

THE DEVELOPMENT OF KINETIC MODELS AND SIMULATION METHODS TO STUDY
MOLECULAR FLUCTUATIONS, MODAL RESPONSE, SHOCK-LAMINAR SEPARATION
BUBBLE INSTABILITIES

BY

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DISSERTATION

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Abstract

The study of laminar to turbulent transition of hypersonic flows typically includes investigation of instabilities generated in the boundary-layer and laminar separation bubble (LSB) induced by shock-wave/boundary-layer interactions (SBLIs), without reference to the internal structure of shocks or instabilities potentially generated in them. However, the predictions of shock structure based on the Navier-Stokes equations increasingly deviate from those delivered by kinetic theory as the degree of rarefaction in shock's interior nonequilibrium region increases with the Mach number. Therefore, a kinetic approach is required to resolve the internal structure of shocks, such as the Direct Simulation Monte Carlo (DSMC) method that approximates the solution of the more-general Boltzmann equation of transport. Kinetic modeling requires resolution at molecular length and time scales, which vary by order of magnitude from the freestream to the vicinity of compression surfaces inducing SBLIs. A three-dimensional DSMC solver is developed to overcome these computational challenges, known as the Scalable Unstructured Gas-dynamic Adaptive mesh-Refinement (SUGAR), which employs algorithms for adaptive mesh refinement of a computational octree mesh and its linearized representation using the Morton-based space-filling-curve approach. Performance studies have shown 87% weak scaling efficiency for 8192 processors and 24 billion computational particles for simulating a strong shock created by flow over a hemisphere. This good performance is achieved by implementing algorithms for assessing the computational load of a processor by the use of profiled run-time data, creating exchange maps for optimization of processor point-to-point communications, efficiently generating new DSMC particles every time step, and optimizing the run-time memory usage. In this work, the SUGAR solver is used to investigate the role of finite-thickness shock layers in the dynamics of complex three-dimensional SBLIs, characterize molecular fluctuations in shock's internal nonequilibrium region, and obtain fully-resolved, one-dimensional, steady shock layer profiles for their linear modal analysis.

Linear three-dimensional instability is analyzed in the shock layer and laminar separation bubble induced by SBLIs in a Mach 7 nitrogen flow over a $30^\circ - 55^\circ$ double-wedge configuration. At a freestream unit Reynolds number $Re = 5.2 \times 10^4 \text{ m}^{-1}$, this flow exhibits rarefaction effects and has shock-thicknesses comparable to the thickness of the boundary layer at separation. DSMC simulations have been fully resolved using 60 billion computational particles and

4.5 billion computational cells to capture the flow evolution from the inception of three-dimensionality, through linear growth of instabilities, to the early stages of nonlinear saturation. It is shown that the laminar separation bubble sustains self-excited, small-amplitude perturbations that originate past the primary separation line and lead to spanwise-periodic wall striations inside the bubble and downstream of the primary reattachment line, as known from earlier experiments, simulations, and instability analyses. A spanwise-periodic instability, synchronized with that in the separation zone, is identified herein for the first time, which exists in the internal structure of the separation and detached shock layers, and manifests itself as spanwise-periodic cats-eyes patterns in the amplitude functions of all linear flow perturbations. The growth rate and the spanwise-periodicity length of linear disturbances in the shock layers and laminar separation bubble are found to be identical. Linear amplification of the most unstable three-dimensional flow perturbations leads to synchronized low-frequency unsteadiness of the triple point formed at the intersection of separation and detached shock layers and the separation bubble, with Strouhal number of $St \approx 0.028$.

Investigation of molecular fluctuations in the internal nonequilibrium region of monatomic shock layers revealed two orders of magnitude lower frequencies than the flow upstream. The presence of low-frequency fluctuations is shown to be a direct consequence of the bimodal nature of the probability density function (PDF) of gas particles in the shock, as opposed to their Maxwellian form in the upstream. Inside the shock-layer, the strong correlation between perturbations in the bimodal PDF and fluctuations in the normal stress suggests the development of a novel two-energy-bin Lotka-Volterra-type model to describe the reduced-order dynamics of a large number of collision interactions of gas particles. The model correctly predicts the differences in fluctuation frequencies in the shock versus those in the upstream and is consistent with the small-amplitude fluctuations obtained from DSMC computations. The variation in dominant low-frequency fluctuations with changes in upstream conditions revealed that they could be described by a Strouhal number that remains practically independent of Mach number, upstream temperature, and number density. Furthermore, PDFs of particle energies in the upstream and downstream equilibrium regions, as well as inside shocks, are analytically derived and shown for the first time to have the form of the non-central chi-squared (NCCS) distributions. Linear correlations are proposed to relate the change in average low-frequencies of fluctuations obtained from DSMC with the change in the shape of analytically-obtained bimodal PDFs in shocks and the most-probable-speed inside shocks at the location of the maximum bulk velocity gradient. These correlations are used to construct a semi-empirical relationship to predict average low-frequency of fluctuations in shocks for a wide range of Mach numbers ($3 \leq Ma \leq 10$) and input temperatures ($\sim 90 \leq T_{tr,1}/(K) \leq 1420$), which can be used in receptivity and linear stability analysis studies of laminar-turbulent transition in high-speed flows.

A framework for studying modal analysis of finite-thickness normal shock layers has been developed, and linear temporal analysis is conducted to study the stability of $Ma = 1.2, 3$, and 5 shocks obtained from DSMC against

two-dimensional, small amplitude, harmonic perturbations having wavelengths smaller than the shock-thickness. Two sets of constitutive equations are used to obtain closure of the compressible governing equations used for modal analysis: the traditionally used Navier-Stokes-Fourier (NSF) equations, applicable only at the lowest Mach number, and equations derived based on Mott-Smith’s bimodal approximation for the velocity distribution functions inside a shock layer, which are better than the former in terms of approximating the DSMC-derived transport flow quantities at high Mach numbers. Comparison of two formulations allows for quantifying the effect of the resolution of internal shock structure on the stability of shock layers.

Duck and Balakumar [1] conducted the temporal analysis of one-dimensional shock layers satisfying the Navier-Stokes equations three decades ago and found only stable continuous branches in the eigenspectra. However, they did not explore their key characteristics, such as the parameters governing the temporal decay rates of ‘continuum’ modes and the far field behavior of corresponding eigenfunctions. In this work, we find the least stable continuous branches exhibiting both stationary and traveling modes and show for the first time that their eigenfunctions decay monotonically and sinusoidally in the far field of the shock layer, respectively, while exhibiting an order of magnitude lower spatial decay rate in the upstream than the downstream. These characteristics of eigenfunctions are shown to be governed by only one physically possible root of a septic characteristic equation derived by simplifying $O(\epsilon)$ normal mode equations in far fields of a shock layer. An approximate equation for this root is obtained in terms of specific gas constant γ , upstream Reynolds and Mach numbers Re and Ma , respectively, spanwise wavenumber β , complex eigenvalue Ω , and far field flow quantities. Using this relationship, it is shown that these modes are stable in the entire parametric space and become less stable by the decrease in Re , increase in Ma , decrease in γ , and increase in the degree of translational nonequilibrium. This is consistent with the predictions of slower decay rate at higher Mach numbers by the kinetic-based constitutive equations compared to the NSF equations.

To my mother - Prajakta, father - Satish, sister - Rutuja, & aunt - Shobha

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List of Abbreviations

AMR	Adaptive Mesh Refinement
ACE	Anisotropic Conservation Equations
CFD	Computational Fluid Dynamics
C-mesh	Collision mesh
DSMC	Direct Simulation Monte Carlo
GSI	Gas Surface Interaction
KH	Kelvin-Helmholtz
LB	Larsen Borgnakke
LSB	Laminar Separation Bubble
MFS	Majorant Frequency Scheme
MS	Mott-Smith's
MPI	Message Passing Interface
NCCS	Noncentral Chi-squared
NSE	Navier-Stokes Equations
NSF	Navier-Stokes-Fourier
NTC	No Time Counter
ODE	Ordinary Differential Equations
PDF	Probability Distribution Function
POD	Proper Orthogonal Decomposition
PSD	Power Spectral Density
SBLIs	Shock-wave/Boundary-layer Interactions
SMILE	Statistical Modeling In Low-density Environment
SUGAR	Scalable Unstructured Gas-dynamics with Adaptive Refinement
SVD	Singular Value Decomposition

TSQR	Tall and Skinny QR Factorization
$S^{<\text{label}>}$	Stationary mode on a continuous branch denoted with a superscript of the branch label
$T_{\Omega_r}^{<\text{label}>}$	Traveling mode on a continuous branch denoted with a branch label and frequency Ω_r
VDF	Velocity Distribution Function
VHS	Variable Hard Sphere
VSS	Variable Soft Sphere

Chapter 1

Introduction

1.1 Kinetic Modeling of Three-Dimensional Shock-wave/Boundary-layer interactions - Motivation and Challenges

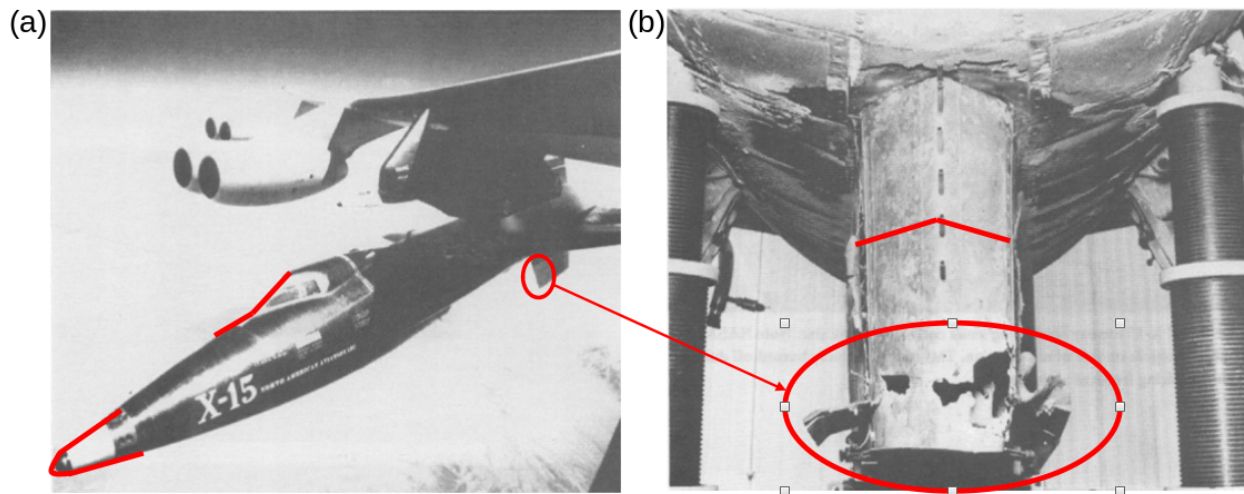


Figure 1.1: (a) The X-15 aircraft separating from the B-52 mothership [2]. (b) Damage to lower ventral fin of X-15A-2 by shock impingement on flight 2-52-97 piloted by Pete Knight to Mach 6.7 at an altitude of 31 km [2].

On October 3, 1967, pilot Pete Knight flew the X-15A-2 aircraft attached with a dummy scramjet at a record-breaking Mach number of 6.7 at an altitude of 31 km. The shock waves off the dummy scramjet impinged on the lower ventral fin of the aircraft, burned off the ablator as well as the surface of the fin (see Fig. 1.1), damaged the instrumentation wiring, control gas line, and bolts used to jettison the scramjet [2]. Since the time of these hypersonic flight tests, we have known that a comprehensive understanding of shock-wave/boundary-layer interactions (SBLI) is paramount to mastering the hypersonic regime ($M \geq 5$). As a result, the study of hypersonic flows over canonical configurations such as a two and three-dimensional ramp and wedge, an axisymmetric and three-dimensional cone,

that make up parts of typical hypersonic bodies, as shown in Fig. 1.1, has been the focus of the last six decades of rigorous research [8–18]. Since the past decade, there have been efforts in studying more complicated configurations such as a double-wedge or double-cone because they form the most complex SBLIs [19–23]. Yet, we are far from reliable predictive capabilities in this flow regime, and one of the main reasons can be attributed to our lack of thorough understanding of the first ingredient in SBLIs, the shock. The work presented here is an effort to explore some of the key aspects of shocks in such complicated flows, such as a sharp-angled $30^\circ - 55^\circ$ double-wedge, as well as some fundamental aspects in simplest monatomic shocks, which will, in turn, help us better understand the complicated shock-dominated flows.

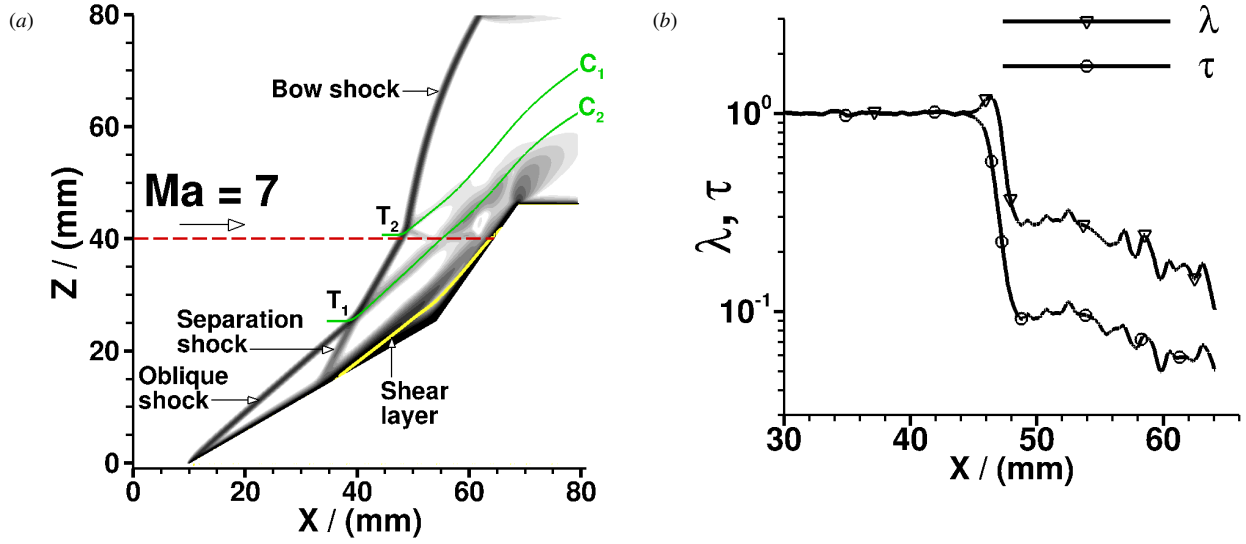


Figure 1.2: (a) Shock-wave/boundary-layer interactions in the contours of density gradient magnitude of Mach 7 nitrogen flow over a double-wedge. (b) Variation of local mean-free-path, λ , and mean-collision-time, τ , normalized by respective upstream values along the red dashed line shown at $Z = 40$ mm in (a).

The computational study of SBLIs is fraught with challenges in terms of both flow physics and computational intensity. One of the defining features of SBLIs over the aforementioned double-wedge configuration is a separation bubble, as seen in figure 1.2(a) for a two-dimensional flow, which contains a shear layer in the vicinity of the interaction of two wedge surfaces. The separation shock formed at the point of separation intersects with the leading-edge oblique and detached bow shocks at triple points T_1 and T_2 , respectively. Depending on the lengths and angles of the slant surfaces and the strengths of shocks, the interaction pattern changes, which can be typically classified into six types, denoted as Edney I-IV [24–26]. Here we see a variation of an Edney-IV type interaction, the defining feature of which is a supersonic flow between two slip lines, C_1 and C_2 , as shown in figure 1.2(a). The study of such SBLIs involves at least three major aspects: predictions of aerothermodynamic loads on surfaces [21], modeling

of thermal nonequilibrium or internal energy relaxation of polyatomic species and chemical reactions [27–29], and characterization of instabilities generated in the flow, either self-excited or surface-induced, may cause an initially laminar flow to become turbulent [22, 23, 30, 31]. Each of these three aspects affects the other two; however, in this work, we mainly focus on understanding flow instabilities while doing due diligence to quantification and modeling of the first two aspects when required.

The computational challenges in high-fidelity modeling of SBLIs include accurate modeling of the internal structure of a shock wave [32, 33], surface rarefaction effects [34–36], and resolution of multiple length and time scales in the problem. For Mach numbers greater than 1.4, the viscous normal stresses and heat fluxes in the interior of strong shocks are significantly underpredicted by traditional continuum formulations such as the Navier-Stokes equations compared to the kinetic methods such as the Direct Simulation Monte Carlo (DSMC) method [32, 37], used in this work, that represents the solution of the more-general Boltzmann equation of transport [34]. Modeling of these rarefaction effects may be crucial to the overall dynamics of these flows, especially when the origins of instabilities and the intimate interplay of shock waves and separated flows are in question at conditions where shock layer thicknesses are comparable to the boundary layer thickness at separation. However, kinetic modeling of these flows comes with its own set of challenges because it requires spatial and temporal resolutions at the molecular length and timescales of mean-free-path, $\lambda \sim O(10^{-4} \text{ m})$ and mean-collision-time, $\tau \sim O(10^{-9} \text{ s})$, respectively. These quantities vary by at least an order of magnitude from the freestream to the regions inside the shock and in the vicinity of the surface, as shown in Fig. 1.2(b), and therefore these simulations demand billions of computational particles and cells used to select colliding pairs. Yet we must resort to such computational investigations because experimental test times [20, 38] are typically an order of magnitude lower than the characteristic times of the development of instabilities $\sim O(10^{-3} \text{ s})$ [23, 30].

When it comes to the stability of a flow, three-dimensional SBLIs can be significantly different from idealistic two-dimensional SBLIs, where flow is assumed to not depend on the span [39]. Tumuklu *et al.* [30] previously conducted two-dimensional simulations of flows over the double-wedge mentioned above at $Ma = 7$ and $Re = 5.2 \times 10^4 \text{ m}^{-1}$) and demonstrated that the flow reaches steady-state through decaying modes identified by linear stability analysis as well as proper orthogonal decomposition (POD). However, the steady-state of a two-dimensional base flow does not guarantee that the flow will be stable if it is allowed to evolve in the spanwise direction. The three-dimensional relaxation of a two-dimensional laminar flow may result in a different steady-state, or it may even transition to a turbulent state [40]. The three-dimensional relaxation of the flow can be studied over a finite length of span, which leads to spanwise acceleration of the flow towards the free edge of the wedge, known as the ‘pressure relief effect’ [30]. Or, it can be over a periodically repeating section of a span where the pressure relief effect is negligible, but the flow may exhibit small-amplitude, three-dimensional perturbations that are harmonic in the spanwise direction having wavelengths

smaller than the periodicity length of the span. The questions regarding these three-dimensional relaxation effects that have motivated the current work on three-dimensional simulations of SBLIs at the same conditions as Tumuklu *et al.* [30]. Note that it is more complicated to analyze the underlying instability mechanisms in the presence of strong pressure relief effects which cause variation in the size of the separation bubble along the span, known as an ‘open separation bubble,’ while such flows are also computationally expensive because one needs to model the flow over an entire span [39]. The spanwise-periodic simulations are simpler in comparison and help us analyze the stability characteristics of the flow using the well-established linear stability theory [40].

1.2 Role of Shocks in Stability of High Speed Flows - Motivation and Challenges

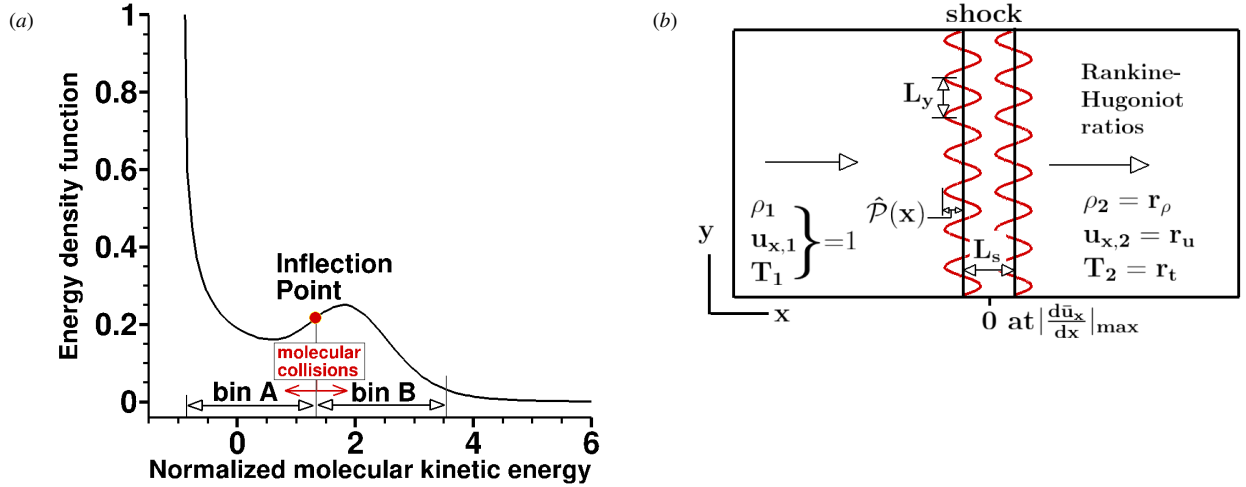


Figure 1.3: (a) Bimodal energy density function inside a shock layer. (d) A sketch showing a shock of finite-thickness L_s propagating in the X -direction subjected to 2-D harmonic perturbations in Y of wavelength L_y and amplitude function $\hat{P}$ (not drawn to scale). ρ , u_x and T are mass density, bulk velocity, and temperature, respectively, where subscripts ‘1’ and ‘2’ correspond to the up and downstream regions, respectively. Quantities shown are nondimensional.

The behavior of three-dimensional laminar separation bubble induced by SBLIs has been the subject of intense experimental [41, 42] and numerical [43–47] investigations. These works have shown the presence of striations in the laminar separation bubble past a primary separation line and have associated them with a global linear instability mechanism which leads to the linear amplification of small-amplitude, stationary, three-dimensional, self-excited perturbations. However, high-fidelity kinetic simulations may help us answer the relatively unexplored question of the dynamic behavior of the shock layer which drives the interaction with the boundary layer and the subsequent

appearance of striations in the laminar separation bubble. In such flows, when the shock thickness is comparable to the boundary layer thickness at separation, we would like to know how the internal structure of the separation shock is affected by the presence of linear instability of the bubble. Also, if the separation shock is affected, then naturally, we expect such effects to propagate to the detached shock as well as the shear layer in the vicinity of slip line C_2 , shown in Fig. 1.2(a). Such yet-answered questions have been the focus of the kinetic simulations explored in this work.

Furthermore, the vast majority of research on how laminar supersonic or hypersonic flows transition to turbulence focuses on boundary layers, not the shock. Linear stability theory has been successful in predicting whether a boundary layer is stable against small-amplitude disturbances or whether it is susceptible to transition [48–50]. However, when it comes to the prediction of the Reynolds number of transition, many experimental observations have shown a strong correlation between this quantity and the level of freestream noise, which includes atmospheric or tunnel-induced turbulence, acoustic, vorticity, and entropy fluctuations, and particulates [16]. The processes that cause excitation of boundary layers through small external disturbances are grouped under the term, receptivity [51]. Numerical research in receptivity and ‘natural’ transition, as opposed to an induced-excitation of a boundary layer, has focused primarily on the development of models to account for freestream disturbances [52,53] and their interaction with shocks through shock-capturing [54] or shock-fitting [55] schemes. In addition, the receptivity studies of Fedorov and Tumin [56] and Luchini [57] have also highlighted that equilibrium molecular fluctuations in the compressible and incompressible boundary layer can also trigger laminar to turbulent transition. However, these works do not account for the internal dynamic structure of a shock wave or the nature of molecular fluctuations in their internal nonequilibrium region. Since freestream noise inevitably passes through a shock before interacting with a boundary-layer, the role of the internal dynamic structure of a shock may not be ignored in the study of receptivity. This is true even when the level of freestream noise is minimal, *i.e.* only containing equilibrium molecular fluctuations, because the leading-edge shock interacts with boundary-layer formation.

To understand the nature of molecular fluctuations inside a shock layer, we need to rely on kinetic methods that provide insight into the particle velocity and energy distribution functions. For example, the energy density function of normalized x -directional molecular kinetic energy inside a Mach 7.2 one-dimensional shock, shown in Fig. 1.3(a), is bimodal, and it exhibits an inflection point where a majority of particles in the low energy bin A have collided with particles in the downstream subsonic region, while those in the high energy bin B come from the hypersonic flow upstream. Kinetic methods facilitate the analyses of intermolecular collisions, which cause perturbations of distribution functions and, in turn, dictate the frequencies of molecular fluctuations. However, understanding detailed molecular collisions in two- and three-dimensional flows is challenging because of the tremendous length and time scales related to boundary-layers, instabilities, and unsteadiness of SBLIs. Therefore, as a first step, investigating fluctuations in

one-dimensional monatomic shock layers is the best way to close this theoretical gap.

Apart from the characterization of molecular fluctuations inside a shock, whether the profiles of macroscopic flow quantities of a finite-thickness, steady shock layer governed by compressible mass, momentum, and energy equations are stable, and under what circumstances do they may become unstable is a vastly unexplored topic. Past works on the interactions of an isolated shock with external disturbances focused on understanding how do acoustic, vorticity, and entropy waves amplify, reflect, or transmit through an inviscid shock treated as a discontinuous jump [58–61]. However, to the best of the author’s knowledge, the question of intrinsic stability of a finite-thickness shock layer was only last attempted three decades ago by Duck and Balakumar [1]. These authors imposed small-amplitude, harmonic perturbations to the macroscopic solution of a shock layer governed by Navier-Stokes equations obtained using the method of Gilbarg and Paolucci [7] and studied the stability using temporal amplification theory, which, in a nutshell, assumes that the spatial structure of harmonic perturbations remains unchanged while their amplitude may grow or decay in time. Their analysis showed only decaying modes that are a part of continuous branches of eigenspectra; however, it did not explore some of the key questions. For example, it was inconclusive whether the amplitude functions or eigenfunctions are physically possible in the sense that they decay in far fields, *i.e.* in up and downstream regions of a shock layer. It is also of great significance to find out the parameters that govern the temporal decay rates and the spatial variation of physically acceptable eigenfunctions. To answer these questions, we must revisit the modal analysis of finite-thickness shock layers, but first start with the study of the temporal analysis of one-dimensional shocks. Also, as stated earlier, it is long known that the predictions of the shock structure based on the Navier-Stokes equations increasingly deviate from those delivered by kinetic theory [37, 62, 63] as the Mach number increases ($M > 1.4$). Therefore, to study the stability of shock layers obtained from DSMC at higher Mach numbers, we require better constitutive equations for transport flow quantities, *e.g.* the stress tensor and heat flux vector. Furthermore, note that even if the temporal analysis predicts decaying eigenmodes, it is possible that there is a short-time initial transient growth due to the effect of possible non-orthogonality of eigenvectors. Such analyses could not be examined here but may provide a better picture of the stability of finite-thickness shock layers, which can then be extended to curved or oblique shocks or complex shock systems interacting with a boundary layer.

1.3 Scope of the Work and Main Contributions

Sections 1.1 and 1.2 highlighted that there is merit in exploring the origins and dynamics of instabilities in SBLIs as well as simple one-dimensional monatomic shocks using kinetic approaches that account for the internal structure of shock layers. The SBLI problems are computationally expensive but can be simulated with strategic use of growing

state-of-the-art computing facilities, while the study of one-dimensional shocks is computationally inexpensive, yet comprises many aspects that are mathematically challenging as well as instructive for gaining insights into more complex problems such as laminar to turbulent transition over hypersonic vehicles. To that end, we define the following four major goals in this work:

1. Development of a highly-scalable DSMC solver that makes use of the petascale computing facilities to resolve multiple length and time scales in SBLIs at near-continuum flow conditions.
2. The study of the stability of 2-D flow of nitrogen over a $30^\circ - 55^\circ$ double-wedge at conditions studied by Tumuklu *et al.* [30] against small-amplitude, spanwise-harmonic, three-dimensional, self-excited perturbations. Exploration of the coupling between the fully-resolved internal structure of shocks with the laminar separation bubble.
3. Characterization of the nature of molecular fluctuations in the internal translational nonequilibrium region of a monatomic shock layer. If the frequencies of fluctuations are different from the frequencies in the equilibrium flow in far fields of a shock, understanding the reason for this difference.
4. Performing the temporal analysis of one-dimensional shock layer profiles obtained from DSMC by imposing harmonic small-amplitude perturbations in the plane of the shock. Development of constitutive equations that account for the bimodal nature of PDFs in a shock layer, and as a result, approximate the DSMC transport flow quantities better than the traditional NSF constitutive equations. Using these sets of equations, assess the role of translational nonequilibrium on the stability characteristics of a shock layer.

The major contributions to these four primary objectives are briefly described in the following Secs. 1.3.1, 1.3.2, 1.3.3, and 1.3.4, respectively.

1.3.1 A highly scalable DSMC computational framework

We have developed an octree-based, three-dimensional DSMC solver known as Scalable Unstructured Gas-dynamic Adaptive mesh-Refinement [39]. The code takes advantage of an adaptive mesh refinement (AMR) strategy where each cubic cell, known as a ‘root’ cell, of a coarser uniform Cartesian grid is recursively subdivided into eight parts until the smallest cells, known as ‘leaf’ cells, are smaller than the local mean-free-path. Accessing these leaf cells in a traditional pointer-based data structure was found to be expensive [64], and therefore, the solver is equipped with a linearized data structure, where all leaf cells are stored in a continuous array that can be accessed using bit-wise

operations using the Morton encoding algorithm [65–67]. To make use of existing petascale facilities, the solver makes use of the message-passing-interface (MPI) for parallel communication. However, excellent strong and weak scalings to thousands of processors were achieved only after implementing a series of systematic strategies for improving the computational load distribution across processors, reducing the point-to-point communications of particle information between neighboring processors by creating exchange maps, and optimizing the introduction of new particles in a domain at every time step. Simulations of billions of particles and computational cells required the rethinking of several strategies for reducing the run-time memory usage of processors. Furthermore, the solver employs a cut cell algorithm to accurately compute the part of the cell cut by the surface that faces the flow so that the collision frequency in the vicinity of the surface is accurately computed. The thermal non-equilibrium accounting for rotational and vibrational relaxation of diatomic species was achieved through the accurate computations of collision temperatures on a sampling grid designed to be compatible with the above approaches. The capability of the solver was demonstrated by simulating complex 3-D SBLIs forming on a finite span double-wedge configuration having the same cross-sectional profile and input conditions as used by Tumuklu *et al.* [30] in their 2-D calculations. The solver was later extended to model spanwise-periodic, two- and one-dimensional flows while making use of the aforementioned strategies, which required substantial development efforts.

1.3.2 Instabilities in three-dimensional shock-laminar separation bubble interactions

The 2-D Mach 7 base flow of Tumuklu *et al.* [30] was indeed found to be unstable self-excited, small-amplitude, spanwise-periodic perturbations due to a linear three-dimensional instability. At a freestream unit Reynolds number $Re = 5.2 \times 10^4 \text{ m}^{-1}$ ($\sim 60 \text{ km}$ altitude), this flow exhibits rarefaction effects and has shock-thicknesses comparable to the thickness of the boundary layer at separation. Flow features have been fully resolved using the SUGAR DSMC solver simulating ~ 60 billion computational particles and ~ 4.5 billion computational cells over 19,200 MPI processors to capture the flow evolution from the inception of three-dimensionality, through linear growth of instabilities, to the early stages of nonlinear saturation. DSMC has been shown to capture spanwise-periodic flow structures that form past the primary separation line inside the separation bubble and downstream of the primary reattachment line, as known from earlier experiments, simulations, and instability analyses. It is shown for the first time that the linear instability in the separation bubble is synchronized with the instabilities in the internal regions of the separation and detached shock layers. The growth rate and the spanwise-periodicity length of linear disturbances in the shock layers and laminar separation bubble are found to be identical. Linear amplification of the most unstable three-dimensional flow perturbations leads to synchronized low-frequency unsteadiness of the triple point formed at the intersection of

separation and detached shock layers and the separation bubble with a Strouhal number of $St \approx 0.028$.

1.3.3 Characterization of molecular fluctuations in a one-dimensional monatomic shock layer

We have shown for the first time using DSMC simulations of one-dimensional argon shock layers in the Mach number range $2 \leq M \leq 10$ that the translational nonequilibrium zone of strong shock waves exhibits two orders of magnitude lower molecular fluctuations than the upstream equilibrium flow. This difference has been shown to be a consequence of the bimodal nature of the probability density function (PDF) of particles in the shock, as opposed to their Maxwellian distribution in the freestream. Inside the (finite-thickness) shock region, the strong correlation between perturbations in the bimodal PDF of particle energies and fluctuations in the normal stress has led us to introduce a novel two-energy-bin model to describe the reduced-order dynamics of a large number of collision interactions of gas particles. Our model correctly predicts two orders of magnitude differences in fluctuation frequencies in the shock versus those in the freestream and shows that in the shock, the low frequencies correspond to relaxation of high energy particles coming from the upstream in the background of low-energy particles that have collided with particles in the subsonic region. We have also shown that the average low-frequencies of fluctuations can be described by a nondimensional Strouhal number defined based on the bulk velocity upstream of the shock and the shock-thickness based on the maximum density-gradient inside the shock. This Strouhal number is practically independent of Mach number, upstream number density, and temperature.

Furthermore, we have also derived PDFs of particle energies in the upstream and downstream equilibrium regions and inside shocks and shown for the first time that they have the form of the non-central chi-squared (NCCS) distributions. A linear correlation is proposed to relate the change in the shape of analytically-obtained bimodal PDFs in shocks as a function of Mach number with the average low-frequencies of fluctuations obtained from DSMC at a specified upstream number density and temperature. For cases where the Mach number and upstream number density is constant but upstream temperature is varied, the low-frequencies are found to be proportional to the most-probable-speed at the location of maximum velocity gradient magnitude. Using the proposed linear functions, it is shown that average low-frequencies can be estimated at an input number density of 10^{22} m^{-3} for a wide range of Mach numbers ($3 \leq M \leq 10$) and input temperatures ($\sim 90 \leq T_{tr,1}/(K) \leq 1420$). In the future, a similar approach can be used at other input number densities, and for other gases of practical importance, where the DSMC-derived low-frequencies can be obtained for a few selected input conditions and using those, a broader database of low-frequencies can be generated through linear correlations with analytical PDFs.

1.3.4 Computational framework for modal analysis of one-dimensional monatomic shock layers

Development of a computational framework for the modal analysis of normal shocks required complete derivation of $O(\epsilon)$ normal mode continuity, momentum, and energy equations from the compressible conservation equations that use traditional Navier-Stokes-Fourier (NSF) constitutive equations as well as a newly-derived set of constitutive equations using Mott-Smith's (MS) bimodal approximation [68]. These two formulations are referred to as the Navier-Stokes equations (NSE) and anisotropic conservation equations (ACE). The motivation for using the latter stemmed from the fact that these constitutive equations are substantially better than NSF equations at approximating the DSMC-derived normal viscous stresses and the x -directional heat flux at high Mach numbers ($M > 1.2$). As a result, the comparison of these two formulations for linear stability analyses of DSMC-derived shock layers at $Ma = 1.2, 3$, and 5 allowed for monitoring the effects of translational nonequilibrium on the stability of shock layers.

This work shows that consistent with the observations of Duck and Balakumar [1], eigenspectra obtained from both formulations contain decaying eigenmodes belonging to only continuous branches. It was shown for the first time that the eigenfunctions of the stationary and traveling modes of the least stable branch decay monotonically and sinusoidally in far fields of a shock, respectively, while the spatial decay rate was found to be an order of magnitude lower in the upstream than the downstream. This spatial decay behavior was shown to be governed by only one physically possible characteristic value (α_1) of out seven, predicted by a septic characteristic equation obtained analytically by simplifying normal mode equations in far fields of the shock. We could also derive an approximate formula for α_1 , denoted as α_1^{appx} , which provides a number of insights into the behavior of the least damped modes. We showed that there exists a range of temporal decay rates for which physically acceptable values of α_1^{appx} exist, meaning that the eigenfunctions can spatially decay in both far fields. The temporal decay rates of the first and second least damped branches of eigenmodes obtained from the linear stability analysis are close to the bounds of this analytical range. We show that these modes are always stable and address the question of the dependence of temporal decay rate on perturbation wavenumber, freestream Reynolds and Mach numbers, specific gas constant, and far field flow quantities. The analysis also shows why the ACE formulation, which uses a better constitutive equation for the stress tensor than the NSF equations, predicts a less stable decay rate than the NSE formulation, consistent with the observations of linear stability analysis at high Mach numbers.

1.4 Dissertation Structure

The remainder of the dissertation is organized as follows: Chapter 2 gives an overview of the DSMC method and describes the development strategies in the computational framework of the SUGAR solver, demonstrates its strong and weak scaling performance, as well as its capability in simulating SBLIs formed in three-dimensional Mach 7 flow of nitrogen over the double-wedge of finite span. Chapter 3 describes the spanwise periodic simulations of the same double-wedge configuration to study the stability of the 2-D base flow of Tumuklu *et al.* [30] against self-excited, spanwise-periodic perturbations. It also documents in detail the analyses of synchronized linear instabilities in the laminar separation bubble and the interior of separation and detached shocks. Chapter 4 is dedicated to the analyses of molecular fluctuations in the argon shock layers, the development of the two-energy-bin model to explain low-frequencies observed in shock layers, and characterization of a Strouhal number to scale the average low-frequencies at different input conditions. The analytical derivations of PDFs of particle energies in equilibrium freestreams, as well as shocks, are documented in Chapter 5, along with the established correlations to predict average low-frequencies of shocks for a wide range of input parameters. Chapter 6 presents the framework for modal analysis of monatomic shock layers based on compressible equations governing macroscopic flow quantities using traditional NSF as well as kinetically-derived constitutive equations. Comparisons of eigenspectra obtained from the two formulations, the characteristic temporal decay rates of eigenmodes, and the spatial decay behavior of their eigenfunctions are also presented in detail in this chapter. Finally, Chapter 7 offers a summary of major findings of these works and suggests possible topics for future research.

Chapter 2

Kinetic Modeling of Three-Dimensional Shock-Wave/Boundary-layer Interactions using the SUGAR DSMC Computational Framework

In this chapter, an efficient, new DSMC framework based on AMR/octree unstructured grids is demonstrated for the modeling of near-continuum, strong shocks in hypersonic flows. The solver is able to capture the different length scales in such flows through the use of a linearized representation of the unstructured grid using Morton-Z space filling curve for efficient access of collision cells. Strategies were developed to achieve a strong scaling of nearly ideal speed up to 4096 processors and 87% efficiency (weak scaling) for 8192 processors for a strong shock created by flow over a hemisphere. To achieve these very good scalings, algorithms were developed to weight the computational work of a processor by the use of profiled run time data, create maps to optimize processor point-to-point communications, and efficiently generate new DSMC particles every time step. Rigorous thermal non-equilibrium required for modeling high Mach number shocks was achieved through the accurate modeling of collision temperatures on a sampling grid designed to be compatible with the above approaches. The three-dimensional simulation of a nitrogen flow over a double wedge configuration for near-continuum conditions of Mach 7, unit Reynolds number $Re = 5.2 \times 10^4 \text{ m}^{-1}$, and Knudsen number $Kn = 3.4 \times 10^{-3}$ revealed complex hypersonic shock-wave/boundary-layer interactions as well as three-dimensional gas-surface kinetic effects such as velocity and temperature slip. The simulations showed that three-dimensional effects influence the size of the separation bubble, and in turn, the gas-surface measurements such as pressure and heat flux. The flow was found to be unsteady, although the two-dimensional flow at the same conditions had reached steady state.

2.1 Introduction

Hypersonic compressible flows are characterized by significant gradients in density, high temperatures, and thermochemical non-equilibrium. Because simulation of such flows requires consideration of the shock structure, chemistry of diatomic molecules, and the interactions of gases with embedded surfaces, the inherent multi-scale nature makes it challenging in terms of both flow physics and computational intensity. This work has been motivated by the development of a computational kinetic tool that can be applied to shock-wave/boundary-layer interaction (SBLI) problems which are known to involve complex flow physics such as flow separation, three dimensional effects, shear layers, and instabilities. All of these effects play a significant role in determining aerothermodynamic quantities such as heat transfer, skin friction, and pressure loads over flight vehicles with geometries that contain flares and corners. The particle based Direct Simulation Monte Carlo (DSMC) method [37] is a good candidate to simulate such flows because it solves the Boltzmann transport equation, and hence is valid even in strong shock regions where the continuum assumptions inherent in the derivation of Navier-Stokes equations fail. Recent three-dimensional DSMC simulations have been performed by Tumuklu et al. [69] of a nitrogen flow over a double wedge and a series of double cones [70] for a near continuum Knudsen number using the two-level Cartesian based Statistical Modeling In Low-density Environment (SMILE) code [71]. These simulations incur a computational time of approximately a million core-hours, and when used in a time-accurate manner to perform linear instability analyses [72] the need for efficient state-of-the-art peta-scale resource will only grow. As is well known, the use of DSMC to model such problems is limited by the high computational requirements arising from the need to simulate a large number of particles to satisfy DSMC requirements such as having a cell size comparable to the mean free path, using a time step that is smaller than the mean collision time, and having enough particles per cell to perform collisions [37]. Therefore, to solve such computationally demanding cases in an efficient manner, it is important to have a code that scales well on thousands of cores.

Among the well-known heritage DSMC codes, NASA's DSMC Analysis Code (DAC) has been demonstrated to scale linearly up to 256 processors for a flow over a hemisphere, however, beyond that the speed-up diverges [73]. Some new existing DSMC tools make use of parallel computer architecture with the Message Passing Interface (MPI) protocol to perform communication between the processors and a dynamic division of computational work to improve parallel efficiency. However, many new implementations show scaling for only 32 processors and for simulations with less than a million particles without consideration of embedded bodies in the flow [74–77]. The recently developed open source DSMC tool, SPARTA [78], has provided the DSMC community with an important tool for running compute intensive problems. Gallis et al. [78] have shown strong and weak scaling of SPARTA for many billions of particles for homogeneous heat bath cases which do not include embedded bodies or strong flow gradients. They have extended the scaling study to simulate a free molecular flow over a hemisphere [79] using about 64 million particles,

a problem that still does not encounter the difficulties involved in efficiently simulating strong gradients. White et al. [80] have reported a near ideal strong scaling for up to 10× processors with 200 million particles using the modified open source solver, dsmcFOAM+, for a lid driven cavity problem. When an embedded geometry is modeled in a high density hypersonic flow, however, the distribution of the computational work among processors becomes more difficult and can pose hurdles in achieving optimum performance efficiency for both structured and unstructured grids.

In addition, GPU-based implementations of DSMC have demonstrated good potential for simulating complex flows [65,81–83], however, there are limitations in using these architectures for high density problems. Such problems are memory intensive due to the requirement of billions of computational particles and cells, whereas GPUs are presently limited in terms of their device memory (about 6 GB on Bluewaters). In addition, the communication requirement is significant in such hypersonic flows and in the current generation CUDA architecture, direct GPU-GPU communication is not typically available on many high performance clusters. The information, therefore, has to be communicated to other GPUs through CPUs, which is limited by low bandwidth between CPU to GPU. Therefore, the focus of current implementation is to develop a highly scalable CPU based DSMC code and the lessons that we learned from linearization of the collision cell data structure from our CHAOS DSMC code [65] have strongly influenced the strategies developed in this work.

Furthermore, as the choice of the grid structure is one of the important factors in determining the accuracy and performance of the solver, it is instructive to understand how the aforementioned DSMC tools differ in their approaches. The SMILE [71] system uses a two level rectangular grid structure, where the particles are first initialized on a uniformly distributed Cartesian grid, labeled as “level-1”. Then, during run time, the level-1 grid cells are refined in regions of higher density into sub-cells denoted as “level-2” cells. This approach, although straightforward, is not optimal when it comes to resolving strong gradients [84–86]. Extending this strategy, SPARTA [78] uses a multi-level grid refinement, where each cell is subdivided to N_x , N_y , and N_z sub-cells. The DS2V [87] and dsmcFOAM+ [80] solvers, on the other hand, use a 2-D rectangular grid with a capability to generate transient adaptive sub-cells (TAS) [88], which exist only during the collision phase. The idea behind this method is that the coarser Cartesian cells typically used for sampling could also be used for selecting collision pairs, although the sampling cells are larger than the local mean free path. However, due to the transient existence of sub-cells, such an approach poses challenges in terms of load balancing since grid partitioning can only be done at the level of larger Cartesian cells and does not guarantee that the sub-cell size is smaller than the local mean free path in strong gradients [88].

To that end, we investigated the use of unstructured octree/AMR grids, to improve scalability in a manner that can accommodate complex geometries for both internal and external flows [3, 64, 84, 89]. This DSMC tool, known

as Scalable Unstructured Gas-dynamics Adaptive Refinement (SUGAR) was first applied to the study of ion thruster plumes by Korkut et al. [84–86], where it was demonstrated that a rectilinear octree/AMR [90] grid could capture the large gradients in the supersonic flow to vacuum much more efficiently than a two level Cartesian grid approach. Consistent with the plasma environment, the code used species dependent time steps to accommodate the large difference in velocities for neutrals and ions, an octree collision grid to model neutral-neutral and neutral-ion collisions, and an octree electric field grid to resolve the Debye length. In this method, the computational domain is first uniformly divided into cubic cells, known as roots and particles are initialized uniformly among them. As the flow evolves through collisions between DSMC computational particles, mesh refinement, based on the criteria that the cell size should be smaller than the local mean free path and there must be more than five particles per cell to perform non-reacting collisions, occurs. After the refinement, eight new cells are formed which are called the children of the root. The particle positions in the root are mapped onto these children and now the children are checked to see whether they satisfy the refinement criteria. The children that do not meet the requirement are refined further and when the refinement stops, the final cells are known as ‘leaves’ of the octree structure, and are ultimately used to perform collisions. This strategy was chosen since it has the advantage that mesh refinement is performed only in regions where the ratio of the cell size to the local mean free path is larger than unity, thus minimizing the number of required cells in the domain.

However, the unstructured nature of the mesh poses domain decomposition challenges to achieve good load balance for modeling *compression* flows using DSMC. To achieve high efficiency in a general manner, the collision mesh should be decomposed such that each processor has an equal amount of computational work and communication between processors is minimized. Figure 2.1(a), obtained for a flow over a double wedge shows how nonuniform the grid is and the large variation in the maximum depth of the octree. Roots A and B, as shown in Fig. 2.1(b) and Fig. 2.1(c), have three and five levels of refinement, respectively and roots near the surface have seven levels of refinement to capture the sharper gradients compared to those further away from the geometry. *The objective of this work is to develop algorithms that take advantage of the adaptability of octree grids for different geometries and length scales to model hypersonic, compression flows using the DSMC approach with good performance on petascale computers.*

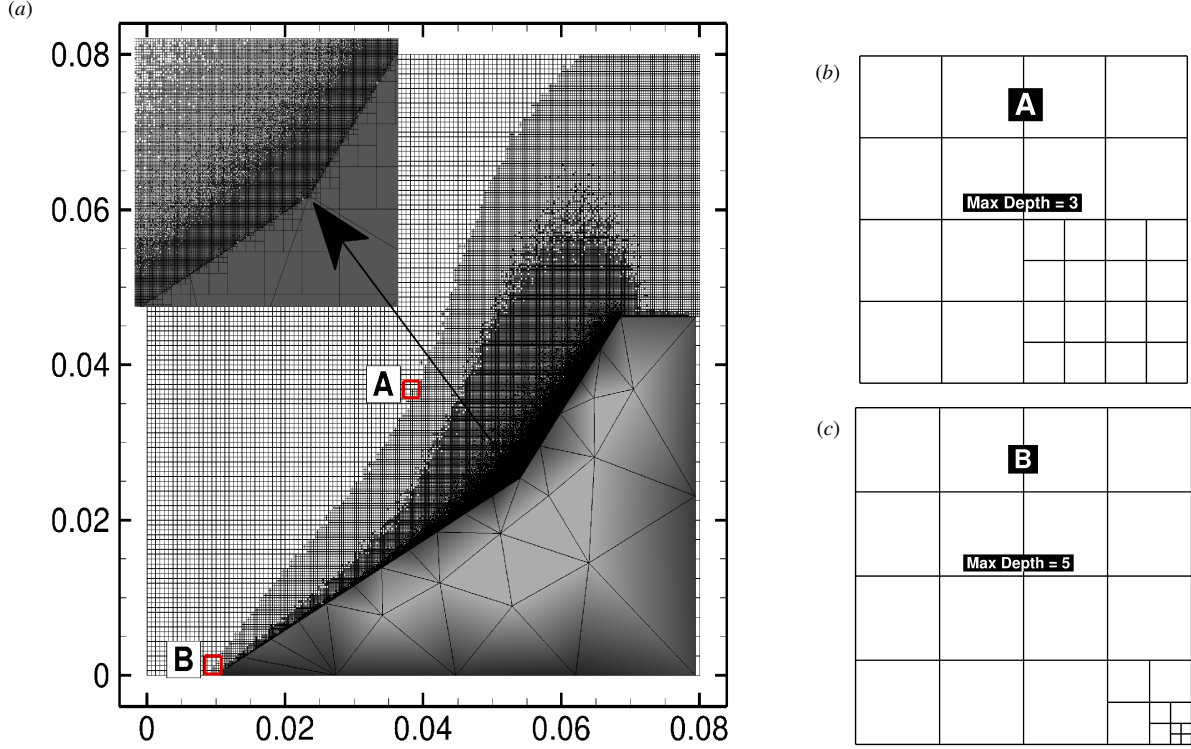


Figure 2.1: Collision mesh shown in (a) and the variation in the levels of refinement of root A in (b) and root B in (c). Flow has a freestream Knudsen number, $Kn = 0.04$ [3].

The outline of this chapter is as follows. Section 2.2 provides a brief description of the DSMC method. Section 2.3 describes the problems with the performance of the SUGAR code for compression flows, prior to this work, and the steps taken to improve the single-processor performance are presented. Section 2.4 describes the three important strategies that played a major role in the improvement of scalability and parallel efficiency of the code and the step by step effect of these strategies on the strong and weak scaling studies performed for a nitrogen flow over a hemisphere. The development of these strategies are constrained by the physics of hypersonic flows, namely, thermal non-equilibrium caused by insufficient collisions in the shocklayer. The strategies used to map DSMC computational particles from the octree/AMR grid to a collision temperature grid that is used to calculate thermal relaxation rates as the flow evolves are also discussed and steady state flow macroparameters are presented. The strong and weak scaling achieved in Sec. 2.4 allows us to consider the final demonstration case of the SUGAR code in Sec. 2.5, the simulation of SBLIs for a flow over a double wedge geometry for near-continuum Knudsen number conditions.

2.2 Overview of the Direct Simulation Monte Carlo Method

The particle-based DSMC method [37] is a computationally powerful tool, based on the decoupling of molecular motion and intermolecular collisions, in which each simulated particle represents a finite number, F_n , of actual gas molecules. When all numerical parameters are satisfied, the time-accurate flowfield represents a solution of the Boltzmann equation of transport of the molecular velocity distribution function, $f(t, \mathbf{r}, \mathbf{v})$ with respect to time t and position vector $\mathbf{r}$, as

$$\frac{\partial f}{\partial t} + (\mathbf{v} \cdot \nabla)f + \left(\frac{\mathbf{F}}{m} \cdot \nabla_v \right) f = \left[\frac{df}{dt} \right]_{\text{coll}} \quad (2.1)$$

where $\mathbf{v}$ is the instantaneous velocity vector and ∇ and ∇_v are gradient operators in physical and velocity spaces, respectively. The first, second, and third terms on the left-hand side describe the change of f with time, convection of molecules in space, and convection in velocity space as a result of the external conservative forces per unit mass $\mathbf{F}/m$, such as gravity or electric field, which are ignored in this work, respectively. The right-hand side term accounts for changes in f in an element of space-velocity phase-space due to intermolecular collisions. Vincenti and Kruger [91] provide a thorough description of the Boltzmann equation.

The DSMC algorithm typically comprises four major steps of particle mapping, selection for collision partners, evaluation of collision outcomes, and movement. Based on the choice of boundary conditions, particles are introduced, removed, or reflected from the domain boundaries and interacted with the embedded surfaces using gas-surface collision models during a timestep. They are then mapped to a mesh that encompasses the flow domain with cell size, Δx , that is smaller than the local mean-free-path of molecules, λ . Particle pairs are selected for collisions based on the appropriate elastic or inelastic collision cross-section and are then assigned post-collisional instantaneous velocities and internal energies in each computational cell. Macroscopic flow quantities of interest such as pressure, velocities, and temperature can be derived from the microscopic properties of simulated particles using the statistical relations of kinetic theory. Finally, based on the post-collisional velocities, particles are moved for a timestep, Δt , that is lower than the local mean-collision-time, τ . Conveniently, this physics based approach provides accurate modeling of the internal structure of shocks, their mutual interactions, and surface rarefaction effects. This warrants the use of DSMC for detailed modeling of SBLIs, compared to ad-hoc techniques of modeling shocks in numerical solutions of the Navier-Stokes equations that fall short of accurately capturing the internal structure of the shock [62].

Parameters	Single processor study	Multi processor scaling study	Verification study
Geometry	Hemisphere	Hemisphere	Double wedge
Species	Ar	N ₂	N ₂
Viscosity index	0.81	0.74	0.74
Number density [m ⁻³]	9.33×10^{20}	1×10^{21}	1×10^{22}
Knudsen number	0.138	0.05	3.4×10^{-3}
Mach number	8.46	8.46	7.02
Free stream velocity [m/s]	4200	4200	3812
Free stream temperatures [K]	200	200	710
Stagnation enthalpy [MJ/kg]	9.19	9.19	8.0
Free stream mean free path [m]	1.38×10^{-3}	1.29×10^{-3}	1.64×10^{-4}
Reynolds number [Re]	128	321	2652
Reference length [m]	0.01	0.025	0.0508
Surface temperature [K]	200	200	798
Time step [s]	1.0×10^{-7}	5.0×10^{-8}	4.0×10^{-9}
FNUM ^b	4.0×10^9	8.8×10^9	2.5×10^8
Domain size (x,y,z) [m]	0.02 each	0.09 each	(0.08, 0.06, 0.08)
Adaptation start time step	1000	1000	500
Adaptation period	500	1000	500
Adaptation end time step	2000	8000	24,500
Sampling start time step	2000	9000	25,000
Sampling end time step	4000	10,000	27,000
Maximum level of refinement	5	4	5
Average number of particles	3.21 million	96 million	23.96 billion
Average number of collision cells	0.26 million	2.04 million	2.154 billion

^a Surface accommodation coefficients of unity, VHS collision model.

^b FNUM is the number of actual molecules represented by one computational particle.

Table 2.1: Input conditions and numerical parameters for the hemisphere and double wedge simulations.^a

2.3 Performance Improvement on a Single Processor

Our starting point was the original SUGAR code which used a recursive pointer based traversal of the leaf cells during mapping and storage of the octree structure and a linked-list based storage of particles [3, 64, 84, 89]. For parallelization, the SUGAR code uses the CPU-based distributed memory systems and employs Message-Passing-Interface (MPI) for communication of particles between the processors. Korkut et al. [84], used a two dimensional (2-D) blocking algorithm which divides the available roots equally among all the processors to decompose the mesh across processors. For a single thruster expansion flow, the code demonstrated a strong scaling speed-up of 400 for 1024 processors having 10 million particles in the simulation domain [84, 92]. With the use of the Parmetis [93] graph partitioner the speed-up improved a bit but it was still sub-optimal (50%) for 1024 processors [92]. Using the same 2-D blocking partitioning scheme, a strong scaling study performed for a hypersonic flow over a double wedge only showed a linear speed-up for up to 128 processors but beyond that it diverged from the ideal curve and a maximum speed-up of only 335 was observed for a case with 512 processors [64, 89]. Similarly, for a hypersonic flow over a hemisphere, only 50% scaling

was observed for an eight times increase in the number of processors [3,64] and even with the use of the state-of-the-art SCOTCH [94] graph partitioner, where the roots were partitioned among processors based on dynamically assigned weights [3,64], the scaling did not improve.

