XSEDE helps the nation's most creative minds discover breakthroughs and solutions for some of the world's greatest scientific challenges. Through free, customized access to the National Science Foundation's advanced digital resources, expert consulting, training and mentorship opportunities, XSEDE enables you to Discover More.

XSEDE also provides the following tools to help researchers make the most of their allocations:

- Extended Collaborative Support Services (ECSS) pairs XSEDE users with computational science experts to maximize their research potential.
- The XSEDE Cyberinfrastructure Integration (XCI) team provides advanced hardware and software architecture for a more integrated user experience.
- The XSEDE User Portal helps users access XSEDE resources, manage jobs, report issues, and view results.
- The XSEDE Resource Allocations Service (RAS) team helps coordinate allocations of NSF's high-end resources and digital services.
- Specialized community services, provided through the XSEDE Federation, allow for rapid innovation and experimentation (e.g., gateway development, education, training, etc).
- Training, education, workforce development, and campus engagement provided by the Community Engagement & Enrichment (CEE) team.
- A fellowship program that brings Campus Champions to work closely with XSEDE advanced user support staff.
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IT IS ALWAYS WITH A GREAT SENSE OF PRIDE AND ACHIEVEMENT that we present the annual Extreme Science and Engineering Discovery Environment (XSEDE) highlights book. This sixth edition provides a snapshot of key research funded in part by the National Science Foundation (NSF) and supported by XSEDE in areas such as genomics, artificial intelligence, drug design, environmental conservation efforts and so much more. The research published in this book works toward solving some of the greatest issues facing the world today. With XSEDE, the research community that our staff collaborates with is working to find answers to these challenges and to pursue the opportunity to discover more about the future of science. As a significant entity within the broader community, XSEDE has continued to grow and surpass our expectations. In addition to enabling the great science represented in this publication, XSEDE has continued to incorporate and refine a multitude of services into the XSEDE infrastructure to accelerate scientific discovery. This has been complemented by further development of the technical skills of XSEDE staff to stay on the leading edge of technological developments that can be harnessed by the community.

In addition to the scientific achievements enabled by XSEDE this year, the Campus Champions program celebrated their 10th anniversary, growing to now include over 450 champions, reaching over 200 institutions spanning all 50 states, the District of Columbia, Puerto Rico, Guam and the U.S. Virgin Islands. XSEDE also continued to engage with the student community, offering opportunities for undergraduate involvement in technical aspects of XSEDE such as networking, system maintenance and support, and visualization through the XSEDE EMPOWER (Expert Mentoring Producing Opportunities for Work, Education, and Research) Program. This program provides students with a stipend and resources for their experiential work and training through engagement in XSEDE projects. XSEDE EMPOWER successfully completed its first full year of support and mentorship to young scientists with outstanding results. These community efforts are cemented in our fundamental commitments and high aspirations for the future of XSEDE.

From its inception in 2011, the XSEDE project has allocated over $270 million in research-enabling resources and services including access to computational systems, data analysis resources, visualization environments, resources supporting data-intensive science, and access to critical technical expertise. These resources have helped the Laser Interferometer Gravitational-Wave Observatory (LIGO) detect gravitational waves, helped identify cancer DNA changes using very high resolution brain imaging, enabled promising new research that will engineer an enzyme that can break down plastics and help put an end to plastics pollution worldwide, as well as countless other scientific breakthroughs and discoveries. While these achievements were made possible through the hard work of many, I am deeply grateful to the number of individuals whose hard work made providing resources, services, and technical expertise all possible through XSEDE.

In short, today’s research requires the resources, services and technical expertise represented by XSEDE. It is our mission to continue to enhance the productivity of scholars, researchers, and engineers by providing access to advanced digital services that support open research and add significant value to the broader cyberinfrastructure ecosystem. As we move forward, I am proud of what XSEDE has accomplished and am excited about our future. The XSEDE community is strong and vibrant, and together we will continue our efforts to accelerate exciting research.

Sincerely yours,

John Towns
XSEDE PI and Project Director
"I started working at the facility in August 2014," says Megan Justice, who was working as an undergraduate at the time, in Marshall University's Genomics Core Facility. "About a year later, I was helping with the work on the Sumatran rhinoceros and Narcissus flycatcher genome assemblies." Now, Justice is a Ph.D. student, studying Genetics and Molecular Biology at the Dowen Lab at the University of North Carolina at Chapel Hill.

The two assembly projects, led by Herman Mays, an evolutionary biologist at the Huntington, WV, university; and Jim Denvir, co-director of Marshall's Genomics Core Facility, promised critical advances in our understanding of evolutionary processes. The rhino and flycatcher genomes, the scientists expected, could shed light on how species respond to climate change and other environmental stresses. The rhino, a tropical species, was nonetheless more closely related to the ice age wooly rhinoceros than to other modern species. The flycatchers are a rare example of a species that have populations that are migratory and some that are not.

"He asked me if I’d be willing to work on [the allocation submission]," she explains. "I said, ‘Yes.’"

"The first thing I did was get on the XSEDE User Portal and read a lot of examples of allocations," she says. "I researched the different centers to see which was the best fit for us … The examples online were very specific, and included a genomics assembly example. It’s a step-by-step process that shows you what you’ll need for the next step before you even get there."

"XSEDE continues to streamline and refine the allocations policies and processes," says Dave Hart, director of XSEDE’s Resource Allocations Service. One upcoming innovation will be a series of submission templates for users which have the dual benefit of clarifying what the reviewers are looking for and splitting material in submissions into fields that can be searched and analyzed more effectively.

"This will give [users] somewhere to start," Hart says. "It won’t be mandatory at first and will roll out over time as we get feedback from XRAC members. And for experienced users it will be OK to still use their successful prior submissions as a starting point." The aim, he explains, will be to give first-time users in particular a greater chance at success.

