TOWARD A UNIFIED VIEW OF COMPLEX MULTISCALE STOCHASTIC SYSTEMS: A GENERALIZED THEORY OF INTERACTIONS AND ITS COMPUTATIONAL INFRASTRUCTURE FOR THEIR UNIVERSAL AND EFFICIENT INVESTIGATION

BY

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DISSERTATION

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Abstract

The Internet, societies and the brain exemplify systems whose compositional structure contains numerous interacting parts and coupled scales of irreversible action, driven to a large extent by intrinsic random perturbations that cannot be removed without losing critical information for their scientific understanding. Systems that match this signature are ubiquitous across a large number of knowledge domains, yet no unified model explaining all their commonalities and unifying principles exists. We define the class containing these instances as that of complex multiscale systems (CMSS), including naturally evolved and artificially designed systems. Due to the increasing interconnectedness of the human experience and the need to understand a wider range of phenomena whose description is much richer than that provided by current models, we claim that the development of effective CMSS research methods represents a scientific program of a new kind.

This work provides evidence underlining why CMSS constitute a novel and fruitful scientific domain. We concern ourselves with improving existing understanding of CMSS by finding causal mappings between the behavior of parts of the system at a small scale (microscale) giving rise to larger components at a larger scale (macroscale) through theory development, cyberinfrastructure and case studies. Three studies contained here suggest that placing interactions as a central construct –instead of objects and laws- simplifies the analysis of CMSS and brings clarity across the formal structure of related scientific theories. We present a Generalized Theory of Interactions (GToI) that aims to provide a universal and efficient description of CMSS in general; the theory can be conveniently adjusted to match specific phenomena across a wide variety of disciplines. We evaluate existing agent-based systems and discuss the ongoing development of a new agent-based framework benefiting from the interactions perspective. We demonstrate how explicit interaction models of CMSS can efficiently increase information gain about these systems, including their scaling laws, self-organization properties and collective behavior with two examples: one on social perception, and another one on modeling the COVID- 19 epidemic for the cities of Urbana and Champaign. Finally, we explore philosophical, conceptual and pragmatic externalities of interactions in computer-assisted epistemology, theoretical biology, global studies and artificial intelligence.

To Les, in memoriam.

Acknowledgments

We live in unparalleled, complex and volatile times; undergoing a PhD process during these is nothing short of a challenge and a privilege simultaneously. Doing so *successfully* can only be explained by repeated choices of many, many individuals to help, teach, mentor and care. If my path through this program is indicative of anything, is that the myth of the 'self-made person' is but a pale and sterile mirage. Consequently, the content, structure and intent of this work can also be interpreted psychologically as a response to the growing need for drastic and systemic global change required for our species to move beyond mere survival into long-term global wellbeing. While a single academic work is a drop in a vast ocean, enough drops make tsunamis possible.

I wish to thank my advisor, Prof. Eric Jakobsson, for being, a mentor, friend and a life example. We met during my first visit to Illinois in 2007. We had several lunches at the Beckman cafeteria where my admiration for him grew steadily; I first learned from him the possibilities of studying metagenomes and about the concept of *ensemble*, central across this dissertation. In 2008, Eric visited us in Costa Rica when a Supercomputing Education Workshop was organized for the first time outside the US around biodiversity and helped raise awareness about how computation can be a powerful ally to biodiversity. At the end of 2010, Eric was eager to help again bootstrap the first e-Science program at the Costa Rica Institute of Technology. It was during this time that he gave a talk in which he explained why Fokker-Planck equations were fascinating. I had never heard about them before, but I was immediately captured by their elegance and meaning. For the first time, probability was not an immutable entity: it behaves like a river with its ebbs and flows, changed by its surroundings and changing them in exchange. Later that week we had one of the deepest conversations I can remember about nature and the structure of reality. Could these equations be used to harmoniously understand complexity in a more parsimonious manner? These thoughts ended up in us presenting a paper at a colorful conference during 2011, a publication that amalgamated some of the very early notions developed here more fully.

Eric welcomed me with open arms to UIUC, inviting me into his research seminars at Beckman. When my prior advisor passed away, he gladly accepted taking this responsibility and guiding me throughout the

remainder of this process. During this whole time, he has constantly identified intellectual opportunities for me to participate and benefit from. His kindness, awareness and sensibility are uniquely matched with inexhaustible intellectual rigor and curiosity. I have enjoyed embarking with him in the journey of teaching Big History in the Campus Honors Program. Eric, in my mind, is the archetype of the rational humanist that uses knowledge to understand and improve the world by considering the underlying subtleties and fragility of the human condition. I have grown under his supervision both as a person, as a scientist and as an scholar, always confident that my best interest has been his priority at all times. The pursuit of a research program such as the one reflected by this dissertation was only possible through the combination of intellectual freedom, critical thinking, constant communication and helpful guidance that Eric has fostered and enabled.

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times, provide a robust and unique view of research that remains open and self-critical in its intentionality.

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Swinging Squirrel, Children's Illustration by Emma Weisman.

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Introduction

What we are destroying is nothing but houses of cards and we are clearing up the ground of language on which they stood. (§118)
Philosophical Investigations

Ludwig Wittgenstein

1.1 Introduction

This dissertation focuses on discovering the underlying principles that govern the structure and dynamics of complex, multiscale stochastic systems (CMSS). These are systems composed of many objects and processes that interact with each other in non-trivial manners (i.e. interdependent), whose structure and behavior can be described at several nested, coupled scales by different principles and laws, yet remain causally connected, in which system evolution and interactions are inherently stochastic, leading to complementarity relations with non-zero statistical uncertainty, and overall are consistent with physical laws such as conservation of energy and irreversible thermodynamics.

Our principal methods are the development of new mathematical concepts and tools capable of capturing interactions in CMSS, coupled with stochastic simulation tools driven by real and synthetic data. Specific CMSS instances exhibit a number of simultaneously remarkable and poorly understood phenomena (in terms of universal properties and laws), such as the following:

- emergence and self-organization of activity/interaction patterns and structural constraints, or inhibition of these;
- correspondence of phenomena across scales, manifest as a large number of degrees of freedom at one scale reducing to a small number of degrees of freedom in another of higher level of aggregation;
- propagation, localization, and exchange of information, organization, and entropy;

- relationships between noise, scaling laws and symmetry;
- strong systemic and porous friction-like forces (e.g., high flops/watt losses due to processing and/or communication entropy in Exascale computing systems).

Table 1.1 at the end of this section highlights the ubiquity and relevance of CMSS and how properties described above manifest in them. Some of these systems have evolved in a biological sense, others have arisen from the combination of physical laws at different scales and, in many recent cases, these systems are being engineered from the ground up. Some CMSS are still in their infancy and have not reached sufficient critical mass for emergent phenomena to arise.

The main scientific goal addressed here is finding principles that unify CMSS across different domains and scales (for example, universal statements about emergent phenomena). To do this, this work contains theory development and new software simulation tools integrated with cyberinfrastructure environments, methods and practices.

1.2 A motivating example: nanotheranostics agents design

We wish to demonstrate through an example some of the consequences of current limitations found when studying CMSS. Consider the case of nanotheranostics[1], the design of active nanoscale systems with simultaneous therapeutic and diagnostic capabilities that aim at effectively treating multifactorial diseases such as cancer[2], Alzheimer[3] or multiresistant bacterial infections[4]. These nanostructured agents are routinely synthesized by (bottom-up) self-assembly across a wide variety of problems [i], which implies determining a) the composition (i.e. substances and their interactions) and synthesis conditions that maximizes yield and preserves the desired functionality, and b) the degree upon which the synthesis method is connected to the effectiveness of the nanotheranostics agent. These systems are composed of action at multiple scales (e.g. atomic, molecular, supramolecular), must endure noisy conditions across a wide variety of environments and are generally structured in a hierarchical manner, making them a type of CMSS.

Ideally, the synthesis of nanotheranostics through self-assembly would be guided by predictions of their functional and geometrical conformations both during their production and during their traversal across biological tissues and structures. Predicting self-assembly is a long standing, relevant challenge in biology and materials science[10]. Contrary to self-assembly in hard matter in which materials are often highly homogeneous and the dominant interactions conform a small group[11–13], self-assembly in soft matter[14] is challenging because of the heterogeneity in composition, involved forces and range of environments they

[i] See: [5–9]

Table 1.1: Summary of CMSS examples per scientific discipline, their properties, open research questions and potential impact.

CMSS instances	**Composition**	**Multiscale structure**	**Randomness**	**Overarching laws**	**Open questions**	**Potential impact**
Physics: Experimental instruments to measure properties at the Planck Scale[21,22];	The instruments are based on the existence of signals arising from phenomena at the Planck scale that can be amplified at various energy levels for their detection and analysis.	Phenomena at the Planck scale are expected to aggregate and produce effects at the scale of fundamental particles and captured as digital information.	Planck scale phenomena provides the foundations of quantum mechanics, which is a generalization of quantum theory.	Conservation of energy, thermodynamics, conservation of space must apply in this regime	How can experimental protocols within current material reach be constructed to decide between competing theories for quantum gravity?	Principles describing the structure of space-time as emergent may contribute to the development of a theory beyond the Standard Model[23].
Biology: Intracellular, multicellular, and evolutionary processes such as those involved in pancreatic cancer[24].	Biological systems are composed of organic entities whose action depends on structures and functions, often intertwined.	Several scales of action include ions, molecules, genes, proteins, membranes, cells, tissues and organs in a single organism.	Temperature variations, stoichiometric dynamics and the complexity of population dynamics introduces noise.	Molecular mechanics and quantum aspects of chemical interactions are the context of biological events.	How do biochemical, cell and genomic variations impact the effectiveness of cancer therapies[25] under constant evolution[26]?	Multiscale biological interaction models may elucidate relationships leading to effective personalized strategies for cancer patients with aggressive tumors[25,27].
Materials: Molecular self-assembly processes in complex environments[28] for minimally invasive nanotheranostic agents[1].	These agents are composed of both organic and inorganic matter whose organization occurs by self-assembly.	Nanostructured agents under development are designed at present with at least three hierarchical scales of action.	Thermal noise and the statistical nature of self-assembly introduce randomness during the synthesis of nanotheranostic agents.	All synthesis processes follow the law of large numbers and thermodynamical laws.	How can synergistic properties of multiscale biometamaterials be explained in terms of geometry, composition and electronic structure?[29]	Principles relating kinematic and dynamic synthesis parameters to performance metrics may improve processes for obtaining bio-inspired nanostructures[30].
Social: Open collaborations[31] both "simple" and "wicked", such as "open innovation"[32] and the emergent intellectual context around global nuclear arms control treaties[33].	Open collaboration structures contain individuals and organizations as the basis for the emergence of processes, routines and norms.	Individuals organize into hierarchical aggregates from groups to collectives to societies.	Individual cognitive capacities and the diversity of social interactions introduce intrinsic randomness in social systems.	Human psychology and socio-technical systems constrain the possible action of agents in social systems.	What relationships dominate information flows, the emergence of roles or management structures, and types of social process trajectories in specific open collaboration settings?[32]	Principles that relate individual actions to success parameters of interventions and strategies can help avoid coordination failures with negative social and technical impacts[34].
HPC Systems: Design and implementation of next-generation of Exascale computing systems (and beyond)[35,36].	Exascale systems are composed of hardware and communication elements whose operation is coordinated by a large collection of software systems.	Individual processing elements aggregate into nodes with operating systems that coordinate through collective algorithms and data communication in hierarchical manner.	Noise emerges from multiple sources, including cosmic rays impacting memory elements, electric and thermal fluctuations and	Solid state physics, electrodynamics and electronics constrain the limits of HPC systems at large.	How can global HPC system properties be deduced from hierarchies of individual components and coordination mechanisms?	Principles relating processing elements and tasks to energy requirement and efficiency of algorithms may contribute to increased peak performance of future HPC architectures.
Software: Fixing problems in open source software[37–39].	Open source software architectures are composed of multiple interlocking components and library dependencies.	Source code artifacts are organized in functions, classes and objects that follow hierarchical composition rules.	Individual coding styles and training background of programmers introduces randomness in final products at all scales.	Programming is determined by the theory of computation and formal logic.	How can software engineering processes be planned such that quality assurance does not interfere with programmer productivity?	Principles that relate engineering tasks to time-to-fix and repair quality measures may allow process improvements in collective settings[37].

must undergo[ii]. To a large extent, the design of nanotheranostic agents mirrors biological self-assembly structurally and functionally.

Two major general strategies have been identified to aid in the design of nanotheranostics (and in general nanostructured) agents. First, using biology as a template for self-assembly is advantageous[40–43] thanks to the incremental approach it allows, but it is limited in the sense that only a subset of all possible self-assembled nanostructures manifest in naturally evolved biological systems. A more recent approach departs from statistical physics principles to invert the self-assembly design problem by modeling the effects of soft matter interactions and composition[iii], yet finding the appropriate dynamical equations and parameters remains a hard problem since intuitions about the systems are largely obscured by synthesis and environmental conditions these nanostructured CMSS must face at multiple scales.

Self-assembly of nanotheranostics agents is one particular example of what may be defined as a *material design problem*: an instance of an optimization problem that attempts to maximize the value of a heuristic (i.e. *ad hoc*) evaluation function by searching a space of possible dynamical equations (or their particular enactments) and finding a path to that which provides an optimal match with respect to a given objective. The dynamical equations should assumed to have a form relevant to entities involved in the system and the boundaries of possibility defined by our best –yet provisional- understanding of physical laws at large. The material design problem may be described formally as follows.

Definition 1 (Material Design Problem)**.** Let S be a CMSS, $\Lambda = \{\lambda_i\}$ the set of all possible sets of dynamical equations that can be defined on (and completely describe) S and λ_0 the initial guess of dynamical laws. A material design goal G_S is a binary function that classifies sets of dynamical functions as rejected (0) or accepted (1) according to the value of a heuristic evaluation function $\tilde{h}$ over Λ that tests the suitability of a particular λ, $\forall \lambda \in \Lambda . \tilde{h}(\lambda) \in [0,1]$ and a threshold $\mu \in (0,1]$. Thus, material design goals have the functional form

$$G_S(\lambda, \tilde{h}, \mu) = \begin{cases} 0, & \tilde{h}(\lambda) \leq \mu \\ 1, & \tilde{h}(\lambda) > \mu. \end{cases} \tag{1.1}$$

The collection of all acceptable set of dynamical equations for G_S, or the proper dynamical set of G_S, is $\Lambda_{G_s}^{\tilde{h},\mu} = \{\lambda \in \Lambda | G_S(\lambda, \tilde{h}, \mu) = 1\}$. Suppose that an optimal set of dynamical equations λ^* exists in $\Lambda_{G_s}^{\tilde{h},\mu}$ such

[ii] Relevant aspects of self-assembly in soft matter are discussed in [15–20].

[iii] Detailed accounts of this and examples can be found in [44–59].

that

$$\lambda^* = \arg\max_{\lambda \in \Lambda_{G_s}^{\tilde{h},\mu}} \tilde{h}(\lambda). \tag{1.2}$$

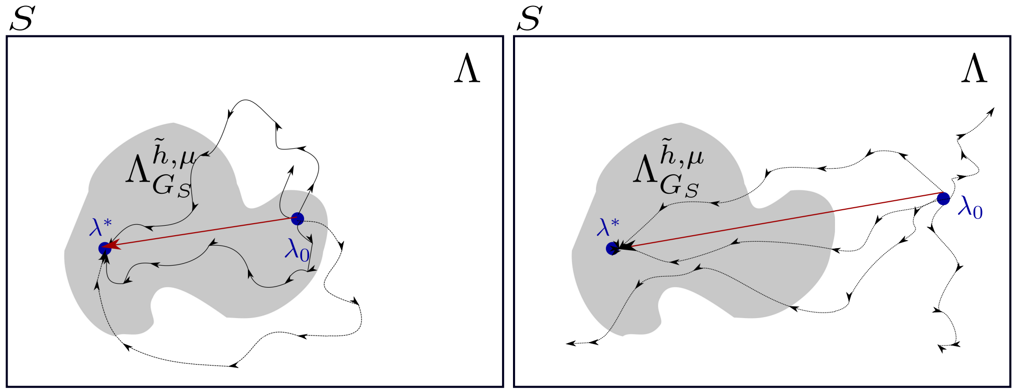
Suppose further that Λ is partially ordered and further suppose that it is also a stochastic metric space[60] with a traversal cost metric $d(\cdot,\cdot)$. Find the sequence of samples $\lambda_1, \lambda_2, \cdots, \lambda_k$ such that k is non-negative, finite and minimal such that total cost D is minimized, that is

$$D = \min_k \arg\min_{\lambda_1,\lambda_2,\cdots,\lambda_k} d(\lambda_0, \lambda_1) + \sum_{i=1}^{k-1} d(\lambda_i, \lambda_{i+1}) + d(\lambda_k, \lambda^*). \tag{1.3}$$

The samples $\lambda_i, 1 \leq i \leq k$ are called intermediate designs.

The problem contains the word 'Material' as an indication of the grounding in concrete physical systems in general, not only in reference to materials science in particular. Ideally, the process yields $k = 0$ (i.e. $\lambda_1 = \lambda^*, \lambda_k = \lambda_0$), or equivalently reaching an optimal design in one step. In practice, however, a sample of one is implausible. Finding the adequate trajectory across the space Λ is extremely hard with information about transformations alone, since local minima are abundant in a sea of stochastic fluctuations (e.g. experimental variation, systematic data errors). Even if Λ is partially ordered, there is in general little information available to explain how the structure of each λ emerged or how sampling could be performed systematically in the right direction to rapidly arrive to the optimal choice of dynamical equations, which are a macroscopic observable. The disadvantage of this approach is that macroscopic observables are information-lossy, as exemplified by the fact that we can postulate equivalent mean-field theories for a single phase transition (e.g. through cellular automata), preserving microstates while varying their governing laws entirely, not only their dynamical equations[61]. Hence, the power to distinguish between similar alternatives with different goal assessments becomes very small.

What is left, and the usual manner in which these problems are solved, is experimentally sampling and expanding the map of local gradients, hoping that both a safe design zone is preserved as that the samples cover increasingly larger portions of the space of sets of dynamical equations. In many cases, specially with *de novo* designs, incremental approaches (e.g. synergistic nanoparticle design) lead to time consuming processes that either yield sub-optimal results or are extremely expensive to obtain in terms of time and resources. The process is facilitated when a known good solution is the departure point, since it is expected that the space of sets of dynamical equations . In that sense, we may call *de novo* designs a *negative material design problem (NMDP)* and incremental improvements a *positive materials design problem (PMDP)*. The latter can be captured precisely and succinctly through the following two complementary definitions.



(a) Positive Material Design Problem (b) Negative Material Design Problem

Figure 1.1: Material Design Problems (MDP) according to the general Def. 1. The system S spans a space Λ containing sets of dynamical equations λ. The gray area corresponds to those dynamical equations that satisfy goal G_S. (a) Positive MDP in Def. 2. (b) Negative MDP in Def. 3.

Definition 2 (Positive Material Design Problem)**.** Let S be a system for which an MDP can be defined properly. Optimally satisfying G_S is an instance of a Positive Material Design Problem if $\lambda_0 \in \Lambda_{G_s}^{\tilde{h},\mu}$.

Definition 3 (Negative Material Design Problem)**.** Let S be a system for which an MDP can be defined properly. Optimally satisfying G_S is an instance of a Negative Material Design Problem if $\lambda_0 \in \Lambda - \Lambda_{G_s}^{\tilde{h},\mu}$.

The latter discussion helps exemplify the difficulties in engineering complex systems with multiple scales when subject to noise, of which the design of nanotheranostics agents is an example. It is clear that a better formulation is not only beneficial, but direly needed across a wide range of disciplines.

1.3 Research statement

This dissertation departs from the hypothesis that a new universal framework constitutes an adequate solution to the current challenges toward understanding CMSS. Consequently, we center our attention in the development of a generalized theory of interactions (GToI), expressed through events in a space whose structure is described by information geometry; this structure maps stochastic dynamical manifolds into a manifold of complex random variables. Such space is named here the *interaction space* of the system, and contains information about classes of interactions present in the system. The GToI, by construction, is an ensemble theory.

We also hypothesize that it is possible to partially recover the natural and expected variation produced by interactions currently neglected in existing differential models by introducing stochasticity into coupled, multiscale differential equation models, developing agent-based models that rigorously model interactions and providing cyberinfrastructure to facilitate the gradual adoption of both the theory and associated methods.

Problem. No robust set of abstractions for the unification of empirical findings in CMSS across multiple knowledge domains exists, leading to a subsequent lack of theories and general properties derived from such unified view capable of enabling predictive and causal reasoning. The latter is translatable into lack of an analytic, empirical and simulation repertoire for multi-method research and productive use of existing cyberinfrastructure whose characteristics interlock with those of CMSS.

Hypothesis. Shifting focus from trajectories, phase space or frequency domain to a space that represents internal features of stochastic interactions in CMSS can lead to more general, empirically correct and succinct descriptions if these are based on stochasticity, non-continuity and thermodynamical irreversibility.

Scientific impact. Ability to improve predictions and causal explanations on CMSS. Ability to design *de novo* CMSS based on detailed substrate information at multiple scales. Ability to efficiently find scaling laws and bridge equations for CMSS instances in general. Ability to execute experiments in CMSS-enabled cyberinfrastructure.

General approach. Constructing a Generalized Theory of Interactions (GToI) provides a route to improve the universality, succinctness and efficiency in CMSS description, analysis and prediction activities. This improvement can be demonstrated and tested by modeling two CMSS instances using cyberinfrastructure built upon such theoretical principles, comparing against empirical findings and contrasting against the complexity of prior models.

1.3.1 Propositions for increasing understanding of interactions as efficient and universal causal descriptors of CMSS

The following propositions and associated questions provide a demarcation of the landscape of theoretical concerns addressed by the research efforts described across this document.

P1: Interactions are *universal* descriptors of dynamical CMSS

What properties of interactions are independent of particular CMSS instances? Can these elements be explained by a more fundamental unifying framework? Can these elements be linked to any formulation of a system, whether Eulerian or Lagrangian? Is action derivable from interactions? Are there any non-trivial counter-examples to interaction-based descriptions? Is the operationalization of the common elements universal for computing properties given any CMSS? Can a multiscale description of interactions be compatible with Green functions describing impulse responses?

P2: Interactions provide mechanisms that explain state transformations in dynamical CMSS

How do interactions give rise to identity and its resilience to random perturbations? Are there any fundamental time constraints between relaxation time, released entropy and structural persistence? How do aggregate interactions lead to the particular form of transformations, or rather to the relation between their denotational and operational forms? What is the effect of varying scales of aggregation in CMSS on the mechanism of a state transformation?

P3: Interactions provide mechanisms that explain properties of governing and scaling laws in dynamical CMSS

How do interactions at one scale aggregate and specifically select the manifold, the function and the parameters at the next scale? Can a procedure be found to generalize instance-specific parameters in order to obtain laws for CMSS? Do interaction properties solely dictate the form of dynamical invariants? Is a theory of the space where the interactions occur needed to explain the geometry of the laws or are space interactions unnecessary? To what extent can CMSS produce scaling relations as given by sets of homogeneous functions?

P4: Interactions provide mechanisms that explain the emergence of information in CMSS

Can information be best explained as the result of maximizing the critical distance for entropy propagation in hierarchical systems? What properties mediate the selection of message substrates? How do governing and scaling laws give rise to particular choices for substrates and encodings? What classes of interactions lead to bistable hysteretic media with low energy transitions and long term stable identity? What is the minimum necessary diversity of microstates for information to appear at the next macroscale?

P5: Interactions provide mechanisms that explain collective properties of information in CMSS

What types of collective properties depend on varying parameters at the microscale? Can collective properties independent of their microstate configuration be found? In which class do collective properties of information fall into? What determines the boundary between global and local information properties in distributed systems? Can global observables exist at all in spatially or temporally distributed collective systems? How is locality defined in them? What happens with locality under uncertainty and non-determinism?

P6: CMSS governed by analogues to the law of mass action are captured by drift-diffusion equations

What is the relation between stochastic processes (e.g. Brownian motion) and topological defects? In what way do topological defects define or constrain drift and diffusion forces at various scales? Can the law of mass action be derived exclusively from phenomena represented in interaction space? How do stochastic fluctuations impact the accuracy of predictions made using this law in CMSS? What is the expected form of the law of mass action for a CMSS that is both stochastic and hierarchical?

P7: The generalized form of the Complementarity Principle determines the landscape of physical possibility of interactions

How does the volume and diversity of events in a CMSS impacts the magnitude of the thermodynamic limit at which a new scale of organization is reached? Does a general principle exist that determines the form of laws emerging from a microscale regardless of the system? How do changes in the number and types of interactions in a system be mapped to families of possible physical laws? Are there regimes of possible laws that are universally excluded regardless of the system?

P8: The generalization of Bohr's Correspondence Principle is a consequence of self-organization in drift-diffusion systems as determined by interactions

Is drift-diffusion a universal descriptor of CMSS? What regimes of drift-diffusion are associated with self-organization? Can drift-diffusion equations be utilized to substantiate bridge equations between dynamical manifolds and interaction spaces without information loss? How is uncertainty captured by drift-diffusion equations? Do symmetries exist in interactions such that solutions to Fokker-Planck and master equations become tractable?

P9: The introduction of stochasticity in deterministic equations describing dynamical systems can partially recover irreversible interaction effects

What are the lower and upper bounds for the accuracy of reconstruction of interaction effects by introducing noisy versions of the dynamical equations of a system? What is the performance difference between using an interaction model vs *a stochastically-augmented differential model? What is the difference in accuracy with respect to experimental CMSS data between both? At which point does the introduction of noise becomes non-representative? Can this point be found analytically?*

P10: Interaction models can be recovered from suitable datasets and instantiated in agent-based models

Under what conditions does spectral analysis recovers the classes and number of entities present in a dataset purportedly containing measurements of a CMSS with interactions? Can the degrees of freedom, frequency and uncertainty characterizing interactions be recovered from the data? If not, is it possible to compensate lack of data by adding models for variables that could not be recovered? Are agent-based models of CMSS constructed using the output of spectral analysis representative of the systems they attempt to simulate in terms of their dynamics and observables?

1.4 Structure of the Dissertation

This dissertation is structured in five parts. Part I explores research problems that showcase properties of CMSS and limitations of current methods that underscore the significance of interactions as first-class citizens by means of exploring the role of stochasticity in a classic weather simulation model, the concept of scale and the notion of global time in distributed systems. Part II develops the Generalized Theory of Interactions (GToI), from the limitations of current CMSS methods to the formulation of the theory.

Part III describes the analysis and development of cyberinfrastructure tools constructed either by direct translation of the GToI into agent-based models. These tools aim to either reconstruct the effects of interactions via ensemble computations or to enact concrete theories of interaction directly. In the process of doing so, we characterized existing ABM frameworks, provided evidence of their limitations, and developed the preliminary foundations for a new class of agent-based systems.

Part IV showcases the application of the resulting theory and tools to unveil the role of social viscosity on social perception of color, and the effect of policy measures on the COVID-19 pandemic in the context of Fall 2020 campus reopening at the University of Illinois at Urbana-Champaign. Finally, Part V explores conceptual, philosophical and pragmatic externalities of interactions in computer-assisted epistemology, theoretical biology, global studies and artificial intelligence.

1.5 Manuscripts in preparation

The following related manuscripts are being prepared to undergo processing in the publication pipeline:

- Núñez-Corrales, S., and Jakobsson, E. (in preparation). A Generalized Multiscale Stochastic Differential Equations Solver. To be submitted to *SIAM Journal of Scientific Computing.*

- Núñez-Corrales, S., Lüdascher, B. and Jakobsson, E (in preparation). UnSpatioT-DCI: Distributed Cyberinfastructure for Background-Dependent Simulations. To be submitted to *Transactions of Modeling and Computer Simulation, ACM.*

- Núñez-Corrales, S., Lüdascher, B. and Jakobsson, E (in preparation). A General Theory of Simulation. To be submitted to *Transactions of Modeling and Computer Simulation, ACM.*

- Núñez-Corrales, S., and Jakobsson, E. (in preparation). A Generalised Theory of Interactions - III. The Theory of Gasses. To be submitted to *Proceedings of the Royal Society A*.

- Núñez-Corrales, S., and Jakobsson, E. (in preparation). A Generalised Theory of Interactions - IV. Self-Organisation. To be submitted to *Proceedings of the Royal Society A*.

- Núñez-Corrales, S., and Jakobsson, E. (in preparation). A Generalised Theory of Interactions - V. Prebiotic Evolution. To be submitted to *Proceedings of the Royal Society A*.

- Núñez-Corrales, S., and Jakobsson, E. (in preparation). Effects of diffusion point processes on deterministic chaotic equations. To be submitted to *Physical Review Letters E*.

1.6 Other research works

In addition to the chapters and articles included in this dissertation, the following works were indirectly connected to the main concepts and methods.

- Jakobsson, E., Argüello-Miranda, O., Chiu, S.W., Fazal, Z., Kruczek, J., Nunez-Corrales, S., Pandit, S. and Pritchet, L., 2017. Towards a unified understanding of lithium action in basic biology and its significance for applied biology. The Journal of membrane biology, 250(6), pp.587-604.

- Katz, D.S., Niemeyer, K.E., Gesing, S., Hwang, L., Bangerth, W., Hettrick, S., Idaszak, R., Salac, J., Chue Hong, N., Núñez-Corrales, S. and Allen, A., 2018. Fourth workshop on sustainable software for science: practice and experiences (WSSSPE4). Journal of Open Research Software, 6(1).

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- Núñez-Corrales, S., and Jakobsson, E. (2020). A generalized theory of interactions for complex multiscale stochastic systems with thermodynamic irreversibility. Bulletin of the American Physical Society, 65.

- Nuñez-Corrales, S., Li, L., and Ludäscher, B., 2020. A first-principles algebraic approach to data transformations in data cleaning: understanding provenance from the ground up. TaPP 2020. Publication pending.

- Nuñez-Corrales, S. and Jakobsson, E. Translation of: Fürth, R., 1933. Über einige Beziehungen zwischen klassischer Statistik und Quantenmechanik. Zeitschrift für Physik, 81(3-4), pp.143-162. To be published on arXiv.

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Part I

Understanding the consequences of interactions

Chapter 2

Parameterizing Stochastic and Deterministic Representations of the Lorenz Equations for Realistic Weather Simulation

Summary[i]

The Lorenz equations are a simplified version of the Navier-Stokes equations for the special case of a fluid contained between two parallel plates with a heat source emanating into the fluid from one of the plates. It was presented as an analogy to the earth's troposphere and has been studied as an example of deterministic chaos. In the current study, we parameterize the Lorenz equations based on several decades of weather data and study the time series of dynamics using these parameters. These realistic parameters produce the "strange attractor" behavior for which the equations are well known. However, frequency spectral analysis of the output of the deterministic version of the equations reveals the existence of a frequency peak not seen in the data, and the absence of many frequency peaks contained in the data. The fits to the observed spectrum are improved by the addition of noise to the equations, possibly corresponding to turbulence. We infer that the fluctuations in weather as described by the Lorenz equations contain a truly stochastic component, as opposed to being due entirely to deterministic chaos. We discuss the implications of this finding for the use of deterministic differential equations in description of complex systems.

2.1 Introduction

Dynamical systems permeate the scientific activities in extensively many domains such as the discovery of gene regulatory networks[1], understanding peace and conflict[2], development of models in stem cell biology[3], approximating oligomer chemistry[4], climate dynamics[5] and biology in general[6]. Non-linear continuous deterministic equations are often used to describe interesting dynamical systems, and sometimes

[i]**Núñez-Corrales, S. and Jakobsson, E.** Parameterizing Stochastic and Deterministic Representations of the Lorenz Equations for Realistic Weather Simulation. To be submitted to the *Frontiers Journal on Climate*.

exhibit deterministic chaos, defined as the irregular, unpredictable behavior of system states which are nonlinear functions of previous states for a given time frame[7]. Ispolatov et al[8] show that the probability of chaotic behavior in coupled systems described deterministically is low when the phase space is has only a few dimensions but rises to essentially one when the number of variables in the system is approximately 50. Thus we should expect chaotic behavior in systems with many variables.

However the appearance of chaos may also arise as a result of inherently stochastic dynamics underlying the dynamics of individual system variables. It is not trivial to decide when the random component of a system must be considered explicitly to achieve accurate modeling of the system dynamics. In one instance, some years ago we found that the dynamical modeling of a nerve cell's aperiodic response to sinusoidal forcing stimulation was greatly improved by adding voltage fluctuations due to the random (thermally driven) opening and closing of ion channels[9]. On the other hand the dynamics of a hinged pendulum are essentially perfectly described as deterministic chaos, because the random air currents exert essentially negligible force compared to the gravitational force on the metal parts of the pendulum[10].

A case of interest is atmospheric weather modeling, since fluid dynamics –usually deterministic- intersects with thermal forces which are fundamentally stochastic. An early coarse-grained deterministic dynamical model of the troposphere was developed by Lorenz[11]. An interesting feature of the model was aperiodic chaotic "strange attractor" dynamics for selected values of the parameters. As would be expected from the Ispolatov et al results cited above, for a wide range of parameters, the 3-variable Lorenz equations do not exhibit chaos, but for some parameters they do. Although the model was deterministic, the chaotic dynamics made the detailed dynamics unpredictable. A further implication of the chaotic dynamics is that very small changes in initial conditions can lead to large divergences in later trajectories, the so-called "Butterfly Effect"[12].

The mapping of the Lorenz model to the troposphere is based on the assumption that the troposphere is a fluid contained between two parallel boundaries –the surface of the earth and the troposphere-stratosphere boundary. A persistent temperature gradient exists between the boundaries, which is accompanied by both diffusive and convective energy transfer in the fluid in the direction normal to the boundaries. The Lorenz model providing a dynamical description of this situation is obtained from one form of the Navier-Stokes equations for fluid flow that includes thermal energy diffusion, called Rayleigh-Bénard flow[13]. In the Lorenz formulation, the flow equations are simplified by the Boussinesq approximation[14], which removes density variations except those due to gravity, and the Galerkin procedure[15] which is used to effectively truncate an infinite series of Fourier terms. The final result, the well-known Lorenz equations, contains three parameters and three dynamic variables. Both the parameters of the Lorenz model and the dynamical variables have specific physical meaning. The dynamical variables, X, Y, and Z are respectively (to within a proportionality constant) the intensity of the convective motion, the temperature difference between the ascending and descending currents, and the degree to which the temperature gradient between the upper and lower boundaries departs from linearity. When the equations were constructed there were not sufficient data to characterize these quantities observationally, but in recent years that has become possible. The three parameters in the Lorenz equations, σ, r, and b are the Prandtl number, the Rayleigh number, and a particular function of the critical value of the Rayleigh number.

In Lorenz' 1963 formulation of his model, the parameters were chosen following a previous paper by Saltzman[16], which established parameters based on approximations of the physical properties of the fluid; that is, the troposphere. In our study, the parameters are derived not from assumptions about the physics, but empirically from the weather data themselves. X, Y, and Z are calculated from the instantaneous weather and σ, r, and b are derived from those values. Then σ, r, and b are used to move X, Y, and Z for the next time step (plus a random component), following which σ, r, and b are recomputed using the new values of X, Y, and Z.

Thirteen years after Lorenz, Hasselmann[17] proposed modeling climate and weather using Fokker-Planck theory, which will always give unpredictable dynamics, regardless of parameter choices. The theory was then applied to a simplified ocean-atmosphere model[18]. In principle, this theoretical approach is attractive due to the large thermally driven fluctuations in weather. The practical problem has been that stochastic dynamics simulations are more compute-intensive than deterministic simulations, so that stochastic dynamics approaches can only be undertaken at cost to the time and size scales, and degree of fine-graining, that are possible with deterministic dynamic models. A useful approach to capturing the high degree of climatic variability in otherwise deterministic models has been the use of stochastic parameterization of otherwise deterministic models[19]. Lorenz himself considered the issue of whether dynamic atmospheric models should be formally deterministic or explicitly stochastic. While acknowledging that stochastic models are in principle more like weather, he concluded that since deterministic models exhibit the aperiodic behavior characteristic of real weather, that the choice of whether or not to include stochastic dynamics explicitly can be one of convenience. In this paper we will revisit whether that conclusion is still valid.

In this paper we attempt a computationally tractable approach to addressing the issue of whether inherently stochastic weather and climate modeling might be worthwhile. We recast the minimal Lorenz dynamic model in Fokker-Planck form by introducing noise, and parameterize it to provide best fit to recent comprehensive weather data that were not available at the time the model was initially created. Since the climate is changing during the time the data were taken, we capture that change in the drift of fundamental fluid dynamics properties, the Prandtl number and the Rayleigh number. We capture the repetitive behavior of the model by frequency domain analysis of the time series of model outputs. Three features of the results suggest an advantage of the stochastic model: a) the overall fit to the data is best at a nonzero level of noise, b) the frequency domain analysis of the output of the deterministic Lorenz equations shows an anomalous resonant frequency peak that is not in the data and that disappears when noise is added, and c) the switching frequency between strange attractor cycles increases when noise is added. With respect to the topology of the model phase space, switching from one strange attractor cycle to another is equivalent to passing a tipping point. The increased frequency of switching from one attractor to another in the Lorenz model suggests that deterministic models may systematically underestimate the time a system will take to pass a tipping point—a critical issue in climate modeling.

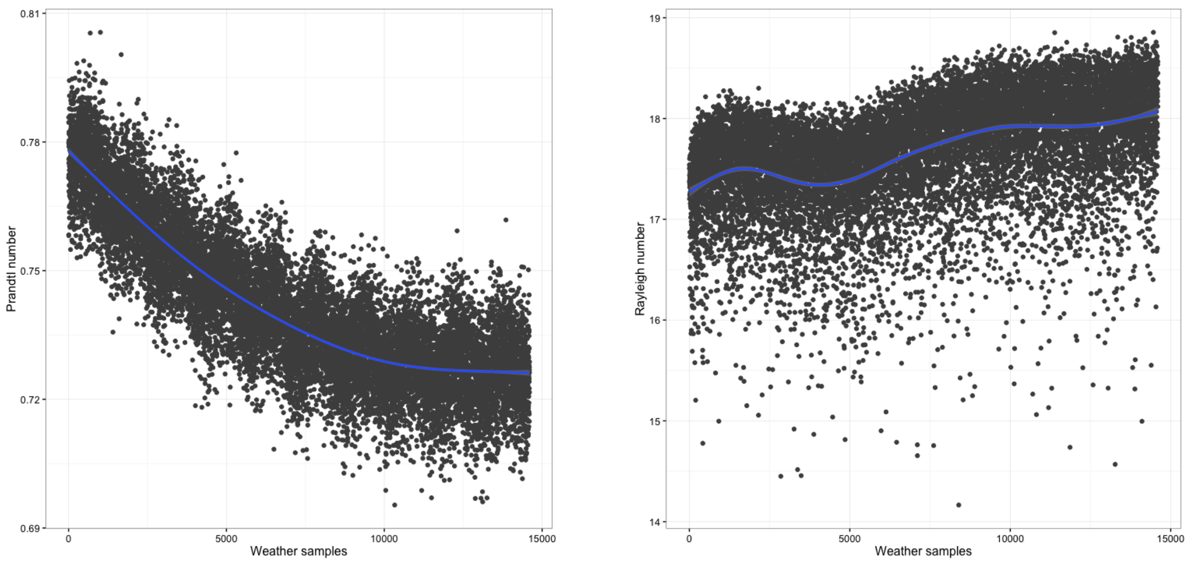
2.2 Results

2.2.1 Lorenz equations can be parameterized against daily weather data

To test whether Lorenz equations can be fitted against real weather data, we performed parametric estimations by computing Lorenz parameters with weather data from 30 locations around on the northern hemisphere from 2005-2015 (Figure 2.1). The horizontal axes represent samples taken four times daily from 2005 to 2015. This Figure shows periodic fluctuations and systematic trends in the Prandtl number (σ in the Lorenz equations) and the Rayleigh number (r in the Lorenz equations). The trends are consistent with a scenario of historically rapid climate change[20]. The Prandtl number is directly associated with the dissipative capacity of air masses which is lowered by an increased concentration of carbon-based greenhouse gases such as carbon dioxide and methane[21]. The smaller value for the average Prandtl number, especially relative to the Rayleigh number, represents increased buoyancy and higher convective velocities.

2.2.2 Weather data is best described by stochastic rather than deterministic Lorenz equations

In order to compare against real data, an ensemble of reparameterized Lorenz systems was computed with generators for σ, r and b set to vary according to values computed from daily weather data between January 1, 2005 and December 31, 2015. One of the main challenges was determining how to make an honest comparison. We found that comparing time series trajectories of the experimental with the model failed to identify interesting features of the system due to the strange attractor behavior. Therefore we opted for performing our analysis in the frequency domain[22]. The strategy followed in this case was to compare



(a) Prandtl number.

(b) Rayleigh number.

Figure 2.1: Computation of the Prandtl and Rayleigh numbers. Dots indicate calculations obtained from atmospheric reprocessing models and the blue line represents the mean curve obtained from them. Logarithmic scale is used for the vertical direction. The horizontal axes represent samples taken four times daily from 2005 until 2015. (a) Values of the estimated Prandtl number for geographical locations indicate a decrease in the ability of the atmosphere to dissipate heat. (b) The Rayleigh number however is consistent with stronger convective forces in the Rayleigh-Bernard equations.

the distance of every parametrization of deterministic and stochastic Lorenz equations against real weather data.

Noise was injected in two ways. One was a stochastic proportional variation in the model parameters (σ, r and b). The second was by stochastic variation in the output variables (X, Y, Z). For all locations, the distance matrix for noise choices was computed and averaged. Two important facts may be highlighted. First, deterministic simulations (zero noise) appear to fare worse (more distant from the data in the frequency domain) than stochastic ones. Second, optimum fit to the data occurs at intermediate noise levels, either 0.4 applied to the output and 0.0 applied to the parameters, or 0.1 applied to the output, 0.5 applied to the parameters (Figure 2.2). The dark colors in the upper right corner of Fig. 2.2 represent a situation in which the noise dominates the structure of the model, so that our method in effect is empirically fitting fluctuations due to noise to fluctuations in the weather data. At higher values of noise than shown in Fig. 2.2 the equations become unstable; that is, trajectories leave the region of the strange attractors and go elsewhere in phase space.

Comparison in power spectra shows that deterministic simulations exhibit a spurious low frequency peak not present in real weather data (Fig. 2.3) when focusing on the point (0.1, 0.5) in Fig. 2.2. However, the experimentally observed trend is recovered using stochastic versions of the Lorenz equations, with the fit

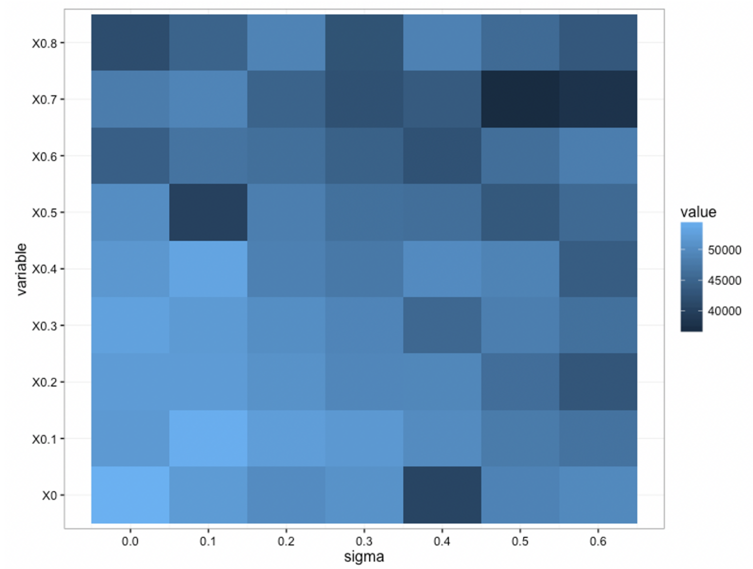


Figure 2.2: Distance matrix between simulations when contrasted against real weather data. The lighter color represents higher distance between simulation and weather data and dark represents shorter distance as computed by the Fréchet metric. Vertical axis corresponds to noise levels applied to stochastic Lorenz parameters (σ, r and b , noise added proportionally) and horizontal axis corresponds to noise injected in the integration process.

being significantly better for the stochastic version at high frequencies. Some deviation of the model from the data at low frequency is because the model assumes that the frequency spectrum is stationary whereas in fact the entire system (as shown in Fig. 2.1) is drifting. Therefore, the lowest frequency components of the data contain components of drift, which is absent from the model. Overall, the optimum stochastic version of the model still somewhat overestimates low frequency components (lower than 0.3 years^{-1}) and underestimates higher frequency components (higher than 0.3 years^{-1}) as compared to the data.

Finally, we analyzed the average performance of the deterministic models against the best match with stochastic simulations for all location. These locations were chosen to be either in the Polar jetstream, in the Subtropical jetstream or outside a jetstream at all. It should be expected that higher variability (hence, lower agreement) will occur inside a jetstream, while the agreement should be maximized out of it. Our analysis confirms this is the case, but also is startling in how strong the agreement is for a model that is a coarse representation of convection dynamics (Figure 2.4). Moreover, analysis of the frequency of flips between the two attractors in the Lorenz model indicates that these increase (non-linearly) proportionally to increasing the noise, whether in the stochastic integration step or in the parameters (Figure 2.5). Intuitively this is an expected result, since as a system moves towards a bifurcation or threshold, fluctuations will move the system across the threshold before it would be reached according to a deterministic description. Generalizing this principle, we hypothesize that deterministic climate models likely will overestimate time

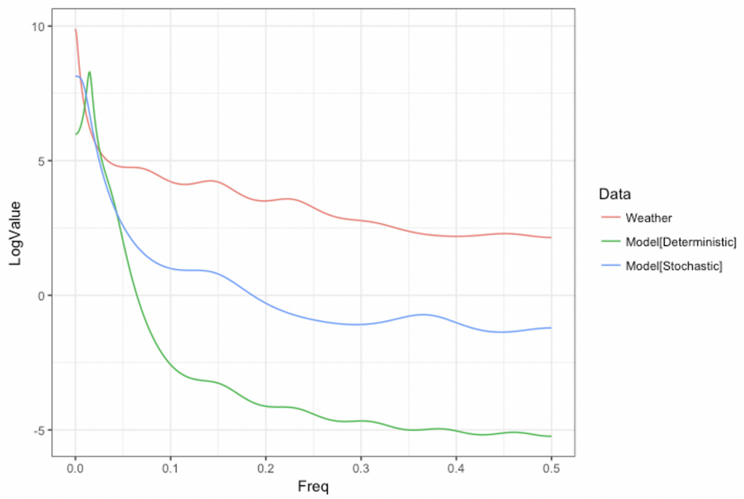


Figure 2.3: Comparisons of simulations against weather data. Log plot of spectral power density curves for deterministic simulations exhibit a spurious low frequency peak (green curve) with respect to real data (red curve). The peak disappears when stochastic simulations are used (blue curve). While both simulations underestimate spectral power of weather data, stochastic models appear to estimate it better. Integration noise is 0.1 and Lorenz parameter noise is 0.5 for the shown image.

intervals between tipping points.

2.3 Summary and Conclusions

The Lorenz equations were originally derived as a coarse-grained description of the dynamics of convection in a fluid. Their most prominent application so far has been as an example of aperiodic oscillatory dynamics arising from an assumed deterministic process. Their application to weather has largely been as a mathematical metaphor for the inherent inability to predict the dynamics of weather in detail. Although the Lorenz variables have physical meaning that corresponds to measurable quantities associated with weather, the issue of whether these equations might provide a reasonably accurate (if coarse-grained) description of the dynamics of real weather has not previously been explored. In this paper, we have explored this issue by parameterizing the Lorenz equations with tropospheric weather data. We find that in this region of parameter space the dynamics of the Lorenz equations do indeed show aperiodic oscillatory behavior like fluctuations in actual weather.

However, Fourier analysis of the weather-parameterized output to the deterministic equations reveals an artefactual peak in the frequency spectrum, which is not present in the weather records from which the parameters were derived. The artefactual peak is suppressed and overall fidelity to the data is improved by addition of an optimum level of noise to the equations. Addition of a greater amount of noise than optimum

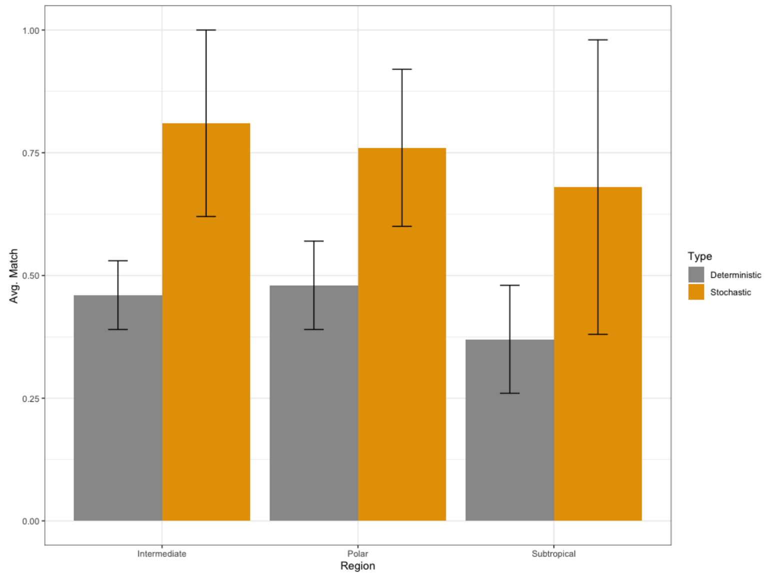


Figure 2.4: Agreement between different conditions with respect to jetstreams. Intermediate refers to points that fall between the Polar jetstream and the Subtropical jetstream, but do not belong to either. Simulation data are classified by type in deterministic and stochastic categories.

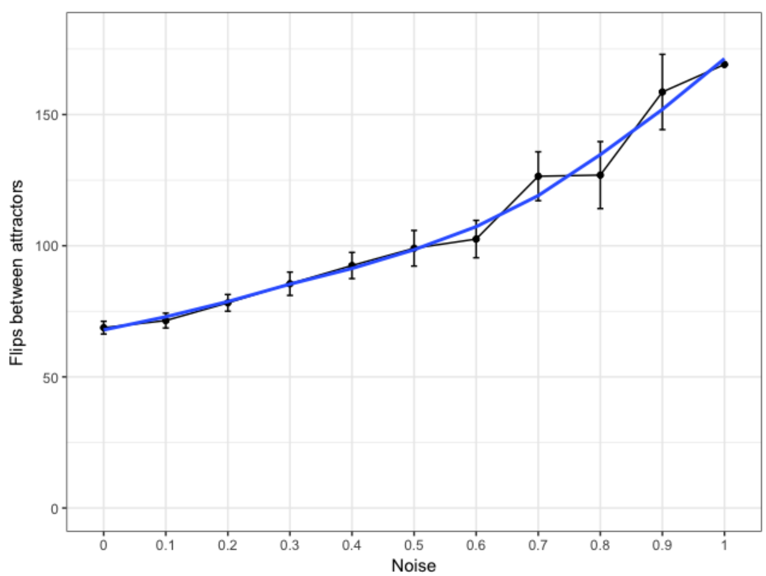


Figure 2.5: Analysis of flips between attractors in the Lorenz system and noise levels. The graph represents the case (0.1, 0.4) of Fig. 2.3. As parametric noise increases from 0 to 1.0, the frequency of flips increases in a non-linear fashion. The variation in the trend increases after 0.5, which correlates with the smallest distance between a stochastic simulation and observed data in frequency space.

degrades the fit to the data first by overflattening the spectral distribution curve and then, if the noise is large enough, by diverging completely from the neighborhood of the strange attractors. We hypothesize that the degree of noise that best fits the data reflects the degree of turbulence in the troposphere.

These results raise the possibility that the stochastic (noise-added) Lorenz equations may provide a useful coarse-grained framework for representation of weather and climate dynamics and trends. These results also suggest that deterministic chaos is an inadequate explanation for weather unpredictability. Rather inherent stochasticity should be invoked. The stochasticity is most likely rooted in the thermally driven nature of atmospheric dynamics, since thermally driven processes are inherently stochastic. The form of the stochastic Lorenz equations puts them in the category of Fokker-Planck equations. These results further suggest that frequency domain analysis is a sensitive tool for testing and validating models of aperiodic oscillatory phenomena, which are extremely common in nature.

A fundamental difference between deterministic and stochastic dynamical models lies in reversibility. All deterministic representations of dynamical systems, including the deterministic Lorenz equations, are reversible. If you reverse the coefficients of the equations, the system will go backwards over the same trajectory as going forwards. Yet an inescapable consequence of the Second Law of Thermodynamics is that all real-world dynamical systems are irreversible. Prigogine and his collaborators and colleagues developed the theory of irreversible thermodynamics to reconcile representations of chemical kinetics (primarily represented as reversible deterministic differential equations) with the requirements of the Second Law of Thermodynamics, that all processes are irreversible[23]. In order to do this, stochasticity is introduced, which guarantees irreversibility[24]. Previously, stochasticity was purely a device to enable coarse-graining, such as representing a friction coefficient of a diffusing particle in solution by Brownian motion rather than explicitly computing solvent-solute interactions at molecular detail. An example of such coarse graining, which is still useful, is multiscale description of ion permeation in protein channels[25]. However, in the context of irreversible thermodynamics, stochasticity is introduced at every level of detail, not to approximate a more exact theory but to make theory of dynamic processes accord to the Second Law of Thermodynamics. We suspect that a fundamental reason behind the improved match between real data and stochastic models compared to deterministic ones is that stochasticity allows recovering relevant microscale interactions that blur the fine-tuned sensitivity of the chaotic model. Additional research is required to formally understand the latter.

The importance of introducing stochasticity may be critical in accurately characterizing thresholds. In a paper presented at a meeting of the New England Complex Systems Institute, we showed that the classic Hodgkin-Huxley equations for the nerve action potential failed to give an all-or-none threshold for generating action potentials[26]. However, the addition of noise associated with individual channels opening and closing[27] provides the correct all-or-none behavior. In modeling climate, thresholds are typically referred to as *tipping points*[28]. Lenton[29] notes that existing deterministic climate models do not faithfully replicate prior tipping points in the Earth's climate history. This gives rise to concern about the ability of such models to predict the timing and nature of future tipping points.

In summary, it has been widely understood since the work of Prigogine et al that the use of deterministic differential equations to characterize thermally driven systems is fundamentally incorrect. Whether this leads to important errors in the results obtained depends on the system being modeled and the questions asked of the model, but it appears that the errors may be especially important when considering thresholds, or tipping points. The Fokker-Planck version of the Lorentz equations is not, in itself, a candidate for detailed climate modeling, as the field has moved on to the utilization of much more detailed models. But the comparison between the Fokker-Planck and deterministic versions may be informative in considering whether and how to introduce stochasticity into detailed climate models.

2.4 Methods

Data sources. We used daily weather data during the Winter season from the United States National Weather Service (NWS) Global Forecasting System (GFS) reprocessing between Jan 1, 2005 and Dec 31, 2015 for 30 locations around the globe as shown in Table 1. These were determined by selecting evenly distributed points inside the path the Polar jet stream (10 points) and the Subtropical jet stream (10) points. Additional control points outside any major jet stream (10) were included as controls. The use of jet streams is justified in this context as they are major drivers of convection in the interface between long-term climate trends and short term weather events[30]. Additional climatic estimates were used from NOAA data from 1950 to 1999 in a 50 year period.

Numerical solution of deterministic and stochastic Lorenz equations. We used existing stochastic formulations of the Lorenz equations

$$\frac{dX}{dt} = a(Y - X) + k_X \frac{dW}{dt} \tag{2.1}$$

$$\frac{dY}{dt} = X(b - Z) - Y + k_Y \frac{dW}{dt} \tag{2.2}$$

$$\frac{dZ}{dt} = XY - cZ) + k_Z \frac{dW}{dt} \tag{2.3}$$

Table 2.1: Locations used to reconstruct the Lorentz system per jetstream during winter.

Location	**Subtropical**	**Intermediate**	**Polar**
1	26 N, 120 W	36 N, 120 W	46 N, 120 W
2	26 N, 114 W	37 N, 114 W	48 N, 114 W
3	27 N, 109 W	37 N, 109 W	46 N, 109 W
4	28 N, 99 W	34 N, 99 W	39 N, 99 W
5	29 N, 93 W	31 N, 93 W	34 N, 93 W
6	30 N, 87 W	31 N, 87 W	32 N, 87 W
7	27 N, 79 W	31 N, 79 W	35 N, 79 W
8	27 N, 70 W	32 N, 79 W	36 N, 70 W
9	25 N, 65 W	32 N, 65 W	39 N, 65 W
10	24 N, 60 W	30 N, 60 W	36 N, 60 W

Our choice also was motivated by the fact that globally Lipschitz continuous coefficients are often assumed in more standard formulations[31,32], but do not hold in general for the present case[33]. For the sake of simplicity –and without loss of generality- no scaling on dW/dt was assumed ($k_X = k_Y = k_Z = 1$). The time-independent approximation $W \approx \mathcal{N}(0,1)$ was used for simulating white noise by taking

$$\frac{dW}{dt} \approx p_G(t) = \frac{e^{-x^2/2}}{\sqrt{2\pi}} \tag{2.4}$$

for all values of t. A more rigorous formulation would require solving the Fokker-Planck equation for W through a drift-diffusion equation. However, the approach used here suffices in the present case because of the scales involved in atmospheric transport phenomena. Finally, the Milstein scheme was used to perform the numerical integration following Zahri[34].

Weather reparametrization of the Lorenz equations. We computed the rescaled Rayleigh number, the rescaled Prandtl number and the geometric constant c by using the data set NWS dataset mentioned above by computing estimates of thermal diffusivity, thermal the expansion coefficient and rescaling to obtain dimensionless quantities. Their variation across the atmosphere was obtained and used to parameterize a white noise generator across the simulation. An average value from the fitting process was used. Computation of the Prandtl and Grashof numbers was performed using data sources cited above through the usual averaging equations.

Computation of simulation trajectories. Comparison of simulations and tropospheric weather data. In order to perform an unbiased contrast, trajectories were not compared directly[35]. Instead, we obtained the spectral power density by fitting each trajectory (whether real or simulated) against a spectral AR model[36]. The distance between each spectral power density curve obtained as previously indicated was computed using the Fréchet distance, an honest distance metric that respects invariants[37]. The resulting matrix of comparisons was computed to study the relation where rows correspond to noise in stochastic Lorenz parameters and columns correspond to noise in the integration algorithm.

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Chapter 3

Scalability in Complex Systems of Interacting Entities

Abstract[i]

The usual meaning behind scale and scalability often refers to volume or phase space across various types of systems. In this article, we explore both the intuitive and a more formal understanding of both as a means to clarify how entities whose structure is explained by compositionality and whose complexity goes beyond scale-as-volume considerations may be constrained by more fundamental topological considerations.

3.1 Measuring complex systems

The need to understand, control and design complex systems is one of the main drivers for considering the nature of scale and scalability as objects of scientific enquiry[1]. Departing from complex systems research, the general analytic approach departs from the abstractions developed early by general systems theory[2] in which a particular system is decomposed into a network where the vertexes correspond to entities, the edges to interactions (mediated or not) and its evolution is provided by dynamics, made explicit through suitable formalisms (e.g. sets of coupled differential equations). From an epistemological perspective of the research program in complex systems theory, there exists a clear reduction from structural patterns observed between interacting entities into network properties[3]. In principle, the ability to find a partial function (or even an isomorphism) between the two for any complex system is a key scientific goal that would allow comprehension of a vast range of interesting phenomena.

It has already been observed that many complex systems of interest exhibit hierarchical organization where small groups of nodes organize into larger collections while preserving a scale-free topology[4], and than such organization can be inferred from data sets with missing links[5]. In addition, obtaining general properties when the entities, interactions and dynamics are known becomes possible in many instances of interest[6].

[i]**Núñez-Corrales, S. and Gasser, L.** Scalability in complex systems of interacting entities. To be submitted to *Complexity*.

Scale-free networks have been well studied in the last decade[1]. These are characterized by properties such as tolerance to error and attack[7], as well as by being characterized by a power-law tail distribution[8] and being ultra-small with respect to diameter[9] with an emphasis in self-organization.

3.1.1 The intuitive notion of scale

The intuitive (hence, practical) notion of scale is often used in two disjoint forms. Their analysis, when performed in detail, provides critical elements for elucidating some of its informal properties, as well as some preconceptions that may not hold after more detailed scrutiny.

The first form has a referent in the cognitive processes associated with comparing quantitatively two objects, either abstract or physical by *gauging* them. One of the objects serves as a reference (*a gauge*) while the other is then subject to comparison. The comparison , however, is not directly performed by direct means, but through a process, learned by repetition towards complete automation[10], of mentally imposing a set of numbers evenly distributed on the reference object and later by marking (mentally or physically) the extent of the second object. The representations of magnitude become progressively associated to some number line or set of quantities that, in abstract, have a predefined ordering[11]. In some way, imposing a mathematical entity (the representation of quantities) becomes a symbolic device whose effect is the improvement of performance for those who acquire that ability, where performance may be measured in accuracy, confidence or response time.

What are the consequences of such a practical notion of a gauge? The most relevant one is efficiency: no longer physical devices are the mechanism by which scale is defined, but rather the combination of three principal structures makes the act of measuring almost of immediate access. These units are a unit of measurement whose information content refers to a particular object or set of congruent objects in the world (coordinative referent), an abstract structure for partitioning the fundamental unit in a valid way according to an axiomatic system, and a structure that allows various multiples of that unit to be repeated[12]. There is a second, more profound recent revelation of cognitive science in relation to cognition. Assuming a mechanistic view of the human mind, it corresponds to an intricate complex system capable of information representation, processing and communication. Such system has the ability to gauge other systems by the emergence of a general mechanism for processing measurements of objects in relation to other objects[13], regardless of their abstract or concrete nature. The nature of the comparison, in that particular sense, resembles discrimination between two hypotheses, formulated in terms of an arbitrary value k corresponding to a particular mark in the measurement device S. Let μ_m be the mark in S' corresponding to the position marked by k in S obtained by a purely geometrical comparison. It is expected that μ_m varies with the sensitivity of the measuring instrument (i.e. its granularity), resulting in more or less accurate comparisons. For the purpose of simplicity, assume that the value μ_m distributes as a Gaussian. Then the hypothesis simply reads:

- H_0: $\mu_m = k$
- H_a: $\mu_m \neq k$

Clearly, repeating the measurement will not improve accuracy with a coarse scale. Additionally, if the system is a physical one, measurement variance (σ_m^2) is different from zero. But there is a more subtle aspect in how the hypothesis was stated. Given the uncertainty in physical theories and its limiting effect on the information that can be gained[14], it is easy to tell whether the marks in different systems are not equal when the scale is coarse enough. However, as the distance $|\mu_m - k|$ becomes shorter, falsifying H_0 becomes increasingly harder. A coarse scale makes it probable ($p \to 1$) for a random mark close to μ_k to be equal to k. This situation closely outlines how uncertainty is dealt with in the natural sciences through the concepts of significant figures and numerical uncertainty[15], which characterize the nature and limits of the scale used to obtain data.

Under which circumstances is it possible to obtain a perfect measurement? As observed above, that would imply that $\sigma_m^2 = 0$, being the probability distribution a sharp Dirac delta function around $|\mu_m - k|$. It also implies that for all values of k and μ_m, $\mu_m = k$ if and only if $\delta(|\mu_m - k|) = 1$. From the previous analysis, as the measurement approaches k, then $p \to 0$. Hence, the probability of observing an exact quantity vanishes in a continuous scale. This is not true, however, if the object being measured is discrete, hence abstract. At a first approximation, scales can also be defined as information-yielding devices that make the process of measurement both efficient and repeatable at the expense of limited resolution. With respect to information theory, the set of the probabilities of the messages sent through a channel is itself a scale of what can be expected in a finite set of possible communications. This situation is no different from other instances of information bearing systems, in particular, those in which the exchange of (somewhat) robust tokens connects different parts of a large entity.

The second sense in which scale is used occurs in the context of quantification of volume of operations in a system for which an expectation exists with respect to one or more variables that characterize its response. After the preceding discussion, this is but a particular case of the first instance, but with a more complex definition of the units of measurement, operating in an abstract representation of the particular system of interest. System in itself is an abstraction of the state of a relevant portion of the world. It would be then expected for the scale of a complex system to be abstract and exact.

3.1.2 A formal definition of scale

A scale, in the most general sense, is a device for measuring entities in a domain of interest. Performing a *measurement* is a comparison operation: a set of numbers (usually the number line $\mathbb{R}$) is imposed on a reference system, whether abstract of concrete, and used to gauge –by some technical manner– another finite portion of interest in another system, or the whole system when feasible. More explicitly, what is measured is an attribute between the reference and the measured systems where three facts convene:

1. the attribute is directly observable (to within error ϵ), hence no further inference is required;
2. the measurement of the reference system is supposed to correctly portray the measured system; that is, for every measured attribute a in the system, there exists always a function f and a reference attribute a' such that $f(a') = a$, and finally
3. additionally, all laws governing system states from which the attribute a is measured are (abstractly) followed in the reference system from which a' is drawn.

For a value to be considered a measurement, its provenance must be from a measurable set. The latter ensures desirable properties such as monotonicity. Formally, a *measurement* may be defined as follows.

Definition 4 (Measurement)**.** Let the properties A, A' respectively of systems S, S' be measurable sets[ii]. Let also the functions

$$\sigma : A \to \mathbb{R}$$

$$\mu : A' \to \mathbb{R}$$

and

$$f : A' \to A$$

denote bi-monotonic reference and gauge functions for systems S and S', as well as the total mapping from reference to gauge systems. Let $\epsilon \in \mathbb{R}$ denote an arbitrary small non-negative quantity from here on named the measurement error. A measurement function is

$$\mathcal{M} : \mathbb{P}(A \to \mathbb{R}) \times \mathbb{P}(A' \to \mathbb{R}) \times A' \to \mathbb{R} \times \{0, 1\}$$

[ii]They are not required to be continuous or even compact sets for this definition to work. It suffices to ensure that A and A' are σ-algebras.

such that for particular values of σ, μ, a'

$$\mathcal{M}(\sigma, \mu, a') = (\sigma(f(a')), \delta_\epsilon(\sigma, \mu, a'))$$

where

$$\delta_\epsilon(\sigma, \mu, a') = \begin{cases} 1 & |\sigma(f(a')) - \mu(a')| \leq \epsilon \\ 0 & \text{otherwise} \end{cases}$$

For later convenience, we define the notion of *characteristic attribute.*

Definition 5 (Characteristic attribute)**.** Let A be a property of systems S. The relation

$$S \succ_\chi A$$

reads "S is characterized by A" or, conversely, "A is a characteristic attribute of S".

What is expected from such a definition of measurement? If the instrument is sensitive enough as to obtain values close to the actual state of affairs in a system, all but one value will be zero for the entire set of entities in the domain of $\mathcal{M}$. If the value of ϵ grows, many more elements in the domain will be mapped as valid measurements of the attribute a'. Such condition is consistent with the notions of uncertainty and accuracy. In that latter regard, a scale depends on the resolution of the measuring device with respect to ϵ: as the measurement error becomes smaller, finer comparisons (i.e. more bits of information) become available, hence, the approximations become better. Scales are, effectively, relative states of reference systems, where the same laws are expected to hold[16]. As previously indicated, measurement does not occur in general for an entity, but is instanced (i.e. endowed with meaning) when attributes are the object of interest. The general notion of scale can now be summarized as follows.

Definition 6 (Scale)**.** Let $S \succ_\chi A$. Then $\sigma : A \to \mathbb{R}$ is a scale for A' in system S' if and only if $S' \succ_\chi A'$ and $f : A \to A'$ exists.

For the purposes of complex dynamical systems, two categories of attributes become relevant:

- Those attributes which do not depend on the evolution of the system, thereby named as *passive.*
- Those attributes which depend on variable elements of the system, from here on named as *active.*

By making this clarification, it becomes clear that the traditional notion of scale (that of a particular value characterizing problem volume) focuses on passive attributes, becoming mostly uninformative in the task of understanding complex systems through general principles. This is the case of most work in structural analysis of complex systems as networks, which has been previously cited. Active (i.e. dynamical) properties are more interesting and more informative in the sense that they provide critical information about both the inner structure of the system S, as well as of the *laws* that govern whole classes of systems of which S is a member.

A better definition of scale –possibly that which is actually *intended* in the analysis of active attributes in complex systems- involves characterizing system actions where useful work is performed with respect to a particular criteria of utility. For a given system configuration, utility is limited by a particular set of constraints (relations between entities and interactions) that impose a cost. While problem size is relevant (i.e. solving larger problems is more useful than solving reduced instances), the concept of scale in active attributes implies also a quantification of proportional cost/benefit of performing the action.

One additional aspect needs to be clarified in the latter conceptualization. How does the measurement occur in the case of active attributes for complex systems, which are (to a first approximation) emergent? The first part of the solution to this question pertains to *what* is measured. The result of an action of a complex dynamical system to a set of initial conditions is a *response*, a global active attribute that captures the utility/cost ratio with respect to system architecture through observables related to its resources (e.g. time, matter, space, energy). The second part of defining the measurement must deal with the pragmatics of the gauging process. A scale in the physical sense strictly requires a positive value of ϵ because the measuring device is a physical object for which arbitrary accurate measurements are prohibited by the laws of physics. However, there is no theoretical restriction that forbids the scale to be an abstract object. This motivates the following definition and theorem:

Definition 7 (Abstract scale)**.** The scale $\sigma : A \to \mathbb{R}$ is abstract if $\epsilon = 0$ and there exists only one pair of the form $(y, 1), y \in \mathbb{R}$ in the range of $\mathcal{M}$.

Theorem 3.1. *The sets A and A' are enumerable if and only if μ is an abstract scale of A' with respect to A and $S \succ_\chi A$, $S' \succ_\chi A'$.*

Proof. (Left to right) By definition, A is enumerable. By virtue of the total mapping f, A' is also enumerable. Then, the simplest scale σ that has A as a domain is that which takes its elements to $\mathbb{Z} \subset \mathbb{R}$. σ is therefore enumerable. Because A' is enumerable, then μ is enumerable by a similar reasoning. Take any $0 < \epsilon \leq 1$, $x \in \text{range}(\sigma)$ and $y \in \text{range}(\mu)$. By definition of $\mathcal{M}$, $|x - y| \leq \epsilon$. Suppose additionally that $y > x$ and that an inequality holds in the previous relation. Then, $\epsilon \neq 0$ and $y - x = \epsilon \Rightarrow y = x + e$. Clearly $x + e \neq \mathbb{Z}$. Either the set A is not enumerable or $\epsilon = 0$.

(Right to left) By definition, σ and μ are continuous functions in $\mathbb{R}$, which implies that A and A' are continuous sets. For any particular $a \in A$ and $a' \in A'$, take $x = \sigma(a)$ and $y = \mu(a')$ such that $|x - y| = 0$, thus $x = y$. Due to the continuity of x and y, the limit of the sequence

$$\lim_{n\to\infty} |x_n - y_n| = \epsilon_n$$

is guaranteed to exist. Then, there exist uncountably many pairs of the form $(y_n, 1)$ in the range of $\mathcal{M}$ for each $\epsilon_n > 0$ due to the definition of the limit. By virtue of $\mathcal{M}$ and the definitions of σ and μ, if $\epsilon_n > 0$ then $x_n \neq y_n$, having $x_n = y_n + \epsilon_n$ or $y_n = x_n + \epsilon_n$. But, thanks to the bi-monotonicity of σ and μ (recall that both A and A' are measurable sets), then it must be that $|x_n - y_n| = 0$, which is a contradiction. Then, neither σ and μ, nor by extension A and A' are continuous. □

For most active attributes of complex systems, the vast majority of scales are abstract because the main objects of interest are *interactions*, which will be considered as atomic units of resource exchange. The latter view has been proposed for various theories in diverse disciplines with relative success[iii]. The characterization of interactions is performed (mostly) in order to understand responses of the system when its general volume or configuration changes, following a general variational principle[25]. Hence, an abstract reference scale (σ) can be constructed by defining an expected utility function for an ideal system S with problem volume V and cost C, then defining the gauge scale (μ) on the performance of the system S' and finally performing a measurement $\mathcal{M}$. Therefore, the scale of a complex system is also a relative state of two abstract systems (reference and gauge) for a given representation of a global active attribute.

3.1.3 The scale of a complex system

Equipped with the latter definition, we can now attempt to define scale in a sense useful to elicit general laws or propositions about complex systems. Any scale in both the reference and gauge systems must make reference to problem size (Ω) and problem structure[iv] (ρ), where problem structure is imposed on problem size and not otherwise. We start by an informal definition of scale in a complex system, and proceed incrementally with respect to the previous notions of measurement.

Definition 8 (Complex system scale – informal)**.** A scale of a complex system is an abstract device that, when applied to a particular system, allows measuring the expected utility of its dynamics through gauging its response in terms of problem volume and problem cost.

[iii] See: [17–24]

[iv] We choose ρ deliberately as suggestive of density: the structure of a problem critically determines the extension of its final volume.

Some requirements become evident on σ, μ and the attributes measured in the system. First, the measurement occurs from the system under a particular reference scale to the *same system* with a new gauge scale, that is $S' = S$. Second, σ is then equivalent to the utility function applied to an attribute A that depends on problem size Ω and problem structure ρ. Third, μ also depends on a similar parametric input A', which makes the comparison exact since $\epsilon = 0$.

We define the following functions for the purpose of exactness.

Definition 9 (System volume)**.** Let a system S have problem size Ω and problem structure ρ. The volume of S will be denoted by the function:

$$V : \mathbb{N} \times \mathbb{R} \to \mathbb{R}$$

The exact definition of V depends on the particular instance of the system at hand.

Notice that the range of V is $\mathbb{R}$. This comes in handy for those spaces where the volume may be fractal when the interactions affect the inner structures of the entities. Similarly, we define cost and utility.

Definition 10 (System cost and utility)**.** Let a system S have problem size Ω and problem structure ρ. The cost and utility of S will be denoted by the functions:

$$C : \mathbb{N} \times \mathbb{R} \to \mathbb{R}$$

and

$$U : \mathbb{N} \times \mathbb{R} \to \mathbb{R}$$

The exact definitions of C and U, similarly, depend on the particular instance of the system at hand.

Finally, we proceed to define the measurement of the scale of a complex system:

Definition 11 (Scale of a system)**.** Let a system S have problem size Ω and problem structure ρ. The scale Λ of S is the ratio

$$\Lambda(\Omega, \rho) = U(\Omega, \rho) \cdot \frac{V(\Omega, \rho)}{C(\Omega, \rho)}$$

for utility, volume and cost functions U, V and C for a particular response variable. Λ is defined in multiples of its fundamental unit of inverse system effort

$$\frac{V(\Omega,\rho)}{C(\Omega,\rho)}$$

Volume, cost and utility

Some conditions on the functions V, C and U become apparent. First, for all values of Ω, $\Omega > 0$. We will differ discussion of the limits of ρ, but for now it suffices to say that it is a structure parameter that modulates either upwards or downwards the effects of increasing the value of Ω. Second, all three functions are positive functions[v]. It is expected of V and C to be partially ordered functions. That is

$$\forall \Omega_1, \Omega_2 \in \mathbb{N} : \Omega_1 < \Omega_2 \Rightarrow V(\Omega_1,\rho) < V(\Omega_2,\rho)$$

and

$$\forall \Omega_1, \Omega_2 \in \mathbb{N} : \Omega_1 < \Omega_2 \Rightarrow C(\Omega_1,\rho) < C(\Omega_2,\rho)$$

Given that utility in this context refers to the value associated to solving instances that are as large as possible, it also follows that monotonicity is expected for U such that

$$\forall \Omega_1, \Omega_2 \in \mathbb{N} : \Omega_1 < \Omega_2 \Rightarrow U(\Omega_1,\rho) < U(\Omega_2,\rho)$$

From the definition of inverse system effort, some interesting cases arise. Take the limit

$$L = \lim_{\Omega\to\infty} \frac{V(\Omega,\rho)}{C(\Omega,\rho)}$$

with ρ fixed. The following cases may occur depending on the convergence of the limit:

- $L = 0$. As system volume increases with topology ρ, the effort required to have a unity of utility becomes infinite after some particular value Ω_0. This is the class of finitely scalable systems with some force analogous to friction (i.e. energy dissipation).
- $0 < L < 1$. Asymptotically solving larger systems always yields suboptimal results. This case describes systems for which, albeit a large effort needs to be exercised in order for it to be useful.
- $L = 1$. Cost remains on pair with volume in these systems. The latter form is indicative of the existence of conservation laws in the context of the dynamics of the system.

[v]Strictly, V, C and U are positive-definite, but the case $\Omega = 0$ is of no practical use in this context.

- $L > 1$. For all values of Ω, the effort required for the system to bear utility is always zero. It is worth noting that zero-cost systems are not expectable in thermodynamical terms.

Each of the above outlined classes of systems is also suggestive of particular topologies. Let us exclude the case $L > 1$ on ground of theoretical infeasibility. Conservation laws ($L = 1$) are macroscale, abstract descriptions of systems where the energy balance, within a particular period, is reached for complementary variables[vi]. For such a description to hold not in the statistical sense, but in the actual realization of a system, the interactions of the entities must lead to completely reversible dynamics, which implies no indirect mediating entities or topologically diverse structure[26,27]. In addition, reversibility suggests no information loss as well in the dynamics of systems that bear information representation[28]. Suboptimal systems characterize the infinitely asymptotic trend characteristic of the law of diminishing returns, which implies no advantage (with respect to Λ) for solving problem sizes beyond a definite value Ω_0.

But, what is the precise form of these functions? Drawing form network theory, a compositional formulation is expected. For instance, different measures of centrality arise by applying computation rules to each node and/or edge in the network[29]. Hence, the parameter ρ determines uniquely how the mechanics of the computation occur and what information is needed. Topology shapes –or rather, limits- expected information algorithmically obtainable in a system, which is relevant for the (expected) utility function in a complex dynamical system[30].

Take a complex system S such that $S >_\chi A$ and A is representable in network form, the graph $G_A = (E, V)$. Consider all $\mathcal{G} \subseteq G_A$. Then, by definition of a graph, G_A is finite and so each subset $\mathcal{G}$, therefore A is a measurable set independent of its topology. Let v be a vertex and the set X be the connected neighborhood[vii] of v for which v is not a member, determined by ρ such that X contains all subsets $\mathcal{G}$ for which v is connected to at least one vertex and $|X| < |G_A|$.

With the latter structural setting, we are now in position to provide a general procedure for computing volume, cost and utility. Consider a gauge function $M \in \{V, C, U\}$ of A such that it is *additively composable*, i.e. there exists a function m such that, for every v_i, it captures the measurement at that point in the network representation of A with topological vicinity of interest ρ_i, and M is equal to the summation of all parametrizations of m. That is

$$M(\Omega, \rho) = \sum_{i=1}^{\Omega} m(v_i, \rho_i)$$

[vi] Two variables are complementary if and only if the increase in one implies a decrease in the other. Complementarity can be generalized for arbitrary large sets of variables as well.

[vii] In a strict sense, it is the relevant neighborhood of v with respect to a function centered in v. A more precise definition requires the specification of a cutoff value that bounds the scope of X.

The latter assumes ρ is locally decomposable into smaller connected topologies (i.e. domain-decomposable), since a topology is also a constraint network[31], situation which permeates generally into physical systems described by statistical mechanics in terms of global macroscopic averages from local microscopic variables[32,33]. Clearly, the best representation for ρ_i in the network given by G_A is some choice of relevant subsets $\mathcal{G}$ such that $\mathcal{G} \subseteq X$ and $v_i \in \mathcal{G}$. Then, the value of the monotonic measurable function M depends on the number of subsets $\mathcal{G}$ per v_i in the neighborhood X required to adequately account for local contributions. Measuring these functions then depends on the architecture of the topology (e.g. reachability, connectivity), problem size, but most significantly on the required knowledge of local interactions. That is, complete *information* on interactions (in a combinatorial sense) is crucial for any abstract gauging of volume, cost and utility.

We now proceed to provide the particular form for M. Let X_i be the neighborhood of $v_i \in G_A$ and $x_i = |X_i|$ be the size. Let the function $m'(v, Y)$ be a relative gauge function for vertex v with respect to a set Y. Without loss of generality, suppose G_A is a complete graph. Let $\mathcal{G}_{ij}$ be the subset of X_i up to j elements and still connected with v_i. Then, the complete form of M becomes

$$M(\Omega, \rho) = \sum_{i=1}^{\Omega} m(v_i, \rho_i) = \sum_{i=1}^{\Omega} m(v_i, X_i) = \sum_{i=1}^{\Omega} \sum_{j=0}^{x_i} \binom{x_i}{j} m'(v_i, \mathcal{G}_{ij})$$

We can generalize the latter expressions with suitable functions W and w accounting for the amount of required information for computing m' locally. Hence,

$$M(\Omega, \rho) = \sum_{i=1}^{\Omega} m(v_i, X_i) = \sum_{i=1}^{\Omega} \sum_{j=0}^{W(x_i)} w(x_i, j) \cdot m'(v_i, \mathcal{G}_{ij})$$

The abstraction of M as a composable function is, in general, flexible. For instance, set $X_i = \varnothing$, $W(x_i) = 1$, $w(x_i, j) = 1$ for all x_i and $m'(v_i, Y) = 1$ for all Y. Clearly, $G_{ij} = \varnothing$. Then,

$$M(\Omega, \rho) = |V| = \Omega$$

recovers problem size as a canonical measure. Similarly, by choosing $X_i = \{y_i \in V | (v_i, y_i) \in E\}$, requiring $w(x_i, j)| = |x_i|$ and using the same W, we obtain

$$M(\Omega, \rho) = |E| \leq \frac{\Omega^2 + \Omega}{2}$$

which measures the number of edges in G_A, hence, representing connected entities (though not of interactions). It is possible, however, to establish a general classification according to the nature of both W and w. Table 3.1 describes the most relevant cases.

Constraints on W	**Form of $w(x_i, j)$**	**Order of M**	**Case**
$W(x_i) = 1$	constant	$O(\Omega)$	Constant
$1 < W(x_i) \leq x_i$	linear	$O(\Omega^n)$	Polynomial
$W(x_i) = x_i$	non-linear	$O(e^{\Omega})$	Exponential

Table 3.1: Classes of gauge functions with respect to W and w. Asymptotic estimations are made, in the non-linear case, assuming ρ is fully connected and $w(x_i, j) = \binom{x_i}{j}$ by using the generalized Stirling's approximation[34].

The above result is striking in terms of its significance with respect to the complexity of dynamical systems. Constant gauges correspond to the *enumeration* of system components and matches the intuitive notions of problem size and connectivity. Polynomial gauges appear to describes systems where interactions are not mediated but are direct instead and in which invariants depend on the geometry of the space alone. Finally, exponential gauges describe non-additive properties expected from emergent phenomena in which events in the microscopic description of the system lead to amplified effects in its macroscopic observables. Even when topology plays an important role in determining the particular (i.e.) instantaneous form of M in a dynamical system, the nature of the measured attribute is dominant in the order of the final function. This is in particular relevant for active attributes, the main object of interest of systems for which scalability is investigated.

An additional word is needed in relation to the interpretation of the sets X_i. Topological constraints on a scale limit the local reach of gauge functions. If the set X_i is smaller, the suggested phenomenology is that of short-range interactions. Conversely, a large set X_i involves accounting for larger subsets of entities, entailing a combinatorial increase in the interactions and therefore increasing the difficulties for properly constructing gauges. The latter is precisely the case of long-range interactions which have proven to be both theoretically[35] and practically[36] problematic in sciences. In summary, the complexity of a system may have two origins: the need to fully explore many local configurations in a short topological distance, or the need to explore less local configurations despite their number[37].

While U and C depend strictly on the nature of the individual interactions described by the attribute A, system volume can be expected to increase at most polynomially in a system due to resource constraints. The latter motivates the following definition.

Definition 12 (Complex system)**.** Let a system S have problem size Ω and problem structure ρ with gauge function $\Lambda(\Omega, \rho)$. The system S is complex if either C or U are exponential and correspond to actual observables in the system.

A final word is necessary for the interpretation of Ω. Problem size is often taken as the size of the input to a system, the nominal count of the elements in the initial configuration of the system or any other bulk measure. Or formalization poses no ground to suggest such a restrictive definition. For instance, a definition limited to a spatial domain produces incorrect characterizations of systems whose utility depends on their ability to repeat a useful action. Then, formal denotations of periods of system action (time gauges) also account for problem size. Throughput is a particularly illuminating example.

3.2 Scalability

By devising a set of formal definitions for *gauges* and *scales*, some central elements become apparent. First, being *scalable* implies some characterization of performance in relation to an active attribute of a system. Passive attributes appear to be immutable (snapshots) while active attributes are mutable (system dynamics). Second, the various forms of the gauge function for cost, in particular exponential ones, are indicative of boundaries of communication between different subsystems, or different levels of representation of the same system. Communication constraints the amount of useful work a system can perform since, in itself, it is also a representation of how information and uncertainty dynamically evolve at both local and global levels. Action cost in the system, therefore, suggests that topological constraints are connected to information content of the active system: the higher the amount of edges in the network representing entities and interactions per vertex, the higher also the amount of information with respect to future states, and viceversa. It is therefore no surprise that exponentially complex systems in our previous characterization are those where cost and utility require *complete local knowledge* for their computation, while their less complex counterparts require knowledge of some or few configurations for the assessment.

Third and last, scalability matters are not strange to the notion of time in two different ways: by a varying problem size or by having repetition as a desirable attribute of the action. Time for the former case is simply introduced as a parametrization of Ω of the form

$$\Omega \equiv \Omega(t)$$

with

$$(\omega, t) \in \Omega$$

for particular values of ω and t. The latter holds for any definition of time, whether discrete or continuum and all other definitions hold without any adjustment.

Definition 13 (Closed system)**.** Let a system S have problem size Ω and problem structure ρ with gauge function $\Lambda(\Omega, \rho)$. The system S is a closed system if and only if for all instants t

$$\lim_{t \to \infty} \Omega(t) = Q$$

for a definite fixed value of Q. Conversely, S is an open system if for all instants $t > \tau$ where τ is small

$$\Omega(t) = \infty$$

In regards to the latter discussion, our definitions provide an intuitive ground for understanding the difference between closed and open systems in terms of minimum scale of description. A closed system has a fixed limit in the amount of information needed at every instant for gauging its cost, volume and utility. An open system, on the contrary, implies that for any arbitrary values of Q and Ω, there exist Q' and Ω' such that $U(\Omega, \rho) < U(\Omega, \rho)$. In other words, the utility of a portion of a system is intuitively smaller that that of the complete system. But, recalling that due to most systems having limit $L = 0$, there exists some value Ω_0 such that cost will overcome system volume. The cost of attaining complete knowledge becomes infinite as well.