Characteristics	SMILE (Cartesian mesh, array based)	SUGAR (Recursive octree, linked-list based)	SUGAR improved^b (Linearized octree, array based)
Total time:	5665 s	11,400 s	4804 s
Time per particle:	1.74×10^{-3}	3.55×10^{-3}	1.49×10^{-3}
Number of cells:	262,144	260,119	260,119

^a based on 2000 samples and using CPMAT [95] profiler on Bluewaters.

^b the final version of the code with improved algorithmic performance.

Table 2.2: Performance improvement of the SUGAR code on a single processor.^a

Clearly further algorithmic improvement were required, but, before considering performance on multiple processors the *single processor* efficiency was closely examined by choosing a case, where the entire simulation could be fit on a single processor so that all the DSMC procedures could be profiled to find the performance bottlenecks. The input and DSMC numerical parameters for this case of a hypersonic flow over a hemisphere are shown in column one of Table 2.1. Comparison of columns one and two of Table 2.2, shows that the original version of the SUGAR code took about two times more time per particle compared to the two-level Cartesian grid code with mesh adaption, SMILE [71]. To understand the source of this large difference, both the codes were profiled to compare the time taken by the major DSMC tasks such as movement of particles, mapping (*i.e.*, the search for the destination collision cell), sampling, or the calculation of macroscopic properties using particle velocities in a cell, and the computation of binary particle collisions. Surprisingly, it was found that the time taken per collision was more or less the same and the performance bottleneck was due to the differences in the way particles were accessed from the memory and mapping was performed in the SMILE versus the recursive pointer based SUGAR code. Since particle access and mapping is performed extensively in DSMC, the use of the recursive pointer approach was unacceptably high.

In our earlier investigations of AMR/Octree for DSMC modeling of flows through porous media on GPU architectures, using a code called CHAOS [65], we investigated the use of linearized data structures based on Morton-Z space filling curves. In this approach, only the leaves of an octree are stored and each leaf cell is assigned a unique Morton index [65–67] with which it can be accessed in a balanced tree structure and in a sequential fashion thus allowing

direct access of the leaf cells in a root. This method has been extended to an unbalanced tree structure by creating a ‘location code’ array [65, 66]. Such an array uses the Morton index as the input and gives the destination leaf cell index as the output, as explained by Jambunathan et al. [65]. To investigate the possible benefit of the space filling curve approach in SUGAR, a CPU single processor version of the CHAOS code was developed and run for the same case and the absolute compute time was reduced significantly to 4832 s. This comparison proved that it was possible to match the mapping time of a simple two-level Cartesian grid with an unstructured one using the Morton indexing strategy.¹ When the Morton-Z space filling curve was implemented in the SUGAR code the absolute time was reduced from 11,600 s to 8000 s.

Further improvements in the single processor SUGAR code, bringing the compute time down to 6300 s, were obtained by implementing efficient gas-surface interactions. When the original SUGAR code was modified to include embedded geometries, a cut-cell approach similar to the work of Zhang et al. [96], that allows for an accurate calculation of the fluid portion of the volume of the intersected cells was implemented. However, to further improve the efficiency, instead of performing geometry detection for each particle at every time step, particles are checked for possible gas-surface interactions when they are sufficiently close to the geometry. This spatial region is formed by marking the root cells intersected by the geometry and its neighbors in the streamwise direction, as shown for a double wedge configuration in Fig. 2.2(a). Furthermore, instead of checking for all possible interactions, the code loops over only a subset of surface panels that are in the vicinity of the particle. This is achieved by creating a grid much coarser than the collision cells, known as the ‘Gas-Surface Interaction (GSI) Grid’, which contains surface panels, as shown in Fig. 2.2(b). Particles in a GSI cell that intersects the geometry, shown in pink, are checked against a list of panels that belong to that GSI cell as well as panels that belong to the neighboring root (blue) GSI cells. This strategy always identifies the correct interaction panel because the mean free path near the geometry is very small and particles do not move far from its position before colliding with the surface. If the geometry to be simulated is a simple shape, such as a hemisphere or the double wedge, then the potential looping over multiple panels and mapping of particles to the separate GSI grid can be eliminated. This is achieved by identifying the intersection point using well-known computational geometry algorithms to locate the GSI cell containing the exact gas-surface interaction panel.

¹The 17.85% reduction in time compared to the Cartesian SMILE code was due to optimizations in gas-surface interactions by taking advantage of the hemisphere geometry and by checking for gas-surface interactions only for particles having positive streamwise (X) velocity if they were downstream of the peak of the hemisphere.

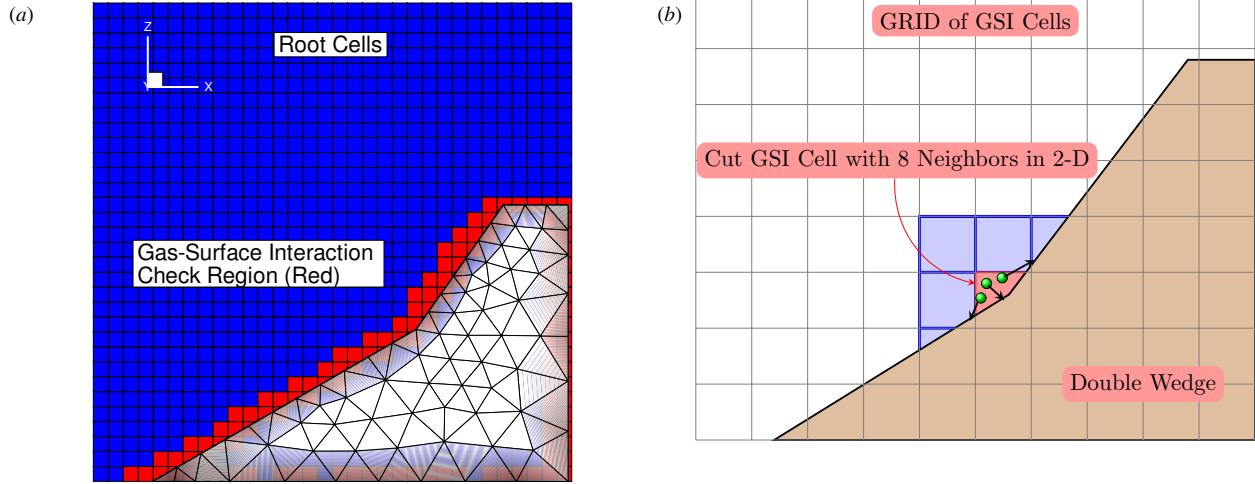


Figure 2.2: Efficient gas-surface interaction strategy. (a) The red region in the vicinity of the wall where particle-surface interaction procedure is performed. (b) Neighbors of an intersected GSI cell (pink).

Even after these modifications the time taken by the SUGAR code was still 30% greater than the CPU-based CHAOS code. The effect of the difference in the particle data structure on compute time was investigated. Both the SMILE and CHAOS codes used an array-based data structure to store particle information such as location and velocities whereas, the SUGAR code was using linked-lists to facilitate the dynamic changes in the number of particles throughout the simulation. Such a structure can lead to inefficient use of cache memory because neighboring particles are not necessarily stored close to each other in memory. Therefore, while accessing particles for collisions, movement, mapping, and sampling, the processor has to access the global memory most of the time, which incurs a larger time penalty than when accessing cache. Table 2.3 clearly emphasizes the effect of using arrays as opposed to linked-lists for millions of particles. Since, the flow was hypersonic and collisions were switched off, particles moved across the collision cells very fast requiring extensive re-mapping, compared to a normal DSMC simulation. The first row in Table 2.3 shows that the D1 cache was well utilized by both linked-list and array based versions of the code, however, the D2 cache, which is the next closest memory to the processor, was poorly utilized by the linked-list based data structure. The third row (D1+D2 Cache Utilization) shows that for the case of linked-lists a cache miss occurred, on average, after every 35 data accesses. At every cache miss the processor has to access the main memory, which is quite often in case of linked-lists. For arrays, the cache utilization ratio was about 62 times larger (2137/34.74). The fourth row shows that the Translational Lookaside buffer (TLB) utilization was about 34 times more for arrays. After implementing the array-based data structure for storing particles, SUGAR was re-run for the original case and comparison of column three with one of Table 2.2 shows that the execution time for SUGAR was 15% lower than SMILE and comparable to CHAOS.

Observations	SUGAR	SUGAR
	with linked-list	with arrays
Total time [s]	1460	275
D1 cache hit ratio [%]	94.5	99.3
D2 cache hit ratio [%]	47.5	92
D1+D2 cache utilization [refs/miss]	34.74	2137
Translation Lookaside Buffer utilization [refs/miss]	74.67	2470

^a Gas surface interactions, collisions, and sampling are deactivated. The number of particles and profiling duration are ~ 7.4 million and 1000 time steps, respectively.

Table 2.3: Effect of arrays storage versus linked-lists in a flow without collisions.^a

2.4 Performance on Multiple Processors for Flows with Strong Shocks over a Hemisphere

For transitional to near-continuum free stream Knudsen number cases, even flows over a simple hemisphere require multiple processors. We start this section describing the thermal nonequilibrium predicted by SUGAR through the accurate implementation of a collision temperature grid to efficiently calculate collision temperatures prior to sampling or steady state on the octree/AMR grid in Sec. 2.4.1. However, the freestream Knudsen number and geometries that we wish to consider impose even more stringent DSMC numerical requirements. Therefore, with an efficient single-processor code for modeling strong shocks, we turn towards the strategies that we developed to model the flows with strong non-equilibrium with near-continuum conditions requiring ~ 24 billion particles. Such strategies must be developed in the context of efficient domain decomposition for DSMC computations on octree/AMR grids. Following our previous work on GPUs [65], we partition the linearized octree structure across processors. Since all the leaves are stored together in an array in the Morton-Z approach, these arrays can be divided among available processors as a first step towards achieving good load balancing. For strong shock problems we use the preferential direction of the flow to assign leaves that lie in the streamwise direction to the same processor compared to those that are in the transverse direction. This reduces inter-processor communications time because roots contained by a processor are

mostly adjacent to each other in the bulk flow direction. As beneficial as the Morton-Z approach is however, additional work was required to achieve efficient parallelization in a dynamically evolving flow.

The main strategies that will be discussed in this section are (1) processor weighting factors for load balancing (Sec. 2.4.2), processor maps for point-to-point communications (Sec. 2.4.3), and efficient introduction of particles into the domain (Sec. 2.4.4). As we discuss these strategies we explain the relative improvements that were obtained in terms of strong scaling, which is difficult to achieve. For the strong scaling analyses the baseline case is given in column two of Table 2.1 where all the 32 processors of one XE node on Bluewaters cluster were used.² Figure 2.4 shows the step by step effect of different implementations on the strong scaling performance of the SUGAR code and in Sec. 2.4.5 we summarize the performance for weak scaling as well.

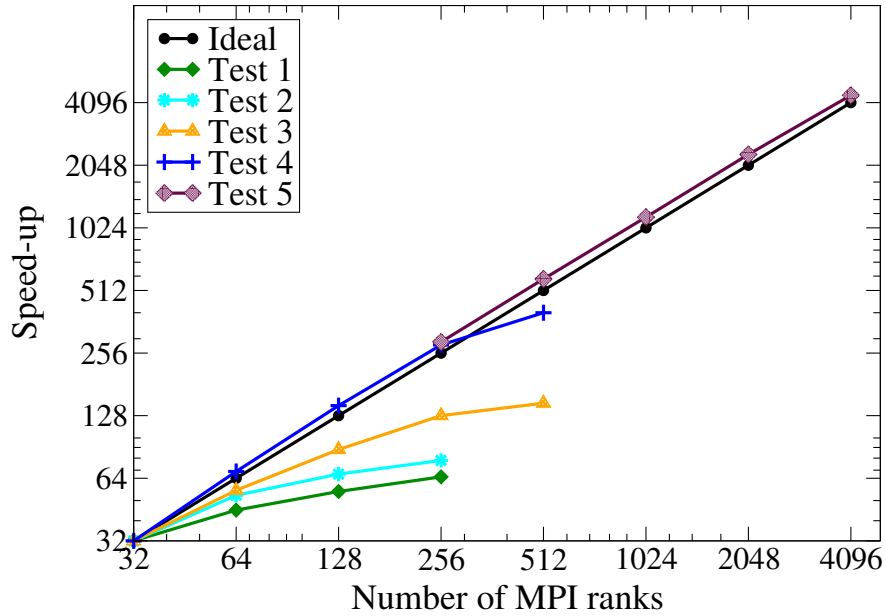


Figure 2.3: Speed-up comparisons for a flow over a hemisphere. Tests 1 and 2 were performed before implementing any new strategies. Tests 3-5 demonstrate the cumulative, successive improvements of Strategies A, B, and C, as described in Sec. 2.4, respectively. Execution times for 1000 time steps and 32 processors were 2793, 2413, 2541, and 1402 s for Tests 1 - 4, respectively. For the purpose of speed-up calculations, the 32-processor case for Test 5 is assumed to take the same amount of time as Test 4.

2.4.1 Thermal non-equilibrium in strong shocks

An important benefit of the octree unstructured grid formulation is to be able to resolve the large translational, rotational, and vibrational temperature gradients in the shock overshoot and near the wall. To demonstrate this capability a non-

²One node on Bluewaters has 32 processors and about 64 GB available memory.

reacting molecular nitrogen flow over a hemisphere of radius 0.025 m is embedded in a computational domain of size (0.09 x 0.09 x 0.09) m, with its base centered at (0.09, 0.045, 0.045) m in the X, Y, and Z-directions, respectively. Note that the simulations described in Sec. 2.3 and the first column of Table 2.1 did not correspond to a physically correct DSMC simulation because our goal in that case was to perform the main DSMC algorithms on a single processor with a high level of refinement. A true physical solution would have required a much larger computational domain size.

A number of collision models and pair selection procedures have been implemented in the SUGAR code. To model elastic collisions, one may choose the variable hard sphere (VHS) [37] or variable soft sphere (VSS) model [97] and to model collision frequency, the options of using the No Time Counter (NTC) [37] or the majorant frequency scheme [98], which is derived using the Kac stochastic model, are available. In the simulations presented here the VHS model and the majorant frequency scheme [98] were used. Other collision schemes such as simplified Bernoulli trials (SBT) [99, 100] and intelligent-SBT (ISBT) [101], could also be implemented in this framework. In terms of thermal relaxation, the Larsen-Borgnakke (LB) method [102] for the continuous rotational relaxation was used assuming a rotational probability, P_r , of the form [103],

$$P_r = \frac{1}{Z_r} = \frac{\zeta_t + \zeta_r}{\zeta_t Z_r^C} \quad (2.2)$$

where Z_r is the rotational collision number, ζ_r is the number of rotational degrees of freedom of the particles participating in collision, $\zeta_t = 5 - 2\omega$, is the number of relative translational degrees of freedom, ω is the viscosity index, and Z_r^C is the rotational number used in continuum simulations. The Parker model for the temperature dependence of the rotational probability [104],

$$Z_r^C(T_e) = \frac{Z_{r,\infty}}{1 + \frac{\pi^{3/2}}{2} \left(\frac{T^*}{T_e}\right)^2 + \left(\frac{\pi^2}{4} + \pi\right) \frac{T^*}{T_e}} \quad (2.3)$$

was used, where the values of constants $Z_{r,\infty}$ and T^* for nitrogen are 18.5 and 91, respectively. To model vibrational relaxation we followed the approach of Ivanov et al. [71], who extended the LB method assuming that the temperature dependent vibrational relaxation probability is given by the semi-empirical expression of Millikan and White [105] with the high temperature correction of Park [106],

$$P_v = \frac{1}{Z_v} = \frac{\zeta_t + \zeta_r + \zeta_v}{(\zeta_t + \zeta_r) Z_v^C} \quad (2.4)$$

where ζ_v is the number of vibrational degrees of freedom of the particles participating in the collision and Z_v^C is the vibrational number used in continuum simulations. Note that $\zeta_i = \zeta_{i_1} + \zeta_{i_2}$, where $i = r, v$ and subscripts 1 and 2

represent the internal number of degrees of freedom for the two particles in the binary collision.

The collision temperature, T_e , used in Eq. 2.3 and the Millikan and White expression [105] must be computed as the flow evolves even though general macroparameter sampling has not started. A separate uniform grid, known as the collision temperature grid, that can be related to the unstructured collision octree grid was created to compute this temperature by sampling the translational collision energy of colliding pairs for typically 500 time steps. This grid is typically finer than the Cartesian grid used to define the roots but coarser than the collision cells to ensure that there are sufficient particles to give an accurate collision temperature required to compute internal energy relaxation probabilities. The probabilities are updated based on the collision temperature sampled from the previous 500 time steps and these probabilities are used for all the collision cells that lie within a given sample cell. Finally, the gas-surface interactions were modeled using Maxwell's model [37] with full momentum and energy accommodation.

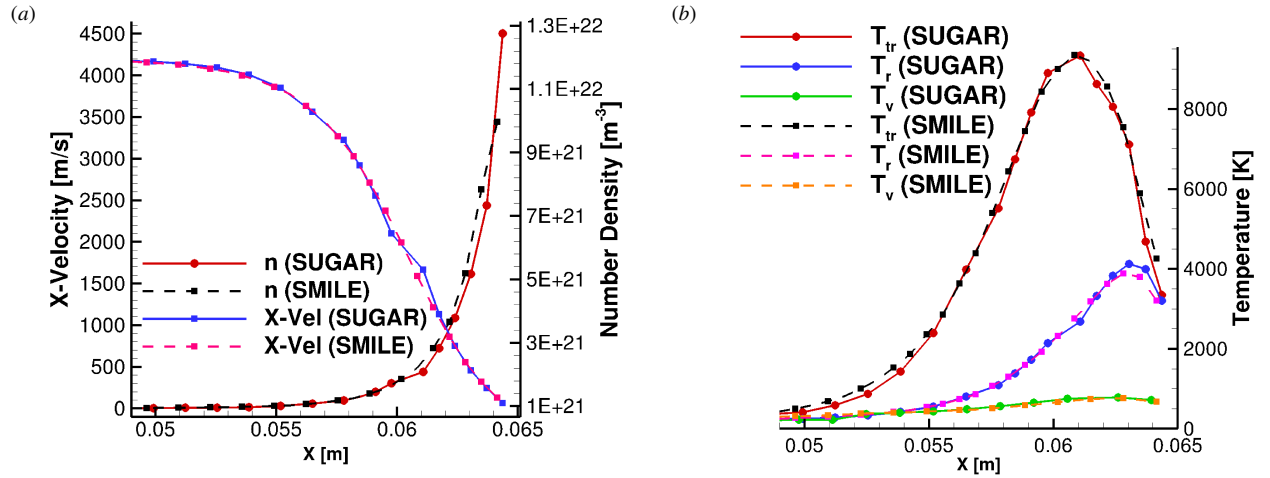


Figure 2.4: For a flow over a hemisphere, the comparison of SUGAR and SMILE results for number density and X-directional bulk velocity in (a) and temperature in (b). Line plots are compared along the stagnation line. The stagnation point on the wall of the hemisphere is at $X = 0.065$, $Y = 0.045$, and $Z = 0.045$ m and the hemisphere is embedded in a domain of length 0.09 m in each direction.

Figure 2.4(a) shows the number density and the streamwise velocities predicted by SUGAR and its comparison with SMILE. The convergence of these results is verified by ensuring that the mesh resolution in the vicinity of the geometry is sufficiently fine such that the size of the collision cell is smaller than the local mean free path and the chosen time step of 5×10^{-8} s is at least two times smaller than the mean collision time in each collision cell. Satisfaction of these criteria justifies the decoupling of the collision step and the movement of particles in DSMC [37]. Also, the smallest collision cells have at least four computational particles, which is sufficient since the majorant frequency scheme [98] is employed in the selection of collision pairs. To accurately compare the results with SMILE, which uses a two level

Cartesian grid, the level-1 grid cells were equal in size to the root cells in the SUGAR code and each level-1 cell was allowed to be subdivided into 16 parts to match the maximum refinement of the four levels observed for the collision mesh in SUGAR. The classic strong shock behavior of a bow-shock stand-off distance 60% of the hemisphere radius and the thermal nonequilibrium observed in Fig. 2.4(b) is demonstrated. Downstream of the shock the flow becomes subsonic and the peak translational temperature of 9400 K is observed. Due to the free stream Knudsen number and the use of molecular nitrogen, the vibrational mode is essentially inactive. Agreement with the SMILE DSMC code is very good but note the improved resolution of the SUGAR predicted number density of about 20% and the translational temperature gradients at the wall of 25%. These differences at the wall are attributed to the accurate calculation of the volume of cut-cells in the SUGAR code, which can affect the computation of heat flux, an important quantity in comparing simulations with experiments.

2.4.2 Strategy A: weight criterion based on profiled time for load balancing

An important part of achieving good load balance is the accurate assessment of the computational work of each processor also known as its weight. During the transient phase, the SUGAR code uses the total number of particles in a leaf cell to assess the processor weight during a period of typically 500 time steps during which leaf cells are re-partitioned among processors. However, this criterion is not optimum and cannot be guaranteed to succeed in flows with high gradients where for example, some processors may have to perform more tasks if they contain the region with many cells near the geometry or a region with a relatively higher collision frequency. Such a high collision frequency region is downstream of the bow shock where the temperature is about 50 times higher than that in the free stream. A weight criterion based on equal division of number of collision cells, or leaves, would also fail because the volume of the collision cells in the free stream region is larger than those near the geometry and therefore, the cells in the freestream contain more particles. For example, in the hemisphere case, the cells in the free stream will typically have 64 to 256 times more particles than the cells near the geometry. These points are demonstrated in Fig. 2.5(a) which shows the distribution of the number of particles, profiled time, and the number of leaf cells for each processor on the final AMR mesh, partitioned based on the number of particles. The profiled time for each processor is obtained by collecting the time taken by each of its collision cells to perform the major DSMC tasks such as collisions, gas-surface interactions, and sampling for a period of typically 500 DSMC time steps once the flow reaches steady state.

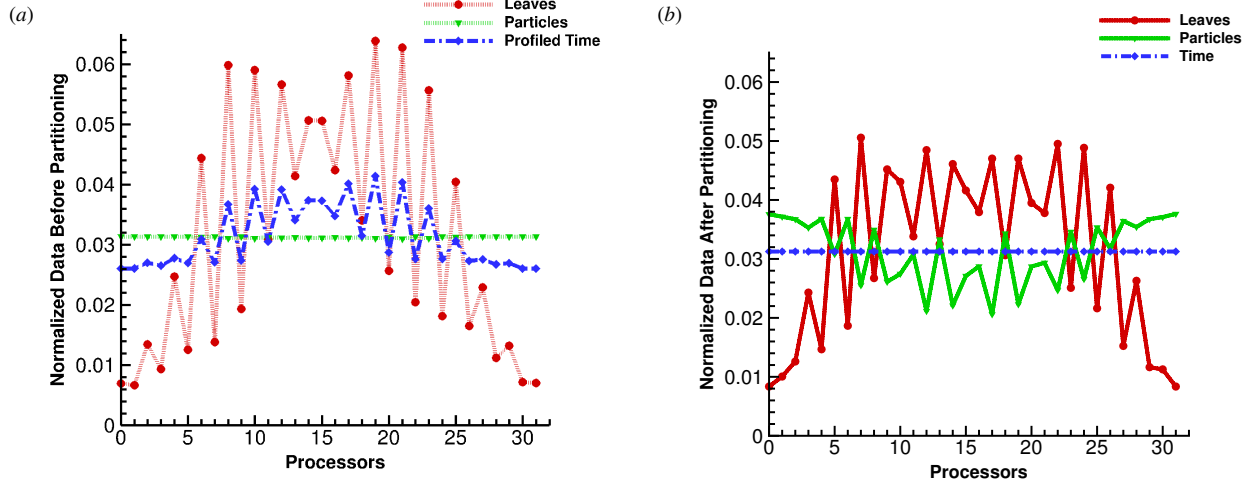


Figure 2.5: (a) Profiled data for 1000 time steps using 32 processors before partitioning. (b) Statistics taken after final partitioning. Data shown is normalized by the total corresponding quantity on the entire mesh.

It is seen that for a case with a domain decomposition criterion based on the number of particles, the distribution of leaf cells is not uniform across processors. Specifically, processor 9 has a smaller number of leaf cells because it contains most of the cells that are further away from the geometry which are larger in size and contain more particles per leaf, whereas, processor 10 has a larger number of cells since it contains most of the cells lying in the post shock region and near the geometry. Processor 11 has fewer leaf cells than 10 because it contains many leaf cells further away from the geometry. Furthermore, processor 10 spends relatively more time than 9 and 11 because its cells have a higher collision frequency and its particles perform more gas-surface interactions. To overcome these limitations in the most general manner, the SUGAR code uses profiled time to assess weights once the flow reaches steady state and the mesh is finalized. Figure 2.5(b) shows that after the final partitioning, every processor takes more or less an equal amount of time in performing the required DSMC tasks and that indeed the number of particles and leaf cell distribution is uneven.

The effect of the weighting strategy on speed up is demonstrated in Fig. 2.4 in terms of speed up results for Tests 1-3. For the criterion based on the number of leaf cells (Test 1), the relative weights of the leaf cells were varied based on their level of refinement with the coarser leaf cells being given higher weighting since they contained more particles than the refined leaf cells. As seen in Fig. 2.4, the weight criterion based on an equal number of particles (Test 2) or leaf cells (Test 1) among processors did not give good speed-up. As the number of processors was increased, the code did not continue to scale well because the number of leaf cells (or particles) per processor decreased and some of the processors only contained the post shock region (with a higher collision frequency) or the free stream. However, the weight criterion based on the profiled time (Test 3) gave relatively better speed-up, up to 256 processors. The lack of

speed up beyond 256 processors was suspected to be due to the inherent serialization in point-to-point communications (Sec. 2.4.3) and the introduction of particles by a single processor (Sec. 2.4.4).

2.4.3 Strategy B: optimization of processor point-to-point communications

In the present DSMC application, MPI point-to-point communication of particles takes place at each time step to exchange particles that move out of a processor's domain. Each processor needs to know the number of particles that will be leaving its domain as well as their destination processor IDs. This *Send* information is computed on each processor when a particle moves out of its domain and is mapped on to the domain of another processor. Processors also need to know the reciprocal information, *i.e.*, the *Receive* information. To achieve this, all processors first communicate their *Send* information to an assigned 'master' processor, which serially sorts through this data to determine the *Receive* information of each processor. The problem with this method is that all the other processors remain idle during this sorting step, leading to a loss of efficiency.

This bottleneck can be completely avoided by taking advantage of the "steady state" nature of the flow. That is, after the final mesh is created, the *Send* Information and *Receive* Information for each processor does not change and each processor can keep track of the potential list of processors it would receive information from and send information to. Sometimes a processor may receive a few particles from a distant processor only for a period of a few time steps. To take this possibility into account, the potential list of processors is formed from the data collected for typically 500 time steps and modified accordingly. Once this map of possible processor IDs for sending and receiving information during point-to-point communications is created, the inherent serialization of the mapping process has been removed. The improvement in the speed-up is shown as Test 4 in Fig. 2.4, where the speed-up was close to ideal for 256 processors, but, for 512 processors, the curve degraded from the ideal.

2.4.4 Strategy C: optimization of particle introduction

In DSMC, particles are introduced at the inlet planes of the domain every time step in order to maintain a constant inlet flux that corresponds to the free stream conditions. For the large numbers of particle that we consider, a single processor cannot perform the task of *generating* particles from directed Maxwellians in the bulk flow direction; therefore, particle generation is usually divided equally among all processors. However, if the task of generating particles is assigned to every processor in the domain, then the performance of the code will be sub-optimal because the simulation will incur extra communication time as those processors that contain collision cells far from the inlet planes send the information about the newly generated particles to processors that contain the inlet planes. Therefore, the task of generating particles was assigned to only those processors that contain at least one of its root cells adjacent to the inlet planes.

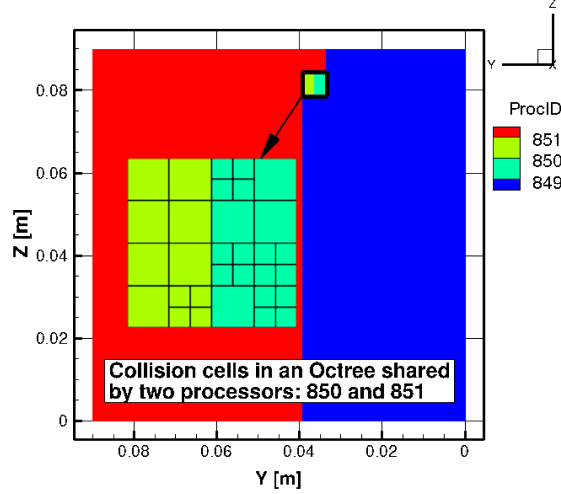


Figure 2.6: Conflict (shown on an X-inlet plane) when the collision cells in a root are shared by two processors.

One difficulty in the implementation of this approach is that when the leaf cells belonging to a root are shared by more than one processor, one of the processors must be selected to generate particles. Such a case is demonstrated in Fig. 2.6, which shows a highlighted root on the X inlet plane, where the collision cells from same the root are divided among two processors, 849 and 850. In such a case, processor 849 was given preference (based on the fact that its ID was lower) to generate particles and the newly generated particles that were mapped to leaf cells contained by processor 850 were communicated from processor 849 to 850. Note that this strategy complements Strategy B because it reduces the potential list of senders for each processor, whereas without the modification such a list would have to include all the processors adjacent to the inlet. With this implementation (Test 5) a speed-up close to ideal was obtained for up to 4096 processors as compared to the 32 processor baseline case, as shown in Fig. 2.5. These current improvements in the strong scaling were found to be very good in comparison with the speed-up for the old SUGAR version.

2.4.5 Weak scaling study for a flow over a hemisphere

Ideally, for weak scaling the execution time should remain the same as the baseline case, as described in column two of Table 2.1. However, it is challenging to achieve this scaling because the amount of communication increases with an increase in the number of nodes. For this study, the number of processors was increased in proportion to the total number of particles in the domain because the latter plays a major role in the compute time for high density flows. Figure 2.7 shows the parallel efficiency, which is defined as,

$$E_N = t_{32}/t_N \quad (2.5)$$

where, E_N is the parallel efficiency for N processors, t_{32} is the time taken to run a baseline case on 32 processors, and t_N is the time taken to run with N processors. Note that in this study, the mesh was kept the same as for the baseline case and the execution time for 1000 time steps on 32 processors was 1402 s.

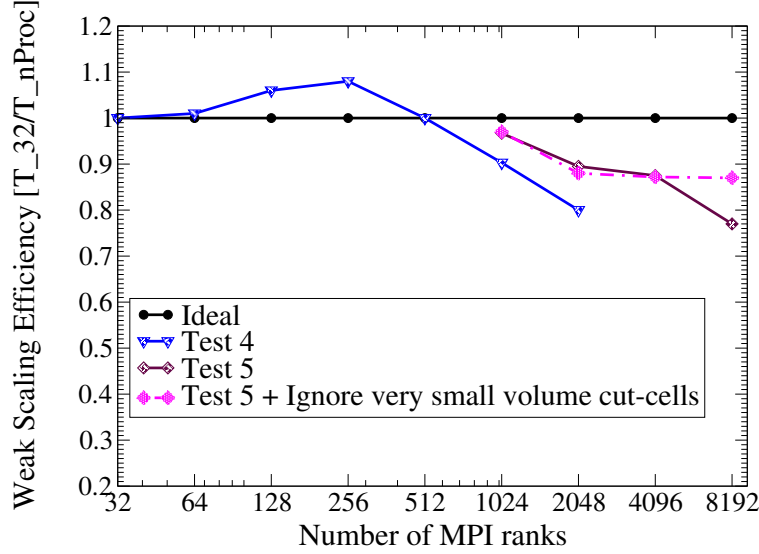


Figure 2.7: Weak scaling for a flow over a hemisphere. See Fig. 2.4 for definition of Tests 4 and 5.

Figure 2.7 shows that in general the SUGAR code achieved good weak scaling. During Test 4 (blue curve, but particles generated by all processors) the code performs close to ideal up to 512 processors and for 64, 128, and 256 processors it exhibits super-linear scaling due to the fact that as the number of computational particles increases in proportion to the number of processors, each node has fewer cells since the mesh was unchanged. This results in better cache utilization during the stages of sampling, collisions, and mapping. However, after 512 processors the efficiency started to decrease, due to the increase in the communication time. The communication time was slightly reduced by the implementation of Strategy C (Test 5) of Fig. 2.4 and the parallel efficiency for 1024 processors improved from 90 to 96%, as shown by Test 5 in Fig. 2.7. Because the flux of incident particles increased with the increase in computational load the manner of particle introduction does play an important role. However, for 2048 processors the efficiency decreased to 87% because the overall number of root cells had to be increased to assign more than two roots to each processor in the streamwise direction. For test 4 the efficiency flattened out and remained same up to 4096 processors, but decreased for 8192 processors.

This decrease in efficiency was determined to be due to the creation of leaf cells having extremely small fluid volume close to the geometry, *i.e.*, the ratio of the fluid to cubic cell volume was less than 10^{-9} . Such a small fluid volume results in a spuriously high collision frequency. If these cells have two-three particles, then they keep performing collisions, leading to a very large weighting factor based on profiled time. Note that the probability of

occurrence of such cells is negligibly small, however, it can have a detrimental effect on performance. For example, for the simulation on 8192 processors with about 24 billion particles, 24% more time was taken by about 10 processors causing an imbalance even after final partitioning based on profiled timings. However, when such cells were not allowed to perform collisions, the time taken by each processor was found to now be equalized within 4 %. With this improvement the efficiency went back to 87% for 8192 processors in Test (5 + ignore small volume), where the code took 1611 s for 1000 time steps.

2.5 Shock-Wave/Boundary-Layer Interactions of a Hypersonic Flow over a Double Wedge

Satisfying the DSMC requirement for the SBLI case at a Knudsen number of the order 10^{-3} requires billions of computational particles and cells, which necessitated additional memory optimization tactics discussed in this section. The results for the actual case presented in the next subsection correspond to a free stream Knudsen number of 0.00324 simulated using 20,000 processors.

2.5.1 Root size, level of depth, and processor assignment

First we consider the number of roots for which the location code array is stored, which is required by every processor during the mapping procedure to find the destination leaf cell of particles. For a root with a maximum depth d , the size of the location code array is equal to 8^d integer elements [65]. Therefore, the memory requirement increases rapidly with the depth of roots, for example, a root with seven levels of refinement needs 8 MB of memory (4 bytes per integer). The required memory per processor is lowered by storing this array for only those roots that lie in the portion of the domain assigned to the processor and their neighboring roots, as shown in Fig. 2.8. This is justified because even if a particle moves out of a processor, it is typically not going to travel any further than a neighboring root cell. Note that the location code array information for a root is computed during the AMR procedure by the processor that root was assigned to during the initial 2-D blocking root partitioning. However, after the load balanced partitioning, the portion of the domain that the processor contained can change. Therefore, the processor needs the location code array of roots refined by other processors, which is obtained by a point-to-point communication procedure where each processor has the *Receive* information and the *Send* information is obtained by sorting performed by the master processor. Note, however, that this is not performed every time step, but only after AMR refinement. Furthermore, the maximum depth of a root (8^d integers), which is dictated by the local Knudsen number, can be reduced by creating finer root cells. The root cell size should be such that the maximum depth of roots in the freestream is not more than one. In this way, the

refinement in the shock structure usually does not exceed more than seven.

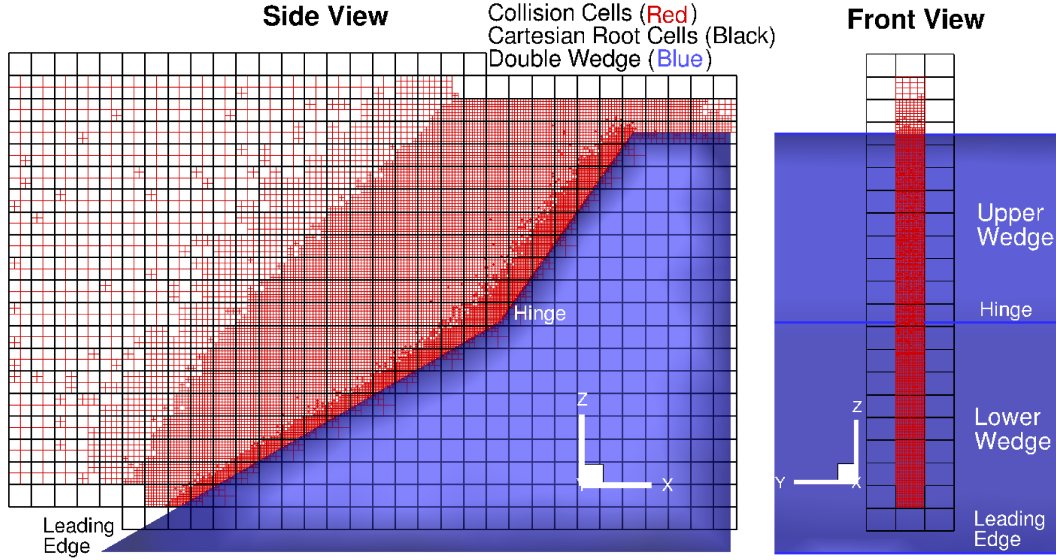


Figure 2.8: Decomposition of the computational domain held by a single of the 32 processors used to run a simulation over a double wedge geometry. Collision and root grids are shown in red and black, respectively. Root grid elements that are blank represent roots held by neighboring processors. The processor needs the location code array data held in both filled and blank roots.

Secondly, to further reduce the memory consumption, only a local part of the collision temperature grid is stored on each processor, which is used to sample collision temperature to compute rotational and vibrational probabilities. The boundary of this local part of sample grid closely coincides with the boundary of the collision cells contained by a processor. However, after load balanced partitioning the local domain boundary of a processor changes, therefore, the corresponding set of sample cells contained by that processor also changes. This means that a processor may contain a new set of sample cells after the partitioning step for which it did not sample the collision temperature. Therefore, prior to partitioning, one of the processors designated as the master processor, gathers the information of collision temperatures computed by the sample cells of every processor. After partitioning, when each processor identifies its new set of sample cells, the master processor scatters or sends the corresponding information of the collision temperature. One important point to note is that sometimes the local sample grid boundaries of two adjacent processors may overlap. This situation arises because the domain decomposition is performed at the leaf level among the processors without heeding the sample cell boundaries. For such shared sample cells, the master processor gathers the collision temperature from the processor that has more collision events.

2.5.2 Double wedge flow and gas-surface results

After implementing all of the aforementioned modifications, the capability of the SUGAR code was demonstrated by simulating the high density, compressible flow of nitrogen over a double wedge configuration [107]. This case was chosen in particular to show that the SUGAR code can overcome the performance challenges typically posed by such cases due to large density gradients in the flow, thus extending the capability of the time-accurate DSMC method to capture thermochemical non-equilibrium and rarefaction effects such as temperature and velocity slip, where the continuum approaches may potentially fail. The geometry of the double wedge has forward and aft angles of 30 and 55 degrees, respectively. The first wedge has a slant length, L , of 50.8 mm, which is considered as the reference length to calculate the free stream Knudsen and Reynolds numbers. In the computations, the symmetry of the flow is taken into consideration, and only half of the wedge in the lateral direction (Y), 50.9 mm wide, was modeled. The flow conditions and the DSMC numerical parameters are given in the third column of Table 2.1. Note that the present work does not consider any chemical reactions as it was shown in earlier work [108] that the number of dissociation events is negligibly small for the Mach 7 flow.

In order to ensure the numerical convergence, the parameters were selected to satisfy the DSMC criteria such that the chosen time step of 4×10^{-9} is smaller than the mean collision time, the ratio of local mean free path to collision cell size is greater than unity throughout the domain except for a small region in the vicinity of the separation zone where it is 0.8, and the number of particles per collision cell in the shock interaction region are four, and more in the rest of the domain. To further test the effects of collision mesh resolution on the surface parameters, another DSMC simulation was run with two times less number of particles, keeping the time step the same, which resulted in 1.26 times less number of collision cells. It was observed that the surface parameters were within 1% by this change thus proving the numerical convergence of the results presented below.

The simulated schlieren of the complex shock structure formed in the symmetry plane on the double wedge at 0.1 ms (25,000th time step) is shown in Fig. 2.9. In order to obtain flow field values with reduced noise, the instantaneously calculated values are time averaged from time step 25,000 to 27,000. A short sampling duration is selected because the flow is still unsteady. It can be seen that an oblique and bow shock are formed at the leading edge of the lower wedge and in front of the upper wedge, respectively. As the flow moves up the lower wedge, an adverse pressure gradient is formed and the boundary layer separates, thus generating a separation shock. These three shocks meet at the triple point and with their interaction a reflected shock, also known as the trailing shock, is formed. As the reflected shock reaches closer to the boundary layer, the compression is nearly isentropic with a continuous transition to subsonic velocities [109]. At the reattachment location of the boundary layer, a succession of compression waves are formed which coalesce into a secondary shock [110]. As the flow passes through the oblique, separation, and the reflected

shocks, the increase in density and temperature results in a reduction in the thickness of the boundary layer [110] downstream of the reattachment location. Strong recirculation is observed in the separation zone embedded between the hinge, separation point, and the reattachment point. Note that the flow downstream of the bow shock is subsonic but the flow going through the oblique, separation, and reattachment shocks remains supersonic. Therefore, a contact surface, also known as the shear layer, is formed across which the pressure is constant, however, the velocities and temperatures differ.

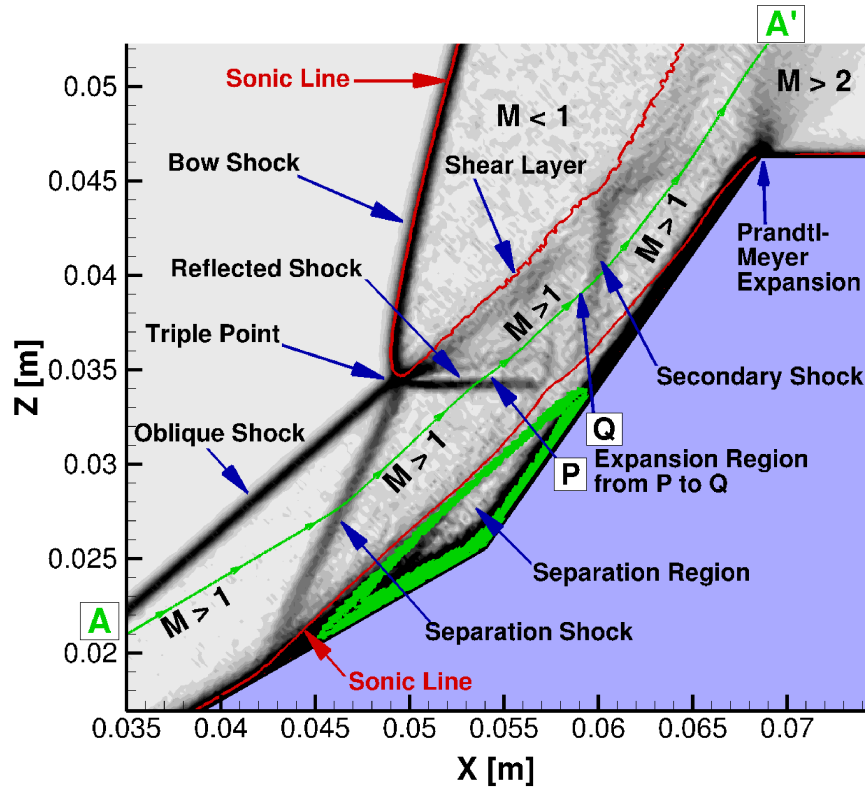


Figure 2.9: SBLI features shown based on gradient density magnitude in the symmetry plane (at $Y=0.06$ m) based on flow field parameters sampled from 0.1 to 0.108 ms (i.e., from the time step 25,000 to 27,000) here and in subsequent figures.

Figures 2.10(a) and 2.10(b) show the Mach number field and the effect of different shocks on selected streamlines. The Mach number of streamline AA' is reduced to 2.2 as it experiences the oblique shock. It further goes through the separation and reflected shocks, which are weaker and have almost equal strength. The region downstream of the reflected shock is supersonic. This pattern is also known as the ' λ -shock pattern', as defined by Déleroy et al. [109]. Downstream of the reflected shock, the flow goes through a very weak expansion and a secondary shock originated from the reattachment point. The Mach number variation along the streamline downstream of the trailing shock can

be analyzed in Fig. 2.10(b), where point P ($X = 0.054$ m) marks the end of the reflected shock. Then, the streamline goes through a weak expansion region up to point Q ($X = 0.059$ m), where it experiences the secondary shock. Note that for this flow, the length of upper wedge is small to notice a series of compression and expansion waves, which are typically observed downstream of the λ -shock pattern. As the streamline approaches to the shoulder of the wedge, it passes through the Prandtl-Meyer expansion. By observing the behavior of streamline BB', it is seen that at the triple point the flow becomes subsonic and then the streamline passes along the sonic line before experiencing expansion. For the streamline, CC', passing through the bow shock, the Mach number decreases from 7 to 0.8 and remains relatively constant through most of the subsonic regime.

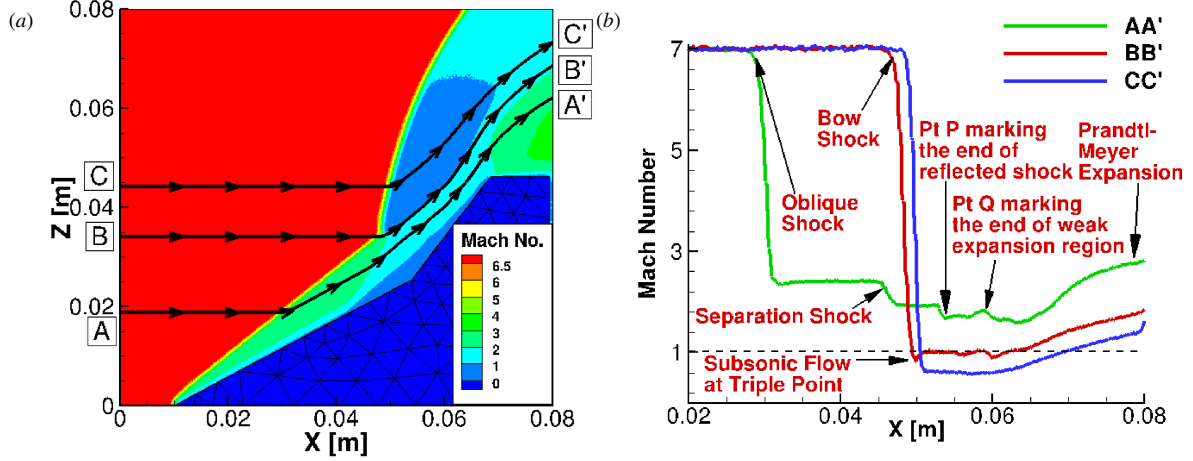


Figure 2.10: Mach number contour field is shown in (a) and Mach number along different streamlines are shown in (b). Note that the streamline A – A' is also shown in Fig. 2.9, where the location of point P and Q is marked.

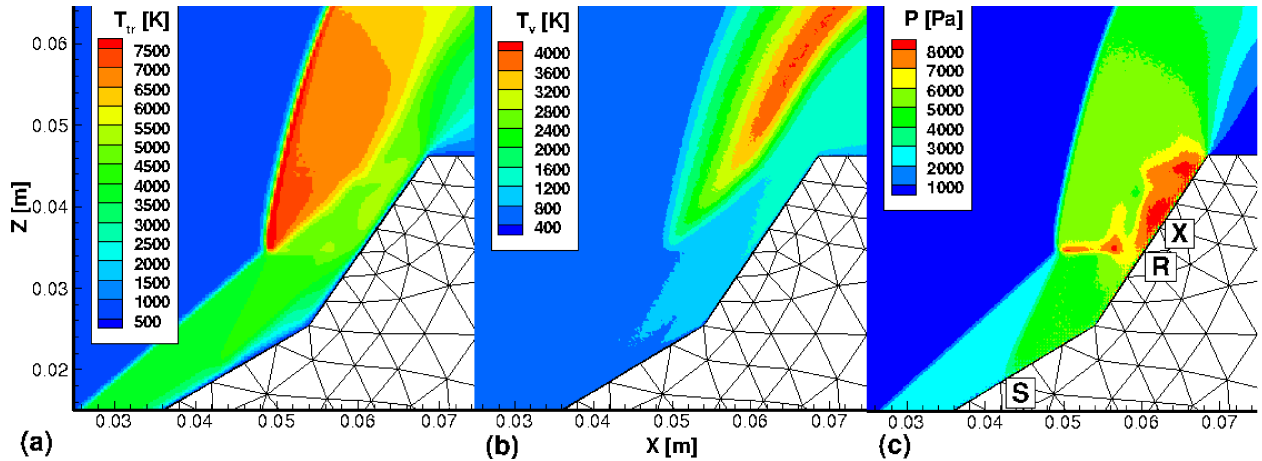


Figure 2.11: Flow field contours in the symmetry plane (at $Y = 0.06$ m). Figures show (a) translational temperature, T_{tr} , (b) vibrational temperature, T_v , and (c) pressure, P .

Figure 2.11 shows the flow translational and vibrational temperatures and pressure fields in the symmetry plane. With respect to temperatures, it can be seen that the vibrational temperature is much lower than the translational temperature, indicating non-equilibrium. Note that the rotational temperature (not shown) is essentially equilibrated to the translational temperature. The pressure contour shows that an adverse pressure gradient is formed on the lower wedge after the separation location ‘S’ and downstream of the reattachment point ‘R’, at location ‘X’, it reaches its peak value (also seen in Fig. 2.12(b)). Also, the pressure remains the same across the shear layer.

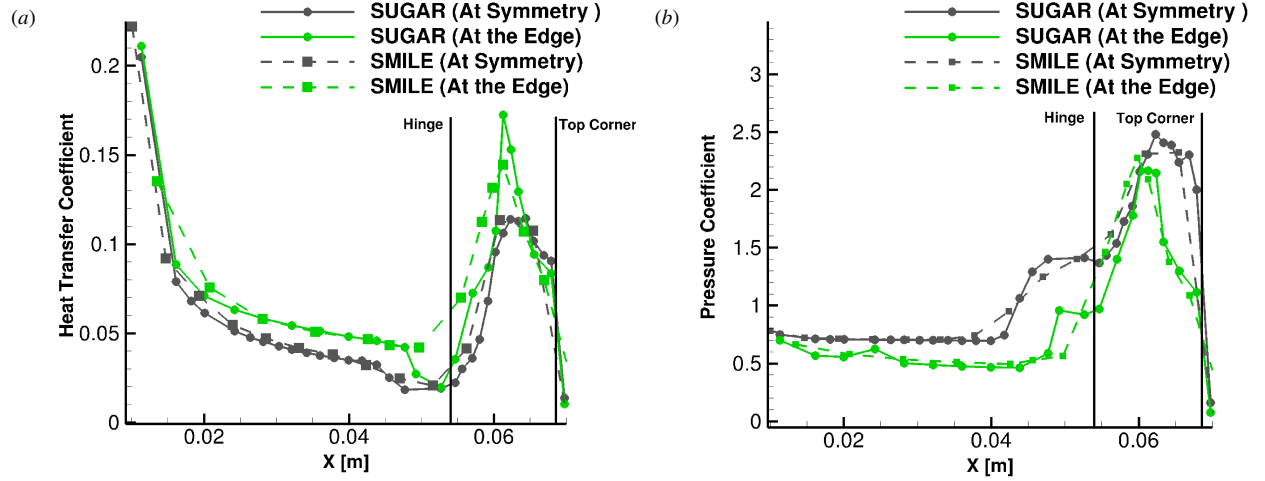


Figure 2.12: Comparison of SUGAR with SMILE for predictions of (a) heat flux coefficient and (b) pressure coefficient along the surface.

Since surface measurements are an important diagnostic of these complex flows, DSMC predictions are crucial. Figures 2.12(a) and 2.12(b) show close agreement of the heat flux and pressure coefficient predicted by SUGAR and SMILE along the surface in the symmetry plane. The heat flux coefficient decreases smoothly from the leading edge along the lower wedge and downstream of the separation point ($X=0.0478$ m) it reaches its minimum value. It then, increases rapidly and peaks after the shock impingement point on the upper wedge, *i.e.*, location ‘X’ shown on the pressure contour in Fig. 2.11. The heat flux coefficient, along the surface in the plane passing through end of the span ($Y=0.0094$ m), matches well with the SMILE prediction on the lower wedge, however, the SMILE result does not capture the decrease in the heat flux in the separation region because of the lack of refinement in the surface panels. For the same reason the SMILE peak heat flux coefficient is about 12% lower than SUGAR, at $X=0.0614$ m. Note that the heat flux at the end of the span is more than that in the symmetry plane because the temperature slip leads to a larger temperature difference between the surface and the gas. The pressure coefficient starts increasing after the separation point and attains a peak value downstream of the shock impingement point, where the boundary layer thickness is reduced. In the plane passing through the end of the span, the SUGAR code captures the increase in the

pressure coefficient in the separation region better than SMILE. The pressure coefficient along the surface is highest on the symmetry plane as compared to the end of the span.

Furthermore, the SUGAR code has the capability to compute velocity and temperature slip along the surface panels of a 3-D geometry, as shown in Fig. 2.13. Figure 2.13(a) shows that the streamwise velocity slip, V_{st} , along the lower wedge is larger in magnitude by about 24 m.s^{-1} in the plane passing through the end of the span ($Y=0.0094 \text{ m}$) as compared to the symmetry plane. The negative slip region indicates the size of the separation bubble, which is shown along the entire half span in Fig. 2.13(b). It is seen that the separation is delayed along the span towards the edge of the wedge due to the increase in velocity slip and temperature jump as a result of the pressure relief effect. The size of the separation bubble may be calculated as the difference of the reattachment point and the separation start at each X-location, which can be seen to decrease by 60% at the edge compared to the symmetry plane. The comparison of V_{st} in the symmetry plane with SMILE 2-D reveals the 3-D effects on the upper wedge, where the peak slip value seen in SUGAR downstream of the shock impingement point ($X=0.064 \text{ m}$) is absent in SMILE 2-D. However, the size and the location of the separation bubble in SMILE 2-D is close to that observed from SUGAR at 0.1 ms. On the lower wedge, the tangential slip, V_{st} , predicted by the two codes, agrees within 10% except at the leading edge, where the difference may also be attributed to the differences in panel size. The lateral slip, V_{sl} , is observed in Fig. 2.13(a) to be small and nearly uniform for the plane passing through the end of the span. A separate examination of V_{sl} along the span (not shown) was only found to be non-zero within about 5.5% of the span length from the edge ($Y = 0.0094 \text{ m}$). With respect to the temperature jump, Fig. 2.13(c) shows that the two codes are in agreement within 3% on the lower wedge, however, the peak value downstream of the shock impingement point ($X=0.058 \text{ m}$) appears to be shifted towards the hinge in SMILE 2-D, a difference that seems to arise from the lack of 3-D effects in a 2-D simulation. The average temperature jump along the surface does not change along the span except within a small portion near the end of the span, where it is about 18% higher on the lower wedge and 14% higher downstream of the shock impingement point.