"Marshall is not a very large university," she explains. "When it was time to apply to grad school, I wanted to take a step to a larger institution. At the University of North Carolina Chapel Hill, they were so impressed I had worked on a project like this, that I had worked independently on writing this application. I think it really gave me an edge … When I accepted their offer of admission, one of the researchers who interviewed me even called to ask if I would be interested in doing a rotation in their lab."

The actual wet-lab sequencing of the species’ DNA fragments went well, Justice says. But the assembly step, using the computer to combine the sequence fragments into the two full genomes kept crashing their campus computing cluster. That’s when their Campus Champion, Jack Smith, told them about XSEDE.

"Through working with XSEDE, an undergraduate student gained a competitive edge for applying to graduate school — and helped assemble the genomes of two biologically important species."
HOW TO SEE LIVING MACHINES

Every cell in our body has identical DNA, the twisted staircase of nucleic acids uniquely coded to each organism. These molecular machines are so complex, yet so tiny, that scientists are just starting to understand their structure and function using the latest microscopes and supercomputers. Biological molecular machines could lay the foundation for developing cures to diseases like cancer. How small can one see, and what will one find?

For the first time, structures have been detailed of the complex groups of molecules that open up human DNA,” said study co-author Ivaylo Ivanov, associate professor of chemistry at Georgia State University. “And for us, XSEDE has been absolutely essential,” said Eva Nogales, professor in the Department of Molecular and Cellular Biology at UC Berkeley and also Senior Faculty Scientist at the Lawrence Berkeley National Laboratory and Howard Hughes Medical Investigator.

Cryo-electron microscopy combined with supercomputer simulations have created the best model yet, with near atomic-level detail, of a vital molecular machine, the human pre-initiation complex (PIC). The PIC finds genes associated with making a specific protein, pulls apart the two strands of DNA and then feeds the coding strand to the transcription, where DNA bits are copied by RNA polymerase II into a single strand of messenger RNA, and makes its way to ‘protein factories’ in the cell called ribosomes that take them as orders for which protein to make. If DNA is like the blueprint for building a house, RNAs are instructions to the ‘contractors’ at the ribosome work station. The manufactured proteins are like the nails, wood, plaster, and just about everything else in the house.

The experiment began with images of PIC ‘freeze frames’ of PIC were processed using supercomputers at the National Energy Research Scientific Computing Center to sift out background noise and reconstruct three-dimensional density maps that show details in the shape of the molecule that had never been seen before.

“Cryo-EM is going through a great expansion as are all the computer softwares used to generate both the density maps and also to interpret them like we’ve done in this study,” Nogales said. “It is allowing us to get higher resolution of more structures in different states so that we can describe not just one picture of how they look, but several pictures showing how they are moving.”

Study scientists next built an accurate model that made physical sense of the density maps of PIC using XSEDE. Ivanov’s team has run over four million core hours of simulations on the Stampede1 supercomputer at the Texas Advanced Computing Center (TACC) to model complex molecular machines, including those for this study. Ivanov’s broader molecular machine work also includes an XSEDE allocation of 1.7 million core hours on the Comet supercomputer at the San Diego Supercomputing Center (SDSC), putting water and counterions in addition to the PIC complex in a molecular dynamics simulation box, we get the full story of the structure and function of the protein complex of molecules.

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The goal of all this computational effort is to produce atomic models that tell the full story of the structure and function of the protein complex of molecules. To get there, Ivanov’s team took the twelve components of the PIC assembly and created homology models for each component that accounted for their amino acid sequences and their relation to similar known protein 3-D structures.

XSEDE was “absolutely necessary” for this modeling, said Ivanov. “When we include water and counterions in addition to the PIC complex in a molecular dynamics simulation box, we get the full story of the structure and function of the protein complex of molecules.”

One of the insights gained in the study is a working model of how PIC opens the otherwise stable DNA double helix for transcription. Nogales explained that one could imagine a cord made of two threads twisted around each other. Hold one end very tightly. Grab the other and twist it in the opposite direction of the threading to unravel the cord. That’s basically how the living machines that keep us alive do it.
While computers have beaten human champions at a number of games—like checkers, chess or Go—these games offer perfect information. No information is hidden from the contestants and they have limited ability to deceive each other.

Poker, on the other hand, is an imperfect information game. Unlike in chess, in an imperfect information game the opponent’s hand is secret, and he or she is trying to mislead. Imperfect information games are like many real-world problems, including cybersecurity, terror defense, negotiation, and medicine. This paves the way for AIs to help transform how humans approach real-life problems in security, negotiation, and medicine.

Tuomas Sandholm of Carnegie Mellon University and his Ph.D. student Noam Brown have created a series of artificial intelligence programs (AIs) capable of optimizing how to play essentially any imperfect information game. The scientists wanted to find out whether the AI’s strategic reasoning had finally reached the point at which humans couldn’t beat it, even under imperfect information. To find out, they took on the world’s best specialists at heads-up, no-limit Texas hold’em poker—a benchmark game in which hidden information and deception are paramount. The AI would have to learn how to deceive—and how to win despite deception. In 2015, the team’s earlier AI, called Claudico, narrowly lost to top human players.

Before contending with poker champions, Libratus, an artificial intelligence program developed by Carnegie Mellon University School of Computer Science, would have to figure out its own strategies by playing itself, without human advice. In developing Libratus, Sandholm and Brown worked with XSEDE ECSS expert John Urbanic at the Pittsburgh Supercomputing Center (PSC). Urbanic helped them to write the parallel algorithms in earlier versions of their AI such as Claudico. As they refined their software, he helped them manage the huge database the AI required as well as the large number of nodes necessary for it to run on Bridges.

“We didn’t actually look at any data, just the rules of the game,” says Sandholm. “It was like practicing by shadow boxing and then stepping into the ring with Mike Tyson.”