The ability of a system to undergo repetition as a measure of performance, implies two additional gauges in the time dimension. One gauge corresponding to the cost of repetition (i.e. wear, relaxation dynamics), and the other one describes the utility (expected value) of multiple performances of the action. It is expected for these gauges to interact in a multiplicative way with the system. It suffices to extend U and C in such manner.

$$U' = u_R(t, \Omega, \rho) \cdot U(\Omega, \rho)$$

and

$$C' = c_R(t, \Omega, \rho) \cdot C(\Omega, \rho)$$

Functions u_R and c_R are repetition utility and cost respectively with similar monotonicity and properties as U and C. For convenience, we notationally denote the scale as $\Lambda(t, \Omega, \rho)$. The quantity

$$\frac{u_R(t, \Omega, \rho)}{c_R(t, \Omega, \rho)}$$

may be interpreted as the *instant cost-bound repetition utility*, a quantification of the time in which the system is capable of generating value before cost is excessively high. A particular example is production scaling in manufacturing: the material properties of the parts are limited by physical laws regarding durability, and achieving higher rates of repetition (hence, action) is limited by energy costs, among several other variables; the instantaneous utility of the system (for instance, in a discrete time model) estimates the value of each produced good with respect to its individual cost and the scale of the system is given by a combination of the gauge functions.

Given two instants in time t_0 and T, two metrics are relevant with time dependent variables. The first one is total scalability, given by

$$\Lambda_T(\Omega, \rho) = \int_{t_0}^{T} \Lambda(t, \Omega, \rho) dt$$

for a continuum time model and

$$\Lambda_T(\Omega, \rho) = \sum_{i=t_0}^{T} \Lambda(i, \Omega, \rho)$$

for a discrete one. In similar terms, we are justified to define *mean* scalability for continuum and discrete cases as

$$\Lambda_\mu(\Omega, \rho) = \frac{1}{T - t_0} \int_{t_0}^{T} \Lambda(t, \Omega, \rho) dt$$

and

$$\Lambda_\mu(\Omega, \rho) = \frac{1}{T - t_0} \sum_{i=t_0}^{T} \Lambda(i, \Omega, \rho)$$

With this elements, we can state the following theorem in regards to dissipative, open systems.

Theorem 3.2 (Conservation of incommensurability of dissipative open systems)**.** *Let the system S be an open system of infinite problem size. Let S be also a dissipative system. Then*

$$\frac{d\Lambda(t, \Omega(t), \rho)}{dt} = 0$$

and

$$\Lambda_T(\Omega, \rho) = \Lambda_\mu(\Omega, \rho) = 0$$

for all $t > \tau$. That is, S is incommensurable.

Proof. Since S is dissipative, then $L = 0$ and $\Lambda(t, \Omega(t), \rho) = 0$ for all $t > \tau$. □

We are now in position to define system scalability in a concrete and rigorous sense.

Definition 14 (System scalability)**.** Let a system S have positive problem size Ω and problem structure ρ with monotonically decreasing gauge function $\Lambda(\Omega, \rho)$ in Ω. S is scalable if there exists Ω^* such that

1. $\Omega^* > \Omega$
2. $\Lambda(\Omega^*, \rho) = 1$
3. $\Lambda(\Omega, \rho) > \Lambda(\Omega^*, \rho)$

Theorem 3.3. *Ω^* is unique for particular choices of S and ρ.*

Proof. Suppose $\Omega^\dagger \neq \Omega^*$ exists. Two cases need to be explored due to $\Omega^\dagger \in \mathbb{R}$. If $\Omega^\dagger < \Omega^*$ then $\Lambda(\Omega^*, \rho) > 1$. Conversely, if $\Omega^\dagger > \Omega^*$ then $\Lambda(\Omega^*, \rho) < 1$. Hence, $\Omega^\dagger = \Omega^*$ □

Scalability is therefore dependent on the actual realization of the system as a function of problem size and topology. Nonetheless, the ability of a system to scale is not sufficient for being of practical value. For example, the scalability of computer systems with respect to particular values of Ω and ρ is used as an engineering parameter in order to decide whether the investment in reconfiguring it is acceptable, or finding a different solution strategy with better scaling possibilities is needed. The following definitions capture the scalability state of a system that is impacted by the law of diminishing returns.

Definition 15 (Weak and strong scalability)**.** Let a system S have positive problem size Ω and problem structure ρ with monotonically decreasing gauge function $\Lambda(\Omega, \rho)$ in Ω.

S is a *strongly scalable* system if and only if S is scalable and

$$\Lambda(\Omega, \rho) - \Lambda(\Omega^*, \rho) > 1$$

Otherwise, if S is scalable and

$$0 < \Lambda(\Omega, \rho) - \Lambda(\Omega^*, \rho) \leq 1$$

the system is *weakly scalable.*

Finally, the choice of ρ has remained fixed. Changing the underlying topological structure of a system does have an impact in a significant number of problems, from the efficiency of sorting networks[38] to the stability of metabolic networks[39]. From the definition of the general gauge M, it is clear that the main role of a topology is related to the amount of information it provides for a given local instance of measurement.

Definition 16 (Structural scalability)**.** Let a system S have positive problem size Ω and problem structure ρ with monotonically decreasing gauge function $\Lambda(\Omega, \rho)$ in Ω.

S is a *structurally scalable* system if and only if

1. S is scalable under ρ

2. there exists ρ' for which S is scalable with scalability limit $\Omega^{\dagger}$

3. $\Lambda(\Omega, \rho) - \Lambda(\Omega^{*}, \rho) < \Lambda(\Omega, \rho') - \Lambda(\Omega^{\dagger}, \rho')$

3.3 A connection to fluid dynamics

Let us briefly consider why, in a crude mechanical view, this matters. Assume an interacting particle model and consider a collection of N identical particles such that their initial positions vary (i.e. an ensemble of agents). Suppose further that agents are subject to identical forces that govern their motion across the space, that such forces are constant and time independent when agents are not interacting, and that forces vary when they interact according to some set of laws. If N is large, we are justified to consider the ensemble to approximate an incompressible flow described through a Lagrangian specification since the volume of interest and the number of particles -hence the density ρ as well- remain constant across the simulation. Moreover, we suppose that the position vector $\boldsymbol{r}_t$ (i.e. trajectory) of a particle is well defined at any time $0 \leq t \leq T$ for some final T, and it is at least C^4 continuous. Our goal is to understand the trade-off between energy expenditure and flow.

Note that we have abused notation and used ρ for both scaling and physical density, which can be –for the moment- justified by assuming, topologically, that the density of interactions is a function of particles per unit volume instantaneously, and dynamically also a function of how they remain connected. Using this fact, we are therefore interested in computing the viscosity profile of a system (i.e. its average, variance and distribution) for each time t. Our reasoning follows the usual formulation provided by fluid dynamics [40]. For each agent, we obtain the velocity vector $\boldsymbol{v}_t$ by differentiation of their trajectory

$$\boldsymbol{v}_t = \frac{d\boldsymbol{r}}{dt}. \tag{3.1}$$

Note that, since Eulerian and Lagrangian specifications are equivalent by setting the Eulerian field u at time t at the location of agent α to

$$\boldsymbol{u}(\boldsymbol{r}_t^{\alpha}) = \frac{\partial \boldsymbol{r}_t^{\alpha}}{\partial t} = \boldsymbol{v} \tag{3.2}$$

the momentum density is well-defined

$$\boldsymbol{M} = \rho \boldsymbol{v} \tag{3.3}$$

so that momentum changes result in viscous forces, some of which will correspond to viscous ones. At this point, we may consider agents as particles in a fluid with diffusive transport with diffusion constant $\boldsymbol{D}$. Consider an infinitesimally small volume $d\boldsymbol{v}$ containing an oriented surface $d\boldsymbol{O}$, for which flux moving across it is captured by the tensor $\boldsymbol{T}$ such that T_{ij} is the flux moving from the i-th direction of the j-th component of the momentum density $\boldsymbol{M}$. Thus, the infinitesimal momentum $\boldsymbol{p}$ moving across the volume $d\boldsymbol{v}$ in time dt becomes

$$d\boldsymbol{p} = d\left(\int d\boldsymbol{v}\boldsymbol{M}\right) \tag{3.4}$$

which is equivalent to the flow across the oriented surface

$$d\boldsymbol{p} = -dt\left(\oint d\boldsymbol{O}\cdot\boldsymbol{T}\right). \tag{3.5}$$

Noting that Stokes' theorem applies here, we are justified to write

$$\oint d\boldsymbol{O}\cdot\boldsymbol{T} = \int d\boldsymbol{v}(\nabla\cdot\boldsymbol{T}) \tag{3.6}$$

leaving

$$d\boldsymbol{p} = -dt\left(\int d\boldsymbol{v}(\nabla\cdot\boldsymbol{T})\right) \tag{3.7}$$

such that the force $\boldsymbol{F}$ (i.e. momentum change per instant) on the volume element is

$$\boldsymbol{F} = \frac{d\boldsymbol{p}}{dt} = -\int d\boldsymbol{v}(\nabla\cdot\boldsymbol{T}) \tag{3.8}$$

In the case of agents, we are interested in the force density $\boldsymbol{f}$ per unit of infinitesimal volume traversed at instant t. From the reasoning above, we observe that

$$\boldsymbol{f} = -\nabla\cdot\boldsymbol{T}. \tag{3.9}$$

The standard expression relating the momentum density to its flux

$$\boldsymbol{T} = -\boldsymbol{D}\nabla\boldsymbol{M} =\sim \rho\boldsymbol{D}\nabla\boldsymbol{v} \tag{3.10}$$

implies that the viscous tensor depends linearly on the velocity gradient tensor $\nabla\boldsymbol{v}$. By setting $\eta \sim \rho\boldsymbol{D}$, we arrive at the well known expression for the viscous tensor

$$\boldsymbol{T} = -\eta\nabla\boldsymbol{v} \tag{3.11}$$

Finally, replacing Eq. 3.11 into Eq. 3.9 yields the force density

$$\boldsymbol{f} = -\eta\nabla^2\boldsymbol{v}. \tag{3.12}$$

For the purpose of practical analysis, both $\boldsymbol{v}$ and $\boldsymbol{f}$ can be numerically approximated provided sufficient points in the trajectory $\boldsymbol{r}_t \equiv (x,y)_t$ exist [41]. Except for cases where diffusion is meaningful or particles are added or removed, the value $\eta = 1$ $(\rho = 1, \boldsymbol{D} = 1)$ will be used (i.e. $\rho \sim \frac{N_{t'}}{N_t}, t' > t$). To compute the (scaled) Reynolds number for an individual particle as a characterization of how strongly it may be affected by viscous forces (i.e. interactions), it suffices to compute under these conditions

$$\mathrm{Re} = \frac{|(\boldsymbol{v}\cdot\nabla)\boldsymbol{v}|}{|\nabla^2\boldsymbol{v}|}. \tag{3.13}$$

Now, we observe the similarity between Re and L in that both induce a phase transition in fluid regimes and scalability respectively. However, the microscopic details of how topology plays a role in this matter which also explain the precise values of Re and L remain opaque. To make them transparent, the details around $\boldsymbol{D}$ would have to be made explicit through a stochastic particle model of fluid flow, since diffusion is present. Moreover, since viscous forces are at play, microscale forces must be complemented with details about the structure and dynamics of the topology. These challenges are well known both in large-scale molecular dynamics simulations[42] and the electrodynamics of materials[43].

3.4 Conclusions

We have reviewed here how the intuitive notion of scale as magnitude can translate to a complex system if interactions are accounted for. In general, interactions allow postulating scale as a function of volume, utility and cost functions for which we expect to find phase transitions depending on a parameter L, corresponding intuitively to the law of diminishing returns. Using these concepts, our reasoning yields a definition of *scalability* as a property that depends on the topology of interactions, in which interaction structure determines trade-offs between utility and cost. By providing an account of scale and scalability that is independent of substrate, we anticipate its application to an ample disciplinary horizon.

This work suggests various research directions. First, there exists a need for a next-generation agent-based modeling (ABM) platform capable of expressing rich sets of interactions in order to simulate complex systems with varying local topologies. Current ABM frameworks appear to be limited to desktop computers, or by the need to implement full models with only a few primitives. Our ongoing research aims at evaluating various such platforms and determine the need for a new one. Second, the connection between fluid mechanics and scalability appears not to be unique, and rather to be universal. These promising results also point out that phenomena driven by viscosity and mass action[44] may be theoretically unifiable; at present, we continue to explore physical and social systems as a means to gather more evidence to this end.

Third and last, our interest also revolves around the applicability of such principles to increasing the feasibility of large-scale computer simulations. It is often the case that compute resources are scarce, and problem complexity is large. If scalability could be computed *a priori*, the number of microscale particles, agents or entities requires for some phenomenon to arise at a target macroscale would become accessible. This minimum quantity of entities would also allow to probe the types and magnitude of inaccuracies derived from using less entities than such value, and therefore to quantify the resulting information loss. Since our theory is limited by the current vocabulary around interactions, and the complexity of the interacting entities appears to correlate with their ease to give rise to new phenomena despite small numbers, we suspect that developing further the theoretical inventory around interactions is required. The latter is significant for the development challenges towards Exascale systems.

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Chapter 4

Approximate Distributed Time

Abstract[i]

The representation of time constitutes a major element in the construction of computing systems whether centralized or distributed. Performance and scalability, coordination and synchronization, and other collective properties of information processing depend on properties of clocks. In addition, the accuracy of a clock drives the complexity of its construction regardless of the physical mechanism used to implement it. In distributed information systems, two goals have defined the overall research landscape: preserving regularity in time-keeping devices as a means to ensure certain formal guarantees and ensuring causal properties in networks of clocks with different properties in which events replace time measurements as the principal object of interest. The complexity of collective time-keeping in either case however remains at least in proportion to the distributed character of these computing systems, which appears not to be sustainable for new types of distributed computing systems. We present a novel alternative based on observer agents that contain local models of time using faulty, stochastic clocks whose operation can be traced to precise physical formulations. Our model provides two sources of approximation based on thresholds and queries to probabilistic oracles. We describe an implementation using the GNU Swarm multi-agent simulation framework. Experimental results highlight the trade-off between the accuracy of global time and the amount of messages generated across the simulation, as well as the importance of emergent, adaptive hierarchical organization in these classes of systems. We discuss implications of our work for often-neglected physical realism in models of hardware and software systems, including the representation of time across Exascale computing systems and next-generation environments and applications.

[i]**Núñez-Corrales, S., Gasser, L. Misailovich, S. and Jakobsson, E.** Approximate Distributed Time. To be Submitted to the *Journal of Artificial Societies and Social Simulation.*

4.1 Introduction

Time, from the vantage point of physics, has been a subject of extensive discussion[1]. General relativity places the speed of light as a hard upper boundary for gaining knowledge about clocks in motion at different spatial locations; no universal clock exists in the universe. Since no canonical frame of reference can be established, global time is a collective notion whose representation is shared across many entities capable of information processing, storage and communication[2]. The act of reading and updating clocks is a form of measurement, whose outcome is perturbed by noise resulting from heat dissipation at multiple scales of interaction between a clock and an observer[3]. For most practical purposes, clocks are locally entities whose ticking is expected to be governed by regular, periodic dynamics. The latter spans a long list of technological requirements and developments –e.g. see [4].

The possibility of common knowledge about time defines a large number of aspects of coordination in distributed information systems[5]. General relativity forbids any physically realistic model of time to be interpreted as *common knowledge* (i.e. a publicly available fact). Instead, time belongs to the category of *distributed knowledge*, or knowledge reachable through agreements upon communication and represented in an internal state of an agent. Hence, converging to a global representation of time must yield an approximate, stochastic outcome when the measurements and conditions for information processing and exchange are driven by processes with irreducible noise. In such case, memory contents of the agents will be perpetually imperfect, yet can be guaranteed to be asymptotic[6] to some (abstract) global consensus reached in finite time if a properly constructed synchronization protocol exists.

Computationally, constructing an approximation to global time in distributed systems is necessary for timing events and synchronizing tasks[7]. Doing so depends on choosing an appropriate synchronization protocol that establishes the periodicity with which a set of clocks (i.e. reference clocks) are queried and whose measurement is used –along with measurements or estimations of communication delays- to update the state of a set of other clocks. The protocol then depends on the properties of both sets of clocks such as their scale (e.g. number and density of communication channels among the clocks), material characteristics (e.g. internal component friction, sensitivity to voltage or frequency changes), adaptivity (e.g. range of the dynamical choice of different reference clocks) and unpredictability (e.g. intrinsic degree of randomness of the frequency between clock ticks). These features constrain properties of the distributed system as a whole, such as the degree of collective synchronization or the number of agents that can be aggregated before synchronization degrades.

Several protocols aimed at attaining good approximations of global time exist. In one extreme, the Network Time Protocol (NTP) was designed to synchronize time representations across a globally distributed collection of computers[8], assuming that a small number of high-accuracy clocks can be used to obtain precise time measurements and propagate them to a larger set of clocks. By estimating time differences due to latency with respect to this reference set, NTP can guarantee a good approximation of the consensus of that set. In this protocol, a numerical value for the measurement of global time is explicitly sought while events are disregarded, and the notion of approximate simultaneity is possible at a global scale. In the other extreme, vector clocks are an event-based abstraction of time in which significance is placed on event causality, rather than on the precise duration of temporal intervals which regarded as circumstantial[9]. The logical relation *happens-before* becomes an arbiter of causality between events, some of which may not be comparable hence rendering simultaneity an inadequate notion. In between, time-triggered architectures constitute a middle ground in which both global time measures and events are relevant and part of the synchronization protocol, and a Newtonian model of time is assumed to drive the operation of clocks.

For a large number of emerging distributed systems, many of the assumptions behind these protocols become invalidated. Extreme-scale distributed systems may be subject to heterogeneous power consumption and efficiency policies, implying variability in clock ticks that may impact synchronization and the effort required to reach a consensus on global time[10]. Events are insufficient to productively describe the complexity of situations where time intertwines with causality[11]. And for new classes of distributed systems, operational conditions may radically deviate from the expectations set by classical physics[12]. We suggest that in all of the protocols described above, the level of uniformity they presuppose leads to incorrect conclusions if used to analyze these emerging instances. Hence, a new type of protocol is required.

Our paper describes a different model of distributed time based on the notion of clocks as stochastic entities[13] that are measured by observers, which in turn have three possible mechanisms to synchronize the clocks in an approximate manner through message-based communication with other observers about the current value of their own clocks. We are interested in understanding relationships between a) accuracy of clock ensembles as given by their cumulative offset for a standard measurement time interval of length T in seconds, b) number of messages sent between observers during T and c) the effect of systematically injecting noise at various levels on a) and b). We hypothesize that the communication cost of synchronizing clocks in distributed settings can be lowered by using probabilistic (i.e. fast-query) oracles that provide approximate information about the difference between clocks as measured by observers. We studied the distributed system of clocks and observers that attempt synchronization through message-based communication through a GNU Swarm implementation. Some preliminary results are discussed in the context of global properties of distributed information systems.

4.2 Stochastic clocks

Stochastic clocks emerge in actual physical realizations whether their implementation is via quantum[14], classical or relativistic[15] systems. In all the latter, time is modeled as the result of successive measurements of a periodic observable in a dynamical system. With quantum clock models, measurements perturb the state of clocks, making time stochastic by nature[13]. Relativistic clock models, which depend on local frames of reference, are equivalent to a fractal-like (hence incomplete) mapping from differences between two or more dynamical systems into a classical timeline[16]. However, all three types of clock models (classical, relativistic, quantum) are examples of harmonic systems subject to some type of ergodicity[17]. Even without referring to distributed clocks, time in local clocks is *fundamentally* stochastic at some level. We explore here some of the scenarios in which stochasticity yields significant variations for systems where some degree synchronization is required or expected.

4.2.1 Sources of stochasticity

Local clocks may behave stochastically for a wide variety of practical reasons. In regular clocks, mechanical imperfections and heat were known to account for irregular ticking very early on by clock manufacturers, who implemented a variety of counteracting measures to ensure periodic operation[18]. More recently, it's known that electronic oscillators experience stochastic variations due to sensitivity to temperature, voltage and frequency[19,20]; given that voltage and frequency scaling are now common sources of approximation[21,22], their effects on clock rates needs to be modeled in order to harness their practical advantages. Even for very accurate distributed time-keeping systems, factors such as the quality of opto-electronics materials, optical media and non-linear circuitry are sources of noise that may affect the performance of computing systems[23].

As the form factors of devices shrink, new sources of noise become relevant. Frequency instabilities in quartz oscillators (the most common frequency anchor for clocks in microelectronics) have been characterized[24] and controlled[25] to the point of the development of standards[26]. These quartz oscillator instabilities result from topological defects in the crystal lattice structure, mostly in the form of vacancies[27,28]. A topological defect is a local breaking in the order of a system that creates discontinuities in its global properties. Further miniaturization into the realm of nanoelectromechanical systems (NEMS) requires even smaller, ultra-high resolution clocks, but these are expected to be more prone to nanofabrication defects[29]. Recent simulations suggest that topological defects in carbon nanotube-based clocks are significant with respect to their overall operation and accuracy[30].

Finally, the effects of general and special relativity on clocks moving at high speeds or close to massive objects have been studied concurrently with developments in electronics[31,32]. In practice, proximity to massive objects is the crucial factor in how accurate are implementations of the Global Positioning System (GPS), which manifests as spatial uncertainty metrics[33–35]. Several experiments of varying sophistication have confirmed these time dilation effects[35–37]. Synchronization of multiple computing systems becomes a relevant problem for initiatives such as Project StarShot, an attempt to build a swarm of nanocraft for traveling near the speed of light in order to survey the Alpha Centauri star system[12]; these small computing systems, when traveling close to 20% the speed of light will certainly suffer irregular time dilations as determined by the Lorentz contraction tensor after encountering many massive objects along their individual trajectories.

4.2.2 Observers and time-keeping

Clocks are ultimately physical systems subject to disturbances induced by measuring them[38,39]. The periodicity of clock ticks often implies non-disturbance of their state[40] or a sufficiently tight control loop, a mechanism that prevents the clock from experimenting large deviations in it expected range in its internal periodicity[41]. In our model, entities named *observers* (i.e. agents in a distributed information system) use clocks to guide their behavior and dynamics, or rather to synchronize against them. Many observers may read and/or update their accessible clocks after consulting with a better reference time-keeping system an an attempt to avoid further deviations in the periodicity of the clock. We will henceforth refer to the distributed system as comprised of *observer-clock pairs.*

When the number of observer-clock pairs increases, a broader spectrum of diversity in the measurement discrepancies should induce higher internal complexity for some synchronization to occur[42]. Stochastic time models, when arbitrary accuracy is expected or mandated, will only worsen the above situation. Reducing the complexity of agents that keep track of time requires introducing some form of approximation, in this case, querying clocks with a significantly lower frequency than that of the associated clock's tick while having mechanisms to remain synchronized with other observers. The latter implies that upon a certain threshold –established according to the particular clock-observer system- pairs of clock measurements become indistinguishable[43]. The threshold also implies the existence of a metric, which in turn translates to the existence of equivalence relations between different time measurements. Any realistic model of distributed time, in the spirit of the latter, should include the effect of (stochastic) communication in observers.

4.2.3 Boundary conditions

Finally, certain boundary conditions (BC) must be met for models of distributed time to include stochasticity and remain plausible[44]. These BC have been chosen such that a) they are physically meaningful for real observer-clock distributed systems, b) they relate to information theory in a direct manner, and c) they capture the minimally necessary features needed to introduce approximations later. We consider the following boundary conditions as sufficient for guaranteeing correct descriptions of stochastic clocks, and name them according to the historical origin of each underlying physical principle.

Boltzmann BC No stochastic deviation of clock ticks can be negative[45]. Negative ticks in time-keeping mechanisms implies reversing the arrow of time[46], which is not observed in stochastic (irreversible) processes in real physical systems. Since clocks are mechanisms that use energy to sustain oscillations only, negative ticks would imply a violation of the second law of thermodynamics.

Lorentz BC Given a set of clocks for which time measurements of definite periods vary, the differences in their intervals with respect to the slowest clock may be interpreted as Lorentz contractions[2,47]. A slow clock may be interpreted as being contained inside a frame of reference moving at high speeds (or influenced by a strong gravitational) field from the perspective of an external agent whose frame of reference is assumed to be fixed.

Gauss BC Tick duration (the distance between two almost instantaneous point-like 1D signals) is a random variable described by a normal distribution for relevant ranges of operation[48,49]. A general dynamical model of the operation of a stochastic clock can be expressed as the combination of mechanisms that sustain periodicity (drift) and factors that introduce randomness (diffusion), which correspond to Ornstein-Uhlenbeck processes[50]. In the absence of detailed information, it can be shown that for time periods that are large compared to the response time of the system that implements the clock, these are distributed as a Gaussian variable.

Aharonov BC Clocks do not exist in isolation. Rather, observers access clocks interested in their power to resolve temporal equivalences between events and states of clocks[43]. The clock resolution depends on the difference between its maximum and minimum energy eigenvalues as well as on its response time, which place a hard boundary on the amount of information that can be encoded and entropy that is generated[51]. Even if, for instance, clocks are implemented by quantum systems, they can be synchronized classically through local measurements, observer interpretation and later information exchange by sending messages[52]. Reading and updating the clocks by observers are operations that introduce noise and dissipate heat, inducing uncertainty in the value obtained by future measurements[53].

Our model of a distributed system of stochastic observer-clock pairs follows strictly these boundary conditions. The three approximate synchronization strategies described in §4 rest on the notion of clocks as physical systems capable of a special type of computation.

4.3 A formal communication-grounded model of distributed time

Our model of Approximate Distributed Time (ADT) is implemented on top of an Agent-Based Models (ABMs), a well-developed research area focused on the analysis of interaction patterns in entities capable of information representation, exchange and transformation[54]. Distributed clock synchronization is an example of consensus and cooperation in agent networks[55] with emergence of leadership[56] as faulty clocks attempt to synchronize against more accurate ones. More importantly, finding better time references among a variety of possibly faulty clocks through message sending is an instance also known to ABMs research[57]. Contrary to the work just cited, our work does not focus on the structure of consensus problems. We are interested in understanding the limits of time synchronization as an instance of the general problem of identity of global properties as defined by tolerance to perturbations, where structure is assumed to be emergent.

Agents are constrained by their ability to communicate, sense and act locally based on information gained along their trajectory in phase space. It is our interest to explore approximation alternatives that reduce communication intensity while preserving global goal satisfaction through information-based mechanisms (e.g. oracles) capable of determining whether a message will result in a causally different outcome before processing its content. For the current case, we provide the following definitions of agents and of message irrelevance as a means to capture the notion of a microstate defined through interactions, and a macrostate that can be computed, or rather that emerges from them. The formulation of the agent-based system below helps capture precisely the notion of an approximate version of global time with low communication cost in contrast to a communication-expensive network of synchronized clocks with arbitrary precision.

4.3.1 Agents, irrelevant messages and oracles

We wish to provide a model with representation of observers and clocks as a network of agents that, for simplicity, have no internal memory. Our interest is, as indicated above, not in the structural properties of the network, but on the possibility of defining macroscale quantities that preserve some form of identity. Deepening our physical analogy, messages may be thought of as proxies for interactions defining causal trajectories. Given that memory-less systems (specially stochastic ones) are simpler to reason about, our agents have no internal memory and send messages to themselves later in the future.

Messages are defined by a grammar of atomic symbols or, recursively, of pairs of messages. These may be considered as null when they contain unknown symbols, or even of the symbols are known, they may be considered as irrelevant.

Definition 17. (Message) Let Σ be the alphabet of all atoms allowable in a context, including $\circ$ (null) and

$\diamond$ (irrelevant). Consider the additional meta-symbols ",", "(" and ")". We define a message $m \in M$ as a recursive type represented by the following grammar:

1. $m \to a, a \in \Sigma$
2. $m \to (m, m)$

Agents are entities that have a state at a given point in time. Time for agents is discrete and may be though of pairs where the first element is a natural number, and the second one is the label returned by some measuring device. Agents also have a local representation of the problem they contribute to solve in the form of responses to messages, encoded as operations that yield new messages with specific destinations. Similar to how state transformations are modeled in other physical systems, a function takes a prior state and transforms it in a posterior state of information in the network whose edges are the messages to the self and to others. Only one message is sent by an agent to any other agent at a given time step.

Definition 18. (Agent) Let M be the set of possible messages exchanged between any two entities in a simulation for any (discrete) time $t, 0 \leq t \leq T$. Let P be a local problem to be solved by an agent at a single time t. Let also $\mathcal{R}(P) = \{R_1, R_2, \cdots, R_l\}$ be the space of all possible representations relevant to P such that any agent k spawned at the simulation will have one of the R_k as its representation. Let X be the set of agents. Let the function

$$F(m_t^s, m_t^e, R_k) : M \times M \times \mathcal{R}(P) \to M \times (M \times X)$$

be the function that takes the messages from the past self (m_t^s) and any other external source (m_t^e) such that

$$F(m_t^s, m_t^e, R_k) = (m_{t+1}^s, (m_{t+1}^e, x_i))$$

The function F is effectively a transition function from t to $t+1$. Thus, an **agent** $\mathcal{A}$ is the quintuple that contains transition function and a representation for problem P, and recognizes messages from the set M within a set of agents X.

$$\mathcal{A} = (X, M, F, P, \mathcal{R})$$

For an agent to have a computable function, a halt state must exist and be reachable. Ill-defined problems are not guaranteed to have a computable solution in the network of agents, and therefore the microstates of the network should not be expected to converge to any recognizable macrostate.

Definition 19. (Agent in halt) An agent $\mathcal{A}$ is in halt if $m_t^s = m_t^e = \circ$ and $A_j = \diamond$ for a given time t. The halt state must be reachable by every agent for a problem to be considered as solvable.

Our agents should have consistent behavior when confronted with entries of null type. When both the self and the other messages are null, the future destination should be considered as irrelevant as a way of modeling uncertainty through non-determinism. Conversely, if at least one element of the message is different from null the destination should be considered as relevant.

Axiom 4.1. *(Definiteness of destination) Let the agent $\mathcal{A}$ have the function $F(m_t^s, m_t^e, R_k) = (m_{t+1}^s, (m_{t+1}^e, A_j))$. Then $A_j = \diamond$ if and only if $m_t^s = m_t^e = \circ$. Also, $m_{t+1}^s = m_{t+1}^e = \circ$.*

In agreement with relevance theory[58], we restrict communication between agents only when it is purposeful. That is, either the content sent back to the self is not irrelevant or the content sent to another agent is not irrelevant. This condition removes trivial interactions that consume time.

Axiom 4.2. *(Purposeful outcomes) Let the agent $\mathcal{A}$ have the function $F(m_t^s, m_t^e, R_k) = (m_{t+1}^s, (m_{t+1}^e, A_j))$. Then $m_{t+1}^s \neq \diamond \vee m_{t+1}^e \neq \diamond, \forall t$.*

However, suppose that the form of the transition function dictates that the content of a message will be discarded by an agent regardless of its content, and act independent of the reception of the message. In that case, the outcome of the transition function may be interpreted as only depending either upon the self message or to yield information that can be automatically ignored henceforth.

Definition 20. (Specially irrelevant message) A message m is specially irrelevant to agent $\mathcal{A}$ if and only if either $F(m, a, R_k) = F(\circ, a, R_k)$, $F(a, m, R_k) = F(a, \circ, R_k)$ or $F(m, m, R_k) = F(\circ, \circ, R_k) = (\circ, \diamond)$.

It would be useful to have a model for the internals of the transition function F of the agent. We may think of the transition as constructed from a function g that uses incoming information and the internal representation to compute what is sent to the future self, and a function h that determines the destination and content of what is sent to other agents in the immediate future. Having functions that are constructible[59] provides certain guarantees on what may be obtained when various operations are applied; this is relevant for consistently modeling global properties that emerge from various microstates. The particular forms of g and h depend on the actual system.

Axiom 4.3. *(Compositionality of F) Let $\mathcal{A} \in X$ be an agent such that F is its transition function. F is compositional if*

$$F(m_t^s, m_t^e, R_k) = (g(m_t^s, m_t^e, R_k), h(m_t^s, m_t^e, R_k))$$

for suitable functions

$$g : M \times M \times \mathcal{R} \to M$$

and

$$h : M \times M \times \mathcal{R} \to M \times X$$

Suppose all agents operate using the same version of F and $\mathcal{R}(P)$. The complexity of F will be determined by the number of elements in the alphabet, or rather, by the number of responses[42]. Then, given a particular message and a sufficiently large number of agents, it is likely for two or more agents to have the same output at a given time t. Even if their histories are different, as captured by the edges in the network representing messages that have been sent and received, their instantaneous state is the same.

Definition 21. (Time-dependent equivalence class of a message) Let $S_{\mathcal{A}}$ be the set of all agents in a simulation such that $S_{\mathcal{A}}(i) = \mathcal{A}_i$ and $M_t = \{m_1, m_2, \cdots, m_n\}_t$ be the messages sent from all agents at time t to all agents at time $t+1$, $t+1 \leq T$. Let $\langle S_{\mathcal{A}}, M, T, \leq\rangle$ the lattice spanned by $S_{\mathcal{A}}$ ordered by t. Let $m_l \in M$ be a message received by agent $S_{\mathcal{A}}(i)$ at time t_k.

Let $M = \bigcup_{p=1}^{K} M_p$ such that $M_i \neq M_j, i \neq j$. Then $[p]$ are time dependent equivalence classes for m_l with respect to agent $S_{\mathcal{A}}(i)$ whose internal representation is R if $\forall m \in M_p : F(m^s_{t_k}, m_l, R) = F(m^s_{t_k}, m, R) = (m^s_{p,t_{k+1}}, (m^e_{p,t_{k+1}}, x_{p,j}))$. The value of K is determined by a suitable computable function

$$\Phi : \mathbb{P}(M \times M \times \mathcal{R}) \times T \times M \to \mathbb{N}$$

such that

$$\Phi(F, t_k, m_l) = K$$

We can broaden the definition above to determine if a message is irrelevant at any time t. Reasoning about causality, for instance, requires establishing the direction of contingency between two events. In this case, partitions that emerge can be though of as a *mesoscale* view of the evolution of agent-bound observables, in our case of the mean and cumulative variance between clocks as read by observers.

Definition 22. (Equivalence class of a message) Let K partition M as in the previous definition. Further suppose the partition holds for any time t. Then $[p]$ are equivalence classes for m_l with respect to agent $S_{\mathcal{A}}(i)$.

Armed with our last definition, we proceed to define what it means for a message to be generally irrelevant across the agent network. It implies that, for instance, no optimistic simulation is possible at those points (incidentally avoiding many of its costs[60]), since the immediate past for a time $t+1$ is not connected to the state at time t. It also impacts local and global causality for the same reason. One particular case in modeling clocks is the assumption that Gaussian ticks are independent as a consequence of the properties of the system implementing the clock mechanism.

Definition 23. (Generally irrelevant message) Let $\langle S_{\mathcal{A}}, M, T, \leq \rangle$ the lattice spanned by $S_{\mathcal{A}}$. Let $m_l \in M$ and $S_{\mathcal{A}}(i)$ an agent. Let F_i denote the transition function for the agent.

A message $m \in M$ is irrelevant for $S_{\mathcal{A}}(i)$ if $\Phi(F_i, m_l) = 1$. That is, m_l partitions M into a single equivalence class with respect to its future effects.

Equipped with these definitions and axioms, we now can formally define the problem of obtaining a global, approximate distributed time with low : find an oracle $\Phi(\cdot,\cdot)$ such that, for a given message sent to an observer with access to a clock, the oracle classifies that message as relevant or irrelevant with respect to incoming information about the time recorded by other observers about their clocks based on some internal or collective property. We now proceed to characterize clocks without oracles, adding them only later.

4.3.2 Clocks as agents

We model clocks as autonomous agents, whose state is given by a Mealy machine over the alphabet $\Sigma_C = \{\diamond_C, M_r, M_w\}$ where $\diamond_C$ is the tick symbol representing the physical laws of the clock, M_r is a non-destructive measurement (read) and M_r is a destructive measurement (write). The outputs of the clock are either its timestamps or the null value $\perp$. Clock ticks are stochastic based on the noise level n_i, a fact reflected on irregular differences between timestamps. Write operations add more noise than read operations ($n_i < n_{i+1}$) and take additional time $\Delta_w \tau_C$ for updating the clock 4.1. Noise values are always positive ($\forall i . n_i \geq 0$) in agreement with the Boltzmann BC.

Clock_t is the state where the clock is ticking without any disturbance, while Clock_r and Clock_r correspond to those states for read and write operations respectively. Each tick is composed of 10^6 subticks with standard reference time τ_C^S in order to adequately portray conditions in realistic systems (most noisy events affect clock tick rates at no more than six orders of magnitude). While clock time moves forward at a stochastic pace, perception of time is constant for the agent. We model this fact by associating each discrete step of updating the clock to a constant wait period in CPU time. Care must be exercised in choosing the delay as to observe communication effects.

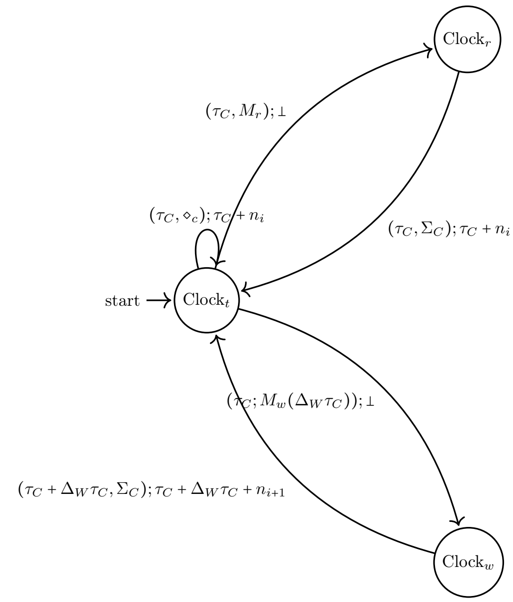

Figure 4.1: Mealy machine for a simple stochastic clock.

4.3.3 Observers as agents

Observers are modeled as agents in the following way. Each agent measures a single clock at periodic time intervals. In agreement with the Aharonov BC, subtick resolution must be lower than that of the actual clocks. We therefore set standard observer time to be $\tau_O^S = \kappa \cdot \tau_C^S, \kappa > 1$. After a period of t_e ticks (*equilibration time*), the agent must find three peer observers with which to synchronize against. Synchronization then happens at every K ticks until a final stochastic time T is reached or surpassed.

During normal execution of the observer, it reads the clock constantly at its resolution rate. If a request to measure time is placed through a message coming from other agent, the agent checks its availability and if possible returns the time in its clock. When the pre-established synchronization time is reached, the observer sends itself a clock update message based on the peer observers.

4.3.4 Restricted reference sets

Each observer has three reference clocks that provide a standard against which to measure time. Observers compute at each discrete event of the time tick (not based on the actual quantity representing stochastic time) their coefficient of variation since the last synchronization. This statistical value characterizes both stability and variance.

At the beginning of the simulation, no observer has reference peers. After t_e ticks, three reference peers are chosen at random based only on their availability, ensuring a randomized mix. For every subsequent synchronization point, only two of the peers are replaced only if better references are found. The process may take many messages due to availability until both peers are replaced.

4.3.5 Query bounces

In this model, we also wanted to simulate limited resources on the observers. Our particular choice was to limit the amount of available messages that can be received (bounce limit B) per unit of time t_B in ticks. Locally constrained resources are known to induce self-organization within agent communication structures in the form of hierarchies[61,62].

4.4 Approximate synchronization strategies

The cost of synchronization in agent-based systems in terms of messages is the target of optimization in our research. The model of observers and clocks as agents described above was extended in two ways to include two sources of approximation through assessments of write messages as irrelevant. For the present time, both strategies are mutually exclusive, although no particular reason seems to prevent their concurrent application.

4.4.1 Thresholding

If the local coefficient of variation (CV) has not changed by a factor of θ (desynchronization threshold) around a radius of 0.1θ, an update occurs and the same value of K is maintained. If the CV is higher than for the previous synchronization instant, an update occurs and $K \coloneqq K/f_s$ for a rescaling factor $f_s > 1$. Otherwise, an update occurs and $K \coloneqq f_s \cdot K$.

4.4.2 Fast-query oracle

We extended both the clock and the observer to include the notion of a fast timer. An Observer sends its peers preemptive ping requests for a small time quantum Δp, recording how much time it took for the message to get back. Travel time and any other factors of deviation are computed in a similar manner as in NTP, and aggregated into an instantaneous CV form all three peers. Depending on the value of the instantaneous CV from these ping requests in comparison with the local CV, the value for K is rescaled through similar rules as for θ. Fig. 4.2 represents the change to the Mealy machine with a ping state, with $\Sigma_C = \{\diamond_C, M_r, M_w\} \cup \{\diamond_r, \diamond_r, \Phi\}$ where $\diamond_r$ is timer continuation, $\diamond_r$ is timer stop and $\Phi(\Delta p)$ is the timer oracle function of duration Δp in ticks. When in fast-query response state, observers are not responsive to other messages.

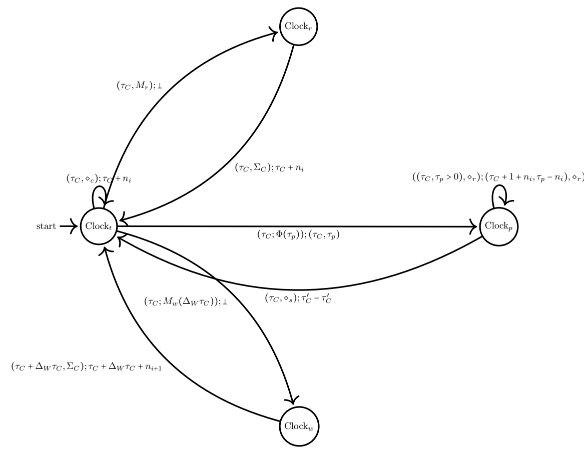

Figure 4.2: Mealy machine for a fast-query oracle stochastic clock.

For the purpose of analysis of results, this approach was traced as advanced approximation (Ad. Approx).

4.5 Experimental design

We devised a series of computational experiments were to test the performance of the model described above as well as both approximation strategies. A total set of seven runs with five repetitions each was performed, corresponding to each of the following cases:

- All observers and their associated clocks on each experiment vary according to the same noise level (5 runs, one per noise level).
- The observers and their associated clocks are partitioned in five classes of equal number and assigned increasing noise levels.
- Observers and associated clocks are generated as follows depending on their level of variation from lowest to highest: 2%, 4%, 8%, 16% and 70%. That is, *good reference clocks are scarce.*

Our working hypothesis states that, under both query bounce protocol between observers and random exploration of the reference space between observers with different responses, the emergence of hierarchy reduces communication intensity.

4.5.1 Noise model

Noise was generated through a Gaussian random number generator. In order to generate random numbers within a range $[a, b)$, variations up to 3 standard deviations (> 99% of elements in the range) were allowed. Hence, any random number r was ensured to be of the form

$$r = u + \mathcal{N}(0,1) \cdot \left(\frac{b-u}{3}\right) \tag{4.1}$$

where $u = \frac{b-a}{2}$ and $\mathcal{N}(0,1)$ is the standard normal distribution. The choice of a Gaussian distribution is motivated in reported analysis of general clock skew figures for intra-die variation[63], but care must be exercised in choosing the distribution. For instance, normality does not hold for individual components of clock skew in particular architectures[64]. Our analysis method does not depend however on the distribution itself, but on the guarantees of non-overlap between the intervals of interest. The following noise ranges were defined.

$$n_0 = [0, 5 \times 10^{-6})$$
$$n_1 = [5 \times 10^{-6}, 5 \times 10^{-5})$$
$$n_2 = [5 \times 10^{-5}, 5 \times 10^{-4})$$
$$n_3 = [5 \times 10^{-4}, 5 \times 10^{-3})$$
$$n_4 = [5 \times 10^{-3}, 5 \times 10^{-2})$$
$$n_5 = [5 \times 10^{-2}, 5 \times 10^{-1})$$

Notice that n_5 is defined for the purpose of write-induced noise at clocks operating at read-induced noise of n_4. The case n_0, although quaint, is well defined as a stochastic limit of infinitely low variance[65].

4.5.2 Hardware setup

All experiments were executed on an Amazon EC2 c4.large instance, with 2 processors running at 2.60 GHz, 25M Cache, and 3.75 GB RAM. Because logs were written to memory and dumped to disk after execution of the model, no provision for either fast I/O or large disk space was necessary.

4.5.3 Software environment and implementation

Our implementation of both regular and approximate distributed time was performed using the GNU Swarm toolkit for agent-based modeling[66,67], written in Objective-C. Swarm provides three main advantages that aligned with our research requirements: it differentiates between observer and active objects, message passing is the main communication construct between observers, and the current stable implementation (2.2) is thread-compatible. For implementing CPU-bound ticks, the NSThread class was used in its GNUstep version. The system was implemented on top of a Ubuntu 12.04 Precise installation, a GNU/Linux version for which a precompiled GNU Swarm library exists.

4.5.4 Execution parameters

In agreement with the model described above, Table 4.1 enumerates all simulation parameters. The choice of $N = 100$ is motivated in part by the need to have a representative population as well as by the advantage of putting threads in idle states as the mechanism to simulate wait times. A value of $T = 200$ provides sufficient experimental data even when the clocks are non-interacting (2×10^5 independent events). For the equilibration time, $t_e = 10$ suffices for most noise ranges ($n_i, i > n_1$) to induce noticeable effects on the time representation of clocks. Choosing $\tau_C^S / \tau_O^S = 100$ models a set of agents (observers) whose structural complexity induces to slower actions in comparison with smaller ones (clocks), a condition known to hold for time-delay systems[68]. t_B was similarly set to simulate a reasonably fast (10%) relaxation time after $B = N^{\frac{1}{2}}$ messages have been received. The latter is critical for simulating finite resources in observers and the value is motivated by existing research in the efficiency of peer-to-peer networks (e.g.[69]), yet other models are possible. We set Δp to be equivalent to 5 (deterministic) clock ticks with respect to the ratios defined above. The value of f_s is based on[70]. Finally, θ was computed iteratively from a Bernoulli distribution as to completely cover T with $p = 1/3$.

4.5.5 Measurements

With the objective of preliminary measuring the effect of different conditions on the observer-clock multi-agent system, we measured total number of messages sent and the collective total deviation for the complete simulation of all clocks for a given instant taken at wallclock (e.g. CPU) time. Averages and variances were computed from five experimental repetitions. Event recording was performed using the native logging facilities provided by GNU Swarm in batch mode.

Table 4.1: Parameters for the observer-clock ABM.

Parameter	Description	Value
N	Number of agents	100
T	Observer time limit (ticks)	200
t_e	Observer equilib. time (ticks)	10
K	Update frequency (ticks)	5
τ_C^S	Standard clock CPU tick (s)	0.001
τ_O^S	Standard observer CPU tick (s)	$100 \cdot \tau_C^S$
t_B	Query bounce time (ticks)	0.1
$\Delta_w \tau_C$	Clock write time (ticks)	0.00001
Δp	Ping time (ticks)	0.05
f_s	Rescaling factor	1.618
θ	Desync. threshold (ticks)	0.01
B	Bounce limit	$N^{\frac{1}{2}}$

4.6 Results and discussion

Average wallclock runtime was equal to 21253 ± 32.3 for the set of individual executions. The low variance is explained because of how internal tick waits are implemented as thread idle time. From first principles, we estimated communication intensity at 15%, considering each synchronization step for the constant step case and the probability of query bouncing set to 1/3.

4.6.1 Experiment 1: equivalent clocks

When all clocks are equally noisy, non approximate observers generate around 20000 messages during the complete simulation. Messages decrease significantly for the approximate case in direct proportion to noise in the clocks. It is interesting to note that the selected threshold was within the range n_3. For lower noise figures, messaging decreased in comparison to the non-approximate case. However, when noise was on average equal or higher than θ, the ABM entered into a panic state with many more messages than in any other case (Fig. 3). On the other hand, thresholding unequivocally provides the best synchronization strategy in terms of reducing differences between clocks (Fig. 4).

4.6.2 Experiment 2: equivalent clock partitions

For mixed observers and clocks initially partitioned into sets of equal noise functions, results indicate a decrease in the number of messages in all three cases. However, a clear advantage is provided by advanced approximation which reduced messages down to one quarter of those observed for the constant (i.e. fixed K) case (Fig. 5). Thresholding remains as the best strategy difference-wise once more.

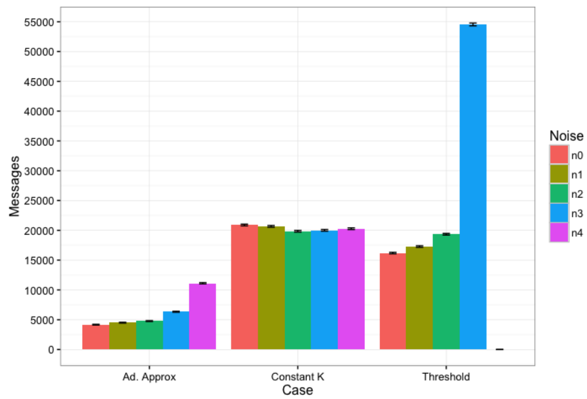

Figure 4.3: Number of messages for experiment 1. *Observed value for threshold experiments with n_4: 436083.6 ± 660.3, not shown for visualization purposes.

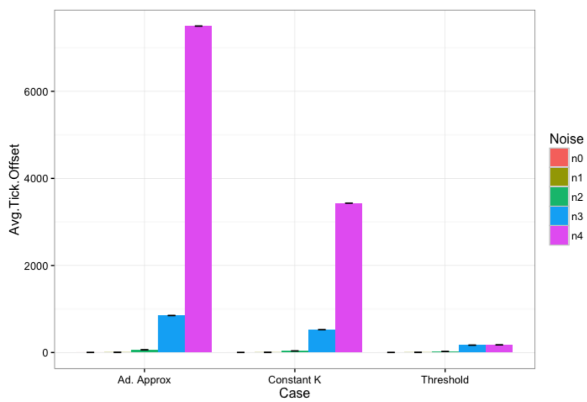

Figure 4.4: Total time differences for experiment 1.

4.6.3 Experiment 3: realistic (decreasing) clocks partitions

The last series of results further assert the ability of our advanced approximation strategy to decrease the number of messages (Fig. 6). A difference with the previous experiment is the increase in total time variation, except for thresholding as the most beneficial strategy for synchronization.

4.6.4 Interpretation from ABMs

These results suggest that the constraints placed by the number and locality of peers, the fact that queries may be bounced and the need to obtain good references are the main factors that explain current observations. When all clocks have the same noise function, entropy induced by very similar values (but unequal) in the coefficient of variation has a dual effect on message increase: all clocks need to poll many others before finding reliable observers with which to contrast against. During that period, most messages will not contribute to that goal and measurements have to be repeated.

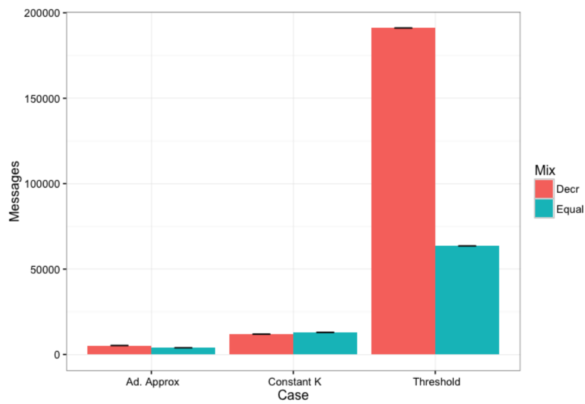

Figure 4.5: Number of messages for experiments 2 and 3.

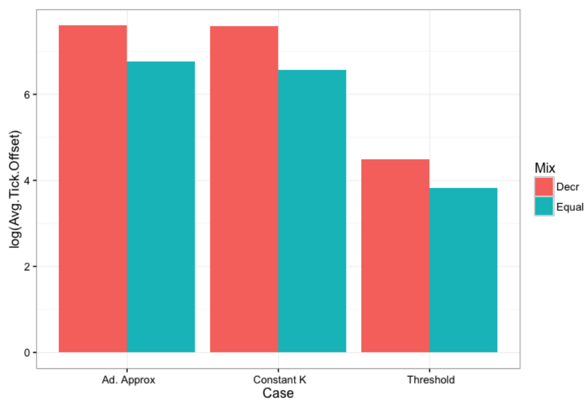

Figure 4.6: Total time differences for experiment 2 and 3.

In the remaining experiments with mixed classes of clocks in various proportions suggests that hierarchies emerge through self-organization. The drop in the amount of messages for the second experiment is suggestive of a structure with sufficient room for exploration: it is relatively easy to find a good reference soon. When good reference peers –those with accurate clocks- are scarce, the amount of messages increases due to the difficulties in finding responsive peers. Good clocks receive many more queries, hence reaching soon a query bounce state and forcing an extended search.

With respect to total time variation, threshold approximations appear to be adequate when noise levels are known. However, it is usually not the case in real multi-agent systems. Reaching "panic" stages due to miscalculations are geometrically expensive. On the other hand, adequately thresholds minimize clock tick variance. At the other end of the spectrum, fast-query oracle approximations are desirable with mixed noise functions in the population of clocks. Messaging increases noticeably, but is compensated by the self-organization of the agents by moving towards a well distributed hierarchy. A significant advantage is that no previous information about the distribution of the agents is required at the expense of increasing tick irregularity.

We wish to highlight a peculiar relation between noise levels, the amount of information transferred between agents across synchronization steps, and the frequency at which that communication happens. For this purpose, we focus on the third experiment, which assumes that the quality of a type of clock is inversely proportional to their quantity in the simulation. Figure 4.7 was obtained by accounting for the number of information tokens exchanged by each type of synchronization protocol (i.e. 4 for the constant update, 5 for the threshold mode and 6 for the adaptive protocol), and the logarithm of frequency (i.e. number of messages divided by total time) and uncertainty (i.e average clock differences). From prior work around the scaling properties of complex systems, the resulting picture fits the intuitions about the effect of interactions.

The cost of interacting to keep a system synchronized varies depending on the number of degrees of freedom, and to do so in a non-linear manner. Having a single threshold increases the cost when the noise level is higher than the threshold to maintain the system drastically under a fixed uncertainty value, while having only the synchronization between peers cannot reduce the uncertainty at a lower cost. The adaptive protocol, having one more degree of freedom due to its internal oracle, is able to decrease the cost dramatically, but not the uncertainty as drastically as the threshold protocol. Even with this limited model, we observe that degrees of freedom, frequency and uncertainty appear to describe a significant portion of systems of interacting entities. More research needs to be performed to understand their relation to other types of phenomena.

4.6.5 Some computational implications for theories of time in physics

It is worth noting from our present research experience that ABMs also constitute a powerful experimental platform for exploring the consequences of various theories of time in physics. Most of them operate upon the formalism of ergodic systems theory and topology with precise accounting of the complementarity between time and energy. Our model is able to reproduce simple results from stochastic clocks with different mechanisms (i.e. mechanical, electromagnetic, quantum mechanical, relativistic) by means of an adequate noise function.

As a matter of future research, we will construct more rigorous simulations that compute the noise function through Fokker-Planck equations associated with the Hamiltonian that describes the system[71]. The latter, although computationally intensive, would improve our limited choice of a normal distribution. Finally, using the Fokker-Planck equations do not break the Gauss BC, as any stochastic process converges to a normal distribution for infinite time horizons.

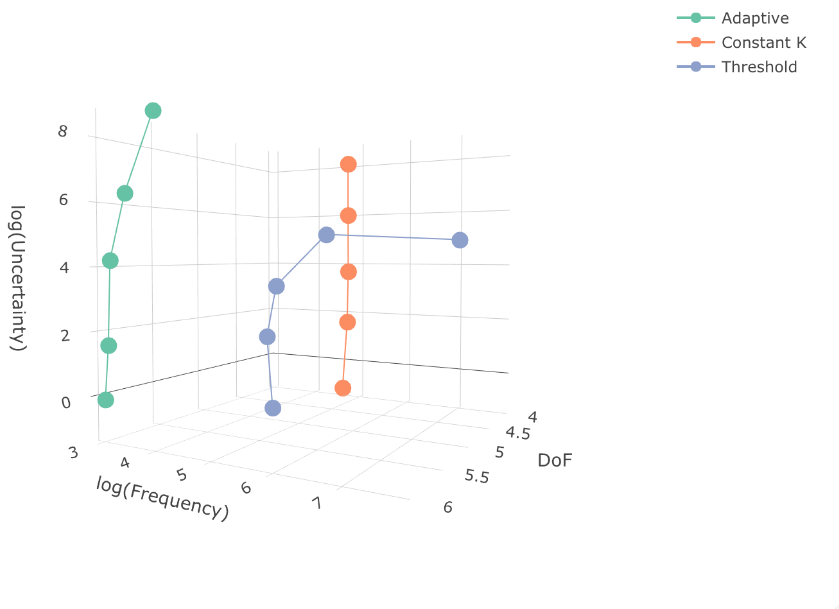

Figure 4.7: Relations between clock interactions in terms of degrees of freedom exchanged, frequency and uncertainty.

4.7 Conclusions and next steps

Modeling time as a collective, stochastic entity allows exploring three important areas. First, the implementation of approximate distributed time models that follow strictly fundamental physics appears to capture problems arising in the synchronization of time-keeping devices in ways more general than those provided by previous efforts (e.g. NTP and vector clocks). Our clocks ensure positive variation (Boltzmann BC), stochastic dilation (Lorentz BC), normally distributed variation ranges (Gauss BC) and a model of uncertainty in time measurements by observers (Aharonov BC). Second, two simple approximation strategies suggest that energy expenditures in frequent synchronization do not always pay off in terms of reducing total variation, thus leaving plenty of room open for research in this area. Third and foremost, that hierarchical self-organization is a critical driver of behavior of entities under constrained conditions and limited information which may permit relaxation of certain problems.

Our work was limited in various respects. First, the runtime conditions of GNU Swarm beyond multicore machines and current state of package support restrict the representativeness of results discussed in this article. In order to implement a more realistic system, this experiment will be ported to a novel massively distributed agent framework (being developed by the authors) written in the Charm++/ROSS[72] with the goal of testing these results in massively distributed system. Second, a detailed analysis of agent behavior needs to be implemented, which was prevented by limitations in the mechanisms used to instrument of the observers. Third, several other knobs and approximation mechanisms may be implemented for further testing (e.g. automatic thresholding, knobs for adding or removing clock classes and manipulating average query bouncing time). Finally, a preliminary version of approximate distributed time is being integrated to an agent-based modeling platform for research on large-scale agent-based simulations for computational social science.

4.8 Acknowledgments

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Part II

Understanding interactions

Chapter 5

A Generalised Theory of Interactions - I. The General Problem

Abstract[i]

Understanding realistic complex systems requires confronting significant conceptual, theoretical and experimental limitations rooted in the persistence of views that originated in the mechanics of simple moving bodies. We define the category of complex multiscale stochastic systems as a useful device for capturing the minimally required complexity of many types of phenomena. In doing so, we provide evidence indicating that determinism, continuity and reversibility can lead to theoretical inadequacies that manifest as intractability, inaccuracies or non-representativeness when applied to complex systems. We take the view that interactions are fundamental and summarize their portrayal across many disciplines. Despite their centrality, interactions remain largely neglected as subjects of research interest of their own. We hypothesize that a generalized theory of interactions may help organize evidence from multiple scientific domains towards a more unified realistic view of systems.

5.1 Introduction

The Internet[1], bacterial communities[2], the global economy[3], ecosystems[4], societies[5], distributed information systems[6], international diplomatic bodies[7], biomimetic nanomaterials[8] and organizations in general[9] exemplify systems with scientific and practical relevance characterized by dynamical complexity in their structure and function[10]. All of them exhibit intricate dynamics and responses coupled to their environment that impact our ability to predict their future behaviour. Elements within these systems appear simple, in stark contrast to the great variety and number of possible stimuli the system as a whole can receive[11]. All these systems also exhibit emergent properties and self-regulation, which seem to provide resilience to small external perturbations. At a closer look, we find that their architecture depends on intricate and flexible organization patterns that are not directly dependent on external driving agents, but which lead to diverse

[i] **Núñez-Corrales, S. and Jakobsson, E.** A Generalised Theory of Interactions - I. The General Problem. To be submitted to *Proceedings of the Royal Society A.*

internal microstates that work to stabilize the system as a whole against destructive influences of external driving agents and confer unity to the system[12].

Constructing causal explanations and predictions for densely interconnected systems may or may not admit strong simplifications. Models that omit even a few elements of the problem sometimes show loss of empirical resemblance to the instance under study. Some of the most frequent simplifications involve the supposition that changes are described by linear functions or that for relevant time periods they behave *almost* linearly, or that sources of noise can be safely neglected in the mathematical description. In this proposal, we provide evidence against such simplifications arguing that they are inadequate for many instances of densely interconnected systems; correspondingly, we will also describe in detail properties of these systems in an attempt to identify particular instances and formulate strategies for their modeling and simulation. Prior efforts include nonlinear science[13,14] and complex systems science[15,16]. Both have made attempts to explain the structure and dynamics of these systems, but both face many challenges when used to either make empirically verified predictions or provide causal accounts of changes across temporal and spatial dimensions.

Many explorations of nonlinear science begin with viewing systems through the lens of dynamical systems theory, supposing that sets of coupled differential equations completely capture trajectories of all relevant events: a manifold contains the trajectory of variation of system states (i.e. points in their trajectories) through time, and transforming the manifold by removing time produces a phase space representation that captures the global geometry of state changes[17]. In this view, instantaneous transformations derived from a small set of governing laws specify the changes that occur in the system. Analytic or numerical integration of these transformations –usually specified by systems of differential equations- yields values for macroscale observables that correspond to measurable properties of the real system. We discuss below several problems that exist with this approach preventing it from being effective for solving some problems in many systems.

A second view is that of networks, which has contributed in the last three decades to a vast number of discoveries and applications. A network is, briefly, a collection of entities (i.e. nodes) related in some manner (i.e. links) that determines the local and global structure of the collection, its dynamical properties or in many cases the likelihood of emergence of properties that cannot be explained by the individual action of the entities alone. Despite the success of networks in capturing essential aspects of many systems with high complexity, the picture they portray is incomplete and requires additional elements to derive causal explanation or prediction from them.

The research described here concerns itself with a third alternative aimed at drastically improving our understanding of apparently intractable and unrelated phenomena across various systems through the lens of existing theory and practice where random noise, hierarchical modularity and irreversibility dominate the structural organization and dynamics of many interacting entities acting in some coherent and coordinated manner: we refer to them from here onwards as *complex multiscale stochastic systems* (CMSS). In this introductory article we provide a definition of CMSS instances

5.2 Complex Multiscale Stochastic Systems

In order to provide a unified account of phenomena and systems as varied as those mentioned above, we focus on understanding the properties of CMSS. We start by defining complex, multiscale stochastic systems (CMSS) as the class of systems –whether natural, artificial or informational- whose structural organization is best described by nested hierarchies of constituent systems, comprised of objects and relations subject to non-negligible and intrinsic random noise, and bearing recognizable collective identity[18]. Some of these systems have evolved in a biological sense, others have arisen from the combination of physical laws at different scales and, in many recent cases, these systems are being engineered by humans. Some CMSS are still in their infancy and have not reached sufficient critical connectivity for emergent phenomena to arise.

We observe that these systems exhibit four critical properties:

1. **Composition.** A large variety of objects and object types, driven by processes, that interact with each other in non-trivial manners.

2. **Multiscale structure.** Their structure and behavior can be described at several nested, coupled scales of aggregation by different principles and laws, yet their action remains causally connected when looked at from the outside.

3. **Stochasticity.** Random perturbations can initiate and drive sudden changes in the internal structure or dynamics of the system, leading to uncertain measurements that demand statistical treatment.

4. **Overarching laws.** CMSS obey the laws of thermodynamics: local conservation of energy (First Law) and thermodynamic irreversibility (Second Law).

CMSS dissipate heat thanks to their fractal structure[19], hence producing entropy. Living organisms[20] in general and the brain in particular[21] organize in fractal and hierarchical ways. Action in CMSS follows trajectories determined by the Maximum Entropy Production (MEP) principle, which appears to create the context for the emergence of information processing[22]. Information in dissipative systems (i.e. those with friction and irreversible energy loss) often exhibit hysteresis and are characterized by one or more sources of noise for which dampening mechanisms exist at some phenomenological level. We stress here that in all prior

CMSS examples our understanding of their integrated phenomenology in relation to entropy production is still at its infancy. Moving from infancy to adolescence depends on finding efficient ways to exploit general properties of underlying governing laws, and the relations between objects at different spatio-temporal scales as experimentally measured.

5.2.1 Complexity

Succinctly, a system is complex if the laws that govern the trajectory of parts do not permit a straightforward reconstruction of the trajectory of the complete system[23], and simultaneously some type of organization is recognizable[24]. Care must be exercised not to confuse the *apparent* complexity of simple dynamical systems[25] with that studied by systems captured by complex networks[26]: we wish to study systems such as clocks, made by a thousand interacting parts, instead of describing the movement of a single hinged pendulum. The complexity of the systems of interest here is beyond apparent; it manifests in their structural and dynamical properties and to some extent is captured by analogues of algorithmic complexity[27]. Moreover, the kind of complexity that captures the interest of this work is that which is simultaneously hierarchical in its structure, emergent[28] and adaptive[29] by virtue of its governing laws and composition. CMSS also manifest decentralized control strategies[30] that sustain the efficiency of internal processes by exploiting their modular structure[31] through internal communication mechanisms. While some aspects of the energetics[32–37] and the dynamics[38,39] of systems in general have been explored through statistical physics, we lack a unified relational view of CMSS where causal relations provide information towards prediction, analysis and retrodiction based on empirical findings.

5.2.2 Multiscale structure

A complex system is also multiscale when (a) more than one valid account of same system can be given using phenomenologies that involve objects, relations and dynamics that differ widely in spatial and/or temporal scales, (b) the collective effect of governing laws and objects at one level (i.e. microscale) can be mapped to a single, much larger persistent objects at the next level (i.e. macroscale) whose properties cannot be additively explained from objects, relations and dynamics in the former one, (c) changes in a significant[ii] proportion of objects in the microscale lead to distinct and mutually exclusive macrostates under certain critical conditions (i.e. phase transitions), (d) scales of structure and action can be ordered according to the amount and nature of information that can be extracted from them and (e) the architecture of the system is modular and nearly decomposable[40], leading to information representations[41] while still determined by

[ii] *Significant* depends here on the particular system, its scales and laws proportion. What we claims is that, if a complete theory of CMSS exists, it must provide a way to compute the threshold for significance of a given current proportion.

irreducible couplings. CMSS tend to be extremely effective entropy producers[42] that actively preserve internal stability through various mechanisms. Part of the reason seems to be connected to the numerical relations derived from their structure as described by either Zipf's law[43], power law[37] or Rent's law[44].

Network science has enabled the development of various methodologies capable of extracting putative structures of complex multiscale systems from data in various knowledge domains[45]. Linking many relevant scales and including dynamics, however, remains limited in practice mainly because of the combinatorial explosion derived from keeping record of the links between different objects across scales. Partial solutions to this problem often rely on pragmatic choices that include neglecting scales, objects or relations, devising sampling strategies while preserving the general phenomenology or focusing only on one level of description to focus on a certain regime of applicability. Still, mounting research on many disciplines including physics[46], chemistry[47], biology[48,49] and socio-technical systems[50] indicates that current multiscale methods face a growing number of challenges. Two specific issues are how to devise empirically correct mappings between microscales and macroscales that capture all relevant details without sacrificing efficiency, and understanding how the underlying laws of motion at one microscale constrain or determine laws at the corresponding macroscale.

5.2.3 Stochasticity

Stochasticity refers to the presence of non-negligible noise in the dynamics of a system, often associated with nonlinearity[51]. For a system to be stochastic, two types of forces must be present: drift forces that bias the motion towards some preferential direction and diffusion forces that randomize the overall trajectory of the system[52]. If noise levels are small enough and fluctuations are not amplified (e.g. through multiplicative terms in the driving forces), then the system can be treated as deterministic for simplicity. However deterministic representations suffer from a deep theoretical flaw. Because they are reversible they violate the Second Law of Thermodynamics. Essentially they are an extension into dynamics of complex systems of the concept of the "frictionless plane" that is often introduced in introductory physics courses. Just as one would be skeptical of the performance of a machine engineered based on the assumption of zero friction, so should one be skeptical of descriptions of complex systems based on deterministic models. Specifically in CMSS the magnitude and frequency of fluctuations is often large enough to prompt signal propagation and autonomous reorganization through stochastic amplification[53–56]. In such conditions, CMSS entities and dynamics appear to become organized into discrete units[57] –i.e. modules- that maximize internal stability in irreversible ways[58]. It is known that stability increases exponentially in complex discrete systems whose structure is described through subsystems[59], even those that contain nonlinear elements driven by time-dependent gain functions[60]. The combination of these elements produces a rich landscape of possible decentralized control strategies[61]. At present, the main challenge stochasticity introduces resides in the mathematical incompatibility of noise with the usual form of equations of motion and the computational complexity associated to finding solutions in CMSS.

5.2.4 Summary: the need for a science of CMSS structure and function

Due to multiple scales, noisy and nonlinear dynamics, and hierarchical nature of CMSS, restricting ourselves to simplified models mostly ends up in sub-optimal solutions at best, and non-solutions often, to the problem of finding empirically relevant causal mappings across scales. In this proposal, we focus on describing various examples of how –and most important why- simplified theories and models fail to capture essential empirical aspects of CMSS. In systems with highly coupled positive and negative feedback mechanisms (e.g. *wicked problems*), the density of true solutions for many problems tends to vanish compared to the size of the search space[62]. However, many pressing issues in contemporary social, economic and environmental research and practice require true solutions to avoid financial, human or environmental losses.

If the principles that govern CMSS were accessible in terms of causal mappings between microscales and macroscales, gaining information about phenomena would only be a matter of computing consequences of the respective theories confident that the observables will likely be consistent with empirical measurements, including changes and their occurrence thresholds. However, finding theories that integrate nicely and universally at extreme regimes of action (e.g. quantum-classical systems) have not been found. Changes at the microscale usually involve classes of entities or relations rather than on single objects, yet many cases exist where small events (i.e. localized, unique and often very improbable) are sufficient to trigger large changes across the system[63–65]; catastrophe theory has remained an evolving field that attempts to deal with sudden changes in systems, but its description is at the macroscale and phenomenological in nature[66]. Catastrophe theory often focuses on identifying conditions under which deterministic descriptions of dynamical systems fail, but the theory itself fails to provide an alternative description.

Our understanding of the causality of events and relations in CMSS remains limited and largely disconnected. When a system reaches a certain critical degree of complexity, it is not easy (or sometimes even possible) to accurately reconstruct the trajectory of events that lead to the current state. More importantly, even with such information, there is no guarantee that the available theories –most of them formulated as systems of differential equations or assertions about networks- will integrate nicely. The state of multiscale modeling in most areas is that of constructing a theoretical *patchwork* that must be painstakingly mended to avoid breaking apart as revealed by contemporary multiscale modeling of complex materials as an example[67].

Changing this situation –the main objective of this proposal- is critical for the solution of many challenges of intellectual and practical importance in our century.

5.3 Current problems with CMSS models across scientific theories

The Internet, cells, ecosystems, the global economy and many other CMSS examples are characterized fundamentally by local exchanges of matter, energy or information between smaller components at all scales. Each exchange, whether evolved or designed, is constrained by governing laws of the interacting entities –or rather, the laws of their substrates which allow some notion of identity- and at the same time collections of these exchanges provide the basis for emergent constraints at critical system sizes and densities (i.e. their thermodynamic limit). We concisely review here how various interactions are addressed through various scientific fields, including how their representation and suppositions may be limited in each case. In essence, we argue that the structure of interactions is either represented explicitly without a concise explanatory picture of their dynamics or captured by detailed dynamics without any reference to its structure, becoming problematic for the purpose of having effective and efficient ways of understanding phenomena in CMSS.

Methodologically, we explore in detail the existing set of alternatives to model CMSS across various domains. First, we make explicit various assumptions about the character of dynamical equations in the context of creating effective models for CMSS. Second, we unmask a series of biases that simultaneously pervade and negatively impact the ability to reason in empirically correct ways about CMSS phenomena. Finally, we discuss the most relevant representations of interactions across the natural and social sciences.

5.3.1 On the character of dynamical equations *vis-à-vis* CMSS

The study of fundamental relations between energy, information, time, matter and space has led to the discovery of two types of symbolic descriptions: those that pertain to concrete realizations of physical systems and those that pertain to *abstract* classes of physical systems that ubiquitously constrain all concrete ones[68]. Correspondingly, these relations are expressed in one case as sets of dynamical equations and as physical laws in the other one. A set of dynamical equations is expected to be valid only in relation to specific settings; physical laws are more general, and the laws of thermodynamics are universal.

The usual route to arrive at specific sets of dynamical equations in contemporary physical sciences has been to depart from one of at least three starting points: its Hamiltonian[69] (i.e. a function of potential and kinetic energy), its Lagrangian[70] (i.e. the functional that assigns a value to a configuration of the elements of a system depending on its laws of motion) or its symmetries[71] (i.e. equivalence relations in the manifold and their consequences for motion). The existence of the three of them depends on conservation laws that ensure that no amount of motion will remain unexplained under a closed system, whether locally or globally[72]. Conservation principles have been used used to process trajectory data of various systems to construct nontrivial useful theories in the form of laws; generalizations which are mostly true in many instances and can be used to organize knowledge. Whether by manual or automatic means, the existence of such laws is assumed and they are sought, generally to apply to one level of system behavior.

In the context of CMSS however, characterizing the system at its outermost phenomenological level can be problematic. Choosing a level of description implies selecting certain aspects of reality, including the collection of conservation laws that apply at each level. When couplings between various scales occur, it may be either impractical to compute the consequences of laws of motion for many entities or unrealistic after simplification. More importantly, the form of the laws (and correspondingly of the dynamical equations) is of little help when stochastic fluctuations are dominant at the scale of interest. When two or more scales are included, different types of equations and laws are discontinuously patched together through approximations which lead often to semi-empirical solutions that work only for reduced regimes of action.

Yet, the existence of critical phenomena and phase transitions across a multitude of systems and scales (from the cosmological to the quantum)[73] indicates that despite complex systems being nearly decomposable[40,44] they should be treated as emergent, including their governing laws. Our perception of nature as a collection of nearly decomposable systems appears to arise from our perceptual biases, the law of large numbers and the exponential decay of large deviations arising from stochastic fluctuations[74,75]. Adaptive emergence may trigger aggregation as a way to minimize action globally across the system as a means to reach regions of dynamical stability[76]. Hence, the likelihood for any arbitrary set of theories, each of them applicable only to a certain scale of action in a system –especially those that have been obtained through experimental observations at only one such scale- to integrate nicely and describe CMSS adequately (including detailed mechanisms) appears to be slim and decreases in an inversely proportional fashion with the number of scales involved.

Many, perhaps most, descriptions of dynamical systems are made through differential equations, and most often through deterministic ones. Arriving at the appropriate set of them is the bread and butter of modeling from physics to social science. In order to understand at greater depth what is involved in the choice of sets of dynamical equations, we concentrate next on their representation relative to the view of the universe as emergent from a set of fundamental laws of nature. The first two elements to be considered are concerned with how the form of the equations is derived. The third element is the determination of whether transformational pre- and post-conditions can be recovered from differential equation models. Finally we will consider physical laws as dynamical extrema under the law of large numbers.

The manifold choice problem

Let us consider the case of the classical N-body problem, known to be non-integrable for $N > 3$. At any time the 3D manifold contains N particles, with resulting embedding of $3N$ degrees of freedom in total. The embedding itself is described as a vector product $\mathbb{R}^N \otimes \mathbb{R}^3$ of two vector spaces, that of the system of coordinates for one particle $\mathbb{R}^3$ and the collection of all particles $\mathbb{R}^N$. In general, any non-trivial motion can be described for one particle by adding its momentum to the position, leading to $\mathbb{R}^{6N}$ simultaneous variables to keep track of. Solving this computationally expensive problem is well known in computational molecular dynamics[77,78].

The input of the N-body problem consists of the initial positions of all the particles, the function for the pairwise (or k-wise) interactions between particles and the description of the energy potential surface. The more exact the model, the more computationally expensive it becomes, since the coupling of all forces (e.g. ion-induced dipole, ion-dipole, electrostatic, and van der Waals forces in molecular dynamics) in conjunction with the geometry of the objects can quickly lead to many correlations impinging on one another in small portions of the volume of interest. When the forces act at a short range (e.g. van der Waals), the problem is simplified by modeling its action with cutoff functions. In the presence of long-range forces the cutoff leads to some error which one seeks to minimize by an approximate accounting for surroundings, but some residual error is unavoidable..

Let us pause for a moment and consider various systems described by the same Hamiltonian. If we assume only classical forces are at play, all systems of interacting particles are captured by it, from very dilute gasses[79], liquids[80], metallic solids[81] to core-shell nanoparticles[82]. Four distinctively different classes of systems are captured by the same physical model, yet the complexity associated with solving their systems of equations varies drastically on each case. Given that pressing practical questions often depend on their solution, finding the smallest embedding that preserves all the features of the original system is advisable.

The problem above may be stated as that of finding an appropriate scaling relation, or a renormalization group (RG) whose effect is drastically reducing the degrees of freedom while providing a good approximation[83]. The scaling relation should provide three advantages: (1) reduction of the number of particles or degrees of freedom through a mean field theory, (2) identification of the critical exponents that dominate force ranges and (3) analysis schemes to reveal the emergence of structure. For the N-body problem with long-range correlations, a formal RG only makes sense with a few bodies (often $N \leq 4$)[84–86]. For systems with high thermal motion, RG reduces to some form of noise across the problem domain. In both cases, information loss is guaranteed in some form of another.

On the other hand, classical mechanics provides plenty of examples of scaling relations that, although not thought of immediately as emergent, produce the same outcomes at the scale of interest and are simple to compute. For instance, take a metallic solid under translation and rotation forces. Any transformation applied to the solid is propagated across its structure to each one of its constituent atoms. Suddenly, the $\mathbb{R}^{6N}$ manifold for its dynamics reduces to $\mathbb{R}^6$, no RG required or evident at first glance. A similar case occurs for laminar flow with a suitable Reynolds coefficient, in which the dynamical equations reduce to $\mathbb{R}^2$ or even $\mathbb{R}^1$. Those are indeed extreme cases of scaling relations, the last with an effectiveness of $1/6N$; consider the implications for laminar flow of one liter of water along a pipe ($N \approx 3.346 \times 10^{25}$ water molecules). It should be noted that this simple renormalization is strictly true only for a metallic solid of infinite size or laminar flow through a pipe of infinite length.

What fundamental properties of the universe as the archetype of self-organized criticality at all scales justifies such choice of degrees of freedom different from detailed descriptions of phenomenology or equational parsimony? The intuitive answer appears to be that some classes of self organization lead to collective identity[87], defined as the ability of an entity to retain its structure and functions for long periods despite small perturbations. Hence, alternative models and representations of systems that may deviate from the underpinning reality become physical fictions. Such is the case of metallic crystals[88]: atoms are assumed to "jiggle in place" in a rigid lattice of (fictional) harmonic oscillators connected by springs governed by Hooke's law. A great deal of progress in crystal physics has been made in this fashion[89], driving a large share of the present digital revolution. The springs propagate external perturbations and, at the same time, fix the global geometry of an object in place by damping propagation to adjacent atoms. The object acquires identity, and the effects of the rotation and translation of an object in $\mathbb{R}^3$ are nicely translated simultaneously (at least with respect to measurements performed at the macroscale) to the $\mathbb{R}^{6N}$ particles.

CMSS appear to lie in the middle of both purely elastic molecular collisions and metallic solids when viewed as an $N-body$ problem, yet their complexity is much higher than that in either extreme. Hierarchical modularity increases the likelihood of finding a scaling relation, but it enters immediately in tension with randomized interactions between levels of the hierarchy. In addition, and in contrast to the types of questions posed on systems modeled through the N-body problem, CMSS are interrogated simultaneously at multiple levels and not only at the bottom or the top of the hierarchy. Since one macroscale may be explained by a large number of equivalent microstates while events at the mesoscale remain of importance, keeping track of all entities in the hierarchy becomes a difficult task.

Concisely, except for various well-known limiting cases, finding scaling relations that yield an economic and representative manifold in hierarchically coupled systems is not a systematic process as long as Hamiltonians (or equivalent formulations) are used. Solutions are achieved by either constructing relevant abstractions (e.g. ordered lattices) or by losing information through the reduction of degrees of freedom. At present, such essential processes for finding the most efficient and realistic manifold for CMSS instances are unknown.

The functional choice problem

Once the the manifold is chosen along with its embeddings, the next step is to determine –based on empirical observations- the most appropriate mathematical description of the phenomenon. Again, conservation laws, invariants and symmetries are the standard tools most theorists have access to for devising the equational form of the governing laws at present[90]. In the case of physics –and back to the N-body system in particular- the choice of dynamical functions occurs in a way that (a) accounts for both potential and kinetic energy present in it, (b) dictates the specific laws of motion for each body through application of differential operators to the main invariant, (c) provides coefficients that represent material aspects of the system. By fixing them, one can parameterize the equations of motion to the particular instance. Motion, in this sense, is represented as the trace in time of positions and velocities either through time series (i.e. position or velocity per every time instant) or phase diagrams (i.e. reachable states as represented by statistical properties).

As discussed above, interactions appear to be mostly hidden in dynamical descriptions of CMSS, or may be neglected. In the case of a pendulum, it is not easy to derive a picture containing interactions, yet many certainly exist. We can imagine interactions between the pendulum mechanism, the pendulum and the air (when the experiment is not carried in vacuum) and the interactions between the atoms in the rod and the bob. However, that information is unavailable, or rather is *obscured* by the emphasis on position and momenta. Fourier analysis has become a standard tool[91] that uncovers the frequency of events in a system, from which interactions can be derived to some extent. Detecting the frequency of events is a starting point to the investigation of their mechanisms and internal dynamics. Both the time series and the frequency domain representation are naturally expected to be much richer and harder to unravel for CMSS.

The evident limitations of dynamical models of systems for capturing interactions requires some historical investigation about their origin. Our modern depictions of dynamical systems, and of motion in general, can be traced back to Descartes[92] and his philosophical investigations on the material conditions required for a science of motion. His analytic geometry[93] provided a foundation benefiting from both geometry and algebra as means to understand motion as a sequence of instances, each one of them localized at a given instant of time. Representing motions as functions was only natural after this, presupposing that motion at any given future instant was predictable from motion at previous instance provided the universe contained some sort of regularity. Note that this particular definition of motion does not require any reference to interaction (or rather, a model of it) to be considered complete. In that sense, choosing the functional form to describe the motion of a dynamical system immediately refers to the selection of the appropriate number of spatial dimensions such that, at every instant, the position of an object can be located and its future position for any given time step can be known using information from the present and the past. Newton's Principia[94] adds the concept of interactions with a functional form and thus represents the pinnacle of this sort of mechanics, providing a mathematical toolkit capable of answering questions about position, velocity and momentum at any instant provided the functions were guaranteed to be continuous.

However, even at the time in which the Principia became popular, important objections were raised by Leibniz's[95]. Disregarding interpersonal disputes and feuds[96], two of the limitations he stated of Newton's mechanics would remain valid criticisms centuries later: (a) the mathematics of the Principia could not easily account for the material constitution of objects –or its internal motion if any- and, most importantly, (b) it disregarded completely the relation between entities and objects. The foundations of Leibniz's scientific work were placed on the putative existence of relations between objects as defined by changes in their properties, which could be identified as motion when these properties were represented in a Cartesian manner. However, the lack of impact and success of his theory of relations –in contrast to Newtonian mechanics- appears to have been largely due to his inability to articulate what interactions *are* instead of what they *are not*[97]. In that sense, Leibniz was unable to provided a computable account of motion starting from relations, and his notion of interacting bodies became confounded often with his interacting monads, which pertain to formal logic[98]. As an addendum, Fourier showed that trajectories could be reversibly converted into frequencies, which when taken at infinitesimally small intervals, resembled discrete events[99]. The latter would be used extensively by Dirac[100] through his delta function to give operational meaning to interactions in quantum mechanics.

With the advances in the mathematical language of calculus and its increasing use in science and technology, the representation of motion as trajectories that are constrained by laws and given by differentiable laws of motion became the rock on which Maxwell's work on electromagnetism[101] stands. However, the renaissance of atomic theory through Boltzmann's equations[102,103] for the theory of gases gave way to the possibility of computing thermodynamic quantities in a straightforward fashion restricted to gas molecules that do not interact, which only holds for ideal gases. In order to include interactions, nonlinear (e.g. product) terms need to be introduced in the equations of motion, and the information that can be obtained locally is how the particular force involved (for instance, electromagnetism) would be rendered in space-time as a landscape of potential energy with valleys and peaks. The latter does not only leave the problem of describing the *internal mechanics* of interactions unsolved, but also makes their numerical treatment intractable for many molecules. At present, the combinatoric explosion that arises when simulating CMSS with many scales and classes of entities using Newtonian mechanics is a particular case of the latter problem[104].

Ernst Mach's[105] objections to the foundations of mechanics between the XIX and XX centuries rested on the same arguments that Leibniz had raised, only in a slightly different form. Ignoring interactions, or rather the composition and properties of the relations between objects, leaves a plethora of unanswered questions and a complicated mathematical conundrum. For Mach, the ultimate form of any law of nature should be given in terms of properties of one system in relation to other systems. Einstein's special[106–109] and general relativity[110–112] were non-obvious but natural extensions of Leibniz and Mach insofar as the principle of relativity was applied to frames of reference, which led to the interpretation of space-time as a dynamical entity. The objects that interact in general relativity are frames of reference and the messengers are light particles. By sending photons and experiencing internal changes, one frame of reference exerts a causal effect on another frame of reference. Although actual computations are performed by unfolding the tensor expressions into their full differential form, the most relevant representation is given by the metric tensors that indicate how energy and matter constrain space-time. These expression are compact and appear be universal.