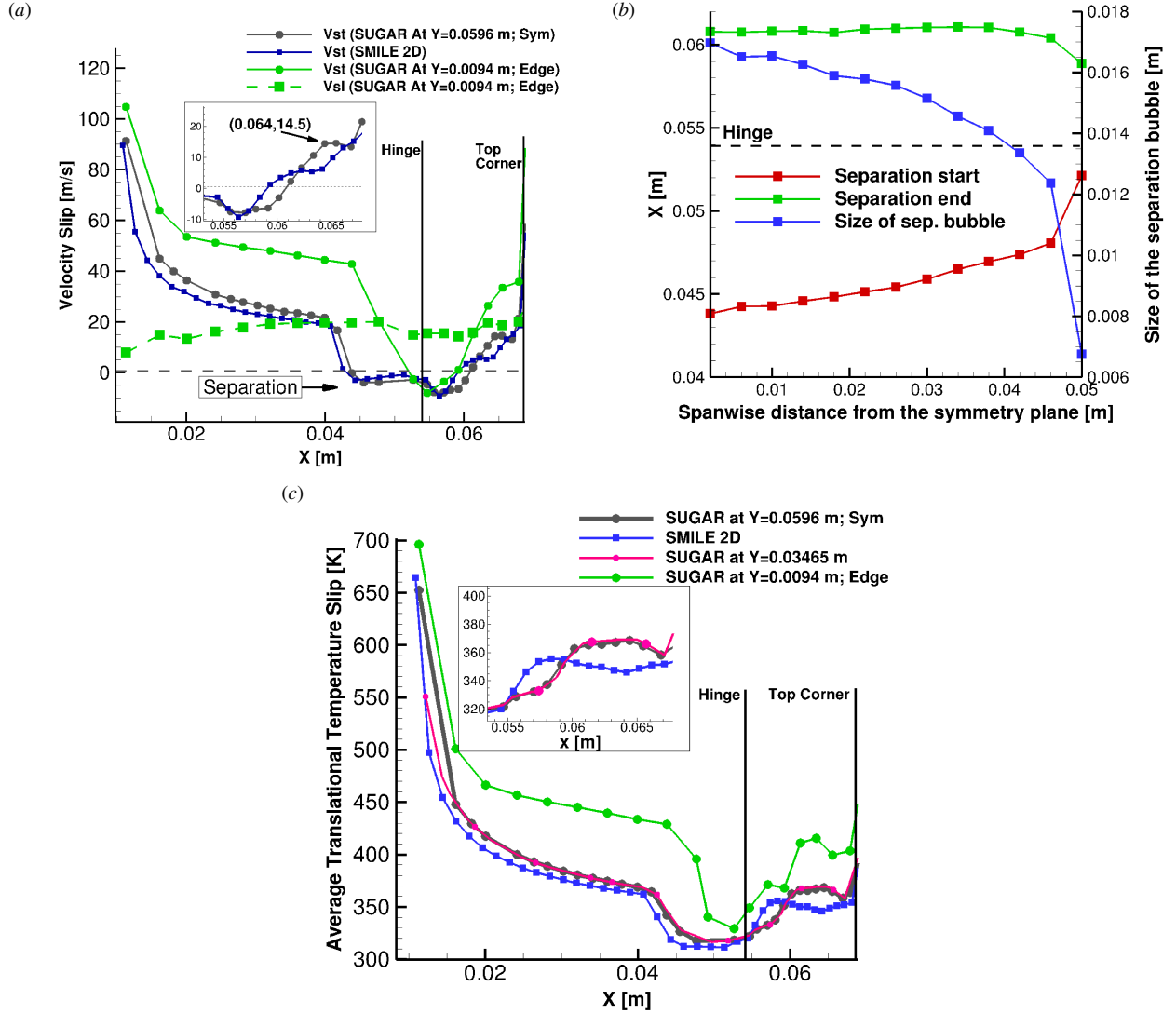


Figure 2.13: Three dimensional aspects of surface slip. Figures show (a) velocity slip, V_{st} and V_{sl} , (b) the size of the separation bubble along the span, and (c) the average temperature slip.

In order to understand the unsteady behavior of the flow, the case was run for 0.4 ms to determine if it had reached steady state. Figure 2.14 shows the percentage difference in the translational and vibrational temperatures, T_{tr} and T_v , respectively, from 0.1 to 0.4 ms at an interval of 0.1 ms. This time interval was chosen in order to observe the potential formation of KH instabilities, which can vary between 10 to 25 KHz [111] for supersonic flows, corresponding to a period of oscillation of 0.04 to 0.1 ms, respectively. The difference for flow quantity $Q = T_{tr}$ or T_v is computed as $[Q(x, z, t_2) - Q(x, z, t_1)]100/\{[Q(x, z, t_2) + Q(x, z, t_1)]/2\}$. Note that each data set at a specific time instant is taken by sampling the results for 0.008 ms (2000 time steps) further. It is seen from Fig. 2.14(a), 2.14(c), and 2.14(e) that the changes in the vicinity of the shear layer are negligible in comparison to those near the separation shock, triple point,

bow shock, and reattachment. As the flow is still developing and the slant length of the upper wedge is small, this may prevent the formation of a well-developed KH instability. The time variation for the rotational temperature (not shown) was observed to be similar to the translational temperature due to the relatively high relaxation rates between those modes. In contrast, the time variation for vibrational temperature is mainly observed after the bow shock, where the vibrational mode is particularly active, as seen from Fig. 2.14(b), 2.14(d), and 2.14(f). However, the difference is negligible for most of the domain for a time interval between 0.3 to 0.4 ms, except for a region in the vicinity of the shear layer, where it is about 20%. In addition, the degree of unsteadiness is much lower for a plane close to the edge of the double wedge ($Y=0.098$ m) as compared to the symmetry plane due to pressure relief effects, as shown in the inserts in Figs. 2.14(e) and 2.14(f). These unsteady flow characteristics will be explored in Chapter 3.

Finally, to compare the performance of the SUGAR code with the three dimensional version of SMILE, the double wedge simulation after 0.1 ms was continued on Intel Xeon E5-2699v3 Haswell processors. For this hardware, SMILE required 1.09×10^{-3} s per time step [69] using 6400 processors, whereas SUGAR only took 8.5×10^{-5} s per time step using 20,000 processors. The scalability of SMILE beyond 6400 processors is not known, but comparing the performance of SMILE with the projected time of SUGAR on 6400 processors, SUGAR was found to be 4× faster.

2.6 Summary

An efficient, new DSMC framework based on AMR/octree unstructured grids has been demonstrated for the modeling of near-continuum, strong shocks in hypersonic flows. The SUGAR code is able to capture the different length scales in such flows through the use of a linearized representation of the unstructured grid using Morton-Z space filling curve for efficient access of collision cells or leaves. This problem is challenging for DSMC solvers using unstructured grids because the high gradients of macroparameters in the shock layer create unbalanced trees. Comparison with a two-level Cartesian grid DSMC solver, on a single processor, showed that for an unstructured approach to be competitive, particle mapping must be performed on a linearized octree structure and close attention must be paid to the particle data structure. It was shown that the use of a linked-list based approach, although responsive to the dynamic variation of particle number densities throughout the simulation domain, can lead to large time penalties when accessing memory cache. If these two general factors are considered, the AMR/octree approach is competitive timewise with multi-level Cartesian grid or patch approaches and offers much more flexibility for flows with embedded geometries and flows that have both compression and expansion regions.

With a competitive single processor version of the code, strategies were developed to achieve a strong scaling of nearly ideal speed-up on 4096 processors and 87% efficiency (weak scaling) for 8192 processors for a strong shock

created by flow over a hemisphere. Rigorous thermal nonequilibrium required for modeling high Mach number shocks was achieved through the accurate modeling of collision temperatures on a sampling grid designed to be compatible with the Morton-Z space filling curve usage of leaf cells and the implementation of an accurate cut-cell algorithm to compute correct fluid volumes for computational cells that intersect the geometry, all across multiple processors. The accuracy of the collision temperature is important because it is used to calculate the rotational and vibrational relaxation rates which have been implemented using the Larsen-Bornakke model. To achieve these very good scalings, algorithms were developed to weight the computational work of a processor by the use of profiled run time data, create maps to optimize processor point-to-point communications, and efficiently generate new DSMC particles every time step.

An important goal of our code development was to enable DSMC simulations in the continuum regime. Our approach was demonstrated in the modeling of the SBLIs in a hypersonic flow at Mach 7, unit Reynolds number $Re = 5.2 \times 10^4 \text{ m}^{-1}$, and Knudsen number $Kn = 3.4 \times 10^{-3}$ over a double wedge configuration having a finite half-span of 50.8 mm. Because the three-dimensional simulations required approximately two orders of magnitude more particles than the hemisphere case and the simulation needed to be run on 20,000 processors, additional consideration of the size of the root cells, the level of depth, as well as, the construction of the local collision temperature grid were implemented. The simulation reproduced the complex hypersonic SBLIs as well as the three-dimensional values of non-continuum effects such as velocity and temperature slip. The simulations showed that three-dimensional effects are important in predicting the size of the separation bubble, which in turn, influences gas-surface measurements such as pressure and heat flux. The simulations were run for a time period of 0.4 ms and found to be unsteady. The simulation was not continued further because it was deemed necessary to understand the reason for unsteadiness by eliminating the effect of spanwise-acceleration of the flow induced by pressure relief, *i.e.* in a spanwise-periodic domain, which is the topic of Chapter 3.

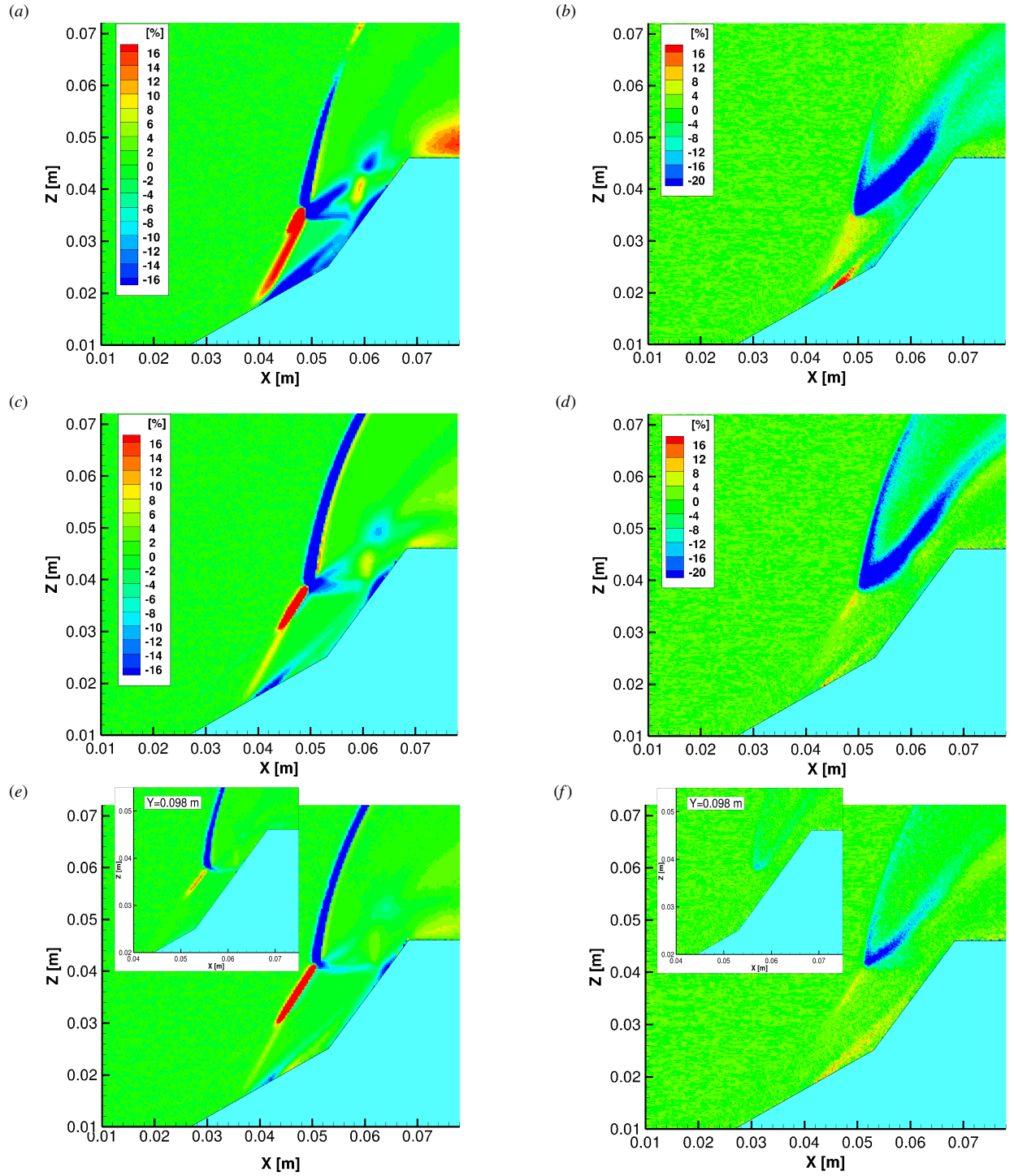


Figure 2.14: Percentage differences in the symmetry plane of temperatures T_{tr} and T_v are respectively shown in (a) and (b) for $t_1 = 0.1$ and $t_2 = 0.2$ ms, in (c) and (d) for $t_1 = 0.2$ to $t_2 = 0.3$ ms, and in (e) and (f) for $t_1 = 0.3$ to $t_2 = 0.4$ ms. Figures 2.14(e) and 2.14(f) have the same legends as Figs. 2.14(c) and 2.14(d), respectively, and the inserts show the differences in the plane at $Y = 0.098$ m, *i.e.* near the side edge of the double wedge.

Chapter 3

Three-Dimensional Shock/Laminar Separation Bubble Instabilities in Hypersonic Flows

In this chapter, linear three-dimensional instability is analyzed in the shock layer and the laminar separation bubble induced by shock-wave/boundary-layer interactions in a Mach 7 flow of nitrogen over a double wedge with a $30^\circ - 55^\circ$ cross-sectional profile. At a freestream unit Reynolds number $Re = 5.2 \times 10^4 \text{ m}^{-1}$ this flow exhibits rarefaction effects and has shock-thicknesses comparable to the thickness of the boundary layer at separation. Flow features have been fully resolved using a high-fidelity massively parallel implementation of the Direct Simulation Monte Carlo method that captures the flow evolution from the inception of three-dimensionality, through linear growth of instabilities, to the early stages of nonlinear saturation.

It is shown that the laminar separation bubble sustains self-excited, small-amplitude perturbations that originate past the primary separation line and lead to spanwise-periodic wall striations inside the bubble and downstream of the primary reattachment line, as known from earlier experiments, simulations and instability analyses. A spanwise-periodic instability, synchronized with that in the separation zone, is identified herein for the first time, which exists in the internal structure of the separation and detached shock layers, and manifests itself as spanwise-periodic cats-eyes patterns in the amplitude functions of all linear flow perturbations. The growth rate and the spanwise-periodicity length of linear disturbances in the shock layers and laminar separation bubble are found to be identical. Linear amplification of the most unstable three-dimensional flow perturbations leads to synchronized low-frequency unsteadiness of the triple point formed at the intersection of separation and detached shock layers and the separation bubble, with Strouhal number of $St \approx 0.028$.

Nomenclature

Roman symbols

C_h	heat transfer coefficient	N_c	number of sampling cells in the entire domain (number of rows of $\mathcal{D}$)
C_p	pressure coefficient	n	number density (m^{-3})
c_r	molecular relative speed (m.s^{-1})	N_r	user-defined rank of the reduced SVD approximation to the input data matrix $\mathcal{D}$ in the POD analysis
d_{ref}	molecular diameter of species at reference temperature of 273 K (m)	N_{r2}	user-defined number of ranks lower than N_r for reconstructing reduced-order data matrix $\mathcal{D}_2$ in the POD analysis
E_i	modal energy of the i^{th} mode in the POD analysis	N_s	number of instantaneous snapshots used for the POD analysis (number of columns of $\mathcal{D}$)
F_n	Number of gas molecules particles represented by a DSMC computational particle	P_{coll}	collision probability in DSMC
f	frequency (Hz)	p	pressure (Pa)
H	wall-normal height (m)	R	specific gas constant ($\text{J.kg}^{-1}.\text{K}^{-1}$)
Kn	Knudsen number	Re	unit Reynolds number (m^{-1})
L_s	length of the separation bubble (m)	S_i	i^{th} singular value in the POD analysis
L_x, L_y, L_z	simulation domain length in Cartesian directions (m)	St	Strouhal number
Ma	Mach number	T	nondimensional flow time defined as the time it takes for the flow to traverse the distance equal
m	mass of species (kg)		
N	number of particles		

	to the length of the separation bubble in the base flow, $L_s=40$ mm, at a freestream velocity of $u_{x,1}$	$\mathcal{T}$	matrix of temporal modes in the POD analysis
Greek symbols			
T^*	a parameter in Parker's model for computing rotational relaxation number	α	scaled angle
T_{rot}	rotational temperature (K)	$\beta = 2\pi/L_y$	wavenumber in the spanwise direction
T_s	surface temperature (K)	Δt	simulation timestep (s)
T_{tr}	average translational temperature (K)	Δx	local cell size (m)
T_{vib}	vibrational temperature (K)	δt	a small period of time (s)
t	time (s)	θ	vibrational characteristic temperature (K)
u_n	local wall-normal component of bulk velocity (m.s ⁻¹)	λ	mean-free-path based on variable hard sphere molecular model (m)
u_t	local-streamwise (wall-tangential) component of bulk velocity (m.s ⁻¹)	σ_T	total collision cross section (m ²)
$\mathbf{u} = [u_x, u_y, u_z]^T$	bulk velocity vector (m.s ⁻¹)	σ_u	standard deviation in bulk velocity u (m.s ⁻¹)
V_s	surface velocity slip	τ_{coll}	mean-collision time (s)
X, Y, Z	Cartesian coordinates of streamwise, spanwise, and streamwise-normal directions (m)	ϕ	matrix of spatial modes of size $N_c \times N_r$ in the POD analysis
$Z_{r,\infty}$	a parameter in Parker's model for computing rotational relaxation number	$\Omega = \Omega_i + i\Omega_r$	eigenvalue in linear stability analysis
Special symbols			
$\mathcal{D}$	input data matrix of size $N_c \times N_s$ in the POD analysis	Ω_i	growth or decay rate (Hz)
$\mathcal{D}_2$	reduced-order, noise-filtered reconstructed data matrix from the POD analysis	Ω_r	frequency (Hz)
$\mathcal{S}$	square diagonal matrix of singular values in the POD analysis	ω	viscosity index of a gas in Variable Hard Sphere model
		$[\omega_x, \omega_y, \omega_z]^T$	vorticity vector along the Cartesian directions
Operators			
		$\bar{Q}(x, z)$	2-D flow or transport quantity in a base flow
		$\langle Q \rangle_s$	spanwise averaged flow quantity Q

$\tilde{Q}(x, y, z, t)$	3-D small amplitude perturbation of a flow quantity Q	1	upstream value
$\hat{Q}(x)$	2-D amplitude function of flow quantity Q	2	downstream value
∇Q	gradient of quantity Q	l	with respect to the lower or first wedge
Subscripts		u	with respect to the upper or second wedge

3.1 Introduction and Overview

Linear instability in the laminar separation bubble generated by shock-wave / laminar boundary layer interaction at supersonic and hypersonic speeds has been the subject of intense experimental and, more recently, theoretical/numerical investigations, owing to the ubiquitous nature of this phenomenon and its potential impact on the design of high-speed vehicles. The appearance of regularly-spaced streamwise-aligned vortices, a.k.a. *striations*, in the reattachment region of nominally two-dimensional supersonic and hypersonic flow over a planar compression corner has been first reported over half a century ago by Ginoux [41], who went on to relate the vortex spacing with the attached boundary layer thickness ahead of the corner and document the quantitative effect that Mach number has on the appearance and spacing of the vortices [112–115]. To-date, the interaction of the three-dimensional shock-wave system associated with the compression corner, also first reported experimentally at around the same time by Holden [13], has not been associated with the process of formation of the striations and motivates the present contribution. However, before turning our attention to the description of oscillations and spanwise modulation in the shock layers, and their association with three-dimensional global instability in the laminar separation bubble (LSB), a brief exposition of current understanding of the physical origins of the streamwise vortices in the compression corner is warranted, in order to set the scene for the present analysis.

Striations in a compression corner generated a long-standing debate regarding the origins of this phenomenon being attributed to (imperfections at) the leading edge of the flat plate preceding the corner [15, 116] and entering the separation region [117] or an intrinsic flow instability mechanism associated with self-excitation of the LSB formed at the corner itself. In recent years evidence has been amassed in support of the latter mechanism: fully-resolved three-dimensional direct numerical simulations by Shvedchenko [43] and Egorov *et al.* [44] over a wide range of Mach numbers demonstrated exponential growth of small-amplitude perturbations, the latter taking the form of spanwise-periodic modulation of the wall-shear and wall heat transfer footprints of the flow; such striations were found to originate inside the LSB formed at the compression corner and extend beyond the primary reattachment line on the ramp wall. Amplification of the spanwise-periodic perturbations was documented beyond a certain value of the corner angle, scaled according to triple-deck theory [118–121]. More recently, global linear instability analyses have unequivocally demonstrated the existence and linear amplification of stationary three-dimensional self-excited perturbations originating inside LSBs formed on account of shock impingement on a laminar boundary layer [45, 122] or that forming in the steady laminar nominally two-dimensional compression ramp flow [46, 47, 123].

In the authors' view the debate regarding the origins of striations need not lead to the search of mutually exclusive instability paths. Fundamental studies of linear global instability of steady LSBs in the incompressible limit have demonstrated that bubbles can act as *amplifiers* which promote exponential growth of incoming disturbances, but

can also become self-excited due to exponential amplification of intrinsic stationary three-dimensional global modes through an *oscillator* instability mechanism [124–126]. Compressibility may alter the relative significance of the two scenarios quantitatively, but not qualitatively. In this context, the interpretation of the experiments of Simeonides [116] and the DNS work of Navarro-Martinez and Tutty [117] would fall in the first category of a bubble acting as an amplifier, while the DNS of Shvedchenko [43] and Egorov *et al.* [44], the global instability analysis of Dwivedi *et al.* [46] as well as the combined analysis and experiments of Dwivedi *et al.* [42] and Hao *et al.* [123] on the compression corner and the global instability analyses of Robinet [45], Nichols *et al.* [122] and Hilderbrand *et al.* [127] in the related problem of shock-generated laminar separation on a flat plate would be examples of the oscillator scenario.

The present contribution is concerned with the relatively unexplored question of the dynamic behavior of the shock layer which drives the interaction with the boundary layer and the subsequent appearance of striations downstream of the primary separation line. Shock unsteadiness and the resulting small-amplitude harmonic spatial corrugations on the shock, generated as a result of flow instability, were first discussed in isolation from the boundary layer by Carrier [58], who addressed the inviscid flow limit and employed linearised Euler equations and Rankine-Hugoniot conditions to study shock interaction with acoustic perturbations. Moore [59] and Ribner [60] also monitored an isolated straight shock wave and used inviscid equations to analyse pressure and vorticity waves interacting with the shock, while McKenzie and Westphal [61] quantified, in terms of the freestream flow Mach number and the shock angle, the amplitude of acoustic perturbations emitted as a consequence of pressure, vorticity, or entropy perturbations transversing a plane stationary isolated shock. Duck and Balakumar [1] introduced viscosity in their study of self-excitation of a finite-thickness steady normal shock, the latter computed by imposing constant upstream and Rankine-Hugoniot downstream conditions in the framework of the base flow computation methodology proposed by Gilbarg and Paolucci [7]. Their modal analysis revealed that the eigenspectrum only contains (several) branches of damped continuous modes, while their solution of the initial-value problem did not yield reliable large-time response of the shock to incoming perturbations, due to the relatively rich structure of the continuous spectrum. Chang *et al.* [128], Esfahanian [129] and Malik and Anderson [130] solved the linear stability eigenvalue problem in the compressible (attached) flat-plate boundary layer [49] including far-field boundary conditions based on the Rankine-Hugoniot equations, to analyse the effect of a shock that is locally parallel at a finite distance to the flat plate. Stuckert and Reed [131] solved the same problem on a cone at very high Mach number, including chemistry effects. Triple-deck theory [118, 121, 132] has been employed to understand separated laminar boundary layer instability in supersonic and hypersonic flows over compression ramps at moderate to high Reynolds numbers [133–138] however instability of the shock layer, or its coupling with instability in the boundary layer, are beyond the scope of this theory.

On the other hand, it is long known that predictions of the shock structure based on the Navier-Stokes equations

increasingly deviate from those delivered by kinetic theory as the degree of rarefaction increases in critical zones such as the internal structure of the shock layer [62,63] and the Knudsen-layer in the vicinity of a solid surface. Liepmann *et al.* [62] computed shock profiles using the Bhatnagar-Gross-Krook model of the Boltzmann equation and documented the systematic departure from Navier-Stokes predictions in the low-pressure region of the shock layer, i.e. up to the location of maximum stress, as the freestream Mach number increases. It then follows that, if the internal structure of the shock is to be resolved, rather than modeled, a numerical approach based on kinetic theory must be used.

Such an effort has been reported by Tumuklu *et al.* [22, 23], who performed Direct Simulation Monte Carlo (DSMC) simulations of Mach 16 nitrogen flow over an axisymmetric double cone configuration at unit Reynolds numbers $Re = 0.935 - 3.74 \times 10^5 \text{ m}^{-1}$ and, within the limitations of a two-dimensional simulation, demonstrated a strong coupling between oscillations of the triple-point and instability of the laminar separated flow region. The amplitude functions of the least-damped global mode computed in these works comprised structures inside the LSB as well as at the shock system, and included the multiple reflections leading to the lambda-shocklet system between the wall and the slip line downstream of the reattachment point; these features of the global mode became increasingly evident as the Reynolds number at which simulations were performed was increased. In the axisymmetric limit addressed, a steady state was reached after this least-damped global mode decayed linearly, at a constant rate quantified by processing the DSMC signal. More recently, Klothakis *et al.* [139] carried out DSMC simulations in which the temporal and spatial development of harmonic perturbations introduced in a hypersonic flat-plate boundary layer were quantified, before applying linear stability analysis to document the synchronization of oscillatory perturbations propagating along the leading-edge shock layer with damped perturbations introduced through a wall orifice into the boundary layer.

The present work addresses the three-dimensional analog of the configuration studied by Tumuklu *et al.* [30], in which the cross-section of the double-wedge is extruded along the third spatial direction. Three-dimensional DSMC simulations are performed to study linear instability of the interaction between the shock and the three-dimensional LSB formed in a Mach 7 nitrogen flow over a 30° - 55° double wedge configuration. Flow conditions are oriented to those of the experiments performed by Swantek and Austin [20] and Knisely and Austin [140] at 8 MJ enthalpy. However, in the present simulations the number density is kept eight times lower than that in the experiments (here $Re = 5.2 \times 10^4 \text{ m}^{-1}$), to ensure that all DSMC numerical requirements are met. The kinetic simulation results are analysed to extract characteristics of the small-amplitude three-dimensional perturbations that emerge from numerical noise and are organized into coherent structures both inside the LSB as well as in the separation- and detached shock layers. Using resources at the limit of present-day massively parallel computing capabilities it has been possible to fully resolve the (comparable in thickness) internal structure of the shock layer and the boundary layer in the separation

region and document, for the first time, the genesis, spatial structure and temporal evolution of small-amplitude shock layer perturbations and their relation to global instability in the laminar separation zone.

The chapter is organized as follows: Sec. 6.2.1 describes the DSMC algorithm, the specific numerical approach, required numerical parameters, and collision models. Details on the initialization of the three-dimensional simulations are provided in Sec. 3.2.1, while the features of the two-dimensional base flow, recomputed here for consistency, as well as surface rarefaction effects, are discussed in Sec. 3.2.2. Results are presented in Sec. 3.3, starting with quantification of the extraction of linear analysis quantities from the DSMC signal in Sec. 3.3.1. In Section 3.3.2 the presence and synchronous amplification of a stationary three-dimensional global mode in the LSB and the shock layer is documented, with emphasis placed in 3.3.3 on the discussion of spanwise-periodic sinusoidal structures arising from global instability inside the internal structure of the shock layer. Section 3.3.4 reports the emergence of low-frequency unsteadiness in the shock/LSB system as a consequence of the nonlinear saturation of the amplified global mode. A short discussion summarising the main findings is offered in Sec. 6.5.

3.2 Flow Modeling Methodology

The particle-based DSMC method using the computational framework of the SUGAR solver [39], described in Chapter 2, is employed to fully resolve the three-dimensional unsteady hypersonic flowfield in question. The satisfaction of the numerical criteria in the flow over the three-dimensional double wedge depends on the free stream conditions, given in table 3.1. Table 3.2 provides a summary of the key numerical parameters for these simulations which were found to require ~60 billion computational particles and ~4.5 billion collision cells of the adaptively refined *C*-mesh octree grid. Here, the Knudsen number is based on the length of the lower wedge, 50.8 mm, F_n denotes the number of actual gas molecules represented by a computational particle, while the wall surface is fully accommodated [37], i.e., isothermal. Section 3.5.1 and the appendix of Ref. [31] describes the DSMC numerical criteria and convergence study for flows presented here.

In terms of collision models, the majorant frequency scheme (MFS) of Ivanov and Rogasinsky [98] derived using the Kac stochastic model for the selection of collision pairs and the variable hard sphere (VHS) model for elastic collisions are used. Appendix 3.5.2 describes an improved strategy for the computations of maximum collision cross-section used in the MFS scheme for accurate spectral analysis of unsteady flows simulated on adaptively refined grids. For rotational relaxation, the Borgnakke and Larsen [102] model is employed with rates of Parker [104] and DSMC correction factors [103, 141] that account for the temperature dependence of the rotational probability. For vibrational relaxation, the semi-empirical expression of Millikan and White [105] is used with the high-temperature correction of

Park [106].

3.2.1 Initialization of three-dimensional flow

The three-dimensional flow studied in this work is initialised using the two-dimensional steady-state solution over a double wedge simulated by Tumuklu *et al.* [30]. The latter flow is recalculated here and then replicated on every octree cell along the spanwise direction (Y) to form the three-dimensional field at the beginning of the unsteady simulation. Note that the Cartesian coordinates of streamwise, spanwise, streamwise-normal directions are designated as X , Y , and Z , respectively. From the inlet boundary at $X = 0$, an inward-directed local Maxwellian flow is introduced at an average number density, bulk velocity, and temperature of n_1 , $u_{x,1}$, and $T_{tr,1}$, respectively. For this work, the SUGAR solver is employed with spanwise-periodic boundary condition in the Y -direction, as described in Appendix 3.5.2. The spanwise extent of the current simulation is $L_y = 28.8$ mm, which will be shown to be sufficiently wide to capture linearly growing spanwise-periodic flow structures. In subsequent sections, contours and isocontours showing the detailed spanwise-periodic structures are presented with two periodic wavelengths for clarity.

Mach number, Ma [-]	7.02
Unit Reynolds number, Re [m^{-1}]	5.22×10^4
Knudsen number, Kn [-]	3.2×10^{-3}
Number density, n_1 [m^3]	10^{22}
Streamwise velocity, $u_{x,1}$ [$m.s^{-1}$]	3812
Equilibrium translational temperature, $T_{tr,1}$ [K]	710
Surface temperature, T_s [K]	298.5
Species mass, m [kg]	4.65×10^{-26}
Species diameter at reference temperature of 273 K, d_{ref} [m]	4.17×10^{-10}
Viscosity index, ω [-]	0.745
Parker model parameters, $Z_{r,\infty}$ and T^* [K]	18.5 and 91
Vibrational characteristic temperature, θ [K]	3371

Table 3.1: Physical gas parameters

In terms of the computational strategy used, it takes $\sim 50T$ (flow through-time, T , defined in the next section) until the onset of linear instability. To minimize data storage, we estimate this time at which the spanwise-periodic flow structures start to emerge such that they can be easily detected in the background of statistical fluctuations in

DSMC. We use an equilibrium criterion along the lines of Hadjiconstantinou *et al.* [142] to quantify the amount of spanwise fluctuations about the two-dimensional base state. For example, the standard deviation in the bulk velocity at equilibrium can be calculated as, $\sigma_u = \sqrt{R\langle T_{tr} \rangle_s / \langle N \rangle_s}$, where $\langle T_{tr} \rangle_s$ and $\langle N \rangle_s$ are local spanwise-averaged translational temperature and number of particles, respectively, and R is the gas constant. The linear instability can be easily detected, when the DSMC-computed standard deviation is larger than the above criterion.

Domain size, (L_x, L_y, L_z) [mm]	(80, 28.8, 80)
Number of octree and sampling cells along X, Y, Z	400, 144, 400
Number of gas-surface interaction cells along X, Y, Z	25, 10, 25
Number of computational particles [-]	$\sim 6 \times 10^{10}$
Number of collision cells [-]	$\sim 4.5 \times 10^9$
F_n [-]	6.1×10^7
Timestep, Δt [ns]	5
Adaptive mesh refinement interval [μs]	5
Relaxation probability computation interval [μs]	1

Table 3.2: Numerical simulation parameters

Finally, to accommodate billions of computational particles and collision cells, 19.2 k MPI processors were used in this simulation. The spanwise-periodic simulation takes ~ 5.5 hours per through-flow time (T) using Intel Xeon Platinum 8280 (“Cascade Lake”) processors of the Frontera supercomputer [143] and ~ 14 hours per flow time using Intel Xeon Platinum 8160 (“Skylake”) processors of the Stampede2 supercomputer [144]. The overall cost of the simulation up to $T=190$ discussed in what follows required ~ 870 k node-hours (~ 43.8 million core-hours) of computing time.

3.2.2 Main features of two-dimensional base flow

Starting with the two-dimensional base flow, Fig. 3.1(a) shows the complex features of an Edney-IV type SBLI system [24, 26]. The base flow results are obtained by spanwise and temporally averaging the DSMC flow fields between $T=48$ to 60, where T is the nondimensional flow time, defined as the time it takes for the flow to traverse the distance $L_s=40$ mm at a freestream velocity of $u_{x,1}$. L_s is defined as the straight-line distance from the separation point, P_s , to the reattachment point, P_R , which mark the origin and end of the shear layer inside the separation bubble, respectively. The SBLI features include the interactions of the separation shock with the leading-edge oblique and detached bow shocks at triple points T_1 and T_2 , respectively. Two contact surfaces, C_1 and C_2 , are formed downstream

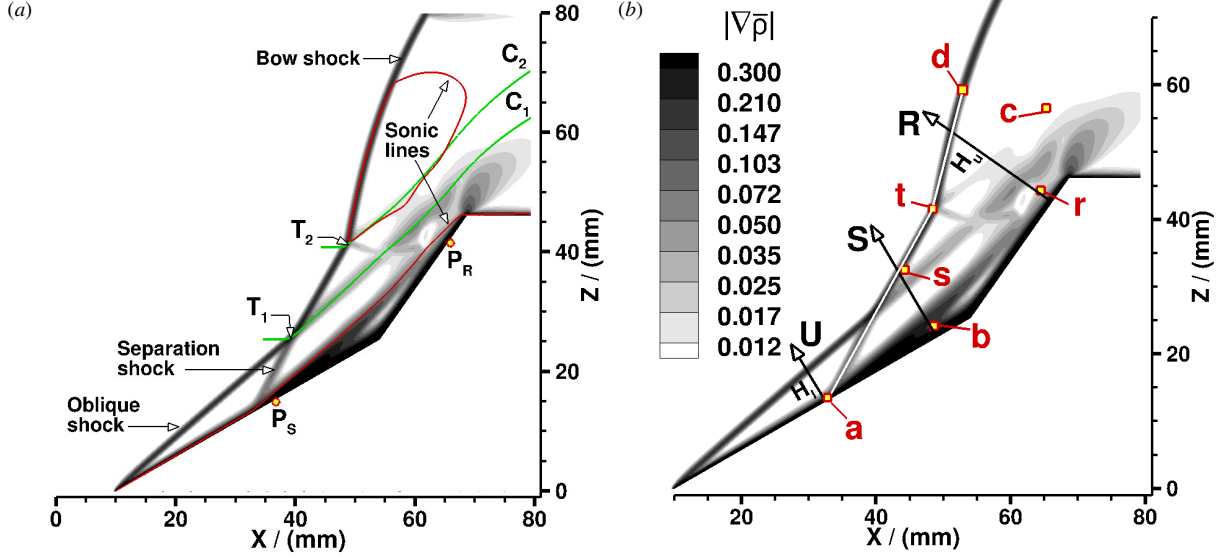


Figure 3.1: (a) Magnitude of mass density gradient of the base flow, $|\nabla \rho|$, normalised by $\rho_1 L_s^{-1}$, where $\rho_1 = n_1 m$ is freestream mass density. (b) Overlaid on the image shown in (a) are the wall-normal directions U , S and R , and the numerical probes a , b , c , d , r , s and t , defined in the text.

of triple points T_1 and T_2 , respectively, where C_1 is between two supersonic streams downstream of the separation shock, and C_2 is between the supersonic and subsonic streams downstream of the separation and detached shocks, respectively. For details about the earlier time evolution of the two-dimensional SBLI features over the double wedge, see Ref. [30].

The image shown in Fig. 3.1(a) is repeated in Fig. 3.1(b), in order to define a number of probes that will aid the discussion of the next sections. Probes are placed at locations a : at the foot of the separation shock, ($X=32.817$ mm, $Z=13.285$ mm), b : inside the LSB, ($X=48.496$ mm, $Z=24.270$ mm), c : at the contact surface, ($X=65.191$ mm, $Z=56.593$ mm), d : on the detached shock, ($X=52.860$ mm, $Z=59.226$ mm), r : at reattachment, ($X=64.396$ mm, $Z=44.358$ mm), s : on the separation shock, ($X=44.165$ mm, $Z=32.597$ mm), and t : at the triple point T_2 , ($X=48.347$ mm, $Z=41.624$ mm). Probes a and d define lines $a-t$ and $t-d$, denoting the intersection with the OXZ plane of two planes passing through the separation and detached shocks, respectively. Wall-normal directions U , S , and R are respectively defined at the foot of the separation shock and either side of the triple-point, T_2 . The vertical projection of the foot of the arrows U , S , and R on the X -axis is at 32.5, 49, and 66.1 mm, respectively. From this point onward, the DSMC-derived instantaneous profiles shown are noise-filtered using the proper orthogonal decomposition (POD) procedure discussed in Appendix 3.5.3.

The use of a particle-based approach permits analysis of surface rarefaction effects; results corresponding to the base flow are shown in Fig. 3.2(a) for the local-streamwise velocity slip, $\bar{V}_s$, normalised by $u_{x,1}$, while the local mean-free-path adjacent to the wall, $\bar{\lambda}$, as well as the translational temperature jump, $\bar{T}_s$, at the surface are presented in 3.2(b), respectively normalised by freestream mean-free-path λ_1 and $T_{tr,1}$.

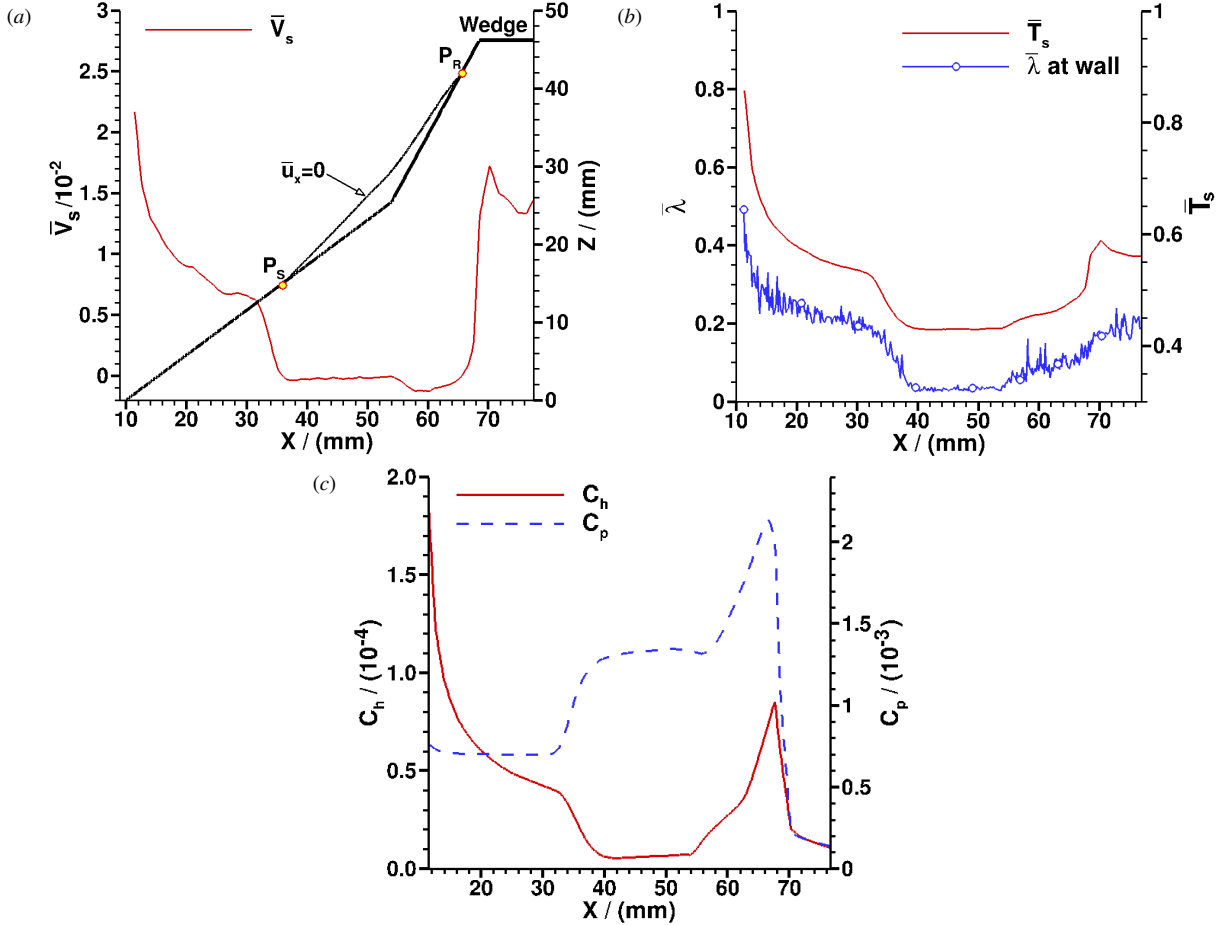


Figure 3.2: Surface macroscopic flow quantities in the base state, where the profiles are time-averaged from $T=48$ to 53. (a) Surface velocity slip in the local streamwise direction, $\bar{V}_s$. (b) $\bar{\lambda}$ adjacent to the wall and temperature jump $\bar{T}_s$. (c) The heat transfer and pressure coefficients, C_h and C_p , respectively.

Figure 3.2(a) shows a maximum $\bar{V}_s$ equal to 2.16% of $u_{x,1}$ at the leading edge ($X=10$ mm), similar to the value of 2.45% obtained by Tumuklu *et al.* [30] in a two-dimensional flow simulation. The large slip at the leading edge is due to the increased rarefaction of gas induced by steep gradients of the leading edge shock. $\bar{V}_s$ decreases along the local streamwise direction to 0.6% at $X=32$ mm, similar to the decrease of $\bar{\lambda}$ adjacent to the wall as seen from Fig. 3.2(b). From $X=32$ to 36 mm in the interaction region of the separation shock with the boundary layer, $\bar{V}_s$ rapidly decreases to zero at the separation point, P_S . Inside the recirculation zone, from P_S to P_R , the point of reattachment, $\bar{V}_s$ is negative

because the flow impinging on the wall is opposite to the local streamwise direction. $\bar{V}_s$ and $\bar{\lambda}$ remain constant on the lower wedge, where the latter is about 3.69% of the freestream mean-free-path, λ_1 . On the upper slant surface, $\bar{V}_s$ and $\bar{\lambda}$ both increase such that the rate of increase is significantly larger downstream of reattachment. $\bar{T}_s$ follows a similar variation as $\bar{V}_s$ and $\bar{\lambda}$, as seen from Fig. 3.2(b). Velocity slip and temperature jump are rarefaction effects that are proportional to the size of the Knudsen layer in the vicinity of the wall [34, 145]. Since the Knudsen layer is approximately of the order of the mean-free-path, which is inversely proportional to number density, n , and directly proportional to the translational temperature, $T_{tr}^{\omega-0.5}$, where $\omega = 0.745$ is the viscosity index of the gas, the profiles of $\bar{V}_s$ and $\bar{T}_s$ are similar to the profile of $\bar{\lambda}$ in the vicinity of the surface, for our assumption of a fully diffuse surface.

The variations in surface heat flux and pressure coefficients, C_h and C_p , respectively, are shown in Fig. 3.2(c). The change in C_h along the local-streamwise direction is similar to $\bar{V}_s$ and $\bar{T}_s$ and C_p is constant on the lower wedge, except for a sharp increase in the vicinity of the separation point from $X=32$ to 38 mm. Inside the recirculation zone on the lower wedge, C_p plateaus, but on the upper wedge it increases rapidly up to the corner of the wedge. It must be noted that although Fig. 3.2(c) shows a small dip in C_p at the hinge equal to 1.36% of the plateau at $X \sim 50$ mm, we do not observe secondary vortices in the separation region. This is consistent with the value of the scaled angle $\alpha \sim 2$ of our simulations, which is much smaller than that required for secondary vortices to emerge ($4 \leq \alpha \leq 5$) [43]. The scaled angle is calculated based on the definition used by Gaitonde [146] (Eq. (1.1)), which was originally defined by Stewartson [147] and Rizzetta *et al.* [120].

3.3 Three-Dimensional Linear Instability Mechanisms

3.3.1 Analysis of the three-dimensional DSMC signal

During the early time of the simulation, when deviations from the imposed steady state are still small in magnitude, perturbations $\tilde{Q}$ of an unsteady macroscopic flow quantity $Q = (n, u_x, u_y, u_z, T_{tr}, T_{rot}, T_{vib})^T$ may be obtained by subtracting from the unsteady three-dimensional full DSMC field the steady, two-dimensional base flow state $\bar{Q} = (\bar{n}, \bar{u}_x, 0, \bar{u}_z, \bar{T}_{tr}, \bar{T}_{rot}, \bar{T}_{vib})^T$ computed in Sec. 3.2.1 and imposed as initial condition in the simulation,

$$\tilde{Q}(x, y, z, t) = Q(x, y, z, t) - \bar{Q}(x, z). \quad (3.1)$$

In the disturbance field vector $\tilde{Q} = (\tilde{n}, \tilde{u}_x, \tilde{u}_y, \tilde{u}_z, \tilde{T}_{tr}, \tilde{T}_{rot}, \tilde{T}_{vib})^T$, $\tilde{n}$ denotes the perturbation number density, $\tilde{u}_x, \tilde{u}_y, \tilde{u}_z$ are perturbation velocities in the X, Y , and Z directions, and $\tilde{T}_{tr}, \tilde{T}_{rot}, \tilde{T}_{vib}$ are perturbation translational, rotational,

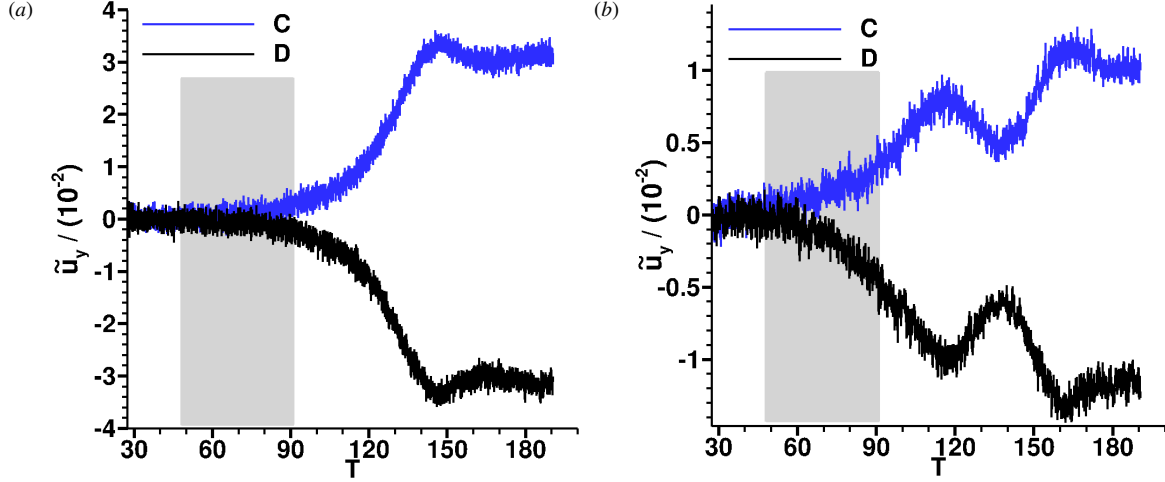


Figure 3.3: Temporal evolution of spanwise perturbation velocity, in (a) the separation shock (probe s) and (b) the bubble (probe b), at spanwise locations C ($Y/L_y = 0.13$) and D ($Y/L_y = 0.63$).

and vibrational temperatures, respectively. The smallness of the perturbations at early times in the simulation permits decomposition of the DSMC-computed perturbation flow fields $\tilde{Q}$ according to linear stability theory into a spanwise-independent vector $\hat{Q}(x, z)$, comprising the two-dimensional amplitude functions, and a phase function, Θ , according to

$$\tilde{Q}(x, y, z, t) = \hat{Q}(x, z) \exp(i\Theta) + c.c. \quad (3.2)$$

where

$$\Theta = \beta y - \Omega t, \quad (3.3)$$

Here $\beta = 2\pi/L_y$ is the real spatial wavenumber corresponding to the spanwise wavelength, L_y , of the global mode, $\Omega = \Omega_r + i\Omega_i$ is a complex quantity, whose real part, Ω_r , indicates the frequency and the imaginary part, Ω_i , is the temporal growth rate, and $c.c.$ indicates complex conjugation so that $\tilde{Q}$ is real. The sign convention in (3.3) indicates that $\Omega_i > 0$ signifies exponentially growing linear perturbations.

3.3.2 Linear instability in the three-dimensional shock layer/laminar separation bubble interaction region

Analysis of the DSMC results was performed during two time windows, $30 \leq T \leq 68$ and $68 \leq T \leq 190$. The lower limit of the first bracket was chosen after initial transients in the solution had subsided, while the upper limit in the second time interval was chosen in order to study the long-time development of the instability, once nonlinear

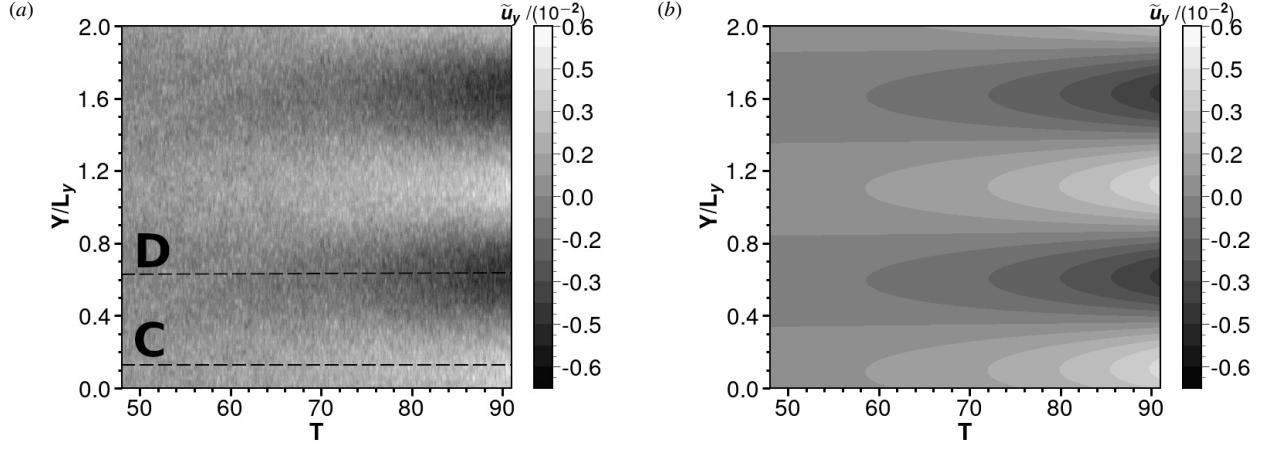


Figure 3.4: Temporal evolution of spanwise perturbation velocity, $\tilde{u}_y$, inside the LSB, along the entire span. (a) Raw DSMC data. (b) Two-dimensional linear fit of the result shown in (a)

Perturbation quantity	Growth rate Ω_i [kHz]	Amplitude $\hat{Q}$
$\tilde{n}$, [m^{-3}]	$4.91 \pm 0.06\%$	$-5.013e+19 \pm 0.24\%$
$\tilde{u}_x$, [ms^{-1}]	$4.90 \pm 0.07\%$	$-0.1613 \pm 0.30\%$
$\tilde{u}_z$, [ms^{-1}]	$4.95 \pm 0.08\%$	$-0.1108 \pm 0.33\%$
$\tilde{T}_{tr}$, [K]	$4.88 \pm 0.04\%$	$0.5111 \pm 0.17\%$
$\tilde{T}_{rot}$, [K]	$4.88 \pm 0.05\%$	$0.5128 \pm 0.19\%$
$\tilde{T}_{vib}$, [K]	$5.15 \pm 0.11\%$	$0.1560 \pm 0.51\%$
$\tilde{u}_y$, [ms^{-1}]	$4.89 \pm 0.10\%$	$0.0762 \pm 0.43\%$
$\tilde{u}_y$ (at s), [ms^{-1}]	$5.12 \pm 0.26\%$	$0.03648 \pm 1.14\%$
$\tilde{u}_y$ (at r), [ms^{-1}]	$4.77 \pm 0.11\%$	$-0.0914 \pm 0.46\%$
$\tilde{u}_y$ (at c), [ms^{-1}]	$5.55 \pm 0.66\%$	$-0.0092 \pm 3.20\%$

Table 3.3: Two-dimensional linear curve fit parameters obtained using Eqs. (3.2) and (3.3). Fit parameters are obtained at probe b unless explicitly indicated otherwise

saturation had been reached. A qualitative change that occurs after $T = 68$ in the shock structure and its long-time ($T > 110$) effect on the LSB will be discussed in Sec. 3.3.4; in this and the next section an in-depth discussion of the results obtained during the linear growth of perturbations is presented first.

The temporal evolution of the spanwise perturbation velocity component, $\tilde{u}_y$, normalised by $u_{x,1}$, within the time of linear growth, indicated by the greyed out box in Fig. 3.3, is presented at probe s inside the shock and probe b inside the LSB, both at two spanwise locations, C and D , to be defined shortly. The immediate observation made is that, both inside the shock layer and in the laminar separation bubble, $\tilde{u}_y$ grows exponentially and, up to this time, monotonically. In order to verify the existence of an underlying linear instability mechanism and quantify its parameters, a two-dimensional linear fit of the full three-dimensional field of the perturbations is performed according to (3.2) using the generalized least-squares method of Python's LMFIT library [148]. The results returned for the mean value of the unknown fit parameters, Ω_i , $\hat{Q}$, Ω_r , alongside the 1σ -uncertainty (standard error) of these estimates, are presented in table 3.3. Consistent with the observation in Fig. 3.3, $\Omega_i \approx 4.9$ kHz is found to be positive, indicating exponential growth of perturbations, while $\Omega_r = 0$, which shows that such a perturbation is stationary. The temporal evolution of $\tilde{u}_y$ at $50 \leq T \leq 90$ over the entire span of the separation bubble is shown in Fig. 3.4(a) as raw DSMC data, while Fig. 3.4(b) shows a two-dimensional linear fit of the data shown in 3.4(a) using Eqs. (3.2) and (3.3). A well-defined harmonic pattern of $\tilde{u}_y$ emerges along the span and the choice of points C and D becomes clear, as they represent the spanwise locations at which $\tilde{u}_y$ attains a local maximum and minimum, respectively.