No-limit Texas hold’em has 10^{40} possible situations—more than there are atoms in the known Universe, and far more than any computer can directly calculate. To master the game, Libratus had to find the optimal way to simplify the game to be computable and how to bluff in ways that tricked some of the most expert human players into holding, and folding, when they shouldn’t.

For their January 2017 “Brains vs. AI” match with the pros, they turned to the XSEDE-allocated Bridges system at PSC, using about 600 of Bridges’ compute nodes. This raw power gave Libratus the capacity to plot each move in real time—and reformulate its strategy each night, even as the four human experts—Dong Kim, Jason Les, Jimmy Chou and Daniel MacIay—were doing the same to try to expose any weaknesses in the AI.

The pros—computation-savvy experts more like mathematicians and computer scientists than the guys in black suits and dark glasses people might imagine—gave Libratus as brutal a competition as they could.

“They did everything I was afraid they’d do.”

In the end, Libratus scored a resounding victory, beating the pros by more than $1.7 million in chips at the Rivers Casino in Pittsburgh. The scientists calculate that an outcome this lopsided or larger was only 0.5 percent likely to happen just by chance. The win marked the first time that an AI had beaten the world’s best players at a game that had emerged over the years as the leading benchmark for solving imperfect-information games. This paves the way for AIs to help transform how humans approach real-life problems in security, negotiation, and medicine.

“The improvement they’ve been able to make over the past 18 months … has been quite extraordinary,” said poker pro Mike Tyson. “It was like practicing by shadow boxing and then stepping into the ring with Mike Tyson.”

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“We didn’t test it ahead of time against professional poker players,” says Brown. “They did everything I was afraid they’d do.”

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“[Libratus] is very beastly—super gangster … Whatever we throw at it, it just figures out … something that shuts us down … We were going after weaknesses, and we’d think, ‘Wow, this is it, we found something’—and as the time went on, those exploits just disappeared.”
CELEBRATING TEN YEARS OF CAMPUS CHAMPIONS

Over the last ten years, the digital research landscape has changed dramatically as campuses across the nation have gained access to local research computing resources and services. Since the inception of the Campus Champions program in 2008, our mission has changed to accommodate the diversity and growth of our community: to promote and facilitate the effective participation of a diverse national community of institutions in the application of advanced digital resources and services to accelerate scientific discovery and scholarly achievement.

What Makes a Champion?

A Campus Champion is an employee or affiliate of a college, university, or research institution whose role is to help their institution’s researchers, educators, and scholars make the most of their computing and data-intensive research. Champions engage in a variety of activities, including educating users on and facilitating the use of advanced digital capabilities, among other things, to improve, grow, and/or accelerate their scientific achievements.

The Champion community is made up of individuals in a variety of roles and disciplines, across all levels, such as system administrators, HPC Directors, faculty, user support specialists and IT staff. The program provides workforce development opportunities, allowing champions to begin early in their academic careers as student champions, or join the community as a Domain Champion providing an advanced level of expertise in a specific discipline.

The Champions are a flourishing, one-of-a-kind community of peer-mentors and facilitators who successfully communicate virtually to share information, best practices and experiences including, but not limited to: asking and answering questions on an active mailing list, sharing technical expertise, participating in video conferences as well as face-to-face meetups at regional and national conferences like PEARC and Supercomputing (SC).

The Champions are experts in a specific discipline.

The Campus Champions program provides an array of professional development and training resources that benefit both the individual Champion, as well as the Champion’s institution. Based on feedback from the community, programming is provided in the form of ad hoc presentations from subject matter experts, with topics ranging from systems-focused technical discussions, resources (XSEDE and non-XSEDE alike), software, education and faculty-focused topics and grant writing. In addition, Champions are given an opportunity to apply to an engaging and challenging Fellowship program that pairs selected Champions with exciting projects and expert mentors that they might otherwise not have access to. The Champions Community welcomed its first fully elected leadership team in July 2018 — providing an opportunity for individual Champions to gain valuable leadership skills while making an impact and giving back to this exceptional community.

What’s next for Campus Champions?

The Campus Champions hope to increase scalable and sustainable access to advanced digital services from providers at all levels. With the rapid growth of the Campus Champions community, the Champions will continue to foster a more diverse nationwide cyberinfrastructure ecosystem by cultivating inter-institutional exchanges of resources, expertise and support. Here’s to the next ten years of Campus Champions!

<table>
<thead>
<tr>
<th>2008</th>
<th>Campus Champions officially started.</th>
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<tr>
<td>December 2009</td>
<td>Champions Leadership Team formed.</td>
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<td>May 2012</td>
<td>Champions Fellows Program began.</td>
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<td>July 2013</td>
<td>Domain and Student Champion Programs initiated.</td>
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<td>August 2015</td>
<td>200th institution joined.</td>
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<tr>
<td>July 2018</td>
<td>First fully elected leadership team in place.</td>
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<td>January 2015</td>
<td>Regional Champion Program initiated.</td>
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<td>2016–present</td>
<td>XSEDE2 / Campus Champions Fellows Leadership Program initiated.</td>
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<td>2011–present</td>
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<td>2007</td>
<td>Planning for Campus Champions began.</td>
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<td>May 2008</td>
<td>First Champion selected.</td>
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<td>August 2011</td>
<td>100th institution joined.</td>
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<td>June 2013</td>
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<td>2014</td>
<td>Campus Champions filled 450th position.</td>
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<td>2018</td>
<td>Champions program has grown to over 450 Champions at more than 240 institutions in every state and EPSCoR jurisdiction.</td>
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HISTORY OF CHAMPIONS:

TERAGRID / 2004–2011

XSEDE / 2011–present

XSEDE2 / 2016–present

Sustained funding from XSEDE and the National Science Foundation (NSF) over the last ten years has helped the Campus Champions support campus cyberinfrastructure and foster a thriving community of practice with nationwide impact.

WHAT IS THE CAMPUS CHAMPIONS PROGRAM?