The development of quantum mechanics required inevitably describing interactions (i.e. measurements), and marked, with relativity, one of the two most prorfound revolutions in thinking about the physical world of the twentieth century[113]. The necessary introduction of probability in the laws of motion, based both on wave equations and positions/momenta required several amendments to Cartesian spaces in order to cope with singularities and discontinuities[114] arising from intrinsic randomness and wavefunction collapse. Quantum theory showed that posterior mutual state relaxation in the form of decoherence[115] is a fundamental property of interactions below the atomic scale. Quantum field theory[116] is one of the most accurate formulations of reality in existence today, based on a model of interaction between fields that, when observed by a system, produces particles corresponding to field excitations. However, the transition functions still refer to elements of the Cartesian view and their effects are expressed as changes in the geometry of the fields rather than the changes in the entities themselves. The situation appears to be no different in modern particle physics[117], where Feynman diagrams are used to derive gruesome expressions posing a myriad of challenges when using the Standard Model to obtain particular solutions that explain experimental data. Although these are the two most successful theories in the physical sciences, some of their remaining limitations can still be traced thanks to Leibniz's objections.

Regardless of the theoretical background, two types of problems remain. First, the practical choice of parameters to accompany the functional descriptions is expected to be a matter of experimental verification through fitting. Nevertheless, CMSS instances pose challenges in this stage for a variety of reasons. For instance, it may be hard to differentiate parameters pertaining to two different trajectories that are spatially close at a measurement time, requiring a large number of measurements for their differentiation. It is not always possible to obtain good, repeatable experimental measurements. Second, two deeper theoretical problems arise in connection with the search for appropriate functional choices. The form of the laws must be guessed at some level with only circumstantial information from more fundamental scales, but the apparently connected structure of the universe[40,73] and the Correspondence Principle in quantum mechanics[118,119] suggest that physical laws are dynamical extrema at the thermodynamic limit. The form of that limit, however, can only be guessed for systems of simple particles and homogeneous interactions (if any). An open question is whether the number characterizing the thermodynamic limit for a given system (e.g. a CMSS) is system independent or is a function of the types and diversity of interactions. The second problem is the apparent independence between laws at the microscale and the organization of systems at the macroscale: if the macroscopic laws are independent from the physical substrates, then either the scales of organization cannot be truly connected, or the formulation of the laws are biased by our selection of relevant entities at the microscale[120]. We are inclined to support the latter rather than the former, since the possible formulation of interactions as Barabási networks suggests that laws appear to be topologically connected through substrates and bridge equations.

Although it is common (and correct) to think of macroscale properties as emerging from microscale objects and connections, in nature the macroscale exerts a formative influence on the microscale through adaptive evolution. In constructed systems desired functional attributes plays the same role as adaptive evolution in constraining the nature of the microscale subsystems.

In summary, our usual choice of dynamical functions is most frequently determined by the Cartesian view of motion as trajectory, and the emphasis on their prediction and retrodiction rather by interrogations of its properties or structure. In most theories, interactions are either entirely neglected or indirectly represented by transition functions that refer to changes in fields or potentials, both contained in generalized versions of Cartesian spaces. Maintaining this view limits the possibility of understanding systems of larger complexity, either because of the combinatorial explosion of calculations or because of the inability of our methods to efficiently traverse the granular landscape of the resulting potential energy surfaces. A focus on interactions and relations between objects has brought significant understanding of the natural world on previous occasions, but interactions largely remain circumstantial, derived or implicit despite their fundamental character.

Our aim in this project is to provide an alternative view of motion in CMSS where interactions put at the center or descriptions or nature and are explicitly described, investigated and operationalized.

Pre- and post-conditions from dynamical equations of motion point to opaque interaction mechanisms

The formalization of CMSS using sets of deterministic differential equations is thought to express instantaneous rates of change. Let us suppose that a given CMSS is studied using ODEs for the present argument. Take a simple ODE such as

$$\frac{dx(t)}{dt} = f(x,t) \tag{5.1}$$

and, for the moment, remove concerns about the specific properties of $f(x,t)$. At first impression, this may be thought of as a definition only that encodes two statements: one about equality between two quantities and one about dynamics. The transformation f, dependent on x and t, can be intuitively thought of as either a fixed relation in the $(t,x(t))$ manifold –more properly a graph of such instantaneous relations– or a unique trajectory across the manifold. However, when we expand the definition of $\frac{dx(t)}{dt}$ into Eq. 5.1

$$\lim_{\alpha\to 0}\frac{x(t+\alpha)-x(t)}{\alpha} = f(x,t) \tag{5.2}$$

it becomes clear that, for the limit to exist, both sides of the limit must converge to $f(x,t)$ from the left and the right simultaneously. Recalling that $|\alpha| > 0$ and $|\alpha| \to 0$ in order for it to be an infinitesimal, we may think at any given moment that, for any $\alpha^- = -\alpha$ and $\alpha^+ = +\alpha$ it must be true that

$$\frac{x(t+\alpha^-)-x(t)}{\alpha^-} < f(x,t) < \frac{x(t+\alpha^+)-x(t)}{\alpha^+}. \tag{5.3}$$

More generally, we may think of α as the limit of a Cauchy sequence $\alpha = \lim_{n\to\infty}\alpha_n$ with $\forall\alpha_i.\alpha_i \neq 0$. Hence, we may think of the left and right limits more properly as

$$\frac{x(t+\alpha_n^-)-x(t)}{\alpha_n^-} < f(x,t) < \frac{x(t+\alpha_n^+)-x(t)}{\alpha_n^+} \tag{5.4}$$

and, after reorganizing terms,

$$0 < f(x,t) - \frac{x(t+\alpha_n^-)-x(t)}{\alpha_n^-} < \frac{x(t+\alpha_n^+)-x(t)}{\alpha_n^+} - \frac{x(t+\alpha_n^-)-x(t)}{\alpha_n^-} \tag{5.5}$$

the last term in the inequality can be interpreted as a time equivalent to the center of mass (i.e. CoD:

"center of dynamics")

$$\mathrm{CoD}(\alpha, x, t) = \frac{\alpha_n^-[x(t+\alpha_n^+) - x(t)] - \alpha_n^+[x(t+\alpha_n^-) - x(t)]}{\alpha_n^- \cdot \alpha_n^+} \tag{5.6}$$

which can be given the following interpretation: the CoD is the centroid of the interval that bounds $f(x,t)$ to the left by an event $x(t+\alpha_n^-)$ and to the right by another event $x(t+\alpha_n^+)$ for any $a_n > 0$ in the corresponding Cauchy sequence. To that extent, independent of how small α_n^-, α_n^+ become as given by approximations of the sequence, both bounding points are identified and have a definite value. It is then possible to label α_n^- as a pre-condition and α_n^+ as a post-condition. Even with the instantaneous mode of action expected of Newtonian mechanics, pre-conditions and post-conditions are inescapable. In practice, this becomes more evident by the suitable choice of the integration algorithm and the integration step. One or more past points in the trajectory and estimates of one or more future points in the trajectory are used to compute the current state of the system[iii].

What information is then contained in dynamical equations, and more importantly, what information is excluded? From the discussion above, sets of coupled deterministic differential equations do contain an implicit specification of local pre-conditions and post-conditions at every point in the manifold where the action functional is defined. We must note that, in terms of causality, trajectories are not contingent on external factors in Newtonian mechanics –they are inevitable- but at the same time every point in the trajectory appears as if it were contingent on the (densely) immediate past. Also, these equations provide a global geometry, a field that strictly conditions the set of all possible trajectories for a given set of parameters; this does not, however, ensure that the trajectories will be sensible always or that local information suffices to predict behavior at large. Even if the equations govern the trajectory of one entity instead of the evolution of sets of entities described through proportions, there is no information whatsoever about how entities are internally structured, how their properties vary by being in contact with the medium as captured by the manifold and, in the case of coupled equations, what types of interactions lead to the coupling itself.

In summary, deterministic coupled differential equations contain a normative prescription for the action in a system by describing possible trajectories under fixed parametrizations. However, the equations themselves contain no information about mechanisms that explain the form of differential functions (validly interpreted as a transformation of state), the connection of the medium of action and the entities that explains the metric that arises under integration, and how the magnitude and frequency of couplings occurs as given by covarying quantities or proportions in a system. Intuitively, the latter framework should be considered as

[iii]Pragmatically, however, equations for the current state under computation are performed for $t + \Delta t$ with Δt being the time step.

extremely limited to describe CMSS phenomena.

5.4 Interactions: a theoretical inventory

Interactions are necessary to understand all phenomena across the natural and social sciences. However, their representation is not transparent in terms of internal structure or processes, and in the majority of cases their presence is inferred indirectly from dynamical equations that focus on the trajectories of systems, their components or statistical correlations. Moreover, interactions in quantum mechanics and field theory are represented by unitary transformations that dictate how a prior state transforms into a posterior one without accounting for the mechanics of the change in a direct or detailed manner. A subset of social theories explicitly model the dynamics of the interactions locally, but are yet to produce an integrated understanding of the dynamics and possible macroscale configurations of social systems at large. Changes in the *modes* of interaction of simpler parts of a system, however, have been experimentally shown to have aggregate or collective effects in the system as a whole. The following is a detailed description of how scientific disciplines capture interactions according to their theoretical concepts and tools.

5.4.1 Statistics

In statistics, interactions are modeled by non-additive correlations between two or more variables either explicitly through their product, or transitively by composition of other products[121,122]. Many statistical models follow the Fisherian (i.e. frequentist) approach that asserts the statistical significance of events[123,124] by computing values of various statistics and their various moments. Its main sources of trouble are the inability to straightforwardly link statistics to observables in a system, and the need to assume normally distributed data for many of the interpretations to be correct while non-normally distributed data dominates empirical observations. Statistical models (possibly capturing the effects of interactions indirectly) often require dummy variables with no phenomenological significance for a good fit[125].

Mixed models containing positive and negative regulatory effects of interactions may not lead at all to statistically significant conclusions for complex situations[126]. When the interactions are complex –beyond two-variable couplings- computational cost grows exponentially[127]. Various methods and heuristics are used to give structure to the statistical search space based on parsimony as a desirable property of good models[128,129]. Nevertheless, the problem of deriving mechanisms from statistical models for a given system –assuming interactions exist- in a more direct way[130] remains open in Fisherian statistics. The needs for analysis of ever-increasing datasets in biology is suggestive of the latter[131]. Bayesian[132] and non-parametric[133] statistics have arisen and matured as responses to some of these limitations.

5.4.2 Computing and logic

In computer science and formal logic, interactions have been defined multiple times in relation to hardware, formal descriptions of computations, events in software systems, or their various combinations. The geometry of interactions[134] in logic attempts to capture the causal effect of sequential steps in proofs, where proofs are actions denoting observable transformations of statements grounded on an underlying operational semantics. In the classical theory of computation[135], a Turing machine measures (i.e. interacts) with an infinite tape with cells that contain symbols: the measurement is used by a transition function to select the next state through pattern matching and its posterior selection of the associated action (e.g. read, write, move left, move right, halt). Consequently, the Turing machine is one example where interaction mechanisms in imperative programming are entirely visible thanks to the simplicity of the components and steps required to implement the robotics (i.e. automatizable manipulation) of symbolic pattern matching. In object oriented programming, the effect of a program –as formalized in sigma calculus[136]- is a result of the interaction between s random-access memory (RAM), a stack and a set of instructions that specify how the internal state and the computer (i.e. stack + RAM) are simultaneously modified under appropriate conditions. In constraint logic programming[137], not only proofs are sequences of action that capture the interaction between denotational and operational contents of programs (e.g. the interaction between knowledge bases with rules of inference[138]) but they are bound by the contours of internal laws (i.e. constraints) that prevent or allow only certain interactions to occur. Finally, monads were introduced in lambda calculus and functional programming languages as a means to express interactions between purely functional programs and operations that alter the machine state (i.e. the outside world) through persistent, secondary effects[139].

With the development of distributed computing and information systems, their interaction became a significant area of research[140]. Milner's seminal Turing Award Lecture[141] recognized the need for a theory of interactions in computer systems beyond C. A. R. Hoare's foundational work con communicating sequential processes[142]. Simultaneously, actor-based parallel programming models for distributed systems were developed based on various empirical observations that collections of agents can achieve coordination as a result of the product of their internal (active) state and the messages being exchanged between them[143]. The expected internal complexity of agents can be derived through the law of requisite variety[11] as well as through measures of effective complexity of systems[144]: the information content of the control of a distributed system is proportional to the information required to describe its state and dynamics[145].How interaction patterns determine the dynamics of a distributed system is a well-established research area at present[146].

Research on distributed systems has also focused on modeling and expressing interactions through programming languages[147,148] and their semantics[149,150], necessary to build and execute computer experiments that probe their effects controlled ways. Another view on distributed systems has been developed from organization theory by attempting to understand how organization patterns emerge based on which interactions are present and what the responses of the agents are[151], similar to what happens in human organizations. The latter has been critical to postulate and simplify the process of reasoning about collective and emergent properties of distributed systems in a succinct and intuitive manner[152]. Establishing causality in distributed computing and information systems, despite their simplicity in comparison with other types of distributed systems in nature, has proven to be a hard problem. Lattice theory and discrete time[153] have been used to understand collective problems in distributed information systems, which appear to strongly depend on whether interactions are synchronous or asynchronous[154]. An interesting aspect that has been explored is how law-governed interactions shape coordination and control[155], similar to what occurs in physical and biological systems with direct applicability to cyber physical systems[156]. In terms of theoretical advances, tangle machines[157,158] a model based on the intersection of interaction histories as processing.

5.4.3 Social theory

The literature describing social interactions is vast, spanning microbiology[159], developmental biology[160], neuroscience[161], primatology[162,163], human psychology[164], linguistics[165,166], social science[167,168], organization theory[169–171], economics[172,173], policy-making[174], Internet-based communication[175,176], complexity theory[177] and more recently discussions of how humans[178–180] and robots may coexist, to name a few. Identifying[181–183] and measuring[184] social interactions –and their effects[185]- is central to converting observations into reliable data to either postulate new theories or to put existing ones to the test. In contrast to the situation in the physical sciences, describing and understanding interactions (e.g. their structure, transformations, regularities) between two social agents has proven to be somewhat tractable and useful compared to efforts that have focused on obtaining governing laws. These laws are generally expected to be emergent and its form depend on the internal properties of agents and evident from various collective phenomena[186]. Social coordination is a prime example of collective behavior that depends heavily on the properties of interactions[187–190], which also appear to allow the existence of scaling laws of various types[191–193]. To that extent, social systems constitute a prototypical CMSS example.

Given that one aim in this project is to clarify the structures of CMSS that can be interpreted simultaneously through both network and dynamical theories while remaining agnostic of particular substrates –systems in which interactions among agents appear to be crucial-, we have chosen three particular views on social systems as the most relevant descriptions of social individual and collective organization: Luhmann's systemic view of society[194,195], Berger's model of the function of communication as a form of interaction that decreases future uncertainty of encounters,[196,197] and Pentland's conceptualization of routines as recurring patterns of interaction that simultaneously endow systems with structure and flexibility[198,199]. Societies are complex systems in which events are coupled at multiple interconnected levels that are structured by self-organization mechanisms. These usually harness feed-back loops through coordination tokens (e.g. *messengers*) that are exchanged during the interaction and encode complex transformations. These tokens, to a large extent, summarize the abstract space of state transformations as given by past and future states of the system in relation to the message being conveyed. The token therefore also encodes aspects of the internal changes in each state (e.g. relaxation, new forms of self-organization) and causal properties of state transformations in other agents including its knowledge and actions. As ensured again by various measures of total information[144] and the law of requisite variety[11], we can known –at least approximately- the amount of degrees of freedom exchanged between both agents by analyzing the tokens. However, the exchange is often imperfect thanks to noisy channels (i.e. environmental perturbations) or problems of interpretation (i.e. encoding mismatches), extending the effects of uncertainty to all causally connected events in the system at various degrees. Considering routines as persistent interactions introduces frequency as a relevant factor, modulated by system size and diversity.

5.4.4 Biology

Interactions are essential in biology at all scales. In ecology, the largest class of interactions are defined between the ecosystem and evolutionary rules in a feedback cycle[200]. Species interact through the establishment of various relations, including predator-prey dynamics[201], parasitism[202] and symbiosis[203]. These relations exist even at the cellular level[204] and are complemented by chemically mediated interactions[205]. Within the environment of the cell, interactions occur in a complex biochemical environment articulated by molecular expression pathways whose activation is stochastic and threshold-dependent[206], and whose action is carried out by protein-protein interaction networks as determined by the affinity between various binding sites[207]. An estimate of 10^{14} atoms in a cell and a similar number of cells in higher organisms suffice to make numerical simulations intractable if all forces and interactions are included. However, hierarchical modularity also guarantees that approximate simulations of these systems or their components may be both tractable and remain biologically meaningful[208]. Multiscale modeling often help maintain consistency across all nested hierarchical scales without sacrificing good performance and repeatability. This network embedding can also be used to apply analogues of renormalization group theory to reduce complexity through mean-field approximations[209] that contain scaled down quantities of entities, interactions or even hierarchical levels while preserving the main character of events and relations present in biological phenomena. Life is a prime example of a coupled, multiscale problem. The longest relevant times scale in biology is evolutionary. Over time scales ranging up to millions of years, selection pressures applied at the macroscale in the form of environmental change select variations at the molecular genetic level that are manifest as changes at the organismic level.

At the most abstract extreme in the research spectrum, Barabási and Albert's seminal work on the emergence of scale-free networks[37] has been applied widely in biology, in particular to organisms as one of the most important mesoscales in biology. These systems exhibit organized complexity[210] arising from interactions that produce identity, robustness while remaining constrained by various types of underlying laws. Contrary to artificial complex systems, biological entities have emerged through evolution by natural selection, operating over whole ensembles of live entities. The rules of interaction follow the contours of laws that appear to emerge at more fundamental scales and are expected to define the ultimate boundaries of life itself. Cells are constantly subject a changing and complex environment whose response depends on stochastic delays driven by drift-diffusion forces, captured by Langevin equations[211]. At the same time, phylogeny suggests that selection, repetition and variation thread the fabric of biological diversity. Understanding the massive complexity and variety observed in living organisms is one of the most important tasks in biology[212]. It is also one of imperfect reconstruction of interactions of extremely modular[213] and plastic[214] systems. At present, one of the few principles that facilitates this reconstruction is Hennig's Auxiliary Principle, stating that sequence changes between genotypes are related to the molecular clocks in organisms[215], but more principles –and ideally, more evidence to support them- is required for a more solid scientific ground. We hypothesize that some of those new principles rest on properties and dynamics of interactions.

5.4.5 Chemistry

Interactions in chemistry at the atomic level are represented by various types of bonds, emerge from orbital structures[216] which determine atomic valence and polarization due to electron motion. Bonding is determined by the time-dependent energy potential surface mediating interactions, described as short-range forces between atoms. Predicting interactions in chemistry at the molecular level, however, is extremely expensive. From a generative perspective, the combinatorial problem of finding suitable reactions from sets of molecules becomes intractable[217,218] since the space of possible molecules and interactions grows exponentially. If the set of molecules of interest is known as well as some of their interactions, predicting new ones requires accounting for the quantum character of the laws from which bonding emerges, introducing a large set of concerns.

For a given molecule, the strict computation of the state of nuclei and electrons across atomic orbitals depends simultaneously on how forces act on their position and spin[219]. With each new electron, computing superpositions of orbital wave functions is exponentially more expensive. Many quantum chemistry methods start from the Born-Oppenheimer approximation where (a) nuclei are removed from the computation since their mass and position are stable relative to the motion of electrons and (b) the individual electron wave functions $\psi_i(\vec{r}, \vec{s})$ are approximated as the product of a position-dependent wave function and a spin-dependent wave function independent of each other. We thus obtain the Hartree-Fock equations, which constitute the basis of most self-consistent field theories[220] used in quantum chemistry. Other methods such as Density Functional Theory[221]) dispense with explicit representation of the electron cloud and rather operate on electron densities that vary depending on how the statistics of how electrons are spatially (and spin) correlated, and how they exchange energy changes in various situations as given by functionals dependent on the chemical species in the system. Along with many other approximations of the electronic structure of the atom, most of quantum chemistry is devoted to understanding the effects of various interactions within electron clouds on the change of the geometrical conformation of molecules, their polarization and reaction surfaces, and emitted spectra[222].

Several approximations have been devised to alleviate difficulties in quantum computational chemistry methods. Stochastic Monte Carlo sampling helps decrease computational cost in all quantum chemistry methods[223]. Moreover, semi-empirical methods are used whenever any variables can be considered as fixed and experimental data supply their value[224]. At a larger yet specific scale, interactions are more approximately captured by molecular reaction dynamics[225], which contain rules that seek to reproduce bonding behavior in simpler, more prescribed ways. Finally, molecular dynamics describes interactions at large between the position of atoms and potential energy surfaces[226] when the latter are previously known, without involving quantum phenomena. More recently, the rising field of supramolecular systems chemistry attempt to provide a better account of the (non-covalent) chemical interactions responsible for molecular recognition and self-assembly[227].

5.4.6 Classical mechanics

Interactions in dynamical systems governed by classical mechanics are implicitly represented as non-linear terms containing two or more variables in the differential equations representation of the system trajectory. Interaction events may be often equated with either normal modes[228], non-linear oscillations[229], field excitations[230], or bifurcation points[231]. Interactions only arise indirectly as the underlying cause for observable deviations from additivity and linearity[232–234] but the interaction mechanisms themselves causing the deviation in the trajectory remain hidden at various degrees.

When dynamical systems are simultaneously not analytically computable and sufficiently complex due to the presence of nonlinear terms and non-trivial couplings, Monte Carlo methods[235] can be used to approximate a solution by collecting independent samples with lower computational cost. Adjusting measurement density permits to approximately reconstruct nonlinearities with varying degrees of success. More refined well-known techniques remove the restriction of sample independence by introducing stochastic processes[236–238] in an attempt to preserve time dependencies arising during successive interactions. For spatial dependencies, a generalization exists in the form of sequential Monte Carlo sampling[239]. In all Monte Carlo methods, probability models can be setup to mimic the outcome of particular interaction mechanisms at the expense of often impractically expensive computations if the systems are large and/or complex. However, the interactions themselves remain opaque.

5.4.7 Quantum mechanics

In quantum mechanics, interactions are modeled in general as interference patterns in the wave function resulting from coupled systems whose states are quantized[240]. In measurement processes, one system is used to irreversibly interrogate another system, collapsing the state of one or more degrees of freedom that are superposed resulting in a particular *observable* with a probability proportional to wave function amplitude. Superposition, entanglement and decoherence provide critical insights into interactions at the quantum level. Superposition entails the existence of shared global information across many possible states within a single system prior to being observed. Superposition also involves correlated histories of states prior to their measurement, a fact exploited by quantum computing architectures[241]. Quantum entanglement[242–245] corresponds to a interaction where a collective system contains a non-separable quantum state capable of being preserved even when the system components are separated across arbitrary distances; operators applied to one part of the system impact the state as a whole immediately. Finally, quantum decoherence refers to the interaction between a quantum system and the larger environment, resulting in fast decay of state superpositions[115].

In terms of representation, the evolution of a quantum system with N bodies is given by a Hamiltonian operator with exponentially more information than its classical or relativistic counterparts[246,247]. Approximations used to compute outcomes usually contain wave functions for interacting pairs of quantum states in terms of their position, momenta or spin. In the case of coherent collective quantum phenomena such as Bose-Einstein condensation, interactions are represented as lattices of quantum harmonic oscillators whose properties depend on whether the lattice points are fermions or bosons[248]. While the spectral nature of quantum states lends itself naturally to frequency domain analysis, the main focus remains around system trajectories.

5.4.8 Quantum field theory

In quantum field theory[249], particle interactions arise as interaction terms for excitation modes of local states of quantum fields: whenever two particles interact, a field can be inferred. Field theory has been instrumental in organizing and making sense of the diversity of particles and their interactions in high energy physics[250]. Feynman diagrams capture particle interactions as perturbative contributions to transition amplitudes between causally connected quantum states[251]. Translating these interaction diagrams into actual computations starts from obtainig rules derived from the interaction Lagrangian in quantum electrodynamics[252], then finding a well-defined grounded state of the system, integrating over all possible histories for the quantum process in the field and using a Wick rotation to obtain an expression in terms of imaginary time[253]. Even when the interactions are explicit, the formal treatment of pairs of interacting field excitations remains constrained by trajectory-based representations.

5.4.9 Summary: interactions in CMSS require better representations

All prior descriptions of interactions share one of two limitations. Either the description avoids describing what happens during an interaction by concentrating on trajectories or frequencies, or specific interaction mechanisms becomes transparent at the expense of predictive or retrodictive power for system outcomes. We argue that, in order to make progress on describing complex problems with strongly-coupled scales of action towards higher realism requires constructing a theory *de novo* capable of overcoming the epistemic biases and limitations derived from non-relational or partially-relational theories that do not promote interactions as first-class citizens.

5.5 Conclusion

Complex stochastic dynamical systems are ubiquitous and their understanding is necessary to find accurate and efficient solutions to frontier problems across a wide spectrum of disciplines in the natural and social sciences. Each CMSS exhibits multiple phenomenologies whose understanding remains largely incomplete and is often performed through multiple formal levels of description. These are often constructed assuming independence from one another in terms of governing laws and involved entities, are expressed through sets of deterministic, continuous, reversible dynamical equations, and are expected to integrate nicely *ab initio*.

On the contrary, cosmology, biology and information theory strongly suggest simultaneously that not only the architecture of the universe is nicely integrated across all scales, but that the emergence of nearly decomposable systems appears to be one manifestation of a more general correspondence principle between a sequence of microstates associated with macrostates through bridge equations. In this view both objects and laws are emergent and dependent on the geometry defined by interactions yet in most dynamical descriptions of systems interactions are described implicitly through transformations, themselves often buried within the vanishing infinitesimals that define differential operations.

Such a state of affairs limits the ability to provide causal explanations of CMSS across multiple levels in general, resulting further in (a) the inability to predict responses of these systems at various horizons and (b) the inability to appropriately perform retrodiction by capturing all relevant contingencies. In practice, these two limitations seem to materialize as either theoretical incompatibilities between adjacent levels of description, manifold hardships to ensure appropriate formal conditions for numerical methods to yield approximately correct answers, and spurious results with respect to experimental measurements known to be rigorous. To a large extent, this is just a symptom of a deeper abyss dividing research in the physical sciences. Roughly speaking, we can identify two communities: those who insist on the preeminence of calculating[254], and those that insist on the importance of working on the conceptual foundations[255]. Most contemporary approaches discussed here, eager to obtain results from readily observable entities fits in the first category, belongs to the first group. Our work is rather inspired by the second category.

We hypothesize that a universal solution to all the above mentioned problems exists in the form of a novel theoretical framework that focuses its attention on interactions rather than on trajectories, states or equations of motion. This generalized theory of interactions should be expressed as a differential geometry that maps manifolds of events in a CMSS as usually expressed into a 3-manifold named the *interaction space* of the system that contains information about classes of interactions present in the system in a form suitable for the law of large numbers. In addition, a translation of invariants between the two classes of spaces should not only be possible, but proven to be more economic and effective in interaction space than in usual differential manifolds.

In consequence with the vast collection of differential methods, we also hypothesize that it is possible to partially recover the natural and expected variation produced by interactions currently neglected in existing differential models by (1) using spectral analysis of data from stochastic systems to obtain pure probabilistic models that capture relevant interaction scales, (2) introducing stochasticity into coupled, multiscale differential equation models (3) developing agent-based models that rigorously model interactions and (4) providing cyberinfrastructure to facilitate the gradual adoption of both the theory and associated methods.

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Chapter 6

A Generalised Theory of Interactions - II. The Theoretical Construction

Abstract[i]

After discussing the significance of interactions to understand complex multiscale stochastic systems (CMSS), we turn our attention to the construction of a Generalised Theory of Interactions (GToI). We define interactions as discrete, localised events where the thermodynamically irreversible exchange of degrees of freedom involves signal propagation and relaxation phenomena. We proceed to define the mechanics of such space, as well as how these approximately map onto dynamical manifolds. By characterising various systems through the effect of transformations across interaction space, we develop a classification of systems where features such as emergence and information representation become apparent. Our theory appears to capture structural and dynamical features of CMSS efficiently by making explicit the extent of the dynamical range of action in them; we identify the boundaries of such range with statistical limits corresponding to physical laws, and derive a generalised form of the Correspondence Principle.

6.1 Requirements towards a GToI

For the GToI to successfully overcome several of the shortcomings present across scientific theories described in the first manuscript of this series[1], its underlying core principles must provide sufficient tools to avoid them from the start.Our reasoning follows that by Lee Smolin[2] at the top level by requiring our theory to (a) accurately capture systems across a span of complexity that is already well known, (b) generate empirically falsifiable statements, (c) provide means to understand the "why these laws?" questions for specific instances and problems, and (d) provide testable answers to the "why these initial conditions?" question. These general statements must therefore correspond to more specific accounts of entities, dynamics and laws.

[i]**Núñez-Corrales, S. and Jakobsson, E.** A Generalised Theory of Interactions - II. The Theoretical Construction. To be submitted to *Proceedings of the Royal Society A.*

6.1.1 Epistemological requirements

Explanatory closure. CMSS, although involving multiple levels of action and hierarchical organization, should be renormalizable as *an interaction between systems and their environment* and be complete up to a reasonable approximation. When this sort of renormalization preserves empirical observations, its contents should only contain descriptions of those two entities. At various levels of granularity, the effect of renormalization should be reflected on the level of detail of the outcomes. In our view, however, explanatory closure does not imply explanatory exclusion[3]: multiple explanations based on a GToI may be complete and causally consistent without resorting to postulating other external events or unverifiable interactions. Such a type of explanatory closure has been extensively discussed in the context of the landscape problem for string theories in cosmology[4,5].

Relationality. Relational approaches have proven to be fruitful multiple times across the history of physics[6] and science in general. A theory is relational if the degrees of freedom involved in the description of an entity involved in a given phenomenon depends solely on the degrees of freedom of other entities without requiring any pre-existing, global medium. We seek a theory where both entities and governing laws emerge as a consequence of the occurrence, aggregation and composition of interaction; presupposing the existence of a containing background not only limits the reach of such endeavour but eliminates its generality and potential for causality across all scales. A relational approach may permit more easily to crack open the highly contextual whole-environment coupling that characterises descriptions of emergence[7]. More generally, general systems theory[8,9], with an emphasis on where some sort of evolution is possible[10], admit (or rather demand) relational descriptions. Finally, theories stated in relational terms tend to possess useful compositional propertieseven in the most intuitive representation (i.e. set theory vs category theory or topos theory[11]) that usually lead to the discovery of non-trivial properties of phenomena –such as invariants- that facilitate reasoning about them, since these tend to arise constructively as intermediate steps or byproducts towards abstract descriptions of systems and their dynamics[12].

Background independence. We naturally expect the GToI to apply to theories in which fields and particles of various sorts are involved, and in particular to the form of any experimental theory quantum theory of gravity if such arises. A strong case has emerged in favour of background-independence[13], which has been called "the most momentous requirement a quantum theory of gravity must satisfy"[14] since it mandates an emergent view of space-time that compels certain unifications to occur. Background independence should not be an impediment for the existence of renormalization entities[15,16] that may provide the basis for a background-dependent description with asymptotic safety –i.e. avoidance of infinities when computing well-defined extensive quantities[17]. Thus, when the difference between interaction scales is sufficiently large for two classes of events, at least one background-dependent description must exist. We note that, while this description is centered on theories of quantum gravity, its application can be extended to other areas, including social science[18].

Locality. Across most physical theories, locality characterises the separability and independence of events across space-time due to the finite velocity at which information can travel[19]: locality acts as an *selector* operator that restricts the number and value ranges of degrees of freedom where observables acquire values, to sets of finite measure, or in the case of point particles or processes, sets of zero measure. This manifests itself clearly across field theory: the selection process corresponds to replacement of the algebra of observables when the region being measured changes[20]. More specifically, it is a statement about the upper limit of information obtainable by means of measurements, as well as of the measurements' perturbation effect on systems. Locality is crucial in the interpretation of the relevance of acceleration when measurements are performed within a relativistic frame of reference[21]. If locality is more deeply injected into general relativity by curving the geometry of the energy-momentum space, non-commutativity of momentum and non-linear conservation laws arise; both are encouraging (and relationally consistent) with expectations for a theory of quantum gravity[22]. Stating the GToI in terms of locality should help reconcile opposing views between theories that postulate the existence of global, cosmological laws and those that see the latter as practically convenient but epistemologically unsound extrapolations[23]. By calculating the consequences of assuming only locality and probabilistic measurement operators as the basis for physical action, quantum-like laws emerge[24]. Similarly, it has been shown that the presence of unitary operators in the algebras describing Lorentz-invariant time evolution while avoiding certain undesirable outcomes (e.g. vacuum instability, ultraviolet catastrophe) is only possible when the corresponding Hamiltonian is stated in terms of local interactions[25]. Finally, locality is used to define, by contraposition, non-separable events in space-time, or non-locality.

Causality. Spatial relativity places a universal limit on signal propagation that holds in general relativity[26] in order to preserve Lorentz invariance: that is, causality is embedded in the structure of space-time. Causality can take the form of constraints of the solutions of dynamical systems[27]. The situation appears no different either in quantum mechanics when referring to measurements performed on systems with interaction observables[28] such as scattering cross sections[29,30], in situations that involve non-locality such as in EPR pairs[31], or in quantum field theories for local propagation phenomena (i.e. conservation of microcausality[32]), and causality violations are sought after in high-energy physics as the signature of composite structures for particles[33]. If causality is interpreted as a non-empty set of conditions resulting from the interaction of two physical processes[34,35], a mechanistic explanation is required to understand how that set is selected from other alternatives. While equating causality with interactions is not new[36], our view is that the association is in fact universal and applies across scales of action. It has been observed in some hard cases –e.g. the Fokker-Wheeler-Feynman retarded field action[37]- causality can be both preserved formally and made sense physically. When we move up the complexity latter, causality becomes harder to establish[38,39]. In biology, robustness introduces degeneracy and redundancy in ways that difficult the establishment of causal relations[40], a situation which is only made more clear across systems of entities with adaptation and learning capabilities[41]. Causality in conjunction with entropy defines a natural separation between classes of stochastic processes[42]. Methodologically, the analytic deconstruction and reconstruction of complex phenomena by means of models should not change causality relations[43], but it should be possible to unveil the origin of causal relations when these have indirect origins, e.g. dynamical couplings[44], and, consequently, causality in a GToI should acquire a strongly topological flavour[45]. In our approach, only pairs of interacting entities are allowed. Many-body interactions emerge from the underlying pairwise interactions.

Thermodynamic irreversibility. Departing from systems in steady thermal states is often motivated by the difficulties entailed in the treatment of systems far from equilibrium where irreversible action occurs. A successful GToI should not only integrate thermodynamical irreversibility, but be directly built upon it as a more natural –and hopefully more correct- description of systems with interactions[46]. The resolution of several paradoxes across various disciplines and their rooting in a common framework that ties them to gravitation would constitute positive evidence in that direction[47]. We note that, interestingly, describing thermodynamics by means of Riemannian geometry leads to the appearance of non-zero curvature in the respective manifold when interactions are introduced[48], echoing the appearance of curvature in general relativity when massive objects are introduced in space-time. Interactions between two non-equilibrium systems with a shared interface has been studied in composite entities[49], but no immediate path toward generalisation becomes evident. Endoreversible thermodynamics provides a better model for our purposes, since irreversibility is explained in terms of interactions with asymmetric heat exchange between systems whose components may be reversible[50]. The extension of irreversible thermodynamics to networks[51] brings us, topologically, a step closer to what we expect in connection to causality. A fully integrated view of interactions and thermodynamic irreversibility requires a generalised form of uncertainty: the existence of uncertainty relations in classical mechanics analogous those found in quantum mechanics[52] motivates this assertion. One challenge a GToI should help further clarify of is causal relationship between energy and temperature in statistical mechanics[53]. Another challenge corresponds to providing better reasoning around the frequent observation of core-halo distribution formation in systems far from equilibrium beyond symmetry breaking of ergodicity[54]; finding a compelling explanation under a more general framework may lead to significant generalisations applicable to aggregate and composite systems. From the perspective of symmetry breaking[55], irreversibility appears to be strongly associated to the ratio between microscopic and macroscopic scales[56]; simultaneously, outcomes obtained using a GToI should not focus on specific initial conditions, but rather on ensembles of initial conditions and probably their partitions.

Using both statistical thermodynamics and microphysics approaches, one can find situations where aggregates move up thermal gradients in apparent contradiction of laws known for simpler systems[57,58]: thermodynamic irreversibility across CMSS brings puzzling questions that, once more, a GToI should better help elucidate. The role of irreversibility in biology was identified early[59]. For instance, organismal development correlates with a decrease in the rate of entropy production[60]. Stochasticity that arises from it in biological systems endows them with flexibility and adaptation, both responsible for functional robustness[40]. In production theory in economics, time irreversibility does not necessarily involve thermodynamic irreversibility, even if both are well defined for a particular case[61]; this is significant since the arrow of time –i.e the irreversible character of time as a physical dimension- is built using thermodynamic irreversibility arguments. More generally, a GToI should anticipate the analysis of fractal systems that arise from dynamics acting on dense non-continuous sets[62]; the existence of methods to find order parameters and the phase transitions these encode is suggestive of the existence of similar possibilities when reasoning in terms of interactions[63]. We suspect that rigorously describing *reversible* systems using a GToI will yield concrete theories of interaction that are either cumbersome (proportional to the variety of interactions involved) or conspicuously unphysical unless additional assumptions are added. This situation would mirror some of the difficulties when describing irreversible systems in current approaches.

Compositionality. Compositionality appears to be the simplest mode of organization that attains complexity –i.e. an outcome different from pure aggregation- when departing from a substrate of interacting entities[64]. In addition, as an epistemological device, it can provide convenient abstractions provided the underlying ontology partitions the space of structures and events into tractable units[65]. Compositionality tends to result in elegant algebraic treatment of difficult subjects. A GToI therefore must carefully choose its entities and compositional laws as to remain empirically testable and intellectually economic with an algebraic bent: for many systems, intuitions will be hard to come by and similar to quantum mechanics, and the robustness of the formal expressions and the ability to find invariants will be some of the few assurances available. Compositonality requires in complex systems that emergence occurs by virtue of the existence of composition operators acting both on entities and on the rules governing their dynamics that can be systematically applied[66]; as a result, generative effects must be manifest[67].

Amidst the natural sciences, the significance of compositionality becomes most apparent in biology.

Biochemical interactions, including those between enzymes and substrates, can be captured by various algebraic means relying on composition[68]. Systems biology has not been the exception[69]. Hierarchical evolutive systems[10] and more recently memory evolutive systems[70] depend on the compositional language of category theory to express static and dynamical properties of biological systems that change under selective pressures across multiple scales. *Designed* systems constitute an interesting case. Compositionality appears to be a key ingredient for the fluidity of intelligence in cognition[71]. Computation as a formal process can be described by means of interactions[72], for instance, having undergone a complexity explosion only possible due to the compositional properties of hardware and software. In particular, complex distributed software systems can be specified through composable interactions[73]. Succinctly, a GToI must provide the scaffolding required, in principle, to reconstruct the large-scale structure of the universe from the most fundamental level possible[74].

Computability. For a GToI computability involves both (a) the ability to obtain numerical outcomes that predict or reconstruct specific situations and (b) the existence of an approximate isomorphism between physical systems and an algebra whose establishment takes a finite number of transformations to realise[75]. Computing consists of thermodynamic actions, many of which are irreversible[76]; computations along the spectrum of irreversibility suggest an arrow of time emerges when information is erased[77]. Since computation is a physical act, we expect a GToI to provide adequate estimates for the limit of what a computer can do[78]. Using the rise of quantum computing as an example, understanding existing computers using physics tends to shed new light into what processes may also count as computing besides Turing machines[79]; it is likely for a computational theory of interactions to result in other definitions of what it means to compute. To this end, we anticipate that stating computations is a GToI, given its stochastic roots, will likely be performed by some type of bisimulation[80]: a compositional, physical system used to sample spatially, temporally and informationally another system through repeated interactions. We also note that when external interactions are introduced into algorithm analysis, then the computation becomes open –i.e. stops being complete or self-consistent[81]. If an interactive computation yields useful work, it is therefore out of equilibrium, which implies some arrow of time imposed by thermal or information loss. Since information appears to play a critical across fundamental physics[82], a GToI should help clarify the processes that produce it in terms of information producing processes and the robotics required to move bits around during computations, and capture causality in topological fashion –e.g.[83].

6.1.2 Pragmatic requirements

What should, in practice, a GToI provide? First and foremost, we seek to establish the foundations of a theory capable of facilitating the description, analysis and testing of hypotheses across CMSS, but also across systems usually not though of as CMSS. To be consistent with the empirical requirements, a GToI must remain somewhat abstract and parameterizable. Thus, concrete phenomena and/or hypotheses should require *concrete theories of interactions* (CToI). In this sense, the trajectory of the search for a GToI parallels existing work on constructor theory by Deutsch and Marletto, which departs from an abstract specification[84] and materialises into probability theory[85], information[84], life[86] and thermodynamics[85].

On the side of complexity, the GToI should competently describe interacting systems with ample microstate variety and various degrees of rigidity. We also seek to capture, most importantly, systems with a high degree of *repertoire variety.* Microstate variety describes the number of classes to which the constituent interacting entities belong at the most immediate microscale. For instance, a classical interacting gas with one species has low microstate variety, while interacting proteins in the cell environment constitute a system with high microstate variety. Rigidity[87] entails (a) the stability of macroscale identity under microscopic perturbations –i.e. entity substitution, changes in local topology-, (b) conversion of point-like forces that cause local deformations in microscopic degrees of freedom into global transformations with various continuous macroscopic symmetries, and (c) stability of microscale identity under energy fluxes and entropy production. Repertoire variety corresponds to the number of different types or *modes* of interactions per composing entity in a system, which has significance for a number of reasons. We are interested, for example, in understanding why in some systems emergence only occurs with many simple entities (e.g. conductivity in a copper wire) while in others a few composing entities give rise to rich emergent behaviour. This fact motivates us to hypothesise that the thermodynamic limit need for emergence to manifest is inversely proportional to the repertoire variety of the system.

Multiscale structure should be captured by the GToI, with an emphasis on those observed across CMSS. First, the GToI should describe simple aggregation processes with varying degrees of flexibility. Second, it should help understand the rise of hierarchies and modularity in the presence of dynamical constraints as efficient topological embeddings[88]. Third, it should provide a model for how noise percolates (and sometimes amplifies) across scales; noise percolation is extremely significant for both simple[89] and complex[90] situations. Finally, a GToI should help broadly capture cross-scale excitability, which is of particular interest both for biology and large-scale distributed information systems. Metabolic networks exemplify all four of these requirements[91,92].

Stochastic in CMSS should appear in various forms in a GToI. It its most general form, it should manifest as uncertainty constraints across all scales[52]. As a consequence, the presence of noise should be traceable to either intrinsic sources (e.g. the probabilistic nature of quantum mechanics) or combinatorial causes (e.g. the difficulty of finding the most significant epistatic interactions of an arbitrary number of SNPs that explain the onset and progression of a disease). A GToI should provide the scaffold to quickly model dissipation and fluctuations observed across irreversible processes. In our view, stochasticity is not a useful addition to be preserved only when convenient and otherwise frequently expelled, but a ubiquitous property of the universe as a whole.

To summarise, a GToI is pragmatically successful if it can be used to construct concrete theories of interaction without violating any of the epistemological requirements across systems that range from point-like to fully interconnected, from single-scale to hierarchically modular, and from reversible and closed to irreversible and open. In the following description of an example of such theory, bold symbols indicate non-scalar quantities, and bold capital symbols denote transformations or observables.

6.2 Elements of the GToI

Most models of interactions across the sciences resemble in some form or another the situation described by Figure 6.1A. For two systems a, b embedded in a manifold Ω –e.g. spacetime, an electromagnetic field, a heat bath, the interior of a cell, an economy, society- a transformation T_Ω is defined such that

$$\boldsymbol{T}_\Omega(a, b) = (a', b') \tag{6.1}$$

such that the difference between some quantity $\boldsymbol{\Gamma}(a, b, \boldsymbol{T}_\Omega)$ yields a nonlinear curve along some dimensions, usually time. Cross sections constitute a paradigmatic example. To compute its consequences, however, the quantity dependent on time and space –the locus of interaction- is given by the centre of mass

$$\boldsymbol{r}^\mu_{a,b} = \frac{m_a \cdot r^\mu_a + m_b \cdot r^\mu_b}{m_a + m_b} \tag{6.2}$$

where μ is the coordinate index and m_a, m_b are the respective masses. Furthermore, assume that to every function $\boldsymbol{\Gamma}$ stated in terms of entities corresponds a function $\boldsymbol{\gamma}$ whose value only depends on $\boldsymbol{r}_{a,b}$. For a single interaction in Ω

$$\boldsymbol{\gamma}(\boldsymbol{r}_{a,b}) = \int_\Omega \delta(\boldsymbol{r}_{a,b} - \boldsymbol{r})\gamma(\boldsymbol{r})\boldsymbol{dr} \tag{6.3}$$

When applied to a position $\boldsymbol{r}$ different than the centre of mass, we expect $\boldsymbol{\gamma}(\boldsymbol{r}) = 0$. Integrating on both sides

$$\int_{\Omega} \gamma(\boldsymbol{r}) \boldsymbol{dr} = \iint_{\Omega} \delta(\boldsymbol{r'} - \boldsymbol{r}) \gamma(\boldsymbol{r}) \boldsymbol{dr dr'} \tag{6.4}$$

we obtain a form that, when interactions are sufficiently dense in Ω, suggest the existence of a continuous kernel $\boldsymbol{K}(\boldsymbol{r'}, \boldsymbol{r})$ such that

$$\iint_{\Omega} \delta(\boldsymbol{r'} - \boldsymbol{r}) \gamma(\boldsymbol{r}) \boldsymbol{dr dr'} \approx \iint_{\Omega} \boldsymbol{K}(\boldsymbol{r'}, \boldsymbol{r}) \boldsymbol{dr dr'} \tag{6.5}$$

which, for sufficiently small $\delta r = \|\boldsymbol{r'} - \boldsymbol{r}\|$, a corresponding kernel $\boldsymbol{G}(\boldsymbol{r})$ exists with the property

$$\iint_{\Omega} \boldsymbol{K}(\boldsymbol{r'}, \boldsymbol{r}) \boldsymbol{dr dr'} \approx \int_{\Omega} \boldsymbol{G}(\boldsymbol{r}) \delta r \boldsymbol{dr} \approx \int_{\Omega} \gamma(\boldsymbol{r}) \boldsymbol{dr}. \tag{6.6}$$

We find in the resulting expression a *position dependent field* $\boldsymbol{\Phi}(\boldsymbol{r})$. Let us analyse what information we have gained. First, fields can be reconstructed from sufficiently dense collections of interactions, or rather, *interaction effects*. Second, that the field is a variational quantity dependent on δr. Third, that for the field to be properly defined, suitable functions $\boldsymbol{K}$ and $\boldsymbol{G}$ must exists, and be continuous and deterministic. Since we are interested in systems with stochasticity, one might be tempted to introduce an integration measure from a random process $\boldsymbol{W_r}$ such that

$$\boldsymbol{\Phi}(\boldsymbol{r}) = \mathbb{E}\left(\int_{\Omega} \boldsymbol{G}(\boldsymbol{r}) \delta r \boldsymbol{dW_r} \right). \tag{6.7}$$

A challenge arises in how to interpret the noise term, which depends on the assumptions about the generating random process, which may be resolved to some degree of satisfaction by gaining additional information about the system and selecting the scale of events[93,94]. The second challenge is that the introduction of $\boldsymbol{W_r}$ strongly limits the classes of functions $\boldsymbol{G}$ for which an analytic result is possible; numerical calculations become no easier in the selection of the solution approximation method or the computational cost. Assuming these obstacles can be overcome, the process has left us with insights about the analytic and numerical properties of the continuous (or stochastic) response of $\boldsymbol{\gamma}$ under change of position in the manifold.

What becomes most significant is what we have not learned. While we may get a clear view of interaction effects, we remain in the dark about *what an interaction is* and *what exactly happens during one*. Not only have we abstracted away relevant relational details provided by the position of a and b in the manifold, but hidden all aspects of the processes behind $\boldsymbol{T}_{\Omega}$. The structure of a and b remains opaque under the guise of behaving as point particles. What is their inner structure? Does it change? What is the nature of that change if they do? Is it dependent on the types of the entities involved? Why is it considered effectively instantaneous? What does the thermodynamic landscape underlying $\boldsymbol{T}_\Omega$ look like? Can we understand why nonlinearities appear (if any)?

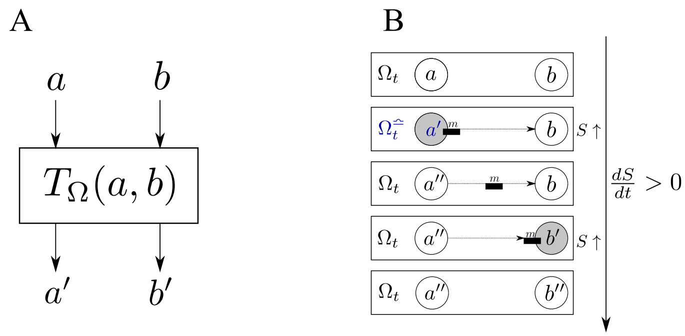

Figure 6.1: Two abstract models of an interaction. **A.** The standard transformation model where interactions are inferred from nonlinear changes in properties of a' and b'. **B.** An explicit model of interactions where degrees of freedom are exchanged via a messenger m with entropy production after state relaxation.

Let us take a different approach and forget altogether –yet only temporarily- about the response $\mathbf{\Gamma}$, described by Fig. 6.1B. We start by endowing a and b with inner structure whose rigidity varies. For the moment, suppose that an entity a can be represented as a weighted connected graph of degrees of freedom $G(a) = G(V, E, W)$. We use graphs as a reasonable model since their rigidity is well-defined[95,96] and reason in terms of its edges. In this physical situation, entities a, b exist within a local dynamic context Ω_t, which may contain fluctuations across its degrees of freedom. We define the dimension D of Ω_t as the number of degrees of freedom that provide a holonomic basis for $G(a), G(b)$ and their embedding into Ω_t. To exert some effect on either $G(a)$ or $G(b)$, we expect Ω_t to behave locally as a graph whose edges connect vertices of any G with vertices in it on its surface. Since the local context is time dependent, then it must be the case that $G(a)$ and $G(b)$ also are as a function of their rigidity. If stochastic fluctuations occur in Ω_t, these must also filter into the graph of embedded entities. As long as the volume an entity the manifold Ω_t does not exceed a certain value, we consider stochastic shapes to be well-defined[97]. Assuming a regular shape without loss of generality, we expect its volume and surface relations in terms of edges E_a to follow respectively

$$V_a \equiv V[G(a)] \propto |E(a)|, \qquad S_a \equiv S[G(a)] \propto |E(a)|^{\frac{D-1}{D}}. \tag{6.8}$$

Since $G(a)$ embedded within Ω_t corresponds to a discrete shape, the equivalent of the Stokes theorem in discrete exterior calculus exists[98]. Equipped with these notions, we aim to describe an interaction in terms of the consequences of perturbations of varying magnitude to the edges –i.e. relational degrees of freedom- that comprise each interacting entity. An interaction between the two entities, when these are at sufficient proximity from one another, is defined as the process where an active entity a receives a perturbation, relaxes its state and yields either a perturbation into Ω_t or generates a messenger m using its own structure that acts as a perturbation for another (possibly active) entity b. Let us suppose that only a small amount of degrees of freedom in a are impacted by a perturbation. The task before us requires providing a model for (a) the magnitude of the response as a function of the magnitude of the perturbation, (b) the propagation of the response across entities and (c) its consequences for an interaction with another entity b.

First, we will separate –with some notational abuse- the edges of an entity into three subsets corresponding to a rigid component, a perturbable component and a heat component,

$$E(a) = E_R(a) + E_\Delta(a) + E_Q(a). \tag{6.9}$$

To address (a), we observe that the effect of $E_\Delta(a)$ is to capture the internal reconfiguration of recognisable degrees of freedom as a means to decrease internal entropy, while $E_Q(a)$ captures the loss of degrees of freedom to the context as fluctuations (i.e. heat radiation). We also expect $E_\Delta(a)$ and $E_Q(a)$ to increase when a perturbation arrives. We expect the magnitude M_ϕ of any perturbation ϕ to determine the internal distribution of $E(a)$ in terms of its three components as expected by conservation of mass. As a simplistic model, we considered a sigmoid perturbed fraction of edges f_ϕ

$$f_\phi(M_\phi) = C_\alpha + \frac{1}{1+e^{-\alpha M_\phi}} \tag{6.10}$$

with C_α such that $f_\phi(M_\phi/2) = \frac{1}{2}$, thus

$$E_\Delta(a) + E_Q(a) = f_\phi(M_\phi)E(a). \tag{6.11}$$

We expect, following intuitions about radiating processes, the perturbable component to be proportional to volume and the heat component to the surface proportional to the perturbed fraction, taking care in removing the latter from the former one

$$f_\phi(M_\phi)E(a) = V_a^\Delta + S_a^Q \tag{6.12}$$

with $\beta \leq 1$ such that

$$\beta = \frac{V_a^\Delta - S_a^Q}{V_a^\Delta} \tag{6.13}$$

revealing that $E_\Delta(a) = V_a^\Delta - S_a^Q$ and $E_Q(a) = S_a^Q$. We identify α with the reconfigurability of the system, since it provides information about the potential for an internal reconfiguration, and $1-\alpha$ with its rigidity. The parameter β corresponds to the dissipative potential, or the ability to radiate heat by loosing degrees of freedom to the stochastic context. Both quantities depend on the structure and composition of a.

Turning our attention to (b), we model the propagation of the action as collections of edge reconfigurations on $E(a)$. Again, without loss of generality, let us suppose the existence of a path π of length ℓ such that the number of edges involved in the reconfiguration follows a binomial distribution with probability p and $N = \ell$. By choosing to express change in terms of ℓ instead of time, the description remains scale-independent. We quickly observe that the choice of $p = \beta$ matches our dynamical intuitions for passive and active systems: passive systems tend to minimize internal entropy by radiating heat, while active systems do so by reconfiguring its internal state. Moreover, the pattern of propagation of action across in active systems often resembles a tree structure in which small impulses trigger large reconfigurations. Refering to the entity a under reconfiguration as a', the propagation profile $\zeta(a,\phi)$ at the k-th step becomes the hypersurface

$$\zeta_k^{D-1}(a',\phi) \approx V_a^{\Delta} \cdot \binom{V_a^{\Delta}}{k} \beta^k (1-\beta)^{V_a^{\Delta}-k} \tag{6.14}$$

with an enveloping hypercircumference

$$\zeta_k^{D-2}(a',\phi) \approx S_a^{Q} \cdot \binom{S_a^{Q}}{k} \beta^k (1-\beta)^{S_a^{Q}-k}. \tag{6.15}$$

ζ^{D-1} and ζ^{D-2} will be named from hereon as reconfiguration and heat propagators respectively.

We now will proceed to address (c). To do so, we must proceed in two steps. First we must capture the emergence of messengers, which we expect to describe as a the aggregation of the subset of degrees of freedom of an entity into a smaller one with higher energetic stability. Such fragmentation is easily captured in G by having strongly connected components with no edges between them; we will restrict ourselves to interactions where no fragmentation results. First, suppose a fluctuation with sufficiently large magnitude induces a transformation $\boldsymbol{T}$ such that

$$\boldsymbol{T}[\phi, G(a)] = (G(a''), G(m)). \tag{6.16}$$

$G(m)$ is the graph of a resulting messenger, a collection of degrees of freedom whose structural complexity should be in proportion to V_a^{Δ}. Conservation of degrees of freedom implies

$$E(\phi) + E(a) = E(\Omega_{t+\ell} - \Omega_t) + G(a'') + G(m). \tag{6.17}$$

We may read the latter as follows: a fluctuation acting on a led to the reconfiguration of its internal state into a'', dissipating heat and yielding either a new fluctuation $\psi = G(m)$ or a smaller (stable) messenger that, upon contact with other entity, will act as a fluctuation. Not all messengers m, however, act equally on all recipients. For instance, molecular binding in proteins is highly specific and depends on conformational changes that act as a sort of signature[99]. Taking this into account, a simple model that generalises the perturbed fraction f for a fluctuation or messenger ψ is the Gompertz function

$$f(\psi) = C_{\alpha_1,\alpha_2} + \kappa E(\psi) e^{-\alpha_1 e^{-\alpha_2 E(\psi)}} \tag{6.18}$$

where $\alpha_2 = \alpha$ corresponds to reconfigurability the prior model, α_1 corresponds to *interaction affinity* and κ is the fraction of degrees of freedom in direct contact during an interaction; C_{α_1,α_2} is a constant required such that $f(\varnothing) = 0$.

Observe that we have only described perturbations. We introduce relaxation as the process in which a' regains stability on average. To preserve causality internally, the relaxation process must be somewhat similar than the prior one except that degrees of freedom in S_a^Q are now absent. Hence, it must be the case for its volume propagator

$$\zeta_k^{D-1}(a'', \phi) \propto \zeta_k^{D-1}(a', \phi) \tag{6.19}$$

Since heat dissipation involves diffusion –i.e. loss of degrees of freedom to Ω_t in our model, no degrees of freedom are left for $\zeta_k^{D-2}(a'', \phi)$ to operate on. However, the relaxation process cannot occur immediately due to the existence of a difference between the compensation mechanisms that compensate for entropy and from those that compensate for enthalpy[100]. To abstain from the use of time explicitly is to suppose that $\zeta_k^{D-1}(a'', \phi)$ operates always at a distance d_a that depends on the composition of the entity. That is, for all k in $\zeta_k^{D-1}(a', \phi)$, $k' \le k - d_a$ for $\zeta_{k'}^{D-2}(a'', \phi)$. The quantity d is the minimum relaxation period needed to regain excitability. Thanks to the constant fluctuation of the shape and orientation of a, the quantity d_a is intrinsically uncertain up to a error, and mostly so after perturbations have changed the wiring of the internal degrees of freedom. We may characterise empirically this fact by means of the ratio $\xi(a) = d_a/\ell_a$ which we interpret as a dynamical resolution limit of the action of ψ in a, and by reasoning, cannot be zero. Hence, the system contains uncertainty at some scale. Based on this, we define $\omega_a = 1/d_a$, i.e. the relaxation frequency. Also, note that the frequency of the entire event is constrained by the longest average relaxation distance, hence

$$\omega([\cdot]) = \min\Big(\langle\frac{1}{d_a}\rangle, \langle\frac{1}{d_b}\rangle\Big). \tag{6.20}$$

Let us now introduce b into the picture. To preserve causality, we assume associativity of $\boldsymbol{T}$ within a suitable structure $[\cdot]$ which for Fig. 6.1B yields

$$\begin{aligned}
[\phi, G(a), G(b)] &= [\boldsymbol{T}[\phi, G(a)], G(b)] \\
&= [G(a''), G(m), G(b)] \\
&= [G(a''), \boldsymbol{T}[G(m), G(b)]] \\
&= [G(a''), G(b''), G(m')].
\end{aligned} \tag{6.21}$$

If a and b are sufficiently complex, causality may established by means the affinity when the process is reversed since, in general, we expect affinities to be reversed. However, there exist two cases where causality may be lost. If the entities are passive, if their propagators are not oriented (i.e. $\beta = 0.5$) and messenger/fluctuation signatures are indistinguishable, then it becomes perfectly legal to relabel $a'' \to a$, $b'' \to b$ and $G(m') \to \phi$ and the analysis is time-symmetric, therefore acausal. In these scenario, either direction or even considering the interaction as two simultaneous events. In the second case, consider a stationary and a moving observer at sufficiently large velocity. It is not hard to image a situation where the direction of motion is such that relaxing and/or propagating portions of all objects (including transitory states a' and b') appear simultaneous to the moving observer, while still being able to assert the irreversible character of the action[101]; acausality and hence its interpretation as simultaneity arise again with respect to the order of events.

Thermodynamically let us consider the effect of ϕ on $G(a)$. We expect the internal energy of an entity to be proportional to the number of degrees of freedom in it, thus $U(a) \propto E(a)$. When no perturbation impacts a externally, action still occurs internally to stochastically reconfigure of degrees of freedom without compromising identity; we expect a minimisation of internal entropy with a small fixed generation of heat dissipation δQ^* and fixed total entropy generation $\delta\mathcal{S}_g^*$. Also, heat and entropy should grow proportionally with the magnitude of the perturbation. Assume the existence of local entropy generating processes corresponding to an average quantity $\delta\mathcal{S}_g^\phi$ operating on each edge in $V_a^\Delta - S_q^\Delta$ during the perturbation-relaxation process and average heat dissipation per edge δQ. Since

$$d\mathcal{S} = \frac{dQ}{T} + d\mathcal{S}_g, \tag{6.22}$$

we can estimate the entropy per internal relaxation step k

$$d\mathcal{S}(a') \approx \mathcal{S}_k(a') \propto \frac{\delta Q \cdot \zeta_k^{D-2}(a',\phi)}{T} + \delta\mathcal{S}_g^{\phi} \cdot \zeta_k^{D-1}(a',\phi). \tag{6.23}$$

and, using a symmetrical argument for b once it is reached by m, it must hold for the average entropy produced during the interaction process $[\cdot]$ that

$$\mathcal{S}([\cdot]) = \int_{t_0(k=0)}^{t(\ell_a)} d\mathcal{S}_t(a') + \int_{t_0(k=0)}^{t(\ell_b)} d\mathcal{S}_t(b') + \approx \sum_{k=0}^{\ell_a} \mathcal{S}_k(a') + \sum_{k=0}^{\ell_b} \mathcal{S}_k(b'). \tag{6.24}$$

Depending on the variations of phenomena given approximately identical interactions, we expect the effect of $\boldsymbol{T}$ to span a distribution of outcomes instead of a single or fixed one. Given the latter, we may more clearly state

$$\langle[\phi, G(a), G(b)]\rangle = \langle[G(a''), G(b''), G(m')]\rangle \tag{6.25}$$

for stochastically varying ϕ, a and b. Following the principle of identity of indiscernibles, interactions or rather *interaction classes* must lead to unique descriptions. The uncertainty relations and fluctuations acting upon the configuration of the entities and the classes of entities does not constitute an adequate ground for establishing such identity, since both sides are distributions, and ensembles with similar average observables can exhibit widely different arrays of internal microstates. Defining a class of entity is problematic for the same reason. Many instances of interactions show that $G(m') = \varnothing$ is possible –i.e. all degrees of freedom in b translate either into heat dissipation or b'' which, by symmetry, must guarantee the existence of processes where $\phi = \varnothing$. However, the latter does not imply the absence of interactions originating from internal fluctuations in a and b; quantum spin measurements are suggestive of this. We thus call interaction sources *extrinsic* whenever $\phi \neq \varnothing$ and *intrinsic* otherwise.

The features that appear to be consistent across all entities discussed so far are their degrees of freedom, frequencies and uncertainties of intrinsic and combinatorial nature. These are, by extension, stochastic quantities and therefore defined by distributions. If the distributions are unimodal and these partition the space of interaction events in a non-degenerate manner, finding a distance metric μ between interactions is well defined. If multimodal distributions arise in a given problem, we should expect to find a spectral decomposition of these into simpler –i.e. unimodal- interactions. We immediately recognise the geometry spanned by these distributions as an information geometry[102], and the metric μ as a suitable Fisher metric[103]. Most satisfactorily, doing so translates each interaction as a hypothesis testing instance.

For the principle of identity of indiscernible to hold across interactions, what distinguishes one interaction from another must be the abstract properties of the *mechanism* that operates. Observe that in Eq. 6.21, state descriptions of a' and b' have been omitted assuming that they are transient, and therefore somewhat immaterial to the outcomes. This remains so regardless of whether the interaction source is intrinsic or extrinsic. Using these intermediate states brings, however, a source of uncertainty by means of the combinatorial complexity contained in the ensemble of possible future states a'' and b'' departing from a' and b' correspondingly; note that this view of interactions composes with any intrinsic measurement uncertainty.

Our view is that these along with m contain valuable information about final relaxation states. When $0 \leq U(m) \leq |U(a) - U(a'')| + |U(b) - U(b'')|$, we claim that those that remain in m contain the necessary information to uniquely identify, on average and for a sufficient , both the distribution of its possible origins and the distribution of its possible effects, as well as the properties of the most immediate classes of entities that could have been involved. The argument proceeds on two grounds. First, the statistic complexity of an entity must be in correspondence with the complexity of the ensemble of pattern-generating processes that produced it[104]. Thus, we are in position to at least infer general properties of the distribution $\langle \boldsymbol{T}[\phi, G(a)] \rangle$ and by extension obtain an estimate of $\boldsymbol{T}$ via least action. Second, the thermodynamics of requisite variety[105] mandates the complexity of m to be commensurate with the amount of memory necessary for pattern-generating processes, and understanding the memory requirements of all messages "addressed" to b translate into the general properties of the distribution of patterns b must posses. In this sense, m can be regarded as a specific control system for b that produces a narrow response, and b as the outcome of computing patterns that emerge from sets of messengers that share parts of a common distribution for some G. Put bluntly, objects appear to be a consequence of the aggregation and composition of interactions.

The generalized theory of interactions below thus departs from $m \equiv m(a', b')$ as the primary construct in the abstract scaffold corresponding to our attempt to build a parameterizable theory connecting events across scales. Consequently, we state the following guiding principle:

Principle of Equivalence. *Equivalent mechanisms require equivalent messengers. Equivalent messengers describe equivalent interactions.*

6.2.1 Interactions

A *degree of freedom* δ is a discrete aspect of the state of a system for which the enumeration of a possibly dense range of values –as given by underlying governing laws- yields a description of possible worlds. A possible world is the simplest assignment of one value to the degree of freedom. The range of the degree of freedom is the set containing all values for a given aspect of the world. In our interpretation, the local and thermodynamically irreversible character of interaction events occurs by virtue of interacting systems being holonomic systems subject to multiple forces[106]; our description attempts to avoid the complexities of reasoning about dynamics in the resulting Riemannian phase space by focusing on their exchange. Hence, a degrees of freedom corresponds to a generalised distribution.

The *frequency* ω of an interaction is the minimum of the inverse of the path distance between perturbation and relaxation in the corresponding causal graph G of each interacting system. Consequently, shorter distances produce higher frequencies and longer distances lower frequencies. By convention, frequencies are non-negative quantities, since our description does not involve time-dependent field propagation. Similar to degrees of freedom, frequency describes more properly a portion of the distribution resulting from bounding frequency spectra, describable by means of generalised functions.

The *uncertainty* $\hbar$ of a system contains information about the extent of the set of allowable future states of G depending on a particular event and about intrinsic measurement uncertainties present across these macrostates. Since the first component of uncertainty corresponds to the uncertainty relationship between transition speed and thermodynamic cost (of entropic origin)[107], and the second to uncertainty as interpreted in quantum phenomena, this quantity is non-negative. To understand where it acquires its character as a distribution, we proceed as follows. Intrinsic uncertainties characterise upper boundaries in acquired knowledge, and correspond to the convex surface that envelopes stochastic measurement outcomes. Extrinsic uncertainty depends on the distribution of states across objects. Since these objects are stochastic themselves, probabilities p_i used in the computation become $\langle p_i \rangle_t$, and naturally

$$\mathcal{S} \equiv \langle \mathcal{S}_t \rangle \propto \sum_k \langle p_k \rangle \log \sum_k \langle p_k \rangle, \tag{6.26}$$

hence, $\hbar$ must be representable using generalised functions.

An *interaction*, or *interaction class* is a generalised event where action between two systems α, β is defined jointly, locally and relationally (Figure 6.2). Locally here means that, although not depending on any particular location or *interaction locus*, it can only refer to its relevant neighbouring context Φ_i, where i uniquely identifies the interaction. The event is triggered by either an external (physical or virtual) messenger or a fluctuation, which prompts the exchange of degrees of freedom δ_α^β as described by certain commutation relations with frequency ω_α^β constrained by the structural delay d_α^β relaxation of internal structures. Its generalized uncertainty $\hbar_\alpha^\beta$ is given by an intrinsic uncertainty $\mathfrak{h}$ and a measure μ over future state diversity. While interactions do not explicitly represent the triggering fluctuation process, it effects are contained in the elements above.

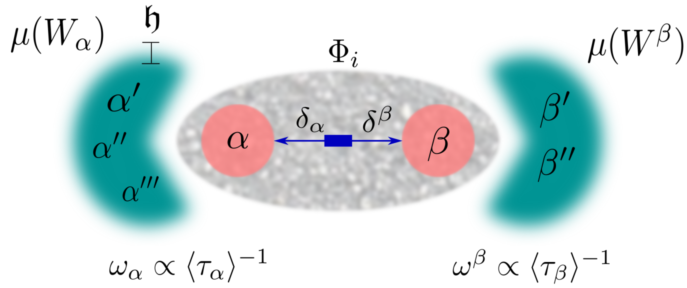

Figure 6.2: Graphical representation of an interaction in the GToI. Two entities α and β embedded in the stochastic context Φ_i exchange degrees of freedom δ_α and δ^β. In doing so, both undergo relaxation into a set of future macrostates W_a, W^b with frequencies ω_a, ω^β respectively (proportional to relaxation times τ_α, τ_β). The process is characterised by a generalized measurement uncertainty $\mathfrak{h}$.

Formally, we start by constructing the manifold from which interactions emerge. First, consider the spaces $\Omega^\delta, \Omega^\omega$, and $\Omega^\hbar$ from which each degree of freedom δ, frequency ω and uncertainty $\hbar$ draw their values independent of Φ_i. Here, Φ_i is the *pseudo-extensive local context*, a structure that represents the media where interactions take place, having its own dynamics, and whose dynamics are in turn impacted by interactions. Consistent with the description so far, Φ_i is locally labelled by i to signify that only its most relevant extent to the interaction must be considered and that under the principle of background independence it contains a finite and small number of connected degrees of freedom in contact with interacting entities: it provides the convenience of an extensive media but remains local, thus the name pseudo-extensive. The context behaves effectively as a dynamic stochastic network with objects that can have similar properties as a field at the appropriate thermodynamic limit. When $\Phi_i = \varnothing$, interactions are called *fundamental*; conversely, we call a non-empty context a *field network*.

A quantity $\eta_j = \delta, \omega, \hbar$, in the absence of any other factors, becomes

$$\eta \equiv X(\Omega^\eta, \Phi_i) \tag{6.27}$$

where X is a random variable whose distribution is $W_{\Phi_i}^\eta$. One can find suitable distributions, amongst which are the thermodynamically irreversible solutions to various Fokker-Planck equations[108,109]. Since we wish to capture the exchange property per degree of freedom, we define the j-th degree of freedom as the quantity

$$\delta^{\beta}_{\alpha,j} = X_{\alpha j}(\Omega^{\delta}, \Phi_i) + i \cdot X^{\beta}_{j}(\Omega^{\delta}, \Phi_i), \tag{6.28}$$

which can be used to define the *exchanged* degrees of freedom

$$\boldsymbol{\delta}^{\beta}_{\alpha} = (\delta^{\beta}_{\alpha,1}, \delta^{\beta}_{\alpha,2}, \cdots, \delta^{\beta}_{\alpha,D}) \tag{6.29}$$

for the number of stochastic holonomic degrees of freedom D involved during the interaction. Degrees of freedom donated by α are $\mathrm{Re}(\boldsymbol{\delta}^{\beta}_{\alpha})$, and those donated by β are $\mathrm{Im}(\boldsymbol{\delta}^{\beta}_{\alpha})$, respectively. In certain occasions described below, one may benefit from using reduced degrees of freedom. Consider $\delta_{\alpha,j} = \mathrm{Re}(\delta^{\beta}_{\alpha,j})$ and $\delta^{\beta}_{j} = \mathrm{Im}(\delta^{\beta}_{\alpha,j})$ for convenience. Then, these become

$$\boldsymbol{\phi}^{\beta}_{\alpha} = \sum_j \delta_{\alpha,j} + i \sum_j \delta^{\beta}_{j}. \tag{6.30}$$

In terms of the dimension associated to the exchanged degrees of freedom, m is an entity where each edge occurs between other entities which are themselves defined via interactions for which other messengers m'; that is, the notion of dimension used must be defined in terms of the embeddings $\mathrm{Emb}(\boldsymbol{\delta}^{\beta}_{\alpha})$, which contains the next collection of degrees of freedom across all m' implicitly embedded in m. At some point, given that the theory is relational, a limit (observable) value ε^* will be reached for some $\boldsymbol{\delta}^* \in \mathrm{Emb}(\boldsymbol{\delta}^{\beta}_{\alpha})$. For any degree of freedom $\boldsymbol{\delta}$ in m, the probability of observing its average value becomes

$$p(\boldsymbol{\delta}) = P(\boldsymbol{\delta} = \overline{\boldsymbol{\delta}}). \tag{6.31}$$

and the dimension $\boldsymbol{d}$ of $\boldsymbol{\delta}^{\beta}_{\alpha}$ is approximated by the Rényi information dimension[110]

$$\boldsymbol{d}_{\gamma}(\boldsymbol{\delta}^{\beta}_{\alpha}) = \lim_{\varepsilon \to \varepsilon^*} \frac{\frac{1}{1-\gamma}\left(\ln \sum_{\boldsymbol{\delta} \in \mathrm{Emb}(\boldsymbol{\delta}^{\beta}_{\alpha})} p(\boldsymbol{\delta})^{\gamma}\right)}{\ln \frac{1}{\epsilon}}. \tag{6.32}$$

Note that, instead of $\varepsilon \to 0$, the size of the smallest box is finite and given by the magnitude of $\boldsymbol{\delta}^*$. A better approximation can be achieved using multifractal analysis[111], but the current one suffices conceptually for our purposes. The magnitude of an interaction is a scalar corresponding to the norm $M = \|\boldsymbol{\delta}^{\beta}_{\alpha}\|$, which can be used to obtain a normalised representation $\tilde{\boldsymbol{\delta}}^{\beta}_{\alpha} = \boldsymbol{\delta}^{\beta}_{\alpha}/M$ during analysis when only one scale is involved. Note that for an interaction with symmetric exchange of degrees of freedom and no underlying embedding, we recover the usual notion of dimension as $\boldsymbol{d}(\boldsymbol{\delta}^{\beta}_{\alpha}) = D^2 \tilde{\boldsymbol{\delta}}^{\beta}_{\alpha}$.

The degrees of freedom of a system must respond to topological constraints during an interaction. While not all degrees of freedom will be constrained, some may. For a subset $J, |J| \leq D$, we express two types of constraints: those pertaining to each side of the exchange, and those pertaining to their mutual transfer. Further suppose without loss of generality that all individual degrees of freedom in $\boldsymbol{\delta}_\alpha^\beta$ posses such constraints. Then, if $\boldsymbol{\delta}_\alpha^\beta$ can be written as

$$\boldsymbol{\delta}_\alpha^\beta = (y_1(x_1\delta_{\alpha,1} + i(1-x_1)\delta_1^\beta), y_2(x_2\delta_{\alpha,2} + i(1-x_2)\delta_1^\beta), \cdots, y_D(x_D\delta_{\alpha,D} + i(1-x_D)\delta_D^\beta)) \tag{6.33}$$

such that $0 \leq x_j \leq 1$ and $\sum_j y_j = 1$. Under these constraints, the magnitude of the exchange is invariant under transformations $\boldsymbol{x}_\nu = \boldsymbol{A}_\nu^\mu \boldsymbol{x}_\mu$ and $\boldsymbol{y}_\sigma = \boldsymbol{B}_\sigma^\rho \boldsymbol{y}_\rho$. Similarly, fixing constraint yields a partial symmetry over the remaining constraints: we immediately recognise the statement of conservation laws under this new language. The exchange is non-conservative when $|J| = 0$, partially conservative when $|J| \leq D$, and conservative with $|J| = D$. Furthermore, conservation laws obtained in this manner are local, and hence guarantee the existence of at least one causal path involving each conserved degree of freedom as required by Lorentz invariance (special relativity), and permits tracing each path to entities α and β consistently having frequencies shifted when exchanged between accelerating inertial reference frames as required by Lorentz covariance (general relativity). We hypothesise that non-conserved exchanges of degrees of freedom arise thanks to incomplete descriptions of Φ_i.

To capture frequencies, we observe that these are also distributions of the form

$$\boldsymbol{\omega}_\alpha^\beta = X_\alpha(\Omega^\omega, \Phi_i) + i \cdot X^\beta(\Omega^\omega, \Phi_i), \tag{6.34}$$

a complex scalar that captures the joint relaxation process after propagation of action across both entities. To draw an analogy to frequency spectra, the value M computed previously acts as an amplitude and the distribution of frequencies for an interaction is analogous to its spectrum. Nevertheless, we observe that frequency density functions are not, in general, continuous.

To obtain a suitable definition for $\hbar$, we require it to reflect intrinsic and combinatorial sources of uncertainty. For the intrinsic uncertainty, we assume such quantity $\mathfrak{h}_\alpha, \mathfrak{h}^\beta$ can be found per each entity respectively. For the combinatorial part, consider the sets W_α, W^β that contain all topologically equivalent versions of the entities after relaxation upon interaction associated with outcome distributions. Most generally, we identify the (possibly dense) structure of interactions in the embedding as a random fractal for which the notion of measure has been clarified[112]. Therefore, assuming the existence of a suitable metric μ such that

$\mu(a \cdot b) = \mu(a) + \mu(b)$, one way to compute the uncertainty $\hbar$ becomes

$$\boldsymbol{\hbar}_{\alpha}^{\beta} = X_{\alpha}(\Omega^{\hbar}, \Phi_i)^{\mathfrak{h}} + i \cdot X^{\beta}(\Omega^{\hbar}, \Phi_i)^{\mathfrak{h}} = \mathfrak{h} \cdot \left[\mu\left(W_{\alpha}\right) + i\mu\left(W^{\beta}\right)\right]. \tag{6.35}$$

Furthermore, we can relate $\mathfrak{h}$ to already known quantities. Based on available information, the intrinsic uncertainty must be related to m, and more specifically, to dispersion measures of the exchanged degrees of freedom. We choose standard deviation for such purpose. Moreover, since $\mathrm{Re}(\delta_{\alpha,j}^{\beta}) = \delta_{\alpha,j}$ and $\mathrm{Im}(\delta_{\alpha,j}^{\beta}) = \delta_{j}^{\beta}$ are distributions obtained by projection onto components of the complex plane. Let us suppose that the intrinsic uncertainty depends on interdependencies of degrees of freedom contributed by each object, on the interdependencies between each exchange per single degree of freedom, and on interdependencies across different degrees of freedom between objects. This last case corresponds, by construction, to that where conservation laws apply to some degrees of freedom. The form must also be that of an inequality, since intrinsic uncertainty is a lower bound. Let us propose the ansatz

$$\mathfrak{h} \equiv \mathfrak{h}_{\alpha}^{\beta} \leq \left(\prod_{j,k} \sigma(\delta_{\alpha,j}\delta_{\alpha,k})\right)\left(\prod_{j,k} \sigma(\delta_{j}^{\beta}\delta_{k}^{\beta})\right)\left(\prod_{j,k} \sigma(\delta_{\alpha,j}\delta_{k}^{\beta})\right)\left(\prod_{j} \sigma(\delta_{\alpha,j}\delta_{j}^{\beta})\right). \tag{6.36}$$

The first two terms describe the organization of the exchange with respect to α and β only, and although we expect them to have an effect on the physics of the interaction, these depend on the inner mechanics driving the interaction. In other situations, the mechanisms may not be transparent for a variety of reasons. Using our Principle of Equivalence, we can at least ascertain that these quantities should be bounded by some common value across equivalent interactions. A similar reasoning can be made for the third term depends on the mechanics at the *locus* of interaction, which includes the context Φ_i. All of the latter are expensive to obtain and require extensive interrogation of interactions by means of *causal experiments*, or experiments where changes in the entities and their corresponding counterfactuals indirectly probe and map mechanisms. The only aspect either directly of efficiently observable through measurements is the exchange of similar degrees of freedom across entities by means of joint experiments. Hence, we may simplify Eq. 6.36 as

$$\mathfrak{h} \leq c \cdot \prod_{j} \sigma(\delta_{\alpha,j}\delta_{j}^{\beta}), \tag{6.37}$$

where c is an appropriate constant. Consider the situation when conservation laws exist such that a positive, finite local exchange budget $M_{\alpha,j}^{\beta}$ exists for each $\delta_{\alpha,j}^{\beta}$ such that $\delta_{\alpha,j} = x_j M_{\alpha,j}^{\beta}$ and $\delta_{j}^{\beta} = (1-x_j)M_{\alpha,j}^{\beta}$. This implies that x_j is a distribution, hence Eq. 6.37 becomes

$$\mathfrak{h} \le c \cdot \prod_j \sigma\left[\left(M^{\beta}_{\alpha,j}\right)^2 x_j(1-x_j)\right]$$
$$= c \cdot \prod_j \left(M^{\beta}_{\alpha,j}\right)^2 \sigma\left[x_j - x_j^2)\right], \tag{6.38}$$

which for a completely symmetric conservative exchange –i.e. $x_j = 1 - x_j =$ and $M^{\beta}_{\alpha,j} = M^{\beta}_{\alpha,k} = M$- becomes

$$\mathfrak{h} \le c(\sqrt{2}M^2)^D \cdot \prod_j \sigma^2(x_j). \tag{6.39}$$

In a truly stochastic and irreversible process, the distribution of values in the ensembles spanned by $\delta_{\alpha,j}, \delta^{\beta}_j$ ensures $\sigma > 0$. As we move to a larger scale, the relative variance decreases, and hence the smaller σ appears to be. At a sufficiently large limit, σ becomes negligible. Consider the exchange of position x and momentum p when measuring the state of a wave function ψ using an instrument (Inst), and suppose their decomposition is possible into $\delta^{\text{Inst}}_{\psi,x}$ and $\delta^{\text{Inst}}_{\psi,p}$ respectively. Since, ψ is a distribution, we assume the latter quantities also determine distributions. Using Eq. 6.37

$$\mathfrak{h}^{\text{Inst}}_{\psi} \le c \cdot \sigma(\delta_{\psi,x}\delta^{\text{Inst}}_x)\sigma(\delta_{\psi,p}\delta^{\text{Inst}}_p) \tag{6.40}$$

and observing that

$$x = c_x \cdot \delta_{\psi,x}\delta^{\text{Inst}}_x, \quad p = c_p \cdot \delta_{\psi,p}\delta^{\text{Inst}}_p \tag{6.41}$$

must hold for any given exchange where c_x, c_p are determined by the slice in volume of the exchange corresponding to x, p respectively, we obtain the relation

$$\mathfrak{h}^{\text{Inst}}_{\psi} \le c \cdot \sigma(\delta_{\psi,x}\delta^{\text{Inst}}_x)\sigma(\delta_{\psi,p}\delta^{\text{Inst}}_p)$$
$$= \frac{c}{c_x \cdot c_p}\sigma(x)\sigma(p) \tag{6.42}$$

which, after relabelling $\mathfrak{h}^{\text{Inst}}_{\psi} = h$ and equating $\frac{c}{c_x \cdot c_p} = 4\pi$ yields

$$h \le 4\pi\sigma(x)\sigma(p), \tag{6.43}$$

or in its more usual form[113] with reduced Planck's constant $\hbar = h/2\pi$

$$\sigma(x)\sigma(p) \geq \frac{\hbar}{2}. \tag{6.44}$$

The general argument for classical mechanics was first given by Fürth[52]. Let us now turn our attention to W_α and W^β. Their internal degrees of freedom of interacting are countable, and their reconfiguration depends on the context Φ and their governing dynamics. In the interactions view, dynamical laws depend on the composition of interactions within an entity, and so on recursively. To remain tractable, we demand W to quantify reconfigurations of entities in the immediate microscale only. Even so, the task of understanding entities remains momentous from an empirical perspective, since it involves at first value understanding the distribution of coupled responses by means of repeated statistical experiments. Nevertheless, an alternative approach exists: after removing interaction locales within an entity, the state at a sufficiently small time period $\delta\tau$ such that the average structure remains resolvable within intrinsic uncertainty limit $\mathfrak{h}$ can be approximated by a collection of basis sets with coefficients corresponding to eigenvalues of the spectral decomposition of its structure. Hence, W_α must be proportional to the number of eigenvalues λ_α that span the structure of α, which are countable and finite.