Table 3.3 also shows the growth rates obtained for other macroscopic flow quantities and for the spanwise perturbation velocity $\tilde{u}_y$ at probes s , r and c defined in Fig. 3.1. It is seen that consistent results for the growth rate are obtained at all locations examined, indicating the presence of global linear instability. The average growth rate of each flow quantity listed in the table is $\Omega_i = 5.0$ kHz, with bounds of $\pm 0.16\%$. Significantly, the absolute magnitude of the small-amplitude of spanwise perturbation velocity, $\tilde{u}_y$, is on the same order at probes r , b , s , and an order of magnitude lower at probe c : the maximum deviation of $\sim 11.4\%$ is found at probe c , which is outside of the region of shock and LSB interaction.

The essential qualitative difference between the present three-dimensional and the earlier two-dimensional results of Tumuklu *et al.* [30] is the discovery of *unstable* three-dimensional perturbations in the three-dimensional configuration, as opposed to the damped eigenmodes in the two-dimensional work, that ultimately led to a steady state being reached in the two-dimensional flow; the present results show that no such steady state exists in the three-dimensional double wedge flow at these parameters. Notwithstanding differences in Mach number, a comparison of the present results with those of instability analysis in the double wedge by Sidharth *et al.* [149], who analyzed a Mach 5 hypersonic flow

of a calorically perfect gas, reveals that the present nondimensional, average growth rate $\Omega_i = 5.7 \times 10^{-3}$ ¹ is nearly an order of magnitude larger than the $\Omega_i = 7.5 \times 10^{-4}$ obtained in the referenced work. This can be explained by the difference in the angles between the upper and lower wedges, which is $\Delta\theta = 15^\circ$ in the present and $\Delta\theta = 8^\circ$ in the referenced work and is consistent with the strong destabilizing effect of $\Delta\theta$ found by Sidharth *et al.* [149], and also known from the related compression ramp flow, *e.g.* Cao *et al.* [47].

Finally, linear instability was found not to affect surface flow quantities. Spanwise variations of the streamwise velocity slip and the temperature jump at the wall were found to be negligible during linear growth of disturbances, such that these quantities are the same as the base state profiles shown in Figs. 3.2(a) and 3.2(b), respectively. The spanwise velocity slip (not shown) was also found to be negligibly small with a maximum spanwise variation of only 0.078% of $u_{x,1}$.

The question of the spatial origin of linear instability and the spanwise periodicity seen in Fig. 3.4 is addressed next. Two locations are selected, U and S , as shown in Fig. 3.1(b), located upstream of the separation shock and in the separation region, respectively. Figure 3.5(a) shows the variation of the local-streamwise velocity, $u_{t,l}$ along the local wall-normal direction, subscript ‘ t ’ standing for the local-streamwise (wall-tangential) component of velocity and ‘ l ’ referring to the lower wedge surface, as a function the wall-normal height H_l . Figure 3.5(b) shows the absolute maximum spanwise variation of $u_{t,l}$ during linear perturbation growth, calculated based on the difference in $u_{t,l}$ at two locations, A , at $Y/L_y=0.88$ and B , at $Y/L_y=1.38$ of the spanwise sinusoidal modulation induced by linear instability; the significance of these locations A and B will be further elucidated in the next section.

¹Growth rate results are nondimensionalised by multiplying Ω_i by the boundary layer thickness at separation, $\delta_{99} = 3.35$ mm, and dividing by the freestream velocity downstream of the leading-edge shock, $u_{x,2} = 2930.8$ m/s, the latter obtained from inviscid shock theory [150] for the observed shock angle of 41°

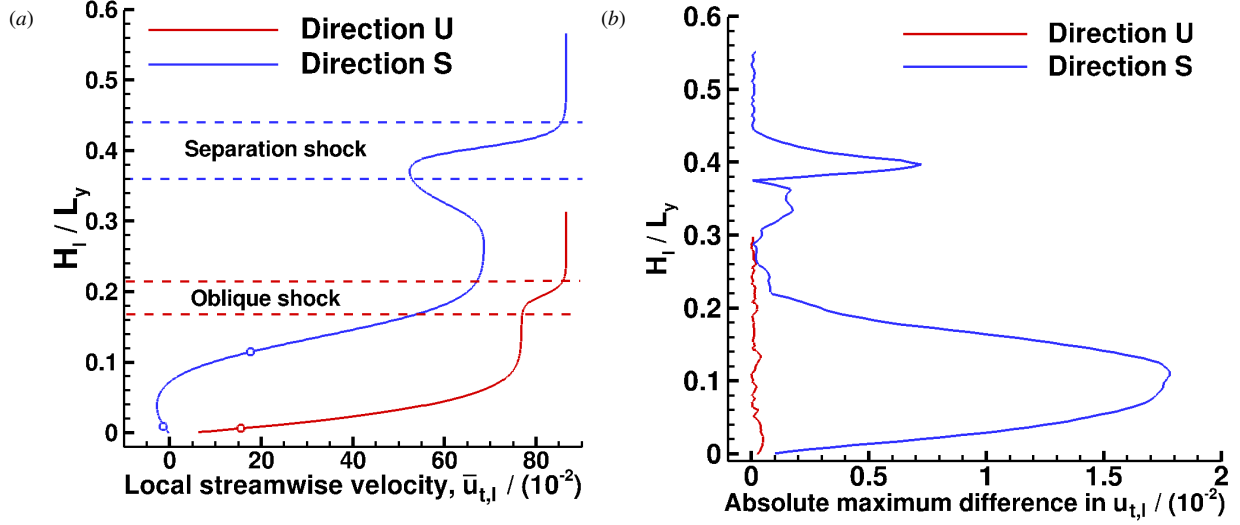


Figure 3.5: (a) Boundary layer profiles in the base state along wall-normal directions U and S . Local streamwise velocity, $\bar{u}_{t,l}$ is normalised by $u_{x,1}$, H_l being distance along the wall-normal. (b) The absolute maximum spanwise variation in $u_{t,l}$ along B and S .

Common characteristics of the boundary layer profiles at U and S are the respective non-zero streamwise velocity component at the wall, due to surface rarefaction effects discussed in Sec. 3.2.2, and the generalized inflection points (GIPs), indicated by open circles. The essential difference between the profiles at the two locations concerns the respective maximum spanwise variation: at U , this is only within 0.05% of $u_{x,1}$, indicating that the flow upstream of the separation shock is essentially two-dimensional. By contrast, at S the maximum spanwise variation peaks at the inflection point, $H_l / L_y = 0.113$, where it is equal to 1.8% of $u_{x,1}$. In addition, a second local maximum of 0.72% of $u_{x,1}$ is observed inside the separation shock layer at $H_l / L_y = 0.40$. Attention is thus turned to correlating this spanwise inhomogeneity inside the shock layer with global instability in the LSB.

3.3.3 Correlation of linear instability in the shock layer and the laminar separation bubble

Figures 3.6(a) and 3.6(b) present probe data of perturbation quantities along specific wall-normal and spanwise field lines, respectively. It should be stressed here that the flow components shown are representative of all perturbation quantities, all of which exhibit the same qualitative behavior, but are not shown for brevity. Figure 3.6(a) shows the variation of the gradient magnitude of the pressure perturbation, $|\nabla \tilde{p}|$, normalised by $p_1 L_s^{-1}$ (p_1 being the freestream pressure) as a function of wall-normal distance, H_l , along the S -direction. Data is shown at the same two spanwise locations, A and B , the choice of which will be discussed shortly. The rapid increase of $|\nabla \tilde{p}|$ at $H_l = 0.36 L_y$ is indicative of the separation shock, inside of which the value of $|\nabla \tilde{p}|$ far exceeds that in the vicinity of the surface. This

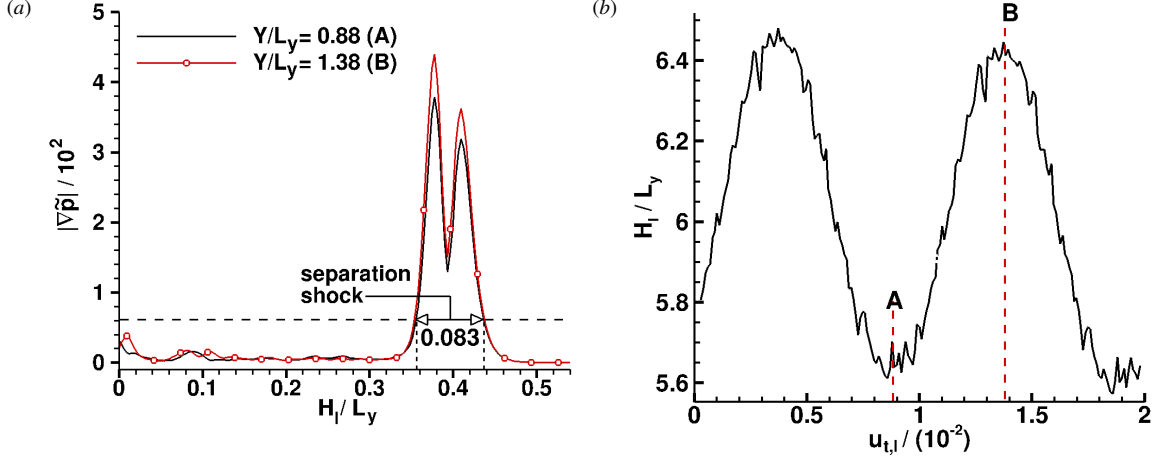


Figure 3.6: (a) Wall-normal probe data for $|\nabla \tilde{p}|$, along direction S as a function of wall-normal height at two spanwise locations A and B defined in the legend. (b) Spanwise probe data for $\tilde{u}_{t,l}$ inside the separation shock at $H_l/L_y=0.4$ on plane S .

criterion was used to indicate the separation shock region in Fig. 3.5(a). It is worth pointing out here that the measured thickness of the shock layer based on this criterion, $0.083L_y = 2.39$ mm, is comparable to the boundary layer thickness at separation, $\delta_{99} = 3.35$ mm.

The choice of spanwise locations A and B can be understood from results shown in Fig. 3.6(b). Here the spanwise variation of $\tilde{u}_{t,l}$ inside the separation shock layer is plotted at a wall-normal height $H_l/L_y=0.4$ along the S -direction. It can be clearly seen that the spanwise locations A and B correspond to the trough and peak of a *sinusoidal modulation* of $\tilde{u}_{t,l}$.

The spanwise structure of small-amplitude perturbations inside the separation and detached shock layers, alongside that inside the LSB, is shown in Figs. 3.7(a) and 3.7(c), respectively corresponding to wall-normal planes at the locations S and R defined in Fig. 3.1(b). Figures 3.7(b) and 3.7(d) show the same spanwise perturbation velocity component on the separation shock plane $a-t$ and the detached shock plane $t-d$ defined in Fig. 3.1(b). On all four of these figures contours of the spanwise perturbation velocity component are shown. This quantity is zero at the start of the simulation and only arises on account of linear instability as time progresses. On Figs. 3.7(a) and 3.7(c) the approximate boundaries of the separation and detached shock regions, as well as the envelope of the LSB and the location of the contact surface are marked by dashed / dash-dotted horizontal lines.

On the S -plane in Fig. 3.7(a), spanwise-periodic flow structures are seen inside the separation bubble between the wedge surface, $H_l=0$, and the outer envelope of the separation bubble, a $H_l \approx 0.15L_y$, where the spanwise vorticity, $\tilde{\omega}_y$, is zero. The outer envelope of the bubble can also be seen to be corrugated sinusoidally, on account of the stationary growing LSB instability, the three-dimensional footprint of which leads to the well-known striations that originate

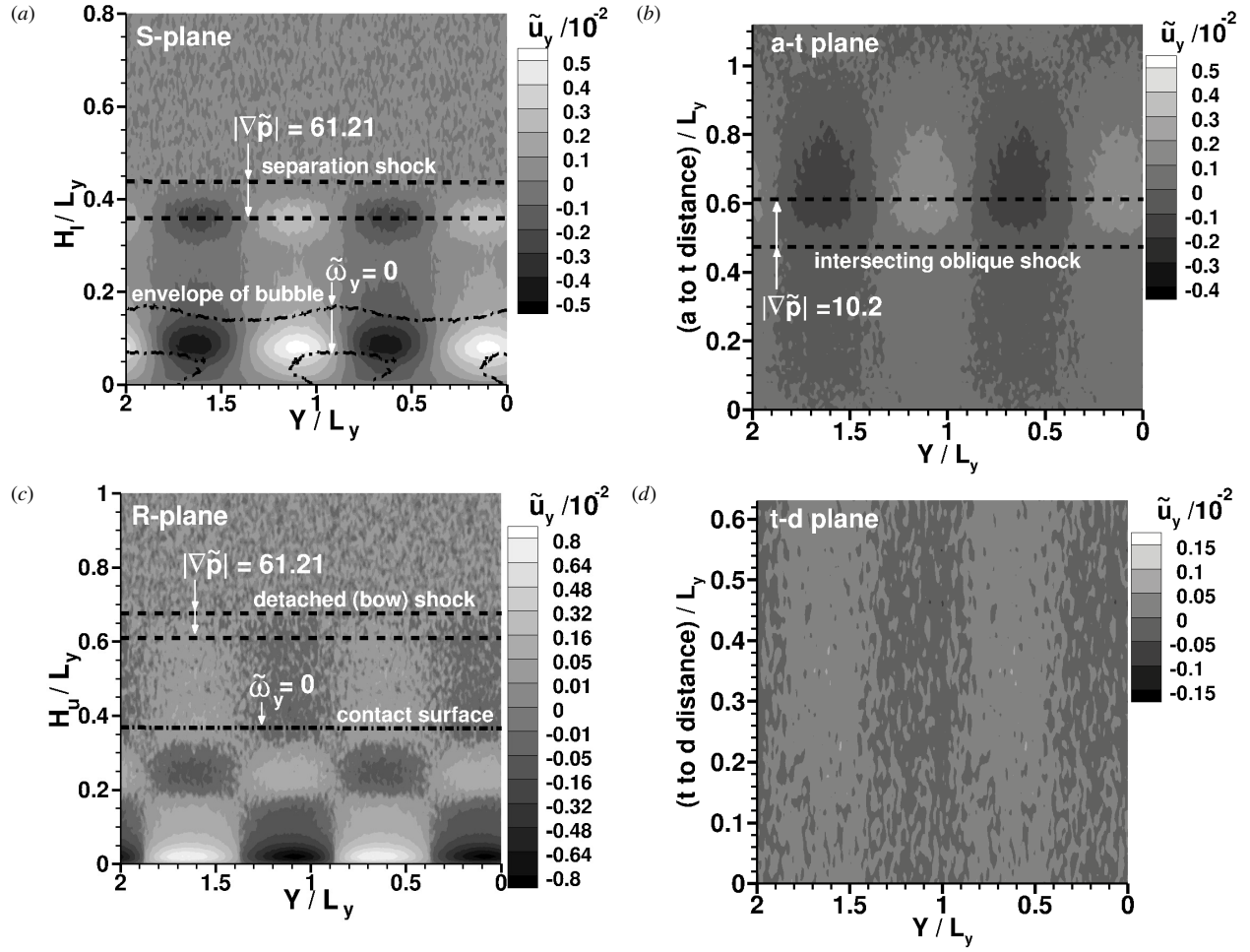


Figure 3.7: Field data of the spanwise perturbation velocity component, $\tilde{u}_y$, normalised by $u_{x,1}$ during linear growth of perturbations, on the planes S in (a), $a-t$ in (b), R in (c), and $t-d$ in (d) as denoted in Fig. 3.1(b). Overlaid line contours: (---) $|\nabla \tilde{p}|$ and (-·-·) $\tilde{\omega}_y=0$.

inside the LSB [41, 43, 46, 123]. *This spanwise-periodic global instability is identified here for the first time in the context of kinetic theory simulations.*

Further away from the wall, Fig. 3.7(a) shows, also for the first time, that spanwise-periodic flow structures form inside the strong gradient region of the separation shock layer, at a height $0.36 < H_l/L_y < 0.44$ away from the wall. These structures are in phase with those inside the LSB and have the same spanwise periodicity length. This result is consistent with the maximum spanwise variation seen in the probe data and the DSMC signal post-processing discussed in the previous section, which revealed nearly identical growth rates inside the LSB (probe *b*) and the separation shock (probe *s*). The conjecture put forward based on interpretation of the probe data can now be further strengthened on the basis of the field data shown, namely that self-excited linear instability leads to spanwise-periodic structures in perturbation flow quantities within the shock layer, with a spanwise wavelength of L_y , identical with that seen in the LSB. On the cut-plane $a - t$ in Fig. 3.7(b), it is seen that the spanwise periodic structures are present in the entire separation shock layer from the foot of the separation to the triple point T_2 . The region of interaction of the oblique shock with the separation shock is marked on the $a - t$ plane at the distance of $0.474L_y$ to $0.613L_y$. In this region, the magnitude of $\tilde{u}_y$ increases and striation patterns emerge further along the separation shock.

On the R -plane, downstream of the triple point, Fig. 3.7(c) shows contour plots of the spanwise perturbation velocity component, $\tilde{u}_y$, which also exhibits spanwise-periodic structures inside the reattached boundary layer; together with the result shown in Fig. 3.7(a) this result shows that the striations originating inside the LSB extend at least up to the location of plane R on the downstream wedge wall. Along the wall-normal direction, H_u , spanwise-periodic structures are also present in the vicinity of contour line $\tilde{\omega}_y=0$ at a height of $H_u = 0.36L_y$, in the vicinity of contact surface C_2 downstream of the triple point T_2 , which clearly points to the contact surface being corrugated by perturbations that are in-phase with the striations on the wall. Further away from the wall, the contour lines of $|\nabla\tilde{p}|$ at $H_u = 0.61L_y$ and $0.677L_y$ indicate the approximate layer of the detached shock. Inside this layer the spanwise periodic flow structures are still noticeable, but their amplitude has subsided compared to that in the separation shock, indicating that the spanwise periodic global mode is concentrated in the zone of interaction between the separation- and detached shock-layer system and the LSB.

The presence of spanwise periodic structures in the detached shock layer from the triple point T_2 to probe *d* is seen on the cut-plane $t - d$ in Fig. 3.7(d). The peak magnitude of these structures is at least a factor of two lower than the structures in the separation shock and an order of magnitude lower than those in the separation bubble. This shows that the synchronization of global instability is strongest between the separation shock and the LSB, and the amplitude of the perturbations in the shock layer declines downstream of the triple point. It can further be seen that the structures inside the detached shock layer are 180° out of phase with structures in the separation shock, shown earlier on plane

$a - t$.

Returning to the analysis of the spanwise structures inside the shock layer and the separation bubble on the S plane, Fig. 3.8 confirms that spanwise-periodic perturbations are present in all perturbation flow quantities, namely number density, $\tilde{n}$, streamwise velocity with respect to the lower wedge (i.e., direction perpendicular to S), $u_{t,l}$, wall-normal velocity with respect to the lower wedge (i.e., direction of S), $u_{n,l}$, translational temperature, $\tilde{T}_{tr}$, rotational temperature, $\tilde{T}_{rot}$ and vibrational temperature, $\tilde{T}_{vib}$. The minimum (negative) and maximum (positive) values of spanwise structures in $\tilde{u}_{t,l}$, $\tilde{u}_{n,l}$, and $\tilde{n}$ are also at spanwise locations A and B , respectively.

Interestingly, closer inspection of the relative magnitude of the perturbation velocity components, all scaled by the same freestream value, reveals qualitatively different results inside the LSB and at the shock layer. In the LSB, the tangential and spanwise perturbation velocity components have comparable magnitudes, while the wall-normal component is an order of magnitude smaller in relative terms. By contrast, the peak oscillation amplitude in the wall-normal perturbation velocity component is *two orders of magnitude higher in the shock layer* than inside the LSB ($|\tilde{u}_{n,l}|_{\max} \approx 0.3$ inside the shock layer, as opposed to $|\tilde{u}_{n,l}|_{\max} \approx 3 \times 10^{-3}$ in the bubble), as seen in the inset graphs that magnify all shock layer results. This behavior, although not as pronounced, can also be seen in the number density and perturbation temperature components.

Furthermore, all three perturbation temperatures have primary spanwise structures adjacent to the wall having minimum and maximum values at spanwise locations B and A , respectively, i.e., they are 180° out of phase with perturbation structures of velocities and number density. Perturbations in the normalised $\tilde{T}_{tr}$ and $\tilde{T}_{rot}$ also exhibit secondary structures immediately above the primary structures within $0.1 < H_l < 0.15$. From a qualitative point of view, all perturbation components inside the shock layer are found to feature the same *cats-eyes* pattern, seen in all insets of Fig. 3.8. The degree of thermal nonequilibrium seen in the perturbation temperatures presented in Figs. 3.8(d) – 3.8(f) is significant, and originates in differences in the base flow temperatures, shown in Fig. 3.9(a), where thermal nonequilibrium is present in the entire region between the shock structure and the wedge surface along the three directions shown. This results in the large differences in the shock, denoted by the blue dashed line at $H_l/L_y = 0.36 - 0.44$ in Fig. 3.9(b), where relatively smaller differences can be seen in the bubble, at $H_l/L_y = 0 - 0.15$, in all three temperatures. Consistent with the faster relaxation between translational and rotational modes, those two temperatures have an analogous spatial dependence.

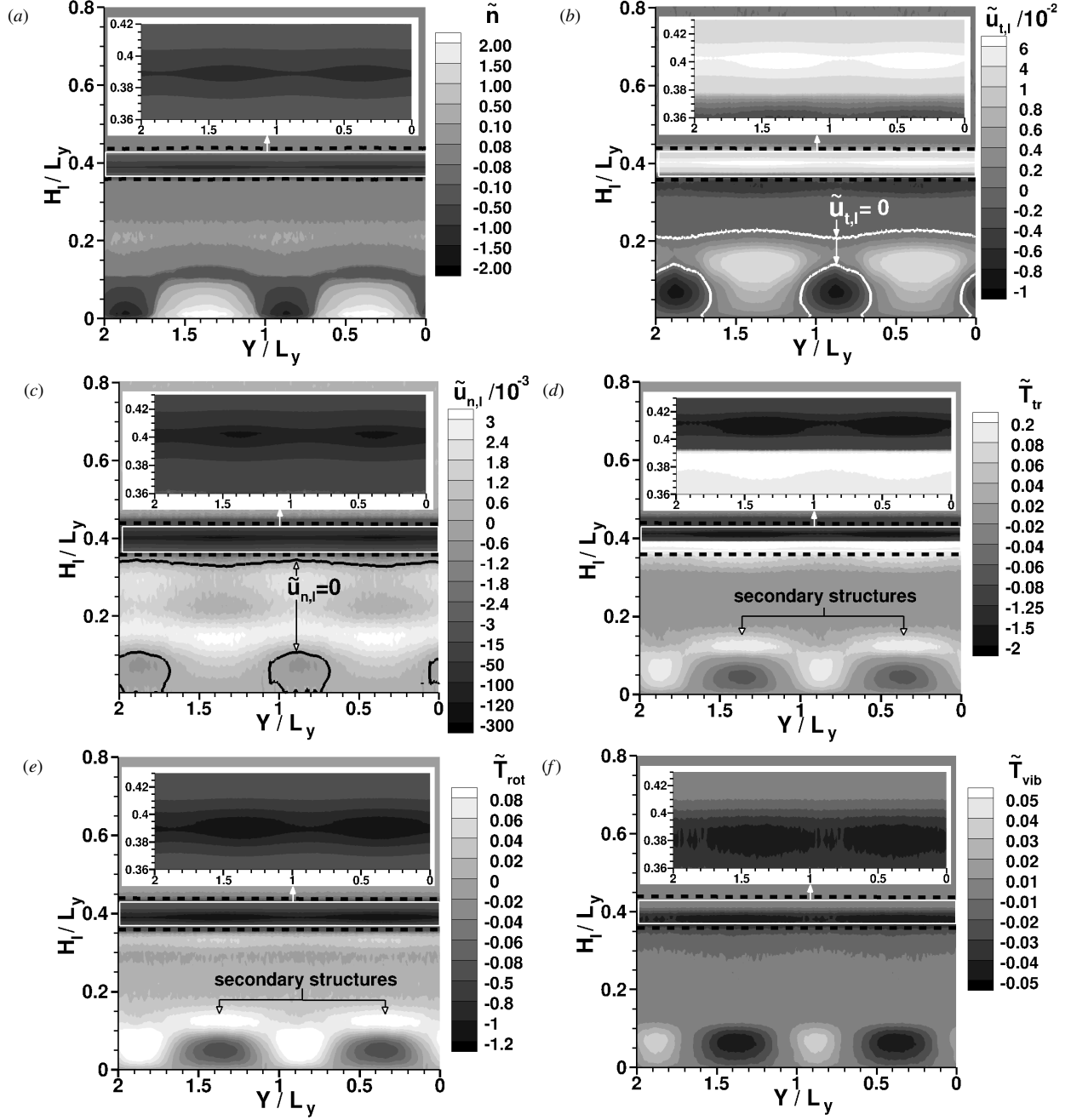


Figure 3.8: Contours of perturbation quantities on the plane defined along S . (a) number density, $\tilde{n}$, (b) streamwise perturbation velocity, $u_{t,l}$, (c) wall-normal velocity, $u_{n,l}$, (d) translational temperature, $\tilde{T}_{tr}$, (e) rotational temperature, $\tilde{T}_{rot}$, and (f) vibrational temperature, $\tilde{T}_{vib}$, showing the cats-eyes pattern of instability in the shock layer. Number density, velocities, and temperatures are normalised by respective upstream values.

Figure 3.10 presents three different views of the spanwise perturbation velocity component over the entire calculation

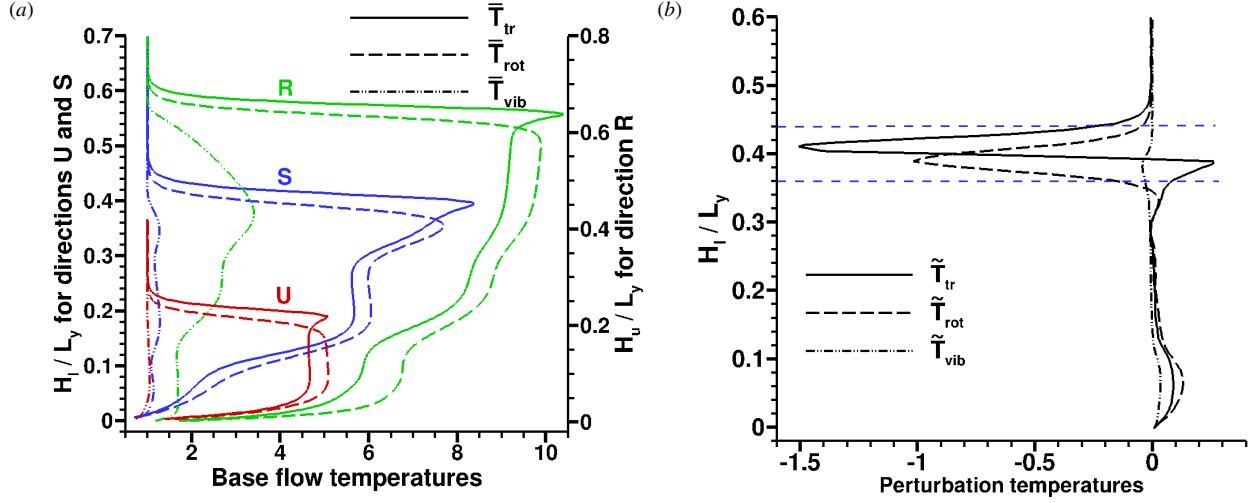


Figure 3.9: (a) Base flow temperatures, $\bar{T}_{tr}$, $\bar{T}_{rot}$, $\bar{T}_{vib}$, along U, S, and R. (b) Wall-normal probe data of perturbation temperatures, $\tilde{T}_{tr}$, $\tilde{T}_{rot}$, $\tilde{T}_{vib}$, along S at the spanwise location A.

domain. In Fig. 3.10(a) the perturbation is shown on the OXZ plane and two characteristic cut-planes, P and Q , defined by their respective normal vectors $[-0.7193 \hat{i} + 0.6946 \hat{k}]$ and $[0.7193 \hat{i} - 0.6946 \hat{k}]$. P is taken approximately tangential to the dividing streamline of the LSB, while Q is taken at a distance from the corner, so as to cross the triple-point of the steady flow. Figure 3.10(b) shows three-dimensional isosurfaces of u_y underneath plane P , while Fig. 3.10(c) presents spanwise periodic structures in the shear layers downstream of triple points T_1 and T_2 defined in Fig. 3.1(a). All of these results, as well as consistent results seen in the isocontours of vorticity components in Appendix 3.5.3, all confirm the three-dimensional, spanwise periodic nature of an instability that encompasses the LSB region in tandem with the separation- and detached-shock layers and the triple point T_2 that connects the latter two.

Summarising, it is seen that during linear perturbation growth the steady two-dimensional base flow becomes unstable to a self-excited, small-amplitude, three-dimensional spanwise-periodic stationary global mode. The spanwise perturbation velocity component, $\tilde{u}_y$, which was zero at the beginning of the simulation, attains a sinusoidally varying amplitude not only inside the separation bubble, as known from earlier work, *e.g.* [41–43, 125], but also inside the separation and detached shock layers and the shear layers formed downstream of triple points. This result extends the findings of Tumuklu *et al.* [22, 23, 30] in the two-dimensional counterpart of this configuration but, contrary to the two-dimensional limit, in the present three-dimensional environment the observed global instability is unstable with synchronized spanwise-periodic small-amplitude perturbations amplifying exponentially within both the LSB and shock layer. Linear growth of the global mode inside the laminar separation leads to striations on the wall, while in the shock layer a spanwise-periodic cats-eyes pattern is formed in all perturbation components. Ultimately, linear growth will lead to nonlinear saturation and attention is turned next to analysis of the three-dimensional DSMC predictions at

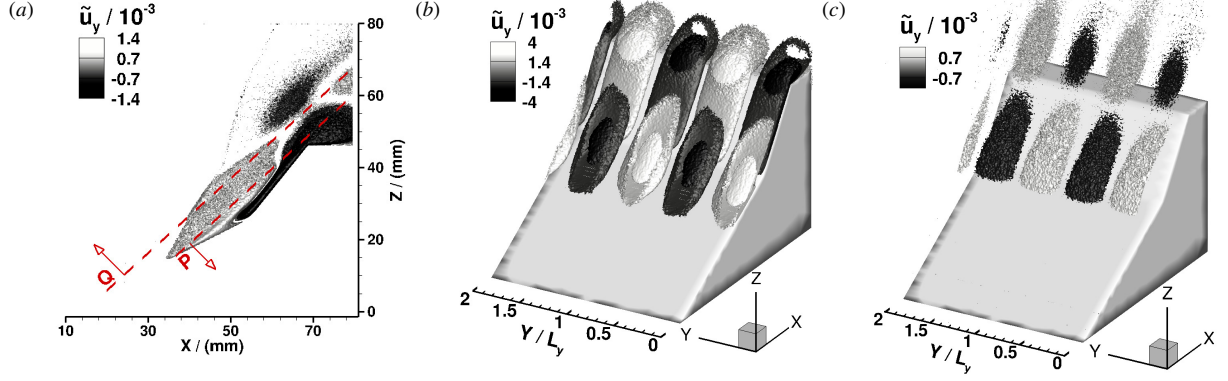


Figure 3.10: (a) Isocontours of spanwise perturbation velocity $\tilde{u}_y$ on the OXZ plane and definition of cut-planes P and Q . (b) Same result for $\tilde{u}_y$, plotted underneath cut-plane P and denoting spanwise-periodic striations inside the LSB. (c) Same plotted upstream of cut-plane Q and denoting spanwise-periodic modulation in the vicinity of contact surfaces (shear layers) downstream of triple points.

later times.

3.3.4 Low-frequency unsteadiness of the shock and separation bubble

Turning to the dynamics of the linear flow instability at times beyond exponential growth of the stationary spanwise periodic global mode, attention is paid to low-frequency unsteadiness, that has been reported over a wide range of $Re \sim O(10^6 - 10^8)$ in a number of numerical solutions of the Navier-Stokes equations, *e.g.* [151–156], as well as many experiments [157], where shock-induced turbulent boundary layer interactions were studied in a variety of configurations. Low-frequency unsteadiness is identified in this context as that corresponding to Strouhal numbers in the range $0.01 \leq St \leq 0.05$, while Strouhal numbers within the same range have also been reported for supersonic laminar and transitional shock / boundary-layer interactions [158, 159].

A qualitative change in the evolution of the signal commences in the triple point at $T=68$. Figures 3.11(a) and 3.11(b) present the spatio-temporal variation of normalised perturbation spanwise velocity, $\tilde{u}_y$, at probe b in the separation bubble, where linearly growing spatial structures start to exhibit sinusoidal oscillations in time with an average period of $46T$. At probe t near triple point T_2 , the variation of normalised perturbation number density, $\tilde{n}$, is shown in Figs. 3.11(c) and 3.11(d) where two timescales with periods of $51T$ and $41T$ (average period of $46T$) can be seen. The corresponding Strouhal number corresponding to these time periods is,

$$St = \frac{fL_s}{u_{x,2}} = 0.0283 \pm 0.003, \quad (3.4)$$

which is defined based on the length of the separation bubble, $L_s = 40$ mm and the velocity downstream of the leading-edge oblique shock, $u_{x,2} = 2930.8 \text{ m.s}^{-1}$. This Strouhal number is within the low-frequency range reported in

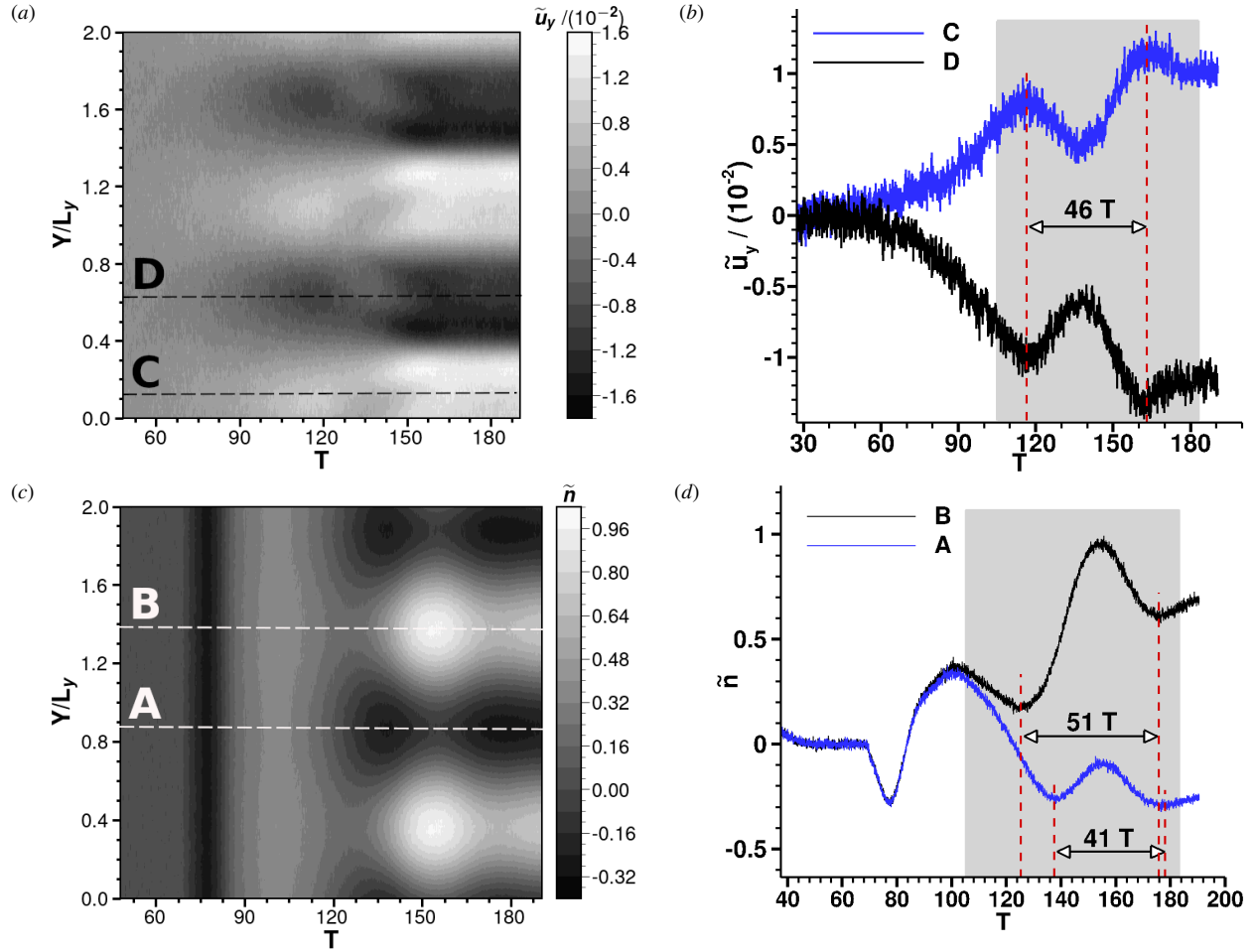


Figure 3.11: Low frequency unsteadiness at probes b and t in the separation bubble and at the triple point, T_2 , respectively. (a) At probe b , the temporal evolution of perturbation spanwise velocity, $\tilde{u}_y$, normalised by $u_{x,1}$. (b) At spanwise locations C ($Y/L_y = 0.13$) and D ($Y/L_y = 0.63$), the normalised $\tilde{u}_y$ indicating the period of unsteadiness. (c) At probe t , the temporal evolution of perturbation number density, $\tilde{n}$, normalised by n_1 . (d) Normalized $\tilde{n}$ at locations A ($Y/L_y = 0.88$) and B ($Y/L_y = 1.38$) as a function of T .

the literature of turbulent SBLI. The triple point starts to oscillate at $T=68$, and its motion remains two-dimensional up to approximately $T=85$, as indicated by the lack of variation in $\tilde{n}$ along the spanwise direction. Past this time, three-dimensional linear instability manifests itself and low-frequency unsteadiness is observed, causing spanwise modulation of structures in $\tilde{n}$ and their oscillations in time.

3.4 Summary

Linear instability mechanisms in laminar hypersonic flow of nitrogen over a three-dimensional double wedge with a $30^\circ - 55^\circ$ cross section have been studied using the particle-based DSMC method, as implemented in the massively parallel SUGAR solver [39]. The temporal evolution of the DSMC field was computed over a span of ~ 200 through-flow time units that included the inception of three-dimensionality, linear perturbation growth and nonlinear signal saturation. The fully resolved kinetic approach permitted space- and time-accurate modeling of the internal structure of shocks, surface rarefaction effects, thermal nonequilibrium, as well as, for the first time, time-accurate description of small-amplitude three-dimensional self-excited perturbations that arise from interaction of the shock system with the three-dimensional LSB both inside the separation and detached shock layers and in the LSB.

In line with the findings of Tumuklu *et al.* [23] for Mach 16 flow over an axisymmetric double cone, and Tumuklu *et al.* [30] for the two-dimensional counterpart of the present double wedge flow, the LSB was found to be strongly coupled with the separation and detached shock system. In contrast to the results in the two-dimensional configuration, linear instability was found to be exponentially amplified in the present three-dimensional context. The origin of instability was traced in the vicinity of primary separation, i.e. the flow region of interaction of the separation shock and the bubble. This finding clearly points out that the observed mechanism is one of self-excitation and not the result of amplification of incoming upstream disturbances, a result which generalises the concept of *oscillator*, introduced in an incompressible context either in weakly-nonparallel [124, 126] or in fully nonparallel flow [125], to include the interaction of the entire separation and detached shock system with the three-dimensional LSB.

The presence of amplified linear instability leads to the formation of spanwise-periodic flow structures in three-dimensional perturbations of macroscopic flow quantities inside the LSB, corresponding to the well-known striation wall pattern. More importantly, the present study showed that spanwise-periodic linear instability also exists in the internal structure of the separation and detached shock layers and in the vicinity of contact surfaces downstream of triple points; this shock-layer instability, which takes the form of cats-eyes patterns, is seen for the first time in the present work. Linear instability in the shock layer and the LSB are synchronized, with the spanwise-periodicity length of the structures forming inside the bubble and in the shock system being identical, and their amplitude growing with

the same average, linear temporal growth rate, $\Omega_i = 5.0 \text{ kHz} \pm 0.16\%$ at the conditions examined. The slow linear growth and long time-scale of low-frequency unsteadiness suggest that experimental test times must be sufficiently long, if differences between the various experimental and numerical results are to be reconciled.

The long time simulation of the flow revealed that, past the stage of linear instability growth, low-frequency unsteadiness of the triple point and consequently of the separation bubble sets in, having a time period of oscillation of 46T. The long-time spatio-temporal evolution of the flow at the triple point T_2 of $\sim 190T$ revealed the presence of spanwise corrugation of the shock as well as sinusoidal oscillations in time. The oscillation frequency corresponds to Strouhal number of $St \sim 0.028$, consistent with the existing literature on turbulent SBLI.

3.5 Supplemental Information

3.5.1 Convergence study

Figure 3.12 shows the DSMC numerical criteria discussed in Sec. 6.2.1 to quantify the solution accuracy of the presented double wedge flow. To justify the decoupling of particle movement and subsequent binary collisions, the two DSMC criteria of collision cell size and mean-collision-time smaller than the local mean-free-path and timestep, respectively, are shown in Figs. 3.12(a) and 3.12(b), at a flow time instance of 0.047 on an $X - Z$ plane of C -mesh. The value of the ratio $\lambda/\Delta x$ is much greater than one in the strong gradient regions of shocks and triple points, however, inside the recirculation region in the vicinity of the wall it is between 0.8 to 1. Note that the collision cells having a ratio of $\lambda/\Delta x < 1$ are blanked to see the extent of this region better. Francis *et al.* [160] had quantified the effect of larger collision cell size on the transport coefficients using the Green-Kubo theory, which predicts an error of 11.8 and 7.1% in shear viscosity and thermal conductivity, respectively, for $\lambda/\Delta x = 0.8$. Note that this error is derived for the rectangular (non-spherical) shaped collision cells and occurs because, in DSMC, the interaction range of particles is equal to the collision cell size instead of the range of the inter-particle force. Note also that their Green-Kubo formulation was verified with the DSMC-derived transverse momentum flux in a Couette flow problem and agreed well for $\lambda/\Delta x > 0.25$. On the other hand, the ratio $\tau_{\text{coll}}/\Delta t$ is greater than one in the entire flow domain, as the blanked region of $\tau_{\text{coll}}/\Delta t < 1$ is absent. In the recirculation region, where the collision cell size is smallest (four to five levels of adaptive refinement), the number of instantaneous computational particles is eight, except for a handful of cells, where it is between five and eight, as shown in Fig. 3.12(c). Additionally, the spanwise independence was ensured for five flow times by comparing the solution with a double wedge span of $L_y = 28.8 \text{ mm}$, discussed in this work, with another case simulated with a span of $L_y/2$.

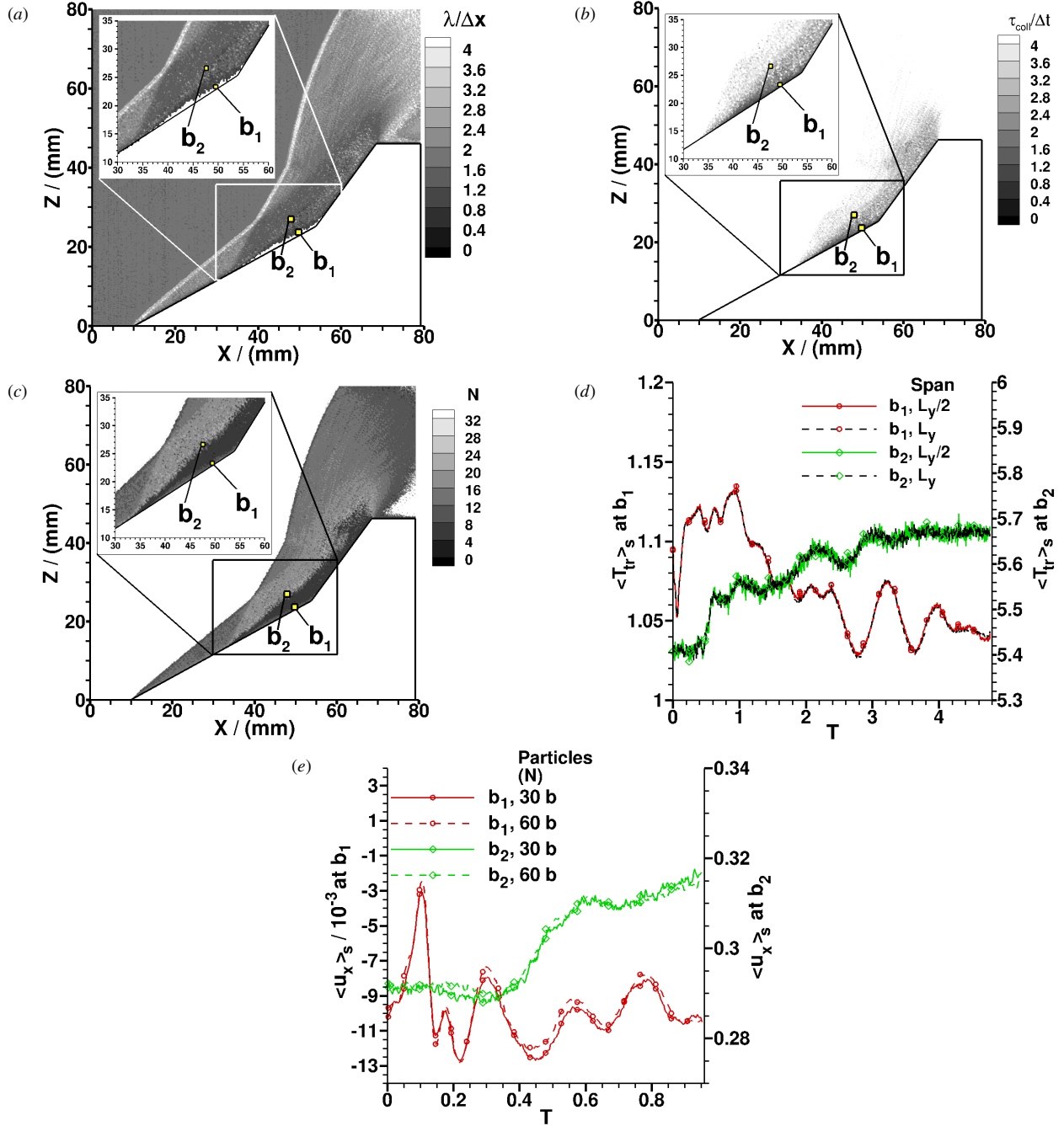


Figure 3.12: (a) Ratio of local mean-free-path to the collision cell size along with numerical probes b_1 ($X=49.177$ mm, $Z=22.963$ mm) and b_2 (47.192, 26.271). (b) Ratio of local mean-collision-time to the timestep. (c) Number of computational particles per collision cell. (d) Spanwise independence in spanwise averaged translational temperature between the 28.8 and 14.4 mm span cases with 60 and 30 billion particles, respectively. (e) Convergence in terms of the number of particles for the 14.4 mm span case of spanwise averaged streamwise velocity, $\langle u_x \rangle_s$, at probe locations denoted in (a). The $X-Z$ Contours in (a), (b), (c) are shown at $Y=14.4$ mm for the 28.8 mm span case with 60 billion particles.

At two critical probe locations inside the separation bubble, b_1 near the surface and b_2 near the shear layer, which are denoted in Fig. 3.12(a), the temporal evolution of spanwise averaged translational temperature, shown in Fig. 3.12(d), is in excellent agreement. Although after 50 flow times of simulation, it became clear that the span of $L_y/2$ is insufficient to capture the largest spanwise structure observed in the case with span L_y , this early time comparison shows spanwise independent initialization of the simulation from a 2-D steady-state solution. The case with $L_y/2$ span was also valuable in testing the convergence of the solution with respect to the number of particles and evaluating the error due to $\lambda/\Delta x < 1$. Due to half the length of the span, using the same numerical conditions, this case required only 30 billion particles to satisfy the DSMC criteria as rigorously as the case with a span of L_y did with 60 billion particles. The case with $L_y/2$ span was repeated with double the number of particles, which satisfies the criterion $\lambda/\Delta \geq 1$. The solution was compared at locations b_1 and b_2 in Fig. 3.12(e). It shows at probe b_1 , the transient profile of spanwise averaged streamwise velocity agrees within 7% at the local maxima and minima, and very well at strong temporal gradients. In contrast, away from the surface at b_2 , the difference is within 1.5%.

3.5.2 Modification to the computations of maximum collision cross-section

A modification to the computation of maximum collision cross-section used in the MFS scheme is described for accurate spectral analysis of unsteady flows. In a typical DSMC simulation, the collision pairs selected using either the MFS or the no time counter (NTC) scheme are allowed to collide with probability,

$$P_{\text{coll}} = \frac{\sigma_T c_r}{(\sigma_T c_r)_{\text{max}}} \quad (3.5)$$

where $\sigma_T = \pi d^2$ is the total cross-section, d is the molecular diameter, c_r is the relative speed, and $(\sigma_T c_r)_{\text{max}}$ is the maximum collision cross-section. The last term is stored for each collision cell and is estimated at the beginning of the simulation to a *reasonably large value* using an expression suggested by Bird [37] (see Sec. 11.1),

$$(\sigma_T c_r)_{\text{max}} = (\pi d_{\text{ref}}^2) 300 \sqrt{T_{\text{tr}}/300} \quad (3.6)$$

where d_{ref} is the reference molecular diameter. As the simulation progresses, this value is updated if a larger value is encountered in the collision cell.

However, care should be exercised at an AMR step during which the old C -mesh is deleted and a new one is constructed, because the newly created collision cells require an estimate of $(\sigma_T c_r)_{\text{max}}$. If the value is arbitrarily guessed based on Eq. (3.6), then the instantaneous temporal signals of macroscopic flow quantities exhibit kinks at the timesteps when the AMR step is performed. These kinks decay in approximately 3 to 4 μs and therefore would

not affect steady state simulations, but for unsteady flows they can spuriously reveal a dominant frequency equal to the inverse of the time period between the two AMR steps. To avoid the corruption of instantaneous signals with such artificial perturbations, at an AMR step each root cell stores the smallest value of $(\sigma_T c_r)_{max}$ among all of its collision cells before deleting the C -mesh. After a new C -mesh is formed, the value stored in the root is assigned as the lowest estimated guess to all collision cells in a given root. Those newly formed collision cells, for which the actual value of $(\sigma_T c_r)_{max}$ must be larger than that assigned as an estimate, quickly update to this value within the next $0.2 \mu s$ and eliminates spurious corruption of the instantaneous residual.

Next, the implementation of spanwise-periodic boundaries in the SUGAR code is performed as follows. Suppose a particle intersects a spanwise domain boundary at $Y = 0$ or L_y , within a period, δt , smaller than the timestep, Δt . In that case, its spanwise position index is changed to the periodically opposite Y boundary index, i.e., $Y = L_y$ or $Y = 0$, respectively. After this translation, the particle continues its movement for the remaining portion of the timestep, $\Delta t - \delta t$. This simple algorithm is implemented in SUGAR's parallel framework by ensuring that the processors containing a portion of the flow domain adjacent to any Y -boundary also store the information of processors containing the periodically opposite portion of the domain. Such information includes the 'location code array' and the triangulated panels of the embedded surface. The location code arrays are special arrays used in the efficient particle mapping strategy based on the Morton-based space-filling-curve approach. Sawant *et al.* [39] provide additional details of these arrays and optimized gas-surface interaction strategies employed in the SUGAR code.

3.5.3 Proper orthogonal decomposition for reduction of statistical noise

Use of the POD method to remove statistical noise in instantaneous perturbation macroscopic flow fields obtained from DSMC is briefly discussed. The basic theory can be found in Ref. [161] while additional details on its application to noise reduction have been provided in a number of resources, *e.g.* [30, 162]. This method performs the singular value decomposition (SVD) of the input data matrix $\mathcal{D}$, in which macroscopic flow field is stacked such that the number of rows and columns are equal to the number of total sampling cells N_c in the DSMC domain and the instantaneous time snapshots N_s , respectively. The SVD procedure performs the decomposition

$$\mathcal{D} = \phi S \mathcal{T}, \quad (3.7)$$

where ϕ is the matrix of spatial modes having dimensions $N_c \times N_r$, N_r is the user-specified rank of the reduced SVD approximation to $\mathcal{D}$, S is the square diagonal matrix of singular values having dimensions $N_r \times N_r$, and $\mathcal{T}$ is the matrix of temporal modes of dimensions $N_r \times N_s$. The i^{th} spatial and temporal modes are stored in the i^{th} column of ϕ and

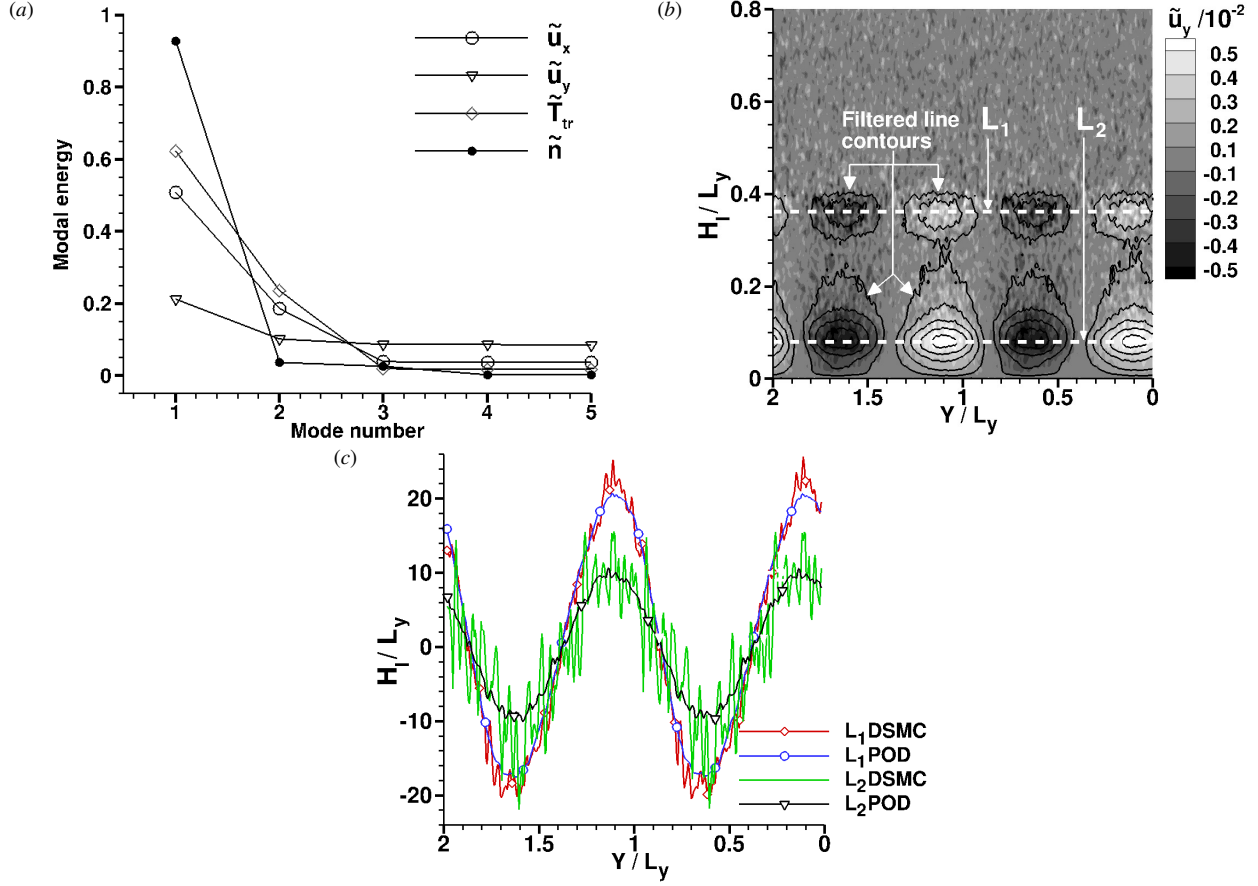


Figure 3.13: (a) Modal energy in perturbation macroscopic flow quantities based on singular values obtained from the POD analysis. (b) Contours of unfiltered raw DSMC data for $\tilde{u}_y$, normalised by $u_{x,1}$ on a plane defined along wall-normal direction S as in Fig. 3.7(a). Overlaid are contour lines of noise-filtered reconstruction of $\tilde{u}_y$ from the first two proper orthogonal modes. (c) Comparison of unfiltered (DSMC) and filtered (POD) $\tilde{u}_y$ along lines L_1 and L_2 denoted in (b).

row of $\mathcal{T}$, respectively. The singular values in S are arranged in decreasing order, and their square corresponds to the amount of energy in each mode. After the decomposition, a reduced-order, noise-filtered representation of $\mathcal{D}$ can be reconstructed by forming a new data matrix $\mathcal{D}_2$ from a user-specified number of ranks $N_{r,2}$, which is smaller than N_r . $N_{r,2}$ is chosen such that the difference between any time snapshot of $\mathcal{D}_2$ and that of $\mathcal{D}$ is within statistical noise.