The Campus Champions program is a community of over 450 members at over 240 research institutions whose role is to help researchers at their institutions use research computing, especially at large scale and high end computing levels. The Champions excel at raising awareness of, and facilitating access to, advanced digital resources, among faculty, researchers, students, and staff within their organizations. Therefore, Campus Champions fill a variety of roles at their home institutions, helping researchers find and use the technologies that best fit their needs at whatever scale they need.

The Campus Champions program provides an array of professional development and training resources that benefit both the individual Champion, as well as the Champion’s institution. Based on feedback from the community, programming is provided in the form of ad hoc presentations from subject matter experts, with topics ranging from systems-focused technical discussions, resources (XSEDE and non-XSEDE alike), software, education and faculty-focused topics and grant writing. In addition, Champions are given an opportunity to apply to an engaging and challenging Fellowship program that pairs selected Champions with exciting projects and expert mentors that they might otherwise not have access to. The Champions Community welcomed its first fully elected leadership team in July 2018 — providing an opportunity for individual Champions to gain valuable leadership skills while making an impact and giving back to this exceptional community.

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The final installment of Arctic maps released in September 2017 by the ArcticDEM project were made possible by the National Center for Supercomputing Applications (NCSA) at the University of Illinois at Urbana-Champaign, the University of Minnesota, Ohio State University, and Cornell University.

Current elevation models for the Arctic have a resolution of one kilometer—Morin’s models offer a resolution of five meters or less, and are much more accurate at gauging height. The jump in detail will help scientists track ice loss better, and enable a host of other research.

Morin estimated he met with Towns sometime in 2014 and Towns immediately introduced the XSEDE project as a potential problem-solver for the massive scale of data that would come from an array of satellites collecting topographic images.

"We did a proof-of-concept pilot that rapidly turned into actual production effort," said Towns of XSEDE’s original involvement in ArcticDEM. "It became clear that the resources necessary to go for the ambitious goals that Paul had—and still has—were simply beyond the capacity and capability to support with XSEDE resources."

"As our project was getting off the ground, we realized that our code was probably far enough along to start putting on XSEDE resources. We got a start-up allocation and got consulting help to allow us to work on that and ran things in relatively small areas of space—like the North Slope of Alaska, those kinds of things," said Morin. "After a while, we knew we needed a bigger resource to do compute and Towns introduced us to Bill Kramer (PI of Blue Waters)."

"With Towns, he’s the ultimate connector. He was able to point us at the right places. When something needed to be goosed, he goosed it. The XSEDE support folks (ECSS) helped do a lot of the initial optimization and grunt work and profiling. That’s what was key for us, because the last time I had touched HPC, it was a different century. I learned to work on Cray-2s."

Morin concluded: "The way that people should start doing research on HPC now is either through their own campus resources or through XSEDE."
What happens on the surface is often given short shrift compared to what goes on inside. But with chemical reactions, what occurs on the surface can mean the difference between a working material and one that refuses to perform its duty.

Tao Wei, an assistant professor of Chemical Engineering at Howard University, studies surface phenomena — also known as “interfacial” — to learn how and why they occur. His research is used in biosensing, designing polymer membranes for water treatment, and creating new ways of generating energy from bacteria, by performing simulations on the Stampede1 supercomputer.

“Computer simulations have become an important tool to complement experimental research for nano-materials and bio-nano technologies. His research is used in biosensing, designing polymer membranes for water treatment, and creating new ways of generating energy from bacteria, by performing simulations on the Stampede1 supercomputer. "Simulations provide atomic-level details and illustrate quantum processes, which are difficult to detect in experiments." From 2014 to the present, XSEDE has awarded Wei’s group several million computing hours on Stampede1. He also used several other supercomputers — including Gordon and SuperMIC systems, Titan and Mira systems — to make progress on a variety of important problems.

We’s work also peers into nano-pores, like polyamide membranes, which have the thickness of only 100 nanometers and the pore size less than one nanometer. Polyamides are the most widely used material to desalinate and purify water, and therefore knowledge of their microscopic structure can lead to significant societal and commercial benefits. "A better understanding of the structure of polyamide membranes will help design future desalination and filtration methods, which will lower energy costs and provide a lot of economic benefits," Wei said. "Running a series of virtual experiments on Stampede1, Wei and his team, working with Dr. Shroll and Murad at the Illinois Institute of Technology, found that the degree to which the benzene rings in the material were cross-linked played a major role in the transport of water.

A third computational project on Stampede led by Wei and his collaborator, Dr. Aiichiro Nakano from University of Southern California, studies the electrical properties of a unique type of bacteria that can harness energy from its environment through the cycling of nitrogen, sulfur and iron. Understanding the long-range electron transfer of the bacterial proteins that enable this process can aid in a variety of applications, including bioenergy production, solar-conversion catalysts, and the removal of toxic hexavalent chromium from water.

"To exploit emergent biomolecules’ electric properties for promising applications in energy and environment, it is critical to understand the interfacial behavior of those conducting proteins," Wei said. "And his team performed simulations on Stampede1 to study the degree to which decaheme cytochrome adheres to a gold surface in water, and the electron transfer efficiency of the process. Their results revealed that dehydration — which reduces the loss of water molecules from the reacting molecule — on the gold surface serves as a crucial driving force for protein adsorption. If we put those proteins on the electron surface and then we transfer the electrons between the outside environment and the inside of the electrode surfaces, we can convert energy or reduce toxic heavy metals through the redox methods," Wei said. "This is very cutting edge, but we are seeing several cool examples already."

Whether through studies of protein-ligand binding sensor, desalinating polymers or bacterial nano-wires, investigating the atomic and quantum behavior of molecules has the potential to help scientists understand new and improved synthetic materials and biomaterials. "These microscopic tools can give you a lot of information," Wei said. "Each type of simulation has limitations, but when we have a strong theoretical background and can connect different scales, we can rationalize experimental structure-function designs and solve important scientific and engineering problems."
The coastal wetlands of Louisiana near the mouth of the Mississippi River in the Gulf of Mexico are at risk. Many factors have played a part in why the state is losing approximately a football-field sized parcel of land every hour, but it’s happening.