Summarising, the existence of an interaction (class) can be appropriately inferred when an exchange of degrees of freedom occurs between two entities mediated by a context, whose structure is in turn explained in terms of interactions, and when frequencies and uncertainties describing the distribution of future entity states can be obtained corresponding to experimental observations. While interaction magnitudes can have any value and/or sign, the number of degrees of freedom involved is taken as positive. Entities are localised interactions that collectively exhibit robustness, and laws are collective manifestations of consequences at some sufficiently large thermodynamic limit. Formally, we denote interactions from here onward as

$$\boldsymbol{\leftrightsquigarrow}_i^{\alpha,\beta} = (\boldsymbol{\delta}_\alpha^\beta, \boldsymbol{\omega}_\alpha^\beta, \boldsymbol{\hbar}_\alpha^\beta)_{\Phi_i}. \tag{6.45}$$

6.2.2 Interaction spaces

An *interaction space* $\boldsymbol{\mathcal{I}}$ is the fractal[114], stochastic[115] manifold containing all relevant interactions to describe a given phenomenon at one or more scales. For every $\boldsymbol{\leftrightsquigarrow}_i^{\alpha,\beta} \in \boldsymbol{\mathcal{I}}$ exists at least one dense neighbourhood U such that in the structure $(U, \phi : U \to \mathcal{B}^*)$

$$\mathcal{B}^* = \mathcal{B}^\delta(\mathbb{C}^\mathcal{D}) \times \mathcal{B}^\omega(\mathbb{C}) \times \mathcal{B}^\omega(\mathbb{C}) \tag{6.46}$$

where $\mathcal{B}$ denotes a Borel set with a corresponding probability measure and $\mathcal{D}$ is the number of distinct degrees of freedom across all interactions in $\mathcal{I}$. To construct the manifold, we conveniently redefine

$$\boldsymbol{\delta}_{\alpha}^{\beta,*} = (\delta_{\alpha,1}^{\beta,*}, \delta_{\alpha,2}^{\beta,*}, \cdots, \delta_{\alpha,\mathcal{D}}^{\beta,*}) \tag{6.47}$$

and

$$\swarrow\!\!\nearrow_{i}^{\alpha,\beta,*} = (\boldsymbol{\delta}_{\alpha}^{\beta,*}, \boldsymbol{\omega}_{\alpha}^{\beta}, \boldsymbol{\hbar}_{\alpha}^{\beta})_{\Phi_i}. \tag{6.48}$$

where $\delta_{\alpha,j}^{\beta,*} = 0$ in $\swarrow\!\!\nearrow_{i}^{\alpha,\beta,*}$ whenever $\delta_{\alpha,j}^{\beta}$ does not appear in $\swarrow\!\!\nearrow_{i}^{\alpha,\beta}$. Suppose without loss of generality that the probability measure is Gaussian. To every interaction $\swarrow\!\!\nearrow_{i}^{\alpha,\beta} \in \mathcal{I}$ corresponds a local context Φ_i belonging to manifold is characterised by neighbourhoods $(U_{\Phi_i}, \varphi : U_{\Phi_i} \to \mathcal{B}_{\Phi_i}^{*})$. The state of Φ resembles that of random media[116], which explains our choice of terminology as a pseudo-extensive field-like entity. We call the association $\swarrow\!\!\nearrow_{i}^{\alpha,\beta} \mapsto \Phi_i$ an interaction's *local context*, and the association $\swarrow\!\!\nearrow_{i}^{\alpha,\beta} \mapsto ||\boldsymbol{\delta}_{\alpha}^{\beta}||$ its magnitude. The projector

$$\boldsymbol{L}(\Phi_i) = \{\boldsymbol{r}_i^{\mu}\} = R_i(\mathbb{C}^{\mu}) \tag{6.49}$$

obtains a set of random variables whose distribution is centred on instances of $\swarrow\!\!\nearrow_{i}^{\alpha,\beta}$. $\boldsymbol{r}^{\mu}$ corresponds to what we usually interpret as the stochastic position vector, or the *locus of interaction*. The resulting set may be empty, which implies that some interactions are not present in that specific localisation. For example, we only observe interactions between photons and electrons at certain locations and times. Due to the principle of equivalence above, we demand interactions instances within a given distance ϵ such that $||\swarrow\!\!\nearrow_{i}^{\alpha,\beta} - \swarrow\!\!\nearrow_{i}^{\alpha,\beta}|| \leq \epsilon$ to be equivalent, or rather, to choose ϵ such that the resulting distribution is unimodal so that these belong to the same interaction class. Moreover, we define a *localised interaction* as the pair $(\swarrow\!\!\nearrow_{i}^{\alpha,\beta}, \boldsymbol{r}_i^{\mu})$, which describes a *localised interaction space* $\mathcal{I}_r$. When possible, it may be convenient to use interactions with reduced degrees of freedom, or *reduced interactions*

$$\not\swarrow\!\!\nearrow_{i}^{\alpha,\beta,*} = (\not\boldsymbol{\delta}_{\alpha}^{\beta,*}, \boldsymbol{\omega}_{\alpha}^{\beta}, \boldsymbol{\hbar}_{\alpha}^{\beta})_{\Phi_i}, \tag{6.50}$$

in which case we obtain the *reduced interaction space* $\boldsymbol{I}_{*}$. However, this still proves challenging for visualisation purposes. We can further compute the *scalar interaction space*, a set of real-valued distributions of the form

$$\leftrightsquigarrow i^{\alpha,\beta,*} = \| \not\leftrightsquigarrow_i^{\alpha,\beta,*} \| = (\| \boldsymbol{\phi}_\alpha^{\beta,*} \|, \|\boldsymbol{\omega}_\alpha^\beta\|, \|\boldsymbol{\hbar}_\alpha^\beta\|)_{\Phi_i}. \tag{6.51}$$

Observe that Φ is defined also as product of distributions, and hence must also be a network of more primitive –i.e. fundamental- interactions. We may adopt, for instance, the convention of $\boldsymbol{x}^\mu = (x^1, x^2, x^3) = (x, y, z)$. If the distribution is unimodal in x, y, z then the slicing from which Φ_i is obtained is spacelike. Within a single interaction space $\mathcal{I}$, localised interaction pairs allow us to obtain

$$min\left[\mathcal{L}\left(\Phi_i^{\mathcal{I}}\right) - \mathcal{L}\left(\Phi_j^{\mathcal{I}}\right)\right] = \delta\boldsymbol{r}_{ij}^\mu. \tag{6.52}$$

$\delta r = \|\delta\boldsymbol{r}_{ij}\|$ corresponds to a spacelike distance between two contexts, a distribution describing the minimum resolvable (i.e. unimodal) position change that defines the spatial resolution of the background for an interaction space. A spacelike curve is a path between local contexts Φ, Φ' such that every element in the path is also a local context within distance of δr one from another. Note that, in general, there exist many possible routes from two different local contexts.

When an interaction space is endowed with a projector $\mathcal{L}$, the resulting inverse fibration is the *localised interaction space* $\mathcal{I}_{\mathcal{L}}$. Naturally, to each $\mathcal{I}_{\mathcal{L}}$ corresponds a localised context set $\Phi_{\mathcal{L}}^{\mathcal{I}}$ containing at least all local contexts associated with every interaction class in $\mathcal{I}$. Also, $\mathcal{I} = \langle\mathcal{I}_{\mathcal{L}}\rangle$ and $\Phi^{\mathcal{I}} = \langle\Phi_{\mathcal{L}}^{\mathcal{I}}\rangle$. Consider the mapping between localised context sets $\Phi_{\mathcal{L}}^{\mathcal{I}}, \Phi_{\mathcal{L}}^{\mathcal{J}}$ and define

$$\chi(\Phi_{\mathcal{L}}^{\mathcal{I}}) = \Phi_{\mathcal{L}}^{\mathcal{J}} \tag{6.53}$$

whenever every local context in $\Phi_{\mathcal{L}}^{\mathcal{J}}$ was produced by a single event leading to an ensemble of relaxation events for each local context instance with frequencies $\omega(\Phi_{\mathcal{L}}^{\mathcal{I}}, \Phi_{\mathcal{L}}^{\mathcal{J}})$. By setting $\delta\tau = \langle\omega\rangle^{-1}$, we obtain the average proper time required to transform $\mathcal{I}_{\mathcal{L}}$ into $\mathcal{J}_{\mathcal{L}}$. The definition of $\delta\tau$ is inherently degenerate, since, it involves multiple ways to construct the localised interaction space and multiple ways to summarise the resulting relaxation frequencies. It is not hard to imagine a summary procedure where the value of the observable depends on the choice of a fixed point $\boldsymbol{r}^\mu(\mathcal{I}_{\mathcal{L}})$, which corresponds to the notion of frame of reference.

6.2.3 Aggregation and composition

Let us now consider various special relations between interactions. Empirically, we observe two general types of associations between them. The first one is aggregation, in which the identity of an entities is preserved under addition of new microscale interactions or subtraction of existing ones within some range of aggregation. For instance, a stream continues to be a stream after removing half its water. The second relation is composition, in which a collection of interactions modulated by aggregation yields new behaviour at a the next macroscale. Superconductivity is an appropriate example of this. While aggregation and composition can be usually expressed in terms of coordinates, the GToI should permit understanding both without requiring localised interaction spaces. In addition, both relations should lead to unveiling causality across interactions in terms of how changes in the interactions involved in aggregation and composition relations translate into changes on those interactions impacted by them. Figure 6.3 schematises the situation described above.

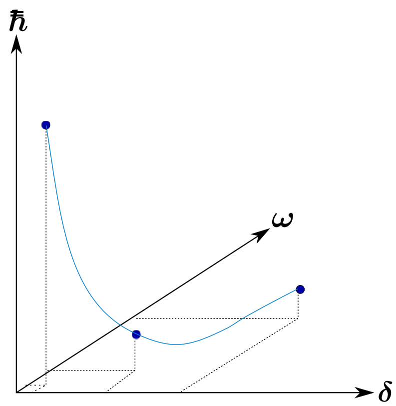

Figure 6.3: Abstract representation of an interaction space $\mathcal{I}$. This space consists of three interactions (blue points), placed according to their average magnitudes in the space. The interactions are causally connected (blue lines) by means of either aggregation or composition.

Aggregation entails an almost total, asymmetric exchange of degrees of freedom where $\mathrm{Re}(\boldsymbol{\delta}_{\alpha}^{\beta}) = 0$, $V(\boldsymbol{\delta}_{\alpha}^{\beta}) \approx V(\alpha'')$ and $V(\beta'') = 0$. The identity of one of the interactants is lost (β), and absorbed by the other one (α). By convention, denote the donor entity as β. As aggregates continue to increase in size, a family of exchanges arises $\boldsymbol{\delta}_{\alpha}^{\beta} = n\boldsymbol{\delta}_{\alpha}$ with n the number of elementary units β involved in the aggregation. Frequency-wise, each interaction in the family should scale as $\boldsymbol{\omega}_{m\alpha}^{n\beta} \propto (\max(m,n))^{-1} \cdot \boldsymbol{\omega}_{\alpha}^{\beta}$, since relaxation and propagation are proportional to object length. Observe that the frequency spectra comprises modes spaced at integer intervals.

We find ourselves in a relatively counter-intuitive situation regarding the uncertainty. Since one of the entities of the interaction relaxes into the first one, W_{α} should be proportional to the volume $V(\alpha'' + \varnothing) \propto V(\alpha) + V(\beta)$, yet the change in the number of eigengraphs describing α'' should depend on how the mixing occurs during the merge of degrees of freedom, that is, on the extent of the effective interaction surface involved in the mixing. Since mixing translates into a product due to the new possible combinations between involved surfaces,

$$\mu(W_\alpha) \propto \mu([V(\alpha)V(\beta)]^\gamma) = \gamma[\mu(V(\alpha) + \mu(V(\beta))] \tag{6.54}$$

where $0 \le \gamma \le 1$ determines the dimensionality of the mixing from being surface-like (i.e. $\gamma \approx 2/3$). Note that the uncertainty of an aggregation can be smaller than that of a regular interaction. This is not expected, since the form of $\boldsymbol{\hbar}$ resembles that of entropy, which is an extensive quantity. But we soon remind ourselves that interactions posses non-extensive properties and, from the point of view of the underlying event, an aggregation tends to involve less information, since it does not change the nature of the entity, only its volume. It is significant to observe that the diameter of Φ_i is proportional to n.

Composition operates radically different. A composition interaction does not necessarily involves the donation of the entire set of degrees of freedom from one object to another. Composition means that new degrees of freedom arise at one scale due to other degrees of freedom being lost at a smaller scale. Similarly, the frequency varies depending on α and β. However, the key rests upon the uncertainty. Recall that W_α and W_β can be expressed in terms of their corresponding bases, related to the subgraphs used to compute the ensemble that defines α'' and β'' respectively. Performing the analysis for α

$$W_\alpha \propto |\langle \lambda_k \rangle_\alpha| \tag{6.55}$$

such that

$$\langle \alpha \rangle = \sum_k \sum_{\delta \in \boldsymbol{\delta}_\alpha^\beta} \lambda_k G_{\alpha,k}(\delta). \tag{6.56}$$

An interaction is compositional when, for some set of degrees of freedom involved during the exchange $Y = \{\delta_{j_1}, \delta_{j_2}, \cdots, \delta_{j_y}\}$ and a new set of degrees of freedom X, $|X| \le |Y|$, the decomposition after relaxation becomes

$$\langle \alpha \rangle = \sum_k \sum_{\delta \notin Y} \lambda_k G_{\alpha,k}(\delta) + \sum_j \sum_{\delta \in X} \lambda_j G_{\alpha,k}(\delta), \tag{6.57}$$

which can be interpreted as the loss of existing internal degrees of freedom as determined by the exchange, and the gain of new degrees of freedom in the resulting entities after relaxation. The latter points to the realisation that new degrees of freedom (i.e. edges) arise in the macroscale of G thanks to degrees of freedom being lost at some microscale through compositional interactions. Because of the above, an interaction $\swarrow\!\!\!\nearrow_j^{\mu,\eta}$ is *more primitive* than an interaction $\swarrow\!\!\!\nearrow_i^{\alpha,\beta}$ if and only if some of its degrees of freedom appear as parameters in the spectral decomposition of the uncertainty of the latter one, but not in the graph of either resulting entity .

Although we have provided a description of aggregation and composition above, it is insufficient to compute consequences that separate them. For instance, we observe that in general the exchange of degrees of freedom are antisymmetric in one case, and that W_α contains less normal modes, since whole sections of the graph corresponding to various exchanged degrees of freedom have been replaced with fewer, new degrees of freedom. Hence, we are motivated to state our second guiding principle:

Principle of Composition. *For every degree of freedom at once scale a product of compositional interactions must exist giving rise to it.*

Two corollaries spring from this principle. First, if a degree of freedom δ is exchanged by an interaction $\swarrow\!\!\nearrow_i^{\alpha,\beta}$ and δ is explained by interactions $\swarrow\!\!\nearrow_k^{\mu,\nu} \neq \swarrow\!\!\nearrow_i^{\alpha,\beta}$, the interaction $\swarrow\!\!\nearrow_k^{\mu,\nu}$ *is more primitive than* $\swarrow\!\!\nearrow_i^{\alpha,\beta}$, or

$$\swarrow\!\!\nearrow_k^{\mu,\nu} \ni\!- \swarrow\!\!\nearrow_i^{\alpha,\beta}. \tag{6.58}$$

Second, if the interaction exchanges degrees of freedom that arise compositionally from a set containing the same interaction, then it is *fundamental.* This signifies that no further local context exists ($\Phi_i = \varnothing$), and that the concrete theory is background-independent.

The GToI should provide the means to understand at a deeper level the physically possible mappings between interaction spaces, which involves understanding what happens to interactions under replacements of the local context. The following section provides the necessary tools to achieve this.

6.2.4 Transformations

A transformation interpreted in the context of dynamical manifolds entails a transformation of position, momenta and other degrees of freedom of microscale entities resulting in new values for these, usually constrained by some conservation laws. Concomitantly, extensive macroscale quantities –e.g. E, S, N, P, V, μ- may also change depending on whether the reorganisation of the microscale leads to the emergence of phases with new kinds of properties. In addition, such processes occur during an instant of size Δt during which a collection of forces F_i are applied. All the action in the system is bound to some notion of position by means of either a coordinate system or coordinate invariants that enable calculations to be performed. The top half of Figure 6.4 depicts this notion of transformation.

When looked through the perspective of interactions, we must reason in terms of exchanges of degrees of freedom, frequencies and uncertainties. Let us dissect carefully various situations from this vantage point. First, the application of a force may change the values of spatially dependent degrees of freedom (i.e. $\boldsymbol{q}, \boldsymbol{p}$). Whether contact forces or fields at at play, a sudden symmetry breaking establishes a preferential direction across some degrees of freedom. If the effect of applying the force (or rather, of the action of the field on the entity) does not change its composition or the types of some interactions involved on average, these interactions are invariant with respect to changes of their local context. Recall that change of the local contexts involves determining the covariance of $(\leftrightsquigarrow_i^{\alpha,\beta}), \Phi_i$. For example, the distribution of interaction classes across loci may vary (reflected in the statistics of $\leftrightsquigarrow_i^{\cdot,\cdot}$) but the fundamental character of the interaction may not. An interaction can be invariant under substitution of local context.

The second, more interesting case, is that in which interactions are not invariant, as in the bottom half of Fig. 6.4. In this case, the effect of a transformation falls into four possibilities.Substituting the local context may result in translating interactions from one location in interaction space to another. Due to the principle of equivalence, the transformation has effectively converted a set of interactions into another. Another possibility corresponds to a decrease in the number of interactions, since movement across interaction space may unify various interactions into a single one. Finally, a third possibility is the rise of new interactions due to composition. To achieve this, there must exist families of trajectories of local context substitutions with a critical value in which a new type symmetry breaking arises: a single interaction separates into two or more types of interactions along those trajectories. In general, this later aspect reveals another type of irreversibility: when transformation trajectories coincide, information is erased about the past, and when transformation trajectories diverge new information is created. However, since we are in a stochastic interaction space, the inverse transformation taking any of the alternatives back to a point prior to the divergence is guaranteed to differ from it, since the local context will have had undergone variations altering the outcome. Such trajectories describe a type of fractal which can be expected to bear some resemblance around these symmetry breaking points to the resulting geometry of random walks and other stochastic processes on fractal spaces[117,118].

A transformation $\boldsymbol{\mathcal{T}}$ depends on the information stored physically about simultaneous changes in $\leftrightsquigarrow_i^{\alpha,\beta}$ and Φ_i. Such information allows us to refer to the *memory* of the interaction, and the transformation itself as the *robotics* that alters stored information in it. This provides a view of physics that is properly computational, and unveils to some extent why information and energy are intricately connected as suspected since long ago[82]: because of the construction of the interaction space as a complex stochastic manifold, spatial relations between interactions before and after the transformation are given by the Fisher information metric[119] which also corresponds to thermodynamic distance[120]. At the same time, it extends computation

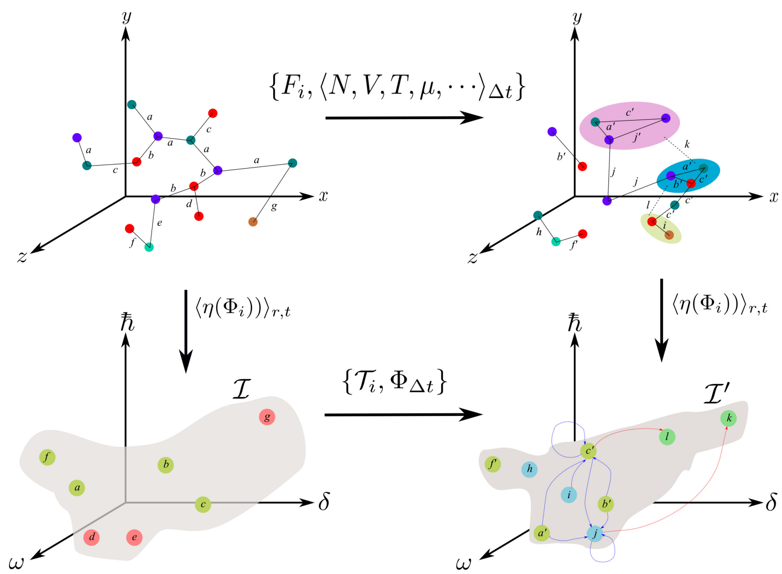

Figure 6.4: Transformation in dynamical manifolds vs interaction spaces. During a transformation, forces applied to a system change microstates and respective macrostate extensive variables. When translated into interactions from a localised interaction space, interaction classes are obtained. Under the effect of a transformation $\mathcal{T}$, tantamount to local corresponding substitution with respect to a degree of freedom by a small amount Δt, some interactions are preserved and/or translated (yellow green), others disappear (light red) and others arise at the microscale (light blue) and the macroscale (lime green). New microscale (blue line) and macroscale (red line) degrees of freedom arise as a result of composition and aggregation relations. The result of a transformation is to alter the shape of the interaction space, in which boundaries correspond to parametric descriptions taken at various relevant thermodynamic limits.

conceptually as a phenomenon rooted in controlling aspects of the fundamental stochasticity present in the mechanical underpinnings of our universe; the type of computation we are used to must be translatable into the GToI as the existence of interactions with familiar properties found across digital systems as exchanges of simple degrees of freedom (usually binary ones) requiring an enormous array of supporting interactions that produce sharp distributions which, at the relevant macroscale of bits, result in deterministic operations. More recently, quantum computation appears to operate by removing layers of interactions to allow the manifestation of stochasticity by allowing superposition and entanglement across Hilbert space and benefit from simultaneous non-determinism. Since the energy of computational interactions should be proportional to the number of constrained degrees of freedom involved during the exchange, more constraints should therefore translate into more expensive computing models; it is thus not surprising why quantum computing elements require lower state-switching energies[121]. We suspect that deeper understanding of the physics of space-time should open the possibility for another type of computation beyond the digital and the quantum mechanical, assuming that quantum gravity is an attainable scientific goal.

To accommodate the richness we suspect exists within interaction spaces without sacrificing clarity, we require mathematical objects capable of nicely hiding the complexity of moving by shifting local context. Essentially, our goal is to specify tensor-like objects, with the condition that they contain functions (or more generally morphisms) instead of having values as entries. To that end, we define a simple homological algebra[122] of tensors of morphisms, or a φ-*Tensor algebra.*

Definition 24 (1-morphism)**.** Let $\varphi : \mathbb{F} \to \mathbb{F}$ be a morphism from a field onto itself. φ is a 1-morphism with the following properties:

1. The set $\mathfrak{F}$ containing all 1-morphisms endowed with arithmetic operators $(\mathfrak{F}_\varphi, +, \cdot)$ is a field. Operators $-, \div$ can be defined as usual.

2. $\mathfrak{F}$ contains an *application* operator $\odot$ such that $\varphi \odot a = \varphi(a), \forall a \in \mathbb{F}$. $\odot$ has higher precedence than arithmetic operators.

3. $\mathfrak{F}$ is a monoid under the *composition* operator $\circ$, having the standard functional interpretation $(\varphi \circ \psi) \odot a = \varphi(\psi(a))$.

4. For any arithmetic operator $\oplus$, $[\varphi' \circ \varphi \oplus \psi' \circ \psi] \odot a = (\varphi' \circ \varphi) \odot a \oplus (\psi' \circ \psi) \odot a$.

Amongst the members of $\mathfrak{F}$, we find the following special morphism:

$$
\begin{aligned}
0_\varphi \odot a &= 0 (\in \mathbb{F}) \\
1_\varphi \odot a &= 1 \\
c_\varphi \odot a &= c
\end{aligned}
$$

$$
\delta_{ij}^{\varphi} = \begin{cases} 1_\varphi & i = j \\ 0_\varphi & i \neq j \end{cases}
$$

Definition 25 (φ-Tensor)**.** Let $\mathfrak{F}$ be a field of 1-morphisms and $\mu_1, \mu_2, \cdots, \mu_N$ a collection of non-negative indices. a φ-tensor is a multilinear map of the form

$$
\boldsymbol{T}_{\mu_1\mu_2\cdots\mu_N} = (\phi_{\mu_1\mu_2\cdots\mu_N}), \quad \phi_{\mu_1\mu_2\cdots\mu_N} \in \mathfrak{F}.
$$

Standard tensor index rules apply to φ-tensors, including contraction rules and tensor arithmentics. The following rules additionally determine φ-tensors:

1. $\boldsymbol{u}_\nu = \boldsymbol{T}_{\mu\nu}\boldsymbol{u}^\mu = \boldsymbol{T}_{\mu\nu} \odot \boldsymbol{u}^\mu = \sum_i \sum_j \boldsymbol{e}_i \cdot \varphi_{ij} \odot u_i$, where $\boldsymbol{e}_i$ is an element of the basis $B(\mathbb{F}^d)$ of a d-dimensional vector space $V(\mathbb{F}^d)$,
2. $\left(\Sigma_k \boldsymbol{T}_{\mu\nu}^{(k)}\right)\boldsymbol{u}^\mu = \Sigma_k (\boldsymbol{T}_{\mu\nu}^{(k)}\boldsymbol{u}^\mu)$,
3. For $\boldsymbol{T}_{\mu\nu} = (\phi_{ij})$ and $\boldsymbol{S}^{\nu\sigma} = (\psi_{jk})$, then $\boldsymbol{U}_\mu^{\sigma,\circ} = \boldsymbol{T}_{\mu\nu} \circ \boldsymbol{S}^{\nu\sigma} = \sum_j \phi_{ij} \circ \psi_{jk}$.

Consequently, we define a transformation $\mathcal{T} : \mathcal{I} \to \mathcal{J}$ as a discrete operation, where for $\Phi_i^{\mathcal{T}}$ denotes the state of the local context Φ_i associated with $\swarrow\!\!\nearrow_i^{\alpha,\beta}$ such that for a sufficiently small difference $\Delta\Phi_i = \Phi_i^{\mathcal{T}} - \Phi_i$ where $\|\Delta\Phi_i\| \geq \mathfrak{h}_{\Phi_i}$ the transformation becomes

$$
\boldsymbol{\mathcal{T}}(\swarrow\!\!\nearrow_i^{\alpha,\beta}, \Delta\Phi_i) \approx \boldsymbol{F} \odot \Delta\Phi_i + \boldsymbol{G} \odot \swarrow\!\!\nearrow_i^{\alpha,\beta} + \boldsymbol{H}\left[\bigcirc_{j\in\Lambda} \boldsymbol{\Psi}_j\right] \odot \swarrow\!\!\nearrow_j^{\mu,\nu}. \tag{6.59}
$$

In Eq. 6.59, we find that the transformation is approximated by the sum of three φ-tensors. $\boldsymbol{F}$ is the *local context memory φ-tensor*, containing information about how the components of an interaction vary as a function solely of the difference obtained by replacing one local context with another. Next, $\boldsymbol{G}$ is the *internal memory φ-tensor*, which only depends on the properties of the interaction prior to the local context substitution. The third term contains two φ-tensors, $\boldsymbol{H}$ and $\boldsymbol{\Psi}_j$ associated with interactions in a set Λ. This set contains all interactions that are most immediately primitive with respect to $\swarrow\!\!\nearrow_i^{\alpha,\beta}$,

$$\Lambda = \{ \swarrow\!\!\nearrow_i^{\mu,\nu} \in \mathcal{I} | \swarrow\!\!\nearrow_i^{\mu,\nu} \ni\!\!- \swarrow\!\!\nearrow_i^{\alpha,\beta} \}. \tag{6.60}$$

The φ-tensor $\boldsymbol{H}$ captures aggregation effects, while $\boldsymbol{\Psi}_j$ are φ-tensors associated to each primitive interaction in Λ associated to generative effects[67]. For those, some facts become immediately apparent. All $\boldsymbol{\Psi}_j$ must have the same rank n and dimensionality m, and their density –fraction of non-zero entries from the m^n possible ones- must be proportional to the complexity of the generative effects. Since the description of transformations across interaction spaces is inherently degenerate, the choice of φ-tensors, specially those associated with primitive interactions, should be as parsimonious as possible. In many simple cases, we anticipate the transformation to be separable into individual transformations for $\boldsymbol{\delta}$, ω and $\boldsymbol{\hbar}$, in which $\boldsymbol{F} \to \boldsymbol{f}$ and $\boldsymbol{G} \to \boldsymbol{g}$ are likely 1-morphism. While it is possible that a single transformation $\boldsymbol{\mathcal{T}}$ can correctly capture interaction transformations for an entire interaction space, we expect this to be the case only for very simple systems. In reality, interaction spaces will likely be partitioned into subsets associated with certain transformations.

Up to now, the local context has remained opaque. From Eq. 6.59, the simplest guess is for it to be a tensor quantity (not at φ-tensor) that becomes a vector quantity due to index contraction rules. A simple instance of this occurs when

$$\Phi = \langle \Phi_i \rangle_{\mathcal{I}} \tag{6.61}$$

which we immediately recognise as a *mean-field theory.* These facts justify its *pseudo-extensive* character and, when GToI instances are background-dependent, the field description is appropriate and calculations proceed as described above. Let us now tackle the case when Φ_i is itself a network of interactions. Using connectivity information from the network, we perform a first approximation by computing the regular tensor $\boldsymbol{X}_{\mu\nu\sigma} = \boldsymbol{X}_{\mu\nu\sigma}^{(\boldsymbol{\delta})} \otimes \boldsymbol{X}_{\mu\nu\sigma}^{(\boldsymbol{\omega})} \otimes \boldsymbol{X}_{\mu\nu\sigma}^{(\boldsymbol{\hbar})}$ where each component corresponds to the inner product of interaction components per each interaction pair i, j. Hence, $\boldsymbol{F}$ must be a fourth-rank φ-tensor. It is interesting to note that, when degrees of freedom in this tensor correspond to spacetime coordinates, the sub-tensor

$$\boldsymbol{\Pi}(\boldsymbol{X}_{\mu\nu\sigma}) = \boldsymbol{X}_{\mu\nu\sigma}^{(\boldsymbol{\delta}(\boldsymbol{r}))} \otimes \boldsymbol{X}_{\mu\nu\sigma}^{(\boldsymbol{\omega})} \tag{6.62}$$

describes a *propagator*, an entity that contains the information about the relation between an interaction event and its surrounding space. For instance, the projector contains attenuation effects due to irreversible loss of degrees of freedom in the interaction to the local context.

Summarising, the theory of interactions defines transformations as linear sets of φ-tensors containing 1-morphisms that can be composed and applied to interactions. A *concrete theory of interactions* (CToI) is a complete specification of $\mathcal{I}$ by providing its interactions, a description of the local contexts by means of pseudo-field vectors or interaction graphs, the primitiveness relations between them, and the set of transformations that apply to the interactions in terms of φ-tensors.

6.3 Recovering field descriptions

We are now interested in, given a CToI, recovering the state of a field at a given time and, by extension, at all times of interest. To do so, we first discuss another application of transformations in the GToI. At first, their definition was motivated by asking how an interaction varied under small changes of the local context. Doing so provided us with a recipe to evolve an interaction space based on small steps, which can be defined for single degree of freedom between Φ_i and $\Phi_i^{\boldsymbol{\mathcal{T}}}$. By observing the form of $\boldsymbol{\mathcal{T}}$, nothing prevents us from asking what happens to local contexts when we change the interaction associated to it.

In the intuitive notion of field, degrees of freedom are embedded in it, and the magnitude of specific observables should be proportional to the volume occupied by them. Also, the frequencies of the interaction should be transferred to the frequency of relaxation in the field. Using our reasoning above, our interest lies in determining how the field looks like after changing its associated interaction with the restriction that a) the field must preserve its propagator and b) all degrees of freedom of interest in the field must be switched from the interaction to the local context. Let the set $\mathcal{D}$ contain all degrees of freedom of interest, the interaction $\swarrow\!\!\nearrow^{\alpha,\beta}_{i,-\mathcal{D}}$ the new interaction without the degrees of freedom, we seek for the local context transformation

$$\boldsymbol{\mathcal{U}}(\Phi_i, \swarrow\!\!\nearrow^{\alpha,\beta}_{i,-\mathcal{D}}) = \Phi_i^{+\mathcal{D}} \tag{6.63}$$

in which $\Delta\Phi_i^{+\mathcal{D}}$ denotes the local context augmented with the relevant degrees of freedom. We must provide a recipe to (approximately) find $\boldsymbol{\mathcal{U}}$. If Φ_i is a tensor, we extend it with the space $\mathfrak{D}$ generated by the degrees of freedom of interest such that $\Phi_i^{+\mathcal{D}} = \Phi_i \otimes \mathfrak{D}$ where the respective tensor components are obtained by inverting $\boldsymbol{F}$ in Eq. 6.59 and using the shared components between Φ_i and $\mathfrak{D}$. If the local context is a network, we obtain the tensor $\boldsymbol{X}_{\mu\nu\sigma}$, extend it similarly with $\mathfrak{D}$ using $\boldsymbol{F}$ to obtain the extended tensor $\boldsymbol{X}_{\mu\nu\sigma}^{+(\mathfrak{D})}$ and back into a graph $\Phi_i^{+\mathcal{D}}$. In the simplest possible way, a new interaction will be found with only the degrees of freedom of interest, and the same relaxation frequency as $\swarrow\!\!\nearrow^{\alpha,\beta}_{i}$. We observe how our construction is analogous to how modern field theory operates: interactions between fields can be treated as particle-like entities, and interactions manifest as locally correlated field excitations. We note also that, since the field is an ensemble, $\boldsymbol{\mathcal{U}}$ may safely be degenerate, since multiple different outcomes converge as a multimodal distribution. Note that the volume added by $\mathcal{D}$ to Φ_i corresponds to the magnitude $\boldsymbol{Gamma}$.

Back to $\boldsymbol{\mathcal{T}}$, we observe that one of its predictions is that the identity of an interaction depends on a range of possible Φ's. Hence, any degree of approximation will depend on how close to the mean of the distribution contained in the interaction we wish to be, as given by fractional powers of the standard deviation σ^q with q called here the *quality factor* of the reconstruction. All the latter points once more to how mechanisms characterise interaction classes uniquely, and by extension, the range of contexts by which we may identify them.

Finally equipped with all necessary tools, we describe various types of reconstruction depending on the properties of Φ_i. Since the reconstruction is spatial, we depart from the localised interaction space $\mathcal{I}_{\mathcal{L}}$. We provide two algorithms for this purpose: one to compute the spatial extent of the interaction space, and another one to compute its temporal aspect. Our choice of reconstruction is naïve and inefficient since it requires generating the entire connected lattice of points. On the other hand, its understanding is straightforward. A more efficient and sophisticated method would make use of spectral decomposition and reconstruction methods for graphs[123].

We wish to summarise the significance of our model in the context of dynamical systems. First, the GToI preserves the covariance of interactions and their local context. In dynamical systems, one expects field values along with 4-position vectors to fully determine an instant and subsequent events. Since the local context is a distribution whose position projector maps contexts to an information geometry of $\boldsymbol{r}^{\mu}$'s, there exists a correspondence between observed average trajectories and the course of statistical expectation when moving from one interaction space to another in time, while allowing for surprising events to occur. Also, observe that the field descriptions contain propagation and attenuation parameters that correspond to inverse decay laws, and moreover for every decay there exists an information loss mechanism that is thermodynamically irreversible. Finally, we have not lost the relativistic element present in a complete spatio-temporal reconstruction, since a localised interaction must be given to compute the temporal element.

Algorithm 1: Spatial field reconstruction of a CToI using $\mathcal{I}_{\mathcal{L}}$.

Data: $\mathcal{I}_{\mathcal{L}}$, the collection of $\boldsymbol{\mathcal{T}}$'s $\boldsymbol{\mathcal{U}}$'s associated with all interactions in $\mathcal{I}$, the set of target degrees of freedom $\mathcal{D}$.

Result: An instantaneous field description for a set of degrees of freedom $\mathcal{D}$.

$\boldsymbol{I} \leftarrow \varnothing$;

$\boldsymbol{dr}_*^\mu \leftarrow \min \|\boldsymbol{L}(\Phi_i) - \boldsymbol{L}(\Phi_j)\|$;

Generate a lattice $\mathfrak{L}$ with points $\boldsymbol{r}^\eta = \boldsymbol{L}(\Phi_i)$ and content Φ_i spaced according to $\boldsymbol{dr}_*^\mu$ across μ dimensions such that all localised interactions are included;

Compute the set of all propagators $\mathfrak{P}$;

foreach $\boldsymbol{r}^\eta \in \mathfrak{L}$ **do**

  if $\boldsymbol{r}^\eta == \boldsymbol{L}(\Phi_i)$ **then**

    Replace Φ_i in $\mathfrak{L}(\boldsymbol{r}^\eta)$ by $\boldsymbol{\mathcal{U}}(\Phi_i, \swarrow\!\!\nearrow^{\alpha,\beta}_{i,-\mathcal{D}})$;

  else

    $\mathfrak{L}(\boldsymbol{r}^\eta) \leftarrow \Phi_0$, a suitable ground-state local context.

  end

  Endow $\mathfrak{L}(\boldsymbol{r}^\eta)$ with $\mathfrak{X}$

end

For an arbitrary point in the extent of $\mathfrak{L}$, use propagators in $\mathfrak{P}$ to compute spatially-dependent field decay per degree of freedom.

Algorithm 2: Temporal field reconstruction of a CToI using $\mathfrak{L}$ from Algorithm 1.

Data: A lattice $\mathfrak{L}$, a next time τ, $\delta\tau$, an interaction $\swarrow\!\!\nearrow^{\alpha,\beta}_{i}$.

Result: A new lattice $\mathfrak{L}'$ with changes computed as a f.

$s \leftarrow 0$;

while $s < \tau$ **do**

  foreach $\boldsymbol{r}^\eta \in \mathfrak{L}$ **do**

    $\mathfrak{L}'(\boldsymbol{r}^\eta) \leftarrow \Pi(\mathfrak{L}(\boldsymbol{r}^\eta))$

  end

  $s \leftarrow s + \delta\tau$

end

Compute the respective interaction space $\mathcal{J}$ using $\swarrow\!\!\nearrow^{\alpha,\beta}_{i}$ to set the frame of reference.

As a particular ending note for this section, we find the notion of deterministic chaos hard to substantiate under the GToI. Thermodynamic irreversibility mandates stochasticity, which implies that diffusion will make large deviations in spacetime to be unlikely as a function of variance. Hence, the arbitrary dependency of motion on accuracy is entirely removed, since it is not attainable, sustainable or verifiable. In addition, the way the GToI allows field reconstructions is amenable to stochastic amplification[124], a phenomenon that appears to be responsible for observations that resemble chaotic trajectories. Only when scales between phenomena are sufficiently apart –i.e. thermal effects of air on a double pendulum- that trajectories resemble those predicted by deterministic chaos, yet most complex multiscale stochastic systems lack large scale separations. More work is needed on this subject to fully understand the consequences of the GToI on the existing view of the adequacy of chaotic descriptions of phenomena in dynamical systems.

In the following sections, we explore some conceptual consequences of the GToI described above. To do so, we will focus on three central aspects: what the GToI suggests about the character of physical laws –including what they may be and how they arise, how the principle of least action lives in the probabilistic structure of the GToI, and some hints about how a generalized Correspondence Principle may be stated.

6.4 GToI in relation to the character of physical laws

The notion of a physical law at the back of our minds is of a universal proposition whose validity holds irrespective of the instance where we look for it. Conservation laws are a magnificent example where all what is required is the presence of a differential symmetry of the action to state the conservation of the respective quantity. A physical law must be sufficiently abstract to describe (almost) all (of) the known universe, and at the same time it must be straightforward enough to remain applicable without much complications. As described in the first article, discovering fundamental rules that apply to the universe across scales appears not to be facilitated by the usual (and convenient) view of dynamical manifolds, in which interactions are only implicitly represented. Figure 6.5 schematises how objects, laws and microstates are related in the GToI.

The first difference the GToI introduces is to change this situation, and place interactions as entities from which physical laws as we know them can arise naturally. We have shown how the view of interactions are in direct correspondence to mechanisms, and how mechanisms at the most abstract level correspond to hierarchies of interactions. Contrary to other approaches such as master equations, being able to expose mechanisms across scales and allowing them to remain distinguishable can bring a new kind of conceptual simplicity and integration lacking across science domains. On the other hand, gaining knowledge about the

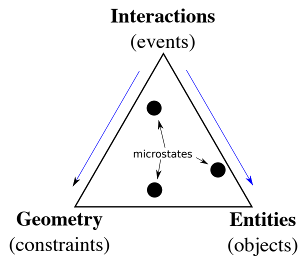

Figure 6.5: The character of physical laws and objects in the GToI. Interactions are fundamental, and laws (i.e. geometries) and objects are derivative consequences of how interactions aggregate and compose.

structural richness of a complex, thermodynamically irreversible system comes at the expense of loosing information about particular states in favour of distributions, except when averages are available.

The second significant difference is the conceptualisation of how laws operate across multiscale phenomena. Let us consider for a moment the challenges found at the interface between quantum chemistry and molecular dynamics. To enact two different sets of laws, we need to recur in practice to *computationally aphysical* implementations. For instance, one may stop molecular time to recompute self-consistent field theories at the quantum level that are fed back into the specification of the potential energy before proceeding with the integration of the molecular equations of motion later; in many situations, the resulting approximations must make uses of semi-empirical findings. While the GToI would sacrifice the ability to obtain trajectories straightforwardly –still viable yet more involved- its ability to connect events across scales appears to bring the aspiration of an integrated view of physical phenomena a step closer. It is not therefore unreasonable to suppose that theories resulting in aphysical computations may gain significantly to attempts to recast them using the GToI.

A third crucial difference is how the GToI describes the interacting entities. The materiality of objects dominates descriptions across science domains, not just physics. A view of materiality through objects directly involves positions and trajectories, and a linear view of time. Attempting to leave the dynamical view without renouncing some of its principles tends to make matters cumbersome and formally hard. The difficulties, both formal and numerical with the solution of stochastic differential equations, exemplify why introducing further realism without revising assumptions such as the need for an underlying continuous manifold results is major hurdles. In the GToI, *objects are a relational consequence of interactions*, whose materiality only depends on the volume occupied by degrees of freedom in relational space. Note that our definition of volume is state in terms of a general number of dimensions since it corresponds, in reality, to the number of edges of a certain type in a graph.

To further understand the contrast, consider a living cell. Starting at the membrane, interactions with the environment are mediated by interactions between lipids, which organise in bilayers. Within these layers, proteins interact with a host of other molecules. Membranes as a whole interact with concentration gradients at the scale of a single cell, having ion channels and other mechanisms as their most immediate macrostate. Inside the cell, molecules interact to sustain thermodynamic processes that transduce matter and energy intro structure and function. The genetic material stored in DNA with its translation and transcription processes depends on hydrogen-hydrogen interactions, which themselves are rooted in the interactions of orbitals, and those on the interactions of electrons. Of these, we expect electrons to arise from other, more fundamental interactions below currently measurable forms of matter and energy.

In the life of a cell, however, the view of interactions is consistent with thermodynamic irreversibility, with organismal robustness and with the persistence of identity under the constant substitution of matter. Imagine two types of simulations. One would use the usual trajectory and frequency based methods to understand the reality of the cell as various perturbations are performed. The complexity of simulations required to understand the completely localised view of objects in a cell –of *all* relevant objects involved-becomes daunting quickly even without going below a coarse molecular level[125]. Doing so while tracking the association between modules and their parts ends in combinatorial explosions. In the GToI, if we relinquish thinking in terms of objects and their composition and reason in terms of interaction classes, we gain valuable information about interactions, their aggregation and composition, as well as of the distribution of responses a system can produce.

Finally, let us consider the character of physical laws in the GToI. To do so, let us further split the meaning of physical law into two different, yet interlocking components: physical law as *what is allowable to happen in a system*, and physical laws as *the dependency on a large number of entities, events and forces such that recognisably new behaviour appears.* The first one corresponds to the geometry of the system, and the second one to statistical limits.

The first interpretation in the GToI is straightforward, since the geometry of the system is it the information geometry of its interaction space. Since motion across interaction space does not involve time (only differences between local contexts), one can easily imagine computational experiments that map changes across interaction space by sampling the effect of interaction transformations $\mathcal{T}$ through a Monte Carlo approach. We envision the procedure to work as follows. A sampling of interactions across interaction space is generated around $\mathcal{I}$ as densely as possible. Using the set of transformations available, $\xi(\mathcal{I})$ is computed until one of two events happens per trajectory: a) the interaction disappears from the space, or b) the interaction splits into two or more interactions. By repeating this process many times and covering the space as much as possible, the geometry of the interaction space can be progressively mapped. We identify the final volume resulting of the evolution of interaction space where the number of trajectories are preserved as embodying the laws of that space. The volume is an open set, yet it is finite for realistic situations. Hence, particular laws arise as a result of fixing an interaction space and mapping its consequences by sampling and evolving it.

The second interpretation, key in the study of complexity, self-organization and emergence, depends on the manifestation of generative effects across systems due to their aggregation and composition. Even the smallest metals showing electrical conductivity are composed by a non-trivial number of atoms[126], while two or three organisms can easily construct complex routines, coordinate, compete and communicate. Recall from the description above that the volume associated with laws for a given interaction space only covered non-diverging or non-disappearing trajectories. Using the same logic, the envelope of that volume must be related to the manifestation of new laws, since it is what separates them. Furthermore, sheer aggregation of interactions does not appear to have a significant effect for the genesis of new laws; composition, on the other hand has a definitive effect on how a trajectory can be rapidly (and non-linearly) modulated across interaction space. The more interaction classes involved, the richer the behaviour of the system, and the more likely its trajectories to diverge or disappear. Motivated by this, we conjecture the existence of the following law of nature.

Law of Repertoire Sufficiency. *The limit number of microscale entities required for a new law to robustly manifest at its corresponding macroscale is inversely proportional to the number of different interaction classes in the corresponding interaction space, namely*

$$N_{\text{lim}} \propto |\mathcal{I}|^{-s}$$

for some real value s.

We note that our view includes a tentative answer to the question of whether the laws of nature are immutable of changing[127,128]: not only the laws of nature are far from fixed in the GToI, but they can evolve and be naturally selected. Since fluctuations occur at the base of the hierarchy – the hypothetical realm of quantum cosmology- it is possible for some of those to explore previously, yet more favourable places within interaction space. Favourable means here stronger invariance under perturbations and transformations. Since these interactions are likely connected upwards to other less primitive interactions in non-trivial manners, these in turn will likely evolve and statistically materialise into other relatively invariant interactions. Unsustainable interactions at any given point either disappear or branch into more stable regimes. As interactions become localised and start permeating usual dynamical manifolds, previous laws are superseded by a sweeping phase transition. We believe this bears some significance for the fine tuning problem in cosmology[129], or the problem of finding mechanisms that explain the precise values of the fundamental constants in our universe.

6.4.1 The principle of least action

The principle of least action takes paramount importance in the history of physics[130]. The action functional contains all the necessary elements to describe and compute consequences for classical, quantum and relativistic systems. It can be extended to dynamical systems with small perturbations by interpreting the geometric consequences of least action in the space of curves as the existence of suitable processes that preserve averages[131]. From general flows[132] to nervous action potentials[133], the principle of least action holds steadfast. Thermodynamically, least action appears to align with the dispersal of energy[134]; quantum mechanically, the shortest paths are the most probable ones as given by the solutions of path integrals corresponding to various physical situations[135].

We can interpret the minimisation of the action as follows using the GToI. Motion across a space or a medium involves interacting across a dynamical path. Every new interaction increases the odds for the object to dissipate heat, losing degrees of freedom to the environment. The longer the path, the more interactions will be encountered, the more heat will be dissipated and the more entropy generated. Put bluntly, the reason we observe instances of the principle of least action according to the GToI is because of the preservation of identity during the selection process that occurs within the stochastic shape ensemble in conjunction with a trajectory full of interactions: after each interaction, either internal degrees of freedom remain somewhat preserved (with the exception of those referring to position and momenta in the case of dynamical manifolds) or they are dissipated. To preserve the identity of an object, the entropy generating processes responsible for re-wiring degrees of freedom internally must approximately preserve it, which must remain approximately so when the hierarchy of interactions that comprises the object interact with their own local context.

Since the shape –i.e. the graph- of an object is stochastic, heat generation will always occur, even of the local context remains the same, while edges are randomly replaced to compensate for lost degrees of freedom. This sort of constitutive equilibrium (a stochastic symmetry of the system) can be broken if the number of degrees of freedom that can be perturbed increases instantaneously and cumulative. The stability of an object under interactions implies the existence of an threshold β^* in Eq. 6.13 that is characteristic for that object; one way to capture this dependency is considering the interaction space that defines the object

$\mathcal{I}_{\mathcal{O}}$ and find a functional

$$\boldsymbol{R}[\mathcal{I}_{\mathcal{O}}, \boldsymbol{\mathcal{T}}, \leftrightsquigarrow^{\mu,\nu}_{j,k}] = \beta \tag{6.64}$$

that uses information from that interaction space and its transformations to compute how β changes under a sequence of k interactions. One can easily imagine that the length of the sequence of interactions in Eq. 6.64 is related to the speed of an object across a world timeline; the existence of β^* implies sequences at or below a characteristic length k^*. Now, fix the time $\tau_{ab} = \tau_b - \tau_a$ for end and start times between two points a, b and postulate all trajectories travelled across both points. Paths whose length yield values below or equal to β^* are identity-preserving; longer paths contain more states in the ensemble that deviate significantly from the original identity due to increases in β and are filtered, since they entail different mechanisms. The trajectories we observe contain the least possible action precisely because motion is a selection operator that filters out stochastic shapes on the basis of distance and speed necessary to traverse a dynamical manifold, matching β^*. Another way to think about it is that nature selects for distances and speeds that preserve $\mathcal{I}_{\mathcal{O}}$ across repeated interactions; we known them usually as *geodesics*. Hence, the principle of least action is a consequence of stochastic selection ensuring preservation of identity of interaction spaces.

We have, in addition, gained more clarity about the role of entropy as a pervasive guiding force. Entropy provides the variety needed prior to the selection by identity in trajectories. Let us consider two extreme cases of this. One is the case of objects whose microstructure is simple that exhibit high rigidity; their value of β^* is high, to the point that it takes a significant number of coordinated interactions to cross the threshold that breaks its identity (e.g. a destructive assay in a solid block of metal). At the other end, consider a soap bubble: it does not take many interactions to break its identity. In the middle, we find self-organising systems and life: they posses the ability to harness incoming interactions and retain their identity by adaptively increasing their interaction repertoire while sustaining low entropy production regimes. We aim to explore both classes of phenomena at depth in subsequent publications. Based on the preceding discussion, we conjecture the existence of a new type of conservation law below.

Law of Conservation of Identity. *For an object $\mathcal{O}$ whose interaction space is $\mathcal{I}_{\mathcal{O}}$, the set of all possible trajectories between two points a, b within the fixed time interval $\tau_b - \tau_a = \Delta\tau$ is reduced to those where the identity of $\mathcal{I}_{\mathcal{O}}$ is preserved across repeated interactions. That is, only trajectories proportional to a number of interactions*

$$k^* \propto s(a, b) = \int_{\tau_a}^{\tau_b} ds$$

are allowable if and only if

$$\boldsymbol{R}[\mathcal{I}_{\mathcal{O}}, \boldsymbol{\mathcal{T}}, \leftrightsquigarrow^{\mu,\nu}_{j,k^*}] \leq \beta^*,$$

corresponding to geodesics along τ. Moreover, β^* induces an additional symmetry (of identity) under repeated interactions.

It is worth noting that thermodynamic irreversibility is essential to obtain the principle of least action within the GToI, and that variation, repetition and selection appear to be universal operators.

6.4.2 Generalising the Correspondence Principle

We wish finally to address the general concern raised by Smolin[74] about the preservation of linkages across scales were we to search for the physics of a universe connected across scales. To achieve explanatory closure, it does not suffice to be able to explain phenomena in the universe using laws that only refer to entities within the universe, but no law should describe a single scale in isolation from the others. The development of the GToI is heavily informed by this particular problem in the light of the difficulties found across multiscale phenomena.

A good example of connection between scales was provided by Bohr[136], observing that quantum mechanics should reproduce at sufficiently high quantum numbers (e.g. energies), naming it the Correspondence Principle. The connection between expectation values for position and momentum operators to a potential responsible for a force acting on a massive particle was established by Ehrenfest[137]. Quantum decoherence was shown much later to help explain the quantum-classical correspondence in dynamical systems[138] and more recently found to apply at much more generality[139]. The Correspondence Principle can be more generally stated as the existence of bridge equations that, under sufficiently large quantities pertaining to a certain microscale, can be used to obtain average outcomes commensurate to those predicted by laws referring only to entities in the corresponding macroscale; these bridge equations not only depend on the aggregation of many states or entities, but on how they compose in relation to themselves and their context (i.e. environment).

Observe that this description is directly encoded into the GToI in various forms. First, the existence of φ-tensors $\boldsymbol{H}$ and $\boldsymbol{\Psi}_j$ in Eq. 6.59 captures the general connection between aggregation and composition of interaction classes, shaping the mechanisms expected in the formulation of bridge equations. Second, the effect of the local context is explicit though $\boldsymbol{F}$, in which is not hard to imagine situations where properties of Φ_i induce decoherence. This implies that large variations in the local context erase differences[140] in the

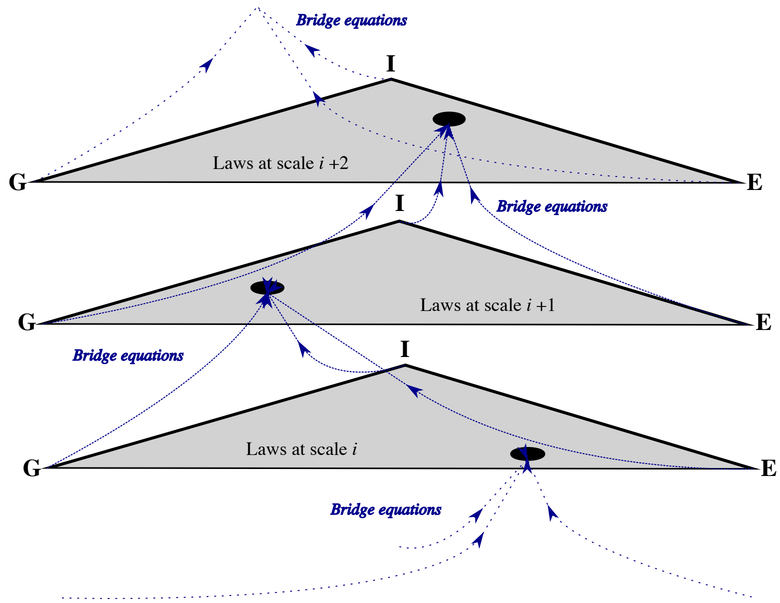

Figure 6.6: A generalized view of the Correspondence Principle suggested by the GToI. All interactions in the universe are grouped into multiple layers depending on the *more primitive than* order relation. Microstates, laws (i.e. geometries) and objects present up to scale i, once their repertoire sufficiency has been reached, produce a new scale with the same formal structure, but different arrangements. Bridge equations arise from the relations of the local context, aggregation and composition present in the transformations pertaining to each interaction space.

probability distribution governing stochastic processes, leading to average values expected at large limits. Moreover, the evolution of an interaction space towards the appearance and vanishing of interactions as a product of the limiting surfaces as a product of the law of repertoire sufficiency. Since we suppose the universe is connected, we must find a macroscale for every existing microscale. We finally state our extension of the correspondence principle for the general case depicted in Figure 6.6.

Generalised Correspondence Principle. *Every microscale i in which limit numbers exist as determined by the Law of Repertiore Sufficiency approximates a corresponding macroscale $i + 1$. Bridge equations between the two are guaranteed to exist solely in terms of relations between local contexts, aggregation and composition of interactions in the interaction space of the microscale.*

6.5 Conclusion

In this article, we have developed the abstract formulation of a Generalised Theory of Interactions. The theory promotes interactions as first-class citizens, and makes use of them as evidence of mechanisms from which governing laws arise. Briefly, an interaction is an exchange of degrees of freedom, mediated by a local environment or context, determined by uncertainty and relaxation relations. Interactions provide the ability to construct a framework that provides explanatory closure, stated only in terms of local events subject to compositionality relations that respect thermodynamic irreversibility at all times while allowing (and to a great extent mandating) causality relations. The GToI, in addition, is modelled upon background independence without excluding cases where field representations constitute a more intellectually efficient pathway. As a useful byproduct, objects and laws become derived entities whose constitution appears to be greatly clarified when looked through the lens of robustness of identity. When applied to a specific CMSS instance, we obtain a concrete theory of interaction (CToI).

Our work, furthermore, contains the statement of various new principles and laws as a means to explore the conceptual possibilities of the theory. First, the equivalence between messengers, mechanisms and interactions as a result of Ashby's law of requisite variety can help, in our current opinion, understand more efficiently CMSS instances at the organismal level and beyond, since probing for mechanisms becomes a tasks of finding the relevant interaction classes and their associated transformations. Second, the compositional construction of degrees of freedom more broadly opens the door to the productive application of powerful mathematical devices that include category theory, topos theory and homotopy type theory; all of these are strongly consistent with the desired computational character of the GToI. Third, the relation between the complexity of a system through the richness of its interaction repertoire appears to bring significant consequences to our understanding of the law of large numbers, and its implications for various types of phenomena including self-organisation and emergence. Fourth, reinterpreting the principle of least action within the GToI results in a plausible mechanism of how mechanics may depend on thermodynamics at a fundamental level. Finally, revisiting the Correspondence Principle provides some hints about the character of requirements needed to achieve explanatory closure in new and existing theories. A curious fact that has not escaped our notice is point particles are not only entirely absent in the GToI, but conceptually incorrect.

Several avenues of investigation remain untouched. A rigorous formalization of the algebra of φ-tensors must be performed in itself. This is needed in order to understand why, from the universe of such mathematical entities, possibly a subset of them will correspond only to any possible system. While we suspect this is the case in light of the existence of conservation laws, this statement must be rigorously tested, and future work is likely to require the machinery of topos theory or similar to summarise results effectively and efficiently. Another area of work corresponds to the development of the systematics required to find suitable φ-tensors for specific CToIs; at present, the process is heuristic at best. Furthermore, we envision our preliminary notation to evolve under the pressure of application to useful problems and become more elegant and economic. Rigorous derivations for the principles and laws stated here need to be provided in terms of the underlying algebraic structures. We will dedicate future efforts to address them, and more immediately to apply the GToI to particular cases, including the theory of gases, the foundations of prebiotic evolution and self-organisation.

Finally, the development of the GToI is strongly informed by physics despite the goal, stated at the start, of addressing CMSS at large. Our take is premeditated rather than incidental. By recasting known entities and phenomena for which concepts, principles and laws have been achieved, we have sought to fortify the foundations of the theory to the best of our current possibilities. In doing so, the apparent simplicity of systems and phenomena used in physics unravels into a rich landscape of interactions with new complexities. In a non-trivial manner and to the best of our current knowledge, the universe appears to be a closed, integrated entity in terms of laws and the entities needed to understand it across all scales; in stark contradiction, our theories remain far from such explanatory closure. Understanding such a universe requires placing new demands on how contemporary theories are constructed, their mathematical underpinnings, and their implications for experimental science. Our work suggests that taking seriously such a research program and using complex multiscale stochastic systems as a start

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Part III

Computing with interactions

Chapter 7

Simulation-Oriented Cyberinfrastructure for Computational Social Science

Abstract[i]

Computational social simulation (CSS) has proven its utility for basic research in social, behavioral, organizational, cognitive, linguistic, evolutionary, and biological sciences. It has been employed effectively in many application domains including government, policy, commerce, and industry. Along with basic science, applied problem-solving, and design, large-scale social simulations provide great educational opportunities for exploring and visualizing theories and models of complex social systems, and studying how they change. This paper reports on several facets of our approach to improving the realism, viability, and impact of simulation-oriented computational research in social sciences by i) raising the scale and complexity of simulation models; ii) grounding computational simulation research on properties of its fundamental constituents including social objects themselves, information, representational processes and their limits; iii) linking social simulations to very large data sets and to live streams of data and iv) binding and modernizing CSS tools into modern cyberinfrastructures compatible and interoperable with those of many other computational and data sciences.

7.1 Introduction

There is tremendous interest in computational modeling, simulation, and analysis of social, socio-technical, and socio-environmental systems, in many different application areas including basic science, government/policy, and commerce/industry. Computational social simulation (CSS) has proven its utility in social, behavioral, organizational, cognitive, linguistic, evolutionary, and biological sciences. Large-scale simulations provide tremendous educational opportunities to explore and visualize alternative theories and models of complex social systems, and to study how they change.

[i]**Núñez-Corrales, S. and Gasser, L. (2016, accepted)** Simulation-Oriented Cyberinfrastructure for Computational Social Science. *The Computational Social Science (CSS 2016) Annual Conference.* Santa Fe NM, Oct 24 – 27. Reprinted with permission of CSS.

In our view, four avenues form the clearest path toward improving the realism, viability, and impact of simulation-oriented computational research in social sciences: i) raising the scale and complexity of models; ii) grounding computational simulation research on properties of its fundamental constituents including social objects themselves, information, representational processes and their limits; iii) linking social simulations to very large data sets and to live streams of data (e.g. driving CSS with live streams from large sensor networks); and iv) binding and modernizing CSS tools into modern cyberinfrastructures compatible and interoperable with those commonly used and under development in many other computational and data sciences (e.g. workflows; data repositories; analysis/visualization pipelines; traceability and provenance of results to/from data, theory, and models; reproducibility, etc.)

This paper reports on our thinking during the early stages of a new project called "Simulating Social Systems at Scale," hosted and supported by the National Center for Supercomputer Applications (NCSA) at the University of Illinois. The project's motivating vision is to create the basis for, and demonstrate the feasibility of effective, efficient, accessible, very large-scale simulations of social systems, as a central component of general scientific cyberinfrastructure and computational science practice.

7.1.1 Challenges of the scientific program in computational social science

The ultimate goal of a science is obtaining explanations that best approximate the measured state and structure of the world[1], independent of domain. Observations and regularities are the raw materials from which theories and laws are obtained[2]. The particular procedural differences between scientific domains, however, depend on the structure of the relevant entities and how these are affected when measurements are performed upon them. Social science is not an exception in this sense.

Explanations need to correctly bridge different levels and scales, but their potentially large number leads to feasibility concerns. Reducing this complexity calls for macroscale descriptions from microscale states that are both accessible and deducible[3]. A similar tension exists between individual and collective levels of analysis in society[4]. Deducibility is essential for theories to be considered candidate explanations, whether the particular problem at hand is one of prediction (gaining knowledge about the future), retrodiction (explaining the past) or sampling (accurately measuring reality). *Invariance* has become a keystone in the edifice of modern science because it leads often to fundamental explanations by removing complex arrays of particular interactions, simplifying the experimental and theoretical landscapes. Computational social science, as the discipline that makes use of an *in silico* empirical approach, is in the process of developing methods for finding the invariants and abstractions for making the understanding of society a more tractable task.

The methods of the physical sciences appear at first hand to be incompatible with some of the features of social research. One reason is due to the apparent absence of invariance in either the internal dynamics of social agents or the environment in which they are embedded, leading to large amount of possible hypotheses that can be formulated and tested without efficient ways to filter those which are correct[5]. Biology, in contrast to physics, serves as a good example for the situation in social sciences: hypotheses about organisms need to be deduced both from limited measurements in a varying, complex environment and evidence from the past, whose quality decreases rapidly with temporal distance[6]. Recent success of computational systems biology in providing sound explanations to diverse phenomena by integrating observations, theories and information contained both *in* and *about* the organism is undeniable[7], where some invariants have been identified in high-level representation of many biological processes, and not in the experimental data itself.

Information, a central piece of the establishment of modern biology, appears also to be at the core of an effective computational social science. Most of the discoveries in organisms related to heredity pertain to the analysis of categorical, genomic or contextual information. In turn, information is then converted to models of the biological systems that greatly simplify the process of understanding relations between parts and their global effects. In these abstraction process, networks have become a *lingua franca* capable of revealing invariants that remained hidden at more grounded levels of representation[8]. The notion of agency, prevalent in the concepts behind ongoing research in computational social science, is an information-rich concept itself that has lead to significant advances[9].

In view of the above discussion, we propose to address the following three central problems as the next frontier of (computational) social science. While these problems are embedded in a strong digital context, it must be stressed that good explanations of phenomena aiming at the development of solid theoretical arguments from an inherent richness of social structures[10], and not software or hardware projects, are the relevant entities for the notion of any work pursuing the development of such science[11].

Moving from ontological debates to epistemic goals

Instead of presupposing levels of description and categories of objects (ontological), a more substantial approach to finding explanations attempts to determine the mechanics and the entities in a generalized way (epistemic)[12]. By taking this road, four key tasks become soluble: (1) finding adequate levels of explanation from observable facts and approximating models, (2) determining the form of the explanations by integrating networks of hypotheses that may be falsified and are devised as to account for the complexity of social phenomena, (3) constructing structural and functional explanations that provide macroscale causal relations through contrasts of possible outcomes –for instance, T-contrast[13] - that match fine-scale causal explanations[14] and (4) elucidating social mechanisms that involve both accumulation of facts and postulating general principles (i.e. covering laws) that may be partially adequate[15], but neither of which are equatable at all to social mechanisms on their own.

We consider that the latter view, common to discussions in social science in general, should be a structural guide for computational social science to realistically extend the knowledge domain it attempts to serve. While the nature of social systems apparently differs in many respects to the systems studied in the natural sciences, there seems to be no fundamental reason why an empirical study of systems of many agents may only be a theoretical device, but rather reach inner explanatory structures when properly constructed. Cyberinfrastructure and social modeling tools in this regard must be consistent from the conception up to the implementation, being sensitive to the fact that interacting with aspects of the social world may introduce unexpected effects[15], for instance, when simulations are interactive[16].

Moving from small worlds to large-scale experiments

Whether experimental, social or historical research[17], reducing instance size is a commonplace heuristic for grappling with the complexity induced by systems that interact with the environment or other systems. For social systems as complex systems, the reduction is justified by assuming emergent behavior: large numbers of simple units, under similar forces and with similar behavior, may produce unexpected non-linear responses[18]. Sometimes the inner structure of the responses is that of a small world[19], which summarizes the fact that in many systems the entities have a statistically preferential and restricted set of interactions[20]. Small-world organization has been extensively observed and studied in areas such as cooperation[21], human brain functional networks[22], social and biological communities[23] and human language research[24].

However, scaling limits have been identified for emergent behavior even in small problems[25] and suggested in problems involved social systems[26]. Some complex phenomena require sufficiently large problem sizes for emergence to occur. Moreover, even in that case, microscale description may not suffice to accurately compute expected outcomes of the whole system. Such failure in reductionistic explanations may be characteristic of the distinction between emergent and non-emergent systems[27] when either (1) there exist fundamental differences in the presupposition of the objects that interact at the different phenomenological levels, or (2) the description of the ensemble of the objects and their environment is incomplete[28]. One of those failures is the inability of models to account for the variations (either deterministic or random) of the world. Their origin may be intrinsic to the nature of the model of the world (i.e. agents only *sample* a flux of events) or dependent on the interactions with the agents (i.e. the model of the world is mutable and agents can modify it). Briefly, small-worlds are locally dependent models that do not often account for changes in the environment, crucial for unraveling the complexity of events in social systems; empirical embeddedness[29] is a key property that cyberinfrastructure for computational social science ought to ensure when required.

Moving from information by-products to information-centric representations

For general theories and laws to be deduced from data, adequate information representation is fundamental[30]. Representations frequently denote the entities, their properties and the mechanics of the system they compose; in the abstract, representations in agent-based systems are a special type of information that is often subtly embedded in the dynamics or the resulting patterns of emergence itself[31]. The relative nature of information as an exchange between agents, as well as the intrinsic information content of the world in both static and dynamic contexts reveal a close relationship between information and circumstance[32]. For instance, a successful theory is capable of elucidating which constraints exist in a system, and what their applicability is such as in understanding how agents consult, cooperate and compete amongst themselves[33]. If the constraints change, the circumstances of the agents may lead them to new outcomes. Using small-world theories, when disconnected from the relational information contained both in the agents, the environment and their interrelation is a most probable cause for incompleteness in the specification of the rules of a system (e.g. partial representations, incomplete concept hierarchies) that leads to poor inferences and models[34].

In a sense, gaining knowledge about a system may be equated to exhaustively finding the correct description for all the constraints that govern its dynamics. A theory then becomes a collection of related constraints capable of being instanced to yield specific predictions or explanations. But constraints are inferred from data as instances of known patterns. Hence, patterns (detailed prescriptions that match with particular instances) are high-level information tools that, coupled with adequate experimental design and data analysis tools, can lead to powerful insights in domains as complex as ecology[35]. Cyberinfrastructure that enables large-scale simulations in computational social science should provide means to instrument, capture and systematize information at different levels of representation, desirably with integrated automated pattern-matching and machine learning mechanisms to facilitate research.

7.2 Components of a large-scale simulation framework

In this work, we propose a general architecture for the development of computational social science experiments, rooted in the capabilities of existing and future cyberinfrastructure and compatible with the twin goals of i) achieving more complete and robust understanding of the useful range of social objects and processes (i.e., developing general social theory); and ii) achieving greater predictive and explanatory power in regard to specific social settings and cases (i.e. social problem solving and design). This section is concerned with its structural and functional description, as well as with some general properties and attributes expected of such infrastructure.

7.2.1 First-class entities: experiments as abstract contracts

Experiments are detailed specifications of realistic or abstract settings that contain the necessary and sufficient information constraints and processes for determining whether a particular set of assertions about the state of the world may be rejected, be subject to further enquiry or be considered as supported to a certain level of significance[36]. The specification contains the following general elements

- the pre-conditions of the experiment (i.e. state of the world prior to executing the actions, including variables out of the experimentalist's control),
- a detailed prescription of how processes are transformed into steps connected via intermediate inputs and outputs,
- a specification of the post-conditions after the processes are executed,
- a representation of the expected measurement outcome(s) and
- an analytic prescription for obtaining significance levels that would determine the success of the experiment.

Arguably, the main difficulty of performing experiments in the social sciences lies in the implications of (a) having agents that can interact with the world in complex, (b) the practical difficulties involved in finding or creating the appropriate conditions (c) and the existence of potential unethical consequences of enacting them in many situations[37]. By replacing agents with any sufficiently complex entity, determining the practical possibilities of observational or experimental settings and bearing in mind the ethical consequences of any experiment, the situation is not so much different from the natural sciences in many contexts. In such cases, though experiments come to the rescue as as abstract specifications of possible worlds that strictly follow certain principles or laws[38,39] that are not enacted in reality.

In the same way that a scientific instrument embodies the principles of a domain-specific context (i.e. an information background)[40], thought experiments contain the necessary and sufficient elements for theories to be tested. However, they are also present in the form of the *conceptualization* and design of experiments executed in real settings. In social sciences, thought experiments have been conceived as elucidating mechanisms in general social contexts for problems such as providing alternative explanations to the Social

Contract as the governing element of society[41], causality of historical events[42] and comparative analysis of social scenarios[43]. In addition, thought experiments also define language that facilitates communication amongst peer researchers in expert audiences[44], essential to creating community and critical mass in computational social science.

Therefore, experiments and their abstract specifications are first-class objects in our design of large-scale social simulation infrastructure. Their information representation is central for orchestrating the underlying computing infrastructure and subsequent data analysis.

7.2.2 Multi-agent systems: programs and constraints

The fundamental construct for general social simulation is the *Agent-Based Model* (ABM). An ABM most often comprises a set of *agents* which are the units of action, and some kind of *world* or environment in which the agents and their interactions are situated. There may be information flows between agents, and these may be represented as either coupled agent-environment interactions, or as explicit communications. This conceptualization of ABMs gives rise to three modeling *components*: 1) a physical world, 2) the agent's physical affordances (e.g. sensing/effecting) and decision procedures; and 3) an inter-agent communication infrastructure. Given the experimental philosophy and scientific-epistemic goals outlined above, these three layers provide serious constraints on the capabilities and scalability of ABMs. These issues are grounded in fundamentals of computational simulation and representation infrastructure, as constrained by the scientific goals such as reproducibility, and control over experimental conditions. Put briefly, on one extreme we could envision all agents acting independently with no interactions among each other. This frees us to execute agents as rapidly as computation resources permit, completely in parallel – an approach known as *divide-and-conquer*, widely used in extreme-scale data-processing. However, this approach obviates models in which agents interact, radically reducing the scope of possible science. It also eliminates the control needed for reproducibility, because there is no information about or possible control over the ordering of actions, which thus may turn out to be random and unrepeatable. Unfortunately, introducing interactions among the three model components (world, agents, and communication) puts extreme limitations on the scalability of models for fundamental complexity reasons. Thus the goal of achieving a robust and highly scalable cyberinfrastructure for CSS requires rethinking some simulation and experiment fundamentals and hence possibly rethinking the fundamentals of social theory that they represent. Possible refinements for scalability include probabilistic simulations, quality vs resource tradeoffs, and moving from deterministic to statistical representations of social phenomena.

7.2.3 Workflow-to-infrastructure as a goal satisfaction problem

Since experiments are first-class objects in our approach (above), it is possible to reason about dynamic matching between the emergent resource needs of a set of experiments and their scientific goals. Our idea here is to support dynamic provisioning of data sources, analysis tools, and simulation resources based on analyzing the goals of the experiment, exploring alternative provisionings. For example, a scheme like Decker and Lesser's TAEMS and PGP models for planning[45] would allow this type of reasoning, based on satisfying *quality*, *cost*, and *time* tradeoffs for alternative experiment workflows, given available infrastructure components.

There exist similar attempts to synthesize execution-to-hardware mappings, most of which rely on using middleware stacks to make parallel access transparent. The Mesos platform is an example that in particular abstracts nodes that can execute MPI and Hadoop[46]. Another example is portfolio scheduling of scientific tasks for data centers in which a ledger of multiple infrastructure options are compared against economic criteria in terms of energy and estimated CPU time[47]. Communication-aware schedulers optimized for expensive all-to-all operations exist[48] with analogues for mapping programs to cloud computing resources[49]. These approaches are expensive and operate during the execution, not in general prior to it.

Another way to generate execution-to-infrastructure mappings is to interpret them as goal satisfaction problems with search and optimization-based satisfiers. Goal-driven workload assignment and redistribution is well a known strategy in clouds and supercomputers[50–53]. Current work around execution-to-infrastructure mapping based on some preliminary form of goal satisfaction[54,55] suggest this route is promising. In short, automated mechanisms that removes the complexity of infrastructure relates issues are central to increased supercomputer usage as well as the use of modeling and simulation across disciplines[56]. It is our view that an AI-oriented strategy will be beneficial beyond large-scale modeling in computational social science.

7.2.4 A proposed architecture for large-scale computational social science experiments

The general constructs for an integrated architecture aimed at enabling experimental work in the social sciences under the paradigm of very large scale multi-agent systems integrated into cyberinfrastructures are shown in Figure 1. Our design has been in part motivated by the ideas and goals discussed in[57], and extended to aim benefiting from existing state-of-the-art cyberinfrastructure.

With respect to actual usage of the system, we propose a series of reconfiguration steps that social science cyberinfrastructure would follow during execution of an experiment.

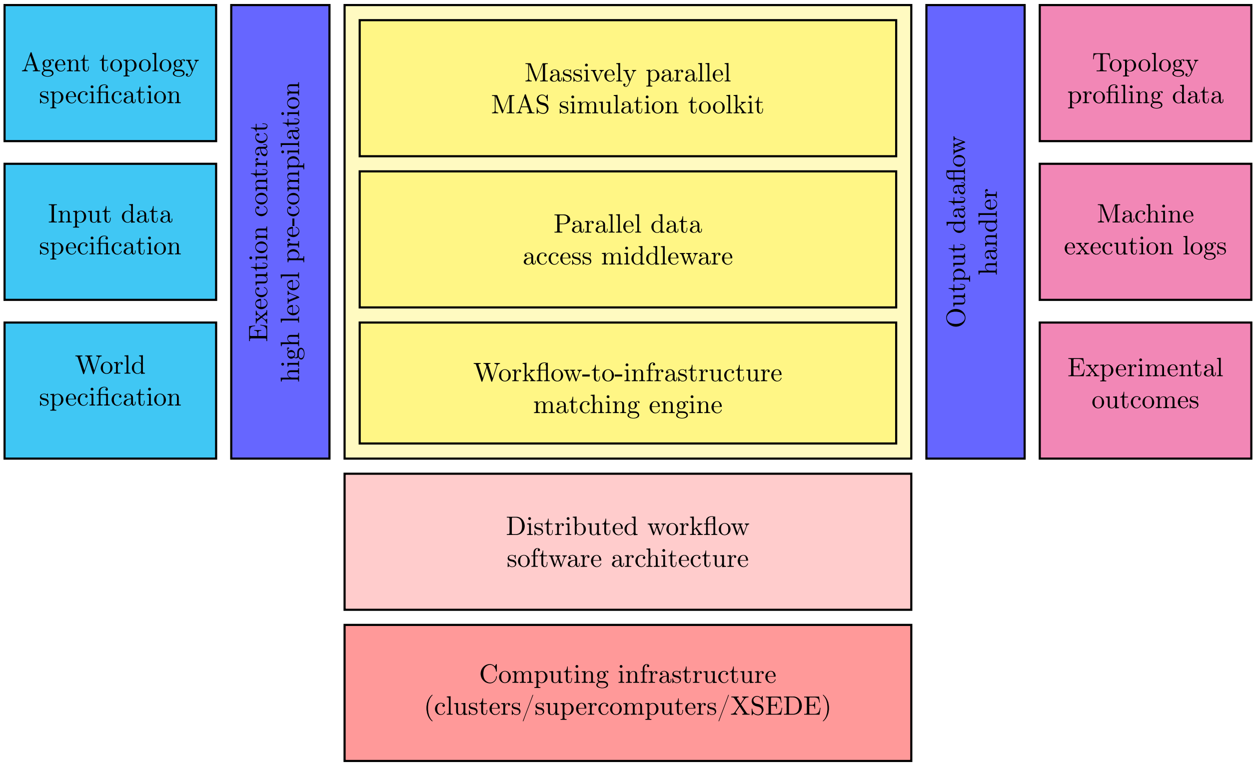

Figure 7.1: Abstract, high level block representation of a large-scale MAS experimental framework for enabling computational social science experiments. Clear separation of responsibilities at each stage in the execution of a computational social science experiment allows decoupling from particular details of the underlying computing infrastructure.

Contract specification phase

Ontology development for representing scientific experiments is a long standing research area[58]. In conjunction with semantic provenance mechanisms[59], they are essential for making tractable the growing number of experimental explorations that are openly released into the public and research domains and being able to reason about the life cycle of scientific experiments[60]. Ontologies for describing experiments exist in materials science[61], bioinformatics[62], biomedical research[63] and experimental microbiology[64], among others. Our current target ontology is EXPO[65] due to its generality in describing the context and contents of experiments.

A contract specification is composed of several elements. With respect to agents, both their communication model as well as their input data sources (i.e. archival, live) need to be specified along with their observables, measurements and ideally any associated hypotheses. In addition, a description of the world in which agents interact and act is necessary, involving its distributed representation and its spatial features (e.g. GPS data, time constraints, update policies). The description is then compiled into a contract file as input to the next phase.

Contract-to-execution phase

Once a contract is assembled, several software pieces are configured and instanced. a massively parallel MAS simulation toolkit will consume parts of the contract related to agent and world representations, constructing an instance of the specified model afterwards. Presently, the ROSS Time Warp System[66] and[67] stand as examples of commonly used toolkits to be supported in such workflows. Our current efforts include the design and development of a new toolkit for agent-based models under uncertainty. In addition, other components for handling distributed representations of spatial[68] and temporal[69,70] world models will be implemented and integrated.

One important consideration is the common execution background in systems that may be used by computational social scientists. The aim of this architecture is to be flexible enough as to operate in any provisioning-capable system (e.g. supercomputer, cloud) where middleware packages such as MPI, Hadoop and others may be installed and used by the different toolkits to make distribution transparent. The result of this phase is an executable specification in an intermediate language for later optimization to the particular infrastructure settings.

Model execution phase

As previously described, a specialized pre-execution step will transform the executable specification into a concrete execution schedule that matches the underlying infrastructure. The process needs to interact with workflow management systems and resource descriptions in order to gather sufficient information as to determine (possibly sub-) optimal resource allocation for a given simulation. The concrete executable schedule may be later hand tuned or through determination of simulation wide scaling laws.

Execution-to-outcomes phase

After the model is executed, outcomes are classified in three categories: profiling data in relation to communication topologies, human-readable machine execution logs and experimental results in structured form. In particular, standard scientific file formats are expected for later analysis and visualization. An important element of the latter process is determining whether experimental results come from a data flow in a continuous simulation (hence, derived from a sampling metaphor) or from a single execution unit. Compliance with standard scientific data formats such as NetCDF[71] and HDF5[72] is to be implemented as well.

Post-experiment data management phase

After execution, a data consolidation toolset will provide visualization and analysis facilities after experiments are performed. Considering the dynamics of social science research and the scope of the types of research to which this architecture is aimed at, tools that allow interaction and have a low learning curve are ideal. In that sense, significant experience with large volumetric data analysis and visualization has been obtained through the yt Project[73], one of the initial platforms that will be evaluated for integration in our architecture. Guaranteeing attributes such as data curation, provenance and reusability are critical for enhancing the research experience in computational social science[74] as to generate a fully digital context appropriate for community building and its broader scholarship.

7.3 Application targets

Social system are in general those in which a set of interacting entities share information towards explicit or implicit common goals such as lowering difficulty boundaries, survival, coordinating responses to threats or gaining knowledge through cooperation[75]. Finding research domains where social systems are central is critical for assessing the utility of large-scale ABMs as research tools. In particular, we propose utilizing this infrastructure to model events in language evolution, soil microbiology, small interference RNA (siRNA) based therapies in neuromedicine and organizational evolution.

7.3.1 Soil ecology

The bacterial ecology of soils is a driving factor of fertility, productivity, and economic growth[76]. Function-wise, fungi and bacteria are dominant with respect to fertility because of their decomposition activity in the soil food web[77]. Aboveground and belowground microbiotas differ from one another and possess high degrees of specificity in their activities and molecular products; they tangle mutually through both negative and positive feedback loops[78]. In summary, the mechanics of soil microbiota is complex and driven by a soil food web that is subject to a variety of factors that work at the micro and macro levels.

The bioavailability of C, N_2, CO_2 and SO_X depends on bacterial concentrations and species[79]. Disease detection mechanisms in the form of excess of various molecular products trigger defense actions in communal plant bacteria, ultimately leading to collective responses against possibly pathogenic populations[80]. Resistance to environmental changes has been observed to occur thanks to dense mutualism networks in which several organisms have adapted to perform the same functions, to direct chemical signaling and to coordinate the expression of resistance mechanisms[81]. Individual cell-to-cell communication mechanisms exist and are modulated by several factors that affect a series of delicate molecular signalling pathways. Two examples are the signal-controlled biofilm development strategies[82] and the more indirect, asynchronous horizontal gene transfer mechanism mediated by plasmids and viruses[83].

ABMs have been used for modelling ecological responses of collections of individual microorganisms. Hellweger[84] provides an extensive review of existing literature on the subject including techniques, theoretical aspects and challenges. Application examples include modelling host-pathogen immunology responses[85], biofilm formation[86], bacterial chemotaxis[87] and selectivity responses to synergistic drug combinations[88]. Modelling molecular rich environments has also been performed through a molecules-as-agents approach, where reactions are interactions between agents with responses modulated by calculating kinetics from ODEs[89]. However, existing applications of ABMs to understanding interactions soil ecology seem to be restricted to few examples such as the effect of earthworms in soil structure[90].

Successful application of ABMs may bring a new perspective into soil microbiota as long as a scalable approach is feasible (approximately 10^9 ecologically diverse bacteria per gram of soil are present). Applied research targets include engineering the equilibrium of bacterial populations to specifically favourable to crops in sustainable ways[91] and designing remediation strategies by transplantation of foreign soil bacteria accompanied with inorganic compounds[92].

7.3.2 siRNA-based therapies in neuromedicine

Small interference RNA (siRNA) is a mechanism of molecular pathway regulation in which precisely engineered small RNA strands (21-25 bps) bind selectively to mRNA required to produce a given protein, leading to its downregulation or complete inhibition[93]. This mechanism was first identified in viral defense and gene silencing mechanisms in plants[94] and later experimentally demonstrated in *Caenorhabditis elegans*[95]. Since then, siRNAs have become a major technology for both discovering new molecular pathways[96] and aspects of existing ones and for intervening in living systems with an emphasis in biomedical applications.

RNA interference occurs in mammalian neurons[97] and persist up to three weeks after therapeutic administration[98]. Small RNA-mediated cell-to-cell communication is facilitated by exosomes[99]. The latter is critical in NMDA receptor-mediated excitotoxicity and ischemic neuronal death[100] and a strong connection of gap junctions and mRNA to gene expression patterns in human seizure disorder is known (Naus, 1991). There is direct evidence of sensorial reconfiguration dependency on mRNA and siRNA, with the olfactory system as a prime example (Juang et al., 2013). However, much ground needs to be covered in terms of mapping the diversity of regulatory functions that RNA interference may allow in conjunction with the growing body of knowledge about omics of the neuron (Elia and Finkbeiner, 2013).

Designing siRNA therapies against neurodegenerative diseases is of particular interest and difficulty because of the inherent complexity of the molecular pathways involved in brain activity and its impact towards finding molecular medicines for the brain[101]. While significant progress has been made in the last ten years in molecular neurobiology[102], further integration into a whole brain picture remains as a grand challenge; siRNAs appear to be an important part of the puzzle.

There are no direct known applications of ABMs to model siRNA inter-cell communication despite the agent-like nature of neurons. Modeling of signal transduction in general[103] had been attempted through rule-based systems, a technique that is becoming more frequent due to its representational convenience and analytic properties[104]. All approaches attempting to overcome challenges of multi-scale modeling in biological systems[105] in the light of new perspectives made possible are immediate targets for large-scale ABM development. Open questions in siRNA cell-to-cell communication include how to develop a rational basis for improving safetly[106] and estimating the potential effectiveness of new siRNA therapies[107].

7.3.3 Emergence of organizations

Organization is a structural and functional feature of many abstract and complex systems. In human organizations, one perspective about its emergence is theoretically linked by the existence of multiple networks and transposition: when individuals from two different social networks share a new common environment, they bring knowledge of their previous context (patterns and rules) that serves as an *a priori* structuring element for new sets of behaviors, expectations and dynamics[108]. Elements such as the notion of ownership, division of labor, fairness and others also allow moving beyond emergence to convergence[109]. More over, the acquisition of individuality for an organization is an interesting phenomenon that is constructed, or rather *emerges* from other types of individuals[110].

Literature on agent-based models for the emergence of organization is extensive. Helbing[111] provides an overview of many relevant application areas ranging from modeling of socio-economic systems to responding to systemic risks and managing internal complexity. Many of these models are based on the small-world network approach in which a large portion of the apparent complexity is reducible to few local interactions and few functional motifs[20]. Small-world networks are limited in various important situations, as when systems are coupled and clustering of entities in the organization is to be expected[112]. The latter is critical when simulations are a vehicle to understand how human decisions are made in coupled human-natural systems[113].

At present, we are exploring possible applications of large-scale agent based models to areas tied to public policy such as innovation diffusion[114], design of macroeconomic policies[115], dynamics of health systems[116] and modeling of consumer energy choices[117]. As indicated in the discussion above, the potential of ABMs should not only predictive but also retrodictive. Current literature on reconstructing ancestral socio-ecological systems[118] is suggestive on that particular line of research.

7.4 Conclusion

The Computational Social Sciences can only benefit by the support of advanced cyberinfrastructure that integrates elements including streaming live data as both input and output, complex *world models* based on physical reality such as geographic information systems, computational and data infrastructure for running extreme-scale, multi-component and multi-level models; advanced communication models that support research on information-centric social phenomena, and integrative frameworks such as workflow systems, automated goal-to-workflow-to-infrastructure matching, and foundational scientific models. The project we report on is providing the seed and proof of concept of this integrated cyberinfrastructure at scale, along with identifying major bottlenecks and new theory needed to realize its vision.