For the double wedge solution, the data matrix for each macroscopic flow quantity was formed by the number of sampling cells, $N_c = 2.304 \times 10^7$ and number of time snapshots, $N_s = 450$. The instantaneous snapshots were collected from $T=48.0312$ to 90.9162 , at an interval of 0.0953 flow time, which corresponds to the frequency of 1 MHz. Initially, $N_r=10$ was chosen; however, $N_{r,2} = 2$ was found to be sufficient as the modal energy of higher modes is less

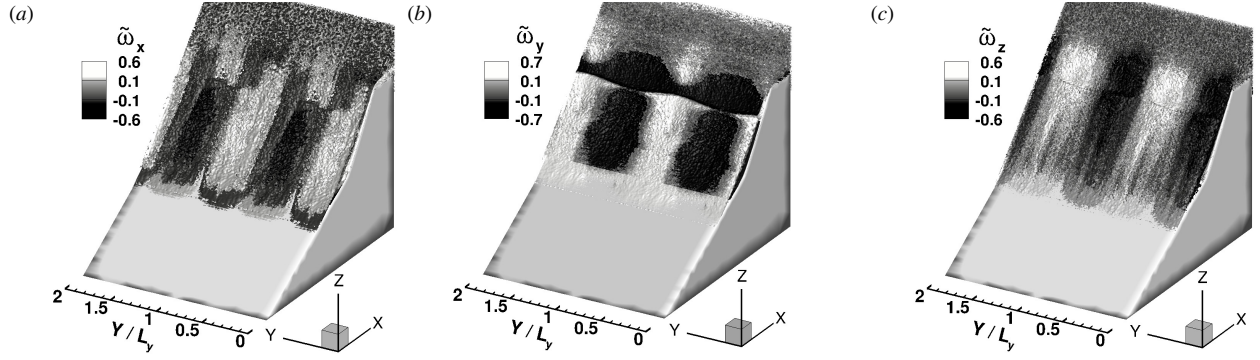


Figure 3.14: Isocontour surfaces of vorticity components during linear perturbation growth, (a) $\tilde{\omega}_x$, (b) $\tilde{\omega}_y$, (c) $\tilde{\omega}_z$, normalised by the local vorticity magnitude. Isocontours are shown underneath cut-plane P , indicated in Fig. 3.10(a).

than 10%, as shown in Fig. 3.13(a). The modal energy, E_i , of the i^{th} mode is defined as,

$$E_i = \frac{S_i^2}{\sum_{j=1}^{N_r} S_j^2} \quad (3.8)$$

where S_i is the i^{th} singular value. The total energy of the first two modes of perturbation quantities other than $\tilde{u}_y$ is almost 70%. For $\tilde{u}_y$, this number is lower than other components because the shock structure has little influence on flowfield of $\tilde{u}_y$, which is composed only of a slowly growing linear mode and statistical noise. Note that the data matrix itself requires 77.24 GBs of run time memory, larger than the typical compute nodes of supercomputing clusters. Therefore, the method was parallelized based on the Tall and Skinny QR factorization (TSQR) algorithm [163] to overcome storage requirements and speed up the SVD procedure. Figure 3.13(b) shows the original noise-contained DSMC solution of perturbation spanwise velocity during linear growth on the S -plane normal to the lower wedge along with the noise-filtered contour lines of the solution reconstructed using POD. The figure also shows two horizontal dashed lines L_1 and L_2 along which the DSMC data is extracted and compared in Fig. 3.13(c). The POD-reconstructed data exhibits the same spatial spanwise variation but contains very low statistical noise compared to the DSMC solution.

The statistical noise reduction using the POD method is sufficient to clearly see vorticity fields in the flow. For example, the spanwise-periodic flow structures in the isocontours of X , Y , and Z perturbation vorticity components are also shown in Figs. 3.14(a), 3.14(b), and 3.14(c), respectively. The X and Z components of vorticity are in phase with each other and 90° out of phase with the Y component.

Chapter 4

Low-frequency Molecular Fluctuations in One-Dimensional Monatomic Shocks

In this chapter, low-frequency molecular fluctuations in the translational nonequilibrium zone of one-dimensional strong shock waves are characterized for the first time in a kinetic collisional framework in the Mach number range $2 \leq M \leq 10$. Our analysis draws upon the well-known bimodal nature of the probability density function (PDF) of gas particles in the shock, as opposed to their Maxwellian distribution in the freestream, the latter exhibiting two orders of magnitude higher dominant frequencies than the former. Inside the (finite-thickness) shock region, the strong correlation between perturbations in the bimodal PDF and fluctuations in the normal stress suggests introducing a novel two-bin model to describe the reduced-order dynamics of a large number of collision interactions of gas particles. Our model correctly predicts two orders of magnitude differences in fluctuation frequencies in the shock versus those in the freestream and is consistent with the small-amplitude fluctuations obtained from the highly resolved Direct Simulation Monte Carlo (DSMC) computations of the same configuration. The variation of low-frequency fluctuations with changes in the conditions upstream of the shock revealed that these fluctuations can be described by a Strouhal number, based on the bulk velocity upstream of the shock and the shock-thickness based on the maximum density-gradient inside the shock, that remains practically independent of Mach number, upstream temperature, and number density.

Nomenclature

Roman symbols	
A	identifier for gas particles in energy bin A .
A_i, A'_i	identifier for the subtype of type- A particles that take part in the i^{th} detailed collision process, p_i . Pre- and post-collisional states are indicated with and without prime.
a	speed of sound (m.s^{-1})
C_i	number of DSMC collisions per timestep per computational volume that take part in the i^{th} detailed collision process, p_i , (s^{-1})
$c(\xi_x)$	cross-correlation coefficient as a function of x -directional energy, ξ_x
d_r	molecular diameter at the reference temperature, $T_r = 273 \text{ K}$ (m)
E_a	activation energy (J)
f	frequency (Hz)
F_n	number of particles represented by one DSMC computational particle
f_{ξ_i}	probability density function of energy ξ_i of particles
$f_{\xi_x}^A$	probability density function of energy ξ_x of particles in energy bin A
$f_{\xi_y+\xi_z}^A$	probability density function of total transverse energy $\xi_y + \xi_z$ of particles in energy bin A
$f_{\xi}, f_{\xi_x}, f_{\xi_y}, f_{\xi_z}$	probability density functions of normalized energies ξ, ξ_x, ξ_y, ξ_z , respectively
F_j	flux coefficient for particles of type ' j ', where $j \in \{A, B\}$ (s^{-1})
$\mathbf{G} = [G_{N_A}, G_{N_B}]^T$	normalized growth rate vector
g_r	relative speed (m.s^{-1})
$J(N_A, N_B)$	Jacobian matrix with arguments as number of particles N_A and N_B
$\tilde{k}_i$	rate coefficient of an i^{th} simplified process Q_i , if different from k_i (s^{-1})
K_i	rate coefficient $K_i = \frac{k_i \Delta V}{F_n}$ ($\text{m}^3.\text{s}^{-1}$)
k_i	rate coefficient for collision processes p_i and P_i denoted by process identifier ' i ' (s^{-1})
K_{th}	theoretical estimate of the rate coefficient ($\text{m}^3.\text{s}^{-1}$)
L_i	i^{th} eigenvalue of jacobian matrix $J(N_{A,\text{crit}}, N_{B,\text{crit}})$ for $i = 1, 2$

L_d	domain length in the direction of shock propagation (m)	T_r	reference temperature of 273 K
L_s	shock thickness (m)	$\mathbf{u} = [u_x, u_y, u_z]^T$	bulk velocity vector ($m.s^{-1}$)
M	Mach number	v_m	most probable speed, $v_m = \sqrt{(2k_b T_{tr})/m}$ ($m.s^{-1}$)
m	mass of species (kg)	$\mathbf{v} = [v_x, v_y, v_z]^T$	instantaneous molecular velocity vector ($m.s^{-1}$)
m_r	reduced mass (kg)	W	total number of time windows used for window averaging for obtaining $c(\xi_x)$
n	number density (m^{-3})	X, Y, Z	Cartesian coordinates in the direction of the shock and two transverse directions
$N(\xi_x, w)$	total number of DSMC computational particles within time windows w to $w + 1$ as a function of ξ_x	B	identifier for gas particles in energy bin B .
N	number of DSMC computational particles	Greek symbols	
N_{init}	initial number of particles in the domain	β	inverse of most probable speed, v_m^{-1} , ($m^{-1}.s$)
N_j	number of particles in energy bin ' j ', where $j \in \{A, B\}$	$\Gamma(j)$	gamma function, $\int_0^\infty x^{j-1} \exp(-x) dx$
$N_{A_i}, N_{A'_i}$	number of particles of subtype A_i or A'_i	$\Gamma(j, y)$	upper incomplete gamma function, $\int_y^\infty x^{j-1} \exp(-x) dx$
N_{crit}	critical number of particles to which the solution of the two-energy-bin model converges	γ	specific heat ratio
p	pressure (Pa)	Δt	simulation timestep (s)
R	universal gas constant ($J.mol^{-1}.K^{-1}$)	Δv	volume of a computational cell (m^3)
Re	unit Reynolds number (m^{-1})	Δx	octree cell size (m)
St	Strouhal number	$\Delta \xi_x$	small region of X -directional energy space ξ_x
T_{tr}	overall translational temperature (K)	δ_{ij}	Kronecker's delta function expressed in indicial notations
$T_{tr,x}, T_{tr,y}, T_{tr,z}$	directional translational temperatures in x , y , and z directions, respectively (K)	δN	a pre-set number of particles used as a threshold to activate stabilization of the shock
t	time (s)		

δx	a small distance from the boundaries	ω	viscosity index in the Variable Gas Sphere model
ε	symmetry factor	Operators	
κ_b	Boltzmann constant (J.K ⁻¹)	$[Q]_{\text{coll}}$	contribution to quantity Q due to particle collisions
λ	mean free path (m)	$\langle Q \rangle_t$	time average of flow quantity Q
μ	mean of the PDF f_{ξ_x}	$\langle Q \rangle_w$	average of quantity Q over time windows W
$\mu(w)$	instantaneous mean of PDF f_{ξ_x} obtained from DSMC by collecting data of ξ_x from time window w to $w + 1$	Subscripts	
ξ_x, ξ_y, ξ_z	normalized X , Y , and Z -directional energies, respectively, where $\xi_x = (v_x^2 - u_x^2)\beta^2$, $\xi_y = v_y^2\beta^2$, and $\xi_z = v_z^2\beta^2$	A	corresponding to energy bin A
ρ	mass density (kg.m ⁻³)	B	corresponding to energy bin B
$\Sigma_{N(\xi_x)}$	standard deviation in fluctuations of $N(\xi_x, w)$ about $\langle N(\xi_x) \rangle_w$	x, y, z	Cartesian components
Σ_μ	standard deviation in fluctuations of $\mu_{\xi_x}(w)$ about $\langle \mu \rangle_w$	1	upstream value
σ_{ij}	component of overall stress tensor expressed in indicial notations (Pa)	2	downstream value
σ_n	standard deviation in functuations of n about $\langle n \rangle_t$ (m ⁻³)	ref	reference value
σ_{u_x}	standard deviation in functuations of u_x about $\langle u_x \rangle_t$ (m.s ⁻¹)	Superscripts	
τ_{ij}	component of viscous stress tensor expressed in indicial notations (Pa)	in	entering into a computational cell
		l	corresponding to the left face of a computational cell
		out	going out of a computational cell
		r	corresponding to the right face of a computational cell

4.1 Introduction

It is well-known that numerical solutions of the deterministic Euler and Navier-Stokes equations (NSE) require special treatment if one is to obtain reliable flow features containing shocks. Solutions of differential equations describing fluid flow motion, in either a shock-capturing [54, 164] or a shock-fitting context [55, 165] can predict both location and unsteadiness of shocks accurately, but the description of the internal shock structure and predictions of the gas properties inside a shock must be modelled in the context of such solutions. Information about the interior of shocks may be obtained from the numerical solution of systems of equations that are more general than the Navier-Stokes equations. The first documentation of differences in shock structure predicted by the Navier-Stokes equations and solution of the more general Bhatnagar-Gross-Krook model for the Boltzmann equation of transport is due to Liepmann *et al.*, [62] who showed that the Navier-Stokes equations are inadequate in describing the internal structure of a shock wave at high Mach numbers ($M \geq 3$) and that the differences between the two solutions increases in the low-pressure region of the shock layer with an increase in Mach number. Soon afterwards, Bird [32] solved the exact Boltzmann equation using the stochastic DSMC method [37] and quantified the level of strong translational nonequilibrium in the interior of shocks.

The significance of the correct description of not only the location and motion of shocks but also of their internal dynamical structure cannot be overstated in fluid mechanics. Amongst other classes of flows, shocks are responsible for the production of sound in supersonic jets as shown by the extensive studies of their interaction with turbulence and isolated vortices. [166–178] The shock-wave/boundary-layer interactions (SBLIs) on compression ramps, cones, and flat plates are widely investigated for their role in generating separation bubbles, unsteadiness, and large surface heat and pressure fluxes. [26, 156, 179] It is also recognized that the study of receptivity of shocks to freestream or induced disturbances is of importance in the investigation of transition in hypersonic boundary layers. [53, 180–183]

However, the vast majority of research in laminar to turbulent transition and SBLIs focuses on the physics of transition in the boundary layer and not the shock. [49, 184–187] In fact, research on the effect of kinetic fluctuations on triggering transition from laminar to turbulent flows has been explored using Landau-Lifshitz's theory of fluctuating hydrodynamics [188] in several works on the receptivity of boundary layers in the incompressible [57, 189] and high-speed compressible [56, 190] regimes. In the phenomenological approach of fluctuating hydrodynamics, stochastic fluxes are added to the stress tensor and heat flux vector in the NSE formulation to account for the effect of molecular fluctuations on the flow field. Using this approach, Luchini [189] showed that the presence of kinetic fluctuations is a non-negligible source of disturbances in a boundary-layer and sets an upper bound on the transition Reynolds number. Fedorov et al. [56] showed that in a compressible flat-plate boundary-layer, the kinetic fluctuations could trigger random wave-packets of Tollmien-Schlichting waves or a Mack second-mode instability. However, this approach cannot be

easily extended to account for the kinetic fluctuations in shocks, where the fluctuation amplitude is known to be larger than the predictions of the equilibrium theory. [191]

Therefore to understand the role of molecular fluctuations in the shock layer, kinetic methods that provide insight into the molecular nature of the shock in terms of particle velocities and energy distribution function are important. However, understanding detailed molecular collisions in two- and three-dimensional (2-D and 3-D) flows is challenging because of the tremendous length and time scales related to boundary-layers, instabilities, and unsteadiness of SBLIs. Our study aims at closing this theoretical gap by examining the origin of molecular fluctuations in the well-known one-dimensional (1-D) shock of a monatomic gas, argon, in a kinetic framework. We show the surprising result that even simple one-dimensional shocks exhibit *low-frequency fluctuations*, that have been, up until now, ignored, yet, their presence may well contribute to laminar to turbulent transition in supersonic and hypersonic flows.

Historically, solutions of the internal structure of strong shocks were sought using kinetic models [62] as they allow for anisotropy of stresses and heat fluxes, which are not accounted for by the traditional Navier-Stokes-Fourier constitutive relations. Bird [32] successfully modelled 1-D argon shock structures using the DSMC method and obtained shock-thicknesses that were in good agreement with the experiments of Alsmeyer. [192] Since then, the method has been widely used for modeling the steady state behavior of strong shocks [33, 193–196] as well as unsteady flows without [197–201] and with shocks [202]. Stefanov *et al.* [191] simulated Mach 26 bow shock over a 2-D cylinder using DSMC and attributed an increase in velocity fluctuations inside the shock layer to ‘thermal nonequilibrium effects’; however, they did not delve deeper into the reason for these effects, the changes in time-scales of fluctuations in comparison to an equilibrium state, and their dependence on the strength of the shock wave. Our work attempts to answer these questions by investigating the fluctuations in molecular velocity and energy distribution functions obtained from the solution of the Boltzmann equation. This work will show that the major role of bimodality in the distribution function inside the shock is to change the dominant frequencies of molecular fluctuations compared to an equilibrium freestream.

Our past work has exploited the fidelity of DSMC to understand the critical role of shocks in hypersonic SBLIs. Tumuklu *et al.* [22, 23] simulated laminar SBLIs in a Mach 16 axisymmetric flow over a double-cone and observed strong coupling between the complex shock structure and the separation bubble. For the freestream unit Reynolds number of $Re_1 = 3.74 \times 10^5 \text{ m}^{-1}$ they found oscillations of the detached (bow) and separation shocks characterized by a Strouhal number of 0.078. In this work, we will show that the Strouhal number associated with the low-frequency fluctuations in an isolated 1-D shock falls within a similar range of $St = 0.001$ to 0.02 . Sawant *et al.* [39] extended the capability of DSMC in modeling the computationally challenging 3-D laminar SBLIs of a Mach 7 flow over a double-wedge at near-continuum input conditions through the use of adaptively-refined octree grids. In addition we have

investigated the stability of the spanwise-periodic laminar separation bubble in the double-wedge flow to self-excited, small-amplitude, spanwise-homogeneous perturbations. [31,203] We demonstrate the existence of the strong coupling of the shock structure with the separation bubble and show that linear amplification of the most unstable 3-D flow perturbations leads to synchronization of low-frequency unsteadiness of the separation bubble with the unsteadiness of the manifold of shock structures corresponding to a Strouhal number of 0.028.

The remainder of the chapter is organized as follows: Section 4.2 describes the DSMC numerical implementation and the nonequilibrium aspects of a 1-D shock structure of argon. It then describes the fluctuations in the overall stress inside the shock with that in the freestream and contrasts the differences in their frequencies. From additional analyses of cross-correlations it is hypothesized that the differences in fluctuations are caused by the long-time collision interaction of particles in two modes of the bimodal energy distribution of particles. To prove this hypothesis, we construct a simplified two-energy-bin ordinary differential equation (ODE) model in Sec. 4.3 similar to the predator-prey model of Lotka-Volterra [204–206] but with modified terms accounting for intermolecular collisions between the two bins. The evaluation of rate coefficients used in the model and the simplification of the collision processes is also described in this section. In Section 4.4 we discuss the dynamics of the two-energy-bin model and compare with the broadband frequencies obtained from the power spectral density (PSD) analyses of fluctuations in the DSMC residuals. Section 4.5 establishes a range of Strouhal numbers for Mach numbers 2 to 10 as well as for variations in upstream temperature at a given Mach number. Using this range, an estimate of low-frequencies is made and qualitatively compared with experiments. A summary of the main findings is provided in Sec. 6.5. In addition, supplementary Secs. 4.7.1 and 4.7.2 respectively describe the STABIL boundary condition implemented to avoid numerical drift of the shock and the additional numerical tests conducted to verify that the frequencies in shocks discussed in this work are not numerical artifacts.

4.2 A Particle Representation of Nonequilibrium Fluctuations inside a One-dimensional Shock

4.2.1 DSMC simulation methodology and properties of a 1-D shock

The DSMC solution of the shock is obtained using a 1-D version of the Scalable Unstructured Gas-dynamic Adaptive mesh-Refinement (SUGAR) DSMC solver [39] which makes use of a binary adaptive mesh refinement structure, where each computational Cartesian ‘root’ cell is recursively refined into smaller cells until its size is smaller than the local

mean-free-path. The smallest cells, referred to as ‘leaf’ or ‘collision’ cells, are used to select neighboring collision partners to perform binary elastic collisions between particles of a monatomic gas using the majorant frequency scheme. [98] The macroscopic flow and transport parameters are computed based on the statistical equations of kinetic theory [37] and shown on larger root cells. In terms of traditional DSMC solvers, each reference to a computational cell in this chapter means a Cartesian root cell. The gas is assumed to follow a variable hard sphere (VHS) molecular model [37] with viscosity index $\omega = 0.81$, mass $m = 6.637 \times 10^{-26}$ kg, reference diameter $d_r = 4.17 \times 10^{-10}$ m at reference temperature $T_r = 273$ K. We compared our DSMC profiles of normalized viscous stress and heat flux along the direction of shock propagation with the results of Ohwada [207] obtained by using a finite-difference Boltzmann solver for a 1-D, Mach three flow of argon and obtained excellent agreement.

The DSMC simulation was initialized using the Rankine-Hugoniot jump conditions at $X/\lambda_1 = 0$, where X is the streamwise direction normal to the shock and λ_1 is the upstream mean-free-path. At the upstream boundary, $X/\lambda_1 < 0$, computational particles are introduced using a directed local Maxwellian flow at a number density, bulk velocity, and temperature of $n_1 = 1 \times 10^{22} \text{ m}^{-3}$, $u_{x,1} = 3572.24 \text{ m.s}^{-1}$, and $T_{tr,1} = 710$ K, respectively to generate hypersonic flow. At the subsonic downstream boundary, $X/\lambda_1 > 0$, a specularly reflecting surface moving at a bulk velocity of $u_{x,2}$, equal to the downstream Rankine-Hugoniot velocity is used (see Chapter 12 of Ref. [37]). The domain length is 0.02 m, i.e. $X/\lambda_1 = -57.45$ to 57.45 , which is sufficiently large so that the boundaries are placed sufficiently far from the shock layer but small enough so that the shock does not move from its initialized central location during the early transient period. The spurious effects caused by the movement of a shock during the early transient period in a very large domain on frequencies observed in this work are explained in Sec. 4.7.2.3. In this domain, the flow takes only $\sim 6 \mu\text{s}$ to transition from the jump condition to form a typical shock structure, a time much shorter than the low frequency molecular fluctuations that we will discuss. Bird’s STABIL boundary condition [37] is used to prevent random walk effects from causing the shock to move, a brief description of which can be found in Sec. 4.7.1. However, because of the high number density and the use of a large number of computational particles ($\approx 475,000$) the drift was found to be very small. Nevertheless, the STABIL algorithm has not been previously used in a 1-D shock simulation where we wish to characterize molecular fluctuations that generate low frequency unsteadiness. For this reason, additional clarification is provided in Sec. 4.7.2.1 to demonstrate that the frequencies that we will observe in the following sections are not influenced by the STABIL algorithm.

Using the aforementioned computational approach, Fig. 4.1 shows time-averaged profiles of macroscopic flow and transport parameters obtained from the DSMC simulation of a 1-D, Mach 7.2 shock in argon. Unless otherwise indicated, subsequent figures and results are based on these 1-D shock conditions. The time-averaged or mean quantities discussed in this work were calculated after the $6 \mu\text{s}$ transient period for additional time steps until ~ 0.2

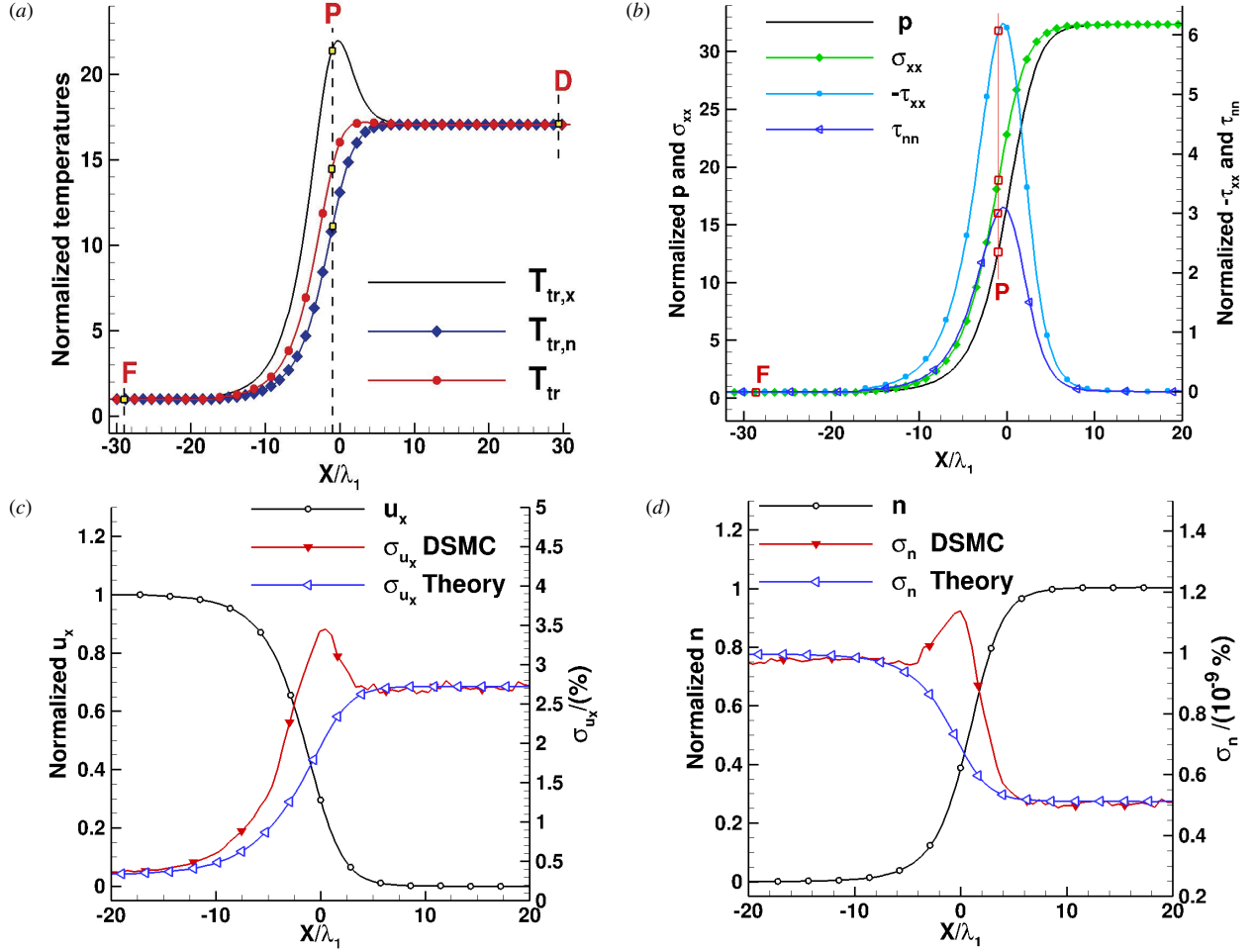


Figure 4.1: (a) $T_{tr,x}$, $T_{tr,n}$, and T_{tr} normalized by the upstream translational temperature $T_{tr,1}$. (b) Normalized p , σ_{xx} , τ_{xx} , and τ_{nn} (see text). (c) and (d) show normalized streamwise bulk velocity, $(u_x - u_{x,1})/(u_{x,2} - u_{x,1})$, and number density, $(n - n_1)/(n_2 - n_1)$, respectively, as well as the comparison of DSMC-derived standard deviation in their fluctuations, σ_{u_x} and σ_n , in percent of respective unnormalized macroscopic quantities with estimates from equilibrium statistical mechanics. Subscripts '1' and '2' denote the upstream and downstream macroscopic quantities, respectively.

ms. Figure 4.1(a) shows deviation of the X - and average lateral directional temperatures, $T_{tr,x}$ and based on axial symmetry, $T_{tr,n} = (T_{tr,y} + T_{tr,z})/2$, respectively, from the overall translational temperature, T_{tr} , within a region of $-16 < X/\lambda_1 < 6$, indicating the presence of translational nonequilibrium in the shock. In the equilibrium regions ($X/\lambda_1 < -16$ and $X/\lambda_1 > 6$), it can be seen that all directional temperatures are equal to the overall temperature. Within the region $2 < X/\lambda_1 < 6$ the gradient of overall translational temperature asymptotes to zero, yet there is a strong deviation of directional temperatures from each other, similar to that in the DSMC simulation of a Mach 8 argon shock by Bird [32]. Figure 4.1 also shows the locations of the numerical probes F ($X/\lambda_1 = -29$), P ($X/\lambda_1 = -1$), and D ($X/\lambda_1 = 29$), based on which later discussions will follow.

Additionally, Fig. 4.1(b) shows the deviation of time-averaged pressure, p , from the X -directional overall stress, σ_{xx} , inside the shock as well as the normal viscous stress components, τ_{xx} and $\tau_{nn} = (\tau_{yy} + \tau_{zz})/2$, calculated based on the relationship,

$$\tau_{ij} = -(\sigma_{ij} - p\delta_{ij}) \quad (4.1)$$

where δ_{ij} is the Kronecker delta function. The pressure and stress components are normalized by the upstream parameter $\rho_1\beta_1^{-2}$, where $\beta = \sqrt{m/2\kappa_b T_{tr}}$ is the inverse of the most probable speed of molecules, m is mass, κ_b is the Boltzmann constant, $\rho = nm$ is the mass density, and n is the number density. The existence of these non-zero stresses leads to a finite thickness of the shock wave, which, when modelled by accounting for molecular thermal fluctuations using a stochastic method, such as DSMC, reveals nonequilibrium bimodal velocity and energy distributions of particles. This chapter will show that these bimodal distributions exhibit a dominant frequency that is two orders of magnitude lower than those found in the freestream.

With respect to the equilibrium regions of the shock, Figs. 4.1(c) and 4.1(d) show excellent agreement between the DSMC-computed velocity and number density fluctuations and theory, as was observed by Stefanov *et al.* [191] For a dilute gas, theory predicts that at equilibrium, statistical fluctuations in macroscopic quantities of bulk velocity, u_x , and number of particles, N , have a standard deviation of $\sqrt{\kappa_b \langle T_{tr} \rangle / m \langle N \rangle}$ and $\sqrt{\langle N \rangle}$, respectively, where the brackets denote time or ensemble average of macroscopic quantities. [142, 188] The DSMC standard deviations are computed for each computational cell of width $\Delta x = 1 \times 10^{-4}$ m for instantaneous data collected at every timestep of $\Delta t = 3$ ns from 6 μ s to 0.2 ms. Note that since the velocity fluctuations shown in Fig. 4.1(c) are expressed in terms of DSMC computational particles, the amplitude of actual thermal fluctuations is obtained by division by a factor of $\sqrt{F_n}$, where $F_n = 10^7$ is the number of dilute gas molecules represented by each DSMC computational particle. Therefore, the 0.344 % standard deviation of velocity fluctuations in the freestream in Fig. 4.1(c) corresponds to an actual value

of $1.09 \times 10^{-4} \%$, a small yet significantly large number on the scale of small amplitude perturbations considered in shock-dominated flows.

4.2.2 Examination of nonequilibrium fluctuations

We are particularly interested in the nonequilibrium zone of the shock layer, where a significant deviation from equilibrium is seen in DSMC-computed standard deviations, as shown in Figs. 4.1(c) and 4.1(d). Note that the standard deviations peak at the location of absolute maximum gradients of respective flow parameters, i.e. at location $X/\lambda_1 = 0$. In contrast to the findings of Stefanov *et al.*, [191] the density fluctuations inside a shock also deviate from the equilibrium Poisson law, although their magnitude is much smaller than the velocity or energy fluctuations.

To understand the frequencies of fluctuations in the shock layer, we focus on probe P located in the vicinity of maximum absolute bulk velocity gradient in the shock to obtain the time history of fluctuations of the normalized X -directional overall stress, $\sigma_{xx}\beta_1^2\rho_1^{-1}$, about the time-averaged mean. This data is important because fluctuations in σ_{xx} correspond to fluctuations in $T_{tr,x}$ given that $\sigma_{xx} = \rho RT_{tr,x}$ and density fluctuations are negligible. The original instantaneous signal is window-averaged with a moving time-window of $0.3 \mu\text{s}$ (100 timesteps) such that frequencies greater than 3.33 MHz are removed. The power spectral density (PSD) of this mean-subtracted, window-averaged signal reveals frequency content in fluctuations of σ_{xx} , as shown in Fig. 4.2. For spectral estimation here and elsewhere in the chapter, Welch's method [208, 209] is used in SciPy [6] library with two Hann-window weighted segments of data sampled with a frequency of 333 MHz prior to the Fast Fourier Transform (FFT) such that the frequency resolution is 0.9 kHz. In Sec. 4.7.2.2 the sensitivity of the PSD obtained using DSMC particle data to the value of F_n is discussed and it is shown that when F_n is set to unity (*i.e.*, no possible numerical amplification of noise), the main features of the non-dimensionalized low-frequency spectrum do not change.

At probe P , the PSD shows a broadband of low-frequencies that goes up to 90 kHz frequency, as shown in Fig. 4.2(a). This upper bound of the broadband is defined as the frequency at which the normalized cumulative energy (NCE), obtained from normalizing and cumulatively summing the PSD spectrum, exhibits an inflection point. This low-frequency broadband is defined by its weighted average of 37.5 kHz and a standard deviation of 21.4 kHz. Figure 4.2(b) shows the contours of PSD plotted on the axes X/λ_1 versus frequency created by interpolating the PSD data at each X/λ_1 location spatially separated by $X/\lambda_1 = 1$ in the Tecplot [4] software using the inverse-distance algorithm with default parameters (exponent=3.5, point selection=Octant, Number of points=8). The figure reveals that such low-frequency broadband is observed within $-6 < X/\lambda_1 < 3$, the region of strong translational nonequilibrium seen earlier in Fig. 4.1.

In contrast to the nonequilibrium region of the shock, Fig. 4.2(c) shows that the PSD at probe F in the freestream

contains widely distributed energy across the whole spectral limit of 166 MHz and does not exhibit a noticeable inflection point within this limit. It also shows that most of the spectral energy is concentrated near the frequency of 3.5 MHz, which is the inverse of the mean-collision-time of $0.284 \mu\text{s}$. This is consistent with the analysis of Kogan (see pg. 82, 124 of Ref. [34]) for a gas in absolute equilibrium (zero bulk velocity, constant temperature and number of particles), which showed that small perturbations to the velocity distribution function and its moments decay exponentially with a characteristic time-scale of mean collision time. Additionally, from the comparison of PSDs in Figs. 4.2(a) and 4.2(c), it can be noted that the low-frequency fluctuations in the shock have about two orders of magnitude larger amplitude than the freestream, and therefore, low-frequency fluctuations of shock may be even more important in laminar to turbulent transition of high-speed boundary-layers than, as commonly believed, freestream kinetic fluctuations. The order of magnitude differences in these time-scales of fluctuations will be explained by the new dynamics model discussed in Sec. 4.4.

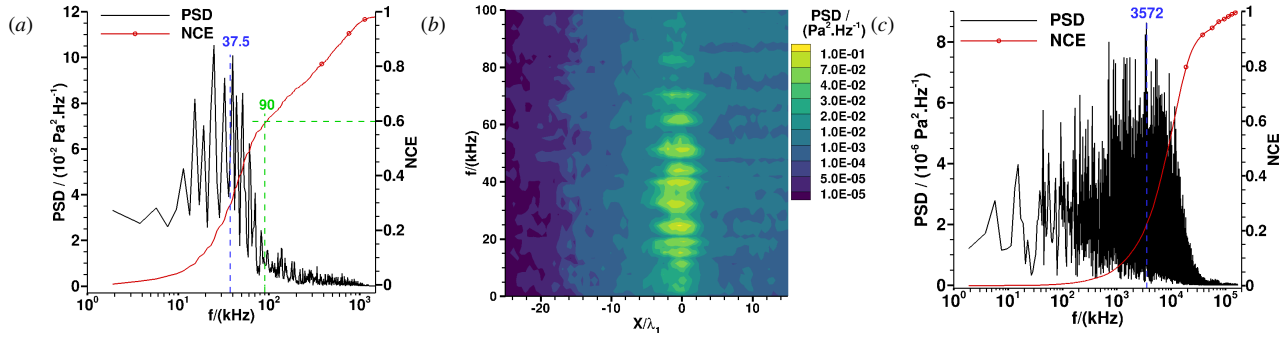


Figure 4.2: PSD of mean-subtracted, window-averaged σ_{xx} is shown inside the shock layer at probe P in (a), in the entire X/λ_1 space in (b), and in the freestream at probe F in (c). (a) and (c) also show NCE (see text).

The key to understanding the fluctuations in the overall stress, σ_{xx} , is to correlate the fluctuations in the PDF f_{ξ_x} of the normalized X -directional energy of particles, ξ_x , and its mean, μ . Note that $\xi_x = (v_x^2 - u_x^2)\beta^2$, where v_x is the X -directional instantaneous molecular velocity of particles, which is the sum of their bulk and thermal components, u_x and c_x , respectively. The mean, μ , is related to overall stress, σ_{xx} , as,

$$\mu = \int \xi_x f_{\xi_x} d\xi_x = \frac{\sigma_{xx}\beta^2}{\rho}$$

Figure 4.3 shows that the behavior of the PDF changes at different locations in the flow, *i.e.*, from the upstream to downstream regions relative to the shock, f_{ξ_x} changes from a nearly symmetric equilibrium distribution (Fig. 4.3(a)) to a one-sided, asymmetric equilibrium distribution (Fig. 4.3(b)). At the location of maximum density gradient in the shock (Fig. 4.3(c)), it can be seen that the density function is bimodal with an inflection point at $\xi_x = 1.33$, where the

portions $-0.86 < \xi_x < 1.33$ and $1.33 < \xi_x < 3.52$ have shapes similar to PDFs in the subsonic and hypersonic regions, shown in Figs. 4.3(b) and 4.3(a), respectively. Note that the bimodal PDF can be expressed as a linear combination of upstream and downstream contributions of equilibrium PDFs, [210] similar to the Mott-Smith model of the bimodal velocity distribution. [68]

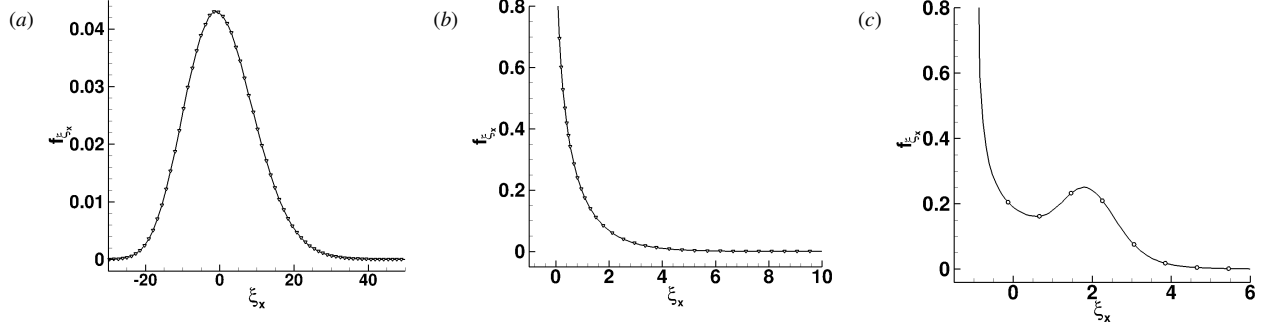


Figure 4.3: The PDF f_{ξ_x} at probes (a) F in the freestream, (b) D downstream, and (c) P inside the shock layer.

Towards that end, the cross-correlation coefficient of μ and the number of particles as a function of ξ_x is defined as,

$$c(\xi_x) = \frac{\sum_{w=0}^{w=W} \sum_{\xi_x=\min}^{\max} [N(\xi_x, w) - \langle N(\xi_x) \rangle_w] [\mu(w) - \langle \mu \rangle_w]}{W \Sigma_{N(\xi_x)} \Sigma_{\mu_{\xi_x}}} \quad (4.2)$$

where

$$\Sigma_{N(\xi_x)} = \sqrt{\frac{[N(\xi_x, w) - \langle N(\xi_x) \rangle_w]^2}{W}}$$

$$\Sigma_{\mu} = \sqrt{\frac{[\mu(w) - \langle \mu \rangle_w]^2}{W}}$$

Note that ξ_x is discretized into 200 energy bins from its minimum to maximum value. $N(\xi_x, w)$ is the total number of DSMC particles within the normalized X -directional energy space ξ_x and $\xi_x + \Delta\xi_x$ from time window w to $w + 1$, $\langle N(\xi_x) \rangle_w$ denotes the number of particles in the same energy space but averaged over time-windows, W . Similarly, $\mu(w)$ is the instantaneous mean of the PDF f_{ξ_x} , from time-window w to $w + 1$, whereas $\langle \mu \rangle_w$ is the mean computed by averaging over all time-windows. $\Sigma_{N(\xi_x)}$ and Σ_{μ} are the standard deviations in the fluctuations of $N(\xi_x, w)$ and $\mu(w)$ about their respective means. Figures 4.4(a) and 4.4(b) show the fluctuations in number of particles $[N(\xi_x, w) - \langle N(\xi_x) \rangle_w]$ in the energy space ξ_x at probes P and F , respectively.¹

¹The movies loop over time windows from -20 to 646, where $w = -20$ to 0 correspond to the transient time, which is not used in the calculation of cross-correlation coefficient and time-averaged means.

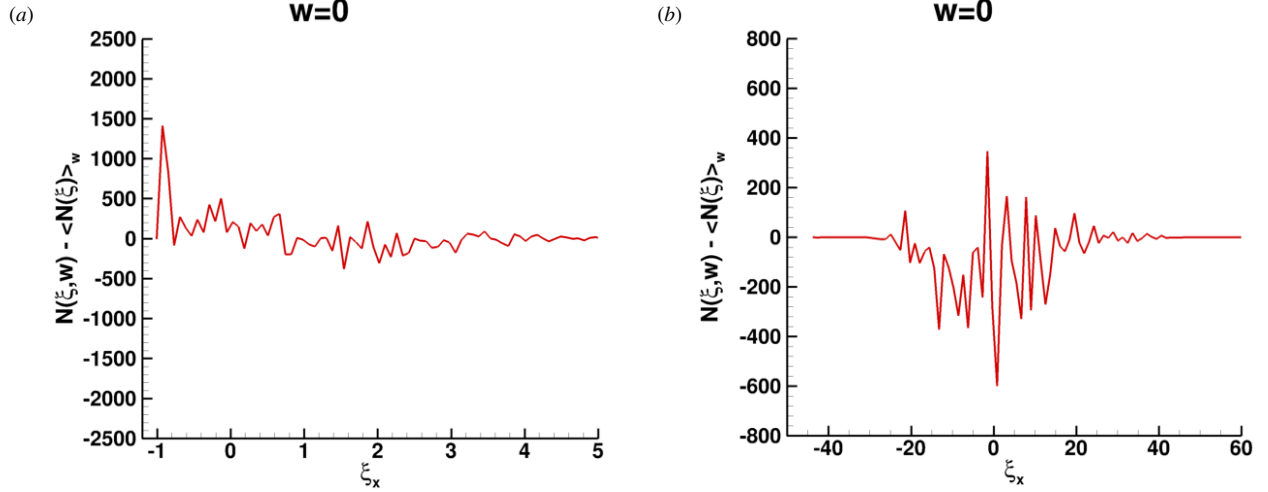


Figure 4.4: The fluctuations $[N(\xi_x, w) - \langle N(\xi_x) \rangle_w]$ as a function of ξ_x at probes (a) P inside the shock layer and (b) F in the freestream. (see multimedia view in the supplementary material of Ref. [227])

The analysis of the correlation functions combined with particle distributions suggests an approach for grouping of particles into a finite number of energy bins whose dynamics can then be further analysed. Starting with Fig. 4.5, the distribution of $c(\xi_x)$ at probes P , inside a shock, and F , in the freestream are compared. $c(\xi_x)$ is calculated using a total number of time windows, W , of 646, each representing a time interval of $0.3 \mu\text{s}$ starting from $t=6 \mu\text{s}$. At probe P , Fig. 4.5(a) shows that $c(\xi_x)$ has a strong negative correlation between $-0.86 < \xi_x < 1.33$ and positive correlation for $1.33 < \xi_x < 3.52$. Opposite signs of $c(\xi_x)$ means that particles in these parts lose and gain particles, respectively, when μ and σ_{xx} increase and vice versa, and understanding the underlying mechanisms in these regions, such as intermolecular collisions and flux exchange with adjacent cells, is necessary to understand fluctuations in σ_{xx} . These two zones in the energy space are denoted as energy bins ‘A’ and ‘B’, which are coarser than the size of the histogram bins, $\Delta\xi_x = 0.0115$, used to obtain smooth variations of f_{ξ_x} . We ignore the energy space beyond $\xi_x > 3.52$, because $c(\xi_x)$ remains negative but small in comparison to other two bins and the total average number of particles in this region is only 3.5% of total particles at probe P , which can be calculated from the cumulative sum of the distribution of average number of particles shown in Fig. 4.6(a). The demarcation between the coarse energy bins A and B is at $c(\xi_x) = 0$, which is also the location of inflection point. Examination of $c(\xi_x)$ for probe F in the freestream (see Fig. 4.5(b)) shows that, in contrast, the maximum magnitude of $c(\xi_x)$ is not more than 0.2, indicating that the fluctuations are random in nature and even if a strong correlation exists, it must be on time-scales smaller than the window size of $0.3 \mu\text{s}$ used to obtain $c(\xi_x)$. Comparison of the correlation functions at probes P and F also shows that the distribution of $c(\xi_x)$ at the latter location is almost symmetric about the inflection point at $\xi_x = 0$, which is consistent with the X -directional energy distribution having a nearly symmetric shape, as shown in Fig. 4.3(a).

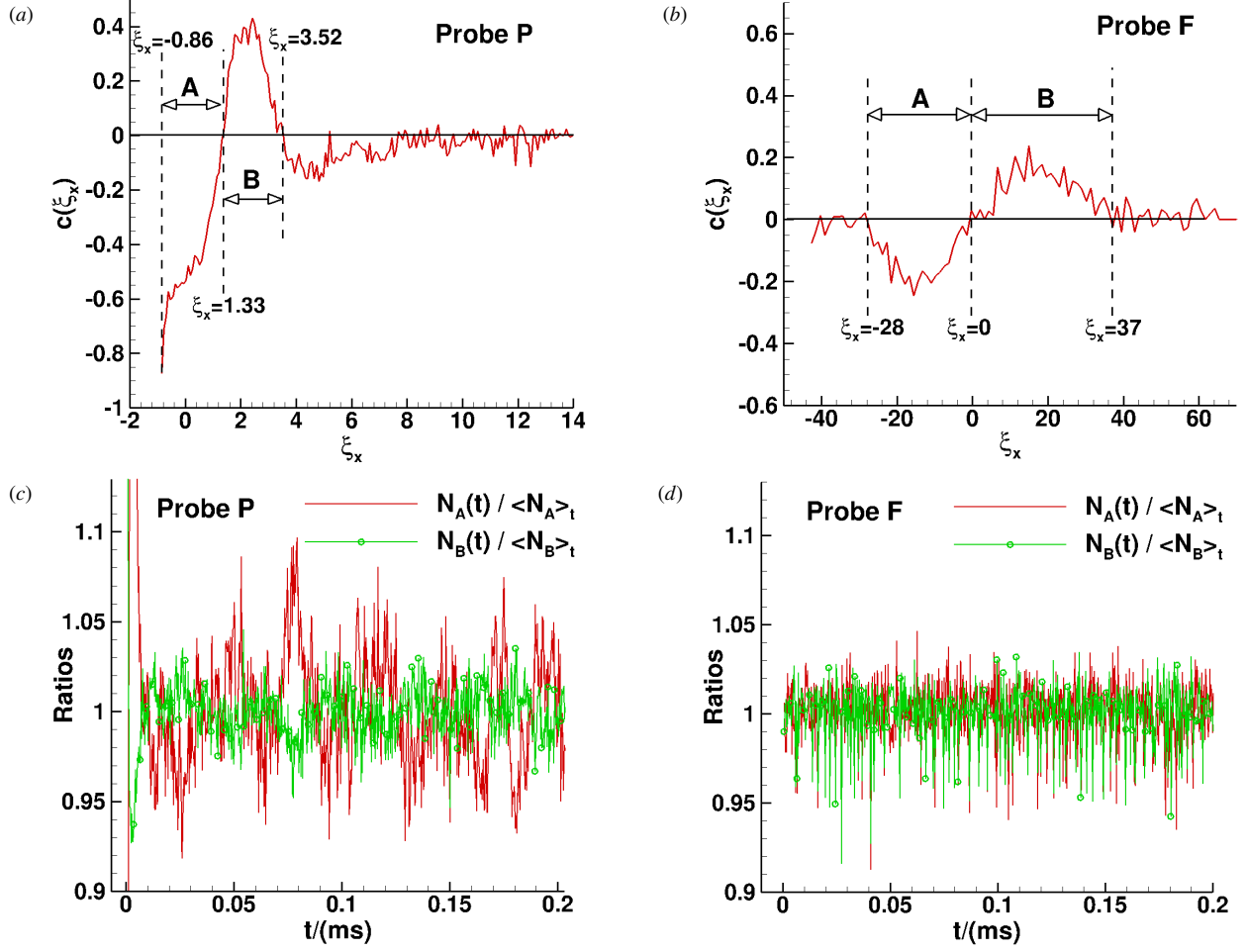


Figure 4.5: (a) and (b) show $c(\xi_x)$ calculated using Eq. (4.2), at probes P and F , respectively. Here and in subsequent figures, the bracket notation, $\langle Q \rangle_t$ denotes the time-average of a macroscopic quantity Q , in contrast to its instantaneous value. (c) and (d) show the ratios of instantaneous to time-averaged number of particles in bins A and B , i.e., $N_A/\langle N_A \rangle_t$ and $N_B/\langle N_B \rangle_t$, at probes P and F , respectively. To reduce statistical scatter, the instantaneous number of particles is averaged over a very small time interval of $0.3 \mu s$, whereas the time-averaged number of particles is averaged from $6 \mu s$ to 0.2 ms.

If we now group particles into two X -directional energy bins, A and B , which are denoted in Figs. 4.5(a) and 4.5(b) for probes P and F , respectively, we can study the ratios of the instantaneous to time averaged particles, $N_A/\langle N_A \rangle_t$ and $N_B/\langle N_B \rangle_t$ as a function of time at these two probes, as shown in Figs. 4.5(c) with 4.5(d). The average number of DSMC computational particles per computational cell in energy bins A and B are $\langle N_A \rangle_t = 1088$ and $\langle N_B \rangle_t = 611$ at probe P , and $\langle N_A \rangle_t = 510$ and $\langle N_B \rangle_t = 493$ at probe F , which can be converted to number density (m^{-3}) by multiplication of an $F_n = 1 \times 10^7$ and division by the volume of computational cell, $\Delta v = 1 \times 10^{-12} m^3$. From the comparison of

these two figures, it can be seen that fluctuations in these ratios are larger in magnitude and exhibit longer time-scales (0.01-0.05 ms) at probe P inside the shock in comparison to probe F in the freestream, where fluctuations appear to be random as their timescales are on the order of mean-collision-time of $0.284 \mu s$, smaller than the time interval used to time-average the signal ($0.3 \mu s$). The standard deviations in the fluctuations of the ratios $N_A/\langle N_A \rangle_t$ and $N_B/\langle N_B \rangle_t$ are 4.5 and 2.1%, respectively, at probe P, versus 1.8 and 1.6% at probe F. Additionally, a noticeable negative correlation between the fluctuations (out of phase fluctuations) of two energy bins at probe P can also be seen from Fig. 4.5(c), while such dynamics are absent at probe F.

Finally, to demonstrate the generality of the difference in properties between probes P and F, Fig. 4.6 shows a comparison of the time-averaged number of particles as a function of ξ_x at probes P and F, and at their respective left-adjacent computational cells. For probe P (Fig. 4.6(a)), two inflection points can be identified at $\xi_x = 1.33$ and 3.52 , where $c(\xi_x)$ changes sign. We can also see that the average number of particles in energy bin A is larger at probe P than in the cell to its left, whereas in bin B it is lower. This is consistent with the fact that from the upstream to downstream region inside a shock, the contribution of the upstream symmetric distribution decreases, while the downstream asymmetric distribution increases. At probe F (Fig. 4.6(b)), however, the PDF of energies does not change between adjacent cells and there is no inflection point.

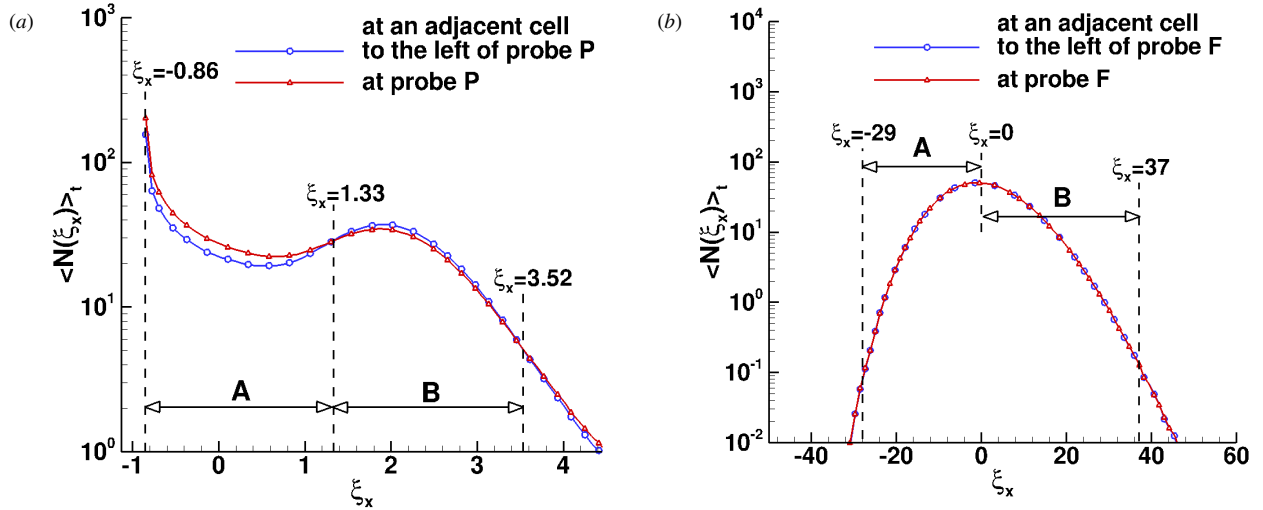


Figure 4.6: (a) and (b) show a comparison of the average number particles as a function of X-directional energy, $\langle N(\xi_x) \rangle_t$, at probes P and F, respectively, with those in an adjacent cell to their left. The time-averages are taken from $t=6 \mu s$ to 0.2 ms.