Since 2015, XSEDE has emerged as an important tool to help stifle land loss thanks to a science gateway called "SIMULOCEAN," which was developed by the Coastal Hazards Research Collaboratory (CHARCOL) led by professor Q. Jim Chen at Louisiana State University (LSU).

Science gateways are web-based "portals" that allow researchers to perform computational science in domain-specific, community-developed interfaces. SIMULOCEAN is one such portal for researchers to investigate water, air and land dynamics on HPC cloud-ready systems like the XSEDE-allocated Jetstream, for example.

One of the defining characteristics of XSEDE is its ability to cater to the researcher who may not be a computational science expert — in the case of SIMULOCEAN, ecologists and geologists (or any other type of scientist) looking at the wetlands loss in Louisiana can use the NSF-funded project to explore, and perform numerical simulations of various coastal weather events like hurricanes and storm surges on large swaths of land like never before. SIMULOCEAN’s easy-to-use interface, along with XSEDE’s ECSS program, can help inexperienced cyber-infrastructure users perform the tasks they need to, which will hopefully lead to land saved.

“We think SIMULOCEAN has three primary goals,” said Jian Tao, former research scientist at the Center for Computation & Technology (CCT) at LSU and developer of SIMULOCEAN. “First, it will increase community and collaboration in this field of study. Second, we want to provide scientists and engineers with easy-to-use computer tools for wetlands restoration and protection. And lastly, we’d like to use and promote NSF-funded resources like XSEDE, which are provided to the greater science community.”

Focusing specifically on the "community and collaboration" goal, Tao said, "it’s important to enhance the collaboration among earth scientists, computer scientists, cyberinfrastructure specialists and coastal engineers tasked with solving the sustainability issues of deltas coast like those in Louisiana."

To make sure SIMULOCEAN is accessed by those researchers without a predisposition to advanced computing resources, it is made to be user-friendly, even allowing a new user to start running applications in mere minutes.

The development of SIMULOCEAN has been supported by the NSF CyberSEES (Cyber-Innovation for Sustainability Science and Engineering) program (CCF-1539567), which "aims to advance interdisciplinary research in which the science and engineering of sustainability are enabled by new advances in computing."

XSEDE fit right in to this project and now offers up the collaborative muscle to hopefully answer important questions about America’s quickly-vanishing wetlands.
PROMISING DRUG LEADS IDENTIFIED TO COMBAT HEART DISEASE

Using a unique computational approach to rapidly sample, in millisecond time intervals, proteins in their natural state of gyrating, bobbing, and weaving, a research team from UC San Diego and Monash University in Australia has identified promising drug leads that may selectively combat heart disease, from arrhythmias to cardiac failure, using the computing power of Gordon, Comet and Stampede1 provided by XSEDE.

Together, the research team performed an unprecedented survey of protein structures using accelerated molecular dynamics or aMD – a method that performs a more complete sampling of the myriad shapes and conformations that a target protein molecule may go through.

“The supercomputing power of Gordon, Comet, and Stampede1 processed hundreds of nanosecond aMD simulations, which are able to capture millisecond timescale events in complex biomolecules,” said the study’s first author Yinglong Miao, a research specialist with the UC San Diego Department of Pharmacology.

Though effective in most cases, today’s heart medications – many of which act on M2 muscarinic acetylcholine receptors or M3 muscarinic receptors that decrease heart rate and reduce heart contractions – may carry side effects, sometimes serious. That’s because the genetic sequence of M2 mAChR’s primary ‘orthosteric’ binding site is “highly conserved,” and found in at least four other receptor types that are widely spread in the body, yielding unwanted results.

For this reason, drug designers are seeking a different approach, homing in on molecular targets or so-called “allosteric binding sites” that reside away from the receptor’s primary binding site and are built around a more diverse genetic sequence and structure than their counterpart ‘orthosteric’ binding sites. Essentially, allosteric modulators act as a kind of cellular dimmer-switch that, once turned on, ‘fine tunes’ the activation and pharmacological profile of the target receptor.

“All allosteric sites typically exhibit great sequence diversity and therefore present exciting new targets for designing ‘selective therapeutics,’” said the study’s co-investigator J. Andrew McCammon, the Joseph E. Mayer Chair of Theoretical Chemistry, a Howard Hughes Medical Institute investigator, and Distinguished Professor of Pharmacology, all at UC San Diego. McCammon was named the winner of the 2016-17 Joseph O. Hirschfelder Prize in Theoretical Chemistry, awarded by the Theoretical Chemistry Institute at the University of Wisconsin-Madison.

In particular, drug designers have begun to aggressively search for allosteric modulators to fine-tune medications that bind to G protein-coupled receptors (GPCRs), the largest and most diverse group of membrane receptors in animals, plants, fungi and protocozia. These cell surface receptors act like an inbox for messages in the form of light energy, hormones and neurotransmitters, and perform an incredible array of functions in the human body.

In fact, between one-third to one-half of all marketed drugs act by binding to GPCRs, treating diseases including cancer, asthma, schizophrenia, Alzheimer’s and Parkinson’s disease, and heart disease.

Though many of the GPCR drugs have made their way to the medicine cabinet, most — including M2 mAChR targeted drugs — exhibit side effects owing to their lack of specificity. All these drugs target the orthosteric binding sites of receptors, thus creating the push to find more targeted therapies based on allosteric sites.

“The problem here is that molecules that bind to these allosteric sites have proven extremely difficult to identify using conventional high-throughput screening techniques,” said McCammon, also a chemistry and biochemistry professor in UC San Diego’s Division of Physical Sciences.