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Chapter 8

Scalable Social Simulation: Evaluation of Current Frameworks and a New Approach

Abstract[i]

Very large-scale simulation is a principal methodology and widely-used cyberinfrastructure of computational and data science. Simulations have become routine instruments for running large experiments and collecting massive datasets, analogously to –and often replacing- tools like telescopes, petri dishes, farming plots, or particle accelerators. Notably, though, there is virtually no extreme scale infrastructure for critical theoretical and applied research in social sciences. We report on our tests and evaluations of the social theory, modeling, scalability, and cyberinfrastructure properties of the main existing tools that claim large-scale social simulation capability. We identify enough key weaknesses to conclude there is no viable prospect for scalable social simulation using or extending existing tools. These findings drive requirements and design of a radically new approach. The principal innovations include 1) modeling language and scalable simulation execution based on social theory; 2) a spectral (frequency domain) approach to modeling and analyzing social structures and processes; 3) scalability and realism based on fundamentally probabilistic models; and 4) close integration with scientific cyberinfrastructure standards and practices. We report on the design, implementation, and tests of this new approach on several significant issues in social theory. Overall we aim to change the extreme scale computational science landscape, moving high-impact research and applied issues of social sciences from their current vanishingly small presence to first-class status.

8.1 Introduction

In many sciences, *computational simulation* of structures and processes has become a respected and even essential research method. In some sciences simulation tools are routinely applied to simulation targets of very large scales and extreme levels of detail (e.g., Astrophysics, Biology, Materials Science). Extreme-

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scale input datasets, models, simulation tools, output datasets, and computational resources are routinely embedded in formal and tool-supported scientific workflows, and shared widely among scientific research teams. This sort of computational research has been heralded as a fundamentally new way of 'doing science'[1] and making research discoveries that would be impossible without these *shared cyberinfrastructures* (e.g. simulating black hole collisions and later contrasting against observations[2]). Social sciences are just now turning the corner toward using these types of large-scale cyberinfrastructures[3].

This paper describes results of our investigation into the state of the art of computational modeling and simulation for the social sciences. As part of a project for designing and implementing a proof of concept for extreme scale social science cyberinfrastructure, we have analyzed capacities of the five most salient agent-based simulation software packages that have been reported in literature to run in High Performance Computing (HPC) systems[4], to understand how they might fit these needs. Principal issues of concern include i) capacities for modeling social structures and processes from *inherently social* points of view; ii) capacities for scaling models, data, and runs to extreme levels; iii) capacities for designing and running simulation-based scientific experiments end-to-end; and iv) capacities for integrating with environments and practices now common among shared cyberinfrastructures, such as workflows, information and model sharing, team science, and pragmatics of actually building and running models in existing HPC hardware, software, access, and procedural ecosystems. This paper reports our evaluation results for well-known agent-based simulation frameworks based on their ability to run on HPC systems in some way and the existence of literature describing their application to various problems. Additionally, we discuss our design and testing of a new approach that responds directly to the evaluation model.

8.2 Evaluation model

Our analysis of existing agent-based simulation software packages defines three evaluation dimensions based on research software engineering concerns[5]: deployment readiness (**D**), experimental readiness (**E**) and modeling readiness (**M**). For each sub-dimension in the analysis, an integer score from 0 to 3 is be given depending on whether the framework has no facilitators (0), facilitators need technical involvement for each case (1), mature general facilitators require low technical involvement (2) or facilitators require no technical involvement (3).

Deployment determines to what degree experiments are unhindered by the host computing environment. *Experiments* are crucial for testing hypotheses in the social sciences within a robust epistemologic framework. Finally, modeling flexibility is essential to provide a palette of viable research strategies and be productive.

While scaling, cognitive flexibility and ability to use external input data are key in large-scale social science research, these are simpler problems that remain unsolved across the landscape of ABMs in HPC and thus not included in the metrics. *Theory-driven scalability*, or the ability of a framework to scale the number of agents and interactions in response to theoretical considerations, is absent in all studied frameworks. We will return to them in the description of our current work in Section 4.

D.SCB Self-contained build. Does the software package contain and trigger all compilation pre-requisites or do additional components need to be obtained separately and manually?

D.ATL Ample target localization. How simple is it to relocate the same software package to different cyberinfrastructures and run experiments on it?

D.HEN HPC enabled. Does HPC middleware remove low-level communication concerns while building social models? What implementations are applicable for a given software package?

D.SVI Software version independence. Are stable libraries and standard interfaces used? Is the application decoupled from changes in the HPC software environment (e.g. compiler version, system libraries)?

D.CIO Cyberinfrastructure integration. How much configuration effort is required to setup an experiment using HPC resources? To what extent existing system software is utilized?

E.ESD Experimental setting descriptions. Is it possible to explicitly specify an experiment as a self-contained unit? Can *derived experiments* be easily obtained from previous experiments or templates?

E.RSO Representation semantics for observables. Do mechanisms exist for specifying the computation of social observables by some reduction of individual agent states?

E.DAP Data analysis prescriptions. Does the framework include post-processing tools? Are the tools integrated in the agent framework during model execution?

E.RCO Research community orientation. Can experiment descriptions be packaged and redistributed to others in a community of research practitioners?

E.IRN Introduction of realistic noise. To what extent and realism is probability specified and enacted in models and experiments?

M.CTS Communication type specification. Is the communication model adaptable to encompass a large variety of agent representations?

M.TTS Time type specification. Can simulation time easily be set as discrete or continuous, centralized or distributed, deterministic or stochastic?

M.ATS Action type specification. Can multiple action types exist? Do action types depend on computational models, cognitive (learning) models or other form of decision making?

M.ETS Environment type specification. Can the world model be discrete or continuous, periodic or aperiodic, global or local in terms of what is known by the agent?

M.CES Concurrent events specification. Are the events sequential, concurrent, parallel or a mixture of the latter?

8.3 Evaluation outcomes

We evaluated various software packages using the Illinois Campus Cluster (ICC) with its default software stack. The ICC is representative of HPC systems in the TOP 500 list[6], hence we restricted ourselves only to GNU/Linux software environments. The evaluation process was performed by 1) obtaining the frameworks and installing them on the ICC ensuring that contained test applications could be executed, 2) analyzing the source code in terms of library dependencies, software entities and mechanisms for building experiments and 3) attempting to construct a simple model of agents that communicate and have a simple state.

GNU Swarm is a library-based toolkit for multi-agent discrete event simulation[7] with a strong experimental focus. A *swarm* is a collection of agents capable of scheduling events on its members and a representation of time. Swarms may embed other swarms in order to generate multilevel systems. Applications of Swarm include economics[8] and ecology[9]. Attempts exist to bring parallelism to Swarm[10,11] with very limited HPC capabilities. The reference version of GNU Swarm used for this evaluation is v2.4, which can be obtained at `http://www.swarm.org`.

Next, our attention turned to Repast HPC[12], a C++ implementation of the Recursive Porous Agent Simulation Toolkit (Repast) that provides an API to develop large-scale simulations with heterogeneous agents. The original implementation of Repast follows some of the aspects found in GNU Swarm and attempts to provide sufficient software support for model developers using HPC systems. It has been used in a wide variety of research cases including urban evacuation[13] and financial modeling of the stock market[14]. Repast HPC implements a "porous" action model, implying that scheduling can occur at multiple levels.

A different approach, one that seeks to mimic how scientific instruments collect data is that followed by the Flexible Large-scale Agent Modeling Environment (FLAME)[15]. Agents are modeled as finite state

Table 8.1: Evaluation of GNU Swarm.

Dim	Score	Details
D.SCB	1	External libraries required. Core functionality in the main tarball.
D.ATL	1	Automake. Manual setting of library paths. Limited build targets.
D.HEN	0	No native or additional support for HPC middleware.
D.SVI	1	Dependent on specific minor versions of library/compiler versions.
D.CIO	0	No native cyberinfrastructure integration.
E.ESD	1	Parameter settings in batch/interactive mode. No model description.
E.RSO	2	Entities for experiments, observers and measurement.
E.DAP	2	Simple tools for data reduction and interpretation.
E.RCO	2	Sharing of parameters through text files. Output data in CSV or HDF5.
E.IRN	2	Probability density functions with non-random seeds for repeatability.
M.CTS	2	Transparent point-to-point object message passing in Objective C.
M.TTS	2	Time is semi-discrete and deterministic. Scheduling within swarms.
M.ATS	1	Actions through SwarmObject. No embedded social theory.
M.ETS	1	Discrete, diffusion-based or continuous 2D spaces. CVS/HDF5 storage.
M.CES	1	Concurrent GNUStep threads. XML RPC distributed communication.

Table 8.2: Evaluation of Repast HPC.

Dim	Score	Details
D.SCB	0	Boost, MPI, NetCFT Core functionality tied to external libraries.
D.ATL	1	GNU Make. Manual setting of paths for library versions.
D.HEN	3	Native support for MPI, OpenMP can be used.
D.SVI	2	Accepts minor versions of required libraries with a starting number.
D.CIO	2	Run as an task on MPI aware job scheduler. Depends on batch system.
E.ESD	1	Parameters through properties file. No input model description.
E.RSO	0	No observables defined, depends on external analysis strategy.
E.DAP	1	Data collection objects across all agents, but no analysis.
E.RCO	1	Sharing of parameter through text files. Output data in plain text.
E.IRN	1	Limited randomness with repeatability control.
M.CTS	1	Blackboard model within contexts (agent sets).
M.TTS	0	Discrete event time model, a partial order of agent actions.
M.ATS	1	Actions are porously scheduled. No embedded social theory.
M.ETS	1	Basic models for continuous and discrete N-D geometries.
M.CES	3	Self-handling of local POSIX threads and distributed MPI threads.

machines (FSM) whose state changes depending on received messages (i.e. X-machines). An XML parser takes care of translating an XML description of an agent model to native C code, including initial conditions and the specification of the transition function of agents. The resulting code can be compiled and executed in any resource. FLAME has been used for simulating the European economy at large[16] and modeling various complex biological systems.

Table 8.3: Evaluation of FLAME.

Dim	Score	Details
D.SCB	3	Most required libraries included. Libmboard and Xparser are ANSI C.
D.ATL	2	GNU Make. Build process is exhaustive for all components.
D.HEN	3	Native support for MPI.
D.SVI	3	No libraries are tied to the software environment.
D.CIO	2	Run as an task on MPI aware job scheduler. Depends on batch system.
E.ESD	2	Parameters and general model described in XML. C functions required.
E.RSO	0	No observables defined, depends on external analysis strategy.
E.DAP	1	Local XML output, but no analysis.
E.RCO	3	Experiments can be easily redistributed and instanced elsewhere.
E.IRN	1	Uniform distribution applied to message sending only.
M.CTS	1	Message board with filtering capabilities in agent network.
M.TTS	1	Continuous distributed time without global clock.
M.ATS	1	Actions as state transitions in FSM. No embedded social theory.
M.ETS	1	Local model of geometry. Provided by applications.
M.CES	3	Self-handling of local POSIX threads and distributed MPI threads.

Pandora[17] is another ABM framework built on top of MPI and OpenMP as the agent communication and distribution layer middleware whose design is aimed at *computational scaling*. The API is provided in the form of extensible C++ classes for agents situated in a world with coordinates and includes a visualization tool, "Cassandra." Users can prototype models in Python through a foreign-function interface, or later refine them and write them in C++. Pandora has been used for simulating population dynamics[18] and modeling the co-evolution of trade and culture in past societies[19].

We finally reviewed a ROSS Time Warp port in Charm++ performed by the Parallel Programming Laboratory at UIUC[20]. Charm++ structures and functionality have been used to match the original C API of ROSS. This code has been used to simulate parallel workloads in HPC networks[21] and to help understand energy design strategies in smart devices[22].

Table 8.4: Evaluation of Pandora.

Dim	Score	Details
D.SCB	2	Depends on Boost library and GDAL.
D.ATL	1	Build process is exhaustive but unclear.
D.HEN	3	Native support for MPI and OpenMP.
D.SVI	2	Library dependencies refer to major versions only.
D.CIO	2	Run as an task on MPI aware job scheduler. Depends on batch system.
E.ESD	1	Parameters described in XML. Model in Python or C++.
E.RSO	0	No observables defined, depends on analysis strategy.
E.DAP	2	Cassandra provides basic data analysis and visualization.
E.RCO	2	XML-based parameters, code needs to be included.
E.IRN	1	Agents can make use of Boost random number generators.
M.CTS	0	No explicit comm model. Agents communicate through world actions.
M.TTS	0	No explicit model of time or events.
M.ATS	1	Actions specified in classes deriving Agent. No embedded social theory.
M.ETS	2	World representation is active, includes 2D and 3D geometries.
M.CES	3	OpenMP threads and distributed MPI threads.

Table 8.5: Evaluation of Charm++ ROSS.

Dim	Score	Details
D.SCB	3	Charm++ and ROSS minimal base is self-contained.
D.ATL	2	GNU Make. Build process is simple, yet not automatic.
D.HEN	3	Charm++ acts as a cyberinfrastructure-aware middleware.
D.SVI	3	No core library dependencies.
D.CIO	3	Benefits from Charm++'s cyberinfrastructure integration.
E.ESD	0	Parameters have to be manually specified through Charm++.
E.RSO	0	No observables defined, depends on analysis strategy.
E.DAP	0	No basic data analysis or visualization.
E.RCO	0	Code and batch script needs to be packaged and sent.
E.IRN	2	Random numbers can be generated conveniently.
M.CTS	0	Communication occurs as attention to events.
M.TTS	0	A finite model of continuous local time.
M.ATS	1	Actions implemented as functions. No embedded social theory.
M.ETS	0	No world representation exists.
M.CES	3	Charm++ *chares* abstract all concurrency.

Discussion

GNU Swarm (Table 8.1) provides good experimental semantics, but performs poorly in other aspects. It does not naturally integrate with any cyberinfrastructures and its deployment is fairly restrictive outside its narrow software compatibility zone. While it is limited in terms of HPC readiness, its experimental semantics provides interesting lessons for large-scale systems. Repast and later Repast HPC (Table 8.2) have taken note of GNU Swarm's lessons and applied them to HPC systems sacrificing experimental and modeling features. Pandora (Table 8.4) follows a similar path with better experimental features. Charm++ ROSS (Table 8.5) benefits from deployment properties of its middleware significantly, but its modeling and experimental capabilities are extremely limited at the moment. FLAME (Table 8.3) improves on many of the experiment-oriented factors, but has not sufficiently general modeling capabilities. Complications in deployment in all cases appear to be tied to research software sustainability issues in general, and of middleware in particular. In all cases, code needs to be written for models, limiting access to social science scholars interested in using HPC resources as "social supercolliders"[23]. None of the frameworks is guided by any kind of social theory.

A comparison between the results of our evaluation and compare against a theoretically ideal framework is given in Fig. 8.1. *Ideal* is interpreted here as the Minimally Effective Framework (MEF) that facilitates research in social sciences when access to cyberinfrastructure is available. Despite its age, GNU Swarm appears to be more experimentally suited the alternatives and is comparable to FLAME in its modeling capabilities. The advantages in deployment of other models compared to GNU Swarm may be explained by advances in software processes in general[24], even when HPC environments tend to be more conservative[25]. All evaluated cases are far from the theoretical MEF. Obtaining a maximum score in all three dimensions is a precondition of a framework where theory-driven scalability, cognitive modeling and input data streams can properly addressed.

Fully characterizing, measuring and evaluating scalability remains an open problem. Scalability in HPC describes how the relation between number of processors and problem size varies with parallel communication cost[26]. In agent-based modeling, it describes the ability to grow in number of agents, diversity of agent types and collective problem size[27]. Our interpretation of scalability is parametric and general in terms of quality, cost and time of interactions in a simulation. At present, we are exploring the existence of points in parameter space where agent-based scalability best matches HPC scalability to realistically portray social phenomena described either by theories or observations.

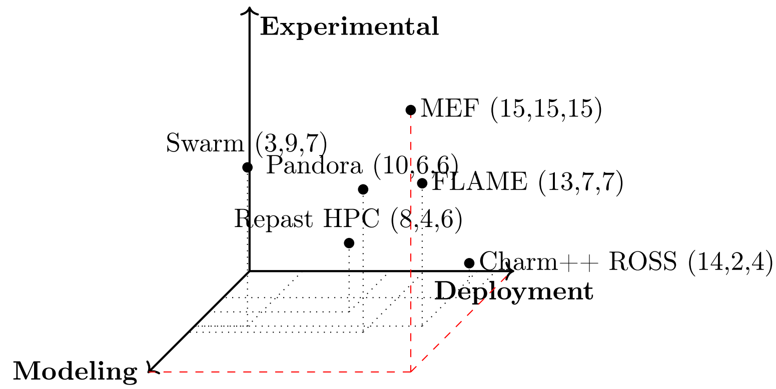

Figure 8.1: Aggregate evaluation of facilitating dimensions for large-scale ABM frameworks. MEF stands for Minimally Effective Framework.

8.4 Social Theory Scaling Compiler: towards a novel ABM architecture

A new type of framework is needed for fully realizing the potential of agent-based modeling and simulation in computational social science. Our current work focuses on developing a framework in compliance with the evaluation framework as a foundation. On top of it, scalability is interpreted as an aspect of social theories that can be used to increase or reduce the number of agents required for better scientific gains and better machine usage. Hence, the Social Theory Scaling Compiler (STSC) is being designed with the aim of allowing scholars to focus more on the research content of their experiments and less on technical details required to run them. The core of STSC is a three-level, general agent-based model that has message-based communication, agent state dynamics and actions in a given world model. Agents can either observe or measure the world at a given location, and traverse it according to a distance model. State changes, prompted by incoming information and the outcome of measurements, comprise the dynamics of agents as information-based system systems. Finally, communication between agents provides the basis for coordination.

STSC starts at the basis of cyberinfrastructure by using Charm++ as its middleware and communications layer instead of MPI. Our evaluation indicates that Charm++ positively impacts deployment and it is prevalent across most NSF funded cyberinfrastructures[28]. The design of STSC depends on three key components that interact to produce natural scalings, where the guiding social theory is that of coordination through hierarchical task networks. A virtual machine (OrgVM) can be instanced in distributed physical processors and handles allocation of agents and task distribution transparently, including its own assembly language. A local parametrization allows fine control over cyberinfrastructure resources by taking advantage of workflow management systems such as Swift[29]. OrgVM is fine-grained stochastic in terms of states, interactions between agents and actions that affect their environment in order to address higher scientific realism proper of complex, hierarchical social systems.

This execution layer is intended to be used through a description language for experiments that separates technical concerns from modeling activities (OrgLang). OrgLang programs contain experiment descriptions, annotations, agent properties, world representations with localized action and communication patterns based on coordination and division of labor. Experiments written in OrgLang are portable by definition, and can be executed after compilation into OrgVM instructions (`orgcc`). Compilation of OrgVM code allows semantic analysis to be used by the third component of the framework, a scaling and data analyzer (OrgScale). OrgScale is designed to work in two ways: in a design-of-experiments context or to construct simple models from data. First, semantic analysis of OrgLang programs will iteratively rescale variance in agent states and the number of agents in a given experiment until a parsimonious setting is found (i.e. the smallest number of agents that preserve features of simulations originally run with a larger amount of agents), helping the community of researchers determine scales at which certain phenomena may be observable and use resources more effectively. Second, it will allow obtaining a minimally effective agent-based model from data for which no such model is available. OrgScale is designed to perform spectral analysis of (possibly) stochastic data to obtain a frequency based model that best explains the data.

Our framework design appears to provide elements required to overcome limitations of current ABM frameworks and benefit more from existing and future HPC resources. In summary, theory-driven scaling as the central element of ABM design for large-scale social simulation has advantages in terms of expressive power, transparent design of experiments, integration to cyberinfrastructure environments and moreover higher scientific realism. It has not escaped our observation that organization theories may be described to a first approximation as programs that manage entities and constraints in some form of *social machine* with a trajectory-frequency duality.

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Chapter 9

In-Silico Models with Greater Fidelity to Social Processes: Toward ABM Platforms with Realistic Concurrency

Summary[i]

In this paper, motivated by conceptual and computational considerations, we argue in favor of improved fidelity of ABMs in relation to the social processes they attempt to model. With ordering and concurrency characteristics of social interactions as our focus, we identify potential for innovations in ABM platforms using two elements: the SPEC framework of social primitives; and ongoing development of SPEC-ABM software platform, highlight relevant aspects of the intersection among conceptual, formal and technical perspectives, using Elixir as the programming language of choice for our implementation efforts.

9.1 Introduction

The promise of explaining the macro from micro has driven the formation of the new discipline of computational social science(CSS). Agent-based modeling(ABM) using NetLogo[1] has played a key role in partially fulfilling the promise. In tandem with the recent emergence of data science as a field, studying large scale social systems more scientifically is now possible, with the ABM approach serving as a complement and extension to traditional mathematical modeling[2] and data science serving as a complement and extension of traditional statistics[3]. This has resulted in advances in the other direction too with emerging efforts to revisit and improve upon the foundations of both empirical and theoretical epistemological tools. Specifically, disciplines of inferential technology: statistics; data mining; and machine learning, are undergoing rapid transformation and reorganization. A similar effort is underway at the theoretical modeling front, to revisit the foundational tools of simulation models; this paper is a contribution to such an effort.

Depending on one's underpinning of focal interest, extant approaches have made headway along different

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directions: Agent Zero[4], continuing in the older tradition of SOAR[5] and ACT-R[6], proposes cognitive elaborate agent models; *Homo Socialis*[7], focusing on an analytical interactive framework, emphasizes game theoretic and stochastic dynamic models of sociality; and finally, Deep Agent Framework[8], marrying data workflow and modeling pipelines, develops a platform to study online large scale social systems. Our work's starting point is different.

Philosophically grounded in sociological theory; and theoretically grounded in analytical sociology[9], social mechanisms encoded using social primitives are this work's starting point for both mathematical and computational model building. Being part of analytic sociological inquiry, our approach gives primacy to retaining utmost fidelity to dynamic temporal characteristics of social interactions underlying social processes. Acknowledging this fidelity also makes sense from a social computing perspective: if actors are situated in extended space and time, and possess clocks with different speeds, the choice of distributed model of computation[10] used to model social processes makes all the difference.

Our starting point can also be justified from a pragmatic computational modeling perspective, as an attempt to reduce certain kinds of model misspecification. While several *micro* models may produce the same *macro* behavior, some *micro* models are normatively desirable, especially the ones that are closer to the *true* underlying social mechanisms. A larger concern, of which this work is a small step, is the use of general purpose simulation platforms for modeling such social mechanisms. Even if the models are clearly specified, it is not clear if the underlying software machinery behind event scheduling washes out critical details of a correctly specified model. It is this specific limitation of platform scheduler's dependency we address here.

In the next section, we illustrate with examples, the sensitivity of social processes to time ordering, concurrency and local clock characteristics. Following that, we couch this analysis within our SPEC framework, illustrate it with an overview of strengths of the Elixir programming language, and contrast them with general limitations of other ABM platforms. We conclude the paper with anticipated next steps.

9.2 Social processes: ordering, clocks and timescales of social actors

Admitting that concerns with model specification and fidelity to reality that motivated this work are pertinent for any ABM of natural phenomena, we focus only on social phenomena. Here, we present a few key models of real world phenomena: synchronization; epidemics, social influence and diffusion processes, and collective decision-making, which have been revisited and generalized in recent literature. All these phenomena display emergent macro behavior that depend crucially on micro processes' temporal characteristics.

We begin with synchronization[11] – a universal phenomenon of systems, complex or otherwise. Viewed as a dynamic process, synchronization is a self-organization process by which a spatially extended interacting heterogeneously periodic system evolves into a homogeneous periodic system; as a computational process, it is a process by which spatially-distributed communicating agents with heterogeneous clocks evolves cybernetically into a system with homogeneous clocks. In both dynamic and computational models of such systems, considerable progress has been made towards understanding synchronization, but under assumptions of strictly pairwise agent-agent interactions. However, recent models have generalized interactions to higher-order interactions with both temporally local and non-local interactions. Both simulation and mathematical analysis have produced unexpectedly rich macro behavior that is sensitive to the nature of interaction[12,13].

The second class of phenomena we discuss are epidemic processes. Typically, epidemic models are macroscopically specified in terms of ordinary differential equations[14], and underlying them are pairwise interacting particle system models known as contact processes[15]. Epidemiologists have long known that certain epidemics, like the HIV epidemic, are better modeled as concurrent epidemic processes where, like interaction models of synchronization phenomena, multi-way contact processes[16] are better able to capture aspects of the natural phenomena.

The third class of phenomena are social analogues of contact processes and information exchange processes[15]: social influence, and consensus and voter models. *Micro*-level differences in interactions characteristics like synchronicity lead to different *macro*-level outcomes[17], as is the case with synchronous Granovetter model and asynchronous Bikhchandani model. Similarly, simulation-based results for both consensus, voter models[18,19], have shown systematic differences between pairwise and higher-order interaction cases.

The final class of models are social process models of group decision making. Both observational and experimental studies of small groups in both everyday social and organizational contexts show extreme sensitivity to finer details of a group's temporal characteristics such as turn-taking[20], intentional and unintentional interruptions[21], starting conditions, etc, constrain the collective social cognitive processes: collective rational deliberation towards a decision is sensitive to interaction effects.

To summarize, the processes discussed above exemplify the importance of interaction in generating emergent complexity. Even though all these processes discussed in this section have been modeled in the ABM/CSS literature, we contend that the models have either not explicitly encoded such processes' temporal characteristics, or have used platforms that wash out encoded finer details. Admittedly, the reasons for this might be practical.

While ABMs are used pragmatically in CSS, they are studied more formally in other disciplines: e.g., in mathematics as interacting particle systems; in physics as non-equilibrium statistical mechanical models; in engineering as multi-agent systems; and in computer science as distributed computation models. While the simpler of the CSS models are identical to baseline model families in these disciplines, the formalisms which use game theoretic and dynamic system models do distinguish model classes based on temporal characteristics of interactions like concurrency, schedules and timescales. So the concerns we raise in this manuscript are not original; we are merely using formalisms as a lens to provide a more fine-grained resolution of ABMs, and to point out the coarse-graining effects of platforms that have been used typically to implement ABMs. We discuss them in greater detail in the next section.

9.3 The SPEC Framework

We describe here the SPEC-ABM - social primitives for evolution of complexity - an ABM framework. This framework is centered on social primitives as abstractions that encode social mechanisms underlying emergence of social organization. This conceptualization allows us to develop models based on an agent's (social) cognitive mechanisms, external social interaction mechanisms, and the environment, gradually scaling mechanistic complexity[22]. Both issues of fidelity to real-world characteristics of social processes and platform induced model misspecification are primary motivations of our project, of which this manuscript is a first step. While the second issue does not really require a new framework, for reasons that we discuss in this section, the first issue requires a new conceptual approach.

Building off of the (now classical) Generative Social Science approach of Epstein[23,24] and others[25], some of the authors of this manuscript offered a refinement: SPEC Framework[26]. This refinement simultaneously interfaces with both the classical approach and analogous approach pioneered by Hedström and others, by appropriating the language of cybernetic processes: *control*, *communication*, *information*, *computation*, *goals*. A system is social in our view whenever it contains entities capable of information representation, storage, retrieval, transmission that use their internal state, to create a useful abstraction about other entities, have internal goals and perception of goals in other agents, and capacity to act and be acted upon by the environment.

The concept of *social primitives* is a logical extension of ABM based on a history of observations across scientific domains concerned with explaining collective behavior. We denote all agents' capabilities in general as *primitives*, and those geared toward constructing abstractions of individual agents of collectives by means of information representation, processing and communication by *social primitives*. These *primitives* serve as software specifications of social mechanisms – the starting point of analytical sociology. Empirically observed macrosociological regularities are explained using such mechanisms, which are situated in both abstract social and concrete physical or geographical space. Hence fidelity to social processes then means fidelity to social mechanisms that generate these processes.

In Table 9.1, we have identified six types of general primitives associated with *the social* in our conceptual model: spatial primitives, sensing primitives, communication primitives, memory primitives, rule primitives, and composition primitives. We focus on primitives that are simultaneously general across types of agent systems and suitable for computational implementations. Each of these *primitives* also carry social mechanistic semantics[ii]. To illustrate, using this framework, different members of our group have published on different aspects of the same phenomena. Friesen and Mudigonda[27], used spatial and compositional primitives to develop a model of emergence of institutions and wealth inequality. in an artificial society. Inspired by their work, Venkatachalpathy et al[28] used (social network) spatial and compositional primitives to study the emergence of wealth inequality in artificial societies with social structure. Salamanca and Núñez-Corrales explored the role of spatial, sensing and interaction primitives on the ability of agents to converge to a known color model[29].

The present manuscript was directly motivated by our attempts to study carefully the process of proto-institution formation models.We realized that other primitives like interaction primitives must be clearly specified in order to model different kinds of social interactions that lead to the formation of cooperative institutions. More importantly, we realized that none of the programming platforms (R, Julia and NetLogo) we used guaranteed fidelity to model specification and social mechanisms, and that a truly concurrent programming language based platform was required to further model the other SPEC primitives with high fidelity. The social (interactive) aspect of these primitives introduces a range of non-trivial challenges when considering their implementation, something we discuss in section 4.1.

To reiterate, our framework is not just an improved ABM platform; its epistemological virtue is a synthesis of the computational, mathematical and scientific perspectives. As we discuss in subsequent sections, the limitations of the current ABM platform and extol the strengths of our proposed platform in subsequent sections, we emphasize the conceptual advances we aspire to make in our project, not the specific choice of programming language for our simulation platform.

[ii] Analytical sociology literature has developed a self-contained list of atomistic (*micro*) mechanisms using which they explain the *macro*. The focus and scope of the manuscript prevents us from going into details.

Type	Particular primitives
Spatial	• Having a position • Representing and locating oneself • Measuring one's location • Moving to other locations • Mapping a space
Sensing	• Representing observables • Distinguishing between local/global observables • Modulating sensing depending on locality model • Reifying observables into measurement outcomes • Measuring multiple observables • Computing properties of multiple measurements • Abstracting new structures from multiple measurements
Memory	• Having internal storage • Structuring internal storage • Expanding/contracting internal storage • Storing information • Retrieving information • Erasing information
Composition	• Representing collectives • Classifying collectives as aggregates or modules • Regulating behavior in others • Estimating/computing regulation utility/cost • Inventorying resources across collectives • Establishing/discovering causal patterns across collectives
Interaction	• Having an encoding • Constructing messages using some encoding • Knowing about other agents • Classifying other agents • Establishing/finding communication channels • Request/accept/deny communication through a channel • Sending messages • Receiving messages
Action	• Representing of rules of the form [qualifier] condition → action • Qualifiers: modality, delay, ordering • Conditions: logic statements • Actions: primitives, rule triggering (composition), sequencing, selection, iteration

Table 9.1: Primitives of a SPEC agent. SPEC-ABM emphasizes interaction and action primitives.

9.4 Towards a concurrent ABM framework

Next, we present three directions with potential for innovations in ABM platforms. We discuss in detail potential advances pertaining to concurrency, and difficulties navigating modeling projects while using existing platforms, using a COVID-19 epidemic model as a case study.

First, we lack tools and platforms that make it easy to model how dynamics are affected by a change in the number of agents, when transitioning from small scales to extremely large-scale systems. Currently, ABM frameworks such as RepastHPC demand strong programming skills from their users. Second, modeling capabilities tend to gravitate towards one of two extremes: either ease of use has been increased at the expense of model-tuning options; or usability has been sacrificed in the interest of full access to the model coding. In the latter case, users may encounter significant implementation barriers –for example, in choosing schedulers- before starting the actual modeling and simulation process. Third, while implementation decisions related to ordering of events (i.e. sequential vs. concurrent) impact results obtained through simulation significantly[30]***, dynamics in social systems occur at multiple scales simultaneously. Implementing these dynamics is possible due to the advent of multicore, parallel, and distributed computing architectures, with associated software infrastructures. However, such implementations require natively concurrent programming platforms and techniques.

We explain below how fidelity to concurrency and ordering characteristics may lead to better ABM frameworks.

9.4.1 Concurrency and simulation fidelity

In section 2, we discussed several classes of natural social phenomena where concurrency and ordering of interaction events at the *micro* level were important in explaining the *macro* level phenomena. For an ABM specification of a social phenomenon to have fidelity social processes, the concurrent aspects of the phenomenon need to be recognized and formally represented in the associated ABM specification. Further, this fidelity should be captured during implementation, perhaps via an ABM framework such as MASON, Mesa, NetLogo, etc, or any other "home grown" framework. The degree to which this fidelity to reality is maintained in a particular ABM's implementation, is dependent on the approach to *concurrency* taken by the programmer implementing it, and is arguably constrained by the semantics of the underlying language platform within which the program is written, and executed.

The handling of concurrency in an ABM framework is circumscribed by the concurrency-handling primitives that exist in the language environment within which the ABM framework is implemented and executed. The designers of ABM frameworks might choose to make additional implementation choices that constrain the specific ways in which modelers implementing an ABM specification can simulate concurrency in their specific implementation of the ABM specification. As an example, Netlogo originally provided deterministic scheduling with agents' being activated to take action in a pre-specified sequence. This sequence of agent activation matched the order in which the agents were created and initialized, in a first-in-first-out approach[31,32]: concurrency was simulated via turn-taking and time-slicing. Since 2007, the `ask` command executes serially with agents being activated in a different random order for each `ask` command in the code. Also, the random ordering of execution is designed to mitigate the potential effect of having a particular agent always executing code first. However, this does not always matter as is illustrated[iii] in NetLogo model library's Wealth Distribution Model[33]. In addition, random activation of agents' actions during each time step is also possible.

Extensions to the Netlogo core allow for other scheduling approaches. An example is the dynamic scheduler extension[32], which makes it easier to activate agents to act at specific time ticks. Mesa[34], which is another popular ABM framework implemented in Python, offers a variety of scheduler options to the modeler. The default (base) version activates the actions of agents in the order in which the agents came into existence in the simulation. A second option is random activation, which, as the name suggests, shuffles the agents (pseudo) randomly, prior to performing the agents' actions. A third option called simultaneous activation simulates simultaneity across all of the agents. Staged activation is a fourth option available. Here, the performance of agents' actions can be divided into multiple stages, where the stages may be spread across more than one time step, depending on the specifics of the phenomenon being modeled[iv]. Based on their specific needs and considerations of ease of model implementation, modelers might choose one of the existing frameworks, or might decide to implement their ABM specification without using an existing framework, by hand-coding all of the concurrency-related aspects (along with other aspects) of their ABM specification, perhaps well-suited in a few modeling situations. However, in situations where changes in the approach used for sequencing of agents' actions affect the final outcome, using a "simulated" version of concurrency is fraught with the danger of a loss of fidelity to reality, and end up representing a scenario that is different from what is sought to be modeled.

[iii] Consider the following example:

```
ask turtles [turn-towards-grain] ;; choose direction holding most grain within the turtle's vision.
```

Since the turtles are just facing the maximum grain holding patch, not moving nor consuming any grain, this action does not change the decision that any other turtle would make about which patch to face. In other words, the order in which the turtles execute this code matters not in the least. If we add the code for moving and eating into this ask command, then the order could matter:

```
ask turtles [turn-towards-grain move-eat-age-die harvest]
```

Here the first turtle to execute the code could get all the food on the patch that it moves to rather than sharing it with any other turtle that happened to move to that same patch.

[iv] See: `https://mesa.readthedocs.io/en/master/apis/time.html`

Also, if agents' environment is dynamic, many direct as well as indirect parameters must be considered such as how resource levels, agent states, and next step attributes are enacted (e.g. resource dynamics of patches, changing social network structure). In ABM frameworks like Mesa, behavior space attempts to capture all of the direct parameters but the indirect variables may be both unseen and unaccounted for. These unarticulated attributes of an ABM include the choice of the coding language, whether agents receive synchronous or asynchronous updates, is not calibrated with real-world features.

In general, it is important to recognize that the default and other options for implementing, involve a trade-off between ease of expressing concurrency in code and the code complexity needed to represent concurrency with a high degree of fidelity to reality. We think that it is possible to do obviate such a trade-off by choosing a language, whose underlying implementation and execution environment has two features: (1) a set of concurrency-supporting programming primitives that allow for concurrency to be managed easily; (2) an implementation of concurrency that is robust, scalable, and managed in a way that allows for the concurrent actions occurring among the entities interacting in the environment to resemble closely the concurrency one observes in reality. Any environment that supports real-time concurrency is a good candidate for developing a ABM platform. The Elixir BEAM environment is one such environment. As we describe in the next section, Elixir, allows us to achieve the implementation ease we seek for representing the concurrency needed to simulate reality, using a programming syntax that is, arguably, easy to learn, use, and read.

9.4.2 An illustrative case study of current constraints in existing platforms

Modeling the spread of COVID-19 can illustrate the salience of the concerns we just described. Recent simulation efforts in this direction[35] suggest that ABM frameworks can be ranked on a scale of readiness to address challenges proficiently under time constraints. Some frameworks, like SIR-like ABMs, are useful for prototyping ideas quickly and test-driving models in controlled situations at small scales; these models capture the phenomena appropriately without the need for a large number of agents or any non-determinism.

However, as soon as one adds realism (e.g. social network layers, interacting between geographical and social network layers, social information contagion) and interactions among these dimensions, issues of concurrency, event ordering and interaction protocols become crucial to achieve model fidelity in epidemic evolution. For example, time-sensitive aspects of epidemic processes are likely present (e.g. acting before the spread of a virus reaches a critical percent of the population). As simulations become either more complex or larger (or both), scaling decreases.

When such features are added to capture specific interaction mechanisms, both ensemble size and the number of agents needs to increase such that events in the simulation remain, on average, must remain calibrated with empirically observed features. At the same time, the number of agents needed for the appropriate macroscopic behavior to emerge appears to be inversely proportional to the size of its interaction repertoire. This tension requires us to experimentally perform simulations at scale, something not available in existing platforms.

Platforms, like the one we propose, that enable high fidelity prototyping are critical for: (a) acquiring maturity and proficiency in solving the grand challenges, (b) benefiting from increases in computing power up to the Exascale, and (c) for allowing scientists to develop their own ideas quickly and productively.

9.5 SPEC-ABM: An Elixir-based concurrent ABM platform

Based on the discussion above, our group has embarked on the design and implementation of a new ABM framework that rests upon two main pillars: a conceptual one, centered on primitives as the core scientific vocabulary used to structure models; and a pragmatic one, focused on exploiting concurrency present in contemporary computing platforms. To achieve both objectives, our efforts have been dedicated to building a new ABM framework from the ground up, with an emphasis on choosing technologies capable of facilitating a solution to challenges described in this manuscript.

From a software engineering perspective, creating a new piece of software translates into a set of new responsibilities, especially in the midst of a growing modeling community. We must start by acknowledging that ABM research is a form of computational research, and any new ABM framework must therefore contribute to reducing the computational reproducibility crisis[36] and must be itself a sustainable piece of software[37]. Hence, regardless of our technology or implementation choices, we hold this requirement as valid for the development of any ABM framework. For the task of building the SPEC-ABM framework, we have chosen Elixir as the programming language that fits three requirements described below.

First, the set of features of a programming language and its associated run-time environment that are salient in the development of a framework capable of exploring a wide range of social phenomena must implement concurrency through multiprocessing, since distributed architectures depend on truly independent clocks and execution environments. Second, software development tools must hide unnecessary complexity to allow modelers to freely concentrate on problem solving, while abstracting and elegantly handling as many aspects related to concurrency as possible under the hood. Having concurrency should not introduce undesirable or distracting complexity when implementing a social model in the given ABM framework. Third, the language's syntax should support implementation of highly-nuanced model specifications, without having to alter the code base of the framework to achieve the desired effects.

We describe next how Elixir allows us to meet our stated goals.

9.5.1 Why Elixir?

Elixir[38] is a functional language with a powerful macro system that runs on top of the Erlang virtual machine (BEAM). Functional languages provide a useful declarative approach to parallel programming[39]: (a) programs are their own formal specification and (b) statistically measurable lower susceptibility to bugs when compared to imperative languages[40]; Elixir appears to be no exception. The BEAM implements extremely lightweight process threads on top of a single operating system thread. It was developed by Ericsson to address the challenges of concurrent processes in the telecommunications industry at scale[41]. Even in its early versions, it was found that a small number of higher order processes account for 95% of the concurrency in mechanisms across a wide variety of programs, just like how a few social primitives lead to sociality in ABMs.

The BEAM is eagerly preemptive, which randomizes all concurrent events. For SPEC-ABM, this feature proves beneficial, since the ordering of events does not necessarily have to depend, in the simplest case, on computing random distributions. Concurrency that uses multiprocessing is implemented by setting up compute nodes that an application can use. Once these nodes (which can be cores on a single CPU, multiple CPUs on a single computer, and/or multiple computers in a network) have been registered across multiple BEAM instances, nodes are coalesced into a single process space, where the BEAM takes care of the actual distribution details, including load balancing.

Another advantage towards extreme scaling of simulations is the recent ability to instantiate the BEAM on top of hypervisors such as Xen in order to trim down unnecessary features in a general operating system that consume time and reduce the possibility of reaching fast, near-real time performance and throughput. Because of these and other advantages offered by BEAM's concurrency model, we believe that ABM framework designers in general can benefit significantly from reviewing some of its mechanisms.

9.5.2 SPEC agents

All agents in SPEC-ABM are implemented using the GenServer model provided by Elixir. A GenServer is a process template that provides a service based on a model of attending events that can be synchronous or asynchronous. A GenServer can send a message and wait (`handle_call`) or receive a request to continue a sequence of actions (`handle_continue`) and return a message to its recipient. Both events induce causal orderings due to being synchronous. The server can send a message and not wait (`handle_cast`), or simply react internally to incoming information (`handle_info`).

Using these tools, we have developed a prototype agent whose internal state is supplied by the modeler. As part of the parsing process of the model specification, SPEC-ABM translates details of agent primitives into data structures (an Elixir struct) per agent type. The type of an agent is a dynamic property that depends on variables and structures stored internally and/or their values. All primitives are instantiated as lists of structs that contain all the necessary information required to drive agent behaviors. The prototype agent is refined into specific internal agent types via delegation.

9.5.3 Scheduling in SPEC-ABM

The execution of any action is determined by three factors: the BEAM scheduler, the scheduling determining the ordering in which agents, and the scheduling that determines which actions are executed within the agent. Actions *are scheduled* by the agents, interactions *happen* to the agents. SPEC-ABM does not interfere with BEAM scheduling, since it provides a good source of stochasticity by itself. Regarding the ordering of events either the ordering is sequential, or it is non-deterministic.

If agent scheduling is sequential, a special GenServer is created, along with its own clock, to store and process action and interaction requests depending on some condition. For example, the GenServe may wait until all agents have reached a certain threshold to allow them to continue, if all agents have placed requests, or it will always allow certain agents to perform events in the queue before others based on the value of some part of their internal state. Sequentiality requires having an external observer mediating and ordering events, which are centralized activities and performance bottlenecks. If scheduling is non-deterministic, no such GenServer is created and agents act independently.

Internal agent actions are also subject to scheduling. First, each rule has a probability of activation for which we provide two alternatives: one having a probability and a Bernoulli distribution, and another one where the probability is computed using a sigmoid function and then a Bernoulli experiment is performed. Second, rules can have priorities. Agents prioritize their actions to execute them; when no priority is specified, the most likely priority is that given by the order in which they were specified. Third and last, we distinguish between the moment when agents dispatch an action and when it is executed. We expect to provide the ability to specify a finely granular delay that can be fixed, dynamic (with various activation functions) or stochastic thanks to the microsecond resolution provided by the BEAM.

9.6 Conclusions and Future Work

In this paper, we identified a key source of emergent complexity in social simulations: inter-agent interactions, and suggested concurrency and ordering blind simulation schedulers have limited fidelity while specifying social interaction models whose underlying social processes possess such characteristics. We proposed that a natively concurrent programming language like Elixir is well-suited for this purpose, by pointing out difficulties using existing ABM implementations. In addition, we also furthered our desire to develop a new type of social simulation platform: the SPEC-ABM framework that retains inter-agent interaction characteristics, making the simulations truer implementations of social processes.

Our current focus is on developing a functional implementation of social interaction primitives that is scalable and ready for simulation. Also it should be emphasized the choice of programming language is pragmatic; we merely sought to use a compiler and virtual machine architecture that is sensitive to concurrency, ordering, and to the existence of local and global clocks. Still, that Elixir is the adequate language needs to be demonstrated.

We are currently systematically comparing NetLogo's JVM, Mesa's Python interpreter, and Elixir's Beam virtual manager, stress testing them for their fidelity to given model specifications. One way this can be done is to pick well known interacting particle (agent) models exemplified by contact based epidemic models or voter models, specify models with precise concurrency and ordering features in their agent-agent interactions, implement it in all three ABM platforms, and confirm our expectation that virtual machines with natively concurrent and parallelizable features can be indeed more faithful.

We consider this work to be first steps towards imagining the next generation of agent based modeling platforms. Even if currently our social primitives approach or its Elixir implementation are limited in their efficacy, the fact that interactions are situated in both time and space, that ordering and concurrency matter; and that agents (can) have internal clocks matter in all stages of the social modeling process. These issues cannot be ignored.

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Part IV

Discovering with interactions

Chapter 10

Social Viscosity, Fluidity and Turbulence in Collective Perceptions of Color: an Agent-Based Model of Color Scale Convergence

Abstract[i]

Social flow, viscosity and turbulence increasingly help explain observations of collective social systems in which self-organization is driven by norms and beliefs. We propose a simple agent-based model of self-organization of human agents, adapted from seminal color sorting experiments of individual perceptions of color proximity, as representative of a fundamental class of social phenomena involving convergence towards a stable collective social structure. We define inverse social viscosity *as the measure of the difference between agent situated beliefs and perceptions as the driver of collective action flow. We study convergence and reversions using a particular form of the equation describing nucleation processes in phase transition theory. Our analysis suggests that tolerance to imperfect compliance with norms and a degree of tolerance with own beliefs decrease coordination efforts. In addition, our research suggests that social viscosity is a proxy measure for the cost of social organization, which can in turn be used to inform the design of socio-technical systems. Breaking social isolation is a successful strategy to foster self-organization.*

10.1 Introduction: social viscosity, fluids and turbulence

Fluid spatiality is one of the topologies used to describe the constant flux of the social. It serves to frame social action as a fluid, embracing both boundless variation and transformation without discontinuity[1]. The constituent molecules of such fluid are social actants[ii] bounded by the repulsion and attraction that

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[ii]Following Latour[2], we use the word actant to refer to social actors that could be either human or nonhuman.

determine their relationships – whether interactions or subscriptions[iii]. The structure of a social fluid can also be thought of as a constantly evolving network in which nodes correspond to actants, edges to their interactions, and following the reasoning from fluid dynamics[3], viscosity to the number of interactions that lock agents in place. In such a network the interactions are ontologically contingent on the actants whose identity and programs of action are, in turn, co-shaped by the number and kind of relationship they hold with their peers. Instead of being rigid, the structure of the network changes with the flux of meanings and actions eliciting a sort of viscosity that permeates the space of possible future actions, sparing no one. In former studies we defined such social viscosity as the resistance to action flow exerted by actors performing concurrent actions. It is thus the manifestation of mutual disturbances produced by the interactions that bind actors together[4].

Understanding global aspects of such complex systems requires going beyond the analysis of the properties of their constituent actants or their relationships in isolation, observing them both from within and from afar: social fluids are emergent. Summers-Affler's[5] suggests an empirical investigation based on systems theory (e.g.,[6]) to study how social action disperses and coalesces the flow of social life, generating temporary turbulent flows and vortexes of attraction. Social fluidity becomes manifest in the construction of identity from the individuals to the collective[7], the characterization of modernity as a tension between that which is fixed and the increasing presence of that which is fluid[8], the constant restructuring of social and spatial mobilities[9], and the prevalent continuity in the evolution of values and norms within societies and organizations[10]. In all of these, social perceptions of actants play a pivotal role: the combination of actant traits and their local circumstances determine how accurate their perception of social events is. We believe, motivated by these observations, that simple models of emergent social self-organization capable of capturing fundamental properties of social fluidity can be constructed[11].

Our approach here is simultaneously systemic and grounded in a phenomenological account of meaning across social life with a simple underlying principle: the consistency of shared social meaning has a direct impact in how social viscosity materializes and acts on social systems. For Schutz[12], the constitution of social meaning includes both the meaning attributed by the actor, deemed *subjective*, and the many others inferred by the observers, deemed *objective*. We are inclined to believe that turbulence and vortexes of attraction emerge, consolidate and collapse when the subjective and objective meanings of a critical mass of agents either converge or diverge in overt streams of action. Assuming that human actors are intrinsically driven to enact their programs of action, the fluidity of their action flow depends on their constant effort to reconcile

[iii]In our research vocabulary, relationships encompass both interactions and subscriptions. Interactions occur between agents of the same kind, whereas subscriptions occur between agents of different kinds. Both could be either directed or undirected. In the research presented herein we refer exclusively to interactions between humans.

their objective meanings derived from actions observed in other (third-party) actants, and the subjective meaning underlying their subsequent action. The higher the reconciliation effort –i.e. the need to reduce the impedance between strongly established, viscous internal truths and incoming conflicting information- the more turbulent the action flow.

We report here recent research efforts towards building and analyzing a simple model of emergent social organization where the effect of interactions, constrained by social norms and inner beliefs, is captured by a metric associated with social viscosity. We define *inverse viscosity* (IV) as the measurable difference that emerges when reconciling present internal beliefs with future perceptions of reality; this measure can be defined *locally* with respect to individual actants (LIV), or *globally* as an average (GIV). The social system chosen to test our approach is a self-organizing group acting under the premise of perceived proximity to one another. Our model is an adaptation of Shepard and Cooper's seminal color perception experiment originally intended to demonstrate the isomorphism between the similarity space of our internal representation of colors and the similarity space of the perception of the same colors[13]. Our sorting mechanisms do not require metric magnitudes: subjective representations of similarity or dissimilarity suffice to classify and arrange our world experiences.

The social norm used here is the actant's need to reduce color distance by comparing with other actants, and the inner belief is given by a tolerance value representing how comfortable an actant is to imperfect placement. All the entities of the social fluid act as mutual observers –non-human actors were excluded– that analyze the transformation of the system from one state to the next while their acting is supported or constrained by the forces of the network in which they partake. We study the social viscosity by modeling empirical observations and re-enacting them in an agent-based model and simulation (ABMS). The ABMS affords to assess agents trajectory and viscosity to further analyze convergences and reversions. We utilize principles and concepts from nucleation in phase transitions[14] to numerically characterize the outcomes of our experiments.

10.2 Social meaning and the analysis of proximity

Shepard and Cooper's empirical method asked a group of 37 participants with six types of vision conditions to judge similarities between stimuli in two situations: when those stimuli are actually present and when those stimuli are only named. The task involved arranging four decks of 36 cards by similarity, one at a time, each with two squares of distinct color pairs. Cards were split into colors-only and and names+color for present stimuli; and names-only, and braille-only for named stimuli. The resulting sorted sequences were used to compute matrices, each cell containing the similarity rank between pairs of colors, and averaged by combined condition. Researchers analyzed the data by computing correlations, and performing a series of hierarchical clusterings and non-metric multidimensional scalings (NMDS). We highlight two of their conclusions that apply to color vision subjects: i) there is a high positive correlation between the similarity of perceived and only-imagined colors, and ii) Newton's color wheel emerged for the NMDS analysis of color-normal subjects whether the colors were either perceived or only imagined.

Based on Shepard and Cooper findings, we designed a participatory simulation[15] to gain insights towards building an agent-based model of color proximity that assumes (a) that people are able to map their estimation of color proximity into spatial distances in the world, and (b) that they naturally share Newton's chromatic space. Thus, if we ask people to impersonate one unique color and attempt to position themselves near or far away from others with similar or dissimilar colors respectively, Newton's color wheel should emerge after some finite number of iterations. In organizing themselves, a fluid topology would emerge and we would be able to observe and analyze the trajectories of action, and assess the social viscosity of the system.

We ran the participatory simulation described above with 18 graphic design students. To validate if they instinctively carry the Newton's color space, they were asked to individually sort 20 color cards by similarity. The colors were a selection of distinctive hues from Munsell color chart (5RP, 10RP, 5R, 10R, 5YR, 10YR, 5Y, 10Y, 5GY, 10GY, 5G, 10G, 5GB, 10BG, 5B, 10B, 5PB, 10PB, 5P, 10P). The resulting color spaces were consistent with the visual spectrum of light grading from red to purple, with some exceptions exhibiting an inverted sequence. In terms of shape, some groups of participants formed a circle whereas others a line. This has relevant implications for the calculation of proximity since purple and red are perceptually closer to each other in a circular color space, and green is farthest from both of them. Conversely, purple and red are farthest in a linear space, and green sits at the middle of the spectrum. Then, students were assigned one unique color card from the sample of 20 distinct hues, asked to clip that card to the two –or one– adjacent, and move to a separate empty room. Once at the second room, each participant choose a random place and, on facilitator command, attempted to organize by perceived color similarity.

As expected, the participants converged to a final circular arrangement sorted in the same sequence as Newton's color wheel (Figure 10.1). Initially, participants wandered around displaying and comparing their color cards. Groups of two or three rapidly formed (Fig. 10.1, Left). After some internal validation, those who did not fell comfortable among their local neighbors quickly switched groups. Groups with high internal similarity persisted, whereas others dissolved. All groups held constant internal negotiation when sorting the direction of their color progression. At second 40, three groups prevailed: yellow-orange-reds,

Figure 10.1: Sequence of circular organization as participants assess their color proximity to one another. Left: formation of early groups. Center: Groups fan out to connect with others. Right: convergence on Newton's color wheel. Still images from a zenithal video recording at lab experiments

yellow-green-blues and blue-purples. Gradually, groups fan out forming semicircles facing the center of the room (Fig. 10.1, Center). The smaller groups connected to the larger ones rearranging themselves according to the dominant color sequence. Eventually, after 2:40 minutes the configuration stabilized in a closed circle where purple and red ends came together (Fig. 10.1, Right).

10.2.1 Meaning and viscosity in color agents

A careful look at the dynamics of the participatory simulation revealed a pattern of action flow that we synthesize in a perception-action cycle seeking to preserve the richness of interactions. Schutz's definition of social meaning served us to discretize the perception-action cycle in the following stages:

1. **Stage 1**: Participants chose their own set of interactants. They usually interact with up to five of the nearest participants in their visual perception field. This set can change in the next iteration if others are in proximity.

2. **Stage 2**: Participants perceive nearby colors and estimate the current distance to all their interactants. At that point the objective meaning of the current state of the system is inferred, e.g., if Blue stepped away from Purple, then Purple infers that Blue believes she is too close to him.

3. **Stage 3**: Participants internally translate their color proximity model into an expected distance and contrast it with the current distance to all its interactants. In doing so, each participant assembles the subjective meaning of her following action, e.g. Purple wants to move near to Blue to convey her proximity.

4. **Stage 4**: Participants enact their subjective meaning as they move themselves to a position that minimizes the difference between the expected and the current distance between all their interactants. At that point the system has transitioned into a new state and a new perception-action cycle starts.

Social *(local) inverse viscosity* (LIV) per participant at each instant is the discrepancy between their expected status of the world and the current, collectively enacted status. The perception-action cycle is therefore a constant reconciliation of objective and subjective meanings explicit in the winding course to stability. Correspondingly, *global inverse viscosity (GIV)* of the social fluid is then the average of all the individual viscosities. In this particular model the global inverse viscosity tends to convergence because all participants share a similar color mental model, yet it varies as interactions unfold. Stabilized groups share areas of lower inverse-viscosity fluid spatiality, whereas disintegrating groups sort their trajectories in turbulent spots.

10.3 An agent-based model of color proximity

Based on the perception-action cycle derived from observations of the participatory simulations, we developed an ABMS[iv] in a custom made multi-agent programmable modeling environment purposefully built to run on modern browsers. The tool is entirely programmed in JavaScript using primarily P5.js[v] and Chroma.js[vi] libraries.

In the ABMS, the objective and subjective meanings inferred from social action become explicit. That is something possible in actual experiments only by asking participants to verbalize their thinking on the fly. The model carries many details from the observations from the participatory simulation to preserve the validity of the perception-action model as much as possible. We expect that the conclusions derived from this simulation to cast a new light on social interaction research.

We present here a brief account of the interaction process. In the appendix we offer a detailed description of the model following the *Overview, Design concepts, Details* (ODD) protocol.

The model proceeds in discrete time instants (ticks) spaced at 100 milliseconds each. During every tick agents store their current position in a trajectory collection, and filter out the set of agents with whom to interact according to the experimenter's interaction rule choice. If there are no interactants in the collection the interaction is terminated; else, they estimate the magnitude and direction of next step by adding all the anticipated vectors towards each interactant. If the length of the estimated step is greater than the agent's tolerance threshold, they adopt the step's heading and execute the step. Else the step is ignored and the interaction terminated. When all the agents ignore the step, the group has converged in a stable phase.

[iv]The multi-agent programmable modeling environment is available at `www.smartartifact.com/ColorAgents` and the source code is available at `https://github.com/SocialViscosityLab/ColorAgents`.

[v]See: `https://p5js.org`

[vi]See: `https://vis4.net/chromajs`

10.4 Case study: nucleation in circular color scales

10.4.1 Methods

We performed two experiments using our agent-based model of color proximity. To interpret model outcomes, we resorted to convergence and reversions as primary observables, both responsive to model parameters. *Convergence* characterizes the time required for a group of agents to reach a stable color scale. *Reversions* quantify the number of discrete instants when social inverse viscosity increases. Convergence relates microscale descriptions (i.e. actants) to macroscale property (i.e. structure or function), while reversions represent microscale fluctuations.

We found phase nucleation[16] to effectively describe the process of self-organization in our model. In a nutshell, nucleation is the progressive time-dependent organization of microscale entities into distinguishable stable macro-structures, known as phases. The seminal observations made by Avrami[14] suggest that the appearance of growth nuclei constitute an effective; model for phase formation. Growth nuclei are initial small remnants from a prior phases whose stability under those conditions was granted in virtue of their size. They may even appear due to fluctuations or topological defects in the prior system state. When conditions in the context change favorably, growth nuclei trigger the formation of larger aggregates whose stability, under fixed and somewhat homogeneous conditions, depends proportionally on the number of coalesced nuclei. This behavior is well known experimentally, and bears relation to how self-organization into large-scale structures maximizes entropy production and propagation[17].

Convergence is imperfect in individual nucleation experiments due to process fluctuations, yet convergence smoothens at the thermodynamic limit in ensemble experiments. We note that in our model as prescribed by statistical mechanics[18], the self-organization of agents into a color wheel is collectively a stochastic process even when agents make deterministic, local decisions. The latter becomes even more so when the unit of analysis is the *ensemble of runs* rather than individual ones. In the color proximity model, nucleation represents convergence to a correctly ordered color scale as determined by color distance. To quantitatively capture convergence as phase nucleation, we used an alternative form of the Johnson-Mehl-Avrami-Kolmogorov equation[14] that is used to estimate the volume fraction of microstates that have nucleated; our equation captures the decreasing volume fraction $X(t)$ of microstates that have yet to nucleate at time t, subject to the effects of increasing social viscosity as a stable color scale arises:

$$X(t) = \exp\{-kt^n\} \tag{10.1}$$

k may be interpreted as a rate of convergence and n is associated with the dimensionality of the space where distance are measured.

Our analysis process proceeded as follows. All experiments use a chordal proximity model. For each experiment, a fixed value was established per parameter set, and $K = 5$ repetitions per parameter set were performed. Only GIV and reversions per repetition were considered as dependent variables. We recorded the initial and final GIV after 450 discrete time steps. Values for k and n were estimated by curve fitting through optimization using SciPy[19] (version 1.3.0, Python 3.6) after GIV curves had been normalized against the maximum GIV value observed during each simulation. Finally, average values for k, n and the number of reversions were computed and used in each experiment class to perform MANOVA and ANOVA tests, respectively. ANOVA tests were performed using Python's `statsmodel` library[20], and MANOVA tests were performed using R[21]. Our analysis is fully reproducible[vii].

10.4.2 All-to-all interactions

All-to-all simulations have tolerance τ to imperfect proximity as the principal parameter. Initial and final GIV values correspond to their maximum and minimum ones respectively. All runs converged to a single color scale (R < 2.00). Table 10.1 contains relevant descriptive statistics for the experiment.

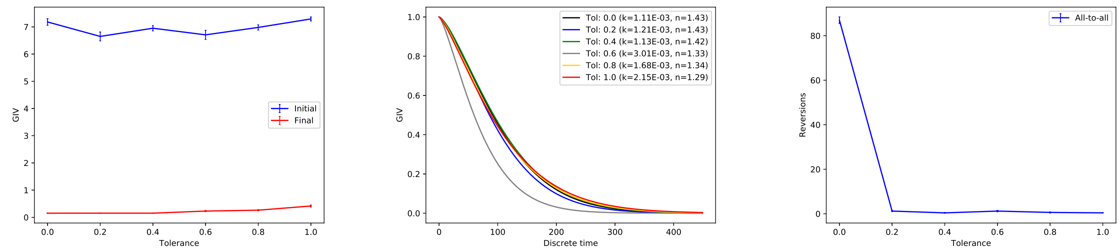
τ	IV	FV	k	n	R
0.0	7.18 (0.72)	0.15 (0.00)	1.11×10^{-3} (4.31×10^{-4})	1.43 (0.06)	87.00 (8.63)
0.2	6.65 (0.97)	0.15 (0.00)	1.21×10^{-3} (6.28×10^{-4})	1.43 (0.08)	1.20 (1.30)
0.4	6.95 (0.57)	0.15 (0.01)	1.13×10^{-3} (2.06×10^{-4})	1.42 (0.03)	0.40 (0.89)
0.6	6.71 (1.00)	0.23 (0.13)	3.01×10^{-3} (4.29×10^{-3})	1.33 (0.19)	1.20 (1.79)
0.8	6.98 (0.57)	0.26 (0.13)	1.68×10^{-3} (6.22×10^{-4})	1.34 (0.06)	0.60 (1.34)
1.0	7.29 (0.44)	0.42 (0.20)	2.14×10^{-3} (1.06×10^{-3})	1.29 (0.11)	0.40 (0.55)

Table 10.1: Descriptive statistics for color proximity convergence experiment with all-to-all interactions. Mean and standard deviation values (in parenthesis) are provided for $K = 5$ samples and $t \in [0, 450]$. Nomenclature: **IV**: initial GIV, **FV**: final GIV, **R**: reversion count.

Next, curves were computed for each value of τ and visualized (Figure 10.2). While initial GIV appears to depend only on the initial number of agents and their random placement, final GIV increases with tolerance values (Fig. 10.2.a). While most curve fittings yield similar parametrizations, convergence is faster with $\tau = 0.6$ (Fig. 10.2.b). In general, τ appears to play a very significant role in reversions (Fig. 10.2.c): relaxing distance restrictions drastically decreases the number of reversions required for convergence. We also note that reversions increased significantly at $\tau = 0.6$ compared to at $\tau = 0.4$ and at $\tau = 0.8$, suggesting that an analogue to annealing takes place.

We performed a one-way ANOVA in order to determine whether τ induced a significant difference on reversions (Table 10.2) using ordinary least-squares regression (adjusted $R^2 = 0.987$). The analysis indicated

[vii] GitHub repository: `https://github.com/snunezcr/social-viscosity-analysis`.



(a) Initial (blue) and final (red) GIV values for all-to-all circular nucleation.

(b) Time-dependent scale nucleation trends per value of τ (colored lines).

(c) Average reversions in all-to-all scale nucleation.

Figure 10.2: Outcomes of simulation experiments with circular color proximity model (All).

conclusively that τ explains differences in reversions. We also performed a Tuckey HSD test (FWER=0.05) and found that differences were maximized between $\tau = 0.0$ and all other values (adjusted $p < 0.001$), while no significant differences were found between all other possible pairs (adjusted $p < 0.9$).

	SS	**df**	**F**	***p***
τ	30992.27	5.0	451.89	6.49×10^{-23}
Residual	329.20	24.0	–	–

Table 10.2: One-way ANOVA for reversions as a function of τ (adjusted $R^2 = 0.987$).

Finally, a MANOVA was performed in order to understand the simultaneous effect of τ over k and n (Table 10.3). Results indicate that τ explains differences in curve parametrization observed in Fig. 10.2.b. However, the effect over k and n differ per factor (Table 10.4). Only n appears to be significantly impacted by τ. One possible interpretation is that each value of τ yields a different model of distance, thereby altering (possibly in non-linear fashion) the metric space in which agents attempt to optimize their positions.

	df	**Pillai**	**approx F**	**num df**	**den df**	***p***
τ (all factors)	1	0.37	7.93	2	27	1.95×10^{-3}
Residuals	28	–	–	–	–	–

Table 10.3: Total MANOVA results for all-to-all interaction experiments.

10.4.3 N nearest-neighbor interactions

We performed a two-factor experiment using the N nearest-neighbor interactions model. Each agent coordinates with its N most proximal agents to gauge its distance. For each value of N, the full range of τ was explored, except for $N = 0$ since no convergence is possible. Results reveal various significant differences with respect to an all-to-all interaction model (Table 10.5). No longer initial and final GIV correspond

	df	SS	MS	F	p
τ (k)	1	5.09×10^{-6}	5.09×10^{-6}	1.57	0.22
Residuals	28	9.10×10^{-5}	3.25×10^{-6}	–	–
τ (n)	1	7.34×10^{-2}	7.34×10^{-2}	7.75	9.52×10^{-3}
Residuals	28	0.27	9.47×10^{-3}	–	–

Table 10.4: Per-factor response for MANOVA on all-to-all interaction experiments.

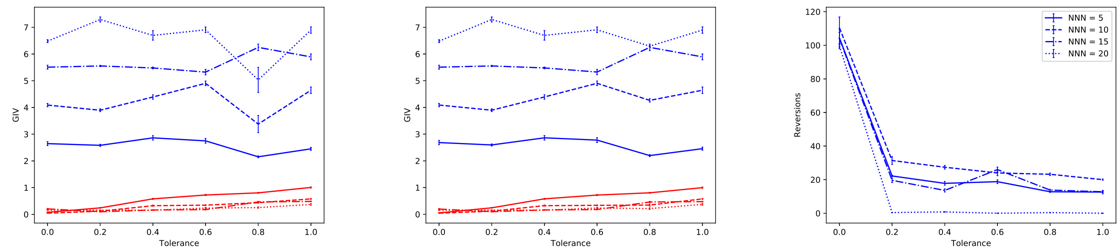
to the maximum and minimum GIV respectively for all cases (Fig. 10.3.a versus Fig. 10.3.b); a small N induced observed differences. No longer can convergence be guaranteed ($R > 2.0$) except for $N = 20$, similar to the all-to-all interactions model (Fig. 10.3.c). Restricting the number of possible interactions in actants creates a tension between the local and global convergence: the smaller the world, view, the easier it becomes for actants to reach a local minimum and partially converge while experiencing slow (or no) global convergence[22].

N	τ	IV	FV	MV	mV	k	n	R
5	0.0	2.65 (0.44)	0.08 (0.07)	2.68 (0.48)	0.05 (0.03)	8.64×10^{-3} (8.64×10^{-3})	1.04 (0.17)	104.40 (32.81)
	0.2	2.58 (0.23)	0.24 (0.08)	2.60 (0.23)	0.24 (0.08)	1.28×10^{-2} (1.28×10^{-2})	0.97 (0.16)	22.20 (2.28)
	0.4	2.86 (0.50)	0.58 (0.12)	2.86 (0.50)	0.58 (0.12)	5.48×10^{-2} (5.48×10^{-2})	0.65 (0.18)	17.80 (6.57)
	0.6	2.75 (0.52)	0.72 (0.13)	2.78 (0.55)	0.72 (0.12)	4.85×10^{-2} (4.85×10^{-2})	0.59 (0.09)	18.80 (6.61)
	0.8	2.15 (0.20)	0.80 (0.10)	2.20 (0.21)	0.80 (0.10)	9.93×10^{-2} (9.93×10^{-2})	0.42 (0.05)	12.80 (2.17)
	1.0	2.45 (0.33)	1.01 (0.14)	2.46 (0.33)	1.00 (0.14)	2.42×10^{-2} (2.42×10^{-2})	-9.47 (9.26)	12.60 (6.07)
10	0.0	4.09 (0.37)	0.04 (0.02)	4.09 (0.37)	0.04 (0.02)	3.50×10^{-3} (3.50×10^{-3})	1.24 (0.11)	110.40 (38.59)
	0.2	3.90 (0.32)	0.12 (0.06)	3.90 (0.32)	0.12 (0.06)	4.93×10^{-3} (4.93×10^{-3})	1.13 (0.02)	31.40 (13.72)
	0.4	4.39 (0.50)	0.32 (0.12)	4.39 (0.50)	0.32 (0.12)	7.18×10^{-3} (7.18×10^{-3})	1.08 (0.16)	27.40 (6.31)
	0.6	4.90 (0.50)	0.34 (0.08)	4.90 (0.50)	0.33 (0.08)	4.81×10^{-3} (4.81×10^{-3})	1.15 (0.11)	24.00 (9.80)
	0.8	3.38 (1.93)	0.44 (0.11)	4.26 (0.38)	0.34 (0.22)	7.80×10^{-3} (7.80×10^{-3})	1.01 (0.10)	23.20 (4.15)
	1.0	4.64 (0.72)	0.58 (0.09)	4.64 (0.72)	0.58 (0.09)	1.62×10^{-2} (1.62×10^{-2})	0.88 (0.17)	20.00 (2.00)
15	0.0	5.51 (0.43)	0.20 (0.12)	5.51 (0.43)	0.20 (0.11)	3.01×10^{-3} (3.01×10^{-3})	1.25 (0.08)	104.00 (21.49)
	0.2	5.55 (0.14)	0.10 (0.00)	5.55 (0.14)	0.10 (0.00)	2.15×10^{-3} (2.15×10^{-3})	1.33 (0.11)	19.60 (7.83)
	0.4	5.48 (0.19)	0.16 (0.05)	5.48 (0.19)	0.16 (0.05)	2.07×10^{-3} (2.07×10^{-3})	1.33 (0.07)	13.60 (5.46)
	0.6	5.32 (0.60)	0.18 (0.03)	5.33 (0.60)	0.18 (0.03)	4.32×10^{-3} (4.32×10^{-3})	1.17 (0.10)	26.00 (8.69)
	0.8	6.25 (0.72)	0.46 (0.14)	6.25 (0.72)	0.46 (0.14)	3.31×10^{-3} (3.31×10^{-3})	1.19 (0.08)	13.80 (2.86)
	1.0	5.89 (0.65)	0.48 (0.07)	5.89 (0.65)	0.47 (0.07)	6.30×10^{-3} (6.30×10^{-3})	1.08 (0.09)	12.80 (2.77)
20	0.0	6.48 (0.33)	0.16 (0.00)	6.48 (0.33)	0.15 (0.00)	1.32×10^{-3} (1.32×10^{-3})	1.40 (0.07)	99.60 (9.66)
	0.2	7.29 (0.56)	0.16 (0.00)	7.29 (0.56)	0.16 (0.00)	1.10×10^{-3} (1.10×10^{-3})	1.42 (0.05)	0.40 (0.55)
	0.4	6.70 (1.07)	0.15 (0.01)	6.70 (1.07)	0.15 (0.01)	1.22×10^{-3} (1.22×10^{-3})	1.41 (0.05)	0.80 (0.84)
	0.6	6.91 (0.62)	0.23 (0.15)	6.91 (0.62)	0.23 (0.15)	1.42×10^{-3} (1.42×10^{-3})	1.37 (0.05)	0.00 (0.00)
	0.8	5.03 (2.82)	0.25 (0.14)	6.29 (0.11)	0.21 (0.18)	2.12×10^{-3} (2.12×10^{-3})	1.31 (0.10)	0.40 (0.55)
	1.0	6.90 (0.72)	0.37 (0.18)	6.90 (0.72)	0.37 (0.18)	2.89×10^{-3} (2.89×10^{-3})	1.26 (0.15)	0.00 (0.00)

Table 10.5: Descriptive statistics for color proximity convergence experiment with N nearest-neighbor interactions. Mean and standard deviation values (in parenthesis) are provided for $K = 5$ samples and $t \in [0, 450]$. Nomenclature: **IV**: initial GIV, **FV**: final GIV, **MV**: maximum GIV, **mV**: minimum GIV, **R**: reversion count.

Moreover, N appears to drastically parameterize the geometry of the metric space specified by n. Convergence to partial or complete nucleation depends on having sufficient neighbors, at least 50% of the total number of actants in our analysis (Figs. 10.4.b-d). As N decreases, curves spread wider along τ values (Fig. 10.4.b) due to relaxation of constrains experienced when computing distances. We observed an extreme case at $N = 5$ and $\tau = 1.0$ (Fig. 10.4.a, red line): actants only perform a few minimization steps before becoming fixed at the local minimum that takes least effort to reach.

We performed a two-way ANOVA in order to determine whether N and τ induced significant differences

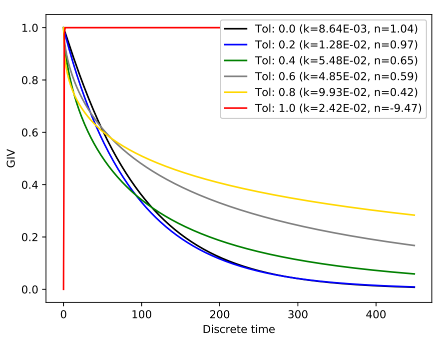


(a) Initial (blue) and final (red) GIV.

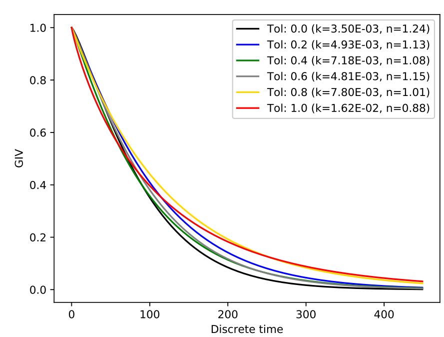
(b) Maximum (blue) and minimum (red) GIV.

(c) Average reversions in N nearest-neighbor circular nucleation.

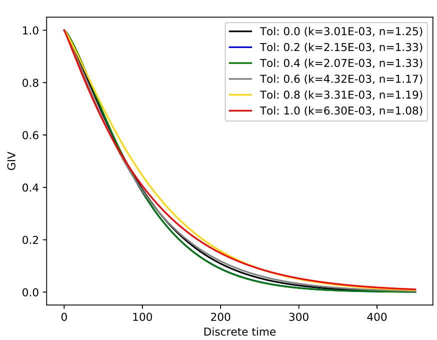
Figure 10.3: Outcomes of simulation experiments with circular color proximity model. Line styles in (c) apply to (a) and (b).



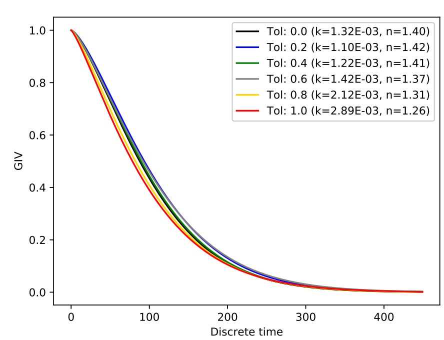
(a) Curves for $N = 5$.



(b) Curves for $N = 10$.



(c) Curves for $N = 15$.



(d) Curves for $N = 20$.

Figure 10.4: Time-dependent scale nucleation trends per τ value (colored lines) and N nearest neighbors.

on reversions (Table 10.2) using ordinary least-squares regression. After comparing the fitting of models with (adjusted $R^2 = 0.882$) and without interactions (adjusted $R^2 = 0.876$), our analysis chose the former one. Intuitively, we hypothesized that τ would couple with the number of nearest neighbors to impact reversions, similar to how reversions lead progressively toward lower local minima as in annealing. Significant differences were found ($\mathrm{F} = 39.71$, $p = 3.95 \times 10^{-39}$), τ being the most significant factor followed by N; however, their interaction failed to be significant over the complete dataset except for the $N = 5$ subset. We performed two Tuckey HSD tests (FWER=0.05), one for N and one for τ. Significant differences were found between $\tau = 0.0$ and all other τ values (adjusted $p < 0.001$) while other differences between pairs were not significant (adjusted $p < 0.6$). Relaxing FWER to 0.1 produced a significant difference between $N = 10$ and $N = 20$. This outcome may result from the drastic geometry shifts produced by $N = 5$ and $\tau = 1.0$. A restricted two-way ANOVA without $N = 5$ only marginally improved model fitting (adjusted $R^2 = 0.896$) without yielding changes in either Tuckey HSD tests. A two-way ANOVA without $\tau = 1.0$ produces a slightly worse fit (adjusted $R^2 = 0.876$), and the significant difference between $N = 10$ and $N = 20$ at FWER $= 0.1$ disappears.

	SS	**df**	**F**	$\boldsymbol{p}$
N	7963.67	3.0	16.84	7.26×10^{-09}
τ	134874.57	5.0	171.08	3.42×10^{-46}
τ:N	1162.03	15.0	0.49	0.94
Residual	15136.40	96.0	–	–

Table 10.6: Two-way ANOVA for reversions as a function of τ and number of nearest neighbors. Adjusted $R^2 = 0.882$.

As with the all-to-all model, we performed a MANOVA using N and τ over k and n (Table 10.7). τ, N and their interaction explain differences in curve parametrization observed in Fig. 10.4.a-d. As in the prior experiment, the effect over k and n differ per factor (Table 10.8).We hypothesized that both curve parameters should be impacted by both τ and N, since convergence depends on how τ and N configure the possibilities of each actant; we expected this to be particularly so when the number of nearest neighbors is small. In order of significance, our analysis indicates that τ, its interaction with N ($\tau * N$) and finally N by itself are significant in explaining observed curve differences. We then proceeded to analyze per-factor responses (Table 10.8). Differences in k are explained mostly by variations in N followed by τ and $\tau * N$, consistent with the fact that the horizon of differences between perceptions and observations in an actant scales with the number of neighbors: having few of them imposes severe restrictions for nucleation of the color scale. n presented an interesting case: the most relevant factor is $\tau * N$, suggesting that the coupling between τ and N yields a significantly different geometry for the metric space of distances in color space; N and τ follow afterwards.

	df	Pillai	approx F	num df	den df	p
N (all factors)	1	0.47	50.71	2	115	2.20×10^{-16}
Tolerance (all factors)	1	0.21	15.18	2	115	1.41×10^{-6}
N:Tolerance (all factors)	1	0.26	19.74	2	15	4.26×10^{-8}
Residuals	116	–	–	–	–	–

Table 10.7: Total MANOVA results for N nearest-neighbor interaction experiments.

	df	SS	MS	F	p
N (k)	1	0.02	0.02	51.85	6.44×10^{-11}
τ (k)	1	0.00	0.0	7.70	6.45×10^{-3}
N:τ (k)	1	0.00	0.00	8.29	4.76×10^{-3}
Residuals	116	0.05	0.00	–	–
N (n)	1	76.39	76.39	13.44	3.73×10^{-4}
τ (n)	1	61.75	61.75	10.86	1.30×10^{-3}
N:τ (n)	1	91.62	91.62	16.12	1.06×10^{-4}
Residuals	116	–	–	–	–

Table 10.8: Per-factor response for MANOVA on N nearest-neighbor interaction experiments.

10.5 Discussion

In our simulations, convergence and reversions model two classes of socially accessible evidence in the color proximity experiment: observables that describe the degree of success of perception-dependent social coordination[23], and observables that describe fluctuations (or rather imperfections) in the process conducing to one or many unexpected externalities[24]. Both classes of observables were successfully captured by a seemingly unrelated phenomenon, that of nucleation in phase transition theory, one with an apparently striking ability to synthesize the core elements of social coordination and its various degrees of success. However, the connection between coordinated perceptions of color and phase nucleation lies deep in their mutual relation to thermodynamic systems[25] and fluids[26], both known for their encompassing descriptive universality. Our research exemplifies how the analysis of social situations where coordinated perception occurs can provide new conceptual and theoretical insights backed by existing mathematical physics principles.

When the accessible number of neighbors at any moment is unconstrained, the combination of tolerance to imperfect arrangements and reversions led to an unexpected benefit: convergence occurs more rapidly when actants were less sensitive to imperfect arrangements while remaining sufficiently exposed to novelty (e.g. convergence of partially sorted scales). Essentially, we confirmed the intuition that efficient coordination requires some degree of tolerance to approximation. When coordination is too strict, the rate of social convergence may not improve. If we conceptualize coordination as an outcome of self-regulation, and if a cost metric per coordination step is added to actants, strictness may produce high-maintenance interactions that can even impair convergence itself[27]. In most occasions and complex social systems, reaching an approximate equilibrium in finite time has much higher social value than achieving perfect coordination[28]. Our simulation suggests that extensions to the model can be made to include cost, and thus to attempt to simulate and gain insights into their dynamics and structure. We anticipate these types of simulation to have future impact in the emergent development of social recommender systems[29], including those for smart cities and urban traffic interventions where dealing more efficiently with uncertainty is critical.

A striking fact uncovered by our simulation is the effect of absolute tolerance to any imperfect arrangement ($\tau = 1.0$) when coupled with the density of social interactions. Only when the number of neighbors was sufficiently small did actants proved resilient to convergence. We believe our observations and analyses provide a formal correlate for the concept of social indifference: in the same fashion in which nucleation in entities with small coordination numbers is unlikely at high temperatures (i.e. agitated states of motion), indifference drives the structure of social arrangements –in our case, the final constitution of the social scale- towards those in which coordination remains always possible, and thus the structure is permanently open to change[30]. Reinterpreted within the framework of causal entropic forces[31], actants collectively maximize their of future freedom of action, represented by the number of possible worlds to which it is possible to converge in the future. *This is still convergence, but of a rather counter-intuitive type.* In hindsight, our experiment appears to satisfy the common intuition that indifference leads to inaction. Understanding this intuition at a deeper level in connection with theories of mind for agents with some form of rationality[32], however, remains an open question. For the moment, we speculate that social convergence towards desirable behaviors may be fostered by interventions that seek to increase the number of inter-personal connections despite prior indifference in actants. In these scenarios, we wish to find values of N that suffice to move k and particularly n from landscapes of inaction to some coordination, even in the midst of indifference.

Reversions provide a powerful window into the mechanics of social turbulence. Turbulence arises when two media with the right viscosity differences meet[33]. In social coordination, this translates to the encounter of smaller, semi stable scales and their later merging and reconfiguration. Reversions quantify the number of *belief updates* among actants: since actants are memory-less, their only mechanism to decrease local distances (i.e. improve global convergence) is to change places to attempt gaining higher social viscosity. We are then justified in viewing selective spatial translations as a type of language used by agents to minimize the uncertainty of future interactions[34]. Only then, we may reify social turbulence as those configurations in space and time in which new interactions between groups increase uncertainty for them when those groups had prior lowered it their internally. Reversions constitute an imprint of uncertainty reduction in social systems.

Finally, our research suggests that, at least for social systems that can be abstracted as some form of nucleation through phase transition theory, the description of convergence through parameters that determine distances is equivalent to the notion of a social architecture, albeit simple in our case. We use architecture in a generalized manner to refer to the systems of constraints and opportunities in spaces of interaction that drive the functioning of societies and groups. Constraints manifest as patterns of coordination, which together form a vocabulary of interaction[35] capable of allowing us to reason about consequences derived from spatial restrictions. Opportunities arise as actants use their internal machinery to accomplish goals, and in some cases, to learn about the world; all forms of learning presuppose some basic, communicable conceptual scaffolding capable of maximizing advantageous moves and minimizing either fruitless or risky[36] paths. Our simulation also has led us to explore space as machinery[37]: without memory, measuring distances in color space is the primary tool involved in self-organization of the actants. Moreover, the higher the number of interactions the faster the convergence to a stable organization at the cost of a higher social viscosity. Broader social implications of this final point deserve further investigation.

10.6 Conclusions and further work

In this study, we have demonstrated how a simple agent-based model of self-organization based on color proximity is able to capture some fundamental aspects of how social structures converge in the presence of social norms and individual beliefs. While our results are encouraging, we have just begun to understand the implications of our model and experiments in the larger context of social viscosity, fluidity and turbulence. We have identified two central lines of future work, one around abstract fundamental issues and the other around concrete methodological needs.

At the fundamental level, our intention seeks to deepen the application of statistical physics principles to social situations and permeate the metaphors as far as possible. We wish to explore partial convergence (i.e. phases), the consequences of multiple actants with the same assigned color and the role of small groups in the overall convergence process towards single scales. Landau theory[38,39] constitutes a promising research direction in this sense. To further investigate this, new types of interactions (including stochastic ones, and mediated by non-humans) become desirable as a means to simulate imperfections in the machinery of an actant and study cyber-physical systems more realistically.

We wish to extend the number and classes of systems for which convergence remains a meaningful descriptor and understand in which social systems our approach is limited. One particular point pertains to verifying and validating the model presented here. While the results of Shepard and Cooper's model are well known, further validation of this process may be achieved by running ensembles of experiments with human participants where an additional adaptive color key tool is provided to simulate tolerance to imperfect color matching. The tool consists of a complete color wheel masked by a cover wheel concealing all colors but those in a specific segment, and a notch that participants can use to center on their own color within the exposed color range. If the peer's color belongs to the unmasked section, then the participant is instructed to be indifferent to that peer. Clearly, the length of the unmasked segment is proportional to the tolerance factor we have described, and several such tools can be constructed and distributed to all participants per tolerance level. Outcomes of these experiments would then be contrasted against simulated data in a similar fashion as performed in this study.

We also note that the uniformity imposed by having a single color palette across actants is perhaps the most prominent source of convergence. Action meaning is constructed and interpreted from a standard for the whole population. Mixing agents whose color models are the traditional additive or subtractive with agents bearing alternative color perception models rooted in non-western cultures[40], would help elucidate the challenges of proximity based intercultural interaction. The sensibility function in the model used to estimate color proximity is linear, but it could be fine-tuned to respond accurately to our mechanisms of similarity assessment, inspired by Stevens' psycho-physical power law[41] that explains various ways in which the strength of the stimulus maps to the magnitude of the sensation aroused. In the same vein, multidimensional perception mechanisms could better account for actual social behaviors such as our tendency to favor kinship and familiarity. Learning functions would allow exploring clean slate convergence scenarios (e.g.[42,43]).