4.3 Collision Processes that Define the Two-Energy-Bin Model

Although the distribution of X -directional particle energies is continuous, we propose a two-bin model to understand the role of particle collisions between the two bins, A and B , and how they induce low-frequency time dynamics in fluctuations of macroscopic flow parameters such as normalized overall stress, σ_{xx} , inside a shock. We first develop a simple two energy-bin model similar to the Lotka-Volterra's predator-prey model. [204–206] We then evaluate the collisions rate coefficients for different energy transfer processes using the DSMC particle distribution data, and show that instead of sustained particle oscillations, the solution to our ODE contains dampening terms that cause the periodic fluctuations to die out on time-scales an order of magnitude longer than the period of oscillation.

4.3.1 The two-bin energy model

The dynamics of the number of particles in energy bins A and B may be written as,

$$\begin{aligned}\frac{dN_A}{dt} &= \left[\frac{dN_A}{dt} \right]_{coll} + F_A N_A \\ \frac{dN_B}{dt} &= \left[\frac{dN_B}{dt} \right]_{coll} + F_B N_B\end{aligned}\tag{4.3}$$

where the first and second terms on the right are the change in number of particles due to collisions and fluxes, respectively. In addition, since the average number of particles in energy bins A and B constitute 96.5% of the total particles, we can assume them to be mutually exclusive and write,

$$\left[\frac{dN_A}{dt} \right]_{coll} = - \left[\frac{dN_B}{dt} \right]_{coll}\tag{4.4}$$

The flux coefficient F_j for bin ' j ' is defined as the difference between the net average influx from the left boundary and outflux from the right boundary of the ' j '-type particles per second divided by the average number of ' j '-type particles,

$$F_j = \frac{(N_j^{l,in} - N_j^{l,out}) - (N_j^{r,out} - N_j^{r,in})}{\Delta t \langle N_j \rangle_t}, \quad j \in \{A, B\}\tag{4.5}$$

where, Δt is the DSMC timestep, superscripts ' l ' and ' r ' refer to the left and right boundaries of the computational cell, respectively, and 'in' and 'out' refer to the incoming and outgoing particles, respectively, as shown in Fig. 4.7 for location P and energy bins A and B .

Flux coefficients are required in the evaluation of Eq. (4.3). Using the values of A and B -type particles given

in Table 4.1, flux values of F_A and $F_B = -1,277,925.8$ and $2,500,681.6 \text{ s}^{-1}$, respectively, at probe P and zero in the freestream (as expected) are obtained. To make sure that the predictions of the model are not affected by instantaneous fluctuations or their numerical amplification, the DSMC-derived fluxes provided in Table 4.1 are temporally averaged from $6 \mu\text{s}$ to 0.21 ms , a time-period ~ 8 times longer than the time-scale corresponding to the average low-frequency observed in the PSD. Note that at probe P , $F_A < 0$ because on average more A -type particles travel to a cell downstream than came in from the upstream, as also seen from Fig. 4.6(a). The opposite is true for type- B particles, resulting in $F_B > 0$. This is synonymous with the fact that if there were no collisions, i.e., $\left[\frac{dN_A}{dt} \right]_{coll} = 0$, the number of A particles, those that mainly represent the subsonic part of the bimodal distribution, would decrease, while the number of B particles, those that mainly represent the upstream hypersonic flow, would increase.

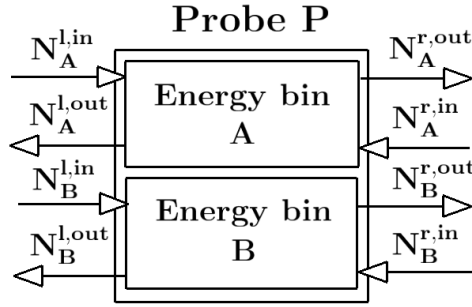


Figure 4.7: A sketch denoting number of particles coming in and going out through the left and right boundary in a two-energy-bin model.

Probes	$N_A^{l,in}$	$N_A^{l,out}$	$N_A^{r,out}$	$N_A^{r,in}$	$N_B^{l,in}$	$N_B^{l,out}$	$N_B^{r,out}$	$N_B^{r,in}$
P	41.46	7.19	47.40	8.96	69.84	0.68	65.37	0.80
F	49.28	0	49.28	0.0	58.63	0.0	58.63	0.0

Table 4.1: Average fluxes of DSMC computational particles per timestep and computational cell area of $1 \times 10^{-8} \text{ m}^2$.

To evaluate the collision terms in Eq. (4.3), we need to identify all possible collision processes that can cause a loss or gain of type- A and - B particles. Note that different collision processes can occur at different rates which could change the dynamics of particle exchange between the two bins and consequently the time-scale of fluctuations in σ_{xx} . Such collision processes are listed in column two of Table 4.2, where the *type* of A particle is labeled based on the collision process that it undergoes, denoted by a subscript ‘ i ’, the relevant pre-and post-collisional states are specified where the latter is denoted by a primed superscript, and the rate coefficient for each *fundamental* collision process, k_i ,

unless it is a “compound” rate which is denoted by a tilde. The table shows that there are six fundamental processes (2nd column) and eight types of A particles, $A_a, A'_b, A_c, A'_c, A_d, A'_d, A'_e$, and A_f , that can cause a net change in the number of particles in energy bins A and B . For example, A'_b particles are the postcollisional particles located in energy bin A that are formed due to the collision process b , while A_c are the precollisional particles in energy bin A that take part in collision process c . Using the DSMC-derived PDFs for all sub-types of type- A particles of the normalized X -directional energy, $\xi_x = (v_x^2 - u_x^2)\beta^2$, and total transverse energy, $\xi_y + \xi_z = (v_y^2 + v_z^2)\beta^2$, denoted by $f_{\xi_x}^A$ and $f_{\xi_y+\xi_z}^A$, respectively (Fig. 4.8), we can reduce the number of types of A particles further, which allows us to write processes p_i (column two) in the form of processes P_i (column three). In what follows, we describe the grouping of processes p_i to processes P_i (column 3) and then their further simplification to processes Q_i (column 4).

Collision process p_a describes a mechanism for type- A_a particles in energy bin A that collide with particles in energy bin B and now belong to bin B resulting in the loss of type- A particles. Simultaneously, process p_b describes the collision process of two bin B particles that causes one of them to move to energy bin A leading to a gain of type- A particles, denoted by A'_b . However, Figs. 4.8(a) and 4.8(b) show that at location P the energy distributions $f_{\xi_x}^A$ and $f_{\xi_y+\xi_z}^A$ for A_a and A_b particles are the same. Therefore, we can group A_b and A_a -type particles and write the second reaction P_b as shown in column three of Table 4.2. The same holds true for probe F as shown in Figs. 4.8(c) and 4.8(d), however, the distributions different from those at probe P .

We can also group all collisions between type- A particles that do not lead to a net change in the energy distribution of particles within bin A as process p_h and see from Fig. 4.8 that the energy distributions of all such type- A particles before and after collisions, A_h and A'_h , is the same at probe P as well as F . Note that at probe F , the distribution $f_{\xi_y+\xi_z}^A$ for A_a -type particles matches with the A_h -type, *i.e.*, in the freestream the transverse energy of particles taking part in processes P_a and P_b is the same as those in P_h . The differences at probe P indicate the role of transverse translational modes in the collision processes P_a and P_b . Similar to process p_h , process p_g , is a bin-exchange process, which causes no net change in the number of particles in bins A and B . Particles simply swap energy bins by exchanging X -directional energies.

Turning to collision processes p_c and p_d , Fig. 4.8 shows that the energy distributions of A_c and A'_d are very similar at probes P and F , so that A'_d -type particles can be considered to be the same as those of A_c . Additionally, although the distributions $f_{\xi_x}^A$ and $f_{\xi_y+\xi_z}^A$ of A'_c and A_d particles is the same at probe F , they are slightly different at probe P at high ξ_x and low $\xi_y + \xi_z$ energies. This occurs because when A_c and B -type particles collide, the B particle loses its X -directional energy which results in the increase of not only the ξ_x of the A_c -type particle but also a noticeable increase in its $\xi_y + \xi_z$ energy, as can be seen in the transverse energy distributions of A'_c -type particles in Figs. 4.8(b) at probe P . Also, when two A_d particles collide, one of them is switched from energy bin A to bin B at the expense

of higher transverse energy of the other A_d particle that remains in bin A . In the freestream, since these two A_d -type particles are the same A'_c -type particles that were generated from process p_c , their transverse energy distributions exactly match, as seen in Fig. 4.8(d). However, at probe P , it is also possible that only one of the two A_d particles is an A'_c -type, and the other one has lower transverse and higher X -directional energy than the A'_c -type particle, as can be seen in the *slightly* larger X -directional energy distribution of A_d -type particles than the A'_c -type in Fig. 4.8(a) between $0.5 < \xi_x < 1.33$. We demonstrate that small distinctions such as this do not affect the dynamics of the system and assume that $A'_c \sim A_d$ to construct processes P_c and P_d given in Table 4.2.

Similarly, we can describe the process p_e , where the particles of type- A'_e have a very different transverse energy distributions shown in Figs. 4.8(b) than the other type- A particles at probes P . This process does not occur at probe F . Ignoring the differences at low transverse energies, the distribution of A'_e and A_f particles is the same, as shown in Fig. 4.8(b), therefore they can be denoted by the same identifier A'_e .

Id	Detailed collision process	Collision process	
		after grouping alike A-particles	Simplified collision process
i	P _i	P _i	Q _i
a	$A_a + B \xrightarrow{k_a} B + B$	$A_a + B \xrightarrow{k_a} B + B$	$A + B \xrightarrow{\tilde{k}_a} B + B$
b	$B + B \xrightarrow{k_b} A_b' + B$	$B + B \xrightarrow{k_b} A_a + B$	$B + B \xrightarrow{k_b} A + B$
c	$A_c + B \xrightarrow{k_c} A_c' + A_c'$	$A_c + B \xrightarrow{k_c} A_c' + A_c'$	$A + B \xleftarrow{\tilde{k}_c} A_c' + A_c'$
d	$A_d + A_d \xrightarrow{k_d} A_d' + B$	$A_c' + A_c' \xrightarrow{k_d} A_c + B$	-
e	$B + B \xrightarrow{k_e} A_e' + A_e'$	$B + B \xrightarrow{k_e} A_e' + A_e'$	$B + B \xrightarrow{k_e} A_e' + A_e'$
f	$A_f + A_f \xrightarrow{k_f} B + B$	$A_e' + A_e' \xrightarrow{k_f} B + B$	-
g ¹	$A_g + B \xrightarrow{k_g} B + A_g'$	$A_g + B \xrightarrow{k_g} B + A_g$	-
h ¹	$A_h + A_h \xrightarrow{k_h} A_h' + A_h'$	$A_h + A_h \xrightarrow{k_h} A_h + A_h$	-
i ¹	$B + B \xrightarrow{k_i} B + B$	$B + B \xrightarrow{k_i} B + B$	-

¹ These processes cause no net change in the number of particles of energy bins A and B .

Table 4.2: Detailed and simplified collision processes.

To complete the dynamical model for particles moving between energy bins A and B , an expression is required for the net change in the number of particles in energy bin A due to collisions from all possible processes related to A -type

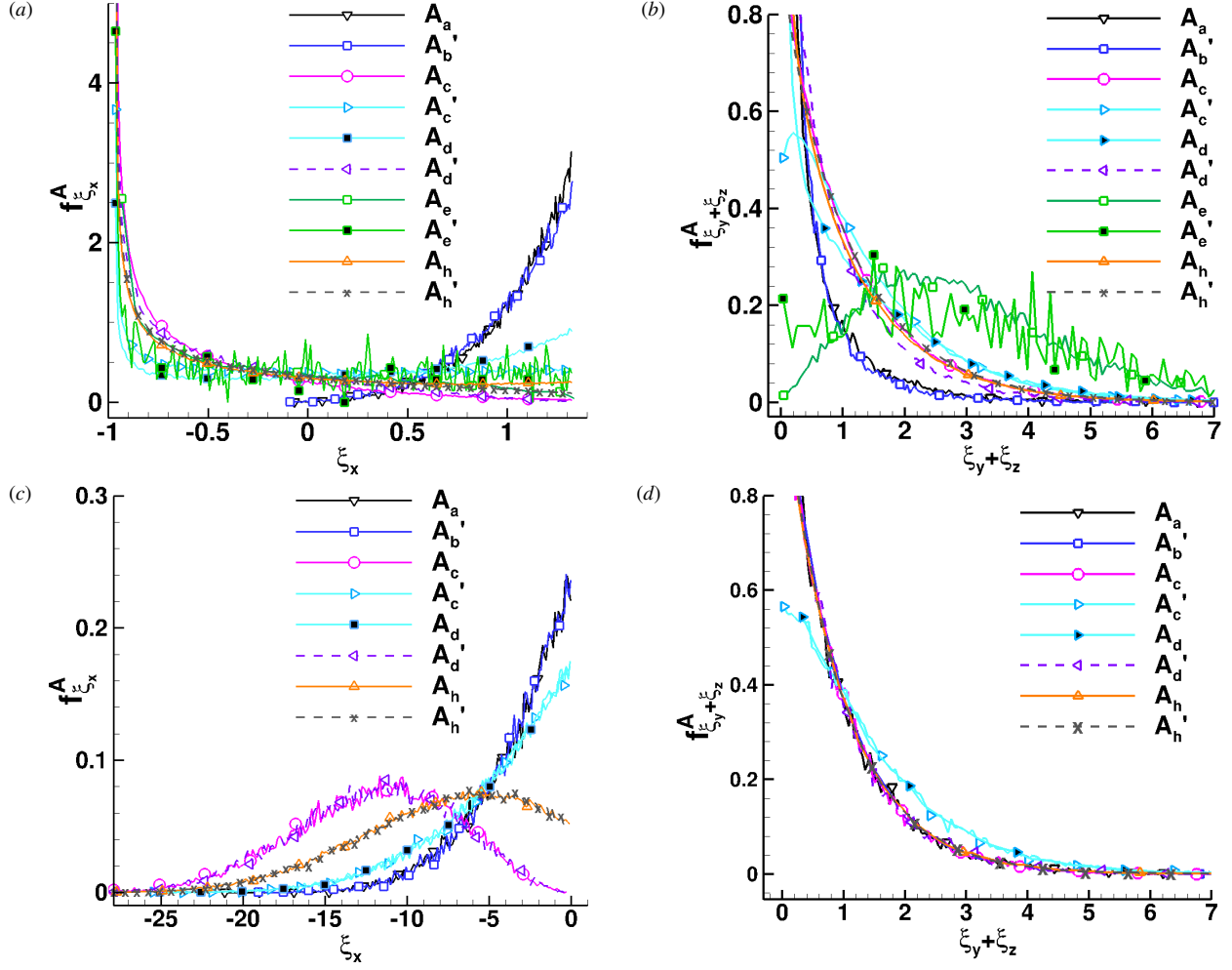


Figure 4.8: (a) and (b) show, at Probe P , the PDFs $f_{\xi_x}^A$ and $f_{\xi_y+\xi_z}^A$ of all sub-types of type-A particles distinguished based on detailed collision processes listed in Table 4.2. Note that $f_{\xi_x}^A$ is obtained by further refining the X -directional energy space of bin A ($-0.86 < \xi_x < 1.33$) with a resolution of $\Delta\xi_x = 0.0115$. Same resolution was used for the transverse energy space. (c) and (d) show the respective plots for probe F .

particles, *i.e.*,

$$\left[\frac{dN_A}{dt} \right]_{coll} = \left[\frac{dN_{A_a}}{dt} \right]_{coll} + \left[\frac{dN_{A_c}}{dt} \right]_{coll} + \left[\frac{dN_{A'_c}}{dt} \right]_{coll} + \left[\frac{dN_{A'_e}}{dt} \right]_{coll} \quad (4.6)$$

where N_{A_a} , N_{A_c} , $N_{A'_c}$, and $N_{A'_e}$ are the number of particles of A_a , A_c , A'_c , and A'_e types, respectively, which are defined based on P_i processes. Using standard rate equation formulations for elementary reactions (see Sec. 16.15 of Ref. andersonModern), the terms on the right hand side can be expressed as,

$$\begin{aligned} \left[\frac{dN_{A_a}}{dt} \right]_{coll} &= -k_a N_{A_a} N_B + k_b N_B^2 \\ \left[\frac{dN_{A_c}}{dt} \right]_{coll} &= -k_c N_{A_c} N_B + k_d N_{A'_c}^2 \\ \left[\frac{dN_{A'_c}}{dt} \right]_{coll} &= 2k_c N_{A_c} N_B - 2k_d N_{A'_c}^2 \\ \left[\frac{dN_{A'_e}}{dt} \right]_{coll} &= 2k_e N_B^2 - 2k_f N_{A'_e}^2 \end{aligned} \quad (4.7)$$

By substituting Eq. (4.7) in (4.6), we obtain,

$$\begin{aligned} \left[\frac{dN_A}{dt} \right]_{coll} &= -k_a N_{A_a} N_B + k_b N_B^2 + k_c N_{A_c} N_B - k_d N_{A'_c}^2 \\ &\quad + 2k_e N_B^2 - 2k_f N_{A'_e}^2 \end{aligned} \quad (4.8)$$

Furthermore, the conditions in the 1-D shock allow us to make additional simplifications to Eq. (4.8) by reducing six collision processes (P_i) given in Table 4.2 to four processes (Q_i) as follows. To construct compound collision processes, Q_i we start with the rate coefficient k_i for process P_i which can be evaluated from the DSMC simulation as,

$$k_i = \frac{\langle C_i \rangle_t}{\Delta t \langle N_{R_1} \rangle_t \langle N_{R_2} \rangle_t} \quad (4.9)$$

where the collision takes place with between particle types R_1 and R_2 . $\langle C_i \rangle_t$ for collision processes defined in Table 4.2 are listed in Table 4.4. Using the definition of rates k_a and k_b , the first kinetic equation in Eq. (4.7) can be written as,

$$\begin{aligned} \left[\frac{dN_{A_a}}{dt} \right]_{coll} &\approx -\frac{\langle C_a \rangle_t}{\Delta t \langle N_A \rangle_t \langle N_B \rangle_t} N_A N_B + \frac{\langle C_b \rangle_t}{\Delta t \langle N_B \rangle_t^2} N_B^2 \\ \left[\frac{dN_{A_a}}{dt} \right]_{coll} &\approx -\tilde{k}_a N_A N_B + k_b N_B^2 \end{aligned} \quad (4.10)$$

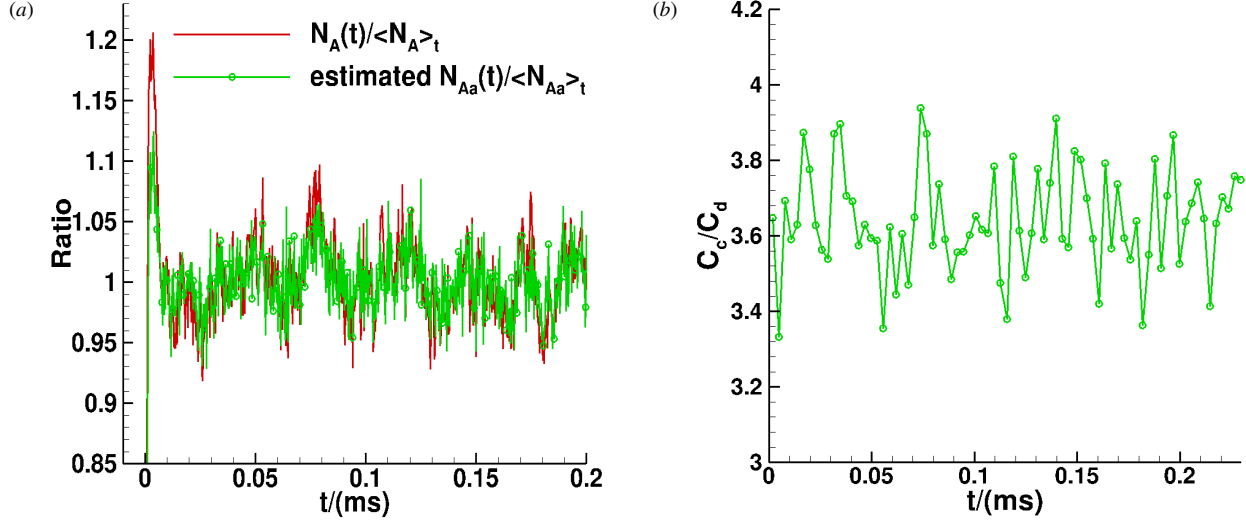


Figure 4.9: (a) and (b) show, at probe P , the comparison of time variation of ratio $N_{Aa}/\langle N_{Aa} \rangle_t$ with $N_A/\langle N_A \rangle_t$ and the time variation of ratio of collisions C_c/C_d , respectively, to justify assumptions in Eqs. (4.11) and (4.13), respectively. The data points in (a) and (b) are obtained by taking time-averages over a time window of 0.3 and 3 μs , respectively, to reduce statistical scatter.

where we have used the fact that,

$$\frac{N_{Aa}}{\langle N_{Aa} \rangle_t} \approx \frac{N_A}{\langle N_A \rangle_t} \quad (4.11)$$

as shown in Fig. 4.9(a). The ratio $N_{Aa}/\langle N_{Aa} \rangle_t$ is estimated from Fig. 4.8(a) by obtaining the number of particles between $0.0 < \xi_x < 1.33$ at probe P . At probe F , the ratio of $N_{Aa}/\langle N_A \rangle_t$ cannot be directly estimated from Fig. 4.8(c) because the distribution of A_a -type particles overlaps with other A -type particles. Yet, Eq. (4.11) is assumed to hold true under the assumption that the entire X -directional energy zone $-28 < \xi_x < 0$ is coarsened into a single bin A .

Using the definitions of rates k_c and k_d , the second kinetic equation in Eq. (4.7) can be written as,

$$\left[\frac{dN_{A_c}}{dt} \right]_{coll} = -\frac{\langle C_c \rangle_t}{\Delta t \langle N_{A_c} \rangle_t \langle N_B \rangle_t} N_{A_c} N_B + \frac{\langle C_d \rangle_t}{\Delta t \langle N_{A'_c} \rangle_t^2} N_{A_c}^2 \quad (4.12)$$

Since the average number of A'_c particles are not known, it is difficult to estimate the second term on the right hand side. However, this term can be simplified by observing from Fig. 4.9(b) that the ratio of rates C_c/C_d does not vary significantly from the average rates at probe P , i.e.,

$$\frac{C_c}{C_d} \approx \frac{\langle C_c \rangle_t}{\langle C_d \rangle_t} \quad (4.13)$$

and the standard deviation in the fluctuation of the ratio of C_c/C_d is only 3.7% of the average ratio of 3.63 for probe P and 4.2% of an average ratio of one for probe F . Using Eq. (4.9) for C_c and C_d in 4.13, and the definition of k_c based

on the average rate, we obtain,

$$k_d N_{A_c}^2 \approx \frac{\langle C_d \rangle_t}{\Delta t \langle N_{A_c} \rangle_t \langle N_B \rangle_t} N_{A_c} N_B \quad (4.14)$$

In addition, we can see from Figs. 4.8(a) and 4.8(b) that the A_c particles have the same energy distributions as the A_h at probe P , which implies that any particle that takes part in process P_c can take part in process P_h and together they constitute 72.37% of total collisions in which the particles in energy bin A take part. Therefore, we can expect the changes in the ratio $N_{A_c} / \langle N_{A_c} \rangle_t$ are correlated with the changes in ratio $N_A / \langle N_A \rangle_t$ and write,

$$\begin{aligned} \left[\frac{dN_{A_c}}{dt} \right]_{coll} &\approx - \frac{\langle C_c \rangle_t - \langle C_d \rangle_t}{\Delta t \langle N_A \rangle_t \langle N_B \rangle_t} N_A N_B \\ &\approx -\tilde{k}_c N_A N_B \end{aligned} \quad (4.15)$$

The same assumption holds at probe F because the A_c -type particles constitute the majority of particles from $-20 < \xi_x < -5$, which is a significant portion of energy bin A ($-28 < \xi_x < 0$), as seen from Fig. 4.8(c).

By using the aforementioned assumptions, the third kinetic equation in Eq. (4.7) becomes,

$$\begin{aligned} \left[\frac{dN_{A_c}}{dt} \right]_{coll} &= 2k_c N_{A_c} N_B - 2k_d N_{A_c}^2 \\ &\approx 2\tilde{k}_c N_A N_B \end{aligned} \quad (4.16)$$

We also drop the second term on the right hand side of the fourth kinetic equation in Eq. (4.7) because $\langle C_e \rangle_t \gg \langle C_f \rangle_t$.

Note that both $\langle C_e \rangle_t = \langle C_f \rangle_t = 0$ at probe F .

By substituting Eqs. (4.10), (4.15), and (4.16), into Eq. (4.8), we obtain,

$$\left[\frac{dN_A}{dt} \right]_{coll} = -\tilde{k}_a N_A N_B + k_b N_B^2 + \tilde{k}_c N_A N_B + 2k_e N_B^2 \quad (4.17)$$

which when substituted into Eqs. (4.3) and (4.4) gives the final system of dynamic equations,

$$\begin{aligned} \frac{dN_A}{dt} &= (\tilde{k}_c - \tilde{k}_a) N_A N_B + (k_b + 2k_e) N_B^2 + F_A N_A \\ \frac{dN_B}{dt} &= -(\tilde{k}_c - \tilde{k}_a) N_A N_B - (k_b + 2k_e) N_B^2 + F_B N_B \end{aligned} \quad (4.18)$$

4.3.2 Evaluation of rate coefficients

Finally, to solve the dynamical system of equations we need to evaluate the rate coefficients in Eq. (4.18). A summary of the expressions for the rate coefficients used in Eq. (4.18) and their values are presented in Table 4.3 for probes P and F based on the DSMC collision data collected during the simulation, summarized in Table 4.4. Note that $\langle C_i \rangle_t$ is

the average number of DSMC collisions per timestep per cell volume that take part in the i^{th} detailed collision process of particle types R_1 and R_2 (see. Eq. (4.9)). Similar to the flux coefficients, $\langle C_i \rangle_t$ were temporally averaged from $6 \mu s$ to $0.21 ms$. The rate coefficients $k/(s^{-1})$ shown in Table 4.3 can be converted to the traditional units of $K/(m^3.s^{-1})$ by multiplying them with the volume of computational cell, $\Delta v = 1 \times 10^{-12} m^3$, and dividing by the parameter, $F_n = 1 \times 10^7$. By this conversion, it can be easily shown that the rates $\tilde{K}_a, K_b$ range from $1.8 - 5.0 \times 10^{-17} m^3.s^{-1}$ at probes P and F .

Rate coefficient	Formula	Probe P	Probe F
$\tilde{k}_a$	$\langle C_a \rangle_t / \Delta t \langle N_A \rangle_t \langle N_B \rangle_t$	188.9	497.0
k_b	$\langle C_b \rangle_t / \Delta t \langle N_B \rangle_t^2$	417.5	513.5
$\tilde{k}_c$	$(\langle C_c \rangle_t - \langle C_d \rangle_t) / \Delta t \langle N_A \rangle_t \langle N_B \rangle_t$	1843.5	0
k_e	$\langle C_e \rangle_t / \Delta t \langle N_B \rangle_t^2$	75.0	0

Table 4.3: Rate coefficients per second for collision processes defined in Table 4.2.

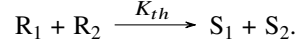
Probes	$\langle C_a \rangle_t$	$\langle C_b \rangle_t$	$\langle C_c \rangle_t$	$\langle C_d \rangle_t$	$\langle C_e \rangle_t$	$\langle C_f \rangle_t$	$\langle C_g \rangle_t$	$\langle C_h \rangle_t$	$\langle C_i \rangle_t$
P	0.377	0.468	5.074	1.396	0.084	0.0079	2.980	8.849	1.481
F	0.375	0.374	0.382	0.383	0.0	0.0	1.028	0.893	0.887

Table 4.4: Average number of DSMC collisions per timestep per computational cell volume, $\langle C_i \rangle_t$.

Note that in the freestream, $\langle C_a \rangle_t \approx \langle C_b \rangle_t$, due to detailed balance in a local equilibrium condition, which dictates that each detailed collision must be balanced by its inverse collision process (see pg. 38-39, 43 of Ref. [91]). Furthermore, the net rate, $\tilde{k}_c$ is nearly zero in the freestream because again by principle of detailed balance, $\langle C_c \rangle_t \approx \langle C_d \rangle_t$, as shown in Table 4.4. On the other hand, in the shock, a factor of 3.63 difference between the average values of these two types of collisions results in $\tilde{K}_c = 1.83 \times 10^{-16} m^3.s^{-1}$. Also, from Table 4.4 it can be seen that both $\langle C_e \rangle_t$ and $\langle C_f \rangle_t$ are zero in the freestream, which means that these processes take place only in conditions of translational nonequilibrium. As a result, the rate K_e is zero in the freestream, whereas in the shock it is two-orders of magnitude slower, $7.5 \times 10^{-18} m^3.s^{-1}$, than $\tilde{K}_c$.

The rate coefficients given in Table 4.3 can be compared with theoretical estimate of a rate coefficient, K_{th} , for a

forward collision process of a quasi-equilibrium gas (see pg. 213-216 of Ref. [91]), which is defined as,



The rate of change of R_1 -type particles per unit volume due to collisions is written as,

$$\left[\frac{dn_{R_1}}{dt} \right]_{coll} = K_{th} n_{R_1} n_{R_2}$$

where n_{R_1} and n_{R_2} are number densities of R_1 and R_2 type particles, respectively. For a gas following the VHS molecular model, the rate coefficient K_{th} can be expressed as,

$$K_{th} = \frac{1}{\varepsilon} \langle \sigma \rangle_t \langle g_r \rangle_t \gamma \quad (4.19)$$

where

$$\begin{aligned} \langle \sigma \rangle_t &= \pi d_r^2 \left(\frac{2\kappa_b T_r}{m_r \langle g_r \rangle_t^2} \right)^{\omega-0.5} [\Gamma(2.5 - \omega)]^{-1} \\ \langle g_r \rangle_t &= \left(\frac{8\kappa_b \langle T_{tr} \rangle_t}{\pi m_r} \right)^{\frac{1}{2}} \\ \gamma &= \left[\frac{1}{\Gamma\left(\frac{5}{2} - \omega\right)} \left(\Gamma\left(\frac{5}{2} - \omega, \frac{E_a}{\kappa_b \langle T_{tr} \rangle_t}\right) - \frac{E_a}{\kappa_b \langle T_{tr} \rangle_t} \Gamma\left(\frac{3}{2} - \omega, \frac{E_a}{\kappa_b \langle T_{tr} \rangle_t}\right) \right) \right] \\ E_a &= \frac{1}{2} m_r \langle g_r \rangle_t^2 \end{aligned}$$

where $\langle \sigma \rangle_t$ is the average equilibrium collision cross-section for the VHS gas, $\langle g_r \rangle_t$ is the time-averaged relative velocity, γ is the fraction of collisions for which the relative translational energy along the line of centers of colliding molecules exceeds the activation energy of E_a (see Sec. 6.2 and Eq. (4.72) of Ref. [37]), and Γ is the gamma function. Also, m_r is the reduced mass (see Eq. (2.7) of Ref. bird:94mgd), d is the VHS molecular diameter (see Eq. (4.63) Ref. [37]), and ε is a symmetry factor equal to two because $R_1=R_2$. Table 4.5 shows that the estimated parameters in Eq. (4.19) and average rate coefficients at probes P and F located inside the shock and the freestream, respectively, are consistent with the values presented in Table 4.3.

Parameters	At Probe P	At Probe F
$\langle T_{tr} \rangle_t / (\text{K})$	10,440	710
$\langle g_r \rangle_t / (\text{m.s}^{-1})$	3326.2	867.6
$\langle \sigma \rangle_t / (\text{m}^2)$	1.81×10^{-19}	4.16×10^{-19}
$E_a / (\text{J})$	1.83×10^{-19}	1.25×10^{-20}
γ	0.351	0.351
$K_{th}^1 / (\text{m}^3.\text{s}^{-1})$	1.05×10^{-16}	6.33×10^{-17}

Table 4.5: Parameters used in Eq. (4.19) for the theoretical estimate of average rate coefficient.

4.4 Dynamics of Energy Fluctuations Inside a Shock using the Two-Energy-Bin Model

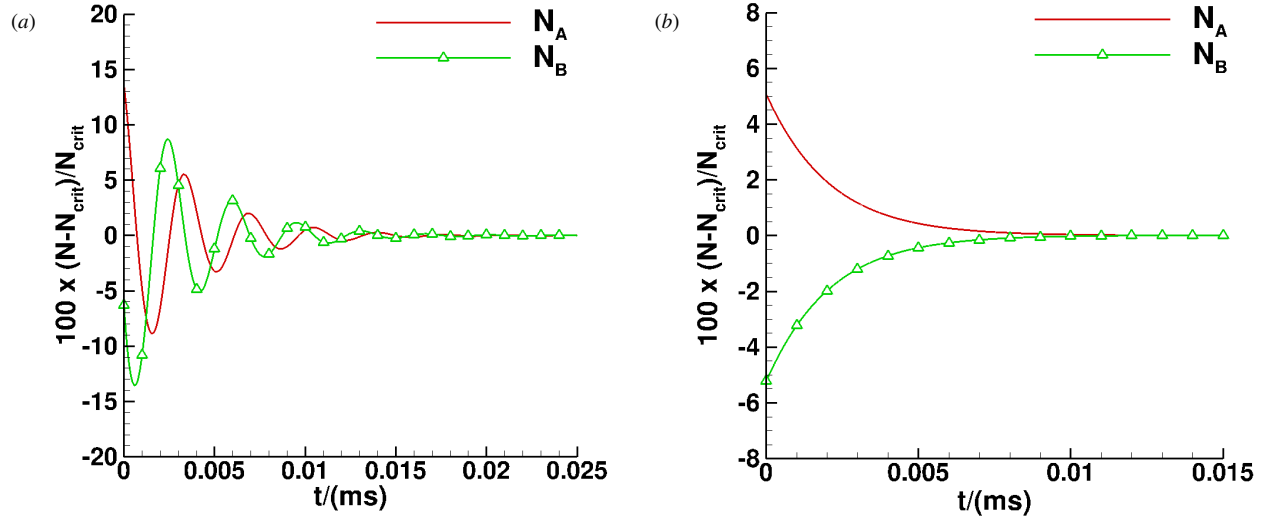


Figure 4.10: (a) and (b) show the solution of the two-energy-bin ODE model at probes P and F , respectively. The initial values of N_A and N_B are taken to be +13.5 and -6.3% of the critical values, respectively, at probe P , and +5.4 and -4.8% of the critical values, respectively, at probe F . These values are three times the percent standard deviation observed from the DSMC simulation in the ratios of $N_A / \langle N_A \rangle_t$ and $N_B / \langle N_B \rangle_t$.

The numerical solution of the ODE system in Eq. (4.18) at probes P and F is shown in Fig. 4.10 as a function of time and in Fig. 4.11 as path-lines in the phase space of N_A versus N_B . Starting with location P , Fig. 4.10(a) shows that

the solution converges to the non-zero critical values of $N_{A,crit}$ and $N_{B,crit}$, obtained by setting $dN_A/dt = dN_B/dt = 0$ which are listed in Table 4.6. There is 18.2 and 7.5% difference between the critical values and the average number of DSMC particles per computational cell volume in bins A and B at probe P , which may be attributed to the simplifications of the two-energy-bin model discussed above. Yet, as will be shown, this simple model reveals two orders of magnitude disparity in frequencies at probes P and F . Figure 4.11(a) shows the streamlines of a vector field defined by the normalized growth rate vector $\mathbf{G} = [G_{N_A}, G_{N_B}]^T$ with components,

$$G_{N_i} = \frac{1}{\|\mathbf{G}\|} \frac{dN_i}{dt}, \quad i = A \text{ or } B \text{ and } \|\mathbf{G}\| = \sqrt{\left(\frac{dN_A}{dt}\right)^2 + \left(\frac{dN_B}{dt}\right)^2} \quad (4.20)$$

We can see from the formation of a stable spiral that the critical point does not depend on the initial values. The figure shows that the streamlines are tangent to the direction of the maximum growth vector at a given location of (N_A, N_B) and show eventual decay to the stable critical point of 1245 and 681. The overlaid path-line in Fig. 4.11(a) describes these dynamics for the instantaneous solution shown in Fig. 4.10(a).

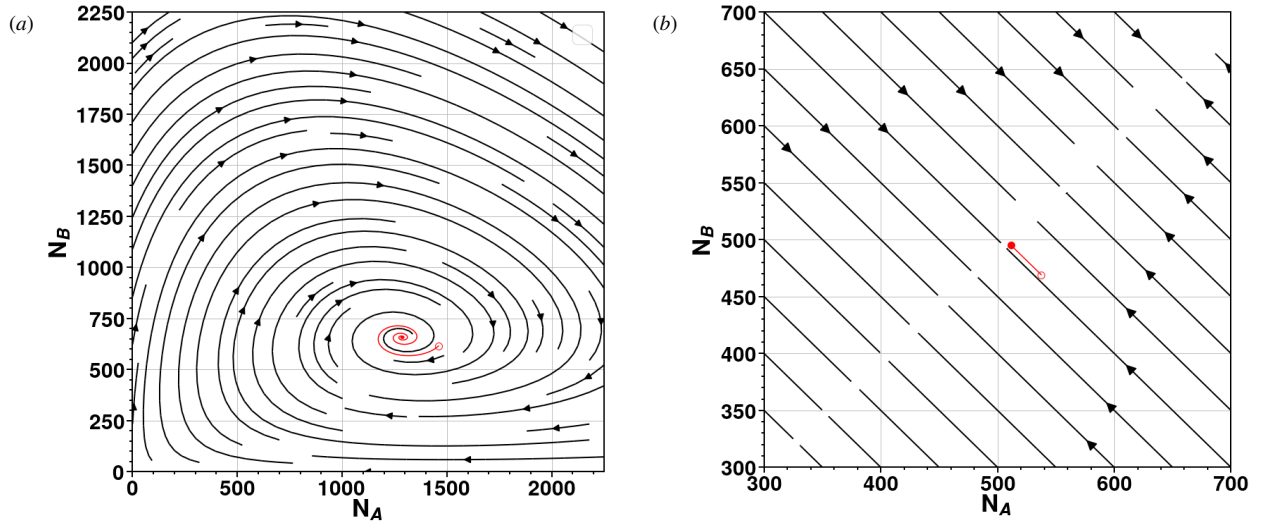


Figure 4.11: (a) and (b) show the streamlines of the normalized growth rate vector defined in Eq. (4.20) along with an overlaid path-line of the instantaneous solution (N_A, N_B) shown in Fig. 4.10 at probes P and F , respectively. The starting and end points of the path-lines are denoted by hollow and filled circles.

The Jacobian matrix of Eq. (4.18) is given by,

$$J(N_A, N_B) = \begin{bmatrix} (\tilde{k}_c - \tilde{k}_a)N_B + F_A & (\tilde{k}_c - \tilde{k}_a)N_A + 2(k_b + 2k_e)N_B \\ -(\tilde{k}_c - \tilde{k}_a)N_B & -(\tilde{k}_c - \tilde{k}_a)N_A - 2(k_b + 2k_e)N_B + F_B \end{bmatrix} \quad (4.21)$$

The eigenvalues of matrix $J(N_{A,crit}, N_{B,crit})$ are listed in Table 4.6. At probe P they are complex conjugates with a negative real part in the shock that gives the rate of decay from the initial to critical values. This is consistent with Fig. 4.10(a), which shows that at 0.01, 0.015, and 0.02 ms, the solution converges to 1, 0.3, and 0.07% of the critical values, respectively. These percentage values correspond to an approximate difference between the critical and instantaneous values of the number of A-type particles of 13, four, and one, respectively.

More importantly, these results suggest that inside the shock, the number of particles are subjected to recurrent microscopic thermal fluctuations which always decay with time-scales on the order of 0.01-0.02 ms with corresponding frequencies on the order of 100 to 50 kHz. These frequencies are close to the weighted-average of the low-frequency broadband of 37.5 kHz observed in Fig. 4.2(a) from the PSD analysis. The instantaneous particles in the energy bins A and B , shown in Fig. 4.5(c), are a result of superposition of responses to recurrent low-frequency microscopic fluctuations. Therefore, even with the underlying simplifications of the two-energy-bin model, it is able to predict the existence of the low-frequencies that originate due to the interactions in the average number of particles between the two modes of the bimodal PDF of particle energies in the presence of translational nonequilibrium in a 1-D shock. Additionally, the imaginary part of the pair of eigenvalues listed in Table 4.6 at probe P also indicates oscillations with a time period of $2\pi/\text{Im}(L_1)$ (frequency of 281 kHz), which may correspond to fluctuations observed in Fig. 4.2(a) in the mid-frequency range of ~ 100 -300 kHz outside of the low-frequency broadband.

Finally, we can relate the two timescales predicted by Eq. (4.18) in the shock to collision processes Q_e and Q_b that describe the relaxation of high energy particles in B to low energy bin A (see Table 4.2). The frequency associated with process Q_e is on the order $f \sim O(k_e N_B)$, or equivalently $f \sim O(K_e n_B = 51 \text{ kHz})$, where $n_B = m\langle N_B \rangle_t = 6.81 \times 10^{21} \text{ m}^{-3}$ is the average number density of particles in energy bin B . Similarly, the frequency associated with process Q_b is, $f \sim O(K_b n_B = 284 \text{ kHz})$. Therefore, it is seen that the two timescales present in the shock are a direct consequence of the bimodal energy distribution function. Also, note that although the analysis in this work is for a steady shock, these results hold for unsteady shock as well, because the PDF inside the shock remains bimodal.

Solution	Probe P	Probe F
$N_{A,crit}$	1286	511.5
$N_{B,crit}$	657.2	495
L_1	$-281,762 + 1,765,303.3j$	0.0
L_2	$-281,762 - 1,765,303.3j$	-499,976

Table 4.6: Dynamics of the ODE at probes P and F .

Turning to probe F in the freestream, we want to demonstrate that the two-bin energy model is able to predict different dynamics than observed in the shock. Since the flux coefficients F_A and F_B and the rate coefficients $\tilde{k}_c$ and k_e are zero, we obtain,

$$\frac{N_{A,crit}}{N_{B,crit}} = \frac{k_b}{\tilde{k}_a} \quad (4.22)$$

which is satisfied by an infinite number of critical points corresponding to different freestream conditions. That is, the number densities are different but the temperature is the same since all solutions have the same shape of the PDF shown in Fig. 4.3(c) and therefore, the same cross-correlation coefficient shown in Fig. 4.5(b). In this case, the solution depends on the initial values of N_A and N_B , and converges to a critical point that satisfies Eq. (4.22). Figures 4.10(b) and 4.11(b) show the solution of Eq. (4.18) as a function of time for a set of initial values of (N_A, N_B) and a streamplot along with an overlaid path-line of the solution, respectively. In Fig. 4.11(b), the dependence on the initial values can be clearly seen. For the given conditions, the solution converges to critical values of $N_{A,crit} = 511.5$ and $N_{B,crit} = 495$, which are within 0.5% of the average number of DSMC particles per computational cell volume, of $\langle N_A \rangle_t = 509.9$ and $\langle N_B \rangle_t = 492.8$, and satisfy the ratio of 1.033 given by Eq. (4.22).

For the freestream conditions, there are two real eigenvalues, as shown in Table 4.6 with the zero eigenvalue indicating again a non-unique solution of Eq. (4.22). The negative eigenvalue of -499,976 gives the linear rate of decay, the inverse of which gives the characteristic time-scale of $2 \mu s$. This fast decay rate is consistent with the PSD at probe F , discussed in Sec. 4.2, which showed that ~94% of the total spectral energy is distributed in frequencies greater than 1 MHz. More importantly, in the freestream the model predicts the absence of two orders of magnitude lower dominant frequencies having significantly large energy, which appear to be unique to the region of strong nonequilibrium inside a shock.

4.5 Strouhal Number Scaling

With the observation of dominant low-frequency perturbations of macroscopic flow parameters inside the shock, a natural question arises as to whether one can define a nondimensional Strouhal number,

$$St = \frac{f L_s}{u_{x,1}} \quad (4.23)$$

that would be constant for different shock strengths. We propose to define the time-scale as that required for the flow to traverse a distance equal to the shock-thickness with the upstream bulk velocity. To justify this time-scale, cases

ranging from Mach two to 10 were run by varying the upstream bulk velocity but keeping the upstream temperature constant ($T_{ir,1}=710$ K). Starting with the selection of frequency, f , the PSD of the instantaneous pressure spectrum at the location of the maximum gradient of bulk velocity in the shock for different Mach numbers is shown in Fig. 4.12(a). A broadband of low-frequencies is seen, the boundary of which is defined by the inflection point in the NCE, shown in Fig. 4.12(b).

The characteristic length, L_s , defined by the density-gradient shock-thickness is calculated as the overall density change divided by the maximum density gradient (e.g. see Chapter X, Sec. 9 of Ref. [91]) and is shown in Fig. 4.13(a). Note that λ_1 , the upstream mean-free-path, is obtained through the VHS model with a viscosity index of $\omega = 0.81$. The SUGAR-1D DSMC shock-thickness values match within 2% with the DSMC calculations of Macrossan and Lilley [193] and Bird (see pg. 294 of Ref. [37]) for the same viscosity index. Note that their results are scaled by 76% to account for the differences in λ_1 , which they defined based on the hard-sphere model. [37] The noticeable discrepancy between the SUGAR-1D DSMC results for $\omega = 0.81$ with the experiments of Alsmeyer [192] is due to the choice of viscosity index, while qualitatively the variation of shock-thickness with Mach number is consistent with the experimental results. Good agreement is observed between SUGAR-1D DSMC and experiment for a Mach 8 shock simulated with $\omega = 0.75$. Based on these values, the calculated ratio of shock-thickness to upstream bulk velocity, $L_s u_{x,1}^{-1}$, decreases with Mach number, as shown in Fig. 4.13(b).

The Strouhal number defined based on the above quantities and the weighted-averaged frequency, f , shown in Fig. 4.12(a), is relatively constant within a range of $St=0.007$ to 0.011 and a standard deviation from 0.001 to 0.02 . For Mach 8 case simulated with $\omega = 0.75$, St was found to be in the same range and equal to 0.0092 . This range of Strouhal numbers is similar to those corresponding to low-frequency unsteadiness of shock and separation bubble, as observed in the literature for highly compressible flows over embedded bodies, indicating that the two phenomena could be related. For example, in the case of shock-dominated separated flows the Strouhal number associated with low-frequency shock motion ranges from 0.02 to 0.05 , e.g. [23, 153, 155–157, 211] assuming that the characteristic length and velocity scales are given by the length of the separation bubble and the upstream bulk velocity, respectively. In the study of oblique SBLIs, Nichols *et al.* [122] defined the Strouhal number based on the upstream boundary-layer thickness and freestream velocity and found it to be within a range of 0.0003 to 0.05 . Therefore, we hypothesize that these fluctuations may play a major role in shock-dominated flows having shock-thickness comparable to other important length scales in the flow, such as the size of the boundary layer in SBLIs and turbulent length scale in shock-turbulence interaction.

To test whether the established range of Strouhal numbers holds for variations in upstream temperature, another set of DSMC cases were simulated in which the upstream temperature was changed from 710 K by fractions of $1/8$,

1/4, 1/2, and 2, while the upstream bulk velocity was varied accordingly to maintain a constant Mach number of 7.2. Figure 4.14 shows a decrease in the ratio of $L_s u_{x,1}^{-1}$ with increase in temperature, due primarily to the increase in $u_{x,1}$ rather than the shock-thickness. The Strouhal numbers obtained using the aforementioned approach is within the range of $St=0.005$ to 0.011 , with a small reduction with decrease in temperature. Nonetheless, the ± 1 standard deviation of broadband frequencies is contained within the limits of $St=0.001$ to 0.02 . Section 4.7.2.2 shows that the Strouhal number remained in the same range for a case run by increasing the freestream number density, n_1 , by three orders of magnitude, where the mean-collision-time of molecules decreased, frequency increased, and shock-thickness decreased by the same order. In Ref. [210], we show that a semi-empirical relationship to predict low-frequency oscillations in shocks can be derived from bimodal probability distribution functions based on noncentral Chi-squared functions for a broad range of Mach numbers and freestream temperatures.

Finally, our Strouhal number formulation was used to qualitatively explain the ~ 300 kHz frequencies observed inside a shock in the experiments of Chynoweth *et al.* (see Fig. 7 of Ref. [212]) of a Mach 6 air flow and $Re_1 = 6.73 \times 10^6 \text{ m}^{-1}$ over a 7° half-angle cone attached with a 10° fin. At freestream conditions experienced by the fin downstream of the leading-edge shock, i.e. $\rho_1 = 4.636 \times 10^{-2} \text{ kg.m}^{-3}$, Mach 5, and freestream temperature, $T_{tr,1}=71.67 \text{ K}$, the normal shock-thickness, $L_s \sim 6.6 \mu\text{m}$, was estimated from Fig. 4.13(a) and λ_1 calculated using the VHS molecular model. Using Eq. (4.23) and estimating St from Fig. 4.13(b), the low-frequency broadband was predicted to have a weighted-average frequency of 1.2 MHz with one standard deviation limit from 0.4 to 2.1 MHz , which was also verified from a separate DSMC simulation. The broadband from the simulation also revealed high spectral energy near 50 kHz frequency, which is also present in the experimental PSD spectrum. This estimate is qualitatively reasonable, even though it ignores factors that could reduce the range of dominant frequencies, such as differences in gas properties, reduced strength of the oblique shock generated by the fin compared to the normal shock, and surface effects.

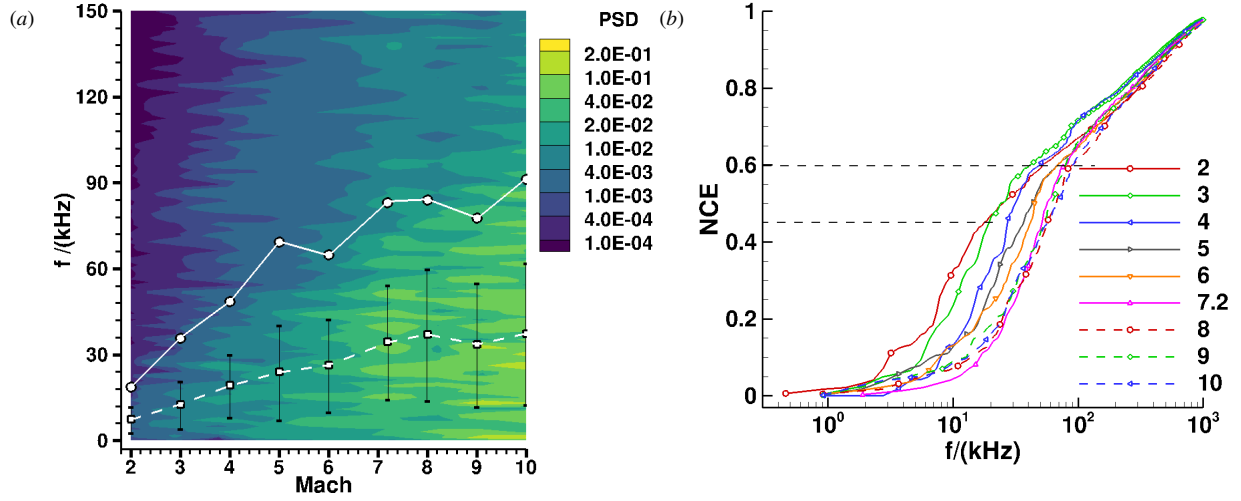


Figure 4.12: (a) The contours of PSD obtained by interpolating the pressure spectrum at the center of the shock at each Mach number. For interpolation, the inverse-distance algorithm in the Tecplot [4] software is used with default parameters (exponent=3.5, point selection=Octant, Number of points=8). The overlaid white solid and dashed lines show the upper limits and the weighted-averages with ± 1 standard deviation of the low-frequency broadbands for Mach 2-10, respectively. (b) NCE of the PSD for Mach 2-10 used to define the upper limit of the low-frequency broadband.

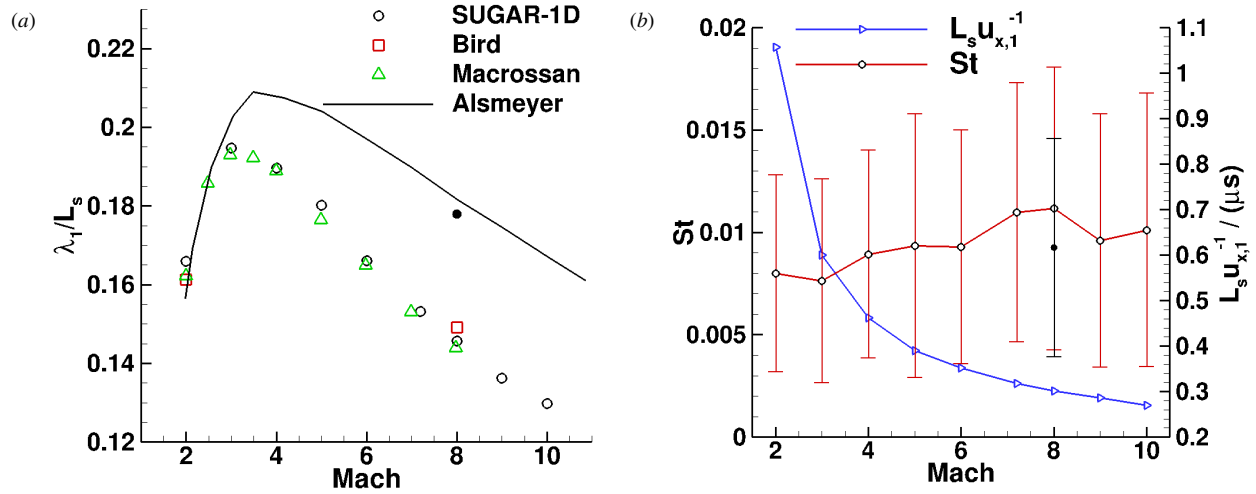


Figure 4.13: (a) Reciprocal of the density-gradient shock-thickness normalized by the upstream mean-free-path as a function of Mach number. The SUGAR 1-D DSMC results use a viscosity index of $\omega = 0.81$ (open symbols) and $\omega = 0.75$ (filled circular symbol) at Mach 8. (b) $L_s u_{x,1}^{-1}$ and Strouhal number, St , as a function of Mach number, including the St at Mach 8, $\omega = 0.75$ (filled circular symbol). The standard deviation in Strouhal number is based on the standard deviation in weighted-average frequency shown in Fig. 4.12(a).

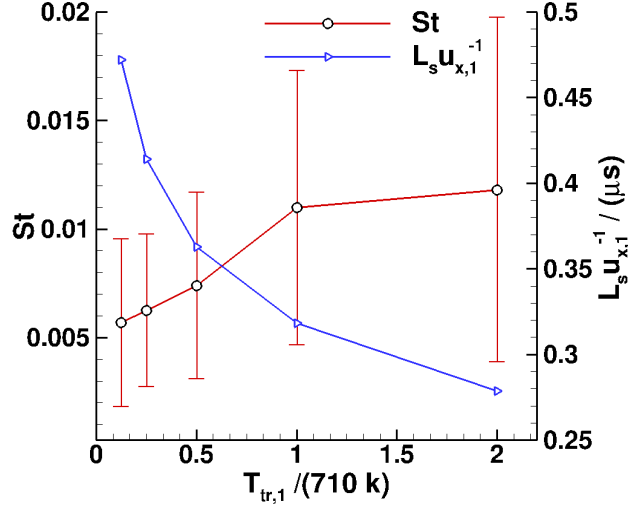


Figure 4.14: Strouhal numbers for a range of cases simulated at Mach 7.2, as a function of freestream temperature $T_{tr,1}$. A viscosity index of $\omega = 0.81$ was used in the DSMC simulations.