Enter accelerated molecular dynamics and supercomputing. As described in this latest study, called “Accelerated structure-based design of chemically diverse allosteric modulators of a muscarinic G protein-coupled receptor”, some 38 lead compounds were selected from a database of compounds from the National Cancer Institute, using computationally enhanced simulations to account for binding strength and receptor flexibility. About half of these compounds exhibited the hallmarks of an allosteric behavior in subsequent in vitro experiments, with about a dozen showing strong affinity to the M2 mAChR binding site. Of these, the researchers highlighted two showing both strong affinity and high selectivity in studies of cellular behavior. These cutting-edge experiments were performed by collaborators at the Monash Institute of Pharmaceutical Sciences.

“This is just the beginning. We believe that it will be possible to apply our combined cutting-edge in silico and in vitro techniques to a wide array of receptor targets that are involved in some of the most devastating diseases,” said Valiant.

HOW DID XSEDE HELP?

The supercomputing power of the Gordon, Comet, and Stampede1 processed hundreds of nanosecond aMD simulations, capturing millisecond timescale events in complex biomolecules in an unprecedented and successful approach.

M. Muscarinic Receptor

G-Protein Coupled Receptor
NEW DRUG CANDIDATE MAY REDUCE DEFICITS IN PARKINSON’S DISEASE

An international team led by University of California San Diego researchers has employed a novel computational approach to design and create a new compound that in laboratory studies has reduced deficits and neurodegenerative symptoms that underlie Parkinson’s disease.

In a study published in the September 27, 2016 Advance Access issue of Brain, researchers describe how their compound, dubbed NPT100-18A, prevents the binding and accumulation of alpha-synuclein or α-syn in neuronal membranes, now considered a hallmark of Parkinson’s disease and a related disorder called dementia with Lewy bodies.

“We’ve demonstrated a novel computational approach to design potential therapies for Parkinson’s disease and related disorders,” said the study’s first author Igor Tsigelny, a research scientist with the San Diego Supercomputer Center (SDSC) at UC San Diego, as well as the UC San Diego Moores Cancer Center and Department of Neurosciences.

Added Eliezer Masliah, the study’s principal investigator and former professor in UC San Diego’s Department of Neurosciences: “It’s a first step, but we believe it’s a big step.”

Parkinson’s disease, which affects more than 10 million people worldwide, is characterized by impairment or deterioration of neurons in the area of the brain known as the substantia nigra. The disease typically occurs in people over the age of 60, with symptoms of shaking, rigidity, and difficulty in walking, generally developing slowly over time and sometimes followed later by impairment in behavior and thought processes.

Since most symptoms of Parkinson’s disease are triggered by a lack of dopamine in the brain, many medications are aimed at either temporarily reversing or slowing the deterioration of neurons in the brain, which many medications are aimed at either temporarily re spaghetti or mimicking the action of the brain chemical. Unfortunately, current drugs have only a limited impact on long-term neurological deficits and mortality.

For this reason, scientists have begun to focus their efforts on α-syn’s role in the disease, based largely on computer modeling describing how mutant forms of this protein penetrate and coil in cell membranes, and then aggregate in a matter of nanoseconds into dangerous ring structures that open pores to toxic ions that ultimately destroy neurons. The modeling has been supported by electron microscopy showing how damaged neurons in Parkinson’s patients are riddled with these ring structures.

Following this discovery in 2012, UC San Diego researchers began an intense search to identify drug candidates that could block the early formation of ring structures. Specifically, the researchers homed in on “hot spots” that block the binding of two α-syn proteins, or dimers.

“Our thinking was that disrupting the formation of membrane-embedded dimers at this early intervention point could reverse the effects of α-syn on synaptic function at a stage before irreversible neurodegenerative processes have been initiated,” said Masliah, now with the National Institutes of Health (NIH).

But the hunt proved highly complex, owing largely to the nature of the unstructured state of α-syn, sometimes referred to as a “chameleon” that constantly shifts its shape, somewhat like a slippery that’s bobbing and weaving on top of an earthquake epicenter.

“Our biggest hurdle was that α-syn doesn’t have any stable conformation,” said Tsigelny. “So long simulations were needed to define a huge set of possible conformations to find clusters of possible compounds that would work.”

Enter several supercomputers—including Trestles, Gordon, and the Triton Shared Computing Cluster, and Blue Gene—to perform simulations that help target and prevent the binding and accumulation of alpha-synuclein (α-syn) in neuronal membranes, now considered a hallmark of Parkinson’s disease.

By using several XSEDE supercomputers—all based at SDSC, and Blue Gene, from the Argonne National Laboratory—that performed molecular dynamic simulations of α-syn ring structures that would displace α-syn from cell membranes.

Based on these simulations, other members of the research team, including Wolfgang Wrasidlo, executive director of medicinal chemistry at Neuropore Therapeutics in San Diego, synthesized a library of 34 potential compounds that targeted the “hot spot” where pairs of α-syn proteins bind, merge, and aggregate in the cell membrane, an early step in the formation of toxic rings and ultimate death of a neuron. Of these drug candidates, the researchers identified one compound—NPT100-18A—as the most promising.

“Essentially, this compound mimics the protein’s amino acids in the place where two α-synucleins come into contact, thus preventing the binding of the second protein,” said Wrasidlo, previously with UC San Diego Moores Cancer Center, and the study’s first author.

Subsequent electron microscopy imaging by researchers at the University of Vienna demonstrated that the new compound reduced the formation of α-syn clusters in cell membranes. Further studies with “transgenic” mouse models prone to Parkinson’s disease, both at UC San Diego and UCLA, concluded that the compound improved behavioral deficits and neurodegeneration. Within an hour after it was administered, imaging studies in these mice further showed that the compound reduced accumulation of α-syn in cortical synapses.

“Specifically targeting the α-synuclein structure that is stabilized in cell membranes also allows for a more specific molecularly targeted drug design,” added Masliah.