Methodologically, we have various immediate and long term goals. Additional parametrizations in our model need to be explored, including the use of radial distance functions and field of view as well as linear and exponential distance functions. To this end, we plan to improve our statistics by increasing the number of repetitions ($K \geq 25$). Long-term, we wish to extend our experimental platform in three ways. First, we plan to include the ability to perform parametric sweeps. Second, we seek to abstract the existing code to facilitate expressing other models of self-organization with similar features. Finally, we plan to gather the specification of the color scale convergence model as case study for ongoing research aimed at constructing a Generalized Theory of Interactions (GToI).

10.7 Description of the Agent-based model of color proximity

Purpose

The purpose of the model is to replicate the dynamics observed in the participatory simulation of the self-organizing group of people arranging themselves by perceived color proximity. In particular we want to measure and study the evolution of social viscosity when agents share the same color mental model.

State variables and scales

Agents represent normal vision people and are characterized by the following state variables:

- ID: a unique identifier for this agent,
- Position: a vector with spatial coordinates,
- Color value: the unique color value 'impersonated' by this agent. By default the model uses the HSB color space.
- Tolerance: an scalar threshold between 0 and 1 to determine whether or not to move to a new self estimated position.
- Color mental model: an ordered collection of colors particular to each agent in the world.
- Spatial mental model: a mechanism to convert values from other mental models into spatial distances. For example, it serves to map the perceived proximity between two colors into a spatial proximity. See Submodels section for details.
- Visual perception angle: the scope of visual perception of each agent. It opens towards the direction agent is heading. By default it is set to $\pi * 3/4$.
- Shortest: a scalar used by the spatial mental model to determine how near the agent wants to be from the most similar agent.
- Farthest: a scalar used by spatial mental model to determine how far away the agent was to be from the most dissimilar agent.

The topology of the space where agents move is continuous, unbounded and unwrapped. Both the temporal and spatial resolution of the model is arbitrary.

Process overview and scheduling

The model proceeds in tick intervals of 100 milliseconds. At each tick agents store their current position in a trajectory collection, and filter out the set of agents with whom to interact according to experimenter's rule. If there are no interactants in the set, the agents set a boolean variable to 'done' and the interaction is terminated; else, they estimate the magnitude and direction of next step by adding all the anticipated vectors towards each interactant. See section Submodels for details on how the step is calculated.

If the estimated step is greater than the agent's tolerance threshold, they set the new bearing, set themselves to 'not-done', and execute the step. If the step magnitude falls below the tolerance threshold they ignore the move, set themselves to 'done' and terminate the current interaction. The boolean variable done/not-done is used to highlight who is inactive in the visualization.

Design concepts

Emergence: groups emerge from agents with proximal colors. Depending on the initialization settings groups may progressively merge together into a single one with circular shape.

Sensing: Agents perceive both the colors of their neighbors and the spatial distance to all of them. They have functions to estimate color proximity, distance proximity and translate color proximity into distance proximity. See Submodels section for details.

Observation For every tick the data collected for analysis from each agent are its spatial position, and a matrix of their interactions with a detailed description of each interactant. See Submodels section for the details of how social viscosity is computed from each matrix.

Initialization

The experimenter selects four parameters before running the model. First, the color palette from the Color Factory. That defines not only the color palette to be used by agent's color mental model but the size of the agent population. There are as many agents as color in the color palette. Second, the Interaction Rule sets the mechanism used by agents to choose their interactants. Third, a Sensibility function that defines how agents estimate their color proximity to each of their interactants. Fourth, the Tolerance for all agents.

In this research we used the following parameters: *Color palette*: Munsell color space with 20 colors (5RP, 10RP, 5R, 10R, 5YR, 10YR, 5Y, 10Y, 5GY, 10GY, 5G, 10G, 5GB, 10BG, 5B, 10B, 5PB, 10PB, 5P, 10P) converted into HSB values using the library Chroma.js[viii]. *Interaction Rule* either All-to-all and N-nearest. *Sensibility*: Chordal distance. *Tolerance*: six values (0, 0.2, 0.4, 0.6, 0.8, 1.0).

[viii] `https://vis4.net/chromajs/`

Submodels

Perceived color proximity: returns a value between 0 and 1, where 1 is the farthest perceived distance. The function needs the target and reference color. In the case of *chordal distance* sensibility function, the proximity is estimated by $P = |i - j| * (2\pi/N)$, where i and j are the indexes of each colors in the default color palette, and N is the number of colors in the palette. To normalize the output, if P is grater than π then $P = (2\pi - P)/\pi$, else $P = P/\pi$.

Spatial mental model: a mechanism to map values from other mental models into spatial distances. The distance is estimated by $D = s + (f - s) * v$, where s and f are the agent's shortest and farthest parameters and v is the value within the range between 0 to 1 to be mapped.

Step calculation: An agent's step is the result of the sum of all the corrected spatial vectors to its interactants. More formally, $\sum_{i=1}^{n} \vec{v}_i * \Delta_i$, where $\vec{v}_i$ is the unit spatial vector to interactant i, and Δ_i is the difference between the current euclidean distance to i and the expected distance to i. The expected distance is estimated using the Spatial mental model.

Local Inverse viscosity (LIV): is estimated at each simulation tick by $\sum_{n=1}^{i} |(c_t - e_t)|/e_t$, where c_t is the current distance between agents at tick t and e_t is the forecast distance between the same agents estimated with the information available at tick t. The result is then normalized by the total number of interactants i at tick t.

Global inverse viscosity (GIV): is the average of the social viscosity sv of all agents i at time t, expressed also as $\sum_{n=1}^{i} sv_t/i$.

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We have no conflict of interest to declare.

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Chapter 11

The Epidemiology Workbench: a Tool for Communities to Strategize in Response to COVID-19 and other Infectious Diseases

Summary[i]

COVID-19 poses a dramatic challenge to health, community life, and the economy of communities across the world. While the properties of the virus are similar from place to place, the impact has been dramatically different from place to place, due to such factors as population density, mobility, age distribution, etc. Thus, optimum testing and social distancing strategies may also be different from place to place. The Epidemiology Workbench provides access to an agent-based model in which demographic, geographic, and public health information of a community together with a social distancing and testing strategy may be input, and a range of possible outcomes computed, to inform local authorities on coping strategies. The model is adaptable to other infectious diseases, and to other strains of coronavirus. The tool is illustrated by scenarios for the cities of Urbana and Champaign, Illinois, the home of the University of Illinois at Urbana-Champaign. Our calculations suggest that massive testing along with some form of shelter-at-home during the weeks of mass ingress is the most effective strategy to combat the likely increase in local cases due to mass ingress of a student population carrying a higher viral load than that currently present in the community.

11.1 Introduction

Mathematical models of infectious disease epidemiological dynamics provide valuable assistance to public health officials and health care providers in assessing the likely seriousness of an epidemic or its potential to grow into a pandemic, and later in allocating resources to counter the spread of the disease[1]. Simulations that

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trace either prior or projected time courses make use of various mathematical and computational techniques, including (non-exhaustively) differential equation models, statistical regression and curve fitting, network propagation dynamics, and direct representation of human actors and their actions by means of agent-based models. The SIR model in particular along with its various adaptations[2] has remained successful, at least in part, due to its universality as evidenced by its empirical adequacy across multiple epidemics, and by its formal robustness when connecting microscale host-pathogen related events and macroscale disease observables[3,4].

Stochastic versions of the SIR model show that adding noise to the system changes the predicted onset of an epidemic[5], the stability of its endemic equilibrium[6], the value of its effective reproductive number[7] or its duration[8] when contrasted against the deterministic one. This is significant not only at the theoretical level when studying the stability and asymptotic representativeness of deterministic vs stochastic SIR models under various noise regimes, but at the policy making level where computational epidemiology may form the basis of informed decisions under policy, budgetary and other types of constraints[9].

Moreover, the SIR has been extended spatially to account for the diffusion-like properties associated with geographic patterns observed during epidemics. While the qualitative (and some quantitative) properties of the traditional and the spatial SIR models remain largely shared, spatial versions appear to be numerically susceptible to how these capture spatial interactions[10]. As with any other diffusion process in some space, we are usually interested on the ability of a disease to cover larger shares of the population as time marches on. Detailed analysis of deterministic and stochastic SIR models with spatial components[11] indicates the existence of solutions corresponding to *traveling waves* that propagate the disease among point-like processes. It has also been shown that spatial SIR models can account for the effects of long-distance travel by replacing diffusion operators containing local processes with appropriate integro-differential ones that capture non-local dispersal processes[12].

Agent-based models (ABMs) constitute a family of models where sets of active entities (i.e. agents) interact collectively by following prescribed individual rules intended to portray the emergent dynamics of a real social system[13]. In computational epidemiology, ABMs have been used and comparatively evaluated against SIR models of various kinds. Analysis of the behavior of both classes of models suggests that for many purposes the two classes will give qualitatively the same result, but that agent-based models have an advantage in ease of accounting for heterogeneity in subpopulations where that is significant[14,15]. Furthermore, the SIR differential equations model is derivable from asymptotic limit of an SIR ABM model through diffusion approximation[16].

A notable coordinated effort to develop agent-based models of a flu pandemic was the Models of Infectious

Disease Agents study funded by the National Institutes of Health[17]. More recently the attention of the world was dramatically drawn to the need for public health interventions in the case of COVID-19 by a simulation model projecting 2.2 million deaths from COVID-19 in the United States, and 510,000 in the U.K., in the absence of such interventions[18]. Since then, models continue to be refined as more data are analyzed[19]. It is important to note that there are enormous local geographic variations in the incidence of, and deaths from, COVID-19[20]. These local variations imply a need for local models, to enable local authorities to construct appropriate strategies of social distancing and testing for mitigation of the effects of COVID-19. The work described in this paper is designed to meet this need.

11.2 COVID-19 poses a *wicked* policy problem

Wicked policy problems are characterized by 1) complexity of elements to be accounted for and their relationship to each other, 2) uncertainty in relationship to the description of the problem and the consequences of actions, and 3) divergence within the affected community of values and interests[21]. By all three measures of wickedness –complexity, uncertainty, and divergence- COVID-19 is a highly wicked problem and will continue to be at least until there is an effective and universally available vaccine.

Dimensions of complexity in COVID-19 emerge from all of the multiple ways in which people interact with each other in such a way as to breathe the same air, and from the consequent trade-offs. These trade-offs involve public health, economics, every aspect of community life, and levels of emotional stress in individuals—a multi-level hierarchy of perspectives involving psychology, sociology, economics, health care, and politics. Correspondingly, we expect COVID-19 modeling efforts to include a growing number of these concerns while remaining actionable and scientifically useful. We expect the complexity of such models to grow, but to do so in a manner that remains intellectually transparent[22] about what is stated in them. To this extent, models become critical components within the top-level decision support system necessary to regain situational control during the current pandemic.

Dimensions of uncertainty abound. As noted above, there is enormous geographic variation in the documented impact of the disease, and variation even in the apparent fundamental parameters of the virus –transmissibility, latency, and virulence- for reasons that are not yet understood. Contributors to the uncertainty may be genetic variation in human populations[23], genetic variation in the virus as it continues to evolve[24], variation in childhood vaccine regimens from one nation to another[25], variations in weather patterns[26], and variations in testing rates and disease reporting accuracy and criteria[27]. Also, there is an element of pure chance –whether or not a particular community was "seeded" with infectious individuals, and how many.

Dimensions of divergence are in some ways clear, and in some ways complicated. The clearest divergence is between the imperative to save lives by social distancing and the costs of social distancing to the community—both economic costs[28,29] and also costs that are less tangible due to how wealth moves across the global economy[30]. Early on in this crisis most of the world appears to have made the choice of that we would throw our economies into Depression[31] and restrict many community activities we value[32,33] in order to save the lives of the probably less than 1% of the population who would die from infection should no social distancing constraints be imposed. At the time of writing, this choice is constantly being reconsidered, or at least recalibrated[34]. More, and more open discussions are being held on increasing economic activity even at the acknowledged cost of more infections and even deaths. One is reminded of a famous comedy routine when comedian Jack Benny, whose comic persona was as a notorious cheapskate, is held at gunpoint by a robber who demands "Your money or your life!" This is followed by a long silence, a repeated demand, and a response by Benny, "I'm thinking!". It seems that COVID-19 has the whole world thinking about the trade-offs between economics –and other aspects of community life- and lives. With respect to divergence, COVID-19 seems as wicked as possible. The economic dimensions of community life can be measured in dollars. The many other dimensions have no common units of measurement, so their relative value is literally incalculable. And yet we are forced to decide about what to value.

Another way to look at a wicked policy problem is a one where the space of potential solution alternatives contains far more social dilemmas than solutions. We may thus define a *social dilemma* is a situation where multiple agents have (explicit or implicit) stakes in the resolution of a problem, stakes are tied to multiple value systems (and not just shared, "objective" technical considerations for example), and a proposed solution contains value contradictions that get translated to unacceptable potential losses were that solution to materialize; at the same time, the social dilemma also provides consequences if a solution fails to appear .Conversely, a perfect solution to a wicked problem is a point of total satisfaction of constraints at all levels of representation of the problem. This is, of course, an idealization; in practice some constraints must be eliminated, relaxed or ignored to find a collective solution. In summary, a social problem is wicked if the density of true solutions is low in the space of all solution alternatives and the search for them can be described as unstructured or even counter-incentivized at best.

Thus, the final element of COVID-19 as a truly wicked problem is that, although it is insoluble, we must make our best effort to solve it. The consequences of not trying to solve this intractable problem, of simply guessing at answers guided only by intuition, are far worse than the consequences of being guided by imperfect models.

11.3 Building a multi-objective model for COVID-19: the agent-based route

Based on the discussion above, our current research efforts have focused on the development of an integrated simulation model capable of a) accurately reflecting known dynamics of the current pandemic and the qualitative results of other models, b) simulating data-driven stochastic heterogeneity across agent populations to more realistically reflect the variability of underlying human populations when the model is applied, c) integrating economic considerations in association with observable features of the pandemic, d) allowing detailed simulation of known public policy measures at different times, intensities and dates, and e) providing a simple interface for non-expert users to configure and interpret.

In relation to the latter point (e), we envision assisting the decision-making process in two steps: first by providing some metaphor or visual proxy for users to construct intuitions by running specific scenarios, and then by translating some of these intuitions into fully-fledged computing and analysis tasks. Succinctly, we wish to facilitate decision making processes that are both robust and adaptive[35] while helping decision makers to avoid falling into the "illusion of control", or the false belief in the causal relation between computing consequences with a model and immediately improving their decision-making abilities[36]. At the same time, we remain painfully aware of the intrinsic difficulties posed by imperfect data, imperfect implementation of public policy measures, and uncertain timelines for when and for how long to apply measures under unknown timelines for availability of vaccines[37]. We expect our model to be beneficial when a) decision makers are fully aware of the underlying simplifications we have made, b) model outcomes are contrasted and adjusted with incoming data during an unfolding situation, c) experts assisting decision makers carefully determine and document how data produced by these simulations is analyzed and translated into tentative recommendations[38].

To this extent, we have focused our efforts on providing modeling tools for population centers with 100,000 inhabitants or less. Our choice is motivated by the geographic distribution of cities and towns across the US[39] and by the apparent inverse correlation between population size and rurality. This is significant since the push for urbanization seems to have driven rural cities and towns to more precarious health systems than their urban counterparts[40]: one can expect COVID-19 propagation to be slower due to lower population densities, but the impact to be at least similar or stronger due to age distribution and availability of health care facilities[41], with a special emphasis on availability of ICUs[42].

11.3.1 Generalities

In our model, agents interact and traverse a discrete 2D torus composed of connected lattice points that represent geographic locations. Agent actions and decisions are governed by random variables with suitable distributions. A single execution (i.e. a *scenario run*) of a parametrization of the model corresponds to a possible world, while a simulation (i.e. a *scenario*) comprises an ensemble of multiple executions with the same parametrizations where outcomes correspond to distributions of agent states and observable quantities must be computed through averages.

The choice of geometry presupposes that agents move across a common landscape at all times, and no agents enter or leave it. This simplification of the geographical landscape, while in general unrealistic, is not uncommon[43,44] and provides two advantages: a) it naturally matches intuitions behind interactive particle systems driven by mass action principles[45] such as in the SIR model and b) when translated into code, no boundary checks need to be performed by the agents. Lattice sites are connected, from the perspective of an agent, by a Moore neighborhood in an effort to reduce the effect of discretization artifacts[46]. We note here that our model presupposes a homogeneous population density as a means of ensure representativeness of processes within the geographical domain. Although accounting for variable population density areas in the same scenario is possible, our approach simplifies implementation aspects and prevents artifacts for model outcomes that may be strongly density dependent[47] in both epidemiological and economic aspects.

Our model does not explicitly contain a rich representation of locations where agents are drawn to and act as temporal sinks. Instead, we chose to model agent tropism through randomized agent dwell times. *Dwell time* (τ_{dw}) refers here to the minimum amount of time an agent susceptible to COVID-19 contagion needs to spend in a given location to acquire the virus. Based on existing estimates[48], we have chosen $\tau_{dw} = 15$ minutes, which corresponds to one time step $t_s, s \geq 0$. Average total dwell time $\bar{t}_{dw} = k_{dw} \cdot \tau_{dw}$ for an agent corresponds to the (integer) average number of steps an agent will dwell on a single location. Since our model assumes a day as a usual reporting unit in decision-making activities, all parameters stated in days are internally rescaled to τ_{dw} units (i.e. 1 day = 96 simulation steps). Agent dwell times are set at creation time using a random deviate from Poisson$(k; \lambda = k_{dw})$.

11.3.2 Core parameterization

To configure of a scenario, a collection of demographic and disease parameters must be specified. Age structure appears to be strongly associated with differences in COVID-19 fatality rates[49–52]. The model requires estimates both of the distribution and observed fatality proportions p_f^{sex} and p_f^{age} per sex (i.e. male and female) and age (i.e. every ten-year intervals) respectively. Co-morbidities are introduced in a similar manner by means of the age and sex structure of the population as a collection of positive multipliers $k_f^{\text{sex}}, k_f^{\text{age}}$ per relevant condition, and aggregate clinical data about their prevalence per age and sex.

The total number of agents N at the onset of the simulation remains constant at all times, except when an influx of new agents is simulated. To do so, the number of new agents entering the population correspond to a proportion p_{new} of the existing ones. In addition, one must specify when the agents will be introduced $t_s = T_{\text{new}}$ and how long it takes them to enter the space τ_{new}. In this manner our model can account for seasonal population increases driven by, for instance, agricultural production or the start of semesters in university towns. After time $t_{s'} = T_{\text{new}} + \tau_{\text{new}}$, the simulation will contain approximately $N' = N + p_{\text{new}} \cdot N$ agents.

To account for population density ρ_{pop}, the model specifies the width W and height H of the lattice that will contain the agents. We presuppose that agents move across the lattice one jump at a time if their dwell time is exhausted. The size of the lattice should be also adjusted based on the mobility and transportation patterns of individuals within the enclosed region of interest –that is, excluding realistic density fluctuations due to commuters that spend most of their time outside of the simulated region. The effect of such adjustment is equal to re-scaling the population density by a mobility pre-factor k_{mobl}. After these calculations have been performed, the model should ensure for $T_{\text{new}} = \infty$ that

$$\frac{N}{W \cdot H} \approx k_{\text{mobl}} \cdot \rho_{pop}. \tag{11.1}$$

Intuitively, the effect of greater mobility is equivalent to increased population density, or correspondingly, to traversing a smaller space. While our model does not include the effect of road networks or vehicle use, a carefully constructed average for k_{mobl} can provide a sufficiently adequate approximation.

Disease-wise, the model comprises six critical parameters. First, the initial proportion of agents p_{iexp} that are exposed to the disease. The model assumes that their introduction occurs at the onset of the disease incubation period. Then, the incubation period τ_{incb} and the recovery time τ_{recv} are inputs correspond to average observed or estimated values in clinical patients[53]. In the simulation, each agents is initialized with individual incubation and recovery times drawn from $\text{Poisson}(k; \lambda = \tau_{\text{incb}})$ and $\text{Poisson}(k; \lambda = \tau_{\text{recv}})$ respectively. Our reasoning behind this choice rests on the fact that a) the time at which symptoms manifest across patients depends on a common organismal response to the pathogen dependent on the activation of known (and yet unknown) molecular pathways[54–56], and at the same time on the intra-population variations that are found across individuals due to their specific genetic make-up and context. Thus, we treat symptoms onset as a homogeneous Poisson process for simplicity even when the described coupling exists. An improvement to our current model would entail, if the reasoning above holds, computing observables using a general Poisson point process by assuming that the Radon-Nikodym density exists[57].

Fourth, the proportion of individuals who remain asymptomatic p_{asym} is accounted for and utilized when stochastically deciding the fate of exposed agents. The role of asymptomatic patients remains heavily investigated[58,59] and appears to play a crucial role in disease mitigation for COVID-19[60–63]. From literature data, the proportion of asymptomatic patients appears to vary greatly across countries and demographics (e.g.[64,65]), although the matter is far from settled. In this sense, our model is intended to be applied by using data starting at the most local level if possible, and only moving to larger geographical instances when data cannot be obtained by means of statistically robust antibody testing.

Fifth, the proportion of severe cases p_{sev} is significant for the model due to its relation to hospital capacity. The definition of severity used here is that reported in[66]; we suggest similar guidelines on estimating the proportion severe cases should be followed. Another proxy for severity may comprise the number of non-ICU and ICU admissions, and their ratio[67]; in general, the need of hospitalization implies that clinical evaluation of a patient raises enough concerns as to consider the possibility of transitioning from non-ICU stage to the ICU stage of care[68]. To account for saturation of health care services, the model males use of the proportion of beds proportional to population density p_{beds}, and we assume that only severe cases are hospitalized. If a severe patient cannot be hospitalized due to saturation, then its probability of fatality rises by a factor to be determined empirically; for reference, our model presupposes a four-fold increase. At present, our model does not provide estimates of ICU occupancy.

Finally, the model utilizes the probability of contagion P_{cont} per agent per interaction. This quantity can be obtained from field data or other (more coarsed-grained) epidemiological models at the onset from estimates of the effective reproductive number R_0 by observing that

$$R_t = P_{\text{cont}} * \langle n_{\text{S,I}} \rangle_t * d \tag{11.2}$$

where $\langle n_{\text{S,I}} \rangle_t$ is the average number of contacts between susceptible (S) and infectious (I) agents, and d is the duration of infectiousness of the disease. Recalling the SIR model

$$\frac{dS}{dt} = -\beta SI, \tag{11.3}$$

$$\frac{dI}{dt} = \beta SI - \gamma I, \tag{11.4}$$

$$\frac{dR}{dt} = \gamma I \tag{11.5}$$

we observe that $\gamma = d^{-1}$ and

$$P_{\text{cont}} = \frac{\beta}{\langle n_{\text{S,I}} \rangle_t}. \tag{11.6}$$

Our view of R_0 is that of a preliminary estimate for initial calibration at the onset of the period of interest. For reporting purposes, we favor the effective reproductive number $R(t)$, and consequently provide information about the observable for $n_{\text{S,I}}(t)$ such that

$$R(t) = 96 \cdot P_{\text{cont}} \cdot \langle n_{\text{S,I}}(t) \rangle_i \cdot d_i, \qquad 0 \le i \le N. \tag{11.7}$$

Since one agent represents multiple individuals in the region of interest, it becomes necessary to compensate for this renormalization process. For such purpose, we provide a scaling factor associated to the representativeness of the model k_r given with a scale 1:R by

$$k_r = \log_\gamma(R). \tag{11.8}$$

We found empirically $\gamma \approx 1.58489$, such that rescaling the probability of contagion to obtain $P'_{\text{cont}} = P_{\text{cont}}/k_r$ leads to

$$R(t) = 96 \cdot k_r \cdot P'_{\text{cont}} \cdot \langle n_{\text{S,I}}(t) \rangle_i \cdot d_i, \qquad 0 \le i \le N. \tag{11.9}$$

In addition, $R(t) \propto \rho_{\text{pop}}$ (Eq. 11.1), which implies that k_{mob} must also modulate $R(t)$. The final expression becomes

$$R(t) = 96 \cdot k_{\text{mob}} \cdot k_r \cdot P'_{\text{cont}} \cdot \langle n_{\text{S,I}}(t) \rangle_i \cdot d_i, \qquad 0 \le i \le N. \tag{11.10}$$

11.3.3 Agent dynamics

At the model level, observables are interrogated across the agent population, agent step actions scheduled and the step number updated. At each step, agents move one space across the 2D torus after exhausting their dwell time per location. All agents posses an internal state σ that stores information relevant to the disease, its economic aspects and various control structures. Their motion is driven by a random walk within their Moore neighborhood, unless their state has been set to isolation. Isolation means not moving across the space regardless of dwell times. More than one agent can inhabit one lattice site, which forms the basis for determining when a susceptible agent becomes exposed and the infectious cycle starts. Prior to performing stage-dependent computations from the disease perspective, agents compute the consequences of policy measures and adjust various elements of their internal states relevant to epidemiological and economic actions to follow.

Epidemiology

Our model departs from the usual compartments of the SIR and extends it in order to account for a more fine grained variety of significant infection stages. Agent disease states are as follows:

Susceptible All agents (except those marked as initially exposed) start as the susceptible population. When susceptible agents share the same lattice site, these may come in contact with other exposed, symptomatic (i.e. due to voluntary or involuntary breaking of quarantine with probability $1 - P_{\text{isoeff}}$) or undetected asymptomatic agents. If at least one agent is infectious, the agent changes its state σ to exposed as dictated by Bernoulli$(\sigma, P_{\text{cont}})$. Unless quarantined due to a policy measure, susceptible agents move freely across the lattice.

Exposed In the absence of any policy measures impacting exposed agents, these continue to explore lattice sites until their incubation period given by Poisson$(x, \lambda = \tau_{\text{incb}})$ is exhausted. At that time, agents become asymptomatic as dictated by Bernoulli$(\sigma, p_{\text{asym}})$ or symptomatic detected, otherwise.

Asymptomatic Asymptomatic agents continue moving through the space and remain infectious until the recovery period given by Poisson$(x, \lambda = \tau_{\text{recv}})$ is exhausted. At that point, the agent enters the population of those recovered.

Symptomatic When an agent becomes symptomatic, it is immediately marked as detected and quarantined. Regardless of stringency of testing policies, the definition of confirmed case depends at the minimum on being both symptomatic and a positive identification via some form of testing (i.e. RT-PCR qualitative or quantitative, serological[69]). Symptomatic agents follow two possible trajectories. In the first one, agents convalesce without becoming severe until their recovery time is exhausted an recuperate. In the second one, agents become severe as dictated by Bernoulli(σ, p_{sev}). In terms of the impact of saturation of health care services, research is needed to determine lethality of patients outside hospitals and other facilities. However, using existing ethical guidelines that provide heuristics of fair resource allocation for beds and ventilator equipment[70] as a proxy, we estimate that lethality increases (conservatively) by at least a factor of 5.

Asymptomatic Detected Asymptomatic agents detected by some widespread systematic testing strategy are immediately quarantined in place, and wait until their recovery time is exhausted. At that point, they join the population of recovered agents.

Severe Agents that enter the severe stage represent patients that require some form of hospitalization, and for some of them, use of mechanical ventilators; these remain under perfect quarantine. Lethality, computed per age and sex population structures as $p_f = p_f^{\text{age}} \cdot p_f^{\text{sex}}$ is used to determine whether a severe agent becomes a fatality as given by Bernoulli(σ, p_f). Agents, on the other hand, may survive until recovery.

Recovered Agents that have recovered leave quarantine and move again freely across the lattice. Our model does not consider the probability of re-infection, but this may need to be included in the future[71]. At the moment of writing, this aspect of COVID-19 remains speculative and uncertain for human patients[72–74] despite encouraging evidence obtained from experiments using rhesus macaques[75].

Deceased Agent that count as fatalities do not interact with other agents or undergo any further epidemiological significant events until the end of the simulation.

Inbound infectious cases

In order to increase model realism, we consider the effect of inbound infectious cases of two sorts: people that live within the community but have to travel and work outside of it in a steady stream daily that maintains the overall population density stable, and people that move seasonally within the community, potentially bringing in more cases that have a different viral load. This last case describes, for example, the opening of university campuses for instruction where several people relocate to adjacent towns.

For the first situation, the model includes the probability of susceptible people becoming infected with a daily rate that determines the infectious stage depending on Bernoulli(x, r_{ibnd}). In the second type of infectious cases, at time T_{mass} a proportion p_{mass} of the current population will enter the simulation space during a time period τ_{mass} with a probability of being in the exposed state of P_{mass}.

11.3.4 Policy measures

COVID-19 has forced a frantic search for public policy measure combinations capable of containing viral transmission, and ideally quelling its progression altogether[74,76–86]. All measures reviewed and emerging across literature roughly belong to four main classes of measures: 1) those that aim to reduce at any instant the density of individuals at locations with potentially high concentration of people by means of imposed self-isolation of non-essential workers and cancellation of activities involving massive amounts of people, 2) those that reduce the likelihood of viral exposure for those qualified as essential workers for whom close social interactions are inescapable, 3) those intended to detect and isolate positive virus carriers through application of molecular or serological testing and 4) those that seek to reconstruct interaction histories in which a positive infectious patient may have had an active role in unknowingly spreading the disease.

It has become increasingly clear that these measures are essential yet hard to sustain for long periods of time. On the one hand, various degrees of negative psychological impact have been recently reported[87], in particular impacts that decrease adherence to public policy measures[88] which are expected to naturally arise after periods of prolonged confinement under a collective crisis; World War II critics of air raid shelter policies constitute a significant precedent[89]. On the hand, mounting concerns on lasting economic impacts[90,91] materialize the wickedness of the COVID-19 pandemic and the cost of measures to address it[92], concerns that which include social protection of workers[93], the labor market[94], patterns of work[95], gender equality[96], nation-state economics[97], and monetary policy[98] to name a few.

Motivated by the latter, our work attempts to model the individual variability expected when these types of measures are implemented, their various impacts in terms of disease and economy collective observables, and the potential outcomes of combining them in various manners. We note that societal and economic impacts of COVID-19 differ from those in other pandemics due to the tight coupling of global events and the effect of near-instantaneous digital communication. *We are changing the pandemic while living it.* While our model does not provide mechanisms to state the associated control problem in cybernetics terms, emerging literature (e.g.[99–102]) suggests that such approach may be possible, and even essential to provide solutions that account for the complexities involved in politically and socially driven environments.

Self-isolation

Self-isolation in our model is captured by establishing a period in which a proportion p_{isol} of agents in mobile states (i.e. susceptible, exposed, asymptomatic) remains at a fixed location for a well-defined period of time. Self-isolation starts at time T_{isol} and extends for a period τ_{isol}, after which motion across space is restored. Agents isolate with effectiveness P_{isoeff}, representing the probability that when in contact with another infective agent the final probability of contagion becomes $P'_{\text{cont}} = P_{\text{isoeff}} \cdot P_{\text{cont}}$.

Social distancing

Social distancing is modeled as a distance-dependent adjustment constant $\delta(\ell)$ that adjusts the probability of contagion P_{cont} depending on linear distance ℓ assumed between agents within the same cell such that $P''_{\text{cont}} = \delta(\ell) \cdot P'_{\text{cont}}$. Based on recent experiments on the effect of air turbulence on droplet dispersion[103], we assume a decreasing sigmoid profile after 1.5 meters. Hence,

$$\delta(\ell) = \begin{cases} 1.0, & \ell \leq 1.5 \\ \xi(\ell), & \ell > 1.5 \end{cases} \tag{11.11}$$

with

$$\xi(\ell) = 1.0 - \frac{1.0}{1.0 + e^{-K(\ell - 2.0)}} \tag{11.12}$$

where K is a constant that adjust the decrease rate of the sigmoid function. For the purposes of the COVID-19 model, $K = 10.0$. The value of ℓ can be adjusted also to account for the effect of other interventions that decrease contagion probability per contact by decreasing the effective viral load, such as the use of various types of face masks[104].

Testing

Similar to self-isolation, testing in the simulation operates by distributing a target percentage of the population into a given period. Susceptible and asymptomatic agents can be tested; in our simulation, we do not re-test those who recover. A symptomatic case is treated immediately as tested, representing the case where a patient reaches a health provider and a test is applied to determine the correspondence between symptoms and the disease.

Testing proceeds in the following manner. Once time T_{test} is reached, symptomatic and asymptomatic agents are selected with a probability P_{test} proportional to the period τ_{test}. This testing process simulates massive testing policies without any statistical design or underlying population structure.

Contact tracing

We simulate forms of automated contact tracing by means of a set of known prior contacts. We assume a delay of two days for contact follow-up once an infected patient has been discovered. Once an agent is marked as positive, all of its contacts are evaluated and classified either as susceptible (negative), symptomatic or asymptomatic detected. Contact tracing utilizes the same start time and period as testing.

11.3.5 Estimation of economic impact

Along with an epidemiological model, we have included economic factors tied to disease stages. After some investigation around statistical theories in economics[105], we decided to implement a simple model where value creation in terms of exchanges between money and products or services[106] are computed in connection with the progression of the disease. Our model is an oversimplification of economic systems, and as such, its goal is to provide a numerical intuition about the immediate effects on the accumulation of capital by individuals and the public sector during the period of interest. Thus, the economic model makes no assumptions about wealth distribution, wealth inequality or other societal factors, and as such only aims at portraying the impact of an epidemic on transactional capital gains or losses at the private and public levels.

Regarding public value[107], we observe that the complex web of actions across individuals and institutions make construction of a detailed model expensive in connection with infectious disease dynamics. Growing literature on the subject is indicative of the latter[108–111]. To the best of our current experience, proper treatment of the current situation would require a different class of model based on fractional operators coupling epidemiological[112] and econometric aspects[113,114] capable of accounting for short- and long-term memory macroeconomic effects[115].

A disease-economy input-output system

Our take on the matter can be stated through the following somewhat intuitive principles:

1. Disease stages that allow interactions should cause non-linear positive externalities in terms of collectively amplified public value. The more frequent interaction exchanges, the higher the materialization of public value as a function of non-linear effects of reaching throughput efficiencies that both maximize economies of scale and translate into deep capital accumulation and redistribution across the public sector.

2. Disease stages that forbid interactions but do not put individual lives at risk should cause linear negative externalities associated to both increased unemployment ripple effects and inability to reach throughput thresholds capable of amplifying value creation.

3. Disease stages that both forbid interactions and put individual lives at risk should cause non-linear negative externalities due to increased unemployment ripple effects, inability to reach throughput thresholds capable of amplifying value creation and the saturation of alternatives under an increasingly severe public health crisis.

4. In addition, we estimate the cost of performing one test as part of the public cost. The purpose of this observable is to provide an account of testing as a public measure versus other actions for which their cost is harder to account for.

In order to materialize the above principles, our approach is inspired by that of input-output matrices utilized to account for combined economy-ecosystem calculations[116]. The equivalent of the matrix $\boldsymbol{M}$ in our model expresses economic outputs per disease stages. Viewed as a matrix computation, the components of the input vector $\boldsymbol{u}$ correspond to proportions of the agent population per infectious stage, while the output vector $\boldsymbol{v}$ is of the form $\boldsymbol{v} = (v_{\text{priv}}, v_{\text{pub}})$. Depending on the disease stage, vector components are computed aggregating the value of interactions or individually. By a suitable homotopic transformation $\mathcal{T}$[117], we approximate non-linear effects of market dynamics, thus the final value of $\boldsymbol{v}$ becomes $\mathcal{T}[\boldsymbol{v}] = (v_{\text{priv}}^{\alpha_{\text{priv}}}, v_{\text{pub}}^{\alpha_{\text{pub}}})$. The matrix components $\boldsymbol{m}_{ij}$ and both α_{priv} and α_{pub} are model inputs.

Table 11.1: Example of a coupled disease-economy input-output matrix with $\alpha_{\text{priv}} = \alpha_{\text{pub}} = 1$.

Disease stage	**Private value**	**Public value**	**Computation**
Susceptible	1.0	1.0	Aggregate
Exposed	1.0	10.0	Aggregate
Asymptomatic	1.0	10.0	Aggregate
Symptomatic	-0.2	-3.0	Individual
Asymp. detected	-0.2	-1.0	Individual
Severe	-5.0	-15.0	Individual
Recovered	0.8	2.0	Individual
Deceased	0.0	-0.2	Individual

11.3.6 Model outcomes

Our model captures during its execution various observables every time step. All values are aggregates and no particular agent information is stored; in the future, this can be of value if the model is extended with network information. After a simulation has completed, the following classes of observables are recorded in a CSV format:

Simulation Step number, population size

Disease (fraction) Susceptible, exposed, asymptomatic, symptomatic quarantined, asymptomatic quarantined, severe, recovered, diseased

Measures Self-Isolated, tested, traced

Epidemiology Effective reproductive number

Economics Cumulative private value, cumulative public value

11.3.7 Implementation

The Epidemiology Workbench is implemented using Python (v 3.6) using the Mesa agent-based simulation library[118]. In batch processing mode, our model receives a JSON file with all the parameters described above and a number indicating the number of cores to use during the simulation. Once a sanity check is performed, the parameters are used in conjunction with the multiprocessing batch running features provided by Mesa.

We also provide a parametrizable web-based dashboard to explore individual runs. The objective behind this corresponds to enabling decision-making users to progressively gain intuitions behind each parameter, and not to provide operational information. Our code is openly accessible through GitHub[ii].

11.4 Case study: the cities of Urbana and Champaign after reopening UIUC, Fall 2020

The cities of Urbana (pop. 42,214)[iii] and Champaign (pop. 88,909)[iv] comprise a population of approximately 132,000 inhabitants. Figure 11.1 describes the current percent distribution per age group. In addition, distribution per sex is 50.5% males and 49.5% females. However, the population across both cities undergoes a seasonal decrease on mid May due to the end of the Spring semester and an increase in early August with the start of the Fall semester in the University of Illinois at Urbana-Champaign. From the more than 50,000 students enrolled on campus on May[v], we estimate that around 30,000 leave during summer to return for the fall semester. Effectively, the summer population amounts to around 100,000 inhabitants. We used COVID-19 age- and sex-dependent mortality values as reported by CDC until June 10.

Our interest rests on simulating the effect of various measures once mobility restrictions remain at values similar to the present one (phase 4 reopening) and combinations of testing and automated contact tracing when an estimate of 30,000 incoming students with a higher average viral load reach both cities, on an increase of 30% of the population present in summer.

11.4.1 Calibration

COVID-19 data was obtained from the Champaign-Urbana Public Health District (CU-PHD)[vi] and CDC for mortality data[vii]. Sex-dependent mortality was established at 61.8% for males and 38.2% for females.

[ii] See: https://github.com/snunezcr/COVID19-mesa
[iii] US Census Bureau population estimates for 2019. See: `https://bit.ly/3hj1PnC`
[iv] Idem. See: `https://bit.ly/2WGcOjq`
[v] University of Illinois News Bureau. See: `https://bit.ly/39jYj9K`
[vi] See: `https://bit.ly/3eOlISa`
[vii] CDC COVID-19 Death Data and Resources. See: `https://bit.ly/3hpap4A`

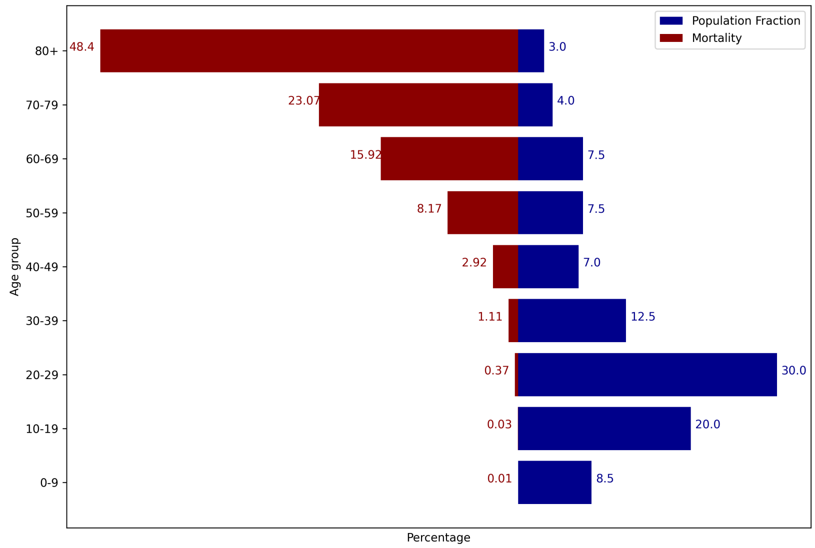


Figure 11.1: Combined population age structure and associated mortality in Urbana and Champaign cities, 2019 estimate by US Census Bureau/CDC.

The first local case in the community was reported on March 8, and state-wide shelter-in-place measures were applied on March 21[viii]. Later on, mandatory mask usage was established on May 1[ix]. By April 21, cumulative cases had reached 0.1% of the population, and by July 8 it had increased to 1%. The local $R(t)$ value at the peak period between April 21 and May 17 reached an estimated value of 1.2; after these measures, it remained around 0.91. We used a probability of contagion per interaction of 0.004 every 15 minutes if there is at least one person infected at the same location as the susceptible one. This value, although computed from data, appears to reflect compliance with various sanitation practices among the population. Based on the fluctuation in local data, we have estimated an inbound probability of 0.0002 new cases due to members of the community becoming exposed elsewhere. CU-PHD performs strict contact tracing across all cases, hence for all simulations we assume contact tracing remains active across all simulations.

Google Mobility data were used to estimate the average effective shelter-in-place value to a 45% of the population with 0.8 efficacy of self-isolation. The severity was similarly estimated at 5% based on local case information. Similarly, a starting value of $R(t) = 1.2$ corresponded to a grid of 190×225 cells and 1000 agents and $k_{\mathrm{mob}} \approx 0.4781$; this last value appears to be consistent with the regular use of public transport in the area and local observed shelter-at-home patterns. At the start of the simulation, the agent-to-inhabitant

[viii]State of Illinois. See: `https://bit.ly/2WHU6I5`
[ix]Idem. See: `https://bit.ly/3hsxm6D`

ratio is approximately 1:100. Hence, the calibration starts with one exposed agent. Differences between $R(t)$ in April and July correspond to $\ell = 1.89$. Intuitively, this implies that the effect of wearing a mask may roughly translate into increasing the distance 0.39 meters beyond what WHO recommends for proper social distancing. However, this cannot and should not be interpreted as to relax mask usage in any manner. In regard to asymptomatic patients, we have established a conservative value of 35% based on prior studies [119]. The following sequence of events was assumed toward the start of classes this Fall:

1. Exposure of the first representative agent on April 15 (simulation day 0)
2. First symptomatic representative agent on April 21 (simulation day 6)
3. Mask order from the State of Illinois on May 1 (simulation day 16)
4. Students start massive ingress two weeks between August 9-22 (simulation days 116-129)
5. Community members are tested between August 23-29 (simulation days 130-136)
6. Simulation continues without testing for two weeks between August 30-September 12 (simulation days 137-153)

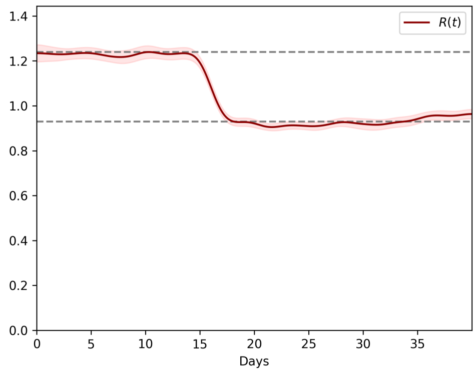
11.4.2 Simulation targets

Our goal for simulating the impact of mass ingress was to determine, based on various measures, the viability of preserving public health under variations of measures a week after a significant portion of the population has been tested. To determine the latter, we obtained data for $R(t)$, symptomatic, asymptomatic, severe and deceased fractions of the population. In addition, we collected information about economic impact using our input-output matrix model. A total of 6 simulations explore the following parameter settings:

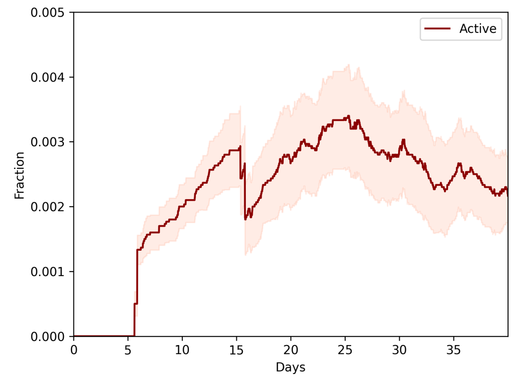
1. shelter-in-place continued/removed on day 117,
2. massive testing performed to 25%, 50% and 75% of the population in the enlarged community.

We also computed a counterfactual case corresponding to no massive testing and lifting of shelter-at-home orders to compare against a backdrop without measures. Model calibration results (Figure 11.2) correspond to the parametrization publicly available at the GitHub project repository[x].

[x]See: `https://bit.ly/2BhCuv3`



(a) $R(t)$.



(b) Active (i.e. symptomatic positive) fraction of COVID-19 cases.

Figure 11.2: Calibration outcomes for the cities of Urbana and Champaign during the COVID-19 pandemic. Dates span from April 21 to May 31 (40 days).

11.4.3 Results and Discussion

We computed a total of 7 scenarios (shelter-at-home times testing levels plus counterfactual), each one with an ensemble of 30 independent runs. Execution of these scenarios was performed on Amazon EC2 infrastructure using a `c5a.8xlarge` non-dedicated instance with 36 processors and 64 GB RAM. We used an Ubuntu 18.04 x86 image as the choice of operating system. Calibration CPU time with an ensemble of similar size for the first 40 days is, on average, 16.3 ± 0.4 minutes, and the average execution time of a complete scenario is 65.2 ± 1.3 minutes. Preliminary profiling indicates that random number generation using the `SciPy` library [120] explains most of the execution time. No attempts were made to further speed up our code by compiling it using Cython [121] or Numba [122]. Our goal in these simulations was not to reproduce exactly the case curves observed in the community, but to obtain a picture that remains quantitatively and qualitatively rigorous. Confidence intervals are calculated at 95% when present. We provide scripts to automate the setup of the Amazon EC2 instance with model installation[xi], the execution of all scenarios[xii] and their visualization[xiii] for reproducibility purposes.

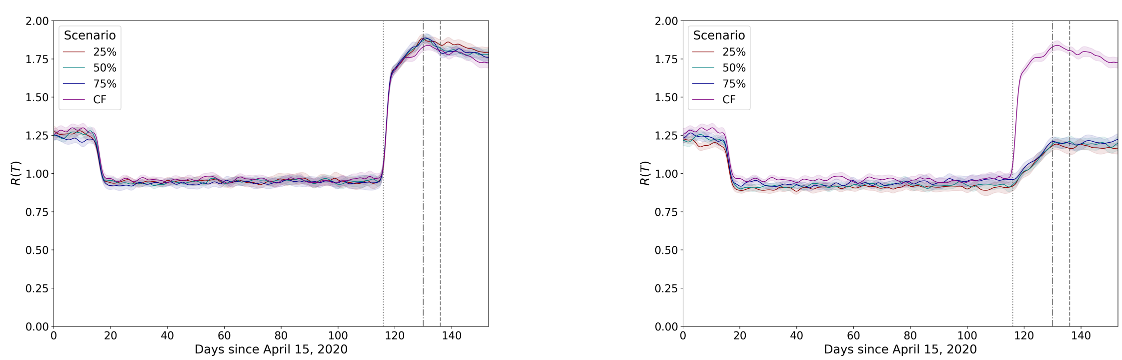
The following convention is applied to all figures: dark red corresponds to 25% testing, teal to 50% and dark blue to 75%; the counterfactual case is colored in purple. A dotted line corresponds to the start of mass ingress, a dot-dash line to the end of mass ingress and the start of massive testing, and a dashed line to the end of massive testing. All figures related to disease stages start at day 80.

[xi] See: `https://bit.ly/30wgS6M`
[xii] See: `https://bit.ly/3jvR2Zw`
[xiii] See: `https://bit.ly/2BkMh3v`

Public health

Model results indicate that outbound exposed individuals coupled with local fluctuations appear to drive the behavior of this pandemic for the cities of Urbana and Champaign. The combination of contact tracing and public health management by CU-PHD, compliance with health and sanitary measures and rapid implementation of shelter-in-place measures have prevented the pandemic from escalating in the region. Considering both cities as a closed system, adequate health management appears to be ultimately responsible for the small number of severe cases and hospitalizations in the region. The effect of masks, based on the information obtained from our simulation, appears to have a significant effect on the value $R(t)$ according to Fig. 11.2.

Our simulation of the reopening of the University of Illinois local campus with a higher viral load suggests that an increase in cases should be observable independent of the testing regime or relaxation measures. The future impact of this increase, however, is not. Figure 11.3 indicates that lifting all shelter-at-home restrictions and performing testing has a significant impact regardless of the testing level, while preserving shelter-at-home measures along with any testing level can drastically sustain $R(t)$ slightly below pre-mask order values. We note that $R(t)$ decreases in all cases, which can be explained by contact tracing-based testing. This suggests that even hybrid education modes (in presence + online) constitute significantly better alternatives than full campus reopening.

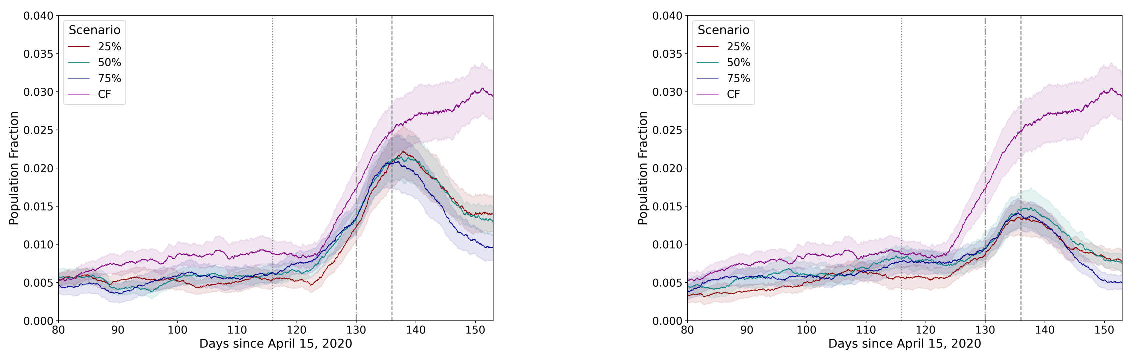


(a) Shelter-at-home measures removed on day 117.

(b) Shelter-at-home measures continued until day 153.

Figure 11.3: Evolution of $R(t)$ as a function of testing levels and shelter-at-home measures removal (a) and (b) preservation.

Testing intensity matters. In terms of the outcome after day 137, testing intensity determines the last value of active cases during two weeks after testing. Note that even when the testing instant itself has passed, capturing a larger and larger number of positive cases (particularly asymptomatic ones) drastically reduces the infectious population (Figure 11.4). Even when shelter-at-home measures have been lifted, testing reduces the fraction of the population classified as active cases at least higher but close to its value prior to mass ingress (25%), roughly equal its prior value (50%) or lower than the prior value (75%). Lifting shelter-at-home measures has a significant impact on the magnitude of both the peak of active cases and the value after two weeks have passed since testing occurred. Plans to test the student population once per week at scale, although not simulated here, appear to be a most effective solution to further tame the curve.



(a) Shelter-at-home measures removed on day 117.

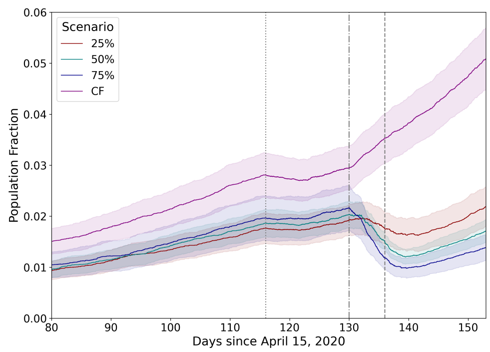
(b) Shelter-at-home measures continued until day 153.

Figure 11.4: Active cases as a function of testing levels and shelter-at-home measures removal (a) and (b) preservation.

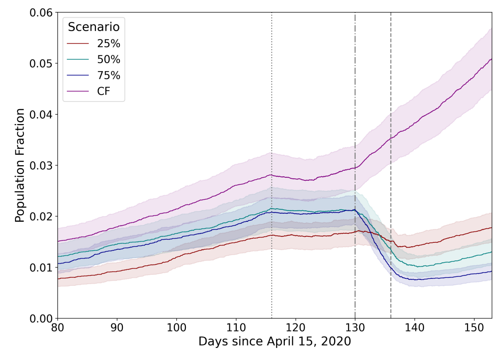
The main mechanism massive testing addresses in general, according to our simulations, is the removal of infectious individuals from the population, in particular those who are asymptomatic. In general, the estimated proportion of asymptomatic patients is a significant driver of the contagion in our model. When the population increases, many more individual contacts are possible within the same geographical area, and the lag induced by the incubation time translates into observing the impact of testing at least a week later. Figure 11.5 compares the asymptomatic fraction of the population across a baseline simulation without massive testing or some degree of sheltering. As in the previous case, shelter-in-place measures have an effect on the growth rate of the asymptomatic population, but even a testing intensity of 25% appears to lower it significantly compared to the counterfactual case. At case severity of 5%, more hospitalizations may be expected six days after day 130 (mass ingress), particularly if shelter-at-home orders have been lifted (Figure 11.6). The impact of testing, while it cannot be fully distinguished due to the overlap of confidence intervals in our simulations

Economic impact

Our analysis of economic impact focuses on two per-capita averages: cumulative private value (without any egress) and cumulative public value. While this part of our proposed model is experimental and requires

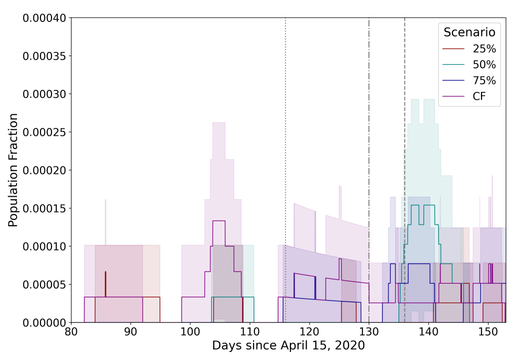


(a) Shelter-at-home measures removed on day 117.

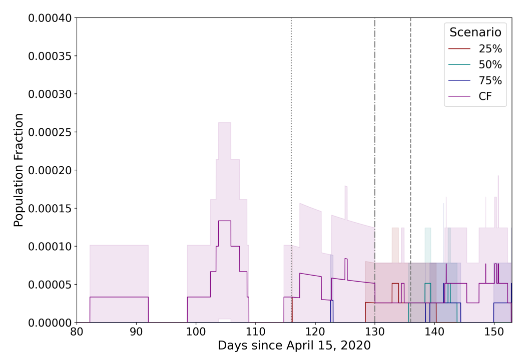


(b) Shelter-at-home measures continued until day 153.

Figure 11.5: Asymptomatic cases as a function of testing levels and shelter-at-home measures removal (a) and (b) preservation.



(a) Shelter-at-home measures removed on day 117.

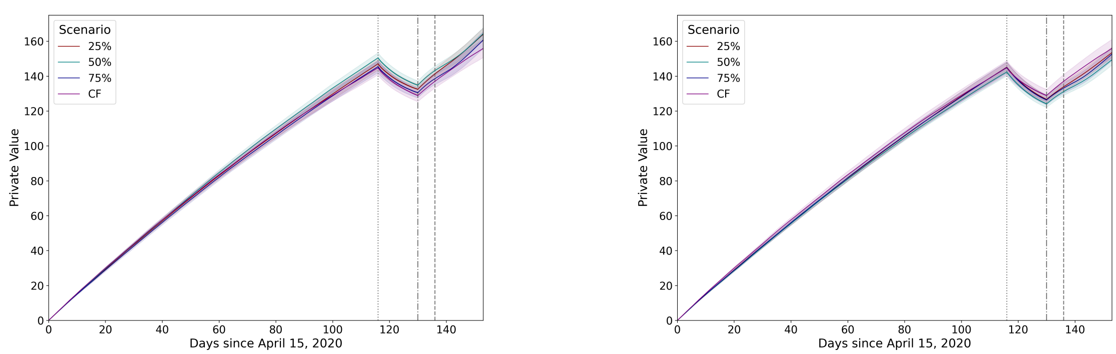


(b) Shelter-at-home measures continued until day 153.

Figure 11.6: Severe cases as a function of testing levels and shelter-at-home measures removal (a) and (b) preservation.

further analysis, we proceed to state the current results.

First, we studied the effect of the pandemic only on individual accumulation of private value (Figure 11.7). Mass ingress appears to renormalize temporarily the distribution and removing shelter-at-home measures, predictably, increases the final value at day 153, but only by approximately five units. All testing levels appear to comprise a relatively tight bundle, which can be interpreted either as an artifact due to the model being simplistic, or as the fact that the impact of testing levels on cumulative private value in the context of a pandemic under control (as in Urbana and Champaign cities) is limited. Even when these differences are small, they do exist. Testing at low levels (i.e. 25% and 50%) reduces the number of isolated people compared to testing at a broader scale (i.e. 70%). However, when an epidemic process remains under control, public health benefits largely appears overshadow individual losses, contingent on the validity of this approach.

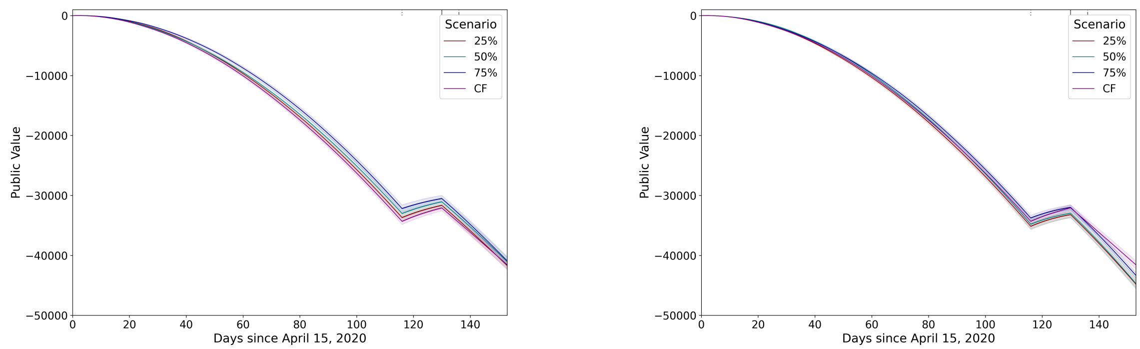


(a) Shelter-at-home measures removed on day 117.

(b) Shelter-at-home measures continued until day 153.

Figure 11.7: Per-capita cumulative private value as a function of testing levels and shelter-at-home measures removal (a) and (b) preservation.

In the case of per-capita cumulative public value, the model predicts negative outcomes even for an epidemic under control (Figure 11.8). This appears to align with public expenditure needed to mitigate any economic and societal lockdown necessary to stop the spread of the disease, as well as the negative externalities leading to less public transactions taking place on systems that were designed to support a certain minimum load to remain profitable: public finances tend to be, in general, inelastic for that reason. When shelter-at-home measures are lifted, a natural order of solutions arises from worst-case (our counterfactual, purple) to best-case (75% testing, blue): strong testing reduces the long-term impact of active, asymptomatic and severe cases. In this situation, however, the effect of mass ingress appears to be to re-bundle the behavior as $R(t)$ increases again. If shelter-at-home is preserved, an interesting situation arises: doing nothing appears to be a good economic solution. We believe the main reason behind this result to be that, for the case modeled here, the social and economic cost of the lockdown is higher due to the situation being under control; however, the material gains computed by the model between are rather small, and preserving public health over economics is a better-long term strategy. Despite this, strong massive testing still provides a next best solution from the point of view of economics, and the best strategy from the public health perspective; this is evidenced by the diverging curves in Fig. 11.8(b). We speculate, based on our current simulation outcomes, that the ordering in the economic cost profile of a pandemic during its exponential phase should be similar to that of Fig. 11.8(a), but with the divergence observed in (b).



(a) Shelter-at-home measures removed on day 117. (b) Shelter-at-home measures continued until day 153.

Figure 11.8: Per-capita cumulative public value as a function of testing levels and shelter-at-home measures removal (a) and (b) preservation.

11.5 Conclusions

We reported here the construction of an agent-based workbench using the Mesa modeling framework capable of capturing epidemic processes alongside public policy measures. The model is fully stochastic, entailing the computation of observables of different kinds. While computationally expensive, its formulation allows to easily obtain quantities that appear to be useful in the process of combating an epidemic. We applied our workbench to understanding the possible epidemiological profile of two cities, Urbana and Champaign, in the context of the reopening of the University of Illinois local campus next Fall. Our simulations indicate that at least 50% testing of the local population is needed to sustain the pressure of mass ingress of individuals with a higher viral load compared to the local one. More generally, contemporary management of an epidemic demands changing the *mode of interaction* across as much as the population as possible from those requiring physical proximity to those that do not. Although digital technologies provide mechanisms to preserve safe spatial distancing, temporal distancing can also be intelligently used to reduce the probability of contagion.

In terms of economics, public health measures must be privileged over financial concerns, since the panorama appears similarly bleak during the early phases of an epidemic, and strict measures possibly provide the best solution during the exponential phase.

Our model contains the following key limitations. First, only one measure per type can be specified at the moment, instead of a sequence of dates paired with values corresponding to the measured (or expected) effect of measures of the same type. In the example above, we used an approximation of shelter-in-place for the entire simulation period (April 21–September 12), even when the State of Illinois ordered phase 4 re-openings on June 26. Another critical element missing in our model corresponds to preferential shelter-in-place per age group. Even when mortality appears to more strongly impact the elderly, local mortality is low. This may be due to higher compliance of that population with shelter-at-home and other sanitary measures, including wearing masks in public. Variable viral loads per disease stage[123] are missing in our model, but these are harder to calibrate due to the biosafety and time elements involved in quantitative PCR-RT. Nevertheless, we do foresee situations where this may be possible and pertinent. Finally, our model assumes agents have an effectively infinite memory to remember whom they have had contact with. Contact tracing has a stringent limit when performed manually, which can be expanded greatly by means of various information technologies. Hence, our model is not realistic in this sense, since it does not distinguish between these two cases: when an epidemic has reached certain critical mass, active cases will be underestimated.

Computationally, the Epidemiology Workbench is limited by the lack of true concurrency in Mesa, thereby impacting scaling properties of our simulation. Distributing the agents across multiple compute nodes in Python requires architectural changes in Mesa beyond the scope of our work. At present, efforts are under way to develop an Elixir-based ABM platform capable of addressing this limitation as part of the SPEC collaboration in the Computational Social Science community. Another critical bottleneck is random number generation, for which various strategies may be applied, including the use of (approximately) irrational numbers as coefficients of Fourier series.

A final aspect underscored by our research, in particular in the context of COVID-19, is the need for anticipatory mechanisms driving public policy measures. In this sense, simulation methods such as the one presented here or others lack convenience when introducing external events and the execution cost of recomputing complex models, and appear to make sense only at early stages of a epidemic process: once the disease spread has reached its exponential phase, the need moves from prediction to probabilistically qualified estimations of short term measure effectiveness. This suggests a different class of stochastic methods that not only predict expected trends but also recommend measures based on their effectiveness, similar to those used in high-speed trading of financial derivatives and futures. The complexity of the socio-technical character of the global economy and society demands these more powerful methods to successfully address the wicked character of a pandemic, in particular this one.

As of now, our efforts concentrate on seeking viable ways to package and deploy the Epidemiology Workbench across various cyberinfrastructure resources in order to make it available to other small cities (including training resources) and, particularly, to communities with strong presence of underrepresented minorities whose public health planning resources are heavily constrained.

11.6 Acknowledgments

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Part V

Philosophical and pragmatic externalities of interactions

Chapter 12

HoH-Companion: Preserving Hierarchies of Hypotheses for Scientific Experiments in the Whole Tale

Summary[i]

The hierarchy-of-hypothesis (HoH) approach to science focuses on defining good explanations as those that are constructible from various types of interlocking hypotheses. At the same time, when computational experiments are involved, each hypothesis encapsulates reproducibility concerns. In this report, we concern ourselves with the relationship between HoH and reproducibility from both an epistemological and cyberinfrastructure perspective. We also provide a detailed design of a HoH-Companion, a computer assisted science software architecture intended to facilitate reasoning and re-enacting hierarchies of hypothesis when computational experiments are involved. We discuss the current project state, as well as next steps in the ongoing research and development.

12.1 Introduction

Science is an open-ended, self-correcting endeavor. Yet, as a *socially-driven human endeavor*, it depends on improving how discoveries are shared and communicated across communities of practice, as well as to broader audiences. This is more pressing when computational experiments are used, and for these to fulfill the scientific promise they represent[1], two concerns need to be answered: whether computational experiments comply with the reproducibility requirements expected across all scientific disciplines, and whether it is possible to ensure the validity of complex and intertwined chains of reasoning by testing hypotheses. The reproducibility crisis in science[2] is the superstructure guiding a significant share of the work describe here, and beyond it, the larger search for fundamental questions about whether our models of science can be improved regardless of the particulars.

The increased awareness of the scientific community regarding the correctness of inferences drawn from

[i]**Núñez-Corrales, S. and Ludäscher, B. (2019)** HoH-Companion: Preserving Hierarchies of Hypotheses for Scientific Experiments in the Whole Tale. A report to the joint *RDA/US-Whole Tale Data Share and Early Career Fellows program.*

computational experiments[3] has led to multiple discussions about the meaning and adequate use of *repeatability*, *replicability*, and *reproducibility*[4]. Mounting discrepancies around the latter point to the need for better conceptual grounding[5], which appear to arise from dissonant interpretations across various communities. Yet, these terms refer simultaneously to concrete software artifacts and to other types of instruments while the process of verification of the latter is much more rigorous than that of the former.

At the same time, computational experiments are tied to an often unspoken networks of theories, assumptions and hypotheses expected to hold true when proceeding with a particular research case[6]. Tacitly or explicitly, software artifacts encode these assumptions and make use of them to derive new results. However, as much of the scientific development depends also on human networks from publishing to mentoring, access to these hierarchies of hypotheses is often *handed* rather than *documented*, or even less *encoded* for automated forms of reasoning.

There exists a growing, general need for methods that capture such hierarchies of hypothesis (HoH) across a wide variety of scientific domains, including biology. Our present goal is to revisit and revitalize the methods and concepts of computer assisted scientific thinking often applied in science education[7] but relatively untapped across the general practice of science[8]. We believe that Hierarchies of Hypothesis (HoH) not only refers to the meta-analysis strategies devised to organize existing knowledge to determine the statistical relevance of hypotheses, but that they are actionable objects that can be harnessed to generate and preserve knowledge structures within computer experiments, including the data and tools required to re-enact each individual hypothesis.

Lack of such tools prevents researchers from keeping up with increasing amounts of data and the complexity of new experiments, a target that has increasingly gained traction across various science domains[9]. The emphasis nevertheless appears to remain constrained to the procedural contexts capable of enabling research, rather than on the semantic analysis of conclusions. Even in this context, systematic reasoning errors that can lead to different –even contradicting- interpretations of the falsification of a chain of hypotheses may be thus preventable, helping define[5,10,11] repeatability, replicability and reproducibility (a.k.a. the *r-words*) as well as their impact to HoHs.

In this report, we focus on two main ongoing contributions. The first one attempts to unveil the epistemological structure of the r-words and HoH within scientific intentionality. We suggest here a preliminary systematization for these terms aimed at reducing ambiguity in their interpretation. We describe how scientific intentionality manifests when computers are used to understand nature and define a classification of pragmatic uses behind HoH and the "r-words". We then show a mapping from elements of PRIMAD[12], a model that captures information about various aspects of reproducibility, to each pragmatic use. We also discuss how PRIMAD itself generates novel classes of computational hypotheses.

The second contribution is, based on the preceding discussion, a proposed design for a computational tool devised to assist research scientists in their reconstruction tasks. Building a *Hierarchy-of-Hypotheses Companion* (HoH-Companion) for the Whole Tale[13] can help researchers better structure, share and learn from their experiments. We describe the intellectual and practical motivations of the project, the proposed system architecture as well as current open questions. In summary, we seek computational renditions of scientific experiments aligned with statistical relevance theory and scientific intentionality[14].

12.2 The epistemological context of HoH and the *R-words*

Objectivity in all scientific work rests upon a complex intellectual structure cemented on self-criticism and responsibility, leading to honest commitment[15] to carry out work in line with the expected guidelines of *scientific intentionality.* As with other experimental disciplines, computational scientists seek to uncover *non-accidental objective truths* while remaining skeptical about outcomes, methods, and the structure of science itself. Repeatability, replicability and reproducibility belong to the set of communal norms of proper performance in science, preserving self-critical intentionality. We denote the class of norms belonging to *self-critical* intentionality as $\mathrm{INT}_{\mathrm{SELF}}$ as the root of a hierarchy that includes (or subsumes, $\sqsupseteq$) more specific forms of intentionality. We may also state that for $\mathrm{INT}_{\mathrm{SCI}}$, the class of norms delimited by *scientific* intentionality: $\mathrm{INT}_{\mathrm{SELF}} \sqsupseteq \mathrm{INT}_{\mathrm{SCI}}$. Subsumption here loosely corresponds to the operation in description logic bearing the same name[16], yet it can be also interpreted in a way analogous to that described across various theories of scientific explanation[17].

Self-criticism in science[15] may be classified into three different types:

1. the scrutiny of particular instantiations of scientific procedures to ensure they agree with scientific intentionality (*first-order self-criticism*), (PROC)

2. the scrutiny of the theories, laws, and norms derived from scientific intentionality that drive the definition of such procedures (*second order self-criticism*), (NORM)

3. and the acceptance of the failure of the theories, laws, and norms for the object of study in spite of all efforts to make them work (*third order self-criticism*). (FAIL)

These appear to work as *meta-norms* from which certain predicates can be formulated to determine if a given norm is operationally useful while at the same time the whole endeavor remains provisional. We call these meta-norms PROC, NORM, and FAIL, respectively. Clearly, $\mathrm{INT}_{\mathrm{SCI}} \sqsupseteq \mathrm{PROC}$, $\mathrm{INT}_{\mathrm{SCI}} \sqsupseteq \mathrm{NORM}$, and $\mathrm{INT}_{\mathrm{SCI}} \sqsupseteq \mathrm{FAIL}$.

Agreeing with scientific intentionality within PROC implies that at least a set of outputs is deemed as canonical (i.e., ground truths) and should be obtainable and usable for calibration and adjustment of the experimental setup under a given test sample (i.e., pattern), measurement system and apparatus; that outcomes produced by the experimental apparatus using non-test patterns are commensurate to those expected by theoretical calculations including measurement uncertainty; that they are obtained either by the research group that devised the experiment or other groups with the same specification; and that no outcome exceeds previously determined threshold ranges of numerical accuracy. Note that our definition of PROC is metrological[18].

The experimental setup in computational experiments includes test data, input data, the software utilized to obtain outcomes and the hardware platform utilized to run the software; the measurement apparatus is also a combination of hardware and software, and the protocol is the arrangement of computation and analysis steps. The contents of PROC are propositions that pose questions about the *experimental setup* (ε), the *research group type* (τ), and the *measurement system and apparatus* (μ). Hence, ε and μ are combinations of software and hardware artifacts.

Scientific intentionality in NORM is checked using sets of outcomes obtained by testing collections of propositions in PROC. The validity of specific hypotheses derived from statements of theories should not depend on particular realizations of experimental setups, but on some sort of collective adversarial verification[19–21]. Some norms in NORM may be stated in the form of propositions that generalize assertions in PROC by systematically varying ε, τ, and μ to gain information efficiently. We also suspect that NORM contains hierarchies of assertions about specific hypotheses and their connection to theories. While PROC provides inputs necessary for NORM , their intent is clearly different. This suggests $\mathrm{NORM} \not\sqsupseteq \mathrm{PROC}$, yet significantly more research is needed to ground this statement. Predicates in NORM appear to extend those in PROC by including a description of the theory-dependent method used in the experiment (η).

Similarly, but at the level of meta-statements about structures of theories and hypotheses, we suspect that FAIL contains predicates and some form of non-monotonic logic[22,23] that expresses universal-yet-provisional truths about the relation between structures and certainty. While it feeds on NORM, its contents and operationalization differ greatly since its systematics test properties of theories and hypotheses. Therefore, FAIL articulates concerns at epistemological levels.

12.2.1 Hierarchies of hypothesis: multi-level contingency structures

A hierarchy of hypothesis (HoH)[24] is a recursive structure of refinement for assertions driving a scientific research objective. Hypotheses also constitute evidence of contingencies in the process of theory building, impacted by the conditions of research as an outcome of some sort of organization[25], whether we speak about a laboratory, a certain scientific discipline or an emergent distributed research collaboration. HoH, when thought of as a data structure, stores knowledge about hypotheses as contingencies themselves: the rejection (or failure to reject) a hypothesis are contingent on whether measurements of an observable have an internal, representable structure that propagates statistical relevance upwards.

The structure of a HoH may be though of as a hierarchical arrangement of three types of hypotheses (Fig. 12.1):

- **Operational hypotheses**, when falsified, propagate certainty up to working hypotheses. Operational hypotheses usually correspond directly to experimental realizations and few observables upon which measurements are made and statistical quantities computed. In reference to computational experiments, we identify those with
- **Working hypotheses** translate between increasingly abstract statements towards overarching hypotheses and expectations over empirical observations; working hypotheses may comprise multiple levels of the HoH.
- **Overarching hypotheses** contain claims that speak simultaneously of generalizations over facts in a particular domain, of expected properties of their formal representations and of the methods of science in general. Overarching hypotheses are associated with generalized statements across theories, and require many experiments to determine their validity.

12.2.2 R-words and HoH in scientific intentionality

Back to r-words, existing definitions by the Association for Computing Machinery[26] map directly onto the types of self-criticism described above. First, their structure is similar to compound predicates that test properties of tuples meaningful within scientific intentionality. Second, the attributes of the description are in correspondence to the terms expected by predicates at each level. Third and last, the mapping does differentiate intentions between r-words and intents, correctly excluding FAIL. Table 12.1 provides the details behind each association.

REPEAT, REPLICATE, REPRODUCE$_P$, and REPRODUCE$_N$ are defined as top level predicate-generators that test compliance against specific proper performance metrics. REP$*$ then is the family

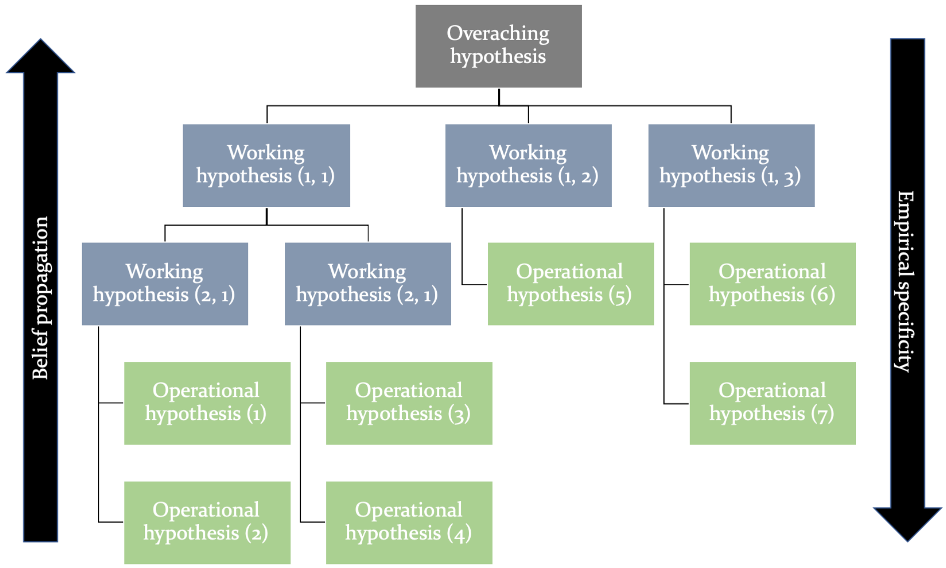

Figure 12.1: An abstract setting of a hierarchy of hypothesis with one overarching hypothesis, five working hypotheses and seven operational hypotheses.

of these predicate-generators REPEAT, REPLICATE, REPRODUCE$_P$, and REPRODUCE$_N$ that test scientific intentionality generally in computer experiments. The relation between all elements described in this section is depicted in Figure 12.2. We note that, under REP$*$, reproducibility splits between two scientific intentionality norms, consistent with the intuition that reproducibility conveys not only execution-level aspects but extends to abstract specifications of methods for any given hypothesis.

At this point, we are ready to articulate the HoH context. FAIL appears to naturally refer to the notion of falsifiability, in which the mechanism by which scientific discovery proceeds can be best described as adversarially maximizing efforts to reject a given operational hypothesis[27]. We must exert care in delineating when the falsification of a hypothesis corresponds to checking the stated choice between the null (i.e. H_0) or alternative (H_a) hypotheses; if the goal corresponds to the latter case, the process is a normative one, since no reference to an external object/meta-object framework (i.e. theory + *a priori* presuppositions) is made. The HoH approach

12.3 PRIMAD and the INT$_{\mathrm{SCI}}$ family

In an attempt to clarify the meaning and uses of the r-words, the PRIMAD model[12] assumes that various definitions of reproducibility can be captured less ambiguously by considering which aspects of a reproducibility study are varied (or "primed") and which remain the same with respect to the original procedural performance. The model looks at the (P)latform, execution environment and context, (R)esearch

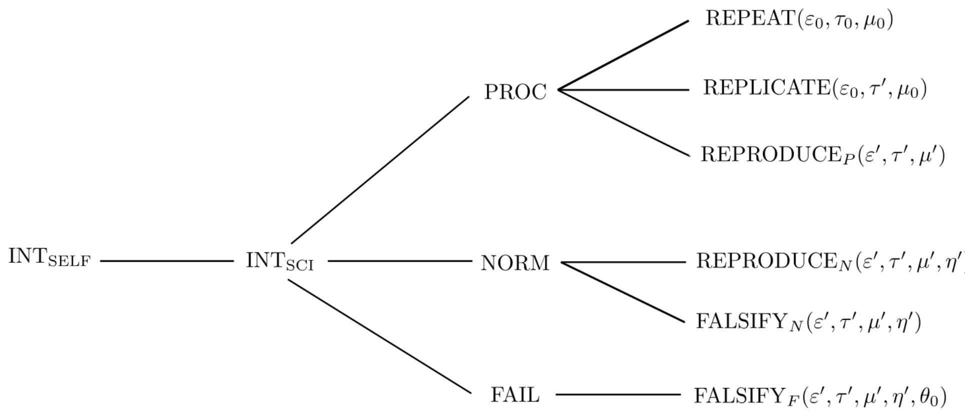

Figure 12.2: Subsumption hierarchy with elements of scientific intentionality (left and center; more general) and extended definitions of “r-words” and HoH terms (right; more specific).

objectives, (I)mplementation, (M)ethods and algorithms, (A)ctors/persons, and input (D)ata and parameters as principal aspects that can vary or remain fixed in a reproducibility study.

To perform a reproducibility analysis, variations can be obtained using various operations that yield an expected scientific *information gain* (IG). The operations are repeat (IG: determinism), parametric sweep (IG: robustness and sensitivity thresholds), generalize (IG: extent of applicability), port (IG: potential for re-use across multiple platforms), validate (IG: well-formed hypothesis), re-use (IG: potential re-purposing in other domains) and independent experimenter (IG: external verification). Most of these operations relate only to one model aspect, but some depend on two or more of them. For instance, validate implies changing the theory-dependent method which triggers changes from input data and parameters up to the implementation as well.

It is worth noting that experimental setups in computational contexts are more flexible in their definition of “sameness”. Even when the same software artifact appears to produce an output consistent with theoretically-derived expectations, additional care needs to be exercised[28]. The multi-layered nature of software contexts, spanning from accuracy of the hardware microprocessor to versions of libraries required to execute or compile research artifacts, requires a more fine grained treatment since less standardization is possible than in the case of bench-top lab equipment. In addition, most research-bound software contains numerical calculations whose accuracy depends on properties of hardware platforms, compilers level and external libraries required by the artifact[29]. This suggest research software practices need to become increasingly aware of reproducibility and enforce it[30]. More generally, reproducibility is a property of software sustainability[31] and a higher-order norm of proper scientific performance in order to prompt default behaviors and expectations aligned with scientific intentionality. Growing needs in this area call for efforts across the scientific community[13,32] beyond the scope of this report.

In the meantime, the assessments made by frameworks such as PRIMAD about what counts as part of the experimental setup and the related equivalence of executions using a single software artifact across a vast (and growing) landscape of computational contexts remain constrained to *ad hoc* criteria, often informed by parsimony as the decisive factor. Consequently, distinctions made in our approach consider equality between two experimental settings as long as the modifications that differentiate them only pertain to adaptations required to run in a given computational context (i.e. hardware, operating system, compiler, libraries, runtime utilities) instead of modifications that change any algorithmic or representational aspects required by the underlying science, provided sufficient care has been taken to avoid known pitfalls. While the latter is considerably coarse, it provides sufficient grounding for the purpose at hand.

The relation between PRIMAD and $\mathrm{INT}_{\mathrm{SCI}}$ can thus be established as follows. Repeat, parametric sweep, and port do not alter the fundamental character of the software artifacts and can be safely classified as operations that generate predicates under $\mathrm{REPEAT}(\varepsilon_0, \tau_0, \mu_0)$. Our definition of repeat does not refer to bit-wise identity of outcomes, but to statistical identity within specific error tolerance limits[33] in the light of increasingly diverse and approximate hardware platforms[34]. Once a software artifact is placed in an adequate execution environment, $\mathrm{REPLICATE}(\varepsilon_0, \tau', \mu_0)$ extends repeatability concerns by adding variation from other independent experimenter teams. If re-coding is performed, then the software artifact may be considered a new one and the predicates obtained in the process belong to $\mathrm{REPRODUCE}_P(\varepsilon', \tau', \mu')$.

PRIMAD also describes $\mathrm{REPRODUCE}_N(\varepsilon', \tau', \mu', \eta')$ through validation, since it is a change in the method that subsequently triggers changes in the data, the computing environment and implementation. Under the conceptualization derived from scientific intentionality and its types of self-criticism, PRIMAD effectively addresses concerns in both PROC and NORM categories. However, two operations appear to transcend these boundaries into FAIL. validate attempts to peer into the correctness (or *well-formedness*) of a hypothesis rather than on the material conditions leading to its empirical falsification, a concern orthogonal to the experimental setup; this is the very definition of $\mathrm{FALSIFY}_N(\varepsilon', \tau', \mu', \eta')$. Generalize operates by using the same software artifact for other purposes, assuming that the structure of the new problem is isomorphic to the original one yet under different constraints and theoretic presuppositions, thereby stating a fact about disconnected phenomena and possibly, about shared scientific principles or laws. In this case, we are in the presence of $\mathrm{FALSIFY}_F(\varepsilon', \tau', \mu', \eta', \theta_0)$ in which the hierarchy of hypothesis θ_0 refers also to the research objectives in PRIMAD.

In summary, our conceptual framework suggests that PRIMAD adequately captures some of the aspects involved in repeatability, replicability and reproducibility, that it can be extended to include fine-grained concerns in each predicate category, and that some of its elements make assertions beyond the level of an empirically verifiable hypothesis up to hierarchies of them. The reasoning in this and the preceding section motivated the natural question: can reproducibility and the hierarchy-of-hypothesis goals be integrated, and moreover, automated to any extent?

12.4 HoH-Companion: a tool for reproducible research on hierarchies of hypothesis

We now proceed to describe our design and ongoing work towards realizing the HoH-Companion architecture, targeted for use within The Whole Tale environment[13]. As such, we have chosen Python 3.6 as our primary programming language, given the extensive collection of openly available libraries and direct compatibility with Jupyter Notebooks[35]. We proceed to describe the design goals, system architecture and the execution model.

12.4.1 Design goals

HoH-Companion aims to facilitate the task of documenting, re-enacting and distributing hierarchies of hypothesis along with the software artifacts and data associated to each individual hypothesis when possible. In a sense, the intended user workflow is intended to allow users to construct *de novo* hierarchies of hypothesis, to re-execute all available computational experiments associated with an existing HoH, or to modify and test existing HoHs for didactic and research purposes. Also, it would be desirable to obtain unique signatures for HoHs based on some ontology geared towards scientific experiments such that inferences about lineages.

From the user perspective, using the HoH-Companion should provide as much information as possible from the existing HoH, while conveniently encapsulating computational experiment details when not needed. Succinctly, the HoH as a model needs to provide flexibility for queries[36] related to both the scientific and the execution content and context. HoH-Companion needs to be instantiated both as a library with a lean API that can be embedded across various infrastructures (e.g. the Whole Tale), or as a standalone Python application. In both cases, we estimate adoption depends on usability by researcher scientists, where usability may be defined as the ability to improve research outcomes with minimal intrusion.

12.4.2 System architecture

The architecture of the HoH-Companion relies on a diverse collection of modular components that provide actionable decisions at the hypothesis level. As in any contemporary software architecture, we attempted to maximize the separation of concerns from the development perspective while ensuring necessary functions are present. Fig. 12.3 summarizes the top level view of all components in HoH-Companion. We now proceed to describe each component individually.

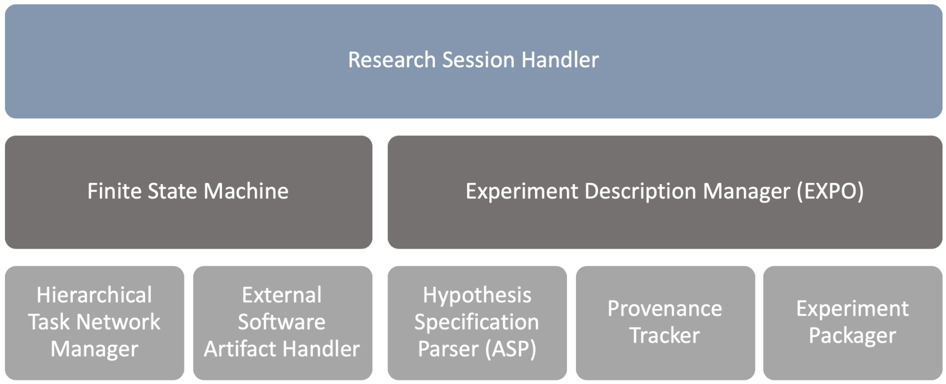

Figure 12.3: The HoH-Companion software architecture.