4.6 Summary

The investigation of macroscopic fluctuations in a DSMC-computed Mach 7.2 shock layer revealed two orders of magnitude lower dominant frequencies of fluctuations than found in the freestream. In the peak overshoot region in the shock a low-frequency broadband with a weighted-average of ~ 37 kHz was observed as opposed to the freestream region where peak frequencies are concentrated at ~ 3.5 MHz corresponding to the inverse mean-collision-time. These disparities were attributed to the differences in particle distribution functions in the nonequilibrium zone of shock versus the equilibrium regime upstream. The fluctuations in the x -directional normalized overall stress component, which is the mean of the PDF f_{ξ_x} , were found to be correlated with perturbations in the entire X -directional energy space of PDF. Two distinct energy bins were identified depending on the sign of the cross-correlation coefficient, and a Lotka-Volterra type two-energy bin ODE model was constructed.

The model accounted for the interaction of two energy bins through intermolecular collisions and particle fluxes from neighboring computational cells. At a location inside the shock, the model predicted two disparate time-scales: a longer time-scale (50-100 kHz) associated with the time of decay of fluctuations in the number of particles in energy bins to critical values and an order of magnitude smaller time-scale (281 kHz) associated with oscillations in the number of particles. In the freestream, the model predicted faster decay of fluctuations, $\mathcal{O}(\text{MHz})$, and more importantly, an absence of low-frequency fluctuations consistent with the DSMC spectral analysis.

Finally, a Strouhal number was defined based on the density gradient shock-thickness and upstream bulk velocity

to nondimensionalize the low-frequency broadband characterized by a weighted average frequency and ± 1 standard deviation across a wide range of Mach numbers from 2 to 10. The Strouhal number was found to range from 0.007 to 0.011 with ± 1 standard deviation between 0.001 and 0.02, consistent with values found in the literature corresponding to low-frequency unsteadiness of shock and separation bubbles in shock-dominated flows. The range of Strouhal numbers was also found to hold for a Mach 7.2 shock simulated with different upstream temperatures and number density, and explain qualitatively the frequencies inside a shock observed in the work of Chynoweth *et al.* [212].

The presence of low-frequency fluctuations of shock layers suggests that these disturbances may play a key role in the receptivity process of transition in hypersonic flows, SBLIs, and shock-turbulence interactions, especially when the shock-thickness is comparable to other important length scales in the flow. Our work implies that the leading-edge shock interactions with freestream disturbances, such as tunnel-induced turbulence, can result in selective amplification of disturbances in the low-frequency range, and consequent excitation of the downstream boundary-layer. Future numerical investigations focused on understanding the effect of freestream disturbances on transition should not ignore shock-induced perturbations in the boundary-layer within the range of Strouhal numbers established in this work.

4.7 Supplemental Information

4.7.1 The overview of the STABIL algorithm

In this section we first explain the origin of the numerical drift of a 1-D shock simulated using DSMC and then give a brief overview of Bird's STABIL algorithm [37] implemented to correct the drift.

On the up and downstream sides of the 1-D shock setup, directed-Maxwellian and moving-piston boundaries are implemented, respectively. To impose downstream subsonic velocity, the moving-piston boundary is given a bulk velocity equal to the downstream Rankine-Hugoniot jump velocity, $u_{x,2}$. The particles colliding with this boundary are specularly reflected and deleted if they lie outside the domain. However, despite the moving-piston boundary, the shock may drift and diffuse over time due to random-walk effects generated at the boundary. These effects arise because we can only maintain the downstream bulk-velocity, whereas in a statistical simulation, particles at the boundary exhibit thermal as well as statistical fluctuations and over time, they may accumulate or deplete near the boundary, which leads to disturbances that are propagated to the shock.

The STABIL algorithm corrects the numerical drift as follows: when the total number of particles in the domain exceeds the number of particles at the time of initialization by a small, pre-set number, δN , then all particles are translated by a small distance, δx , in the direction opposite to the drift of the shock. After translation, molecules

that move outside of the boundary are deleted and those that are within a δx distance from the opposite boundary are replicated. These values are estimated as

$$\begin{aligned}\delta N &= \frac{\sqrt{N_{\text{init}}}}{4} \\ \delta x &= \frac{\delta N F_n}{(n_2 - n_1)A}\end{aligned}\tag{4.24}$$

where N_i is the initial number of particles in the entire domain, A is the cross-sectional area of a 1-D slab, F_n is the number of simulated particles represented by a computational particle, n_1 and n_2 is up and downstream number densities, respectively.

For the Mach 7.2 1-D argon shock case at $n_1 = 10^{22} \text{ m}^{-3}$ presented in this work, δN and δx are 172 and $6.18 \mu\text{m}$, respectively, i.e. 0.036 % of N_{init} and 3.55% of upstream mean-free-path, λ_1 , respectively. Small value of δx indicates that the particles are translated by a very small distance, much smaller than the cell size when the stabilization is performed. Figure 4.15 shows the comparison of the shock drift with and without the STABIL algorithm. When the STABIL algorithm is switched on, the shock remains within $0.2\lambda_1$ distance, as seen in figure 4.15(a); however, when stabilization is switched off, the shock is seen to drift towards the upstream boundary, as seen in figure 4.15(b), because particles keep accumulating in the vicinity of the piston for the present conditions.

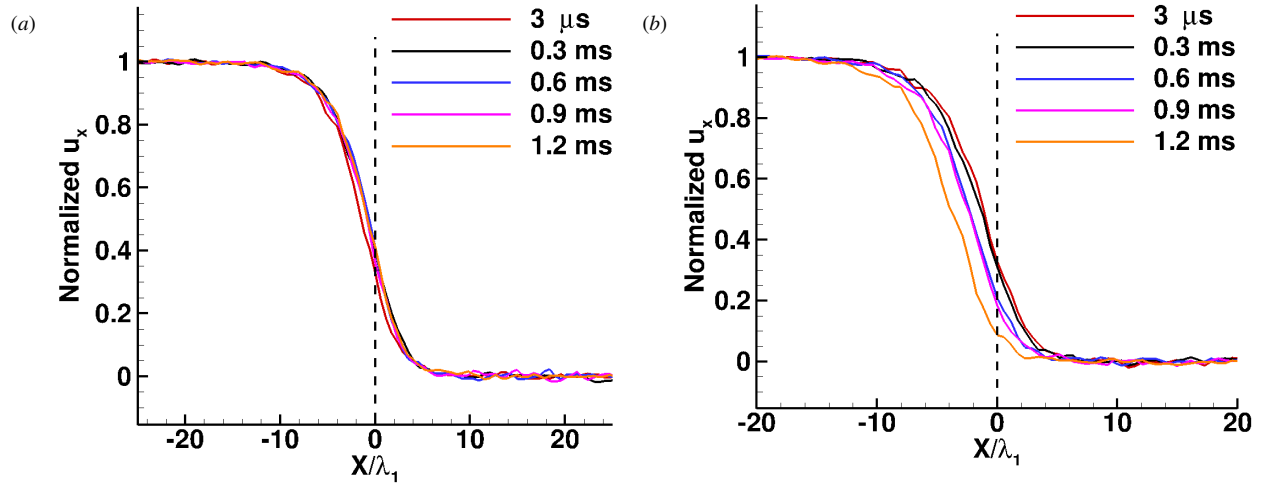


Figure 4.15: Comparison of instantaneous shock location with and without STABIL for Mach 7.2 shock simulated in a domain of 0.02 m, i.e. from $-57.45\lambda_1$ to $57.45\lambda_1$, where shock is centered at zero. (a) STABIL on, (b) STABIL off.

4.7.2 Additional numerical tests

This section describes the numerical tests performed to verify that the observed low-frequencies in the argon shock structure are not numerical artifacts. Section 4.7.2.1 describes the analyses of potential frequencies associated with the

stabilization procedure using the STABIL algorithm as well as frequencies corresponding to disturbances traveling at the speed of sound from shock to the domain boundaries and back. In Sec. 4.7.2.2 we analyze the effect of numerical amplification of fluctuations on our low-frequency predictions. Finally, Sec. 4.7.2.3 shows the effect of increasing the domain by a factor of ten on the observed low-frequencies in the original short domain of 0.02 m ($-57.45 \lambda_1$ to $57.45 \lambda_1$).

4.7.2.1 Analysis of spurious disturbances introduced at the boundaries during stabilization

One way spurious numerical frequencies could be introduced at the boundaries is due to the recurring frequency at which additional particles are added within a δx distance from the boundaries to stabilize the shock. To understand the number and frequency of particles added at the boundaries, we first describe the stabilization process for the Mach 7.2, 1-D argon shock case at $n_1 = 10^{22} \text{ m}^{-3}$, discussed in Sec. 4.2.

Since for this case, the shock drifts upstream, as discussed in Sec. 4.7.1, all particles are translated to the right, *i.e.* towards the moving-piston boundary, during a stabilization step. Let's call this a positive displacement. After translation, the particles outside the domain, *i.e.* further downstream of the piston, are deleted, whereas particles within δx distance from the opposite upstream boundary are duplicated. However, since δx is much smaller than λ_1 , it was found that particles were not added near the upstream boundary during stabilization. After some instances of positive displacement, a negative displacement is needed because shock has moved downstream and translation of all particles to the left is performed. In that case, particles within δx distance from the moving-piston boundary are duplicated after translation. Since the density of the downstream side is higher than upstream, there are some finite number of particles introduced within δx region from the downstream boundary.

Figure 4.16 shows the number of particles added on the downstream side during stabilization as a function of time and time passed since the last instance of particle addition. The mean values of these quantities are 236 (or $\sim 6.2\%$ of the downstream computational particles in a root cell) and 0.0018 ms, respectively. Note that the mean time between adding particles corresponds to a frequency of $\sim 553 \text{ kHz}$, which is much higher than the frequency of low-frequency fluctuations that are discussed in Sec. 4.2. It is possible that the disturbances generated due to these particle additions could propagate to the shock at the downstream speed of sound, but, the frequency associated with such disturbances would be 205 kHz, which is again outside of the low-frequency broadband.

Turning to the upstream side, although there are no particles added within δx distance from the upstream boundary during stabilization, it is possible that the disturbances generated at the shock travel to the upstream boundary at the speed of sound, reflect off and return to the shock. The frequency associated with this phenomenon is 24.8 kHz, very close to the weighted-average frequency of low-frequency molecular fluctuations (37.5 kHz). However, such

reflections of acoustic waves have not been observed in our DSMC simulations. For such wave reflections to occur in the framework of DSMC, in the upstream region, there must be a transfer of particles from the right to left computational cell, *i.e.* towards the upstream boundary. It must be noted that a particle located in the shock does not need to travel all the way up to the upstream boundary for the propagation of acoustic waves. However, since in DSMC, we perform collisions of particles located only within a collision cell, acoustic waves cannot propagate upstream unless some particles move upstream and collide in a cascading manner where a few particles move in the upstream computational cell to collide with particles moving towards the shock and then some of those particles from this cell move further upstream and so on. No such upstream moving particles were detected in the upstream computational cells for the entire duration of the simulation. As a matter of fact, that is the reason why the average number of particles moving from right to left, shown in Table 4.1, denoted as $N_A^{l,\text{out}}$, $N_B^{l,\text{out}}$, $N_A^{r,\text{in}}$, $N_B^{r,\text{in}}$, are exactly zero. Therefore, our analysis supports the conclusion that molecular frequencies at the peak over shoot of the shock are not numerical artifacts of the STABIL algorithm or spurious boundary effects.

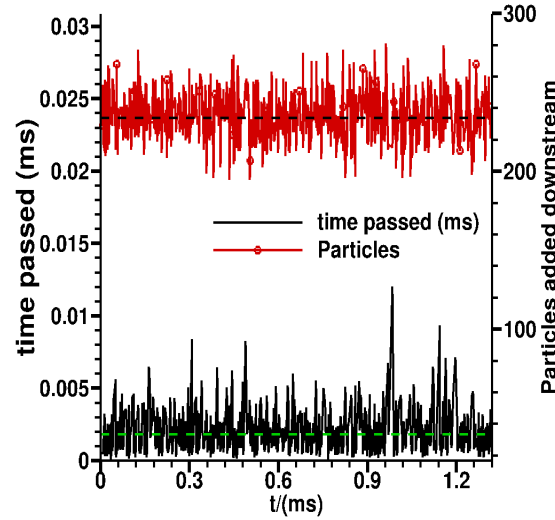


Figure 4.16: For stabilization of the Mach 7.2 shock, additional particles added in the vicinity of the downstream boundary and the time passed since the last instance of particle addition.

4.7.2.2 Effect of numerical amplification of fluctuations on low-frequency predictions

Here we analyze the possible effect of *numerical* amplification of fluctuations on our low-frequency predictions caused by the stochastic nature of DSMC for $F_n > 1$. The best way to assess this is to study its effect on the PSD, as shown in Fig. 4.17. The DSMC simulation, discussed in Sec. 4.2.2, was re-run first with F_n reduced by four orders of magnitude, which now requires 33 million particles, 1.2 million time steps with $\Delta t = 1$ ns, for the same number density of 10^{22} m^{-3} . An additional DSMC simulation was also performed for the case of $F_n = 1$ (*i.e.*, no numerical amplification

of fluctuation amplitudes) with the freestream number density now raised by three orders of magnitude, $n_1 = 10^{25} \text{ m}^{-3}$. Note that we have changed the abscissa from frequency to Strouhal number using Eq. (4.23) because when we change number density we do not expect the “line-by-line” PSD spectrum to remain the same (due to the molecular nature of the flow) but we do expect the mean Strouhal numbers to be similar if we are looking at a phenomena related to fluctuations induced by the motion of the shock and not computational noise. A comparison of the new PSD spectra in the shock with the original case for the 10^{22} m^{-3} upstream condition is shown in Fig. 4.17(a) where indeed we find only a change of 2.7% in the weighted-average frequency of the low-frequency broadband in the shock such that the mean Strouhal number is $St \sim 0.012$. Finally, Fig. 4.17(b) shows the PSD obtained from the simulation run by increasing the freestream number density by three orders of magnitude, $n_1 = 10^{25} \text{ m}^{-3}$ and $F_n = 1$. Comparison of this result with Fig. 4.17(a) shows that both conditions generate PSDs consistent with Strouhal number scaling discussed in Sec. 4.5 and produce similar quantities such as mean Strouhal number and broadband limits.

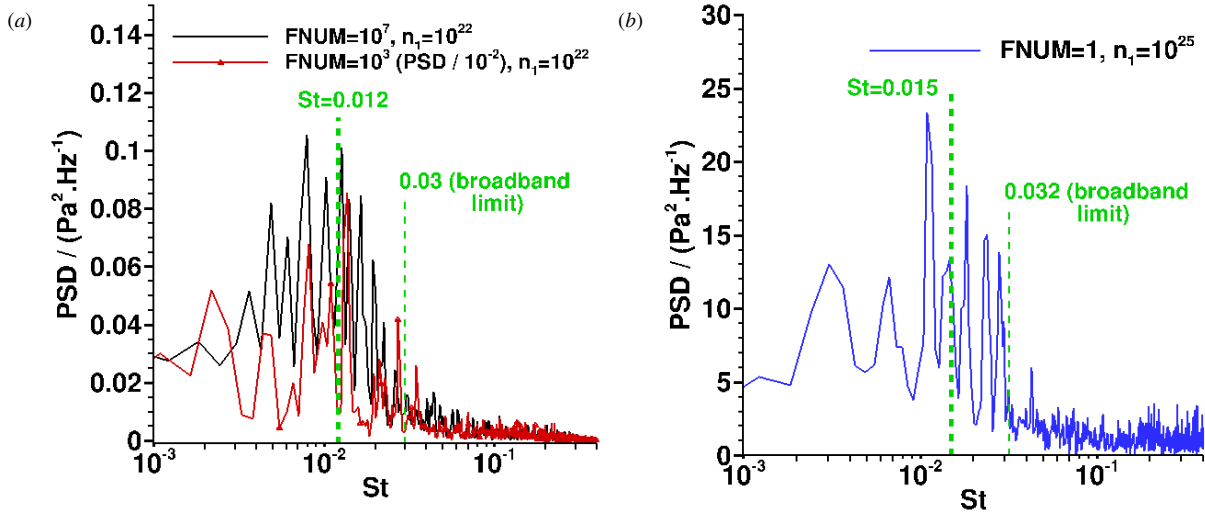


Figure 4.17: Comparison of PSD of the X-directional normal stress, σ_{xx} , inside the shock near the location of absolute maximum velocity gradient, P , for Mach 7.2 argon shock. (a) $n_1 = 10^{22} \text{ m}^{-3}$, $F_n = 10^7$ and 10^3 , and (b) $n_1 = 10^{25} \text{ m}^{-3}$ and $F_n = 1$.

4.7.2.3 Effect of large domain on low-frequencies observed in the original short domain

In this section, we first show that a spurious initial movement of the shock observed in a ten times longer domain, which seems to amplify small acoustic disturbances that might be generated at the upstream boundary during the introduction of directed Maxwellian particles. The amplitude of these disturbances in the PSD analysis seems to be proportional to the initial movement of the shock. To reduce this initial movement, we show further tests carried out by initializing the shock at an off-centered location, where the downstream domain is kept equal to 0.01 m, similar to the original short

domain, while the upstream domain is longer by a factor of ten.

For a shock centered in a domain, as the domain size is increased, shock first moves downstream from its original location, moves back slightly upstream, and then remains at the shifted location. Figure 4.18(a) shows for the ten times longer domain ($L_d = 0.2$ m, i.e. $-574.5\lambda_1$ to $574\lambda_1$), the transient movement of the shock. Shock stabilizes at a downstream distance of $\sim 7\lambda_1$ where it reaches within ~ 0.1 ms. This transient time is roughly equal to 0.097 ms, which is the time required for pressure waves generated at the shock to reflect off the moving piston and return to interact with the shock at the speed of downstream speed of sound. This time has increased ten times from the time of $9.7 \mu\text{s}$ required in a shorter domain, which was fast enough for shock to not leave the initialized $X = 0$ location. Therefore, the initial transient movement was thought to be due to the longer downstream domain size. Figure 4.18(b) shows the comparison of early time history at probe locations $X = 0$ and $X = 7\lambda_1$ in the 0.02 and 0.2 m domains, respectively. It can be seen that large amplitude fluctuations persist in the shock for the long domain case even after 0.3 ms, which seem to have originated because of the initial movement of the shock.

Next, figures 4.18(c) and 4.18(d) show the power spectral density comparison (PSD) in the shock at probe locations close to $X = 0$ and $X = 7\lambda_1$ for short and long domain cases, respectively, the latter figure showing the zoom of the rectangular box denoted in the former figure. The PSD analysis was taken after 0.3 ms for two cases to exclude the transient period from the analysis. PSD shows dominant low-frequencies, lower than the low-frequency fluctuations observed in the short domain. These frequencies seem to correspond to acoustic waves coming from the upstream boundary. For the long domain, it was ensured that there are no upstream travelling particles in the upstream; therefore, these waves must be travelling one-way from the upstream boundary to the shock or rather, the shock must be amplifying small disturbances generated at the upstream boundary when particles are introduced. Such small disturbances, indistinguishable from the thermal fluctuations in the upstream region, must propagate at the acoustic speed of sound. Initial movement and sudden stopping of the shock seems to increase the amplitude of these acoustic waves.

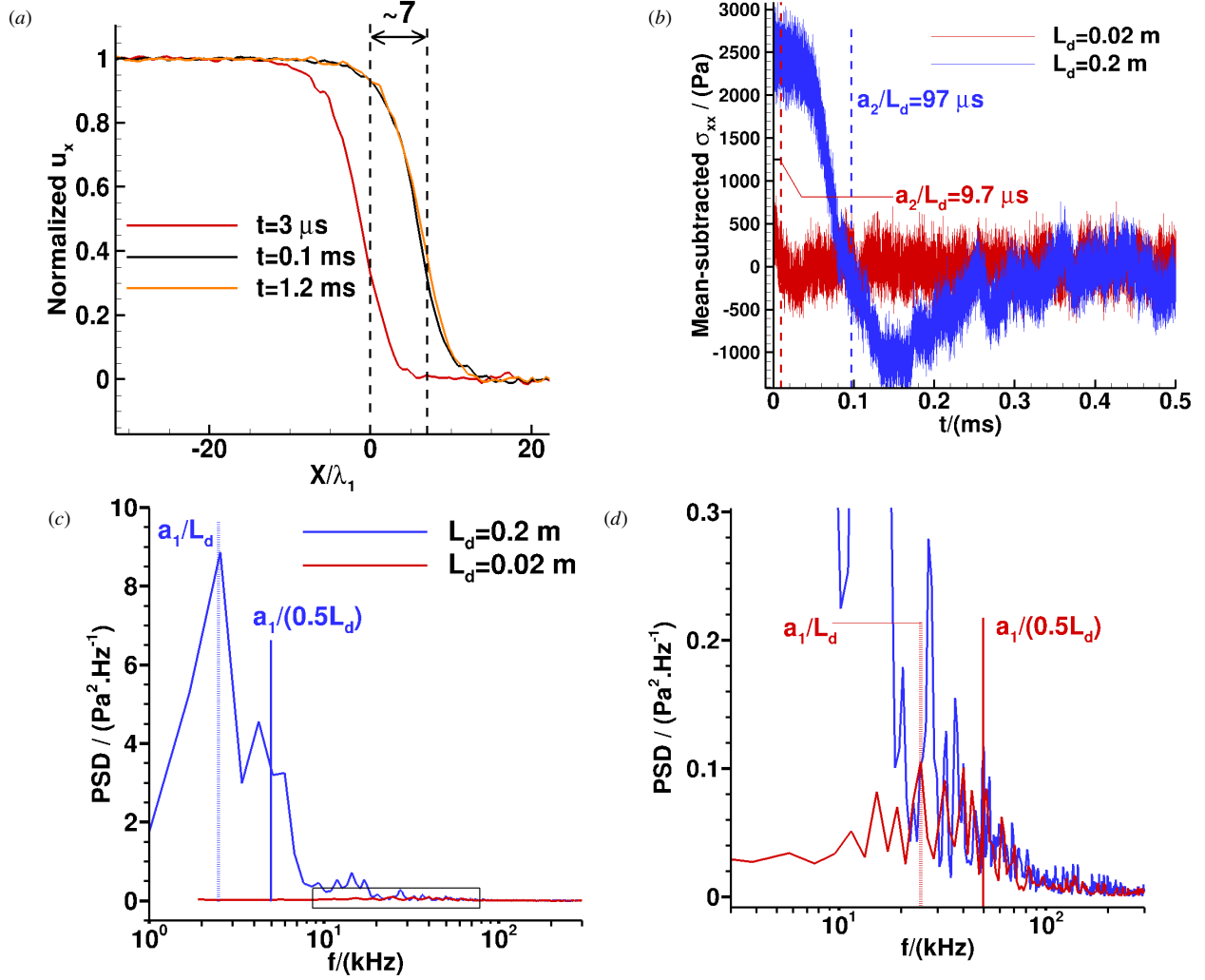


Figure 4.18: Effect of increasing the domain by a factor of ten, i.e. $L_d = 0.2$ m, with shock centered at $X = 0$. (a) Transient movement of the shock. (b) Probe data comparison inside the shock in the vicinity of maximum velocity gradient, i.e. $X/\lambda_1 = -0.86$ and $X/\lambda_1 = 6.14$ for the short and long domains respectively. (c) Comparison of PSD of the probe data signals in the shock starting from 0.3 ms. (d) A zoom of the PSD signals in the rectangular boxed region denoted in (c).

If the acoustic waves are only traveling a distance of $0.5L_d$ then we should expect a peak at $a_1/(0.5L_d)$, instead of a_1/L_d in the PSD shown in figure 4.18(c). However, since the latter frequency is the subharmonic of the former, the PSD analysis cannot distinguish between these two frequencies. One may as well see a peak at $a_1/(0.5L_d)$, if the analysis is repeated for a slightly different duration of the signal. Only by making sure that there are particles travelling upstream in the upstream region, we can say for sure that the disturbances amplified in the shock must have travelled only one way from the upstream boundary to the shock.

Additionally, these acoustic waves seem to persist as time progresses, which was verified by starting the PSD analysis at a later time (1 ms) and yet observing similar PSD (not shown). The large domain case was run for a long duration of 2.76 ms to ensure that the frequency resolution is lower than 1 kHz, even when the PSD analysis was started at a later time instant.

Since the shock seems to amplify acoustic disturbances coming from upstream, one may wonder if the frequencies seen in the short domain case are also amplified acoustic waves. Figure 4.18(d) shows that the frequency $a_1/(0.5L_d)$ and its subharmonic frequency, a_1/L_d , are within the low-frequency broadband region of molecular fluctuations. It is hard to say which of these two effects are present in our original simulation just based on the comparisons made in this section. One can argue that the original frequencies observed in the short domain are still present in the large domain by observing the zoomed figure 4.18(d), where part of the low-frequency broadband is amplified, possibly also due to the shock movement. To find out for sure, another case was simulated, as discussed in the next section, where the shock is off-centered such that the region downstream of the initialized location of shock ($X = 0$) is 0.01 m, as in the short domain case, and 0.1 m in the upstream, as the current large domain case.

Turning to the case where shock is located in a large asymmetric domain of length, $L_d = 0.11$ m (0.1 m up and 0.01 m downstream), the initial transient movement of the off-centered shock is decreased to $1.8 \lambda_1$, as shown in figure 4.19(a). This movement was not zero, as expected similar to the short domain case, indicating some effect of the size of the upstream domain on the initial movement of the shock. The exact reason for this small movement is not known, but the transient period seems to be equal to the time required for the half-Maxwellian flow generated at the freestream boundary to travel to the shock at the upstream bulk velocity, $u_{x,1}=3572 \text{ m.s}^{-1}$, which is equal to 0.28 ms. Figure 4.19(b) shows the comparison of probe signals of mean-subtracted σ_{xx} in the shock, where both signals look similar after the initial ~ 0.3 ms. Figures 4.19(c) and 4.19(d) show the comparisons of PSDs inside the shock and in the upstream region, respectively, for the large asymmetric domain and the original symmetric short domain. For the shock formed in $L_d = 0.11$ m, the amplitude of additional lower-frequencies corresponding to acoustic waves has decreased by an order of magnitude in comparison to the large symmetric domain ($L_d = 0.2$ m), discussed in the previous section, confirming that the amplitude of these frequencies depends on the initial movement of the shock. More importantly, the PSD shows similar low-frequencies that we expect to be due to molecular fluctuations, as seen in the shorter domain, confirming that they are indeed independent of the domain size and are most likely due to the bimodal nature of the probability density function of particles in the shock, as discussed in the manuscript. There is some amplification of these low-frequencies for $L_d = 0.11$ m case, indicating that the initial small shock movement might affect the amplitude of these fluctuations. Turning to the upstream equilibrium region, we see that the PSD spectra are very similar for the two cases and have dominant frequencies closer to the frequency associated with the

inverse of the mean-collision-time, τ_1 , in the upstream region.

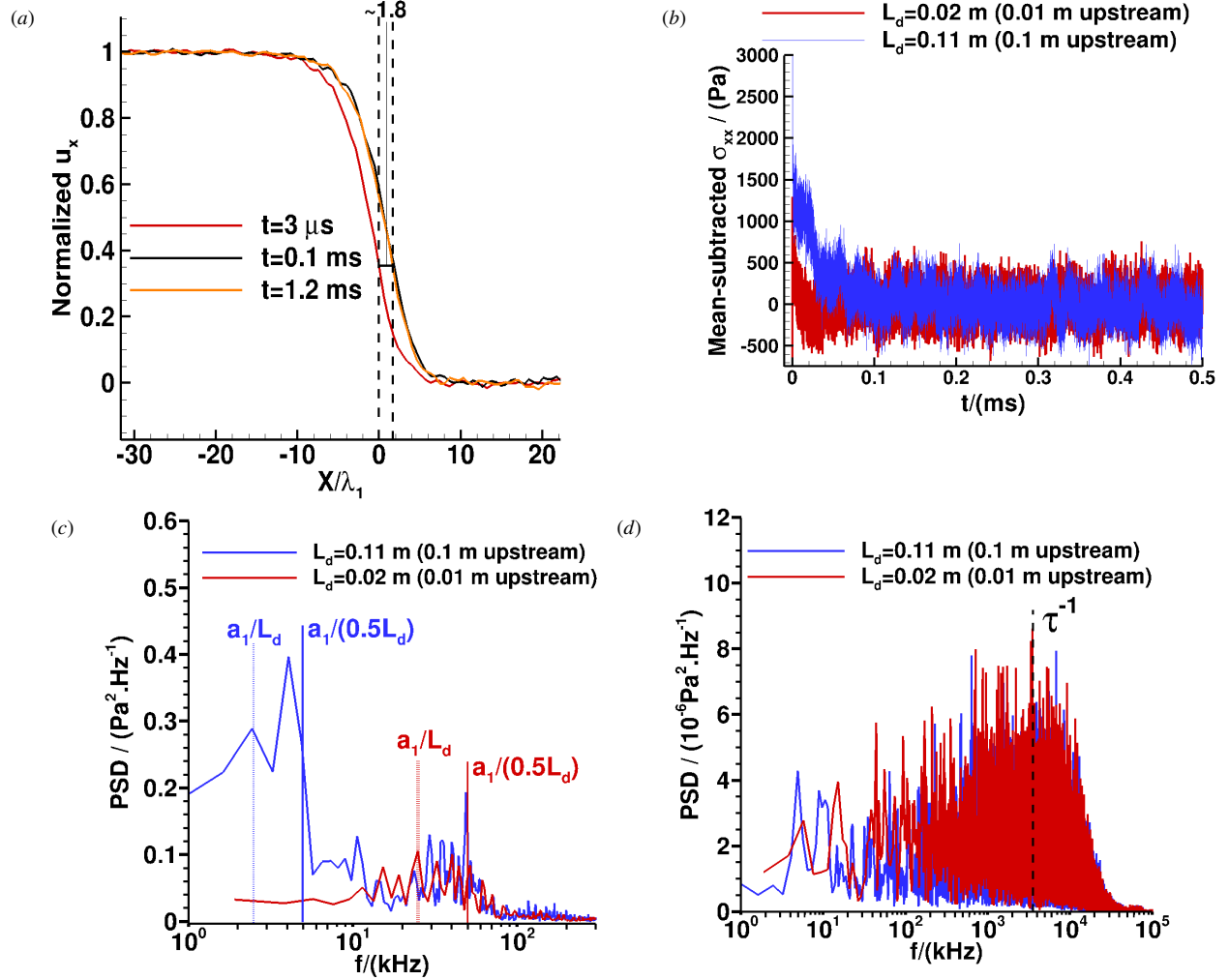


Figure 4.19: Effect of increasing the domain by a factor of ten *only on the upstream side of the shock*, i.e. $L_d=0.11 m$ from $-574.5\lambda_1$ to $57.45\lambda_1$. (a) Smaller initial transient movement of the shock. (b) Probe signal comparison inside the shock in the vicinity of maximum velocity gradient, i.e. $X/\lambda_1 = -0.86$, $X/\lambda_1 = 0.94$, for the short and long domain cases. (c) Comparison of PSD of the probe signals in the shock starting from 0.3 ms. (d) Comparison of PSD of probe signals in the upstream region.

Chapter 5

Analytical Prediction of Low-Frequency Molecular Fluctuations in Monatomic Shocks

Linear instability of high-speed boundary layers is routinely examined assuming quiescent edge conditions, without reference to the internal structure of shocks or to instabilities potentially generated in them. In Chapter 4 we showed that the kinetically modeled internal nonequilibrium zone of straight shocks away from solid boundaries exhibits low-frequency molecular fluctuations. The presence of the dominant low frequencies observed using the Direct Simulation Monte Carlo (DSMC) method has been explained as a consequence of the well-known bimodal probability density function (PDF) of the energy of particles inside a shock. In this chapter, PDFs of particle energies are derived in the upstream and downstream equilibrium regions, as well as inside shocks, and it is shown for the first time that they have the form of the non-central chi-squared (NCCS) distributions. A linear correlation is proposed to relate the change in the shape of the analytical PDFs at a specified upstream number density and temperature as a function of Mach number, within the range $3 \leq M \leq 10$, with the DSMC-derived average characteristic low-frequency of shocks, as computed in our earlier work. At a given Mach number $M = 7.2$ and upstream number density $n_1 = 10^{22} \text{ m}^{-3}$, it is shown that the variation in DSMC-derived low-frequencies is correlated with the change in most-probable-speed inside shocks at the location of maximum bulk velocity gradient for upstream translational temperature in the range $\sim 90 \leq T_{tr,1}/(K) \leq 1420$. Using the proposed linear functions, average low-frequencies are estimated within the examined ranges of Mach number and input temperature and a semi-empirical relationship is derived to predict low-frequency fluctuations in shocks. Our model can be used to provide realistic physics-based boundary conditions in receptivity and linear stability analysis studies of laminar-turbulent transition in high-speed flows.

Nomenclature

Roman symbols

f_v local Maxwell-Boltzmann probability density functions

f_{v_i} probability density functions of instantaneous molecular velocity component v_i , for $i \in \{x, y, z\}$

$f_{v_i\beta}$ probability density function of nondimensional velocity component, $\beta^{-1} f_{v_i}$

f_χ noncentral Chi-squared distribution constructed from any molecular velocity function χ

f_ξ probability density function of total energy ξ of particles

f_{ξ_i} probability density function of energy ξ_i of particles, where $i \in \{x, y, z\}$

f''_{ξ_x} second derivative of f_{ξ_x} with respect to ξ_x

$I_\gamma(x)$ Modified bessel function of the first kind having parameter $\gamma = \frac{D}{2} - 1$ and argument x .

M Mach number

m mass of species (kg)

$N(\xi_x, w)$ total number of DSMC computational particles within time windows w to $w + 1$ as a function of ξ_x

n number density (m^{-3})

p pressure (Pa)

R universal gas constant ($\text{J.mol}^{-1}.\text{K}^{-1}$)

s_1, s_2 scaling factors in the energy distribution functions

T_{tr} overall translational temperature (K)

u bulk speed, u (m.s^{-1})

$\mathbf{u} = [u_x, u_y, u_z]^T$ bulk velocity vector (m.s^{-1})

$\tilde{\mathbf{u}}$ scaled bulk velocity vector, $\tilde{\mathbf{u}} = \sqrt{2}\mathbf{u}\beta$

v instantaneous velocity speed, v (m.s^{-1})

$\mathbf{v} = [v_x, v_y, v_z]^T$ instantaneous molecular velocity vector (m.s^{-1})

$\tilde{\mathbf{v}}$ scaled instantaneous molecular velocity vector, $\tilde{\mathbf{v}} = \sqrt{2}\mathbf{v}\beta$

X, Y, Z Cartesian coordinates in the direction of the shock and two transverse directions

Special symbols

$\mathcal{D}$	degree of freedom in a noncentral Chi-squared distribution	ξ_x^M	location where f''_{ξ_x} attains a local minima
		ρ	mass density (kg.m ⁻³)
$\mathcal{N}_{v_i}$	Gaussian distribution of molecular velocity component v_i , where $i \in \{x, y, z\}$	Σ_χ	standard deviation of noncentral Chi-squared distribution f_χ
$\mathcal{N}_{\tilde{v}_i}$	Gaussian distribution of scaled molecular velocity component $\tilde{v}_i$, where $i \in \{x, y, z\}$	Σ_ν	standard deviation in frequency ν (Hz)
Greek symbols		σ_{ij}	component of overall stress tensor expressed in indicial notations (Pa)
α	constant used in the Mott-Smith bimodal velocity distribution function	τ_{ij}	component of viscous stress tensor expressed in indicial notations (Pa)
β	inverse of most probable speed, v_m^{-1} , (m ⁻¹ .s)	ϕ_1, ϕ_2	weighting functions in the Mott-Smith bimodal velocity distribution function
$\Gamma(j)$	gamma function, $\int_0^\infty x^{j-1} \exp(-x) dx$	χ	any function of scaled instantaneous molecular velocity components
$\Delta\xi_x$	small region of X -directional energy space ξ_x	ψ_1, ψ_2	fractions $\phi_1/(\phi_1 + \phi_2)$ and $\phi_2/(\phi_1 + \phi_2)$, respectively
η	noncentrality parameter in the noncentral Chi-squared distribution		
κ_b	Boltzmann constant (J.K ⁻¹)	Operators	
λ	mean free path (m)	$\langle Q \rangle_w$	average of quantity Q over time windows W
μ_χ	mean of noncentral Chi-squared distribution f_χ	Subscripts	
ν	frequency (Hz)	x, y, z	Cartesian components
ξ_x, ξ_y, ξ_z	normalized X , Y , and Z -directional energies, respectively, where $\xi_x = (v_x^2 - u_x^2)\beta^2$, $\xi_y = v_y^2\beta^2$, and $\xi_z = v_z^2\beta^2$	1	upstream value
		2	downstream value

5.1 Introduction and Overview

Supersonic and hypersonic laminar to turbulent flow transition strongly depends on freestream noise, which includes atmospheric or tunnel-induced turbulence, acoustic, vorticity and entropy fluctuations, and particulates [16]. These freestream disturbances interact with a shock and excite the downstream boundary layer through a process known as receptivity [51]. The importance of understanding this process is evident from several experimental works that have shown a strong correlation between the Reynolds number of transition and freestream noise [213–216]. Numerical research on the process of receptivity and natural transition has focused primarily on the development of models to account for freestream disturbances [52, 53] and their interaction with shocks through shock-capturing [54] or shock-fitting [55] schemes. However, these works do not account for the internal dynamic structure of a shock-wave which, as our recent work [5] has shown, exhibits *low-frequency* molecular fluctuations. The important role of molecular fluctuations in the laminar to turbulent transition is supported by the works of Fedorov and Tumin [56] and Luchini [57] on the receptivity of boundary layers to equilibrium molecular fluctuations using Landau-Lifshitz’s theory of fluctuating hydrodynamics [188]. Since freestream noise inevitably passes through a shock before interacting with a boundary-layer, low-frequency fluctuations in the internal translational nonequilibrium zone of a shock may not be ignored in the study of receptivity. This is true even when the level of freestream noise is minimal, *i.e.* only containing equilibrium molecular fluctuations, because the leading-edge shock interacts with boundary-layer formation.

Some examples of the notable computational fluid dynamic (CFD) literature on modeling the process of natural transition and receptivity include the work of Balakumar and Chou [52], who introduced the experimentally measured freestream fluctuations by Marineau et al. [217] in a Mach 10 flow over a cone at the outer computational boundary of their simulation domain upstream of the detached shock modeled using a shock-capturing scheme. Hader and Fasel [53] simulated a Mach 6 flow over a flared cone geometry following the experiments in the BAM6QT quiet tunnel at Purdue [212]. They constructed a simple free-stream noise model and introduced random pressure perturbations in the boundary-layer downstream of the leading-edge shock to account for the effect of freestream disturbances. Ma and Zhong [181–183] studied the receptivity of supersonic boundary layer to four types of freestream disturbances, fast and slow acoustic waves, vorticity waves, and entropy waves. The unsteady interaction of the freestream disturbance and the shock was captured using the high-order shock-fitting scheme of Zhong [55].

CFD simulations aimed at understanding receptivity do not model the details of PDFs of particles or the internal structure of a shock wave and therefore, cannot properly account for low-frequency fluctuations. Yet it is possible to incorporate the effect of characteristic fluctuations of a leading-edge shock by constructing simple models similar to that of Hader and Fasel [53] to understand the process of natural transition in quiet tunnels. To construct such models, a simple method is needed to estimate the low-frequency of a shock-wave generated at arbitrary input conditions, which

may not have been simulated explicitly using DSMC. Also, the Strouhal number may not be the best way to estimate the low-frequency, especially if the input temperature is not the same as that considered in an earlier DSMC-simulations. In this work, we present a different approach to estimate the characteristic low-frequency of a shock by correlating the shape of the analytically derived PDFs with the DSMC-computed frequencies for the Mach number range of $3 \leq M \leq 10$, upstream temperature range of $\sim 90 \leq T_{tr,1}/(K) \leq 1420$, and an upstream number density, $n_1 = 10^{22} \text{ m}^{-3}$.

The existing literature [37, 91, 218] on the analytic form of PDFs of energy of particles pertains to systems in global equilibrium with zero bulk velocity, i.e. a heat bath, where the PDFs are of the form of chi-squared distributions. In this work, we show that the energy PDFs for a hypersonic flow in local equilibrium at the upstream and downstream regions of the shock have the form of the NCCS distributions (see Sec. 5.3). We also derive the bimodal energy PDFs in the nonequilibrium zone of a shock as the linear combination of the NCCS distributions in the upstream and downstream regions with weighting factors obtained from the theory of Mott-Smith [68] (see Sec. 5.4) and provide a python code to easily generate these PDFs (see supplementary Sec. 5.7.1). The variation of the analytically derived PDFs is studied as a function of Mach number and their shape characteristic is linearly correlated with the DSMC-derived low-frequency of the fluctuations inside a shock for the Mach number range, $3 \leq M \leq 10$ at $T_{tr,1} = 710 \text{ K}$ and $n_1 = 10^{22} \text{ m}^{-3}$ (see Sec. 5.5). At $M=7.2$, $n_1 = 10^{22} \text{ m}^{-3}$, and $\sim 90 \leq T_{tr,1}/(K) \leq 1420$, the change in the DSMC-derived low-frequency fluctuation is also linearly correlated with analytically obtained inverse most-probable-speed. Based on these linear functions, we demonstrate that the average low-frequency of fluctuations can be estimated for any arbitrary input condition within the bounds of the aforementioned parameter space even if it was not computed explicitly in our previous work. For convenience, the estimated average low-frequencies are also provided in this parameter space.

5.2 One-Dimensional Shock Structure and Low-Frequency Fluctuations

The internal structure of a 1-D, steady, Mach 7.2 argon shock simulated using the kinetic DSMC method is shown in figure 5.1, where X is the direction normal to the shock and λ_1 is the upstream mean-free-path, and subscripts 1 and 2 are used to denote freestream and downstream values. Location $X/\lambda_1 = 0$ corresponds to the location where the magnitude of the velocity gradient is maximum. The upstream number density, n_1 , and translational temperature, $T_{tr,1}$, are 10^{22} m^{-3} and 710 K , respectively, and the downstream subsonic conditions are imposed by the Rankine-Hugoniot jump conditions. Figure 5.1 shows the X -directional normal stress, σ_{xx} , normalized by the upstream pressure p_1 , where σ_{xx} is non-zero inside the shock, $-16 < X/\lambda_1 < 6$, and constant in the upstream and downstream equilibrium regions, i.e. $X/\lambda_1 \leq -16$ and $X/\lambda_1 \geq 6$, respectively. Numerical probe locations F , P , and D also marked on the profile of σ_{xx} in the freestream ($X/\lambda_1 = -29$) region, inside the shock in the vicinity of the maximum velocity

gradient magnitude ($X/\lambda_1 = -1$), and in the downstream regions ($X/\lambda_1 = 29$), respectively. The complete details of the simulation and profiles of other macroparameters through the shock are given in our recent work [5].

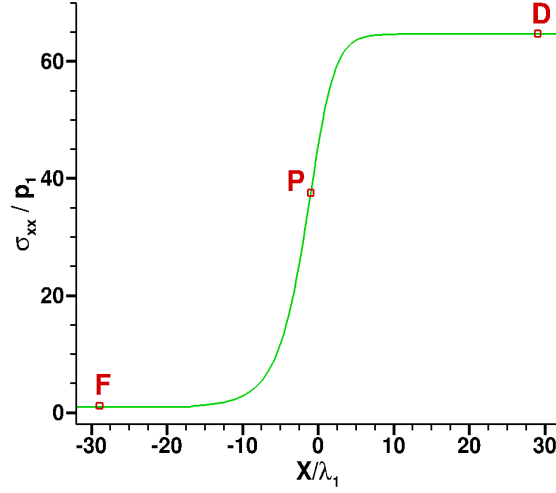


Figure 5.1: Normalized σ_{xx} in a 1-D, $M=7.2$ shock of argon.

To compare molecular fluctuations in the shocks versus that in the freestream, we defined the normalized X -directional molecular energy of particles, $\xi_x = (v_x^2 - u_x^2)\beta^2$, where v_x and u_x are instantaneous and bulk velocity components of molecules. σ_{xx} is related to ξ_x through the first moment of the PDF of f_{ξ_x} defined by mean μ_{ξ_x} as,

$$\mu_{\xi_x} = \int \xi_x f_{\xi_x} d\xi_x = \frac{\sigma_{xx}\beta^2}{\rho} \quad (5.1)$$

where f_{ξ_x} is the PDF of molecules in the energy space ξ_x , $\rho = nm$ is the local mass density, $m = 6.63 \times 10^{-26}$ kg is the molecular mass, $\beta = (2RT_{tr})^{-1/2}$ is the the inverse most-probable-speed, T_{tr} is the local average translational temperature, and R is the specific gas constant. The analytical form of f_{ξ_x} in equilibrium and nonequilibrium regions is described in Secs. 5.3 and 5.4, respectively. Reference [5] shows that based on Eq. 5.1, the fluctuations in σ_{xx} are related to fluctuations in the number of particles in the energy space, ξ_x .

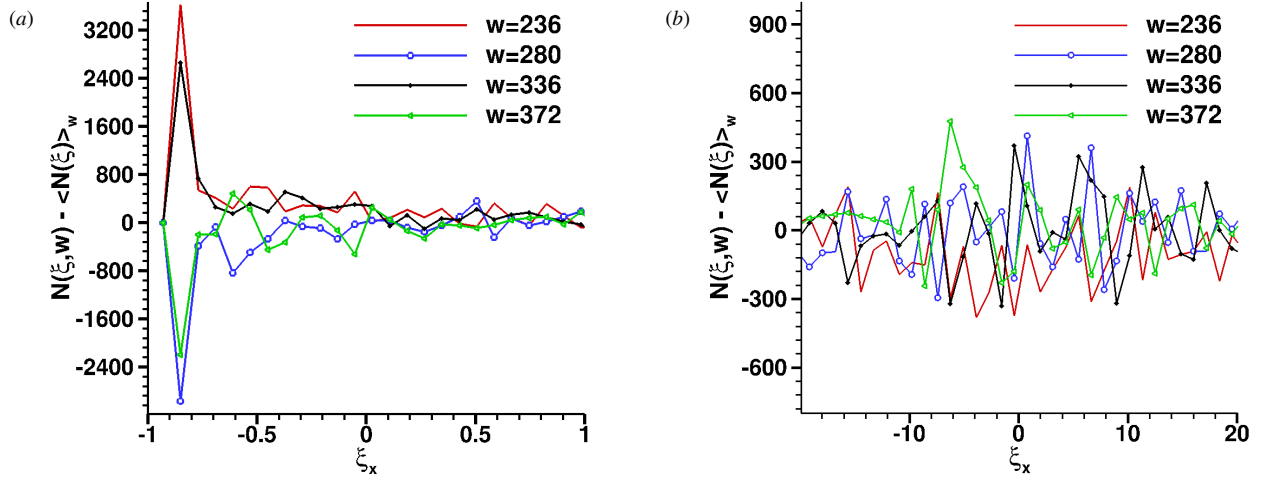


Figure 5.2: Fluctuations in the number of particles in PDF of f_{ξ_x} obtained from DSMC as a function of ξ_x at four time-windows (a) at probe P inside the shock and (b) probe F in the freestream.

The differences in fluctuations in the shock and the freestream are shown in Figs. 5.2(a) and 5.2(b), respectively. The fluctuations are defined by the quantity $[N(\xi_x, w) - \langle N(\xi_x) \rangle_w]$, where $N(\xi_x, w)$ is the total number of DSMC particles within the energy space ξ_x and $\xi_x + \Delta\xi_x$, where $\Delta\xi_x = 0.0115$, from time-window w to $w + 1$ and $\langle N(\xi_x) \rangle_w$ denotes the number of particles in the same energy space averaged over all time-windows, $W = 646$. Each time-window is equal to 100 timesteps of 3 ns and $w=0$ is defined to be the end of transient time of $6 \mu\text{s}$ required to establish the shock structure from the initial Rankine-Hugoniot jump conditions. Figure 5.2(a) shows at probe P inside the shock that the fluctuations within the energy space -1 to 1 have a time-period of approximately 100 time-windows, corresponding to a 34 kHz frequency, a period within which the peak between $\xi_x = -1$ to -0.6 changes sign twice. The low-energy space corresponds to the contribution from the subsonic region. Note that due to the statistical nature of molecular fluctuations the frequencies are distributed over a broadband of low-frequencies, which is characterised by a weighted-average and ± 1 standard deviation. At probe P , these values were found to be 37.5 and 21.4 kHz, respectively. The entire spectrum of frequencies obtained using the power spectral density (PSD) of the mean-subtracted, DSMC-derived data of σ_{xx} are described in Ref. [5]. At probe F in the freestream, however, figure 5.2(b) shows that there are no low-frequencies and the change in the number of particles in the freestream is much lower than that in the shock indicating smaller amplitude fluctuations.

5.3 Formulation of Noncentral Chi-Squared (NCCS) PDFs in an Equilibrium Gas

In this section the PDF of f_{ξ_x} is derived for a gas in local equilibrium using the local Maxwell-Boltzmann (MB) PDF [219] of particle velocities and it is shown that the energy PDF is of the class of an NCCS PDF. For completeness, PDFs of f_{ξ_y} , f_{ξ_z} , and f_{ξ} of the Y -directional (ξ_y), Z -directional (ξ_z), and total energies of particles (ξ) are also derived. The first moment of f_{ξ_y} , f_{ξ_z} and f_{ξ} are related to Y and Z -directional normal stresses, σ_{yy} , σ_{zz} , and pressure, p , as

$$\begin{aligned}\mu_{\xi_y} &= \int \xi_y f_{\xi_y} d\xi_y = \frac{\sigma_{yy}\beta^2}{\rho} \\ \mu_{\xi_z} &= \int \xi_z f_{\xi_z} d\xi_z = \frac{\sigma_{zz}\beta^2}{\rho} \\ \mu_{\xi} &= \int \xi f_{\xi} d\xi = \frac{3p\beta^2}{\rho} = \frac{3}{2}\end{aligned}\tag{5.2}$$

Note that $\xi_y = v_y^2\beta^2$, $\xi_z = v_z^2\beta^2$, and $\xi = (v^2 - u^2)\beta^2$, where v_y , v_z are the instantaneous components in the Y and Z -directions, respectively, u_y , u_z are the bulk velocity components in the Y and Z -directions, respectively, and v , u are the instantaneous and bulk speed of molecules, respectively.