Though highly encouraging, the researchers caution that the compound needs to be refined before clinical trials can be launched in the future.
Recent drops in the cost of batteries have made it possible for those customers to smooth out their need for grid power, potentially saving money for everyone. Michael Fisher, working with faculty advisor Jay Apt at Carnegie Mellon University, set out to understand how different scenarios and assumptions about batteries and energy use would affect the economics of “behind the meter” (BTM) batteries—batteries that belong to users or third parties as opposed to power companies—on commercial users.

“We wanted to investigate how BTM battery systems would be used in a commercial application,” Fisher says. “Residential users just pay energy charges; but commercial users pay for their peak usage as well as how much energy they use. These peak charges can be up to 50 percent of an industrial or commercial customer’s bill. Batteries can make sense in mitigating those charges.”

The CMU researchers used the interim Greenfield/DXC system at the Pittsburgh Supercomputing Center (PSC) and then the XSEDE-allocated Bridges system at PSC to model how a fleet of BTM batteries would behave under different assumptions using meter data from 665 commercial and industrial buildings. With help from XSEDE ECSS expert Roberto Gomez of PSC, they moved their model, which they’d built on personal computers using the popular statistical software MATLAB, onto the PSC supercomputers. Usually, such a transfer from commodity computers to a high-performance computing (HPC) system would require a large amount of rewriting the computer code that runs the computations. But in the case of Greenfield and Bridges, both systems were designed to run MATLAB directly. Fisher didn’t have to rewrite his code—his methods transferred with only minor modifications to the HPC systems, garnering quick results.

“We forecast what the [electric] load would be for part of the day … to see what the optimal step would be for the next 15-minute period … and continued over the whole year,” Fisher says. “That’s 35,000 steps for each of 665 buildings … Each step didn’t take very long, but it adds up. It would have taken months to run on a laptop. With Greenfield and Bridges we were able to do it in an hour.”

The Greenfield run allowed the group to identify the factors most likely to affect the economics of the batteries. In later runs, Bridges’ size allowed the investigators to run computations on many different buildings in parallel, greatly speeding the calculations. The time savings made it possible for the investigators to test many more possible scenarios.

The Bridges work showed that most of the wasted energy associated with battery storage (measured via pollutant emissions) stemmed from internal energy losses in the batteries and not the timing of charging and discharging. This points toward what technology improvements may be necessary to make BTM batteries economical in more markets, and the regulatory environment necessary to encourage their development. The researchers reported their results in the journal Environmental Science & Technology in December 2016.
Through an XSEDE allocation, the Texas Advanced Computing Center (TACC) at The University of Texas at Austin is partnering with the Lamont-Doherty Earth Observatory (LDEO) at Columbia University to host one of the largest data collections for Earth sciences of its type in the country. The data relates to the Ross Ice Shelf, a massive slab of floating ice that is about the same size as the country of France.

Ice shelves, like icebergs, lie mainly below the waterline. This means that the majority of the shelf is not visible without the use of scientific instruments. Studying how the ice, ocean and underlying seabed interact will inform scientists of potential change in the ice shelf from projected climate change.

“The Ross Ice Shelf is of interest because it’s float ing, allowing ocean water to move freely about beneath it and we have seen in other regions like this that they can become unstable and break up,” said Nick Frearson, a lead engineer on the ROSETTA-Ice project whose team designed the Icepod, the data collection system and sensor suite and the radar technology that probes the ice shelf.

“Warming ocean water is getting underneath the shelf that is a significant couple of degrees warmer than the surrounding water and can mean the difference between freezing and melting at the base of the ice,” he said. “The shelf acts like a large cork impeding the flow of incident glaciers and ice streams, and could have far-reaching effects if it changes significantly and releases more ice to flow from the land into the sea raising sea levels globally in the process.”

Over the past four years, researchers at LDEO have been flying over the frozen waters in the polar regions and collecting field data for the ROSETTA-Ice project, which studies the Ross Ice Shelf. The shelf is constantly fed by a flow of ice from glaciers draining from both the East and West Antarctic ice sheets. The field data includes crucial information on the shelf and the underlying tectonics of the Antarctic region.

Frearson says that the data being collected using scientific instruments — hundreds of terabytes in total — is unique. “We take data from a suite of instruments, all sampled synchronously, and bring them together to form a much bigger picture than if we just analyzed data from one instrument,” he said.

Up until now the sea floor under the shelf has only been mapped to a resolution of 50km using a combination of satellite gravity data and a land survey undertaken in the 1970’s. This is low enough to hide whole mountain and valley systems and was not detailed enough for oceanographers to accurately model ocean currents flowing under the shelf. With state-of-the-art radar, gravimeters, which measure gravity anomalies; a magnetometer that measures Earth’s magnetic anomalies; LIDAR, remote sensing of the surface with laser pulses; and high-resolution photogrammetry to map surface structures; ROSETTA has been able to map the interior and ocean floor of the shelf to much higher resolution.

“In the process, we have collected many 100’s of TB’s of data and needed a state-of-the-art solution to manage it. That’s where TACC comes in,” Frearson said.

To collect, process, analyze and store the data, Frearson and other colleagues at LDEO have been using their XSEDE allocations on resources such as Stampede2 for data processing and Ranch tape storage for long-term archiving of data.

“The speed of XSEDE and TACC resources is superior to our existing high-performance computers at Lamont,” said Lingling Dong, a computer software and performance computers at Lamont, “said Chris Jordan, manager of TACC’s Data Management and Collections group. “From the start, they wanted a way to both store hundreds of terabytes of data and to make it widely available on the web as it’s uploaded.”

“We aren’t the only science group having to cope with very large volumes of data and hope that the partnership that we have forged with TACC shows that it is possible to manage and disseminate this level of data in a cost-effective, user-friendly and easily accessible manner,” Frearson said. “We hope that people across the globe, as well as institutions in the U.S., will benefit from this data set.”
NEW 3-D SIMULATIONS SHOW HOW GALACTIC CENTERS COOL THEIR JETS

Some of the most extreme outbursts observed in the universe are the mysterious jets of energy and matter beaming from the center of galaxies at nearly the speed of light. These narrow jets, which typically form in opposing pairs are believed to be associated with supermassive black holes and other exotic objects, though the mechanisms that drive and dissipate them are not well understood.