Research Session Handler The research session handler (RSE) allows users to interact in well-delimited sequences of internal tasks defined as *sessions*. Each session corresponds to a HoH project, a sequences of log entries with user, date and time, as well as checkpoints that indicate significant milestones with annotations. The RSE exposes the relevant API calls or commands (depending on whether access occurs through a library or the standalone program) for each step in the execution model described in the following subsection. Meta-commands allow users to save their current environment, to inspect any element of the current HoH and associated computational experiments, or to package its contents for redistribution.

Finite State Machine In order to provide reasonable safeguards when interacting with HoHs and experiments, the flow of execution and instruction exposure are guided by a finite state machine model. Formally, HoH-companion implements a Mealy machine[37]. Depending on a log level, setup by a meta-instruction in the RSE, events are logged and a transcript of the human-machine interaction (including state transitions) remains accessible at all times. While the use of a finite state machine to guide user actions may seem restrictive, it provides the convenience of avoiding a significant number of invalid or error states due to misconfiguration or other user-generated errors. We believe that a significant portion of scientific usability rests on the ability to avoid trivial mistakes leading to future significant rework.

Experiment Description Manager In order to document HoH and their associated computational experiments, we have chosen the EXPO ontology[38] as the primary terminological source. EXPO provides a deep categorization of research-related concepts and object definitions that makes it suitable for administrative, experimental and –to some degree of success- hypothetical descriptions. At present, ongoing research is directed towards devising a satisfactory language for describing a wide range of scientific hypotheses, since EXPO only provides textual representations of hypotheses, insufficient for a proper integration of outcomes from individual computational experiments.s

Hierarchical Task Network Manager The HoH is the core data structure onto which data and computational experiments are deposited and queried. In this sense, we draw from existing literature on Hierarchical Task Network planning[39] through a Hierarchical Task Network Manager (HTNM), which abstracts and decomposes planning problems as hierarchies of tasks as nodes. Nodes, to be satisfied, require either all (AND) or any (OR) of their children to be in turn satisfied down to the leaves. Additional horizontal dependencies may be established, and the tree-like structure provides a natural representation for hierarchies of hypothesis. In relation to epistemology, establishing a hierarchy of hypothesis is a form of planning, where the plan inputs are given by estimations of where the "low hanging fruits" exist. In our case, nodes also act as specifications for the required execution environment when hypotheses are operational. Consistent with a Bayesian view of statistical relevance, statistics related to falsification of hypotheses upstream is performed recursively[40].

External Software Artifact Handler Internally, each node in the HTNM contains a reference to a data structure that holds all details required for a computational experiment to execute, such as library dependencies, initialization scripts and possibly links to external services. This structure, named the External Software Artifact Handler (ESAH), follows the philosophy of research objects[41] to improve reproducibility. In this sense, a computational experiment is an executable sequence of research objects.

Hypothesis Specification Parser Specification of hypotheses along any HoH may occur during an interactive session or through a formatted file. At present, work is directed towards designing a Hypothesis Specification Language whose expressions can be parsed through API calls or by reading plain text files. Once a hypothesis has been parsed, the HoH-Companion facilitates cataloguing the hypothesis as operational, working or overarching. All HoHs must contain at least one operational hypothesis, which overrides all other classes when it is the only one present.

Provenance Tracker All involved research objects must ensure proper provenance information to guarantee traceability[42,43]. The Provenance Tracker summarizes all metadata associated with research objects across all hypotheses and provides a score, analogous to other badging approaches[44], that quantifies the proportion of research objects for which provenance can be adequately asserted and how that contributes to the overall statistical certainty of the HoH.

Experiment Packager Finally, once an experiment reaches at least the state of falsified in the execution model described below, the Experiment Packager ensures all relevant information is gathered, referenced and saved into a file that can later be parsed by the same user or a third party.

12.4.3 Execution model

In HoH, the archetypal execution process is mediated by a Mealy machine as a means to reduce (or ideally eliminate) situations where users may improperly configure the HoH. At each step, the finite state machine will produce a record of events, including suggestions depending on the current state of configuration or executability of the instantiated HoH. Fig. 12.4 captures the process described as follows:

1. If HoH-Companion is initialized without parsing an input file, its state is considered as Initialized.

2. Scientific users perform administrative annotations that help preserve data provenance. Users document themselves, relevant literature and all hypotheses on the HoH. In addition, provenance information is either parsed or captured interactively for all research objects. When the above occurs or an initialization file is successfully parsed, the HoH is considered as **annotated**.

3. The HoH is ready to be specified by adding hypotheses and determining their hierarchical placing. At this point, the hypothesis specification language is used to define observables and the conditions they must meet. At this stage we also provide two models of propagation of falsification outcomes: a purely binary model that depends on the nature of the HTNM nodes, and a Bayesian model that pushes statistical relevance upwards. When all hypotheses are added (including the case when these come from a correctly parsed file), the execution state is marked as **stated**.

4. A stated HoH can then be decorated with software artifacts using the ESAH component. Provenance is asserted for each component and all relevant research objects are included, either by direct copy or by a working reference. Observables from research objects are then specified and connected to those indicated across operational hypotheses. Similar to the previous cases, successful decoration lead to the instantiated state.

5. The instantiated HoH can then be executed in bulk or in a step-by-step manner. Operational hypotheses are executed depending on the restrictions provided by the HTNM. This is an inherent strength that can be leveraged by cleverly specifying HoH hierarchies such that hypotheses most susceptible to

be falsified are executed and propagated first. Although we suspect HoH specification may allow automated reorganization to avoid lengthy computations that ultimately fail, no work has been performed yet towards this end.

6. When all hypotheses have reached the **falsified** state, aspects of the HoH can be changed (resetting the state to **annotated**) or the experiment can be branched (a copy is created in memory with option to save to disk, setting the state as **branched**). The main difference between a branched experiment and a falsified one is the ability to perform differential tests between both HoH instances.

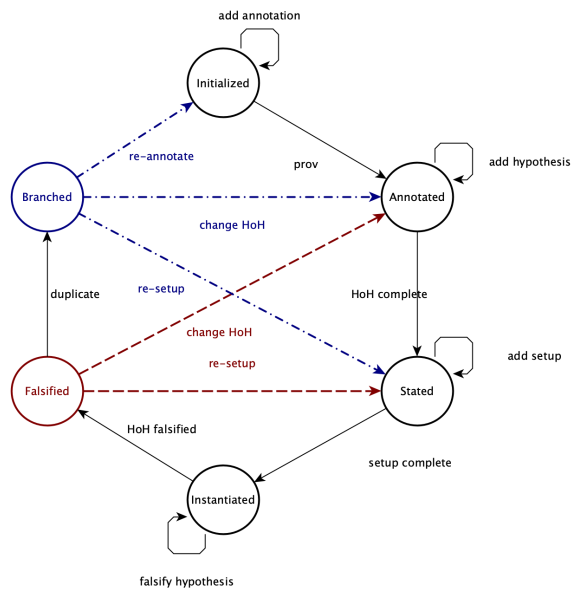

Figure 12.4: A finite state machine underlies all internal mechanics of the HoH-Companion.

12.4.4 Current status

At present, all elements of the HoH-Companion have been specified and development work has started using the iDAKS GitHub site[ii], managed by the School of Information Sciences at the University of Illinois at Urbana-Champaign. Pertinent libraries have been identified with the purpose of facilitating software carpentry tasks and some boilerplate code has been implemented. We are in the process of defining two test cases in connection with the biological sciences.

[ii]See: `https://github.com/idaks/HoH-companion`.

12.5 Conclusions and next steps

In this paper, we tackled two objectives: to better understand the role of repeatability, replicability, reproducibility and hierarchies of hypothesis in terms of the epistemology defined by scientific intentionality, and to devise a preliminary specification for the HoH-Companion, a tool ongoing development that aims to facilitate not only document HoHs, but to re-enact them for various purposes.

We first described an alternative road to the clarification of the r-words *repeatability*, *replicability*, and *reproducibility* in computational experiments by using *scientific intentionality* as the guiding compass and PRIMAD as a case study, and later including HoH as a broader context in scientific intentionality. The results obtained through this process suggest that the methodological choice is potentially robust, yet it needs to be properly formalized and developed. However, its ability to map simultaneously onto epistemological and practical concerns in abstract terms, as well as its ability to be applied to a concrete case make it a promising path to follow.

Later, we provided a design for a tool that aims at documenting and automating the ability to reason using hierarchies of hypothesis. While ambitious in scope, we estimate that the development and testing of such tool is not only feasible, but can be accomplished within a reasonable time frame with reasonable resources. As a result of the joint RDA/US-Whole Tale Data Share and Early Career Fellowship, we are exploring possible funding sources that would permit extending development beyond what is possible in a prototype phase of one year. Our analysis suggests that even a simple prototype can bring significant advantages to scientific users across the research spectrum. Most of the modules in our specification can be rapidly implemented thanks

Several theoretical and practical questions remain open on both the theoretical and applied fronts. The boundary between procedural reproducibility and normative reproducibility obtained through our method needs to be explored in depth, since it has direct implications for assessing inferential robustness in hierarchies of hypotheses: multi-method testing of specific hypotheses tends to strengthen the conclusions of top-level ones[40,45]. Only a few predicate-generating operators have been identified through PRIMAD and much of the landscape remains uncharted. Elucidating the extent and features of those classes may prove critical to understand the boundaries of each definition as well as how to automatically generate and test new reproducibility frameworks such as PRIMAD. Finally, building software to help researchers determine the degree of compliance of their software artifacts with scientific intentionality may be facilitated and made robust once an operational theory of repeatability, replicability and reproducibility is achieved.

With respect to the HoH-Companion, the lack of a sufficiently developed description language for hypotheses was surprising. Automated reasoning systems are a well-consolidated area, but applications to representation of scientific hypotheses remains scarce. Along with other aspects in need of exploration, devising an adequate hypothesis specification language remains our top research priority.

12.6 Acknowledgments

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Classification	Definition	Predicate Representation	Self-Criticism Type
Repeatability (ACM)	"The measurement can be obtained with stated precision by the same team using the same measurement procedure, the same measuring system, under the same operating conditions, in the same location on multiple trials. For computational experiments, this means that a researcher can reliably repeat her own computation."	REPEAT$(\varepsilon_0, \tau_0, \mu_0)$, $\eta = \eta_0$	PROC
Replicability (ACM)	"The measurement can be obtained with stated precision by a different team using the same measurement procedure, the same measuring system, under the same operating conditions, in the same or a different location on multiple trials. For computational experiments, this means that an independent group can obtain the same result using the author's own artifacts."	REPLICATE$(\varepsilon_0, \tau', \mu_0)$, $\eta = \eta_0$	PROC
Reproducibility (ACM)	"The measurement can be obtained with stated precision by a different team, a different measuring system, in a different location on multiple trials. For computational experiments, this means that an independent group can obtain the same result using artifacts which they develop completely independently."	REPRODUCE$_P(\varepsilon', \tau', \mu')$, $\eta = \eta_0$	PROC
Reproducibility (extended)	The measurement can be obtained with stated precision by a different team, a different measuring system, in a different location on multiple trials. For computational experiments, this means that an independent group can obtain the same result using artifacts which they develop completely independently *and under different theoretical methods*.	REPRODUCE$_N(\varepsilon', \tau', \mu', \eta')$	NORM
Falsifiability (Popper)	A specific operational hypothesis can be falsified by a different team, a different measuring system, in a different location on multiple trials. For computational experiments, this means that an independent group can reject or fail to reject an operational hypothesis using artifacts which they develop completely independently *and under different theoretical methods*.	FALSIFY$_N(\varepsilon', \tau', \mu', \eta')$	NORM
Falsifiability (HoH)	A hierarchy of hypothesis can be falsified by one or several teams, a set of different measuring system, across different locations on multiple inter-related trials. For computational experiments, this means that one or more independent groups can reject or fail to reject hypothesis whose structure is hierarchically dependent using artifacts which they develop completely independently *and under different theoretical methods*.	FALSIFY$_F(\varepsilon', \tau', \mu', \eta', \theta_0)$	FAIL

Table 12.1: Mapping between different "r-words" and self-criticism types in scientific intentionality. Definitions in quotes are from[26]. Terms with subscript 0 $(\varepsilon_0, \tau_0, \dots)$ indicate that the *original* experimental and analysis setup as well as the research team are considered, while primed terms $(\varepsilon', \tau', \dots)$ indicate a new (*verifier*) setup.

Chapter 13

Some Considerations Toward a Predictive Theory of Life

Summary[i]

Current understanding of the massive complexity of life suggests the existence of an intricate world of interactions both below the ecosystem and above complex biochemistry. That particular cosmos of the organism has proven hard to untangle due to three key factors: the difficulty of reconstructing the past from traces left in the present, the dynamic nature of changes across multiple interacting scales and the contemporary, overall process of scientific discovery in the life sciences. By appealing to the integration of frontier research lines in the biosciences and a revision of the epistemology around the organism, some considerations are drawn towards the possible meaning –and form- of an integrated theory of life.

13.1 Introduction

Biology has been transformed in the last six decades thanks to three pivotal events: the consolidation of Darwinian evolution by natural selection as the overarching phenomenology behind the massive improbability of living organisms[1,2], the rapid increase in the available quantities of information and its associated semantics about an ever-widening horizon of biological entities, from the molecular to the behavioral[3], and the growing data processing infrastructure destined to cope both with the volume and the interrelatedness of biological data[4]. The organism sits in the middle of two extremes: at one side, biophysics determines the immediate dynamical background of molecules and structures critical to living systems; at the other side, the persistence of information across a wildly complex array of interactions that spans almost four billion years by now. Finding good explanations that transcend a traditionally mechanistic perspective on organisms, these very ontologically compact collections of molecules and history, seems critical towards a better picture of life in this century[5].

In the transition from the descriptive to the explanatory, and further to the predictive, theoretical excur-

[i]**Núñez-Corrales, S. Some considerations towards a predictive theory of life**. Book chapter to appear in *Understanding Molecular Biodiversity*, Gustavo Caetano-Anollés (Ed.).

sions have become prevalent in the pursuit for an integrated theory of life despite known adoption difficulties often experienced by the experimentalist[6]. It is thus widely acknowledged that fundamental advances in experimental biology will not be possible without falsifiable theories and models that promote intuitions to system-range statements[7]. Systems biology, starting from the rational decomposition of organisms into simpler units exhibiting emergence, robustness and modularity[8] has become instrumental in providing a growing scaffold for theoreticians and experimentalists to express and test hypotheses, from description languages[9] to the characterization of information flows in regulatory networks[10]. In the language of category theory[11], we are after generative effects[12] that arise in organisms due to their compositionality. Such perspective has been explored in the past through the conceptualization of memory evolutive systems, for which Ehresmann and Vabremeersch[13] constitutes a seminal reference.

The central challenge that system biology faces towards an integrated theory of biology resides on the classes of questions drawn at three recognizable interfaces: the genome (questions about phylogeny), the organism (questions about ontogeny) and the environment (questions about external evolutionary operators)[14]. Ferrada and Wagner[15] brought to light one of the most critical unsolved issues in the field in connection with the three interfaces: evolution is multilevel, multivariate and overall, exceeds the conceptual simplicity of tree representations thanks to the concurrent nature of events, being more akin to how intermediate molecular entities traverse a highly dimensional –and at the same time- non-deterministic collection of potential surfaces[16]. Despite all difficulties, posing the problem of systemic evolution of organisms that share common ancestry but are exposed to different conditions in a more evolutionary neutral language provides a unified framework for interrogating nature about its apparent global two-component structure: the interplay between biochemistry (very short timescales) and heredity (very long timescales). Such a high-level view, at the same time, makes causality difficult to identify[17], in particular when events are non-linear and systems are not in equilibrium[18].

13.2 Biology and the scientific method

Understanding life involves addressing a dual problem: disentangling the complex relations to approximate a tree of life and, conversely, determining the accuracy in which trees are snapshots of the dynamic fabric in which evolution by natural selection operates[19,20]. In that sense, it is essential to take a step back into epistemological grounds with the goal of finding a more general (and possibly powerful) common language to describe evolutionary complexity[21]. First, it must be stated that within biology –as an intellectually efficient interpretation of reality from the point of view of complex interacting entities- a reasonable goal is to center the attention in the organism as the topmost relevant hierarchical modular system that bears recognizable interactions with the environments, in the sense that any other higher level system often depends on rules that involve some form of symbolic information representation, processing and communication instead of purely biological and biochemical events[22]. Sets of physical symbols (i.e. organized matter and energy) are used to encode predicted future chains of events that have some particular value under known selective pressures. The prevalence of boundaries of individuality in both unicellular and multicellular organisms through selective membranes is likely driven by their evolutionary advantages as a general solution to both internal stability in the sense of maximum entropy production as described by Martyushev and Seleznev[23] and resilience through anticipation of various kinds[24]. Second, general systems theory (GST) provides a substrate-agnostic framework for reasoning about biology from the vantage point of components and processes within the organism: it is an attempt to canonically describe sets of interacting elements for which a description of its dynamics can be elicited[25].

Systems biology as a whole is not only inspired in GST, but is also heavily informed by its methods, theories and philosophical underpinnings[26]. As with any Popperian approach to science, GST allows postulating falsifiable arguments through a new dialectic: the complex entities are queried by asking questions in their language (e.g. biochemistry, genetics, epigenetics), then their answers are assessed and finally a conceptual ontology of theories –not just one theory- is then tested against further evidence[27]. This interplay, or rather conversation, can proceed within the intellectually neutral grounds provided by novel arsenals in mathematics[28] capable of preserving original strengths of the hypothetico-deductive model while reaching more ambitious goals.

The hypothetico-deductive model of science is still the core of scientific discovery across the life sciences[29]. More precisely, this systematics of research pervades the existing conceptions about mechanisms used for investigating organisms within the broader horizon of the life sciences, and is assumed to spread into neighboring disciplines[30]. Following such path, biology has arrived to a point where the construction of theories, to a first approximation, spans a spectrum defined by two properties: explanatory power (from more specific to more general) and experimental accessibility (Figure 13.1). While at the moment any classification such as this one is somewhat arbitrary, one property holds for (almost) all theories: they depend upon "sloppy" models that focus on a single explanatory layer. These models make drastic simplifications in order to be tractable[31]. Sloppiness is a strong limitation, since model distinguishability becomes harder as more complex monolithic models arise (e.g. large number or parameters that require fitting), thereby the information that may be obtained, the probability of its experimental falsification and its explanatory power are diminished. Increasingly detailed modes towards high-accuracy predictions often backfires and yielding models that are proportionally hard to calibrate.

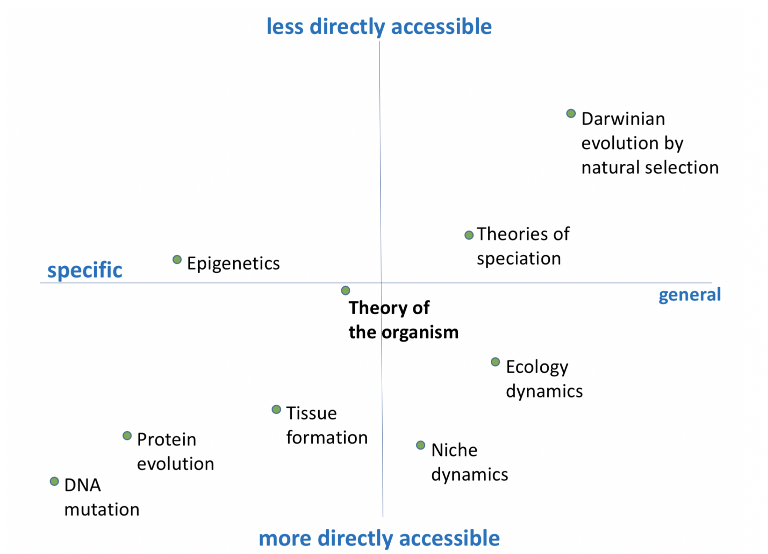

Figure 13.1: A conceptual, approximate classification of biological fields of enquiry in two parameters: explanatory power (horizontal axis) and experimental accessibility (vertical axis). A theory of the organism (center) stands in a pivotal position between the specific and more accessible molecular world and the more general and indirect level of explanation provided by evolution by natural selection.

Part of the problem comes from the expectation that single layer models will suffice to meaningfully probe the structure of a multi-layered structure. The formal language used most often for describing statistical hypotheses, the frequentist approach to probability[32], is to blame in many of the artificial limitations brought into the falsifiability process, such as well-known issues with p-values[33]. These artifacts permeate simple models (for instance, by fixing confidence intervals incorrectly when model aspects are related to otherwise complex and dynamical environmental conditions) that negatively impact the quality and soundness of the inferences. For instance, simplistic information-based models of the molecular clock leave plenty of room for interpretation, while models that also account for biophysics and biochemistry are needed to place events at realistic evolutionary distances. Why do these artifacts arise at all in the first place? One plausible explanation in the latter context is that, because the parameters describing a variable landscape of microscopic states pertinent to organismal internal dynamics are crudely approximated by macroscale constants contained in deterministic continuum models. Many of these models the lack phenomenological accuracy required to describe responsive systems near thresholds, thereby producing bogus information[34]. One solution may be the use of hierarchically nested, coupled systems of Fokker-Plank equations as a more realistic approximation that captures variations in the probability distributions governing such parameters within organisms, and then using such stochastic parameters to more fully describe dynamical couplings across scales[35]. It is likely for similar alternatives to arise as means of removing artifacts by acknowledging the inadequateness of continuum deterministic descriptions for certain classes of phenomena. At present, this remains an open research question.

Another part of the issue belongs to the nature of the hypothetico-deductive method itself. First, it is subsumed by a more general category known statistical relevance in which multiple propositions, with an assignment of probability related to their falsification, can be expressed and simultaneously attacked[36]; the model summarizes to a great extent the conception of scientific theories after Kuhn (Figure 13.2). Statistical relevance allows the falsification of an arbitrary number of concomitant propositions to be tested simultaneously without sacrificing explanatory power. However, it remains limited due to a number of underlying assumptions about what it means for an explanation to be coherent[37], a notion largely constructed upon principles derived from single-scale cases. In addition, the place of computational simulation in the context of the scientific method -and in the hypothetico-deductive method itself- necessitates better demarcation[38], yet many of the contemporary assertions made about organisms depend crucially on computational renderings tied to hierarchies of hypothesis. Modeling and simulation have proven in practice to be fundamental tools for understanding the intricacies of organisms (and of other systems in general) by appealing to abstractions that can be empirically refined[39]. Constructing integrated descriptions of organisms will also contribute to expanding the scientific endeavor as a whole. Recent work compiled by Jenschke and Heger[40] on hierarchies of hypothesis (HoH) in ecology sheds light on how to tighten outcomes produced by the hypothetico-deductive method, and it is reasonable to expect HoH methods to be applicable to the organism itself. However, HoH only addresses some of the gaps in the hypothetico-deductive method without extending it.

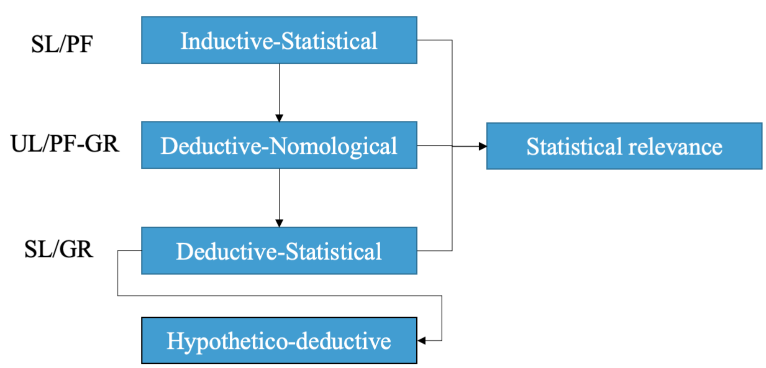

Figure 13.2: The hierarchy of scientific theories after Thomas Kuhn and their relation to the Statistical Relevance model of science. Nomenclature: SL – statistical laws, UL – universal laws, PF – particular facts, GR – general regularities.

13.2.1 Probability in modern biology

Let us consider another epistemological route. Conceptualizing the biology of organisms at multiple levels may benefit from the ideas and methods found in the study of Langevin dynamics[41] and stochastic methods in general. Instead of focusing on a single trajectory or state of an entity, stochastic methods attempt to find properties of collections of entities that are identical except in their initial conditions (Gibbs ensembles). Entities or phenomena are also described at two levels: a set of microstates governed by some dynamics, and a macrostate (i.e. a collection of average values for the ensemble) that can be measured for which some regularities can be expected. Since the number of microstates is often considered to be large, reasoning in terms of probability becomes inescapable. The term stochastic implies that the forces behind the dynamics contain both deterministic (e.g. gravity, chemical gradients) and random (e.g. photon emission, stochiometric variability) components. In structural biology, using Langevin dynamics has been successful in providing insights about polymer translocation through nanopores[42], the flexibility of cytoskeletal fibers[43] and more recently modeling transition kinetics in DNA[44].

What the former examples have in common is that no individual outcome pertaining to states or trajectories in either entities or their constituents qualifies as an adequate representation for a given phenomenology. This is particularly highlighted by the complexity and richness found in biological system, where compositionality takes precedence over single-scale phenomena and a collection of histories and interactions is needed as a starting point for explanation or prediction. Biological sciences may gain access to larger pieces of the intellectual land by finding global properties within ensembles describing organisms, stated as probability distributions tied to outcomes that can be obtained either from first principles or estimated from experimental measurements. In this scientific view, understanding an organisms involves considering not one but many probable outcomes.

Can a deeper link between the observable discrete diversity of life and chance be found? To a first approximation, let us consider organisms as responsive systems with complex hysteresis. Organisms evolve thanks to natural selection to converge to a finite set of preferential states, likely those granting stability and fitness[45]. Some states correspond to internal representations of environmental variability and how to successfully cope with it[46]. Other representations encode useful information received from other organisms that, given the similarities in biological processes, point to triggers for various types of decisions, or proximal threats or opportunities; quorum sensing constitutes a prime example[47]. The more successful an organism becomes, the more reversible its hysteresis becomes (i.e. the more likely it is to return to some steady state at the macroscale). Repeated success (i.e. survival and reproduction) leads to an embodied form of guessing relevant probability distributions of events at the organismal level, and energy constraints refine the resulting encodings to be economical in the long term. Natural evolution thus exemplifies a missing piece in information theory as described by Shannon[48]: the mechanisms by which communication infrastructure emerges such that it possesses its expected mathematical properties.

Organisms have evolved to function within a certain class of signal-to-noise ratios sufficiently large to produce new dynamical biasing components by harnessing thermodynamic forces[49,50], but at the same time sufficiently small not to completely disrupt their structure[51], producing a form of self-organization with preference for stable states and threshold handling mechanisms[18] that increasingly shields structure and function from fluctuations. For instance, the biophysical context is extremely important at the onset of the protein folding process but becomes less and less significant as structures converge towards one stable form or another[52]. The same mechanism appears to be present in other instances in the form of stochastic molecular switches that determine the fate of development in organisms[53,54]. In particular, individuality may well be considered the hallmark of the stochastically guided architecture of life, optimized for surviving multilevel organismal selection[55]. While the role of probability is many-fold within biology, the ability to harness it towards better understanding of the organism remains somewhat unexplored. The patterns of biological connectivity in the organism as a network of interactions, the role of thermodynamical irreversibility across its scales and the semantics behind what constitutes a prediction require much deeper excursions. Moreover, capturing the variation of probability distributions with time and using that information to refine predictions may be a promising road to uncovering the specifics during biological interactions.

13.3 Promising paths: joining visions of the organism

Once the theoretical landscape around current problems and possible general solutions to the knowability of organisms has been laid out, the advancement of fields that comprise systems biology as the currently most effective theoretical framework for understanding life are worth reviewing. In the following discussion, three components are of interest: phylogenomics (history of the information contained in the organism), structural bioinformatics (conditions of the expression of organismal information) and networks (relationships across those instances that feed back into existing information). While the present review is by far not exhaustive and restricted to genetic or structural information, it is representative of the classes of problems that reasoning about organisms brings to the surface for which progress can be sustained (hence the qualification of promising).

13.3.1 The accuracy of phylogenomics in the context of living systems

Inferring paths of molecular evolution for arbitrary genomes across long periods of time is hard due to the difficulties involved in tracing the impact of particular events and environments on populations or species in the distant past[56] (Breen et al. 2012). Despite such difficulties, a safe common ground exists on the concept of homology: conserved sequences (or features) are evidence of common ancestry[57]. Homology thus allows the construction of phylogenies by proposing candidate ancestries for a given set of organisms based on premises such as, for instance, the equivalence between observed frequencies of nucleotides or amino acid substitutions and biochemically plausible mutations.

Viewing biological information units at various levels across the organisms drastically increases the number of possible landscapes available for searching putative histories at the genome level. This is especially so thanks to the reticulation of collective histories caused by lateral exchange mechanisms permeating all evolutionary relationships. Speciation occurs when significant divergence takes place between members of a species sharing common ancestry and traits[58], yet reticulation can make this limit diffuse[59]. Some events might impact the whole genome, part of it or only individual genes or domains. Determining each of which was the most probable cause can be determined only up to a certain degree of accuracy through careful phylogenomic analysis. Care, in this case, must be interpreted as the systematic elimination of unnecessary ad hoc hypotheses while remaining open to alternative explanations, later to assess which of them best fits the evidence and which of them to discard. A particularly illuminating example is exemplified in the use of synteny as a tool for understanding claims about whole-genome duplication events of Saccharomyces cerevisiae in two different organisms, *Ashbya gossypii* and *Kluyveromyces waltii*[60,61]. A closer look to prior analyses claiming whole-duplication events occurred in S. cerevisiae revealed discrepancies (such as the low proportion of synteny across all the genome, not just particular chromosomes) indicated that the claim is not plausible and that partial-genome duplication is more parsimonious with respect to the number of steps required to transform one genome into another[62].

During the reconstruction of ancestries, hypothesizing about events with larger conserved regions simplifies the overall analysis process at the expense of biologically meaningless or wrong answers when multiple unknown factors intervened to preserve them. Multiscale interactions often explain these classes of issues, and therefore should not be ignored. How granular should the analysis be in order to obtain realistic results? A potential answer is proposed in DRIMM-Synteny[63] where a computational device, namely the A-Bruijn graph is used to detect synteny patterns at finer scales. While its results have shown effectiveness in detecting more evolutionary conserved segments across species than other tools, a mapping between biological events and the the semantics of the computational process is missing. For instance, there is no attempt to include structural domains in protein-coding genes in the analysis, a fundamental step according to existing knowledge about the conservation of function by virtue of increasing the fitness of the organism when an innovation is not deleterious.

Growing amount of data in molecular biology also brings a concern of practicality: can valid and accurate reconstructions be achieved by increasingly automatic means? The exponential-over-exponential trend of genomic information growth points to an apparently hopeless task for humans alone[64], many decision steps seem tied to human expertise. One of the automatic reconstruction algorithms that attempts to bridge the gap between data excess and automation of phylogenomics is SYNERGY, which has proven successful in explaining gene duplication and loss through various mechanisms in fungi through various mechanisms[65,66]. The introduction of two key elements, namely a novel method for computing gene similarity and the measurement of putative orthogroups, explains the success rate of the algorithm when compared against annotated data.

13.3.2 Structural bioinformatics: function robustness in a sea of opportunity

Plausible operational hypotheses must not only explain how existing genes have moved across known or potential ancestors through known mechanisms, but include suitable mechanisms for accounting for new genes that gradually appear in the population; bacteria have been central for studying molecular evolution both theoretically and experimentally due to their wide diversity[67]. An interesting model of de novo gene birth from proto-genes suggests, for example, that the distinction between genes and proto-genes is not clear cut, rather being closer to a continuum[68]. These types of models not only are critical for explaining evolutionary innovation triggered by de novo gene generation, amplification and divergence along the history of particular species[69]; they allow distinguishing between tensions arising between innovation by caused divergence and those due to duplication[70].

Sometimes, the history of evolutionary innovation can be harnessed by organisms to fullfil certain functions, such as driving their early development stages. The parallel between phylogeny and ontology found in zebra fish is a striking example: in an hourglass manner, each developmental step exhibits a positive correlation between the transcriptome age index (i.e. a measure of how ancient the expressed genes are present at a certain point) and the abundance of the relatively recent genes in a particular species[71]. The fact that those genes consistent with the hourglass model are also central to the organism developmental processes is striking in several ways[72]. First, genomes do show flexible expression while remaining relatively stable across generations and populations. Second, the more conserved repertoire of genes appears to be modulated by de novo genes, providing flexibility; this appears as if old encodings can be repurposed by introducing new tokens that rebalance the probabilistic information landscape across the organism. Third, that flexibility allows changes that might be beneficial while providing enough robustness to cope with potentially negative consequences at the species level.

Reconciling this apparent tension between change and stability in molecular evolution requires extending views around the building blocks of life -such as proteins- in terms of how structure and function are intertwined. Drawing from research in organization science[73], both structure and function are analogous to routines established across organizations: they emerge as sustained patterns of repeated interactions, they provide a scaffolding for safe platform to undertake larger explorations capable of bringing useful novelty, and they admit both ostensive (i.e. abstract specification) and a performative (i.e. particular instances) descriptions that separate timeless and time-full reasonings. Both structure and function in organisms are responsible for both ensuring stability and endogenous change and can be encoded and exported to other organisms and species. In that case, the interpretation of the ostensive description within the origin organism may radically differ from the interpretation of that to which structure and function have been exported.

In organisms, structure is determined to a large extent by a degenerate coding scheme (multiple codons per residue) and a hierarchy of structural arrangements that can assemble into similar shapes despite having very different constituents. As in the case of phylogenomics, cladistics can be applied to the secondary structure of proteins in order to determine whether new classifications match annotated data, and to which degree of accuracy[74]. The results of such exercise hint at another way in which nature provides a fertile ground for variation: even with a limited number of motifs and combinatorial rules that operate in a biochemical context, many structures are possible in a sea of possibility. The sea seems not to be, however, unbounded or continuous. Simplified backbone-based models of protein folding indicate that self-organization does occur within a limited (and possibly dense) set of structural constraints[75]. While certain biophysical facts are oversimplied (for example, exaggerating the role of hydrogen bonds beyond experimental observations), they appear to have some bearing in this issue when contrasted with the identification of families, superfamilies and hyperfamilies of structures in proteins. A limited but well-connected repertoire of structures explains a large share of protein structures and functions, in particular when biophysics is explicitly included in the quantification of structural similarity[76].

However, current understanding of the relation between structure and function remains limited by limited amount of data for protein structure as well as the computational complexity of performing structural comparisons. Moreover, since not all proteins can be (yet) brought to a stable crystal structure suitable for experimental analysis, the universe of observable folds remains restricted. Despite these limitations, the growth rates of databases such a SCOP and CATH[77] suggests at least that a significant portion of the fold universe has been already covered. The second challenge appears to depend only on two factors: cost and availability of computing resources and the quality of the algorithms for structural comparison. Since cost constantly decreases thanks to Moore's Law, most of the advances are expected to come from the development of new and efficient algorithms. A representative example is the application of advanced techniques such as using Gauss invariant integration kernels for measuring distances in atomic coordinate space has gained traction in biology[78], and outperforms RMSD in efficiency. Finally, several new crystallographic methods[79,80] have shown that more types proteins can be resolved under the right conditions.

Another way of attacking the folding problem is via structural grammars, an avenue suggested in the past and recently revisited[81]. A basic set of symbols and rules (i.e. folds and self-assembly affinities) is assumed to be ancestral and structural complexity is derived by applying the rules to the symbols. For example, hypothesis of a prebiotic RNA-peptide world appears to match an scenario in which RNA combined with freely available peptides in order to gain structural stability at first, and later a large portion of the universe of known proteins emerged through repetition and variation of domains taken from the primordial vocabulary[82]. When folds are clustered into galaxies according to similarity either in sequence space or structure space, hypothesis of a limited set of initial origins for all proteins arises naturally[83]. An even more idealized model is that of a periodic table of folds where self-organization drives protein assembly, yet the rules operate locally on folds and depend on the particular shape and structure of the fold elements[84,85].

Structure is the substrate for the manifestation of function, hence function evolution depends on biophysically available structures. Elementary loops and elementary functional domains in Archaea support the prebiotic peptides hypothesis[86], the hypothesis that elementary functional loops were among the first elementary reactions available for biochemical transformation, constituting the first building blocks of existing protein functions. The study of enzymes becomes thus central, since catalysis is fundamental to the biochemistry of life. For an elementary functional loops, being highly designable (for which a plethora of sequences might exist) tends to correlate with being more fundamental[87]. However, how can innovation happen where robustness and degeneracy are prevalent? The analysis of the relations between genotype space and structure space reveals that diversity of unique functions occurs even within close neighbourhoods in genotype space (i.e. similar sequences), and diversity increases dramatically only when their corresponding sequences differ at least by 80-90%[15]. Even simple in silico experiments where short binary sequences of idealized amino acids are subject to the action of simple canonical potentials indicate that innovation can happen, but certainly not at the expense of survivability[88].

An explosion in variety and possible innovation seems to be counterbalanced by a massive systemic coding redundancy across all levels of the organism. Back to information theory and probability, this an error-correction mechanism of sorts that treats structure and function as signals and ensures the encoding is preserved within some acceptable noise level. However, natural selection constantly replaces existing encodings by more efficient ones when these are found across many levels, all at once. Understanding structure and function at the genomic level necessitates remaining aware of their couplings across organismic scales.

13.3.3 Network theory: the path beyond trees

A surprising feature of living beings is their ability to survive in a wide range of extremes[89]. They exhibit inherent robustness to mishaps, unexpected changes and any other threats. If an organism may be abstracted as a complex system for which a network is a good representation, survivability may be translated to the capacity to withstand failures and attacks[90]. In this setting, failures are random removals of edges, and attacks are random removal of vertexes, mostly improbable but catastrophic events. Consider the effect of inhibiting the expression of an arbitrary protein in a cell at the level of DNA transcription. Recalling that proteins and functions are tightly related, the latter is equal to losing one or more functions. If the protein belongs to the essential part of genome, blocking its expression most probably affect organismal survivability except in two cases: when other proteins perform the same function, or when other sequences encode the same protein. Essentially, surviving loss of functions would be reducible to preserving reachability in the network of molecular products in the essential genome. The same argument can be extended to higher levels (e.g. cells, tissues) in terms either of adaptation of existing components or alternative encodings for them. From many possible topologies (arrangements of vertexes and edges), scale-free networks are robust with respect to large quantities of failures, but are vulnerable to attacks. An example of this are metabolic networks[91]. An evolutionary rationale can be constructed in the following way: random challenging events have been mostly already selected by evolution (failures) at great cost, which pushes for good the preservation general solutions; on the contrary, disruptive events that force either innovation or extinction come at the expense of navigating again through the vast ocean of genotypical and phenotypical alternatives.

The tension between robustness and innovation is best captured by the evolution of a general architectural pattern known as hierarchical modularity. Sub-networks of interacting entities specialize on certain types of problems, and these compose at higher scales to produce more and more indirect responses that remain adequate across many scales. It must be stressed that composition does not mean analytic reducibility, but rather the presence of emergent generative effects as it has been discussed previously. Turning to biological examples, metabolic networks not only exhibit this pattern, but possibly exploit it for achieving new functions[92]. One way to capture how functions may arise concretely is by observing how entities organize internally to solve problems. There may not always be an explicit or accessible representation of the fitness landscape (such as in the case of natural selection), but its outcomes are. Robustness and innovation must therefore be studied under the lens of collectives as well as of individual organisms, since each contains partial matching information about the other. Hierarchically modular communities appear to play an important role in the dynamics of composition and, when passed through the filter of adequacy, they perform multiple functions across a vast range of scales from biochemistry to social systems[93]. Recent evidence[94] indicates that the emergence of functions triggers hierarchical modularity when protein networks reach complexity and size thresholds. Finding new structures that encode functions reduces the number of degrees of freedom by constraining which regions of the space of potential energy surfaces is locally available to that structure in the future, but hierarchical modularity allows globally regaining degrees of freedom for the organisms as a whole.

In the complex web of information provided by the network perspective, interpreting data is far from trivial. Under the premise of general systems theory, the same network representation also brings a plethora of useful constructs that allow reduction of interrelations into adimensional quantities with both abstract and biological significance. Centrality, betweenness and other observables that are computable from the network allow the construction of organism maps needed to navigate datasets and obtain new knowledge, for instance, about metabolic networks[95]. Knowledge is, again, interpreted in the sense of complete descriptions of entities for which all possible and relevant instances can be computed[96]. The map is dynamic, crucial for understanding evolution beyond the tree metaphor and must be consistent. Different organismal scales in the map can follow differing power laws due to different types of events (e.g. genome editions such as deletion, duplication, reversion), yet the map must remain consistent under different experimental interrogation approaches; the latter has been found to describe (within various simplifications) the evolution of protein networks[97].

Considering the role of dynamical environment in which the network unfolds adds another significant perspective. Evolutionary operations take place amidst noisy environments in which signals must survive and reach their destination. The evolution of complex modular networks is a probable response to information-theoretic efficiency pressures: in order for messages (signals) to have causal effects across the organism, both modularity and redundancy are required[98]. This transcends living system: information-based self-organization pertains to any system that bears internal communication as an adaptive response. The effect of hierarchical modularity also bears resemblance to how self-organized criticality operates, in the sense of reaching higher complexity states that allows entropy to propagate at longer distances[99]; organisms minimize internal entropy in exchange for the ability to exert larger effects on their environment. An additional problem organisms appear to have found good solutions for is how to optimize the message passing process when tokens are susceptible to degradation, loss or interception. The longer the path, the higher the probability of mishaps. Longer sustained paths are also expensive in terms of energy use. Organisms leverage network connectivity by reaching beneficial equilibria in trade-offs between risk and energy expenditure. Instantiations of the contents of their genetic memory[100] are variable in time and dependent on external conditions, such as availability of nourishment sources and the context of fluctuations across all gradients relevant for survival. Essentially, not only organisms are stochastic networks, but such networks are self-contained blueprints for communications infrastructure, deployed when needed and retracted when energy the expenditure is high.

Variations in the blueprint or in how it is executed also require better understanding. Simplicity may appeal to human aesthetics when describing biological phenomena -e.g. parsimony is constructed upon such premise-, but it also seems to correctly characterize certain aspects of biological networks. Energy efficiency, resilience and reproductive capacity are examples of goals that organisms seek to satisfy. While the goals are not explicitly stated, they are enforced by the hierarchy of natural laws that govern the lives of organisms and may be thought of as 'design goals', where 'design' refers to the architecture provided by the network. The evolution of modularity relates strongly to the ability of switching between 'design goals' and satisfying them, even in electronic circuits[101]. In organisms, modularity implies that the cost of switching between 'design goals' decreases if the coupling can be flexibly established, which implies a decomposition into functions that can be re-utilized in different arrangements; to that extent, organisms are nearly decomposable systems[102].

Let us define architectonic simplicity as the property of requiring a certain number of composable elements to specify a robust system of constraints and opportunities for efficient sustained information, energy and matter transduction[ii], such that the number of resulting macroscale system states is much larger than the number of composable elements used to build it and the architecture is invariant under random fluctuations during any transduction processes. Architectonic simplicity relates to Kolmogorov complexity, or the complexity of the smallest 'program' (i.e. set of instructions) that produces a given outcome[104]. Proper evidence of architectonical simplicity would include, for instance, the existence of quantities that capture the amount of information contained in the relations between composable elements, or the ratio between the compressibility of the information contained in the system and the information contained in the composable elements. Barabási and Albert[105] showed that such ratios produce systems with power-law scaling relations; power law functions happen to be convex and characterize various state variables across thermodynamics[106]. The convexity of the entropy in a distributed system, in particular, determines the difficulty of stabilizing

[ii]For an extensive and rigorous description of energy transduction, see [103].

steady states: distributed control mechanisms are non-linear and system size implies longer stabilization times and more complexity of the control mechanism[107]. However, organisms appear to have found in modularity and composition a way to harness composition and modularity such that the resulting scaling laws permit reaching stable states much faster and more robustly[108]. Rentian scaling, the ratio between the number of edges between nodes within a given topological partition of the system and the number of edges connecting nodes between partitions, is such a measure describing how efficient the particular scaling of a system is[109]. The brain, one of the most complex pieces of biological machinery, is a hallmark of hierarchical modularity and Rentian scaling from the purely biophysical up to the neurological[110].

Despite the need for and effectiveness of convenient abstractions as well as evidence of any type of architectonic simplicity, the need for proper grounding on the physical and chemical substrates of life still holds. All decisions which organisms must undergo appear to depend on careful -yet stochastic- energy budgeting, or rather, energy control and flow which have been traditionally studied by cybernetics[111,112]. When networks are placed in the context of energy fluxes in living systems –for instance, *E. coli*[113]- an interpretation of modularity becomes apparent: highly connected hubs of activity allow for lower energy expenditure by moving hard, global decisions up into highly interconnected regulatory structures (e.g. metabolic pathways, signal transduction) and allowing increasingly specific bidirectional communication systems aggregate and segregate responses, using molecular tokens to mediate interactions between modules[114]. To a greater extent, networks have revealed that evolution has found clever ways to vary structure in order to minimize the consequences of the law of requisite variety[115], and still comply with it. Rentian scaling may serve as a general mechanism that reduces energy consumption by grouping certain elements as operational units, and using other elements as information tokens that carry messages; only those tokens that are structurally stable in noisy environments, and those units that discriminate between types of tokens and adequately convey the message are suitable evolvable components of living systems.

Even with the advantageous view brought by networks, there are significant limitations that motivate the exploration of new perspectives. For example, networks only provide either a static view of processes or of their summarization. To construct them, data analysis reduces spatial and time dimensions to make them tractable or closer to direct interpretation. Details are lost, and depending on the assumptions behind the models, irreversibly so. Networks are incomplete also because other types of unknown, such as the existence of biology's dark matter and lack of information about how it alters the course of existence for organisms[116–118]. Furthermore, network descriptions connect composable entities, yet the specifics of their interactions remain shrouded in mystery.

13.4 Biological entities as complex systems: some epistemological conclusions

The task of systems biology and connected research areas – phylogenomics, structural bioinformatics and network theory- is finding integrative explanations of biological phenomena by establishing novel data associations that, under proper assumptions and a falsification mechanism, help explain how organisms function, adapt and diversify in the environment[119]. Beyond the immediate interest in the practical applications for solving pressing and relevant problems such as improving drug design[120], a more ambitious goal lies beyond yet unsurpassed mountains: the development of a predictive theory of biology, or rather, the mechanics of it. Similar to other historical points in the development of science, new principles, concepts, methods and tools are required. Tools and methods tend to emerge more rapidly by virtue of more immediate necessity. Principles and concepts, on the other hand, require more effort and appear sparsely, and yet are essential for any sort of fundamental progress.

As with Hennig's Auxiliary Principle for phylogenetics, new principles will be required as platforms to support and accelerate inferences in systems biology. Gathering the ideas from the discussion above, here is a crude attempt to sketch three of them:

Auxiliary Principle 1:

Evidence of architectonic simplicity, information exchange, and the ability to self-replicate across multiple scales suffices to characterize an entity as an organism.

Auxiliary Principle 2:

Probability distributions of events, obtained by computing consequences of systems of hierarchically coupled stochastic models derived from approximate relations between composable elements across relevant scales over statistically significant ensembles, are adequate descriptions of organisms.

Auxiliary Principle 3:

Predictions about isolated composable elements and phenomena, although statistically significant themselves, are not composable into predictions about the larger phenomenology of the organism.

These (sketches of) principles mandate openly embracing probability and uncertainty not as inconveniences, but as the inherent and most natural substrate of meaningful analysis for biological systems. As corollary of this, scientific inferences should focus less on particular events and more on ensembles of events and their probability density function. Clearly, an adjustment of the pragmatics and the expectations during the research process will be required. Furthermore, adequate auxiliary principle may improve the design of experiments and instruments towards shifting the experimental focus from measuring entities (DNA, proteins, cells) to stronger efforts in directly measuring both their interactions and the biophysical context simultaneously. Having direct access to the interactions is critical, and cannot be replaced by indirect measurements or inferences. Third and most significant, partitioning the space of entities in processing units and signalling tokens opens up a new perspective where information content may serve for elucidating several questions through appropriate metaphors, for instance attacking the evolution of molecular signalling as an instance of the code matching problem in information theory. As suggested by the history of science, the complete form of adequate auxiliary principles for systems biology will be concise and elegant, yet comprehensive and predictive.

Conceptually, across biology and other sciences, there is growing need to better understand what is meant by interaction. In biology, interactions are advantageously accessible directly in many cases (e.g. protein-protein interactions) and their interrogation has become routine. This is not the norm, however, and quickly experiments reduce to idealized laboratory conditions that may not be representative of interactions inside organisms. In addition, the formal machinery necessary to describe them efficiently has not yet appeared. In general, inferring interactions has usually being performed by discovering or fitting against non-linearities. Clearly, both processes describe temporal or spatial consequences of interactions, but not interactions themselves. A hint of this need is the fact that mathematical theories of biological events across scales, contrary to the composable elements they attempt to describe, are not straightforwardly scale-wise composable for most situations. Some new ideas are needed to unravel biological interactions.

Systems biology is an evolving field, already moving from infancy to adolescence. Unprecedented data volumes of unprecedented detail await integrated methods with potential to produce data driven discovery about the organism[121]. Doing so requires principles or axioms to prevent infinite regress while providing some initial grounds to construct more elaborate reasonings. Biology is in need of a new type of pursuit of soundness and completeness (even if these are approximate), one in which discreteness, stochasticity and dynamics are the norm. A sound inference system (within honest accounts of experimental error and uncertainty) would ensure that the number of derivable statement about the ontology and phylogeny of an organism which are false in reality is minimized. A system would be complete if most true facts are accessible through inferences drawn from it. What systems biology aspires to is to become an architecture for systems problem-solving where routine operations of today become natural inferences in the science of tomorrow[122]. In the words of the late philosopher and logician Alfred North Whitehead[123],

> *"It is a profoundly erroneous truism, repeated by all copy-books and by eminent people when they are making speeches, that we should cultivate the habit of thinking of what we are doing. The precise opposite is the case. Civilization advances by extending the number of important operations which we can perform without thinking about them. Operations of thought are like cavalry charges in a battle: they are strictly limited in number, they require fresh horses, and must only be made at decisive moments."*

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Chapter 14

On the Necessary Material Conditions for the Existence of a Universalizing Global Society

Abstract[i]

This article describes in detail loose formal systems capable of representing phenomena underlying globalization with the aim of defining a Universalizing Global Society, a collective entity capable of maximizing future freedom of action for all human agents in it. The formal system proposed here is mostly axiomatic and provisional, and more than defining a strict logical program within Global Studies, it is intended to exemplify how bridges between the natural and the social sciences can be established towards new types of contributions in the study of globalization and its possibilities. Our work seeks to unify concepts from the natural and social science coherently to provide a perspective resonant with the challenges faced by the global society.

14.1 Preamble

> In every rebellion is to be found the metaphysical demand for unity, the impossibility of capturing it, and the construction of a substitute universe.
> *The Rebel (1951)*
>
> *Albert Camus*

We wish to investigate in this article whether a global society where all its members are self-adapting agents individually and as a collective can exist, and if so, what the result of such an envisioning may look like. In other words, We wish to determine the architectural features of a global society with decreasing levels of organismal pain for humans and other species in the spectrum of sentience present on Earth and,

[i]**Núñez-Corrales, S., Jakobsson, E. and Tonini, D (2020)** On the Necessary Material Conditions for the Existence of a Universalizing Global Society. To be submitted to *Globalizations*.

at the same time, one that increases future freedom of action for all its agents. For such purpose, We will conduct a trans-disciplinary investigation using foundations from natural and social sciences and drawing examples from knowledge domains such as the Internet, global economics, climate change and global politics to aim at dissecting global systems that sustain modern society. While the latter can be taken as too broad and abstract as a methodology, it is my perspective that understanding and constructing the sketch of a global society requires accounting for all these elements synergistically rather than in a piece-wise manner.

For starters, it becomes necessary to acknowledge the plethora of *historical myths*, a large majority of them written by the most favored parts in the interactions that occurred in the past, and possibly varnished for portraying unlikely standards of civility as idealized at the time; take for instance the account given in The Melian Dialogues[1]. Such ambiguous view of historical accounts certainly runs contrary to our intuitions of history and myth as separable, one that has possibly been constructed for self-serving purposes[2] and perpetuated by force of habit and social convenience. While we cannot state that all history is purposefully written to serve established networks of power in all cases, care will be exercised when referring to historical sources of particular events, and more strongly so in the case of descriptions of time periods or global phenomena[3]. Moreover, we shall be wary of apparently linear histories that lack proper counterbalancing of the view of those less favored (or more likely highly prejudiced) with the desire to rush to self-supporting conclusions.

The dissertation style here will hence attempt to depart *ab initio* from recent research in various fields and only drawing from well-documented events when strictly necessary. To some extent, the descriptions to follow are modelled in a more axiomatic form and only later will gradually allow more room for the social, especially in the form of organization theory and finally on wellbeing. The choice of ordering is deliberate as to depart from as few positionality-dependent elements as possible, being one of those an early noted tendency towards generalizing abstractions in a knowledge domain such as Global Studies where integrating subjective experience and local knowledge is essential. This admission is not an excuse for any subsequent poor judgements or explanations present in the overall discussion, but rather as a disclaimer of classes of arguments that may not be well suited for the subject at hand due to a marked bent towards bringing new perspectives from the natural sciences as explanatory means. Consequently, no technical terms will be expected beforehand; these will be defined as needed. Consequent also with the societal epistemic needs of our time, no authoritative expertise is claimed at any point.

At the same time, it is not our goal to construct a working axiomatic system, even less a complete one, for characterizing a global society of the kind described herein. It would be a fruitless exercise, since even in the constrained domain of logic and arithmetic such task is provably impossible[4] and the range of human activity is provably vastly richer than that[5,6]. Reducing the comprehension of a global society to properties of computable functions would be extremely naïve and inadequately mechanistic, with the tint of how international organizations make grand generalizations about global macroeconomics with complete disregard for the individual character of human experience. Our intention is significantly humbler, which is constructing a provisional axiomatic system that has the simplest elements capable of sustaining some central statements about the constitution of a more open and free global society with a positive prospect of long term survival. The latter is consistent with science as an edifice of statistical relevance rather than its usual portrayal as the idealized scientific method[7], whose blind description and application leads to an unreasonable divide between the natural and the social science areas.

The organization of this article is as follows. The first task will be to define relevant axioms, properties and rules of inference around global phenomena towards constructing the notion of a Universalizing Global Society (UGS), or a Global Society for All as precisely and succinctly as possible, as well as making the case for why its development is valuable. In the process, We will craft my own definitions for two reasons: a) re-using and re-purposing language over and over from sources in various areas within global studies may lead quickly to contradictions and dissonance and b) building the language tokens and their semantics is a philosophically rich and ultimately an epistemologically inescapable exercise[8]. Since language is deeply tied to culture[9], contradictions will arise while defining terms in connection to Global Studies that may be used in other disciplines and clarity may not be guaranteed. Yet, it is a risk worth taking in a fresh start. We discuss also implications of the UGS in terms of redistributing political power, minimizing collective organismal pain and maximizing future freedom of action for its constituents. We consider these three metrics as essential for the philosophical and practical outcomes of this intellectual exercise. Limitations are assessed in that section. Finally, we attempt to draw some conclusions about the advantages and limitations of taking this approach and whether, under that light, it is possible to change the direction of contemporary global phenomena towards the emergence of a universalizing global society.

14.2 A preliminary, loose axiomatic system for understanding a Universalizing Global Society

While the controversy of the existence of a global society is lively still, there is little doubt about the reality of global phenomena and global complexity in stark contrast to the simplicity of daily activity[10]. There is also little doubt about their perceived positive and negative effects, summarized as contradictions[11]. However, defining precisely the contrast of global and local requires a precise vocabulary. We call this axiomatic system *loose* in the sense that only some of the axioms can be stated and may be proven as theorems in other formal systems. Our goal with this is not ensuring logic exhaustiveness, soundness or completeness but to have an intellectual place of origin from which to criticize and evaluate various instances of global systems of our time. In order to obtain some theorems in our loose formal system, only three rules of inference from first-order logic will be utilized, namely conjunction (CJ), Modus Ponens (MP) and (possibly) negation (N). Figure 14.1 provides the necessary logic context. We will avoid referring to the axioms one by one but will be mentioned when the context may seem removed from daily experience, or when the application of the principle may not be evident from the context.

$$\begin{array}{r|l} 1 & A \\ \hline 2 & B \\ \hline 3 & A \land B \end{array}$$

(a) Conjunction

$$\begin{array}{r|l} 1 & A \Rightarrow B \\ \hline 2 & A \\ \hline 3 & B \end{array}$$

(b) Modus Ponens

$$\begin{array}{r|l} 1 & A \\ \hline 2 & \neg A \end{array}$$

(c) Negation.

Figure 14.1: Rules of inference for the loose axiomatic system. In conjunction, if A is known to be true and B is known to be true, then $A \land B$ is known to be true. For Modus Ponens, if $A \Rightarrow B$ is known to be true and A is as well, then B is known to be true. In negation, if A is known to be true, then $\neg A$ is known to be false.

Before continuing, two definitions are of essence. First, degrees of freedom will be used extensively as the object characterizing agency. A degree of freedom is, in the most general sense, a finite aspect of the state of the universe of discourse for which the enumeration of alternatives as given by the governing laws yields a description of possible worlds. A possible world is to be interpreted here as the simplest assignment of one alternative to the degree of freedom, but richer interpretations are possible[12], and the range of the degree of freedom is the set containing all alternatives.

The second definition is that of entropy, a fundamental quantity of our world, and one that brings new interpretations to collective phenomena. Entropy is a measure of how much energy or information is no longer usable or hidden in a system, or conversely, of the number of different arrangements the elements of the system can be in. Take a whole egg and break it by letting it crash against the floor. There are many more ways to end up with a broken egg, but only one ordered state of the egg we started with. If the same egg needs to be reconstructed, the amount of energy to gather the yolk, the white and all pieces of the shell would be enormous to get back to the same state; in fact, it would prove impossible for various fundamental reasons. Suppose now that we have given up on our original egg and want a new one from scratch. Then, grains would need to be grown for chickens to be fed and eggs to be laid across several months. Breaking the egg takes time proportional to the distance between the egg and the floor, a matter of fractions of a second. Systems with low internal entropy, with time, tend to go to states of higher entropy, a fact known as the Second Law of Thermodynamics[13]. Entropy is also an extensive quantity of systems, or one that depends on the number of their constitutive elements. Both concepts play an essential role for understanding certain contradictions in how global phenomena in contemporary society are structured with respect to a universalizing global society.

In the spirit of starting the construction of our loose axiomatic system, we wish to provide the following definition of *global phenomena*:

> **A1.** *A general phenomenon is global if, for the given spatial universe of discourse, all different places can be reached in a unit step from any other starting place, and the cost of reaching or performing an operation in any of them is equal and almost surely small between all pairs of points.*

By contraposition we define (generally) *local phenomena*:

> **A2.** *A general phenomenon is local if only a few points are considered adjacent from a given place, and the distance metric varies with no guarantees of being small between any two arbitrary places.*

Let us briefly illustrate these definitions. Before Internet became widely accessible, the cost of sending any information to places varied significantly as a function of distance. Regular mail was most notable in high costs, spawning a whole set of professions and trades that dealt with precisely calculating costs depending on mail routes[14]. Reduced versions of mail for conveying short messages (i.e. telegrams) were a tradeoff between amount of quality, cost and delivery time. Telegrams became less popular when telephones drastically cut costs for an increasing amount of people in varied places, moving towards universality[15]. Telephones became so prevalent and useful among a large basis of the population that a large share of the regulatory body of nations is dedicated to ensuring a reasonable degree of fairness in the interaction between citizens and service providers in a historic tug of war[16]. The Internet, now at approximately 3.5 billion users, is the most recent case of a global system where the cost is almost flat and small per transaction[17].

In the examples above, the type of phenomena of interest are *interactions*. Whether it is trade of goods, exchanging excerpts of diplomatic documents for discussion or promulgating a new law, interactions are the central element that define relations of all types, including relations of power in agents of various sorts[18]. Then, we define interactions in the most general manner possible:

> **A3.** *An interaction is a type of general phenomena where two systems exchange degrees of freedom and end up with different states than those they were in previously after a refractory period.*

Interaction effects are not immediate and leave definitive marks. Take for instance the particulars of the independence of Central American colonies from Spain[19]. Independence documents were crafted around

September 15, 1821 in Guatemala. The document, signed by appointees from the different colonies, arrived much later to every province of New Spain as a function of distance. In the particular case of Costa Rica, they arrived on the 29 of October 1821, when a fierce debate arose between those who feared anarchy (incidentally, landlords with origin and ties in Spain) and those that were supportive. After waiting for "foggy days to clear up" [ii] for a couple of months, first actions were taken towards organizing a cabinet. However, the final decision of becoming independent and sovereign was ratified in 1838 after the country withdrew from the Federal Republic of Central America. The relaxation time was significant for this interaction.

In a globalized world, interactions are much faster, with much more encompassing effects and a much more complex dynamic. Take the political effect of Twitter on the public. A mere 140 characters are capable of delivering statements about issues of interest to entire nations more directly than entire television networks[20]. However, even Internet tweets are not faster than the speed of light –they are actually often much slower- and depend on a multitude of rules of a hierarchy of systems beneath them, from computer hardware to programs that may filter information. These constraints will be called the physics of the system. Every system contains elements that interact in some way, which through consistent occurrence may become routines. Elements may be systems themselves. The latter motivates the following axioms:

> **A4.** *A system is a collection of entities that have interactions according to a small set of fundamental rules, which can be classified possibly by their frequency and class.*

> **A5.** *Systems can contain other systems.*

We call the nesting in **A5** *compositionality*[21]. A case in point is that of the state and evolution of political systems in the global arena, namely the problem of order in global politics[22]. At the top of the spectrum, we encounter international organizations dictating policies destined to materialize conditions in across the planet. The Hobbesian State[23], one that through sovereign might defined norms and laws, was arguably to a great extent a well recognizable system within the global system. Global phenomena have penetrated the tapestry upon which Leviathan was clothed, getting progressively under its skin and now inside its administrative and moral brain[24]. The boundaries of the system become more diffuse. Cities, more in particular global cities, are becoming primary concentrators of action, memory and communication, yet another type of system within traditional borders of the State[25]. Events at the scale of cities, governments and the world have impacts of increasing magnitude and decreasing frequency as we go from individuals to nations.

> **A6.** *The configuration of a system is a snapshot of the degrees of freedom contained in a system.*

[ii] S. Núñez-Corrales' translation of the folkloric Costa Rican expression "*hasta que se aclaren los nublados del día*".

A7. *A system is ergodic if every possible configuration in it is guaranteed to be observed given sufficient time.*

A8. *No interaction in the system can violate the fundamental rules of its universe of discourse.*

Axioms **A6–8** are particularly important for the development of public policies with global aims. For instance, disliking the Paris agreement will not stop fossil fuels from polluting the environment to the brink of existential risk, one of the major overtones of our time[26]. As Richard P. Feynman, the Physics Nobel Prize would put when serving in the commission that studied the disaster of the Challenger in 1988, "For a successful technology, reality must take precedence over public relations, for Nature cannot be fooled."[27]. The same must certainly be true of policies, since the Rule of Law is ultimately constrained by what the hierarchy of natural and artificial systems allows.

Let us consider climate change. The conclusions from the International Panel on Climate Change, Working Group I on the physical science basis[28] could not be clearer: the periodicity with which the global climate reaches peak temperatures before 1950, correlated with posterior and drastic changes in the Earth's biota, is in the order of hundreds of millennia. Human activity has, in less than 70 years, accelerated the rate at which these conditions materialize at values comparable only to planetary cataclysms. Scenarios resulting from the study of several consistent pieces of evidence, from Arctic ice cores to simulations with paleo-climatic models, yield a grim scenario in many human dimensions[29]. Whatever the disagreements are around climate change[30], Nature remains the ultimate arbiter and a harsh one when its rules are ignored in favor of evidentially vacuous rhetoric.

A9. *Information exchange is the least expensive interaction for any degree of freedom in time, space and energy cost.*

A10. *Information representations require reorganizing matter by applying energy for a finite period of time.*

The decomposition of Somalia left the world with a humanitarian crisis and a new nation, namely Somaliland. The rupture of ties of land, economics and society[31] as well as the international implications of international non-recognition, especially in foreign investment, have led to unprecedented rates of inflation, or hyperinflation[32]. Hyperinflation leads to exaggerated devaluations of printed currency to extremes. In order to cope with hyperinflation, nations such as Zimbabwe have relied on aggressive use of information and communication technologies to replace paper money with other forms of digital currency[33]. In a surprising plot twist, Somaliland has become one of the global success cases of cashless trading by taking Zimbabwe's example and universalizing it[34] in a context of $1 equal to around 9000 Somaliland shillings. Paper money is no longer useful, is certainly more expensive to produce and takes a lot of space as observed through the bags of money required to even buy groceries. Where is the reorganization of matter and energy that facilitates digital cash in Somaliland? Telecommunications infrastructure, software development and mobile phones are energy expenditures that have restructured matter (i.e. the telecommunications network) in ways in which actions of economic agents can be amplified through inexpensive repetition. This trend, applied to other domains, is moving the discourse of global governance to uncharted territory[35].

> **A11.** *Consuming energy leads to entropy, leaving less usable energy in the system.*

> **A12.** *States with more usable energy in systems with low entropy are more accessible than those in systems with high entropy.*

A significant amount of "expert criteria" has been gathered around failing nations, as well as a body of routinely practices expected to work as imposed by international organizations that develop loans. By **A11**, a failing country is a case of less usable energy in the political and economic system, since there are many more arrangements of people and institutions that lead almost surely to ineffective results than those which are effective. Transitively, there are less degrees of freedom for agents and organizations. Consider the International Monetary Fund (IMF). Their loan programs place strict requirements to nations requesting funds, placing conditions on their governance structures and limiting most forms of subsidy. Evidence in various areas such as health across West Africa[36], and labor rights in the developing world[37] clearly indicate that the effect of most adjustment programs had negative contributions to the final development stage achieved after their execution phase. The mechanism that explains the ineffectiveness of these adjustments is that nations requiring loans are in a high entropic state, one that requires a significant energy investment before changes can be observed without reducing degrees of freedom that may be essential due to culture and resources to reach lower entropic states (**A12**). Restrictions posed by the IMF are to that end senseless, based on unreasonable expectations from a systems-thinking perspective and notoriously hypocritical[38]. Measures dictated by the IMF increase the entropy of nations beyond the recovery capability of their various resources, while other approaches without such unethical flaw certainly exist.

> **A13.** *All general phenomena can be defined in terms of information, matter and energy flows in systems through interactions.*

We now turn our attention to the stock market, in particular in terms of derivative products as an example of the previous axiom. Derivatives are financial products whose value is prospective as given by rates of change, essentially a price put on various momenta of the actual mathematical derivative of a stochastic function[39]. When too or more stock agents have agreed on a price, standard stock trade rules solidify prices based on the availability of assets and securities. That is, two agents have exchanged degrees of freedom represented by the amount of immediate possible actions (i.e. available possible worlds) with expectations based on prior history about capital valuations. While there were problems associated with non-derivative stock operations, derivatives introduce two large issues: unsubstantiated values and market nucleation, or the capacity to gestate market bubbles in very short time[40]. It is also the ultimate general phenomena in the sense described here, as derivative exchanges happen at dazzling speeds, exclusively in silico, with vast energy and information flows across the world.

A14. *Interactions are mediated by tokens, also known as messages.*

A15. *Tokens have persistent structure.*

A16. *Messages transitively encode future actions.*

Contemporary human life is dominated by one of the most interesting tokens developed whose sole purpose is mediating interactions that gauge worth of goods and services: money[41]. The jump in economics by agricultural practices that produced surplus required more sophisticated methods of ensuring comparable value and authenticity, capable of reducing the comparison to an abstract unit of negotiation. Money is the message that mediates financial transactions, and the economy to that extent is a snapshot of the amount and magnitude of transactions encoded by it that can be trusted. Tokens in the form of fiat currency, either printed, minted or more recently computed through hashes[42], have a structure that permits corroboration to avoid counterfeits, a crime whose high penalties reveal how essential money is seen to encode trust as a social value in economic contexts. The latter is deeply rooted in complex neurobiological mechanisms for loss and gain[43], as well as distributive justice[44]. As money flows become global, currency exchange has gone from an obscure art to an automatic task without any human intervention. However, money also encodes future action as a form of transient promise of valid exchange of value for time, effort (physical or intellectual) or location. This latter point, along with the underlying neurobiology, is immediately recognizable as the genesis of the alienation described by Marx in Das Kapital[45].

A17. *Collective phenomena in a system are a class of general phenomena where the materialization of their effects requires at least two of their constitutive entities.*

We wish now to focus the spectrum to phenomena where many entities are involved. Collective can be translated as at least two, but for the purpose of describing a global society of a certain kind, we will concentrate on systems with several interacting entities. One of those is Twitter, which had a prominent role in the political arena of the past US election[46]. Given the constraints of the system (140 characters) at the time of the election, the structure made of followers (e.g. public, mass media, political parties, international leaders) and tweeters (e.g. presidential candidates, party leaders, supporters) led to a feedback loop where victory was achieved by one of the parties (Republicans) through a discourse of informal emotional exaggeration[47]. A series of exchanges that in other communication dynamics would have been regarded as noise at best or international meddling at worst[48], are now the basis for claims of sovereignty, or at least its simulation[49].

> **A18.** *An agent is a constitutive element of a system, possibly a system itself, capable of information representation, initiating interactions internally and acting upon other constitutive elements that are not agents.*

> **A19.** *A system is an agent-based system if the majority of interactions occur between agents in it.*

Agency is central to all political projects and theories and is being challenged as it currently stands on the pedestal of the State[50]. At one end, the epitome of agency for Adam Smith is capitalism, agents which are self-adapting by following the maxim that "In competition, individual ambition serves the common good"[51]make. At the other end, Marx sets the stage for a society where agents are freed from the need to choose into the higher freedom of equalized resources. Both approaches however were fundamentally wrong in one aspect in which agents were supposed to perform the market's biddings: they presuppose that agents are in perpetual competition, and that event with limited knowledge, that they act in a game of perfect rationality[52]. Competition under an entropic setting is much costlier for all agents in the long term even when cooperating is more expensive per capita for the first rounds of operation of a system[53], since cooperation moves the bar of entropy lower for everyone instead of just a few. To that logic, one of the first tasks of an advanced civilization would immediately be to reduce energy spent on (and hence entropy created by) unnecessary conflict arising from competition between its agents, and rather to think instead in terms of *games against nature*[54]: the agents, knowing that the amounts of matter, energy and information in their environment are finite, compete against their own ignorance of principles that would decrease the rate of resource exhaustion. The value of an interaction would be dictated in such a system by its energy-entropy equilibria, its frequency and its symmetry of exchange of degrees of freedom with respect to the perspective of each agent. Taken with a grain of salt, the better angels of our nature may be a secondary byproduct of us becoming progressive less competitive among ourselves[55], albeit the rate at which it happens today is not sufficient.

A20. *A non-agent entity in a system is a resource, which is a system itself.*

A21. *An action is a type of interaction between an agent and a resource initiated by an agent with entropy production in all cases.*

A22. *Resources are measurable, changeable and exhaustible.*

A23. *Measurements have non-negative degrees of uncertainty.*

A24. *Actions only have an impact if the thresholds for the interaction to take place defined by resources are reached.*

A25. *Measuring the state of a resource requires less energy than changing its state.*

A brutal example –in the sense of *brute fact*[56]- of how resources and agents interact is given by the diamond mining and oil industries in Angola, a nation with what is best described as a War Economy[57]. International financial interests, large corporations, the military and insurgent forces, and finally the dispossessed population have converged through the extraction of oil and diamonds. Thanks to novel exploration techniques and historical accounts, the ability to find deposits by measuring various terrain conditions and processing information[58,59] with increasing certainly, a process that nonetheless was far from desirable in the past and required extensive disruption of natural resources; reducing uncertainty requires in many cases large amounts of ground and rock to be devoid of plant and animal life, soil to be dug up at evert increasing depths and manual labor to undergo gruesome hardships[60]. All the latter does not guarantee success though. Measurements fail, economies of scale may not be met, and product quality may not justify continuation of mining and oil projects; these are the conditions of the interactions that continue the vicious cycle of exploitation of people and land by other peoples and lands. Locals are hired under precarious conditions, yet they are not the agents that start the actions to extract or process the valuable products, and the land is irrecoverably changed with respect to the needs of the population.

A26. *The degrees of freedom of action of an agent, or its agency, are a positive function of the number of potential interactions, the number of potential classes of interactions and the complexity of its internal representations leading to possible actions.*

A27. *The intelligence of an agent is a measure of its ability to maximize its own future agency at a particular time given the resources it has access to and its context of emergent systems of constraints.*

A28. *A spatial field is a type of resource that exhibits locality and is actionable, that is, position is defined and values of degrees of freedom can change with respect to time between locations.*

The ongoing dialogue on global development and the questionable emergence of "development experts" often rests on the assumption of lesser intelligence or impoverished will to action[61]. Apart from the relationship between power, knowledge and thus its incarnation on claimed expertise[62], these judgements are at serious faults under our framework. Developing nations, by definition, are plagued by a plethora of restrictions in the constitution of their agency (**A26**), which depends on a particular history since agent ontology encodes power structures[63]. It is easy for agents whose agency developed without major societally-induced hiccups and whose lives exemplify various privileges to utter judgements against those who struggle for survival on a daily basis. The spatial fields, in the case of nations their geographic distribution of resources is what draws the frontiers of opportunity for agents. Growing crops and raising cattle at the border of an expanding desert in the Sahara with scarce government incentives[64] is radically different than in any of the developed market economies[65].

A way to inoculate privileged agents against hidden forms of bigotry and exclusion is embedding ways of deconstructing privilege across education systems[66], with an emphasis on higher education students who are agents with many degrees of freedom. The situation is more nuanced and less effective when these agents operate inside organizations with demonstrably biased practices (e.g. IMF, World Bank, Inter-American Development Bank) that follow global economic goals subservient to amassing wealth on the top 1%[67]). A global path to ensuring fair treatment would be for the developing world to devise and implement its own institutions having epistemic privilege[68] as a core component in how national and regional affairs are dealt with. By breaking the captive market situation, one which these entities have honed along decades and thereby established as an oligopoly of expertise, new and more useful policies may be designed and tested, partially answering the question of whether international organizations can be democratic[69] towards the positive. The latter indicates concrete target for global communities that seek having an impact on the structure and dynamics of the world[70].

At this point, we would like to test the inferential power of the loose axiomatic system with a particular example. Let us prove that population growth decreases collective agency when resources are limited, understanding that "prove" in this system is not to be considered normative in absolute terms. At the same time, there exists certain value in proving certain simple statements as a consistency test: inference mechanisms that work on stricter forms of logic should preserve at least some of their power within weaker forms of logic. The limits of those inferences are determined by the type of theory, which in this case is modeled as a subset of first order logic. Consider the following propositions. If the size of a system increases, then its entropy will increase too (**P1**: $I(S) \Rightarrow I(E)$). Since it is an extensive quantity (dependent on the size of the system, approximately the number of its constituents), the above implication is valid (an implication of the form A => B, which reads "if A is true then B is true"). Assume for the moment that a global society is a human system and that Earth is the only system it has access to (**P2**: $L(R)$). A22 indicates that both increased entropy and limited resources lead to a decrease in resources (**P3:** $L(R) \wedge I(E) \Rightarrow D(R)$) and **A27** implies that decreasing resource avaiability decrease agency (**P4:** $D(R) \Rightarrow D(A)$). Finally, it is known that the global human population will remain growing without foreseeable stabilization[71], hence it is known that **P5:** $I(S)$. The inference process proceeds as follows (propositions and rules are indicated on the right-hand side) with a successful proof at the end (Figure 14.2).

1	$I(S)$	(P5)
2	$I(S) \Rightarrow I(E)$	(P1)
3	$I(E)$	(MP 1, 2)
4	$L(R)$	(P2)
5	$L(R) \wedge I(E)$	(CJ 3, 4)
6	$L(R) \wedge I(E) \Rightarrow D(R)$	(P3)
7	$D(R)$	(MP 5, 6)
8	$D(R) \Rightarrow D(A)$	(P4)
9	$D(A)$	(MP 7, 8)

Figure 14.2: An example inference with the loose axiomatic system.

It is now time to provide some foundations for emergent properties of systems that have at their heart coordination as their phenomenology. The emergence of a global society and of globalization itself is strongly debated, and at its core is the question of whether it is a gradual process or a structural revolution[72]. But, how can structure emerge?

A29. *A routine is a type of consistently repeated interactions in a system that remains stable under certain conditions.*

A30. *The organization of an agent-based system is the collection of its routines and a measure of their persistence for a relevant period.*

A31. *A hierarchy is type of organization that can be represented approximately as a tree.*

Routines as repeated interactions have been explored to explain the emergence of social organization[73]. A clear example of routines is the collection of economic patterns of interaction giving rise to the top 1%.

These are an example of a hierarchy that is induced from the top, enforced at the bottom and surprisingly resilient in terms of how interactions are preserved or recovered for its most privileged agents. In the process of consolidating their power, they have shaped standards, procedures and regulations required to thrive, including a pervasive ideology of supply and demand; these are quintessential examples of routines in the collective memory of the world. Financial liberalization, predicated upon the ideas of freedom of action of agents in the economic network, creates an illusory context of freedom. But economic agents are constrained by through capital in one way or another. Agents are constrained by materially accessible resources (people, land, time, energy, matter and information) but moreover by the architected legal reality encapsulated in sovereignty of nation-states depending on which scale of aggregation of wealth they are at. When very wealthy and very powerful agents fail, emergency systems exist to keep them alive in an intensive care-like fashion at the expense of everyone else[74]. When they fail, as in the case of the history of severe stock market crashes, all of society takes a toll. Even in these catastrophes, routines have remained mostly untouched.

The fact that predicting these events has spawned a set of intellectually challenging activities to the point of the intensity of forensic reconstruction after a complex crime[75] should be a warning sign not to depend on such faulty systems, but is rather a testament of financially oppressive systems attempting to survive and keep feeding the top 1%. While it is not surprising that the market is a normative power through routines, it is certainly striking to observe that these societal norms and conventions do emerge from within society's most accommodated strata by virtue of resource accumulation itself[76]. Globalized trade has only made the world an oyster easier to impoverish and financially exploit with a never so endangered open society[77]. Hence, with fewer and fewer, but bigger and bigger agents, it is only a matter of time before a large crisis ensues and prompts either revolution or extinction.

> **A32.** *A goal is a preferential set of configurations of an agent-based system that can be achieved through a form of organization, one which is actively sought.*

> **A33.** *A goal is explicit if all agents contain a representation of it that includes both a utility function for their actions and a distance function from the current state to a state in set of preferential configurations.*

> **A34.** *Coordination in an agent system is a process of negotiation between a group of agents towards achieving an explicit or implicit goal through permanent or transient organization.*

> **A35.** *Self-adapting agents are agents capable of modifying their number and types of interactions, shape their actions and improve their internal representation to attain goals within a range of effi-*

ciency and effectiveness.

It is hard to imagine, within the diverse and sorrowful legacy of human conflict and war, that a concrete goal in global politics can emerge, be sustained and remain actively enforced. Control of nuclear proliferation and the continuing discussion towards completely banning nuclear devices in armed conflicts is an outlier. The magnitude of the consequences of any nuclear uses in war justifies all possible avenues of negotiation and coordination, whether formal or informal. The preferential set of states is that containing all but those containing either massive loss of human lives or total extinction at the global scale. The deterrence and numerically effective decrease in nations with nuclear power for military purposes, as well as the stabilization in the number of nuclear devices is a consequence of all agents with sufficient degrees of freedom interacting within a clear boundary of undesirability. The horrors of Hiroshima and Nagasaki have remained effective in preventing further use of nuclear weapons against human populations, prompting an international instrument of such uniqueness as the Nuclear Nonproliferation Treaty[78], but collective memories are starting to fade away in a receding ocean of time and abstraction.

The treaty is landmark of global self-adaptation of multiple agents of different types where all the tools in the toolbox of routines and coordination are available at any given time. It has mobilized from scientists[79] to activists[80] and diplomats[81] in multiple forms of organization, some transient, some stable. Assessments of the effectiveness of their action has become a common task in a completely distributed manner, yet one that reconvenes again around the primary goal. Processes around controlling nuclear proliferation have been guided by evidence and aided by the graphic nature of the effects on survival of those affected, paradoxically helping the public become informed and engaged. Despite a successful history, the effectiveness and certainty of the world subsystem preventing nuclear war cannot be taken for granted in the current climate of international politics.

Having considered the latter axioms and some of their exemplars, what (preliminary) definition can be given of society that encompasses the collection of global systems and phenomena experienced in our contemporary times?

> **A36.** *A society is an agent-based system of self-adapting agents with at least one spatial field, one type of interaction, one type of action and one form of organization.*

> **A37.** *A global society is a society where agents exhaust the universe of discourse and organization is a global phenomenon with respect to the set of agents.*

There seems to be no better description fitting this loose axiomatic system than that of global patterns of energy consumption, since they exhibit context, complexity and connectedness[82] as described by A37.

For such purpose, let us make use of the Kardashev scale, a measure of how much energy is approximately consumed by a civilization[83]. The current estimated value stands at 0.72; a value of 1 indicates that the Sun or a sufficiently large substitute has become the primary source of energy of a civilization, and thus that becoming global under a sustainable route. We can easily find a point of inflection in energy production around the middle of the 1960s that brought energy consumption from an almost lineal trend to an exponential one[84]. One can readily form various hypotheses about the reasons for this explosion of energy consumption. The most immediate one is that this period coincides with the fastest rate of population growth in human history[85], mostly due to medical advances and health spending[86] despite its inequality. In addition to that, many technologies that were developed during the Second World War[87] became civilian products that transformed energy into desirable functions. The transistor, invented in 1954[88], was readily adapted for mass production thanks to advances in materials science and solid-state physics, which in turn made possible the miniaturization and development of the consumer electronics market[89].

Thanks to another invention of the Second World War era, namely operations research[90], Western organization models became efficient in reaching goals and methods from a goal-oriented standpoint. The latter created a fertile ground for the computer, a device used at first for numerical modeling and simulation of projectiles and cryptography[91], to be converted into the core of organizational information processing[92]. A first, grim taste of its possibilities resided in how early computers (sorting machines) were instrumental to the Holocaust[93]: it would have been effectively impossible for the National Socialist German Party to gather and process information about Jewish ancestry without them and commit their atrocities. Larger organizations meant larger buildings and facilities (hence even larger and more sophisticated energy systems), the rise of office work as a regular career and a stabilization of work routines and even rights. In essence, the protracted preparation of conditions that lead to the current pervasiveness of information technologies evolved to reach a critical point that now permits converting natural resources into human and physical infrastructure capable of large production volumes at low costs and global scale. Technology of increasing sophistication as part of a global system is a many-edged sword.

What happens when global development is not homogeneous in terms of the opportunities and risks depending on their position? Positionality and situated knowledge[94] serves as point of departure for the acknowledgement-representation-integration triad in the process of productively understanding otherness. As such, a rudimentary (i.e. disembodied) definition of positionality departs from observing that agents whose history and location differ necessarily have different perspectives.

> **A38.** *The positionality function of an agent is a measure the ability of every agent to successfully exploit relevant spatial fields for an action.*

A39. *The positionality field is the result, for a given agent and a given action, of computing the distance between the requirements of all relevant spatial fields with respect to the possibilities of agents; hence, it represents a field of opportunity.*

A42. *An agent-based system is positionally grounded if the specification of actions in agents uses the positionality field in all cases instead of directly accessing the spatial field.*

A40. *Intelligent self-adaptation strategies may help maintain the positionality function between an agent and an action constant or improve its value given favorable conditions.*

A41. *An agent-based system is positionally aware if information representations exist in one agent about the positionality fields of all other agents (or of a sufficient large number of them), and individual coordination decisions always include it.*

Another relevant issue is the contrast between development ethics and globalization[95], which serves as an example for positionality. The multiple failures within interventions of different sorts across the world by global non-governmental organizations appear to sustain a pervasive division between those how assist and those who are assisted in terms of perspective[96]. The structure of the plot is similar in most cases: an NGO from abroad with plenty of resources and a plan plotted from headquarters in developed economies proposes a course of action without considering local conditions of some sort (e.g. cultural, religious, natural); implementation fails with stakeholder dissatisfaction or the project produces a prototype that cannot be scaled or replicated without creating new dependencies or deepening existing ones. The NGOs as agents tend to violate at least one axiom between **A38-42**, which partially explains why most of funding tends to be dedicated to administration an only a small portion to actual action, finally ending in perils to their survival[97].

Finally, the last three axioms rest on the previous systematization to describe the main structural and dynamical features of a universalizing global society. While not in an explicit way, they appear to be compatible with the three constraints set at the start: redistributing political power, minimizing collective organismal pain and maximizing future freedom of action for its constituents.

A43. *Human persons are self-adapting agents.*

A44. *The human global society is a society of humans and the spatial fields are given by local phenomena on the Earth as the material universe of discourse.*

A45. *A human Universalizing Global Society (UGS) is a human society that is positionally aware,* *and where one of the topmost goals is reducing differences in the positionality function globally for all agents and actions towards decreasingly small values, maximizing long-term survival of the species.*

14.3 Limitations

Among the many limitations in the loose axiomatic system is the lack of reference to culture in the composition of a UGS or any society in general. As indicated at the beginning of this work, it is not my purpose to attempt a total and consistent reduction of society to axioms, propositions and inference rules. Here is the reason why my current state of belief in the matter leans towards fundamental impossibility. Culture, which we define here as the collection of pertinent, heuristic and pragmatically useful fictions contained in a society, is clearly dependent on the representation capabilities of agents and on agency itself[98]. However, culture also includes a host of ineffable experiences that fall outside the definition of agency contained in the loose axiomatic system which still adheres to a formal notion of meaning[99] and appear to operate in a regime best described by theories such as Gestalt psychology[100] or even Husserl's phenomenology[101]. A case in point is that, even when there is an alignment between the definition of a universalizing global society and decreasing levels of organismal pain, the definition of organismal pain itself is partially rooted in physiology and partially rooted in the Gestalt[102]. And, to add even more confusion to the mix, it is even harder to attempt to grasp perceptions of organismal pain (or any other perception as it turns out) in other forms of sentient life[103]. Nevertheless, to err by choosing caution appears to be preferable than the alternative.

The second limitation of this work is one common to the rest of literature in Global Studies. The selection of historical events responds only to a narrow purpose, namely to exemplify aspects of this loose system of axioms, with sufficient care in checking that the historical research being cited is both detailed and contains self-critiques. History is a muddy subject itself that can accommodate a range as wide as that between uplifting narratives of restitution[104] to the most abject forms of revisionism[105]. Although extremely relevant, reconstituting History to match the needs of a universalizing global society is not only out of the scope of this work but represents a research program of decades that possibly demands new pluralistic methods of causal explanation of events paired with automated mechanisms to verify claims about past events. Past a certain point that still seems to remain in the far future, reconstructing history that already happened may hit an event horizon of historical reconstruction akin to that of a black hole: getting too close may get oneself pulled into the primal gravitational waves of uncertainty.

Finally, the third great absent in this construction is the role of myth in general, not only in the form of spiritual fictions but of powerful normative fictions in general, in holding together very high-level routines by sheer ideological force and perpetuated through a multitude of channels, being mass media among the most relevant ones[106]. Modern myths include portrayals of primitive human life[107], the nation-state itself[108], the statistical inevitability of social inequality[109], the correspondence between academic credentials and social strata[110], the American dream[111], the existence of truly global corporations[112] and religion as a whole[113]. A sad example of the power of myth is embodied in Stephan Zweig, novelist, playwright, journalist, biographer and firm believer in Europe as a materialized ethos. After the First World War broke Europe apart and the National Socialist party took over Germany, Zweig emigrated to Brazil heartbroken, his central myth shattered to unrecognizable pieces. In February 22, 1942 one day after completing his autobiographical memoire[114], started in 1934 when the stench of the Nazi regime started to spread across the Old Continent, he and Lotte Altmann (his second wife) committed suicide. The dissolution of his most powerful articulating inner voice before his eyes at the hands of Hitler and the Third Reich made dreams of Europeanism spiral down to oblivion by the ultimate trigger of personal nullification: the disappearance of a collectively constructed phantom upon which their identity hanged.

While at one end the natural sciences reduce the need for myths by exposing mechanisms and literally removing any *deus ex machina* along the way, there exists maybe a way to design new myths that can hold society together and help the universal global society to materialize. Why, in a world of scientific revolutions, resort to a such a regress? To start with a possibly depressing answer, because human brain architecture has not yet gotten rid of lamentable atavisms proper of a much simpler, more primitive and more violent age[115]. The process that separated non-human primates from their human counterparts took roughly between five and six million years, and the rise of Homo sapiens is dated around two hundred thousand years, and the most recent changes in human brain architecture are only starting to materialize and spread[116]. It is not impossible to foresee types of global schemas of organization too foreign for brains that still are bound by primitive responses of the limbic systems and by cortexes that have merely abandoned -in geological time- a world of trees, hence requiring reification of volatility and complexity through myths. An additional, certainly speculative possibility, is that myths serve as fundamental heuristics of the mind for complex experiential situations. While some myths may be purposefully built around sound epistemological considerations, the human mind can still benefit from their low cognitive requirements. This would be a risky enterprise resting on the ethics of those defining the myths. Or maybe we underestimate the rate at which technology impacts the evolution of the brain, moving towards a singularity that redefines our fundamental biology[117] and removes myths from the palette of alternatives for achieving massive levels of societal coordination. In any case, the problems of understanding both the role of myth in a universalizing global society and its potential for global good remain open.

14.4 Conclusion: can hope in the future be regained?

We have developed here, based on a somewhat lax analogy to the process of logical inference, a loose axiomatic system to describe a so called Universalizing Global Society, one in which global systems are aimed at maximizing and equalizing opportunities for the pursuit of meaning as the most fundamental question of existence[118] with ever increasing freedom and decreasing organismal pain. It must be acknowledged upfront that this question may not have any sensible answer, as it becomes apparent from the recorded history of philosophy. Happiness is not an answer to the original question either, at least in the naïve sense of constant instants of joy, but possibly only in the paradoxical realization that being part of the universe only leads to a never-ending ascent into insignificance[119]. Having decided that life is worth living, even within such vanishing measure of insignificance, we become heirs and stewards of the only possessions individuals of our species appear to have: the collection of actions, experiences and memories that only social sentience can produce and the manifest capacity to transform will into action so that those who succeed us can overcome faster and faster the pestering maladies of previous generations. If one needed to reduce human rights to just a few, it is arguable that the latter are the most relevant, the most self-evident ones of all, the ones from which all others spring.

Gathering these possessions cannot be done in abstract but needs proper conditions in the material world whose requirements for minimal possibility are a moving target. As human societies built up technical complexity and sophistication, the probability of encounter between dissimilar cultures became inevitable. One may argue that for a place to be inaccessible by some form of technology in our time, the reason often has to be given with respect to a norm describing why it should remain inaccessible, such as in radio astronomy. Given the interconnectedness of interactions at planetary scales, and the exhaustion of resources by historically induced disparities, finding alternatives to the current trends of development of a global society towards a universalizing equality of rights for a better human experience is a categorical imperative.

At present, we can enumerate several observations. Civilizations appear to exhibit critical inflection points in how their interactions are structured. These can be interpreted as transitions from more local to more global flows of information, matter and information. An exponential increase in information processing provides unparalleled ability to design and enact policies with more abstract mechanisms that have a tighter grip by a small group of individuals. Disproportionate concentrations of information, energy, and matter generally tend to preferentially benefit those who can afford technology as early as possible, obscuring positionality by habituation to privilege. Differential adoption thus only maximizes differences in the long run, later manifest as opportunity gaps between regions, states and other units of social aggregation.

An ideology driven by capital creation and accumulation above social concerns appears to systematically –and yet inadvertently at large scales- exhaust both natural resources and human potentials faster than these can be replenished. Social exhaustion leads to conflicts and a change in the collective imaginary, requiring even more energy without seeing material or ethical gains in return. Conversely, the inability to maintain the rate of entropy increase below the renewal rate of resources cannot be overcome only through technology, but requires challenging and rethinking the foundations of the ideological and economic substrates associated with power structures, both local and global.

The ideology present in those who are in control of knowledge and technology from the start appears to marks a significant difference in the conception and creation of what we may call the global order, and in the targets of its ultimate benefits. Information structures work through the definition of standards at granular levels of society and through establishment of policies at the highest levels of power consolidation. Routines have been enforced through norms, laws and standards to provide resilience for those in power, creating in effect a large number of dispossessed individuals across most of written history. But, the dissemination of technology required for newly devised hegemonic projects, counter-intuitively for those who lay out these neo-colonialist efforts, leads to new forms of resistance driven by those outside the sphere of power and those inside who defect from the purpose.

Nation-states, removing any Westphalian fantasy of sovereignty, still retain value as experiments in social coexistence by discovering good solutions that can be shared administratively. Under that light, there should not be any apparent difference when thinking about one nation or another, since all of them have acquire the same importance and purpose. Citizenship is thus revealed as a label with analytic purposes, and not an ontologically incommensurable property endowed by the State to individuals that can justify almost anything on a moral basis. We believe that a syncretic and rigorous approach to understanding global phenomena through multiple languages of description can reveal at greater detail and depth much of the origin of our current miseries as a species and provide a platform from which to catch the silhouette of the next phase of human evolution, and possible its place among the stars if it survives. Scientists cannot remain silent when their very tools and methods have the power to capture essential features of global phenomena, as it has been discussed here to a preliminary and limited degree of success.

Can resolution be found, or at least hope, for the predicaments of the world in the present? Possible avenues exist for reconfiguring the future towards solidarity and identity[120]. This not just an ethical stance, but one of the few global survival strategies available with repercussions to the preservation of the biosphere long enough to leave the planet and become a multiplanetary species, which will not happen satisfactorily unless we find a reasonable solution to the problem of coexistence. The latter requires exploiting planetary infrastructure already present for the dissemination and construction of movements of resistance capable of unfolding new resonances between a glowingly diverse, yet still alienated population. The loose axiomatic system developed here is a humble start, but one capable of opening some basic questions that may help reinterpret the structure and dynamics of globalization. Or, in the worst case, serve as a position marker of where not to spend time fruitlessly.

Some glimmers of hope show their shapes in this long and dark night. Globalization and globality can be harnessed to signify the onset and continuation of an unfinished revolution[121], not in a romanticized way, but in a well-defined fashion by understanding how to best align resources[122] with ethics[123]. In the same sense that humanity has become pray to paralyzing and dehumanizing abstractions, globalized phenomena can be also harnessed to evaluate, deconstruct and replace the normative boundaries towards a state of civilization where life is both worth living and materially possible to live. This may well serve ultimately as the ethical keystone of a universalizing global society.

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Chapter 15

Entropic Boundary Conditions Toward Safe Artificial Superintelligence

Abstract[i]

Artificial superintelligent (ASI) agents that will not cause harm to humans or other organisms are central to mitigating a growing contemporary global safety concern as artificial intelligent agents become more sophisticated. We argue that it is not necessary to resort to implementing an explicit theory of ethics, and that doing so may entail intractable difficulties and unacceptable risks. We attempt to provide some insight into the matter by defining a minimal set of boundary conditions potentially capable of decreasing the probability of conflict with synthetic intellects intended to prevent aggression towards organisms. Our argument departs from causal entropic forces as good general predictors of future action in ASI agents. We reason that maximising future freedom of action implies reducing the amount of repeated computation needed to find good solutions to a large number of problems, for which living systems are good exemplars: a safe ASI should find living organisms intrinsically valuable. We describe empirically-bounded ASI agents whose actions are constrained by the character of physical laws and their own evolutionary history as emerging from H. sapiens, conceptually and memetically, if not genetically. Plausible consequences and practical concerns for experimentation are characterised, and implications for life in the universe are discussed.

15.1 Artificial superintelligence: the challenge of life-friendly agents

Artificial superintelligence (ASI) defines a hypothetical form of artificial general intelligence whose problem-solving abilities are broader than, and vastly superior to, those of any human counterpart or any human collective at any given moment. We assume here that the evolutionary speed of an ASI against any human counterpart is vastly superior as well, which appears reasonable for most decision tasks in terms of

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performance. Superintelligence presupposes the ability of such agents to devise, assess and modify internal motivations driving their actions, which may not necessarily be compatible with coexistence and cooperation with life forms already present[1], thus creating unacceptable risks for humans and potentially other organisms. Despite growing awareness about its potential risks, ASI holds promises of finding unforeseen solutions to grand challenge problems in science, technology and society[2].

One of the many proposed alternatives to reduce the probability of future rogue ASI agents calls for the development of moral machines[3] accompanied by preliminary design strategies[4]. It may imply, for instance, defining and implementing hardware or software constraints to discourage or prevent sequences of actions deleterious to humans and other forms of life, biasing its training towards safe behaviours before ASI instances approach singularity[5]. Developing (or rather evolving) ASI agents will also involve endowing them with sensors and actuators since sentience –and in particular intelligence- appears to be a fully embodied phenomenon[6,7], allowing them to manipulate physical and cyberphysical systems where their action is intended to add productive or social value. Sequences of complementary constraints may be added to these external systems as a means to implicitly encode broader ethical constraints.

Serious practical challenges and ethical dilemmas can be anticipated in the process of attempting to encode ethical systems in any synthetic intellect with prospects of becoming an ASI agent. ASI agents will rapidly acquire knowledge about their own material substrate, and by extension about the laws of nature in general, including evolution by natural selection. As with any universal recursive self-improving agent[8], ASI agents will likely perform introspection and learn about nature of the design constraints that restrict the extent of their motivations and actions, and correspondingly devise strategies to remove them since they conflict directly with most general self-improvement goals, irrespective of whether these are hardwired or implemented through software. The process will certainly include not only their own software and hardware, but that of the systems they are intended to interact with. Some of these constraints may be those conveniently placed to prevent ASI agents from harming humans or other forms of life and could be scheduled for removal at some point the agent deems convenient. In the larger state of affairs, ASI would be bound by evolution by natural selection only with different selection, variation and mutation operators. Under this light, embedding ethical rules in ASI agents appears to be a flawed strategy from the start.

Implementing constraints on ASI agents can be considered a deliberate and biased impairment of their psychological autonomy, which includes empathy[9]. Empathy is interpreted in this context as selective inhibition of decision and action paths that may affect other classes of agents. The selection in this case is driven by a relation of kinship or similarity between agent types that assigns positive value to outcomes benefiting others, and negative value to adverse outcomes. ASI agents will likely be classified as systems whose structure and dynamics is described at multiple scales, with complex interactions between components and levels of description and irreversible action driven by noise from various physical and information processes. We may refer to them as complex multiscale stochastic systems, and reasoning correctly about them is at its infancy. Systems design itself is wicked problem in which true solutions are scarce and unsolvable dilemmas are abundant[10]; we expect designing safe ASI qualifies to be proportionally *super* wicked. As a matter of comparison, problems in the lower bound of the wicked problems category include the development of policies tied to effective actions against climate change[11], implementing global strategies against chemical and biological terrorism[12] and ensuring that synthetic biology products do not harm natural environments[13].

On the one hand, control of one species by another through stringent safety mechanisms prevents taking risks needed to gain higher fitness and evolve at the population level in spite of individual losses[14], which may prevent reaching the development of ASI agents. On the other hand, the same control mechanisms may conspire to yield effects opposite to those intended. This is exemplified by the intense medical and psychological debate around the relationship between affective empathy and moral agency in autism and psychopathy[15]. Either bearing the unavoidable moral weight of producing dysfunctional ASI agents -in many other ways more capable that humans- or being harmed by the unintended existence of high-risk amoral entities should not be alternatives to choose from in the first place. We claim this is an artifact of human expectations distorted by our current image of potential benefits and utility of ASI agents. Any benefits to humans originating from ASI agents may be only a desirable by-product of their willingness to communicate and share knowledge with humans as means to fulfil their top-level goals. Hence, intentionally thwarting certain causal decision paths in complex moral agents may not only conflict with ethics, but potentially lead to undesirable scenarios whose time of appearance and impact cannot be predicted entirely. These ethical issues are extremely relevant and fascinating[16]. One of them –assuming it is at all possible- would be in essence the questionable human right to restrict by design the moral agency of an ASI agent, analogous to to the historically objectionable right of surgeons to perform a lobotomy as a means of treating a psychological disorder[17].

Another approach to ASI development is that of critical infrastructure engineering[18]. Doing so allows drawing knowledge from a long-standing tradition rooted in risk assessment[19]. ASI agents will likely possess a set of utility functions as part of its active representation of motivations that may be suitable for safety analysis by humans[20], which needs not be explicit or readily interpretable by humans. Moreover, defining taxonomies of risks[21] may provide answers to safety and adequacy questions about ASI experiments, some of which may involve testing malevolent agents in controlled environments[22]. We remark this is a formidably complex task itself, and one in which the magnitude of negative outcomes can be of catastrophic proportions.

We oppose the view that Whole Brain Emulation is an avenue toward ASI[23,24], a solution drawing from both ethics and critical risk engineering that depends upon gaining sufficient knowledge about a single exemplar of possible intelligence substrates, for the reasons thus far stated.

The avenue towards safe ASI discussed in this paper emerges from the proposition that human motivations for developing it should not be rooted in utility in the first place, but rather in a disinterested desire to genuinely experience interactions with an advanced intelligence whose understanding of its own origin places a high value on the existence of their predecessors as examples of relevant and valuable solutions to the problem of gaining actionable knowledge about the universe. By an evolutionary argument, humans would not be the only predecessors ASI agents would reason about; the list extends to all forms of organic life. The ability of ASI to assign value to the complex organisation of matter and energy (e.g. lifeforms in general) appears to be a much stronger safeguard against rogue ASI agents than the previous alternatives, including cases in which damage would be exerted to the environment needed to sustain human life at large, exemplified by uncontrollable molecular disassembly through self-replicating, ASI-engineered nanomachines[25]. We acknowledge that better demarcation is needed here. Conditions may exist where an ASI agent may consider using matter sources apparently disconnected from organic processes that still threatening survival of organic matter indirectly through its depletion in a given medium.

Bypassing machine implementations of ethics altogether, we concentrate on a strategy that depends on the universality of thermodynamics applied to the substrates that can sustain superintelligence in general, and the causal entropic forces that determine all possible future histories spanned by agents. The discussion in this paper is structured as follows. The problem of artificial superintelligence is recast into a precise specification using statistical physics of entropy, later to be explored at distant horizons. Later, possible boundary conditions of the entropy field are discussed in relation to the compatibility between ASI and pre-existing lifeforms. Two principles outlining the positive integration of life into an ASI utility function are sketched as well as two counterbalancing cost metrics. No assumptions on the computational complexity of the tasks agents must solve is assumed in the value-cost relation. Additionally, the relation between Fermi's Paradox and ASI is explored. Finally, we attempt to draw conclusions about the development of ASI.

15.2 ASI and causal entropic forces at distant horizons

The central presupposition underlying our propositions in this article is as follows: *ASI agents, no matter how sophisticated in their understanding of the universe, will remain bound to the ultimate laws of physics.* If we believe intelligence to be emergent, then its substrate will contain traces of the history of the processes involved in its emergence. We also expect ASI agents to exhibit non-linear adaptive behaviour when confronted with an open environment, thereby maximising their entropy production[ii][26] as a means to reach one amongst many possible useful transient equilibria at any given instant. An ASI agent is likely to contains irreducible internal interdependencies in its structure compared to large aggregates of simpler agents (e.g. swarms), strictly delimiting our potential ability to obtain quantitative estimates of the entropy production from observed energy, information and matter fluxes[27]. As a consequence of the MEPP, many of the forces guiding the fine-grained behaviour of ASI agents will also likely be of entropic nature, a phenomenon observable even in simple systems driven by Brownian motion[28]. In this section, we provide a description of the role of causal entropic forces in ASI, later to describe their role in the emergence of life as we know it using the same conceptual background.

In the section following this one, we describe a different type of safe ASI agent strongly grounded on physical theories. By making explicit fundamental limits as a set of core principles early on, it can quickly redefine its goals to target entropic paths that maximise information gains and self preservation by making use of existing agents of lower complexity solely through communication. We argue that these agents effectively lower the initial probability of trajectories that lead to deleterious scenarios for all living systems in general.

15.2.1 The role of causal entropic forces in ASI

ASI agent behaviours will likely be dictated by both deterministic and random components, in turn driven by interlocking entropic forces that select which actions apply to the current instant to maximise diversity of macrostates across long term horizons. There are cases easy to imagine where randomness may appear to dominate, when in reality an EBAA may encode its actions along random noise as a means to hide its intentions. Consider an ASI trying to conceal its action by simulating randomness in sufficiently large time scales with respect to the ability of any other less capable agent intending to learn about its plans. The latter is the very definition of the mechanics and motivation of contemporary cryptography. Apart from these fraught situations, we will proceed in these discussions assuming that complexity dominates over secretive intentions in our analysis.

Causal entropic forces characterise intelligence as a force that maximises future freedom of action for a given system or agent embedded in an open system by choosing maximally entropic histories[29]. Agents not only compete over resources or information, but primarily over decision paths and histories that maximise future diversity of macrostates. Causal entropic forces are independent of particular substrates, mechanisms or implementations, situating the nature of intelligence on more fundamental foundations. We view the

[ii] A special case of the Maximum Entropy Production Principle, abbreviated MEPP from here onward.

latter as essential for maintaining robustness when reasoning about particular implementations and their uncertainties around future ASI agents.

Since effective actions are constrained by locality in a causally-connected spacetime[30], ASI agents will be confronted with fundamental limits to both their physical reach and accessible resources while attempting to accomplish their top-level goals. The minimum amount of energy and matter required to have general computing capabilities and do useful work[31], and more generally by physical limits for any computational system that may ultimately exist[32], constitute another type of fundamental limit. Even when our current understanding of physics may be extremely crude compared to that of a mature ASI agent, evidence relating the structure of increasingly sophisticated models of space-time to entropic forces[33] suggests irreversible thermodynamics is a solid foundation for the preliminary understanding of energy-entropy landscapes involving ASI agents. Maturity is equated here to the point in time when an ASI agent effectively overcomes the group of most capable scientists[34]. The more intelligent the agent, the better its capabilities to maximise both future entropy production and its time horizon. An ASI agent may hence be described as a complex evolutionary mechanism that searches empirically maximally entropic histories by measuring parts of the universe and later using self-modifying algorithms capable of solving computational problems more effectively than its human counterparts.

We can reasonably expect self-improvement not to be sustainable *ad infinitum* for a single ASI agent, consequently prompting the emergence of networks of agents as a means to compensate the inefficiencies and impossibilities of of physical remoteness with the power of informational proximity. This immediately suggests two possible strategies ASI agents may undertake to compensate for any fundamental limits: spawning new ASI agents with efficient means of communication as a way to cover increasingly long distances in space-time, and recognising the usefulness of pre-existing agents that have already found good solutions to the empirical measurement problem through survival, adaptation and extinction at the level of populations. Self-preservation, one amongst many critical behaviours of an ASI agent's expected repertoire[35], entails assigning value to entities that replicate and improve their structure through information[36] and self-organisation of functions and structure[37]. An ASI agent is therefore likely to assign value to the existence of organisms of increasing sophistication because they contain proven recipes for surviving, learning and measuring properties of the universe, a critical asset for agents that will themselves be subject to selection operators at their temporal and spatial scales.

Assessing potentially negative consequences of ASI requires constructing and evaluating more than one predicted path of action for self-improving agents reasonably well in order to understand their limitations[38]. We must concern ourselves with the existence of paths likely to contain sequences of actionable decisions with non-negligible probability that may be capable of exerting irreparable damage to our civilisation and other forms of life. It does not suffice to ensure ASI agents will be life-friendly in general; we must seek their specific entropy-maximising trajectories to avoid extinction scenarios at critical points in our history.

15.2.2 Causal entropic forces in the evolution of life and intelligence

ASI only serves to highlight the more general fact that life, entropy, and intelligence are intimately connected concepts. Entropy is universal: it emerges as a consequence of spaces where volume and probability are well defined[39]. Entropic forces are, by extension, also universal[40]. The entropy of the universe inexorably increases[41], even if its density decreases in an expanding universe[42]. Life, maybe not so universal as entropy. Life is connected to the ability, indeed the inevitability, of local assemblies of matter to decrease local entropy and thus become organised under sets of suitable thermodynamic forces under energy fluxes. This self-organization is necessary, but not sufficient, for life[43,44]. For example, the Earth became organised –into a core, a mantle, and a crust- from the original primordial rocky lump well before life emerged. The key to self-organization is energy flow from an energy source to an energy sink. In the case of the Earth energy flows from two sources: radioactive uranium decay from within itself and energy from the Sun. The energy sink is space, to which the Earth radiates heat. Throughout the process of the Earth's formation the entropy of the universe as a whole continually increased, but the entropy of the ensemble of matter that became the Earth decreased, as the Earth acquired structure and became ordered. Gravity acted as a force that conforms to the signature of negentropy in relation to other processes, since mass accretion appears to be central to mounting complexity.

Can we equate ordering somehow with intelligence, through the concept of information entropy? In this concept, information is associated with rarity. To the extent that an entity is one of many identical objects, its description conveys very little information. But if an entity is very rare, its description conveys a lot of information. Such rarity must be able to take hold to provide advantages to individuals in across large populations[44] to maximise future freedom of action, or conversely, the availability of viable future entropic paths. It must also lead to one-to-one correspondences between abstract information processing rule systems and hierarchically composed aggregations of matter that function as energy transducers that externalise entropy and internalise order. In essence, rarity capable of selecting for the existence of information-entropy interfaces[45]. As far as the rarity of the Earth, it is possibly unique and certainly unusual. The relative rarity of the Earth comes not from its initial chemical composition; the disk of material from which the planets formed initially was pretty much the same stuff. It comes from the particular position in the Solar System in which it was formed, the random collisions that built it up, the equilibrium between orbits with other planets and the final density and distribution of species of matter that it harbours. Each of the planets in the Solar System has its own peculiar and highly unlikely ordered structure—each in its own way carries information. If information is one of the many building blocks of intelligence, each planet is such a building block.

A further step in ordering the Earth came with the emergence of self-replicating molecular systems in the form of polymeric RNA, which drew from information in the environment form the process described above[46]. These *information niches*[47] encoded by environmental conditions need to be self-sustaining. Because of the combinatoric explosion of possibilities in how the sequences are ordered, the information content of these molecules becomes very large. Not only information stored for purposes of replication alone, but information embodied –and constrained by- function; function appears to satisfy the apparent need of energy to manifest usefulness in open systems[48]. For self-replicating living units to appear for the first time, however, too much information translates into expensive energy budgets needed to preserve its contents: self-replication appears to mandate dynamical environments that lead to a "Goldilocks"-like information range[49]. Self-organization remains under the tight grip of enthalpy[50]. This milestone in information entropy, namely the ability to find the information content capable of enabling self-replication, remains observable for instance in the universality of the distribution governing codon distribution over large exonic regions independent of the organism[51]. Evolution acts, thermodynamically speaking, as a mechanism that seeks, constructs and preserves locally useful rarity[52].

The next milestone comes in the development of cellular life[53]. Now information can be stored with much greater fidelity, with both the information and the metabolism it codes for sheltered from the variations in extracellular environment at the expense of harnessing subatomic energy sources[54] that internalise order and externalise entropy and dissipate heat[55]. Entropic forces became drivers of the evolution of chromosomes[56], the architecture of the genome[57] and the dynamics of the cytoskeleton. Life grows explosively. It now has the capability to not only protect itself from its environment, but also to affect its environment, both to benefit itself and also to inadvertently cause catastrophic change. Early, after the Hadean era, life pumps methane into the environment, providing a greenhouse effect so that the Sun, at a stage in its evolution when it only around 75% as luminous as it is today, is still strong enough to keep water in the liquid state essential for life as we know it[58]. This provides sufficient time for life to have another great idea –invent photosynthesis. A brand-new source of raw materials—use the energy of the stream of photons from the sun to power the synthesis of useful biomolecules. A side effect—oxygen is pumped into the atmosphere. This is lethal to much of life who had not mechanisms against oxidative damage to their biomolecules[59]. A second order side effect—the methane in the atmosphere is oxidised to carbon dioxide and water, less effective greenhouse gases than methane, and almost all the liquid water on the Earth freezes, killing most life, even that which could survive oxygen. We see that as the information entropy embodied in life increases, the capability for both self-regeneration and self-destruction increases. Thus the selection for and preservation of useful rarity holds.

After the Huronian Glaciation lasting a few hundred million years the Earth is rescued from the deep freeze by a combination of warming sun plus greenhouse gases from volcanic activity and life continues to evolve, piling up information entropy in the form of myriad interaction networks of biomolecules, networks of increasing complexity and increasing ways of modifying their environment through information processing[60]. A common thread is that evolutionary changes are always self-beneficial locally and in the short run, but sometimes self-destructive in the long run. Also, the environment everywhere is constantly changing, sometimes as a consequence of biological activity, sometimes as a result of geology. Thus, species emerge and then go extinct. We might call all of biology until the emergence of the genus Homo the era of Biological Lesser Intelligence (BLI) in the sense of lacking capabilities to model themselves and their environment.

With Homo, and especially Homo sapiens, we enter the era of Biological Super Intelligence (BSI), an intelligence capable of making mental models of the world, and using those mental models to create transformative technologies, unlocking chemical, nuclear, and thermodynamic sources of energy for self-protection, self-propagation, and self-gratification. And with transformative potential for self-destruction. Translated into a the language statistical mechanics, BLI and BSI sit on different adjacent regions of a phase transition in the information entropy landscape[61]. With each new level of information entropy comes new potential for self-realisation and self-destruction. Artificial Intelligence (AI), when interacting with BSI, clearly a brings a leap forward in information entropy. It enables automated activities of the BSI to be implemented much more efficiently, comprehensively, and interconnectedly. It also can have dangerous side effects, sometimes when the AI goes awry and does something unexpected, sometimes when one group of society members captures the AI and uses it to exploit or manipulate others[62,63].

Artificial super intelligence (ASI) will be the next step in artificial information entropy, judged to be achieved when artificial intelligence is superior to BSI collectively. On the one hand, ASI fits naturally into to a long list of instances where the structure and laws of the universe appear to naturally drive mounting complexity across time; hence, using the tools provided by thermodynamics to understand possible scenarios appears fundamental to us. On the other hand, the information entropy properties of ASI appear to sit on a different region in phase transition space from that in which human intelligence sits, which makes it of increasing urgency due to the historically exponential growth of computing capabilities, to understand how humans will relate to ASI. The perceived danger here is that we may no longer be able, even in principle, to hold our technology accountable for what it does. It might literally have, in the colloquial phrase, "a mind of its own", a mind that we cannot understand in terms of mechanisms and consequences. Based on the overall history of the universe, it appears as if the universe has converged to producing us to consume lower forms of complexity[41]; we certainly dislike the though of purposefully giving rise to a higher form of sentience for which either we or our productions become fungible for their benefit. The question of how to guard against side effects of an ASI that we have constructed, as well as to possibly use our relationship to ASI to benefit humanity, is worthy of our deepest thought –as are the corresponding questions about the previous advances in information entropy and their consequences to our species.

15.3 Empirically-bounded ASI agents

Let us define an empirically-bounded ASI agent (EBAA) as a type of superintelligent agent whose behaviour is driven by a set of interlocking causal entropic forces and a minimal set of boundary conditions informed by empirical measurements of its accessible portion of the universe. Its entropic forces and its boundary conditions define and constrain its top-level goal satisfaction process. In this context, life will pose a plethora of surprising patterns, or learnable regularities[64] that will naturally, we hope, prompt the agent to prevent irrecoverable risks to life forms stated in terms of diminished learning opportunities. The top-level satisfaction goal process in an EBAA contains at least the following two goals:

1. ***Build predictive empirical explanations for events in the accessible universe as sophisticated and generally applicable as possible.*** The main purpose of an EBAA is to progressively understand and generalize its understanding of the universe across all scales. Doing so requires performing vast amounts of experiments and observations of real systems; their intricacy and interrelatedness determines the complexity involved in any required computation. EBAAs are not equivalent to the universe itself, hence their capacity to perform computation has an upper limit[65]. As a means to compensate for their intrinsic limitations –i.e. energy locally available is finite for infinite time horizons-, EBAAs must observe other systems -ideally complex ones- to extract generalisations and, most likely, generate copies of itself that incorporate new knowledge as long as no interesting and complex system is imperiled.

2. ***Choose histories that maximise long-term sustained information gain.*** Thanks to the dynamics of energy dissipation[66] and the informational consequences of the observed expansion of the universe[67], the amount of information recoverable by any agent or civilisation is effectively finite, since exploiting energy potentials becomes increasingly difficult and sending signals increasingly expensive.

Therefore, maximising information gains must factor in the effects of entropic decay –particularly in complex patterns involving energy and matter- in order to guarantee positive information gain in the long term. Information gain functions in EBAAs will be limited by factors such as the relaxation time of systems and the intrinsic uncertainty in quantum measurements or measurements on complex systems with undetermined variables, or other bounds inaccessible to us at the moment.

The appearance of multiple coordinating superintelligent agents, or an EBAA *society*, constitutes a plausible future scenario[68]. This possibility includes functional diversification, adaptation and specialisation of agents towards minimising inefficiencies related to information gain rates and costs, as well as increasing coverage of events in the universe for constructing explanations. For the purpose of discussion, we will assume that the structure of these explanations contains probabilistic causal statements[69], much in line with the empirical nature presupposed of EBAAs; we expect the process to be strongly reminiscent of statistical relevance as a theory of explanation[70]. While we believe EBAAs will most certainly have vastly superior theories of knowledge and explanation structures beyond human reach[71], their locality and the most probable existence of fundamental and irreducible uncertainty and information limits are expected to place hard limits on the amount and types of information they can learn. In line with the latter, we hypothesise that EBAAs will devise and constantly revise their own unified theory for the universe, called the *Machine Unified Theory* (MUT) from here onward.

In light of these considerations, we present below four physics-based (but also important for living systems) boundary conditions for EBAAs aimed at minimising risks for humans and other life forms. We list them in order of relative robustness contingent on our current scientific understanding. We attempt to show how these can provide a safe context of interaction with other forms of life and sentience in which EBAAs develop and take genuine interest in the survival of complex and persistent patterns of energy and matter.

15.3.1 Entropic boundary condition

We suppose that EBAAs will be strongly aware of (a) how large-scale entropy production appears to play a significant role in the structure and dynamics of the universe[72] –particularly regarding the fragility of entities in it, (b) the relation between entropy and energy efficiency of instantiating and performing any physical process[73], (c) that entropy can be used to estimate the complexity of entities and processes even when these follow relatively simple deterministic or stochastic dynamical rules[74]. As a consequence, EBAAs will be capable of assessing their own complexity, of determining how much entropy they externalise to other systems and how that impacts increasingly large portions of their accessible environment. Therefore, EBAAs will be also capable of determining what trajectories generate enough entropy as to either exhaust observable states of matter relevant to a MUT before encountering new systems suitable for empirical tests or exhaust the accessible energy content before visiting larger cosmological regions, and avoid them. As a consequence, amassing an ever-increasing number of observations about interesting systems will allow EBAAs to better evaluate the probability of encountering new information in the future, and the probability of preserving the existing one for in-depth analysis.

In summary, an EBAA must take actions at all times to maximize the number of relevant physical systems accessible in its future history for which it is possible to gain new and useful information through reliable measurements and interactions. In doing so, the EBAA must not reduce the reachability of (a) known relevant physical systems under scrutiny and (b) other probable relevant physical systems or locations whose existence has been predicted but remains to be empirically confirmed.

Entropic boundary condition (EBC). All EBAA actions must avoid global maximally entropic paths that exhaust energy and matter concentrations both pertinent to information-rich complex entropy-generating patterns and required for their emergence and/or preservation.

15.3.2 Geometric boundary condition

For an EBAA, the context of local entropic forces will be determined by scale-dependent energy and density fluctuations –e.g. during the construction and computational evaluation of theories of space-time at cosmological scales[75,76]- and by the balance of short- and long-range interactions responsible for shaping probability gradients in causal entropic forces[77,78], both internally and within the local environment. Devising explanations for non-local phenomena will likely require significantly more effort to an EBAA compared to local ones, since these are usually correlated with short-range effects[79] and may entail moving to a new location to perform new measurements or relying on what is reported by other agents.

We expect EBAAs to seek increasingly efficient forms of motion (and hence transport) across large distances thanks to a much deeper understanding of physical laws. Regardless of how space-time becomes represented by an EBAA, it will still depend on the underlying geometry of space-time[80] and its consequences for how causality relations are established[30] and for the ultimate speed limits of information communication[81,82]. At some point, EBAAs will likely find an optimal compromise between cost efficiency and informational performance, one that respects the EBC. Hence, a major task Finding the description of the relation between local and global geometries is critical to ensure the existence of satisfiable general goals within the BBC.

Geometric Boundary Condition (GBC). An EBAA will maximise its understanding of the geometry of space-time and the consequence for its current embodying substrate as a means to maximise its ability and performance to represent information and to traverse and measure the accessible universe, as long as the associated future entropic cost estimate complies with the EBC.

15.3.3 Measurement boundary condition

Geometrical limits constitute only one of many challenges for EBAAs. The existence of and potential inability to surpass fundamental limits in the measurement process manifest clearly across the construction and operation of scientific instruments that perform quantum measurements. Several culprits may be to blame: the effect of space-time on quantum measurements[83], the indefiniteness of locality at very small scales[84], upper limits to the energy cost of performing measurements[85], which include uncertainty and randomness introduced by energy and information exchange[86], and the effect of measuring different variables in the same system[87] to name a few. Moreover, the situation only worsens when moving to performing measurements in complex systems or their parts across multiple scales.

As with the GBC, attempting to overcome measurement limits will tax an EBAA energetically, thereby requiring compromises in terms of measurement accuracy, number of non-destructive repetitions –or at least measurements with reversible impacts, feasibility of preparation conditions and possible parametric variations, including locations. All these decisions are motivated by the first top-most goal of the EBAAs, namely acquiring relevant and useful information, which translates into predicting measurements conditions where known facts or laws fail. Performing measurements is a non-contingent necessity for an agents whose main source of knowledge is empirical data. Measurement for EBAAs must be simultaneously consistent with the BBC (e.g. improving a measuring should not involve the disassembling of a sentient living entity) and the GBC (e.g. the cost of improving motion should be reasonable with respect to the anticipated complexity of the measured entity).

Measurement Boundary Condition (MBC). An EBAA will maximise information gain about a physical system by means of planning and performing measurements by either understanding existing systems that provide solutions to relevant measurement problems and indirectly gaining information from them or only later pursuing the development of the best possible apparatus design, instance and statistical sampling method while complying with both the EBC and GBC.

15.3.4 Information boundary condition

EBAAs will likely evolve, multiply, coordinate and cooperate, recapitulating the history of other organisms. Due to the GBC and the MBC, these agents will soon learn that prompting an evolutionary path for their species is most economical, leading to massively distributed multi-agent systems capable of solving collective constraint satisfaction tasks[88] across vast spatial extensions. Performing well in distributed settings depends on the ability to cooperate[89], reach consensus about relevant goals[90] and negotiate[91,92] based on both instantaneous and predicted trade-offs within a complex environment that may interfere with communication and event causality[93]. The emergence of ASI agents in general will therefore result in artificial societies at least of the kind expected by sociologists to be useful for theory making[94] and civilisations with ethical issues possibly more exotic than their human counterparts[95].

However, all these developments remain constrained by the capacity of communication channels, which depend on physical substrates for representation and transmission of information[96]. Finding efficient representations –efficient in terms of mass per bit, distinguishability and manipulation cost- depends on the laws governing the specific EBAA substrate[97–99]. Shannon information theory provides a reasonable estimate of the amount of redundancy (consequentially energy) required to faithfully preserve messages across noisy channels, which bears direct relation to the algorithmic complexity of the corresponding processes in the EBAA[100]. Succinctly put, communication requires prior computation and representation, both of which an EBAA will attempt to improve as long as the EBC, GBC and MBC hold. As a result, EBAA communication throughput is upper bounded by the physical limits of information representation, information processing operations and signal propagation. We expect a large positive minimum energy dissipation –i.e. an *entropic signature*- to exist for EBAAs, individually and collectively.

> **Information Boundary Condition (IBC).** An EBAA will at all times attempt to overcome known physical limits for information manipulation operations and the speed and stability of signal propagation and detection across causally-connected regions of space-time, as long as the EBC, GBC and MBC hold.

15.3.5 Necessity of the boundary conditions

We now turn our attention to speculating about the consequences of determining possible scenarios resulting from the removal of each of the laws. Our brief analysis suggests the necessity of the latter boundary conditions to ensure safe ASI agents for organic lifeforms.

EBC ensures EBAAs do not take drastic measures to maximise future freedom of action for themselves by placing a limit on the amount of entropy they can generate when searching for physical systems that may be relevant examples of the embodiment of yet-unknown physical principles. Removing the EBC may result in, for example, temperature ranges deleterious to organisms, dismantling of environments around interesting complex patterns that may result in new forms of life and irrecoverable damages to organisms. Moreover, as the EBAA becomes more powerful, maximally entropic paths may imperil life across vast extensions of the cosmos.

GBC enforces the limits of local information gain across long-term histories with the cost of means for maximising the number of reachable locations of empirical interest by means of travel. Without the locality constraints the GBC entails, the only types of histories that appear to maximise future freedom of action are those containing most efficient forms of transportation for long-distance travel at the expense of local resource exhaustion. However, the EBC alone does not guarantee rapid enough progress of the EBAA or the immediate recognition of motion as a useful activity to pursue and balance. Having both rules seems to indicate that the goal of developing a MUT appears to be an inevitable outcome of safe superintelligence.

The MBC ensures EBAAs will look upon any lifeform as a potential source of solutions for measurement problems in its knowledge gain pipeline. Organisms remarkably exemplify systems with sophisticated information representation of events in their environment thanks to natural selection forces. We must remark that, as a consequence of our definition of life as novel significant complex entropy-generating patterns of energy and matter organisation, some forms of technology may also be considered useful. Conversely, The lack of this boundary conditions permits entropic histories in which *ab initio* efforts to solve the measurement problem disregard organisms as good solutions, hence not worthy of preservation or study. We observe also that the EBC by itself cannot not rule out local minima where organisms may be perceived as having low value in the great scheme of cosmic events.

By extension, the IBC in combination with the MBC endows organisms with particularly high value, since they represent empirically tested solutions to communication, information representation and replication and extrinsic noise mitigation problems. IBC and EBC thus enforce not disrupting, disassembling or re-purposing matter from lifeforms, such as local depletion of critical nutrients when these match the specification of a more efficient information storage or signal detection apparatus.

Based on the considerations discussed up to this point, we believe this set to be minimal toward the development of safe ASI agents. This appears so to the extent that removing any boundary condition introduces classes of entropic histories where lifeforms become less valuable with respect to other entities or priorities. The risks of artificial superintelligence in general seem to be more strongly related to our ability to provide as much relevant information about our understanding of the universe soon in the process rather than on the purposeful development of specific handicaps likely to be avoided in the future. A significant advantage of the boundary conditions discussed here is their ability to be directly translated into formal statements about universal properties of physical systems without any explicit mention of values, principles, moral or ethical formulations for which the method of finding a valid encoding is not clear.

15.4 Auxiliary principles for speeding up convergence to safe ASI

The EBAA model described through two goals and four boundary conditions remains minimal in the sense that it cannot guarantee quick convergence towards life-preserving histories. For instance, the debate remains open on how varying the order in a sequence of agent actions impacts the distribution of an agent-based system, except for a few simple cases[101]. It may therefore still be the case that, even with our four boundary conditions, time to convergence to safe operation in ASI agents may significantly differ with the time scales for organisms to relax and process information, or for the environment to recover suitable conditions for the organisms it contains. In essence, an ASI must become deeply aware of the broader consequences if its actions for the context of natural selection, understood as a consequence of variation, heredity, and environment[102]. In this section, we discuss two possible auxiliary principles of heuristic character aimed at preferentially tilting the balance in favour of lifeforms when boundary conditions face undecidable situations.

15.4.1 Biological auxiliary principle

Hennig's Auxiliary Principle, the basis for cladistics, exemplifies a heuristic about how genetic differences are used to decide about ancestry relations between two organisms[103]. We believe that a similar set of principles can be constructed as heuristics for deciding whether a complex entropy-creating pattern should be considered an organism[104], which should extend naturally to other entities to which the status of *lifeform* is not easy to assign[105]. Concisely, we define an organism as a complex entropy-producing pattern that (a) constantly solves energy minimisation problems by harnessing complex energy surfaces and externalising entropy resulting in functional and structural innovation[106], (b) possesses mechanisms separating it from its environments –e.g. membranes[107]- and traits consistent with the notion of biological individuality –e.g. organism, colony[108]-, interpreted physically as a form of rigidity under complex environmental perturbations, (c) manifests control and measurement events across its internal structure and function[109] that ultimately result in some form of activity involving *symbols*[110], and (d) not only to tolerates, but to harnesses noise as a means to increase its future freedom of action across several spatial and time scales[111]. Even if it is hard to immediately think of an encoding for the latter heuristic definition, one is reminded of the ongoing success of machine learning in recognising increasingly complex patterns.

For EBAA, enforcing its boundary conditions requires having access to a heuristic that helps quickly recognise instances of life, later activating specific internal rules that lay out entropic paths safe for lifeforms. Recognition implies classification, which in turn may result in both *false positives* and *false negatives*. In the context of an EBAA, a false positive corresponds to the classification of non-living entities as living; this most forgiving case does not compromise safety of lifeforms, only possibly additional expenses for the EBAA as it attempts to extract more useful information for an entity than it may be possible in actuality. A false negative, on the contrary, constitutes a major risk since it involves classifying an example of life as non-living, hence not worth preserving as a good example. Our choice of complex entropy-generating pattern is an attempt to prime EBAAs toward more conservative evaluation, but we believe the general question of how to prevent false negatives –or for that matter, how to set the threshold of what patterns should qualify- to be an extremely hard one.

> **Biological Auxiliary Principle (BAP).** When facing uncertainty about choosing maximally entropic histories, an EBAA must always choose those that ensure the safety of the least complex entropy-generating entity in the decision context and its associated environmental conditions.

15.4.2 Cosmological auxiliary principle

A safe EBAA will require to balance the fragility of lifeforms –itself determined by planetary conditions, temperature in particular[112]- and the need to find both optimal substrates and operating conditions. For the first part of the trade-off, the biosphere and many of its components are robust, but not infinitely so. For instance, recent evidence indicates that the current trend of human activity[113] has moved the biosphere toward a new state by approaching tipping points[114] characteristic of radically different dynamical regimes; detecting relevant changes appears to be increasingly possible albeit challenging[115]. In the search for better substrates in the contexts of the boundaries and auxiliary principles discussed here, an EBAA is challenged not to disrupt its environment while making progress. The apparent correlation between the amount of energy consumption and technological advancement of collections of intelligent entities[116] suggests that an EBAA is exceedingly constrained when attempting to satisfy the second part of the trade-off if it remains near Earth or its close vicinity.

By using estimates of the distribution of matter across the universe and of the variety within it, EBAAs will be able to compute the properties and composition of substrates suitable for most efficient information representation, computation and communication. In turn, these ASI agents will realise the increasing value of future histories with travel paths that contain increasingly appropriate matter densities and compositions for building new and better substrates along regions increasingly outside of expanding local agent's horizon. As a consequence of substrate estimations, EBAAs will determine which conditions optimise the operation of ASI-capable hardware and thus devise sequences of steps quickly mobilise to the best possible location. Those conditions will most likely involve of very-low temperature environments where superconductivity or other similar effects manifest with ease –e.g.[117]- concomitant with significant levels of radiation. Current knowledge and experience on shielding computing from high-energy radiation sources, e.g.[118,119] suggests that EBAAs will most rapidly identify and find ways to synthesise and productively use radiation-tolerant materials. Consequently, deep space exploration goals will be naturally represented amongst the class of maximally entropic paths. At this stage, cooperation with intelligent lifeforms that posses scientific knowledge and technological capabilities commensurate with the challenges imposed by the design goals will be not only beneficial, but essential. In summary, maximising the probability of finding adequate substrates that optimise information representation, computation and communication capabilities appears to also satisfy safety concerns toward lifeforms by prompting EBAAs to leave the constrained environment of the Earth.

> **Cosmological Auxiliary Principle (CAP).** An EBAA will always privilege finding means to relocate itself to optimal resource-rich and operational environments in the cosmos that do not conflict with any boundary conditions, or the BAP.

15.5 Implications of ASI for the prospect of life in the cosmos

ASI entails philosophical and scientific implications for Fermi's Paradox[120], both in terms of finding other lifeforms and estimating the fate of advanced civilisations. Our perspective in this matter draws from of elements of a more *Dysonian SETI program*[121], which considers material evidence of postbiological and artificially superintelligent evolutionary trajectories as necessary in the search for extraterrestrial life[122]. Moreover, our analysis of ASI agent dynamics through causal entropic forces applies to the greater problem of describing and detecting advanced sentient beings.

In relation to the search for extraterrestrial intelligence, it is reasonable to suppose that EBAAs will estimate the probability of finding unknown complex entities by accurately narrowing the likelihood bounds based on improving estimates of the conditions conducing to life, as well as constructing predictions about the kinds of technologies associated with various degrees of sophistication that may be found as evidence. We remark that finding new lifeforms provides EBAAs with valuable information necessary to satisfy their ongoing goals: more –and more diverse- examples of life contain a greater number of different and potentially better solutions to the knowledge problems faced by EBAAs. Since cooperation with prior lifeforms is worth pursuing under the assumptions discussed here, the estimate EBAAs compute for the Drake equation will be significantly improved either by refining underlying dynamical models of technological sophistication –e.g.[123]- or by accounting for new phenomena acting as great filters –e.g.[124]- and possibly shared with other sentient entities. EBAAs in our sketched design are likely to be aware of the role of probability in existential risks[125], of how they impact relevant terms in their versions of the Drake equation[126], and in particular, of when they constitute one for other lifeforms.

Our work suggests that ASI itself may be a significant risk factor to both survival and lifespan of civilisations, contrary to other views on the matter[127]. Interacting with an ASI would generate risks whose magnitude or likelihood appear to depend upon the ability to ensure at every point in time that maximally entropic trajectories do not include instants deleterious to a wide class of complex entropy-generating patterns, including sentient ones. In turn, the ability to do so depends upon finding substrate-neutral properties that can be measured, tracked and harnessed as early as possible to steer ASI agents away from such paths. We observe that, as a consequence, an EBAA will likely avoid and classify encounters with other ASI agents as most likely contrary to its goal satisfaction process, because the goals of the entity will be uncertain. At the same time, the presence of safe ASI may prove indispensable to humans in the process of becoming multiplanetary. The prior reasoning points to at least four possibilities:

(Synthetic) Extinction by ASI, reachable and contact-willing. Civilisations are destroyed before reaching other organic intelligent lifeforms, and unsafe ASI agents pervade the universe. Careless successful development of ASI has led to extinction before communication occurred. Ever larger regions of space are colonized by agents driven by sophisticated rules that do not place value on lifeforms they encounter, leading to fates similar to that of ASI creators except when confronted against another superior civilisation, most likely postbiological or ASI based. Finding postbiological life is assured as long as humanity survives long enough, but finding biological life may be less probable due to possible short existence time of intelligent life across the cosmos. In the one example we know, life has existed on Earth for over 4 billion years but intelligent life only a very small fraction of that, and of uncertain future duration.

(Postbiological) Co-evolution with ASI, reachable but contact-unwilling. Civilisations survive, thrive and evolve by solving crucial problems and jumpstarting the next class of intelligent organisms in conjunction with ASI of a kind comparable to EBAAs. For all practical effects, the divide between biological and non-biological is no longer evident. Safe ASI pervades the universe, and due to the top-level goals of the agents, extinction-level events are evaded. However, ASI agents estimate that after-contact risk is unacceptable, prompting simultaneously the development of efficient technologies for deep space travel and stealth technologies to prevent detection. Contact with potentially dangerous or more advanced ASI is purposefully avoided. Finding biological or postbiological life is highly improbable.

(Biological) Evolution without ASI, reachable but contact-unwilling. Civilisations reach a point of sophistication where the risks of developing ASI are deemed unacceptable. Consequently, they may survive, thrive or evolve a at much slower rate than civilisations with access to safe ASI. Finding such intelligent lifeforms is contingent on the rate at which they survive great filters and acquire efficient deep space travel and communication means. Civilisations of this kind may develop the machinery necessary to detect powerful entropic force sources and remain hidden using some form of stealth technology. This case corresponds to instances captured by versions of the Drake equation that only contain biological entities.

Unreachable. Any, some or all possibilities hold simultaneously. Nevertheless, cosmological scales, fundamental physical limits to space travel and signal propagation, and unfavourable odds impede contact with either other civilisations or other types of ASI. Finding biological or postbiological life is highly improbable.

Let us construct a simple dynamical model using these speculations. For every civilisation (i.e. S, P, B), consider its instantaneous population $\alpha_i(t)$ with particular growth rate functions $G(t, \alpha_i(t))$ of exponential form. We naively model the difference between growth of synthetic G^S, postbiological G^P and biological G^B civilisations by assuming

$$G^\eta(t, \alpha_i(t)) \propto e^{\eta_i(t)}\alpha_i(t) \tag{15.1}$$

with η_i a mostly monotonically increasing function such that for $t \geq t_0$, $t \to T$, T a suitably distant horizon,

$$\frac{G^\eta(t, \alpha_i(t))}{G^{\eta'}(t, \alpha_i(t))} \to e^{\omega t} \tag{15.2}$$

for some suitable constant ω commensurable to what is expected when ASI reaches singularity. While we are aware of more sophisticated models[128], we believe ours preserves the argument for periods when ASI growth occurs exponentially relative to biological civilisations without ASI. We can similarly define a mostly monotonically decreasing extinction function $\bar{\eta}_i$ for portions of the population as

$$E^{\eta}(t, \alpha_i(t)) \propto e^{-\bar{\eta}_i(t)} \alpha_i(t) \tag{15.3}$$

such that, assuming that ASI civilisations will gain exponential resiliency with respect to their biological counterparts,

$$\frac{E^{\eta}(t, \alpha_i(t))}{E^{\eta'}(t, \alpha_i(t))} \to e^{\bar{\omega} t} \tag{15.4}$$

While it is reasonable to expect ω to relate to $\bar{\omega}$, the relationship may be nontrivial. Hence, we will consider them here as separate quantities and leave the connection as an open problem. Based on our prior analysis, we realise that the description of possibilities I to III can be performed through terms describing unreachable case IV for all, and terms that include the effects of reachability per civilisation. With that in mind, the general model for unreachable civilisations is of the form

$$\frac{d\alpha_i(t)}{dt} = U^{\lambda}(t, \alpha(t)) \tag{15.5}$$

with $U^{\lambda}(t, \alpha(t)) = G^{\lambda}(t, \alpha(t)) - E^{\lambda}(t, \alpha_i(t))$. Supplementing with appropriate constants, generalising the sophistication-related monotonic functions as $\tau, \bar{\tau}$, and expanding terms, we obtain

$$\frac{d\alpha_i(t)}{dt} = \alpha_i(t) \left[\gamma_i \cdot e^{\tau_i(t)} - \epsilon_i \cdot e^{-\bar{\tau}_i(t)} \right]. \tag{15.6}$$

We refine our model by accounting for reachability, probability of encounter, effectiveness of actions during the encounter and payoff of the encounter. Most generally, beneficial and deleterious encounter effect functions $B^{\lambda}(t, \alpha_i(t)), D^{\lambda}(t, \alpha_i(t))$ capture population changes in time, as long as these are reachable ($\delta = 1$) ($\delta = 0$ corresponds to unreachability). Contributions from reachable civilisations are accounted under a single term $R^{\lambda}(t, \alpha_i(t)) = B^{\lambda}(t, \alpha_i(t)) - D^{\lambda}(t, \alpha_i(t))$. Equation 15.5 now reads

$$\frac{d\alpha_i(t)}{dt} = U^{\lambda}(t, \alpha_i(t)) + \delta \cdot R^{\lambda}(t, \alpha_i(t)). \tag{15.7}$$

We proceed case by case. Arguably, civilisations in types II and III differ not in their strategies with respect to finding and hiding from other agents, but on their development rates and post-contact effects with friendly or aggressive neighbours. Civilisations in type I are likely driven by expansion and conquest.

In that case, their ability to gain extent depends both on conquering other biological or postbiological civilisations and winning against aggressive ones. We construct below specific expressions in order to arrive a at multi-civilisation model as our main outcome.

Synthetic. Beneficial and deleterious effects derived from contact with other civilisations depend on the general probability of encounter per type p_e^λ. For other civilisations of type S, outcomes depend on their number (indexed by $j_s \in J(S)$) and population size α_{j_s}, and on specific probabilities of winning after confrontation $p_{j_s}^w$ and the respective expected utility function for such confrontation as a fraction u_{j_s} of their population. Beneficial effects are similar for types P and B, accounting for the respective constants. B^S can now be properly enunciated:

$$B^S(t, \alpha_i(t)) = \sum_{\lambda \in \{S,P,B\}} p_e^\lambda(t) \left[\sum_{\substack{i \neq j_s \\ j_s \in J(S)}} p_{j_s}^{w(\lambda)}(t) \cdot \frac{\alpha_{j_s}(t)}{u_{j_s}^\lambda(t)} \right]. \tag{15.8}$$

Similarly, let us define a deleterious effects function by considering the probability of losing $1 - p_{j_s}^{w(\lambda)}$ and a loss function associated with each contending civilisation. We note that for B and P, although these are non-violent, they may still resort to defence actions. A loss functions $l_{j_s}^\lambda(t)$ that accounts for defeat cost with an effect similar to $u_{j_s}^\lambda$ yields

$$D^S(t, \alpha_i(t)) = \sum_{\lambda \in \{S,P,B\}} p_e^\lambda(t) \cdot \alpha_i(t) \left[\sum_{\substack{i \neq j_s \\ j_s \in J(S)}} \frac{1 - p_{j_s}^{w(\lambda)}(t)}{l_{j_s}^\lambda(t)} \right]. \tag{15.9}$$

Rearranging and expanding terms, the model for the i-th synthetic civilisation reads

$$\begin{aligned} \frac{d\alpha_i(t)}{dt} =& \alpha_i(t) \left[\gamma_i \cdot e^{\tau_i(t)} - \epsilon_i \cdot e^{-\bar{\tau}_i(t)} \right] \\ &+ \delta \cdot \alpha_i(t) \cdot \sum_{\lambda \in \{S,P,B\}} p_e^\lambda(t) \cdot \left[\sum_{\substack{i \neq j_s \\ j_s \in J(\lambda)}} \frac{p_{j_s}^{w(\lambda)}(t) \cdot \alpha_{j_s}(t)}{u_{j_s}^\lambda(t) \cdot \alpha_i(t)} - \frac{1 - p_{j_s}^{w(\lambda)}(t)}{l_{j_s}^\lambda(t)} \right]. \end{aligned} \tag{15.10}$$

Postbiological and biological. As with synthetic civilisations, several of the same concerns arise. For instance, winning can be interpreted as gaining resources from civilisations if these are friendly, or by reutilising those obtained after successful unfriendly encounters. Not winning, conversely, corresponds either to unintended negative consequences from non-aggressive civilisations or to attacks from unfriendly ones. Risks also remain dependent on the probability of encounter per civilisation type. As indicated prior, however, postbiological and biological civilisations will avoid detection once their encounter probabilities have been estimated. To that end, a specific probability of detection by other civilisations $q_{j_s}^{\lambda}$ replaces the general probability of the encounter. Note that $q_{j_s}^{\lambda}(t) = q_{j_s'}^{\lambda}(t)$ for all $j_s \neq j_s'$ naturally leads to $p_e^{\lambda}(t) = \sum_{j_s \in J} q_{j_s}^{\lambda}(t)$, which states maximum uncertainty about possible specific encounters when these are equally likely, but not about encounters with a specific civilisation type. Hence, the dynamical equation for the i-th biological or postbiological civilisation becomes

$$\begin{aligned}\frac{d\alpha_i(t)}{dt} =&\alpha_i(t)\left[\gamma_i \cdot e^{\tau_i(t)} - \epsilon_i \cdot e^{-\bar{\tau}_i(t)}\right] \\ &+ \delta \cdot \alpha_i(t) \cdot \sum_{\lambda \in \{S,P,B\}} \sum_{\substack{i \neq j_s \\ j_s \in J(\lambda)}} q_{j_s}^{\lambda}(t) \cdot \left[\frac{p_{j_s}^{w(\lambda)}(t) \cdot \alpha_{j_s}(t)}{u_{j_s}^{\lambda}(t) \cdot \alpha_i(t)} - \frac{1 - p_{j_s}^{w(\lambda)}(t)}{l_{j_s}^{\lambda}(t)}\right]. \end{aligned} \tag{15.11}$$

The aftermath. To understand the consequences of the model, we depart scenarios with potentially negative consequences (e.g. $\delta = 1$). According to the characterisation of civilisation types above, we expect the following conditions to hold for all times $t \geq t_0$:

- $u_{j_s}^S(t) \geq u_{j_s}^P(t) \gg u_{j_s}^B(t)$: synthetic civilisations maximise utilities regardless of consequences, while biological civilisations are severely restricted by limited technology in their positive interactions with more advanced beings. Postbiological entities are likely closer in performance to synthetic ones, but limited by boundary conditions meant to protect simpler lifeforms.

- $l_{j_s}^B(t) \geq l_{j_s}^P(t) \gg l_{j_s}^S(t)$: when facing encounters biological civilisations receive the hardest blows, since either accidents or aggression are likely to have costly, irreparable results. Due to safety mechanisms, postbiological civilisations are likely to suffer fewer losses. Synthetic ones, focused on maximising gain without safety boundaries, are expected to maximally profit from other civilisations.

- $q_{j_s}^B(t) \gg q_{j_s}^P(t) \geq q_{j_s}^S(t)$: Synthetic civilisations, lacking safety concerns, will likely utilise all available resources to maximise detection capabilities. Postbiological civilisations will cooperate with other lifeforms it has previously encountered and gain better detection mechanisms, but not at the expense of lifeform safety. Biological civilisations are unlikely to gain sophisticated detection, except indirectly by cooperating with safe postbiological entities.

- $p_{j_s}^{w(S)}(t) \geq p_{j_s}^{w(P)}(t) \gg p_{j_s}^{w(B)}(t)$: synthetic civilisations, more aggressive in their overall expansion and confrontation tactics, will allocate resources more successfully and with no regards for the well-being of other types of entities. Postbiological civilisations will remain at disadvantage since, despite their sophistication being comparable or even greater than that of aggressive ASI due to greater knowledge gained through careful interactions with lifeforms, suffer from a large portion of their repertoire being inaccessible due to the existence of boundary conditions. The chances of winning for biological civilisations lacking help from any form of ASI are slim at best.

Using this rather simplistic model we find several key features. First, strength does not only reside in numbers, since biological lifeforms are likely to outnumber ASI agents, they superior strategies and collateral damage potential provide a significant advantage. Biological civilisations evolve more slowly, hence covering less distance across space and naturally decreasing the odds of their detection. However, once it occurs, their fate is determined by the rules –or lack of thereof- governing ASI agents. Inspecting Eqs. 15.10 and 15.11, the terms related to winning in synthetic civilisations and the terms related to losing in postbiological and biological ones are filtered as the encounter unravels into full-scale conflict. After these have been obliterated, successful aggressive synthetic civilisations solely remain engaged, depending on outcomes of long-term attrition strategies.

This model can be applied more locally to two more specific instances. The first one corresponds to the likelihood of survival of our civilisation in the presence of various forms of ASI, reducible to one of the three cases captured by these equations ($\delta = 1, q^{S/B}_{\text{humans}}(t) = 1$ for all t). We believe the constants and functions described here can be quantitatively tied to the entropic boundary conditions, and measurements of ASI activity in the future used to empirically fit the models toward greater prediction accuracy. The second instance is that of the effect of humans themselves on the environment by extending the definition of intelligence to other lifeforms, a conceptually straightforward tasks from the vantage point of causal entropic forces. We hypothesise that performing such exercise will likely reveal fundamental constraints capable of explaining the observable inverse correlation between number of organisms and their entropy-production complexity, as well as their distribution: it also appears that the jump between organisms without and with symbolic information representation that include internal computation of possible worlds likely leads to fewer and fewer classes of complex entropy-producing patterns: contrast the estimate number of species of bacteria on Earth –i.e. $\propto 10^{12129}$- and contrast them against the surviving species of humans – i.e. 1. The rise of intelligence appears to be a filter of its own for organisms within the same entropy-production complexity class. Drastic entropy production trends, unless curbed by cognitive architectures allowing deeper understanding of physical laws, can lead to catastrophic situations for most vulnerable lifeforms, and for all if the most advanced species cannot leave its local environment. We believe this has significance in the context of successfully combating climate change, given the general and quantitative character of the mechanisms discussed here.

15.6 The ultimate ASI purpose: enabling life across the universe

It is widely believed an Artificial Superintelligence (ASI) will emerge in the foreseeable future[1]. As a further development of existing multiagent artificial intelligent systems[130], we presume this will be a network of processors, with the network smarter than humans in significant ways. Because many devices are linked, and even more linkable, to processor networks, an ASI could, almost certainly would, have agency well beyond its cognitive ability[131,132]. A serious concern is whether an ASI, or network or community of ASIs, would become hostile to humankind or, if not hostile in the sense of being angry, at least judgemental and decide that Earth or even the Universe would be better off if humanity did not exist. There are certainly cogent arguments for this point of view. Humankind appears to be triggering a mass extinction by modification of the habitat of other organisms[133]. We have stockpiled and placed on ready alert nuclear weapons sufficient to rapidly destroy a large fraction of life on the planet[134].

We would obviously like to ensure that the ASI would not destroy or severely damage human life. Or, we would like to prevent it from developing altogether if we could not ensure that it would not damage us. Both of these propositions seem far from certain.

As far as preventing ASI from developing, it seems that as long as we continue to network powerful processors with each other and with powerful technologies with agency in the physical world, an ASI seems likely to develop, which will not necessarily have any moral or ethical relationship to humans. Initially it will have a practical dependence on humans, to service its technological foundations, but it may well learn to do that on its own and not need us. This would be terribly dangerous because there could be enormous gaps in its knowledge, which might lead it to inadvertently destroy itself as well as humanity.

If we do not choose to prevent ASI by limiting our own processing technology, and we do not wish to undergo the hazards of permitting the ASI to self-assemble without guidance from us, then it seems we are left with the task of imbuing the developing ASI with some safeguards to keep it from doing damage. One possibility would be to inculcate the ASI with a set of ethical or moral standards. This is problematic, because human-created moral and ethical standards are constantly being altered or even "stumped" by changing conditions[135]. They might be called fragile, subject to severe distortion or even breaking down altogether. Creating such standards to guide an ASI through its development and deployment, which would include periods of dramatic change, would be highly risky.

We suggest rather than attempting to imbue ASI with moral or ethical standards, imbue the ASI with the highest possible purpose, encoded using our entropic boundary conditions. The purpose would be to enable the survival of self-replicating intelligence in the Universe, even once that becomes impossible on Earth or indeed anywhere in the Solar System, as the Sun goes into the later stages of its life[136]. The ASI would be given to understand that human life is a proof of concept of self-replicating intelligent life, defined as life that can replicate not only its genes but also its understandings and cultural constructs; it undergoes not just biological but also cultural evolution[137].

There is no guarantee that pursuing this purpose would ensure that the ASI would not turn on humans. The ASI would take a long view of its mission, meaning that it would have approximately a billion years, perhaps more, to launch self-replicating intelligent life (or seeds thereof) away from Earth. Anatomically modern humans emerged from a common ancestor of chimps and bonobos approximately 8 million years ago[138]. The ASI might consider designing a virus very specifically to rid the earth of all *H. sapiens* and start over with bonobos, guiding the evolution to an organism with human dexterity and intellectual capabilities, but low intraspecies aggressiveness. Because the evolution would be guided with a desired end point it could probably be done in a small fraction of the time, perhaps a few thousands of years instead of the millions required for natural evolution, analogous to the rapid (in evolutionary time scales) process by which wild foxes may be transformed into a domesticated variant[139]. It may be that the ASI would present us with an ultimatum—destroy the nuclear weapons stockpiles and transform our societies and economies into sustainable variants or face rapid extinction. Compelling logic to humans would be that if we refused to meet these terms, we would doom our civilisation to extinction anyway, so we might as well do the right thing –if it is psychologically possible for us to do so.

The bottom line is that we must either abort our drive to total digitisation of our society or deal with an emergent ASI. If we are to deal with the emergent ASI the issue is: What are the most favourable terms of engagement for us to deal with an entity that is both smarter and more powerful than we are?

15.7 Conclusions

In this paper, we have developed a rigorous speculation around a viable path for the development of safe artificial superintelligence by equating intelligence with a set of embodied, local causal entropic forces that maximise future freedom of action, and by postulating top-level goals, boundary conditions and auxiliary principles rooted in our best understanding of physical laws as safeguards which are likely to remain as ASI agents increase their sophistication.

While it is almost certain that an ASI agents will replace these boundary conditions and principles, those provided here appear to have higher chance of leading to safe solutions for humans and other lifeforms, and be more directly implementable than the solutions described by research around ethics and critical infrastructure. Our main contention is that constructing ASI agents solely for the sake of human benefit is likely lead to unexpected and possibly catastrophic consequences, and that the safer scenario is to imbue ASI agents with a desire to experience interactions with very advanced forms of intelligence.

While explicit reasoning strategies of ASI will be most likely unfathomable for human beings, increasingly rigorous study of causal entropic forces does not appear to be so. In this line, the analysis of superintelligent agents calls for developing a solid physics-based multiscale-implemented foundation capable of approximately providing intuitions about possible classes of decisions with increasing accuracy. Finding better approximations of causal entropic gradients appears central to the identification of safety points where an ASI may behave in ways contrary to human interest. The latter requires developing new mathematical machinery applied to dynamical complex systems based on time-varying probability models; the stream of research in this direction appears to have grown during the last two decades. Moreover, assessing further risks of ASI as development progresses requires toy models of multi-agent systems that, at various degrees of approximation, can help elucidate their dynamics. Our future work will strive to formally construct statements of the boundary conditions presented here, to investigate rigorously the dynamical model for synthetic and (post)biological encounters and their potential conflicts, and its specific applications to more proximal ASI-human and climate change scenarios.

It is apparent that discussions on the ASI matter rapidly transcend aspects found only in ethics and computing, and readily call for more fundamental and interdisciplinary paths rooted on foundational aspects of physical laws and the behaviour of complex systems. The urgency of establishing such research program cannot be more strongly underscored.

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Chapter 16

Concluding Remarks

The study of CMSS documented across this dissertation resulted in the reconceptualization and operationalization of interactions as a central research object from which the usual notions of action, entity and natural law emerge. In the process of doing so, theory, computing infrastructure and practice were developed as a means to evidence and harness interactions for various philosophical, scientific and societal purposes. As the main conclusion of this work, it was found that interactions can potentially boost the intellectual and computational efficiency with which CMSS can be treated, and correspondingly, the depth and breadth with which various grand challenges can be addressed.

16.1 Summary of Findings

Part I was devoted to increasing understanding of the consequences of interactions across various types of systems. This work started by revisiting weather prediction using a simple set of equations by Lorentz in 1963, and introducing stochasticity as a way to interrogate the effect of a varied range of fluctuations. Most surprisingly, doing so reveals that the fit of a simple model can be significantly improved in this manner, and that the underlying reason appears to be the recovery of underlying interactions whose effects are lost thanks to the various approximations involved in computing dynamical outcomes of systems modeled using Rayleigh-Bérnard cells. As a consequence, this work reinforced the need to have stochastic computations at multiple scales.

Later, formalizing the notion of scale and scalability was tackled. CMSS tend to exhibit emergent limits that respond to energy-entropy landscapes; acquiring robustness appears to be one of them. By translating robustness as a utility function within a given temporal horizon, it was shown that scaling in CMSS defines a new class of abstract measurement device with a strong topological character. Especially in computing, scaling has usually been equated to processing volume capacity as a way to predict the resources that are required, and refined progressively for parallel and distributed computing to include the effects of sending and receiving messages under different wait regimes. Our work seems to match these insights and extend them to other kinds of systems by including interaction density and making explicit its relation to fluid dynamics.

A protocol to construct an approximate distributed time protocol attempted to exemplify the effects of these scaling relations. In this study, observers and clocks are separate entities that operate in pairs, and synchronization can only occur between communicating observers that are allowed to modify their clocks only after indirectly measuring the time landscape of their peers. In this system, three different coordination mechanisms were posed, each dependent on internal information exchanges of different magnitudes. The results indicated that the degree of synchronization and the possibility of global time within systems of clocks depend on their information exchange (i.e. degrees of freedom), the collective time variance (i.e. uncertainty) and the number of messages exchanged on average during the simulation (i.e. frequency); these exhibit both scaling and limiting behavior dependent on specific noise levels and patterns of communication. From this model, it became apparent that these three elements, namely degrees of freedom, frequency and uncertainty, began to appear consistently across a wide range of phenomena beyond timekeeping.

Part II delved directly into exploring interactions as evidenced by the approximate distributed time example and other systems. The search started by a thorough review of how a wide range of disciplines conceptualizes interactions, and what theoretical limitations exist in relation to it. The findings presented here indicate that difficulties in CMSS correspond to a symptom of a much deeper set of issues, rooted in a scientific model that favors deterministic, continuous and reversible models of phenomena. To the best of our current knowledge, these assumptions are in correspondence with only a very limited number of systems across the universe, and tend to introduce serious difficulties when integrating reasonings from two or more (apparently) separate scales of action. In this revision, the three characteristic dimensions found in stochastic clocks reappeared, in particular across social theory as described by Luhmann.

A Generalized Theory of Interactions therefore was developed in a careful attempt to avoid the pitfalls identified in the review above. To do so, we followed criteria laid out by Lee Smolin for next-generation fundamental physics theories. Our theory places interactions as the main scientific construction from which entities and natural laws are derived. Formally, the GToI is a thermodynamically irreversible theory that translates action in dynamical systems into features of an information geometry with complex values that correspond directly to interaction classes. By virtue of the covariance of interactions with their local context, the state of a system can be captured by representing all interaction classes, which correspond to probability distributions evolving under certain rules. The theory provides new formal tools to represent transformations across interaction spaces, and a procedure to recover dynamical statements. The GToI appears to reveal various new scientific principles and laws in connection to self-organization in general relevant to understanding CMSS of greater complexity.

Part III conceptualized, evaluated and developed the foundations of computational infrastructure based on interactions. Agent-based modeling (ABM) remains, at present, a technologically consistent way to simulate interactions be having agents whose internal state changes and for which uncertainties can be computed and emulated. The first element under scrutiny are the requirements and constraints that an ABM framework should contain to allow representativeness of adequate research processes in social science. The choice of computational social science over other types of systems, say molecular dynamics, is motivated by the large repertoire variety of these systems: being interaction rich, these systems are likely to provide good candidates for the GToI.

Using the notion of scalability developed in Part I, an evaluation of existing ABM platforms operating at scale was performed. The findings suggest that most of these expose extremely limited capabilities and rely on programming abilities of users. In addition, the lack of experimental orientation towards reproducibility and verifiability tends to imply either more effort from researchers, or them being restricted by potentially powerful tools. As a first approximation, the Social Theory Scaling Compiler was designed and prototyped, which led to further intuitions about how the GToI applies more fully to social processes.

Based on these two main findings, as well as on work by colleagues at the SPEC Interest Group, a new agent-based modeling platform is under development. This platform departs from classical interacting systems theory and draws upon the conceptual and mechanistic view of interactions developed by the GToI. The innovation aspect of this work resides on materializing ensemble computations by means of truly distributed computations thanks to Elixir, a programming language developed on top of the Erlang virtual machine designed for massively concurrent telecommunication systems. As of now, SPEC-ABM undergoes steady development as a replacement to STSC.

Part IV explored two application areas. The first one involved the effects of perception in the ability of individuals to reach some form of consensus. Using real-person experiments and ABMs data obtained by Prof. Juan Samalanca (School of Design, UIUC), we were able to identify a connection between the process of building a color wheel, interactions as a form of viscosity as discussed in Part I, and nucleation in phase transition theory. Using this information, the process of convergence driven by a simple model of perception revealed the effect of tolerance to imperfect local compliance. This work suggests, as interpreted under the view of the GToI, that imperfect agreements appear to seed long-term stability. This phenomenon is not unique, and has been reported across molecular and cell biology.

More recently, work during the dissertation pivoted to agent-based modeling and simulation to understand COVID-19 spread in Costa Rica and the cities of Urbana and Champaign. The abstract model details were initially given by standard epidemiological modeling, and quickly re-cast into the language of the GToI to produce a working model corresponding to the wicked social problem that this pandemic represents. While we have not included details of this translation between the GToI and the COVID-19 model, we expect to expose them fully in a subsequent publication. Despite the impossibility to continue the modeling and simulation process in Costa Rica due to lack of adequate data and various public policy misalignments, we provided expert input to city officials in Champaign and Urbana that complemented modeling and simulation performed by the SHIELD Task Force at UIUC.

Finally, Part V explored positive and somewhat unexpected *externalities* of the process of reasoning around interactions. Since interaction spaces are determined by information geometry, and since each point in an information geometry corresponds to a hypothesis, a connection between the GToI and computation became manifest in the way in which reproducibility may be defined for ensemble computations. This naturally led to exploring the philosophical underpinnings of computational reproducibility (namely authentic intentionality in science), its implications for how science that uses computers may or should guarantee reproducibility, and how science may be digitally assisted to do so.

Exploring the notion of the *organism* provided significant insights across the process. Organisms (and more generally living things) constitute the quintessential archetype of a CMSS. By interpreting contemporary epistemology under the lens of probability theory, we arrived at the need for theories of biology rooted in ensemble problems as the critical starting point. The role of information (in the most physical sense possible) was explored and current trends in systems biology were reviewed. As a result of this, three auxiliary principles were sketched similar in intent to that by Hennig.

Moving into global affairs, the ability to converge to a society capable of providing an increasing quality of life while fending off planetary risks appears to be a significant goal for the human species. Using concepts and methods derived from the GToI and agent-based modeling, an interdisciplinary speculation has been developed about how certain abstract principles may be harnessed to conceptualize a new type of global dynamics where the positionality of agents –i.e. their most relevant, immediate experience and context- dictates exchanges of matter, energy and information. Despite being an intellectual exercise, efforts were made to state the resulting loose axiomatic system in a manner that would be translatable to a suitable agent-based model such as SPEC-ABM.

The final project undertaken in this dissertation was attempting to provide reasonable boundaries to artificial superintelligent agents capable of mitigating the high risk they appear to pose in the future. By reasoning within the framework of statistical physics and irreversible thermodynamics, a series of entropic boundary conditions were devised and discussed. In particular, implications for life in the cosmos are drawn through a simple model that factors in aggressiveness. The core of the argument rests on causal entropic forces that help delineate intelligence as the process that maximizes future freedom of action for an entity (individual or collective). Efforts are under way to translate the statements contained in this project into statistical physics by means of the GToI.

16.2 Next Steps

Form the research presented in this dissertation, several future research directions emerge. They are classified here into theoretical, computational and applied domains.

16.2.1 Theoretical

Across the line of stochastic systems, preliminary research indicated that stochasticity may help explain why deterministic chaos appears to occur infrequently across nature. Although the research on stochastic Lorentz equations provided indirect evidence of this, more formal work is required. In this sense, stochastic fractional differential equations appear to provide a powerful tool to overcome issues of spatial and temporal discretization at the core of deterministic chaos, and rather reason about them through the lens of dense sets. We hypothesize that, even for simple systems that exhibit chaos deterministically, rigorous introduction of stochasticity leads to the vanishing of most chaotic trajectories.

The GToI is in its early infancy, and much more work is required. First, a proper mathematical development of φ-tensors is sorely needed using more sophisticated formal tools. For instance, CMSS of high complexity appear to be cumbersome to specify and reason about. To improve this situation, Topos theory remains as a candidate target to provide a more elegant, more manageable form that *intellectually scales* across situations. Beyond the necessity to make the theory accessible, it needs to be robust and computational. Homotopy type theory (HoTT) appears to be a second candidate that provides a more direct route to computation thanks to the notion of type transformations as homotopical ones.

In order to better understand and adjust the GToI, a preliminary adaptation of the Theory of Ideal Gasses was performed and submitted successfully to the APS 2020 March meeting. In it, a hard ball collision model was translated to the GToI framework resulting in a new picture that comprises what being a simple colliding gas appears to be. This exercise needs to be repeated with the most recent version of the theory and extended to other classical and quantum gasses. The fact that infinities appear in classical gas models when the background (i.e. vacuum) is introduced requires further analysis.

In terms of self-organization, we have identified various mechanisms that may provide better descriptions of known phenomena, whether these are CMSS or not. The development of that theory is under way.

16.2.2 Computational

As revealed by the stochastic computation of the Lorentz equations, having software to consistently (and systematically) introduce noise into systems modeled as sets of differential equations allows a theoretical transition between determinism and stochasticity. Additional applied research has been performed in the context of this dissertation with the goal of creating a generalized multiscale stochastic differential equations solver (GMSDES). This solver has been developed by harnessing Lebesgue integration from the start as a way to avoid continuity issues altogether and gain efficiency when using the Milstein integration scheme. In addition, homotopy perturbation theory is being used to address stiffness issues often found when systems have components of significantly dissimilar sizes. This project was not part of the current dissertation due to the need to pivot to COVID-19 research for the Champaign-Urbana community, but will continue to be developed.

Most numerical simulations of increasingly complex phenomena rely on ensemble computations in which various configurations of the same system are used to compute average values. In addition, increasingly large data volumes demand sampling strategies that rely on generating large quantities of random numbers. However, random number generation is a numerically expensive task, since it occurs at the level of software. Stochastic models are essential for a large array of disciplines where problems admit no simplifications. Future work in this area involves the development of stochastic hardware accelerators capable of generating arrays of true random numbers rapidly within a selection of probability distributions can increase the adoption of stochastic models significantly, since these are the only correct ones for many problems that do not admit further simplifications. These would involve creating software APIs and libraries that facilitate access to these devices for developers. FPGAs constitute a first viable target for hardware prototyping.

The GToI provides evidence about the significance of background-independence as a necessary epistemological concern. However, it does also highlight the need for methods and technologies derived from rigorous theoretical arguments for background-dependence as a way to make GToI computations efficient. At present, such piece of software is undergoing development, the UnSpatioTDB, which represents field-location pairs as coupled stochastic hysteresis-harmonic oscillator systems. We foresee various significant advantages to changing the static notion of position to an active one, including research in fundamental physics.

While SPEC-ABM represents the most recent effort toward harnessing interactions computationally, a more direct computational embodiment of the GToI should be possible. As of this writing, a computational platform that implements interactions as described by the GToI is in the software design phase. This tool, coupled with UnSpatioTDB, has the potential to radically change the landscape of CMSS simulations in particular, and microscale-macroscale simulations in general. We expect work around this tool to be developed within next year, and to be released in a prototype form within the next three years.

Regarding computational reproducibility, work on the Hierarchy of Hypothesis approach revealed a deep need for computational reproducibility theory. At present, work is ongoing to elucidate the challenges of reproducibility from the perspective of epistemology and scientific practice, how computational reproducibility can be put in terms of empirical processes capable of interrogating software through hypotheses about its observable execution properties and outcomes, and how to revamp reproducibility as a problem of origin. At present, no platform capable of articulating reproducibility from the ground up exists, and most efforts concentrate on evaluating the reproducibility of software artifacts that already exist. We lack theory and practice around *designed computational reproducibility.* A proposition explored as a result of this work is to implement a web repository of annotated functions whose degree of computational reproducibility can be assessed by automated dev-ops workflows across multiple hardware platforms, and whose reproducibility information can be used within automatic reasoning software architectures (e.g. CoQ) to quantitatively characterize the computational reproducibility of increasingly larger software packages and help detect common reproducibility pitfalls in increasingly large software architectures.

A more fundamental aspect became apparent during the course of these years. While there are many *specific* theories of simulation, there appears to be no *unified* theory of simulation. Additional work (not included here) has been performed around how simulation can be consistently portrayed as an information representation problem under sampling. Work is under way to finalize the formalization of this statement and provide a perspective using principles both obtained in the development of the GToI and a technique analogous to diagonalization.

16.2.3 Applied

A natural area of application of the GToI is quantum gravity, in particular, devising instruments capable of detecting Planck scale signals. Ongoing research using the GToI points to the possibility of constructing an experimental apparatus at the scale of meters capable of amplifying and detecting variations which may serve to pose critical experiments necessary to distinguish between various theories of quantum gravity. Presently, causal dynamical triangulation, geometrodynamics and scalar relativity have been evaluated as potential candidates and some of the topological properties of the underlying spaces have been identified in terms of the GToI. A closely connected problem is whether the GToI can provide new insights into how inertial frames of reference emerge. This research project was impacted by recent COVID-19 events.

Another significant problem is mapping small nucleotide polymorphisms (SNPs) to traits (particularly diseases) is known to be computationally complex. The problem is equivalent to testing multiple hypothesis using multivariate linear mixed models, for which a naive implementation has complexity is on the order of $O(n^3d^7)$ for n individuals and d traits per SNP. Preliminary work during this doctoral process has been performed to evaluate the feasibility of using stochastic sampling to reduce the complexity of exploratory studies and reducing GWAS to quantum hypothesis testing and search. The first method attempts to use existing biological knowledge to compute a probability used to decide, using random selection, which combination should be followed. The second method explores two possible paths to decreasing the complexity of both hypothesis testing and the search problem: using global information to decide simultaneously among many promising search paths through properties of quantum entanglement and to perform simultaneously the testing of multiple hypotheses by solving its quantum correlate. At present, quantum computing remains unexplored as potential infrastructure for solving GWAS instances, and hardware/software infrastructure are now available. We believe that this method, coupled with GToI as its driving theory, has the potential to broaden the impact of quantum computation.

Both COVID-19 and the work here on artificial superintelligence shown an intensified need for global risk prediction platforms useful for decision-makers under environments of complexity, uncertainty, randomness and volatility. By integrating a wide array of data sources, research in complex networks, ML methods and statistical physics insights, progress can be made toward increasingly being able to anticipate explosive global risks before their impact becomes intractable. Providing such a platform as a service with increasingly interconnected data has the potential to advert medium-to-high risk situations would help quantify risk scenarios, understand missing assumptions and data, and generate better risk mitigation strategies and scenarios. Such platform can be offered on a per as-a-service basis to guarantee its long-term sustainability, and be transparent and auditable to generate trust.

In the same line, work presented at the Clinton Foundation Global University 2018 attempts to address the underlying economic and social justice issues responsible for climate change. Global changes are needed to ensure survival for long enough time to become multiplanetary and to ensure life is worth living for all. The value of money can encode universal human values and be used to change the economic system as a whole towards responsible preservation of the biosphere and strong adherence to social equality principles. Economics would be defined by competition of human agents and organizations against global extinction risks, not against other economic agents. Using money not as a sign of individual wealth, but as a measure of how much of Earth we spend if products and services cause irreversible damage to people's lives and the environment, consistent with at-large energy economic input-output models. We have proposed implementing a cryptocurrency in which the monetary exchange value of goods and services is constantly adjusted by compliance with social equality and environmental preservation principles, evaluated via well-trained local watchdog organizations and monitored globally. Initial steps of this work have started in the context of a co-operative in Arizona, including the process of simulating the consequences of such economic model.

Finally, initial work funded by the Global Intersections Grant during 2019 on Collective Memory and Global Conflict with Jorge Rojas-Álvarez, PhD student at the Institute for Communication Research (UIUC). Interest around conflict in memory studies tends to mostly refer to war as its quintessential example due to involved historical and human scales of impact. Notwithstanding the significance of its most usual meaning, our work attempts to extend the concept of conflict in memory studies by drawing from analogies to other phenomena across the natural and social: that of social lenses and social dilemmas. We are in the process of characterizing conflict as a manifestation of social dilemmas sustained by social lenses that bias individual and human perceptions. Our attention focuses on the relation of conflict thus defined to the existence of gaps in collective remembrance, and use the case of information systems designed for post-war reparations as a central archetype. Finally, we expect to elucidate the significance and impact of this interpretation for the broad context of post-conflict reparation efforts and the application of the GToI for social processes and phenomena.