With XSEDE-accessed access to a few supercomputers - Stampede2, Ranch, Comet and Oasis, a small team of researchers have developed theories supported by 3-D simulations to explain what’s at work inside supermassive black holes.

"We were finally able to simulate jets that start from the black hole and propagate to very large distances - where they bump into the ambient medium," said Duran, formerly a postdoctoral research associate at Purdue University who is now a faculty member at California State University, Sacramento.

"For a long time, we have speculated that shocks and instabilities trigger the spectacular light displays from jets. Now these ideas and models can be cast on a much firmer theoretical ground," said Dimitrios Giannios, assistant professor of physics at Purdue University.

"With these shocks, the jet is like a phoenix. It comes out of the shock every time," though with gradually lessening energy, Tchekhovskoy said. "This train of shocks cumulatively can dissipate quite a substantial amount of the total energy. The researchers designed the models to smash against different densities of matter in the ambient medium that the jet encounters as it drills a hole [in the ambient medium]."

He added, "Seeing deeper into where the jets come from - we think the jets start at the black hole's event horizon (a point of no return for matter entering the black hole) - would be really helpful to see in nature these 'bounces' in repeating shocks, for example. The EHT could resolve this structure and provide a nice test of our work."
PLASTIC BOTTLES

A plastics pollution problem may have met its match thanks to scientific computing. Polyethylene terephthalate (PET) is the fourth most-produced plastic in the world commonly found in beverage bottles and carpets, but with XSEDE, researchers are using supercomputers to engineer an enzyme that breaks down PET. This computationally-assisted research is a step on a long road toward recycling PET and other plastics into commercially valuable materials at industrial scale.

Supercomputers have allowed researchers to tackle tough science questions about PETase, a plastic-degrading enzyme, such as how it interacts on a molecular scale bound to a substrate, something beyond the scope of what could be determined by knowing its crystal structure.

“Having access to XSEDE resources really opens up the possibility of being able to model and study what type of large-scale conformational or even local, small structural changes occur as a function of both binding to the substrate and, additionally, what are the structural changes that happen or local, small scale structural changes that occur in the enzyme after we make the mutations,” said Lee Woodcock, an Associate Professor of Chemistry at the University of South Florida.

Woodcock explained that they simulated the system using molecular dynamics, in which the motions of the individual atoms in the enzyme, substrate and surrounding water were tracked over long timescales. The work employed two software packages, NAMD (Nanoscale Molecular Dynamics) and CHARMM (Chemistry at Harvard Macromolecular Mechanics), with the forces between the atoms modeled using the CHARMM force fields.

XSEDE awarded study co-author Gregg Beckham, a Senior Research Fellow and Group Leader at the US National Renewable Energy Laboratory (NREL), allocations on the Stampede1 and Stampede2 systems at the Texas Advanced Computing Center (TACC) and on the Comet system at the San Diego Supercomputer Center (SDSC).

“Stampede2 has been a fantastic machine for all the codes we use,” Beckham said. “We get through the queues quickly. We’re producing a lot of great research on the plastics-degrading enzyme, using this machine.”

“What’s great about Comet,” Woodcock said, “is for jobs that you need to get through in a high-throughput fashion, SDSC has a shared queue, which allows you to submit much smaller jobs but do it in a very high-throughput fashion, as they can share cores on the nodes at Comet.”

The study built on a discovery in 2016 by Yoshida et al. of a bacterium, Ideonella sakaensis 201-F6, that feeds on PET plastic as its source of carbon and energy. The PhD students focused on the bacteria’s plastic-degrading enzyme, called PETase. Team members at the University of Portsmouth, led by Professor John McGhee, used X-ray crystallography at the Diamond Light Source in the UK to solve the high-resolution crystal structure of PETase.

“We used computer simulations to understand how a polymeric ligand like PET would be able to bind to the enzyme,” said Beckham. “We also conduct experimental work to show that the PETase can break down plastic bottles, industrially relevant PET films, and another plastic, polyethylene furanoate.”

Next, the authors tried to understand the evolution and look to similar enzymes, a family of cutinases, which degrade the waxy polymer cutin found on the surface of plants.

“When we made it more cutinase-like, the enzyme was modestly improved. That’s actually one of the key aspects of where computation came in, because it allowed us to essentially predict or suggest aromatic-aromatic interactions in the enzyme with the aromatic polymers PET could potentially be responsible for its improved activity. But it was quite a surprise to us,” Beckham said.

“We’re beginning to understand how this enzyme has evolved,” Beckham said. He wants to use computation to take advantage of large databases of genomics and metagenomics on enzymes that can degrade plastics.

“If we’re able to do this at much higher temperature, Beckham said, “it would accelerate the degradation of PET and could potentially be industrially relevant in terms of using an enzyme to degrade PET and convert that into the higher value materials, which could incentivize higher rates of reclamation, reducing the amount plastic waste that goes into the ocean.”

Lee Woodcock sees new computation-al techniques as a game-changer in modeling non-druglike force fields that tackle polymer interactions more realistically than CHARMM and NAMD can today. “I’m working with colleagues at NREL (U.S. National Renewable Energy Laboratory) on making sure that we can improve the force fields more rapidly, to look at various polymers, and put together a modeling strategy in a very short amount of time for a quick turn-around when we have to model many different polymers.”

The scientists are hopeful their work will one day make the world outside of the lab a better place. “Understanding how we can better design processes to recycle plastics and reclaim them is a dire global problem and it’s something that the scientific and engineering community has to come up with solutions for,” Beckham said.
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XSEDE is supported by the National Science Foundation

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