The local MB PDF for particles having instantaneous molecular and bulk velocity vectors $\mathbf{v}$ and $\mathbf{u}$, respectively, and an equilibrium translational temperature, T_{tr} , is written as,

$$f_{\mathbf{v}} = \frac{\beta^3}{\pi^{3/2}} \exp\left(-\beta^2(\mathbf{v} - \mathbf{u})^2\right)\tag{5.3}$$

$f_{\mathbf{v}}$ may change spatially depending on the local values of $\mathbf{u}$, T_{tr} , and applies to particles in equilibrium, i.e. it is valid for $X/\lambda_1 \leq -16$ in the freestream and $X/\lambda_1 \geq 6$ in the downstream. The bulk velocity and temperature are related to the first and second moments of the distribution as,

$$\begin{aligned}u_i &= \int v_i f_{\mathbf{v}} dv_x dv_y dv_z, \quad \text{for } i \in \{x, y, z\} \\ T_{tr} &= \frac{m}{3\kappa_b} \int v^2 f_{\mathbf{v}} dv_x dv_y dv_z\end{aligned}\tag{5.4}$$

The PDF for directional velocity components can be obtained by integrating the differential probability $f_{\mathbf{v}} dv_x dv_y dv_z$ over the remaining two components, i.e.,

$$f_{v_i} = \frac{\beta}{\sqrt{\pi}} \exp\left(-\beta^2(v_i - u_i)^2\right); \quad \text{for } i \in \{x, y, z\}\tag{5.5}$$

Equation 5.5 can be expressed as a PDF of a Gaussian distribution having mean (bulk velocity) u_i , and variance $(2\beta^2)^{-1}$ as,

$$\mathcal{N}_{v_i}(u_i, (2\beta^2)^{-1}) = \frac{1}{\sqrt{2\pi(2\beta^2)^{-1}}} \exp\left(-\frac{(v_i - u_i)^2}{2(2\beta^2)^{-1}}\right)$$

This can be further scaled as a PDF of a Gaussian distribution of a scaled variable $\tilde{v}_i$, having unit variance and non-zero scaled mean $\tilde{u}_i$ as,

$$\mathcal{N}_{\tilde{v}_i}(\tilde{u}_i, 1) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{(\tilde{v}_i - \tilde{u}_i)^2}{2}\right) \quad (5.6)$$

where

$$\tilde{v}_i = \sqrt{2}v_i\beta \quad \text{and} \quad \tilde{u}_i = \sqrt{2}u_i\beta$$

Note that the differential probability of particles lying within a velocity space v_i and $v_i + dv_i$ is the same as them being within the scaled velocity space $\tilde{v}_i$ and $\tilde{v}_i + d\tilde{v}_i$, i.e.,

$$\mathcal{N}_{v_i}(u_i, (2\beta^2)^{-1})dv_i = \mathcal{N}_{\tilde{v}_i}(\tilde{u}_i, 1)d\tilde{v}_i$$

From the scaled Gaussian variables $\tilde{v}_x$, $\tilde{v}_y$, and $\tilde{v}_z$, the PDF for the sum of squares of independent combinations of these variables, χ , can be constructed which are known as the noncentral chi-squared distributions [220],

$$f_\chi = \frac{1}{2} \exp\left(-\frac{\chi + \eta}{2}\right) \left(\frac{\chi}{\eta}\right)^{\frac{\mathcal{D}}{4} - \frac{1}{2}} I_{\frac{\mathcal{D}}{2} - 1}(\sqrt{\eta\chi}) \quad (5.7)$$

They have two parameters, the number of degrees of freedom $\mathcal{D} = 1, 2$, or 3 depending on the number of independent Gaussian variables used in the sum, χ , and a noncentrality parameter η , given by the sum of squares of the respective means of the Gaussian variables ($\tilde{u}_x$, $\tilde{u}_y$, and $\tilde{u}_z$). Note that $I_\gamma(x)$ is the modified Bessel function of the first kind, defined as,

$$I_\gamma(x) = \sum_{m=0}^{\infty} \frac{1}{m!\Gamma(m + \gamma + 1)} \left(\frac{x}{2}\right)^{2m+\gamma} \quad (5.8)$$

The mean, μ_χ , and standard deviation, Σ_χ , of f_χ is given as,

$$\begin{aligned}\mu_\chi &= \mathcal{D} + \eta \\ \Sigma_\chi &= \sqrt{2(\mathcal{D} + 2\eta)}\end{aligned}\tag{5.9}$$

To derive the PDF of f_{ξ_x} , we choose $\chi = \tilde{v}_x^2$. Since only one independent Gaussian variable is required, we have $\mathcal{D} = 1$. The noncentrality parameter for the given χ is $\eta = \tilde{u}_x^2$. By substituting χ , $\mathcal{D}$, and η into Eq. 5.7, we obtain,

$$f_{\tilde{v}_x^2} = \frac{1}{2} \exp\left(-\frac{\tilde{v}_x^2 + \tilde{u}_x^2}{2}\right) \left(\frac{\tilde{u}_x}{\tilde{v}_x}\right)^{\frac{1}{2}} I_{-\frac{1}{2}}(\tilde{u}_x \tilde{v}_x)\tag{5.10}$$

and using Eq. 5.9, the mean and standard deviation,

$$\begin{aligned}\mu_{\tilde{v}_x^2} &= 1 + \tilde{u}_x^2 \\ \Sigma_{\tilde{v}_x^2} &= \sqrt{2(1 + 2\tilde{u}_x^2)}\end{aligned}\tag{5.11}$$

The distribution function in Eq. 5.10 can be scaled by a factor of 0.5 to obtain a distribution $f_{(\tilde{v}_x^2/2)}$ by noting that,

$$f_{\tilde{v}_x^2} d\tilde{v}_x^2 = f_{(\tilde{v}_x^2/2)} d\left(\frac{\tilde{v}_x^2}{2}\right)$$

which means that the probability of particles having normalized energies within energy space $\tilde{v}_x^2$ and $\tilde{v}_x^2 + d\tilde{v}_x^2$ remains unchanged. Therefore, we obtain,

$$f_{(\tilde{v}_x^2/2)} = 2f_{\tilde{v}_x^2} = \exp\left(-\frac{\tilde{v}_x^2 + \tilde{u}_x^2}{2}\right) \left(\frac{\tilde{u}_x}{\tilde{v}_x}\right)^{\frac{1}{2}} I_{-\frac{1}{2}}(\tilde{u}_x \tilde{v}_x)\tag{5.12}$$

This PDF can be shifted by $-\tilde{u}_x^2/2$ to obtain,

$$f_{((\tilde{v}_x^2 - \tilde{u}_x^2)/2)} = \exp\left(-\frac{\tilde{v}_x^2}{2}\right) \left(\frac{\tilde{u}_x}{\sqrt{\tilde{v}_x^2 - \tilde{u}_x^2}}\right)^{\frac{1}{2}} I_{-\frac{1}{2}}\left(\tilde{u}_x \sqrt{\tilde{v}_x^2 - \tilde{u}_x^2}\right)\tag{5.13}$$

This is the PDF of normalized X-directional energy, ξ_x , as seen from the following relation,

$$\frac{\tilde{v}_x^2 - \tilde{u}_x^2}{2} = v_x^2 \beta^2 - u_x^2 \beta^2 = \xi_x$$

Therefore, we can write Eq. 5.13 in terms of ξ_x as,

$$f_{\xi_x} = \exp\left(-(\xi_x + u_x^2\beta^2)\right) \left(\frac{u_x\beta}{\sqrt{\xi_x}}\right)^{\frac{1}{2}} I_{-\frac{1}{2}}\left(2u_x\beta\sqrt{\xi_x}\right)$$

Finally, the above equation can be written in terms of the noncentrality parameter, $\eta = \tilde{u}_x^2 = 2u_x^2\beta^2$, as,

$$f_{\xi_x} = \exp\left(-\frac{2\xi_x + \eta}{2}\right) \left(\frac{\eta}{2\xi_x}\right)^{\frac{1}{4}} I_{-\frac{1}{2}}\left(\sqrt{2\xi_x\eta}\right) \quad (5.14)$$

The aforementioned process of scaling the PDF of $f_{\tilde{v}_x^2}$ in Eq. 5.10 scales the mean and standard deviation in Eq. 5.11 by a factor of half. Furthermore, shifting the PDF by $-\tilde{u}_x^2/2 = -u_x^2\beta^2$, shifts the mean by the same factor but keeps the standard deviation unchanged. Therefore, the mean and standard deviation of f_{ξ_x} can be written as,

$$\begin{aligned} \mu_{\xi_x} &= 0.5 \\ \Sigma_{\xi_x} &= \frac{\sqrt{2(1+2\eta)}}{2} \end{aligned} \quad (5.15)$$

Next, to obtain the PDF of f_{ξ_y} , we follow the same procedure, where $\chi = \tilde{v}_y^2$ and $\mathcal{D} = 1$, however, note that $\eta = u_y^2 = 0$. For $\eta = 0$, the noncentral chi-squared distribution in Eq. 5.7 reduces to a chi-squared distribution and for $\mathcal{D} = 1$, the PDF has the form,

$$f_{\chi} = \sqrt{\frac{\chi}{2\pi}} \exp\left(-\frac{\chi}{2}\right) \quad (5.16)$$

This can be verified by use of Eq. 5.8 in Eq. 5.7, simplifying, and then substituting $\eta = 0$. Use of Eq. 5.9, gives the constant values of mean and standard deviation of one and 1.414, respectively. By substituting $\chi = \tilde{v}_y^2$ in Eq. 5.16, we get,

$$f_{\tilde{v}_y^2} = \frac{\tilde{v}_y}{\sqrt{2\pi}} \exp\left(-\frac{\tilde{v}_y^2}{2}\right) \quad (5.17)$$

To obtain the distribution for $\xi_y = v_y^2\beta^2 = \tilde{v}_y^2/2$, the distribution $f_{\tilde{v}_y^2}$ can be scaled by a factor of half as,

$$f_{\xi_y} = f_{(\tilde{v}_y^2/2)} = \frac{\tilde{v}_y\sqrt{2}}{\sqrt{\pi}} \exp\left(-\frac{\tilde{v}_y^2}{2}\right)$$

or in terms of ξ_y as,

$$f_{\xi_y} = f_{(\tilde{v}_y^2/2)} = 2\sqrt{\frac{\xi_y}{\pi}} \exp(-\xi_y) \quad (5.18)$$

The effect of scaling the PDF by a factor of half reduces the mean and standard deviation to 0.5 and $\sqrt{2}$, respectively. Note that the PDF of f_{ξ_z} has the same form as the PDF of f_{ξ_y} because of axial symmetry in the 1-D case.

Similarly, to obtain the PDF of $\xi = (v^2 - u^2)\beta^2$, we choose $\chi = \tilde{v}_x^2 + \tilde{v}_y^2 + \tilde{v}_z^2 = \tilde{v}^2$, for which $\mathcal{D} = 3$ and $\eta = \tilde{u}_x^2 + \tilde{u}_y^2 + \tilde{u}_z^2 = \tilde{u}^2$. Note that for the 1-D case, $\tilde{u}_y = \tilde{u}_z = 0$, which results in $\eta = \tilde{u}_x^2 = \tilde{u}^2$. By substituting χ , $\mathcal{D}$, and η in Eq. 5.7, we obtain,

$$f_{\tilde{v}^2} = \frac{1}{2} \exp\left(-\frac{\tilde{v}^2 + \tilde{u}^2}{2}\right) \left(\frac{\tilde{v}}{\tilde{u}}\right)^{\frac{1}{2}} I_{\frac{1}{2}}(\tilde{u}\tilde{v}) \quad (5.19)$$

By following an approach similar to that for f_{ξ_x} , the PDF of $f_{\tilde{v}^2}$ can be first scaled by a factor of half to obtain the PDF of $(\tilde{v}^2/2)$ and then shifted by $-\tilde{u}^2/2$ to obtain the PDF of $((\tilde{v}^2 - \tilde{u}^2)/2) = \xi$, which can be written in terms of ξ and $\eta = 2u^2\beta^2$ as,

$$f_{\xi} = \exp\left(-\frac{2\xi + \eta}{2}\right) \left(\frac{2\xi}{\eta}\right)^{\frac{1}{4}} I_{\frac{1}{2}}(\sqrt{2\xi\eta}) \quad (5.20)$$

with mean and standard deviation of f_{ξ} given as,

$$\begin{aligned} \mu_{\xi} &= 1.5 \\ \Sigma_{\xi} &= \frac{\sqrt{2(3 + 2\eta)}}{2} \end{aligned} \quad (5.21)$$

This completes our derivation of the PDFs of f_{ξ_x} , f_{ξ_y} , f_{ξ_z} , and f_{ξ} , which are valid in the equilibrium regions of freestream and downstream. The mean and standard deviation of these PDFs at probes F in the freestream and D in the downstream are listed in Table 5.1. The theoretical estimates of mean and standard deviation (not shown) agree with values obtained from DSMC-derived PDFs within 1%, as expected from the good agreement in PDFs shown in Fig. 5.3.

Equation No.	Parameters	Probes F	Probes D
5.21	μ_ξ, Σ_ξ	1.50, 9.40	1.50, 1.36
5.15	$\mu_{\xi_x}, \Sigma_{\xi_x}$	0.50, 9.35	0.50, 0.92
5.15 with $\eta = 0$	$\mu_{\xi_y}, \Sigma_{\xi_y}$	0.50, 0.71	0.50, 0.72

Table 5.1: The mean and standard deviation of f_ξ , f_{ξ_x} , and f_{ξ_y} using DSMC.

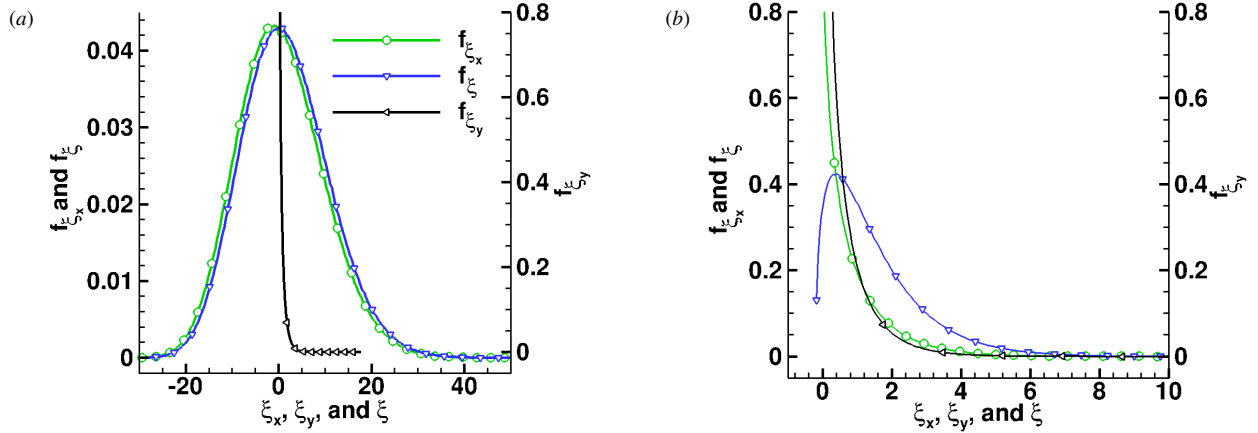


Figure 5.3: The theoretically-derived PDFs of f_{ξ_x} , f_{ξ_y} , and f_ξ at (a) probe F and (b) probe D , respectively. Legends for (b) are the same as (a). The DSMC-derived PDFs are not shown as they agree well with theoretical PDFs.

Figures 5.3(a) and 5.3(b) show the PDFs of f_{ξ_x} , f_{ξ_y} , and f_ξ obtained from the analytical expressions given by Eqs. 5.14, 5.18, and 5.20 at probes F in the freestream and D in the downstream region of the shock, respectively. Since both of these regions are in equilibrium, the theoretically derived distributions agree very well with the numerically obtained distributions from DSMC. The differences in the respective PDFs at the two probe locations are due to the differences in their macroscopic flow parameters. In the freestream, the PDFs of f_{ξ_x} and f_ξ are nearly symmetric about zero, as seen from Fig. 5.3(a), whereas in the downstream they are almost completely to the right of zero, as seen from Fig. 5.3(b). This difference is due to the large noncentrality parameter of $\eta_1 = 2u_{x,1}^2\beta_1^2 = 87.25$ in the freestream, for which the NCCS PDF tends towards a Gaussian, whereas the value in the downstream is only $\eta_2 = 2u_{x,2}^2\beta_2^2 = 0.3538$. Parameter η can be interpreted as the ratio of the bulk flow energy of the gas to its thermal energy defined using the most-probable-speed, β^{-1} . In the downstream, these two energies are expected to be comparable as the kinetic energy of the gas is converted to the thermal energy by the shock.

Also, the differences between the PDFs of f_{ξ_x} and f_ξ are because of the differences in degree, $\mathcal{D}$. In the freestream, this difference is only noticeable as a small shift between the symmetric distributions, whereas in the downstream the

difference in their shapes is quite conspicuous. Note, however, that at both locations the values of μ_{ξ_x} and μ_{ξ} are such that the normalized viscous stress, τ_{xx} , is zero based on the relation,

$$\frac{\tau_{xx}\beta^2}{\rho} = \frac{-(\sigma_{xx} - p)\beta^2}{\rho} = -\left(\mu_{\xi_x} - \frac{1}{3}\mu_{\xi}\right) \quad (5.22)$$

which is also consistent with the DSMC-derived profiles of τ_{xx} (see Ref. [5]).

Additionally, in the freestream, Fig. 5.3(a) shows that there is a difference between the shape of the PDFs of f_{ξ_y} and f_{ξ_x} , although they both have the same degree, $\mathcal{D} = 1$. This difference is because of the difference in η_1 , which is zero for the former and 87.25 for the latter. In the downstream, these two distributions are very close to each other, as shown in Fig. 5.3(b), because the value of η_2 is closer, i.e. 0 and 0.3538 for PDFs of f_{ξ_y} and f_{ξ_x} , respectively. For both equilibrium regions, the mean values μ_{ξ_y} and μ_{ξ} are 0.5 and 1.5, respectively, as shown in Table 5.1, such that $\tau_{yy} = -(\sigma_{yy} - p) = 0$, based on a similar relation as in Eq. 5.22. Furthermore, notice from Table 5.1 that the standard deviations Σ_{ξ} and Σ_{ξ_x} are much larger in the freestream than downstream, because $\eta_1 \gg \eta_2$. Although they are not directly related to any macroscopic flow parameter, they suggest a larger spread of X -directional and overall normalized energies of particles in the freestream, where the bulk flow energy is much larger than the thermal energy, as opposed to downstream where the two energies are comparable. This makes sense because in the downstream, particles collide more and distribute their energy better than the freestream, which causes a reduction in the spread of their energy distribution.

5.4 Formulation of Bimodal NCCS PDFs in Monatomic Shocks

To derive the energy PDFs of f_{ξ_x} , f_{ξ_y} , and f_{ξ} inside the nonequilibrium region of the 1-D shock, $-16 < X/\lambda_1 < 6$, we take the approach of Mott-Smith [68], who approximated the PDF inside the shock of particle velocities as a linear combination of equilibrium PDFs in the upstream and downstream equilibrium regions, i.e.,

$$nf_{\mathbf{v}} = \phi_1 f_{\mathbf{v},1} + \phi_2 f_{\mathbf{v},2} \quad (5.23)$$

where n is the local number density. PDFs of $f_{\mathbf{v},1}$ and $f_{\mathbf{v},2}$ are obtained by substituting the upstream and downstream macroscopic flow conditions of $(n_1, u_{x,1}, \beta_1)$ and $(n_2, u_{x,2}, \beta_2)$, respectively, in Eq. 5.3. The use of normalization condition $\int f_{\mathbf{v}} d\mathbf{v} = 1$ leads to the local number density, $n = \phi_1 + \phi_2$. The weights ϕ_1 and ϕ_2 are functions of X/λ_1 and

are given as [37],

$$\begin{aligned}\phi_1 &= \frac{n_1}{1 + \exp\left(\alpha \left(\frac{x}{\lambda_1}\right)\right)} \\ \phi_2 &= \frac{n_2 \exp\left(\alpha \left(\frac{x}{\lambda_1}\right)\right)}{1 + \exp\left(\alpha \left(\frac{x}{\lambda_1}\right)\right)}\end{aligned}\quad (5.24)$$

where, α is a constant given as,

$$\alpha = \frac{5}{3\sqrt{\pi}} \frac{\sqrt{2RT_{tr,1}}}{u_{x,2}} \frac{u_{x,1} - u_{x,2}}{u_{x,1} + u_{x,2}}$$

Using the above equations, at probe P , the prediction of number density, $n = \phi_1 + \phi_2$, is 0.26% higher than the DSMC-computed value, where ϕ_1 and ϕ_2 are 7.214×10^{21} and 1.053×10^{22} , respectively. By integrating the differential probability $f_{\mathbf{v}} dv_x dv_y dv_z$ over the remaining two components, the PDF of directional velocities, v_i for $i \in \{x, y, z\}$ can be obtained inside a shock. By taking moments of it, the macroscopic flow parameters of directional bulk velocities and directional temperatures can also be obtained as,

$$\begin{aligned}u_i &= \int v_i f_{v_i} dv_i, \quad \text{for } i \in \{x, y, z\} \\ T_{tr,i} &= \frac{m}{\kappa_b} \int v_i^2 f_{v_i} dv_i\end{aligned}\quad (5.25)$$

Figures 5.4(a) and 5.4(b) show the respective comparison of the PDFs of normalized velocities, $v_x\beta$ and $v_y\beta$, obtained from DSMC with the theoretical prediction of Mott-Smith bimodal model and the equilibrium distribution given by Eq. 5.5 at probe P . Figure 5.4(a) shows that the PDF of $v_x\beta$ obtained from DSMC skews towards the high velocity region in contrast to the symmetric unimodal equilibrium distribution. The Mott-Smith model, gives a qualitatively better approximation in terms of bimodality of the PDF, however, it overestimates the contribution of the upstream high velocity particles and shows a second distinct peak. This difference leads to a 1.95% lower prediction of the bulk velocity, u_x , in comparison to DSMC at probe P , although a smaller difference is expected further away from the center of the shock, where the degree of nonequilibrium is lower. Figure 5.4(b) shows a good agreement between Mott-Smith and DSMC except for the region of low Y -velocity, $0.25 < v_y\beta < 0.25$, which is overestimated, but nonetheless, the model correctly predicts $u_y = u_z = 0$. The predicted values of directional temperatures, $T_{tr,x}$ and $T_{tr,y} = T_{tr,z}$, are higher and lower than DSMC by 1.35 and 7.2%, respectively, and the predicted overall temperature, computed as the average of directional temperatures, and the value of β are 2.7% lower and 1.4% higher than DSMC, respectively. Since the Mott-Smith model gives a reasonable estimation of macroscopic flow parameters, a similar idea

can be used to analytically derive bimodal NCCS PDFs inside the 1-D shock.

We start with normalizing the weights ϕ_1 and ϕ_2 by the total weight $\phi_1 + \phi_2$ and use these for constructing a bimodal PDF as,

$$\begin{aligned} f_{\xi_i} &= \psi_1 f_{\xi_i,1} + \psi_2 f_{\xi_i,2} \quad \text{where, } i \in \{x, y, z\} \\ f_{\xi} &= \psi_1 f_{\xi,1} + \psi_2 f_{\xi,2} \end{aligned} \quad (5.26)$$

where

$$\psi_1 = \frac{\phi_1}{\phi_1 + \phi_2} \quad \text{and} \quad \psi_2 = \frac{\phi_2}{\phi_1 + \phi_2}$$

The PDFs of $f_{\xi_x,1}$, $f_{\xi_y,1}$, and $f_{\xi_z,1}$ are generated from PDFs of $\tilde{v}_x^2$, $\tilde{v}_y^2$, and $\tilde{v}^2$ given in Eq. 5.10, 5.17, and 5.19, respectively, by first scaling them by a factor of $s_1 = 0.5\beta^2/\beta_1^2$ and then shifting by the amounts $-u_x^2\beta^2$, 0, and $-u^2\beta^2$, respectively. The local values of u_x , u , and β are obtained from Eq. 5.25. Similarly, to obtain PDFs of $f_{\xi_x,2}$, $f_{\xi_y,2}$, and $f_{\xi_z,2}$ the scaling factor of $s_2 = 0.5\beta^2/\beta_2^2$ is used, while the amount of respective shifting is the same, and the procedure for generating $f_{\xi_x,1}$ and $f_{\xi_z,2}$ is the same as that for $f_{\xi_y,1}$ and $f_{\xi_y,2}$, respectively, because of axial symmetry. The final PDFs of $f_{\xi,j}$, $f_{\xi_x,j}$, and $f_{\xi_y,j}$, where $j = 1$ and 2 correspond to upstream and downstream conditions, respectively, are given as,

$$\begin{aligned} f_{\xi,j} &= f_{(v_{x,j}^2 - u^2)\beta^2} = \frac{1}{2s_j} \exp\left(-2\frac{(v_{x,j}^2 - u^2)\beta^2}{s_j} + \frac{\eta_j}{2}\right) \times \\ &\quad \left(\frac{4(v_{x,j}^2 - u^2)\beta^2}{s_j\eta_j}\right)^{\frac{1}{4}} I_{\frac{1}{2}}\left(\sqrt{\frac{4\eta_j(v_{x,j}^2 - u^2)\beta^2}{s_j}}\right) \\ f_{\xi_x,j} &= f_{(v_{x,j}^2 - u_x^2)\beta^2} = \frac{1}{2s_j} \exp\left(-2\frac{(v_{x,j}^2 - u_x^2)\beta^2}{s_j} + \frac{\eta_j}{2}\right) \times \\ &\quad \left(\frac{s_j\eta_j}{4(v_{x,j}^2 - u_x^2)\beta^2}\right)^{\frac{1}{4}} I_{-\frac{1}{2}}\left(\sqrt{\frac{4\eta_j(v_{x,j}^2 - u_x^2)\beta^2}{s_j}}\right) \\ f_{\xi_y,j} &= f_{(v_y^2)\beta^2} = \frac{1}{s_j} \sqrt{\frac{v_{y,j}\beta^2}{\pi}} \exp\left(-v_{y,j}\beta^2\right) \end{aligned} \quad (5.27)$$

where, $v_{x,j}$ and $v_{y,j}$ are instantaneous velocities of particles that follow PDFs of $f_{v_x,j}$ and $f_{v_y,j}$ in Eq. 5.23, for $j = 1, 2$.

Also, $\eta_j = 2u_{x,j}^2\beta_j^2 = 2u_j^2\beta_j^2$, for $j = 1, 2$. Note that the mean of these PDFs can be easily calculated as,

$$\begin{aligned}\mu_\xi &= \psi_1 s_1(3 + \eta_1) + \psi_2 s_2(3 + \eta_2) - u_x^2 \beta^2 \\ \mu_{\xi_x} &= \psi_1 s_1(1 + \eta_1) + \psi_2 s_2(1 + \eta_2) - u_x^2 \beta^2 \\ \mu_{\xi_x} &= \psi_1 s_1 + \psi_2 s_2\end{aligned}\tag{5.28}$$

however, for higher moments the distributions have to be numerically integrated. A simple Python code to generate the bimodal distributions of energy using Mott-Smith fractions and its moments is given in Sec. 5.7.1.

Figures 5.4(d), 5.4(e), and 5.4(c) show the respective comparison of the PDFs of f_{ξ_x} , f_{ξ_y} , and f_ξ obtained from DSMC with the analytically derived bimodal NCCS PDFs using Eq. 5.26, denoted as ‘Mott-Smith’, and the equilibrium NCCS PDFs obtained from Eqs. 5.14, 5.18, and 5.20 at local macroscopic flow conditions for probe P . The difference between PDFs obtained from DSMC and the equilibrium theory is expected due to nonequilibrium. It is small for PDF of f_{ξ_y} , indicating that the energy distribution in transverse directions is not significantly affected. The DSMC-derived PDFs of f_ξ and f_{ξ_x} exhibit inflection points at $\xi = 0.49$ and $\xi_x = 1.33$, which indicate their bimodal nature.

In our previous work [5], we have used the DSMC-derived PDF of f_{ξ_x} in a Mach 7.2 argon shock at $n_1=10^{22} \text{ m}^{-3}$ and $T_{tr,1}=710 \text{ K}$ to show that the collisions between particles on two sides of the inflection point are responsible for the low-frequency fluctuations inside a shock. Figure 5.4 shows that the Mott-Smith model approximates the bimodality of the PDF reasonably well except for the number of particles in the vicinity of the inflection points. Despite these differences, Table 5.2 shows that the mean and standard deviation of the PDF of f_{ξ_x} obtained from the Mott-Smith model are only 0.6% lower and 4.4% higher than the values obtained from the DSMC distribution, respectively, and the mean and standard deviation of the PDF of f_{ξ_x} are 1.3 and 5.8% higher than DSMC, respectively, whereas for the PDF of f_{ξ_y} , these quantities are 7.8 and 9.2% higher, respectively. We will ignore these small differences and use the analytical PDF in the next section to correlate its shape with the low-frequency of fluctuations obtained from DSMC.

Parameters	DSMC	Mott-Smith
μ_ξ, Σ_ξ	1.50, 1.37	1.50, 1.43
$\mu_{\xi_x}, \Sigma_{\xi_x}$	0.75, 1.37	0.76, 1.45
$\mu_{\xi_y}, \Sigma_{\xi_y}$	0.40, 0.77	0.37, 0.71

Table 5.2: At probe P inside a shock, the mean and standard deviation of f_ξ , f_{ξ_x} , and f_{ξ_y} using DSMC and the Mott-Smith model.

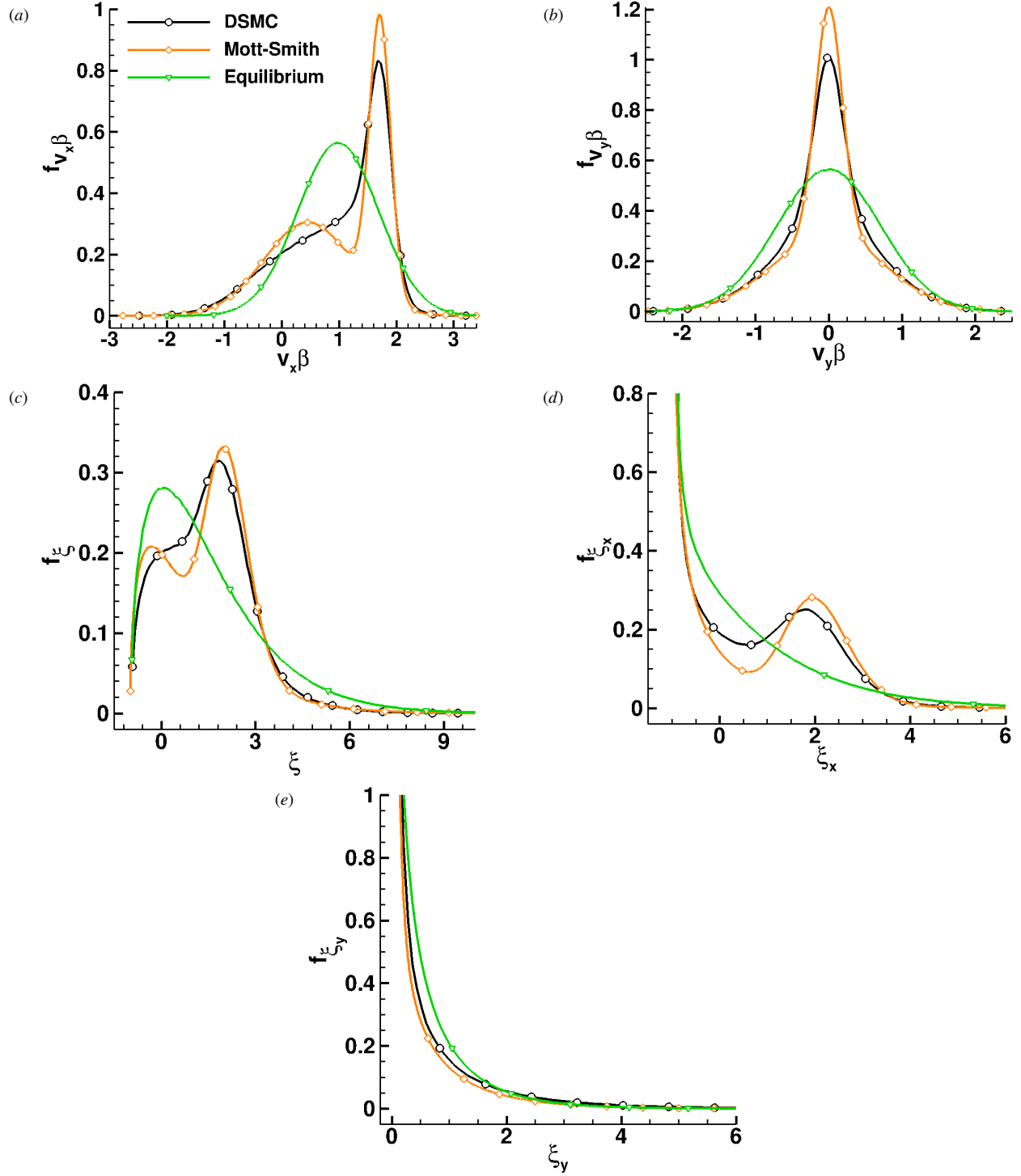


Figure 5.4: At probe P , the PDFs of normalized velocities (a) $v_x \beta$ and (b) $v_y \beta$, normalized energies (c) ξ , (d) ξ_x , (e) $\xi_y = \xi_z$. The DSMC-derived PDFs [5] are compared with the Mott-Smith model and equilibrium theory. The legends shown in (a) also apply to (b)–(e). In (a) and (b), the PDFs of normalized velocities are obtained by scaling velocity distributions as, $f_{v_i \beta} = \beta^{-1} f_{v_i}$.

5.5 Correlation of the Bimodal NCCS PDFs with DSMC-derived

Low-Frequency Fluctuations

This section describes the correlation of the analytical bimodal NCCS PDF of f_{ξ_x} with the DSMC-derived characteristic average low-frequency ν and its standard deviation Σ_ν in argon shocks, obtained in our previous work [5]. Using these correlations, an estimate of ν is made for the Mach number range $3 \leq M \leq 10$ and input temperature range $\sim 90 \leq T_{tr,1} \leq 1420$ at $n_1 = 10^{22} \text{m}^{-3}$. At other input number densities, the DSMC-derived average low-frequencies can be obtained and the following correlation procedure can be repeated. Alternatively, the Strouhal number scaling established in Sec. 4.5 can be used as a rough estimate, which shows that an average low-frequency is inversely proportional to the shock-thickness defined based on the maximum velocity gradient magnitude.

We begin with the correlation of the DSMC-derived average low-frequency of fluctuations in σ_{xx} inside shocks with the change of shape of the analytical bimodal NCCS PDF of f_{ξ_x} for Mach numbers ranging from three to 10 at $T_{tr,1} = 710$ K. Figure 5.5(a) shows the variation of the analytically-derived f_{ξ_x} at the location of maximum bulk velocity gradient in the shock ($X/\lambda_1 = 0$) with Mach number. At Mach 2, the shape of the PDF is very similar to a regular chi-squared distribution, indicating only a small contribution from high-energy upstream particles. However, as the Mach number increases, their contribution increases leading to a prominent peak in the high-energy space, $\xi_x > 1$. The DSMC-derived weighted average frequency is found to be linearly proportional to the location of this peak. This is consistent with the findings in our previous work [5] that the value of low-frequency depends on the collisions of low and high-energy particles from the subsonic downstream and supersonic/hypersonic upstream, respectively. To determine the location of the peak, the second gradient of the PDF is evaluated, f''_{ξ_x} , as shown in figure 5.5(b) for Mach 2, 4, and 10. At Mach 4 and 10, two inflection points can be seen, as defined by $f''_{\xi_x} = 0$, whereas at Mach 2, such an inflection point is absent. Between the two inflection points, f''_{ξ_x} attains a local minimum, denoted as ξ_x^M , which corresponds to the respective peak location of f_{ξ_x} in the high-energy space. It is seen from figure 5.5(c) that the DSMC-derived weighted-average low-frequency ν and its standard deviation Σ_ν at $T_{tr,1}=710$ K and $n_1 = 10^{22} \text{m}^{-3}$ linearly change with ξ_x^M . The data-points with increasing ξ_x^M in figure 5.5(c) correspond to Mach 3 to 10, which are also listed in Table 5.3.

Note, however, that the shape of f_{ξ_x} does not change with changes in the upstream temperature $T_{tr,1}$, at a given Mach number, because ξ_x is normalized by β^2 . Therefore, the change in low-frequency due to the variation in freestream temperature cannot be estimated using only the linear fit in figure 5.5(c). Keeping $n_1 = 10^{22} \text{m}^{-3}$ at Mach 7.2, Fig. 5.5(d) shows the DSMC-derived ν and Σ_ν as a function of the most-probable speed β^{-1} , inside a shock calculated from the analytical Mott-Smith velocity distribution function. The figure shows that ν is linearly proportional to β^{-1}

for $T_{tr,1}/710=1/8, 1/4, 1/2, 1$, and 2 . The variation of β^{-1} obtained from Mott-Smith with $T_{tr,1}$ is also given in figure 5.5(d).

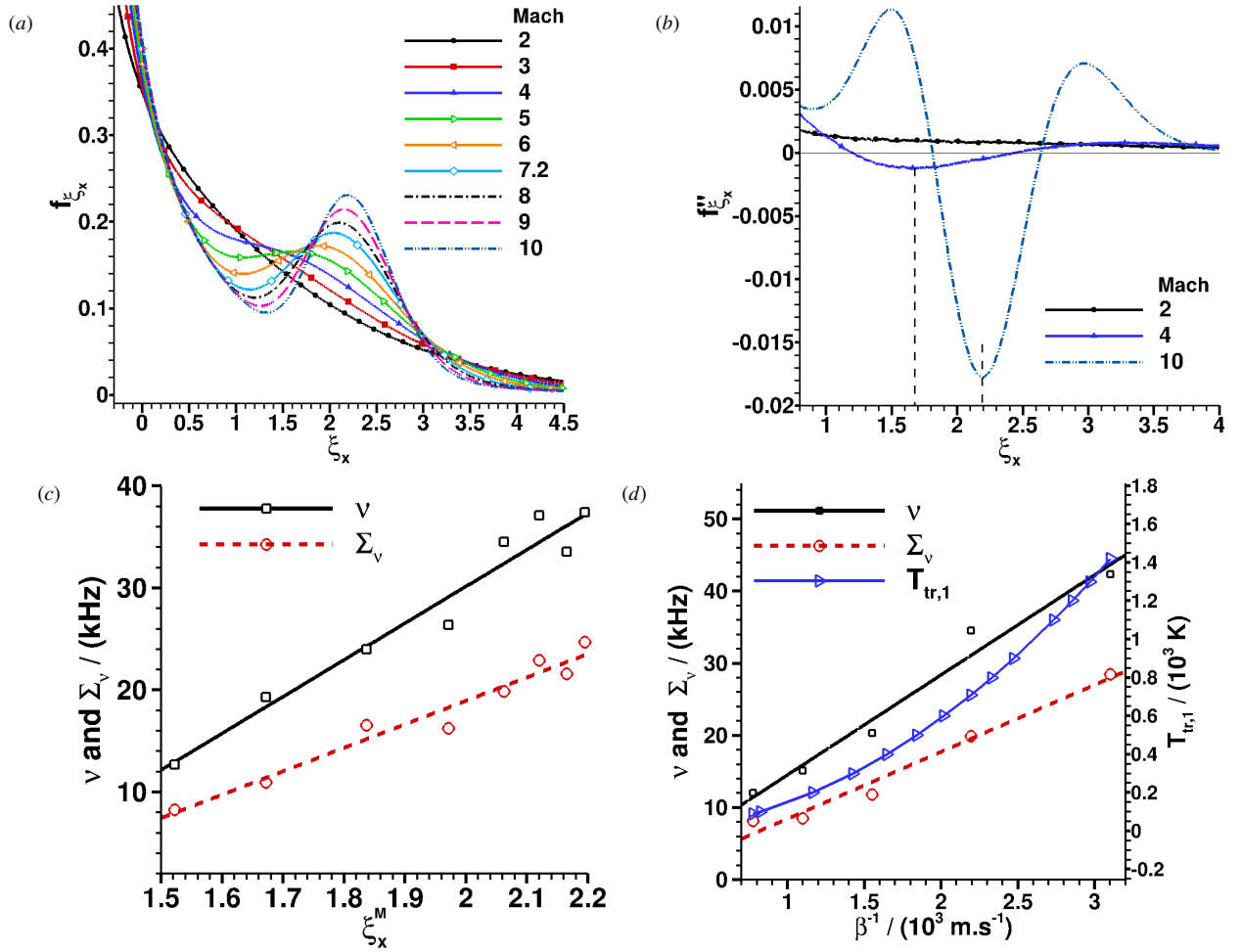


Figure 5.5: At $X/\lambda_1 = 0$, (a) analytical bimodal NCCS PDF, $f_{\xi_x}^M$, for Mach 2–10 and (b) second derivative, $f_{\xi_x}^{M''}$, for Mach 2, 4, and 10 at $T_{tr,1}=710$ K and $n_1 = 10^{22} \text{ m}^{-3}$. Location of ξ_x^M in the energy space is indicated by verticle dashed-lines for Mach 4 and 10. $f_{\xi_x}^{M''}$ is smoothened using the Savitzky-Golay filter provided in the SciPy [6] software. (c) For Mach 3–10, a linear variation of DSMC-derived average frequency ν and its standard deviation Σ_ν with ξ_x^M (open squares) of the PDFs shown in (a). (d) At Mach 7.2, for cases with $n_1 = 10^{22} \text{ m}^{-3}$ and varied input temperature, linear variation of DSMC-derived ν and Σ_ν in the shock with β^{-1} obtained from Mott-Smith bimodal velocity distribution. Also shown the variation of β^{-1} with $T_{tr,1}$.

The aforementioned approach can be combined to write following equations to determine ν and Σ_ν respectively

between Mach 3 to 10 and $T_{tr,1}$ between ~ 90 to 1420 K at $n_1 = 10^{22} \text{ m}^{-3}$ as,

$$\begin{aligned} \nu(M^*, T_{tr,1}^*) &= \nu(M = 7.2, T_{tr,1}^*) \\ &\quad - \frac{d\nu}{d\xi_x^M} [\xi_x^M(M = 7.2) - \xi_x^M(M^*)] \end{aligned} \quad (5.29)$$

$$\nu(M = 7.2, T_{tr,1}^*) = \nu_o + \frac{d\nu}{d\beta^{-1}} \beta^{-1}(T_{tr,1}^*) \quad (5.30)$$

and

$$\begin{aligned} \Sigma_\nu(M^*, T_{tr,1}^*) &= \Sigma_\nu(M = 7.2, T_{tr,1}^*) \\ &\quad - \frac{d\Sigma_\nu}{d\xi_x^M} [\xi_x^M(M = 7.2) - \xi_x^M(M^*)] \end{aligned} \quad (5.31)$$

$$\Sigma_\nu(M = 7.2, T_{tr,1}^*) = \Sigma_{\nu,o} + \frac{d\Sigma_\nu}{d\beta^{-1}} \beta^{-1}(T_{tr,1}^*) \quad (5.32)$$

where M^* and $T_{tr,1}^*$ are the desired Mach number and upstream temperature, respectively. As an example, calculation of ν for $(M^*, T_{tr,1}^*) = (4, 300 \text{ K})$ using Eq. (5.29) is described next. The first term in Eq. (5.29) can be computed from Eq. (5.30), where we read off the value of $\beta^{-1} \sim 1410 \text{ m.s}^{-1}$ at $T_{tr,1}^*$ from Fig. 5(d). The values of the Y -intercept, $\nu_o = 0.6867$, and the slope, $d\nu/d\beta^{-1} = 14.8 \text{ m}^{-1}$, are also known from the linear fit presented in Fig. 5(d). For the second term in Eq. (5.29), we use the slope $d\nu/d\xi_x^M = 36 \text{ kHz}$, obtained from Fig. 5(c), and the values of $\xi_x^M(M = 7.2) = 2.0622$ and $\xi_x^M(M^* = 4) = 1.6715$, given in Table 3. Note that if $\xi_x^M(M^*)$ is not explicitly provided in Table 3 for $3 \leq M^* \leq 10$, it can be linearly interpolated. From this calculation, Eq. (5.29) results in $\nu(M^* = 4, T_{tr,1}^* = 300 \text{ K}) = 6.4 \text{ kHz}$. Similar procedure can be used to obtain $\Sigma_\nu = 4.1 \text{ kHz}$ at $M^* = 4$ and $T^* = 300 \text{ K}$ using Eqs. (5.31) and (5.32), in which $\Sigma_{\nu,o}$, $d\Sigma_\nu/d\beta^{-1}$, $d\Sigma_\nu/d\xi_x^M$ are -0.8226 , 9.284 m^{-1} , and 23.01 kHz , respectively. In comparison, the peak-frequency in the normalized PSD of the DSMC-derived mean-subtracted instantaneous data of $\sigma_{xx}\rho_1\beta_1^{-2}$ is 7 kHz with a standard deviation of $\sim 6 \text{ kHz}$, as shown in Fig. 6(a), in close agreement with our estimate. As discussed in Ref. [5], the PSD is obtained using the Welch's method [208, 209] in the Scipy [6] software with two Hann-window weighted segments of data sampled with a frequency of 100 MHz prior to the Fast Fourier Transform (FFT) such that the frequency resolution is 0.775 kHz . Considering the complexity of this full simulation, Eq. 5.29 is a useful scaling relationship for extension to other Mach numbers and temperatures.

M	3	4	5	6	7.2	8	9	10
ξ_x^M	1.5224	1.6715	1.8366	1.9716	2.0622	2.1202	2.1654	2.195

Table 5.3: ξ_x^M for Mach numbers ranging from 3 to 10.

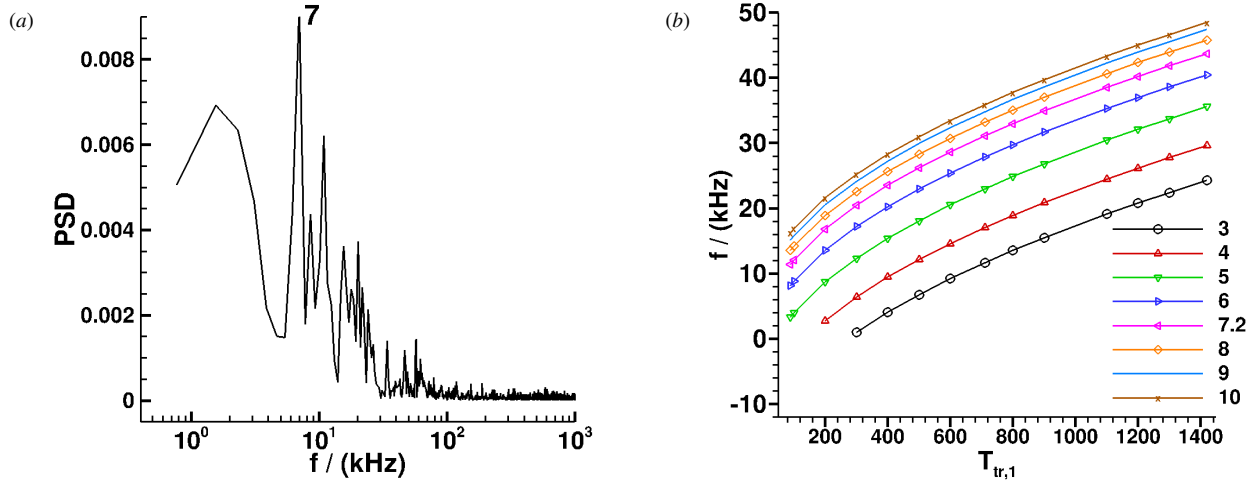


Figure 5.6: (a) At $M=4$, $T_{tr,1} = 300$ K, and $n_1 = 10^{22} \text{ m}^{-3}$, the PSD obtained from the mean-subtracted data of $\sigma_{xx}\rho_1\beta_1^{-2}$ obtained from DSMC at the location of maximum bulk velocity gradient ($X/\lambda_1 = 0$). (b) Predicted characteristic average low-frequencies as a function of input temperature for Mach numbers 3 to 10 and $n_1 = 10^{22} \text{ m}^{-3}$.

Finally, using this approach, the average low-frequencies are predicted for input temperature ranging from 90 K to 1420 K for Mach numbers 3 to 10 at an input number density of 10^{22} m^{-3} , as shown in figure 5.6(b). It is seen that the characteristic average low-frequency increases with increase in temperature and Mach number, however, the maximum range of frequencies is within 50 kHz for the parameter range examined. This figure can be used to read out the average low-frequency fluctuation for a given input temperature and shock Mach number for researchers in hypersonic transition.

Furthermore, for estimating frequencies at some other upstream number density n_1^* , we may first calculate the frequency at $n_1 = 10^{22} \text{ m}^{-3}$, given Mach number and upstream temperature using the above approach, and then use the approximate relation,

$$\frac{\nu(n_1^*)}{\nu(n_1 = 10^{22} \text{ m}^{-3})} = \frac{L_s(n_1 = 10^{22} \text{ m}^{-3})}{L_s(n_1^*)} = \frac{n_1^*}{10^{22}} \quad (5.33)$$

which is derived from the Strouhal number scaling established in Sec. 4.5 and noting that the shock-thickness L_s scales

inversely with the upstream number density, n_1 . Alternatively, one may simulate a number of DSMC simulations at other upstream number densities, obtain average frequencies and their standard deviations from the power spectral density of DSMC signals, as described in Sec. 4.2.2, and derive correlations similar to those given in Eqs. (5.29)–(5.32).

5.6 Summary

This work demonstrates a simple approach to estimate the low-frequency fluctuations in a 1-D shock structure of argon, using analytically derived PDFs of particle energies in local equilibrium. The latter compare well with DSMC-derived PDFs in the upstream and downstream equilibrium regions with respect to a one-dimensional shock. It is shown for the first time that they have the form of NCCS PDFs. Then, using the Mott-Smith model, the bimodal NCCS PDFs inside the nonequilibrium regions of shocks are constructed as a linear combination of the equilibrium upstream and downstream PDFs. ¹

The bimodal NCCS PDFs at the location in the shock where the absolute velocity gradient is maximum ($X/\lambda_1 = 0$) are correlated with the low-frequencies of shock fluctuations previously obtained from DSMC for $3 \leq M \leq 10$ and an input number density of 10^{22} m^{-3} . It is found that the weighted-averaged low-frequency is directly proportional to the location of the peak in the PDF of f_{ξ_x} generated by the contribution of particles from the upstream. For cases where the Mach number and input number density is constant but input temperature is varied, the low-frequencies are found to be proportional to the most-probable-speed at $X/\lambda_1 = 0$ obtained from the Mott-Smith velocity PDF. Using these linear functions, it is demonstrated that one can estimate the low-frequency of fluctuations at an input number density of 10^{22} m^{-3} for a wide range of input temperatures and Mach numbers not explicitly simulated in our previous DSMC simulations. In the future, a similar approach can be used at other input number densities and for other gases of practical importance, where the DSMC-derived low-frequencies can be obtained for a few selected input conditions and using those, a broader database of low-frequencies can be generated through linear correlations with analytical PDFs.

The estimates provided for low-frequency unsteadiness generated at the shock can be used in receptivity and linear stability analysis studies of laminar-turbulent transition of high-speed boundary layer flows, e.g. as boundary conditions in the analyses or to construct simplified models that account for the interaction of leading-edge shock with the boundary layer. The same estimates can also be used to aid understanding of the changes in the spectrum of freestream noise after it interacts with the shock prior to excitation of the boundary-layer.

¹The supplementary section provides a python function to generate these PDFs.

5.7 Supplemental Information

5.7.1 A python code for generating the bimodal NCCS PDFs

This appendix gives the code snippet for generating bimodal NCCS distribution. The values of code variables ‘R’, ‘Ux1’, ‘Ttr1’, ‘beta1’, ‘Ux2’, ‘Ttr2’, ‘beta2’ are 208.243, 3572.24, 710, 1.849×10^{-3} , 944.74, 12120.6, 4.451×10^{-4} , respectively. The values of code variables ‘Ux’, ‘Ttr’, ‘beta’ are obtained from the Mott-Smith velocity distribution and equal to 2012.8, 10149.8, 4.864×10^{-3} , respectively, at probe P . The code variables ‘psi1’ and ‘psi2’ are Mott-Smith fractions and equal to 0.40649 and 0.59351, respectively, at probe P .

```
1 #Code for generating a bimodal NCCS distribution
2 #Note:indices 0, 1, 2 of the following arrays
3 #is for the bimodal PDF of xi_x, xi_y, xi
4 #df1, df2: degrees of freedom
5 #nc1, nc2: noncentrality parameters
6
7 size=10000000
8 size1=int(psi1*size)
9 size2=int(psi2*size)
10
11 Var1 = R*Ttr1
12 s1=0.5*(Ttr1/Ttr) #scaling factor
13 beta1Sq=beta1*beta1
14 Ux1Sq=Ux1*Ux1
15 df1 = [1,1,3]
16 nc1 = [Ux1Sq/Var1, 0, Ux1Sq/Var1]
17
18 Var2 = R*Ttr2
19 s2=0.5*(Ttr2/Ttr)
20 beta2Sq=beta2*beta2
21 Ux2Sq=Ux2*Ux2
22 df2 = [1,1,3]
23 nc2 = [Ux2Sq/Var2, 0, Ux2Sq/Var2]
24
25 UxSq=Ux*Ux
26 betaSq=beta*beta
27 MeanSqBetaSq = [UxSq*betaSq, 0, UxSq*betaSq]
28
29 bins=3200
```

```

30 bin_edges_NCCS = np.zeros(bins+1)
31 bin_center_NCCS = np.zeros(bins)
32
33 i=0 #For the bimodal PDF of xi_x
34 mean, var, skew, kurt = ncx2.stats(df1[i], nc1[i],
35                                   scale=s1, moments='mvsk')
36 r1 = ncx2.rvs(df1[i], nc1[i], size=size1, scale=s1,
37              loc=-MeanSqBetaSq[i])
38 mean, var, skew, kurt = ncx2.stats(df2[i], nc2[i],
39                                   scale=s2, moments='mvsk')
40 r2 = ncx2.rvs(df2[i], nc2[i], size=size2, scale=s2,
41              loc=-MeanSqBetaSq[i])
42 r=np.concatenate((r1, r2))
43 hist_NCCS, bin_edges_NCCS = np.histogram(r,bins=bins,
44                                           density=True)
45 print('mean, stddev', r.mean(), r.std())
46 fig, ax = plt.subplots(1, 1)
47 ax.hist(r,density=True,bins=bins,histtype='stepfilled',
48         alpha=0.4)
49 plt.show()

```

Chapter 6

Effect of Translational Nonequilibrium on the Modal Response of Normal Shocks

A framework for studying modal analysis of finite-thickness normal shock layers has been developed, and linear temporal analysis is conducted to study the stability of $Ma = 1.2, 3$, and 5 shocks obtained from DSMC subjected to two-dimensional, small amplitude, harmonic perturbations having wavelengths smaller than the shock-thickness. Two sets of constitutive equations are used to obtain closure of the compressible governing equations used for modal analysis: the traditionally used Navier-Stokes-Fourier (NSF) equations, applicable only at the lowest Mach number, and equations derived based on the Mott-Smith's velocity distribution function, which are better than the former in terms of approximating the DSMC-derived transport flow quantities at high Mach numbers. Comparison of two formulations allows for quantifying the effect of the resolution of internal shock structure on the stability of shock layers.

The temporal analysis performed by Duck and Balakumar three decades ago of one-dimensional shock layers satisfying the Navier-Stokes equations revealed only stable continuous branches in the eigenspectra. However, it was inconclusive regarding what parameters govern the temporal decay rates of 'continuum' modes or the asymptotic form of eigenfunctions in the far field of the shock layer. In this work, we find the least stable continuous branches that have both stationary and traveling continuum modes and show for the first time that their eigenfunctions decay monotonically and sinusoidally in the far field, respectively, while exhibiting an order of magnitude lower spatial decay rate in the upstream than the downstream. These characteristics of eigenfunctions are governed by only one physically possible root of a septic characteristic equation derived by analytically solving the normal mode equations in the far field. By deriving an approximate equation for this root, it is shown that the least stable continuous branch is always stable but becomes less stable by the increase in Ma , decrease in γ , and increase in the degree of translational nonequilibrium. This is consistent with the observations from the linear stability solver that the noncontinuum effects lead to a less stable branch and that the prediction of decay rates strongly depends on how well the constitutive relations resolve the true translational nonequilibrium region in the shock layer.

Nomenclature

Roman symbols	d	molecular diameter of species (m)	
A_a, A_b	constants used in the Mott-Smith based constitutive equation for viscous stress tensor	Ec	Eckert number
a	y-intercept in the approximate piecewise linear relationship of $\mathcal{L}$ with Ma	e_m	m^{th} nondimensional eigenfunction defined in the far field analysis
B_a, B_b	constants used in the Mott-Smith based constitutive equation for x^* -directional heat flux	f	velocity distribution function
b	slope in the approximate piecewise linear relationship of $\mathcal{L}$ with Ma	h	constitutive function for heat flux vector
$b_m^{(n)}$	m^{th} component of n^{th} characteristic vector $\mathbf{b}^{(n)}$ in the far field analysis	i	imaginary unit, $\sqrt{-1}$
C	constant used in defining power law of viscosity	k_b	Boltzmann constant (J.K ⁻¹)
$\mathbf{c}^* = [c_x^*, c_y^*, c_z^*]^T$	thermal velocity vector (m.s ⁻¹)	k^*	conductivity (W.m ⁻¹ .k ⁻¹)
c^*	thermal speed (m.s ⁻¹)	L_s^*	velocity gradient based shock-thickness (m)
c_r^*	average relative speed of molecules (m.s ⁻¹)	L_y^*	wavelength of perturbations in homogeneous y^* -direction (m)
c_v	coefficient of specific heat at constant volume (J.kg ⁻¹ .K ⁻¹)	$L_{y,\text{min}}^*$	minimum wavelength of perturbations (m)
D_n	n^{th} constant in the general form of amplitude function defined in the far field analysis	L_y	L_y^*/L_s^*
		Ma	Mach number
		m	mass of species (kg)

N_1, N_2	weighting functions used for linear combination of up and downstream distributions in constructing bimodal velocity distribution functions in the Mott-Smith model	T_x^*, T_y^*, T_z^*	directional translational temperatures in Cartesian directions (K)
n^*	number density (m^{-3})	T_n^*	transverse directional temperature $T_n = T_y = T_z$
P^*	Set of dimensional macroscopic flow quantities $P^* = \{\rho^*, u_x^*, u_y^*, T^*\}$	T_x, T_n	x and traverse directional nondimensional translational temperatures normalized by T_1^*
Pr	Prandtl number	t^*	time (s)
p^*	pressure (Pa)	t	$t^* u_{x,1}^* / L_s^*$
Q^*	function of dimensional molecular velocities	$\mathbf{u}^* = [u_x^*, u_y^*]^T$	bulk velocity vector (m.s^{-1})
$\mathbf{q}^*$	heat flux vector (W.m^{-2})	$\mathbf{u}$	$\mathbf{u}^* / u_{x,1}^*$
$\mathbf{q}$	nondimensional heat flux vector $\mathbf{q}^* L_s^* / (k_1^* T_1^*)$	$\mathbf{v}^* = [v_x^*, v_y^*, v_z^*]^T$	molecular velocity vector (m.s^{-1})
R	specific gas constant ($\text{J.kg}^{-1}.\text{K}^{-1}$)	v_m^*	most-probable-speed (m.s^{-1})
Re	Reynolds number	x^*, y^*, z^*	spatial Cartesian components in the direction of, perpendicular to, and along the spanwise direction with respect to shock propagation, (m)
r_ρ	Rankine-Hugoniot mass density ratio across a normal shock	x, y, z	nondimensional spatial Cartesian components normalized by L_s^*
r_t	Rankine-Hugoniot temperature ratio across a normal shock	Special symbols	
r_u	Rankine-Hugoniot bulk-velocity ratio across a normal shock	$\mathcal{A}$	left side linear operator in an eigenvalue problem
$\mathbf{S}^*$	strain rate tensor (s^{-1})	$\mathcal{B}$	right side linear operator in an eigenvalue problem
s	constitutive function of stress tensor	C_{mn}	mn^{th} component of coefficient matrix $\mathcal{C}$
T^*	average translational temperature (K)	$\mathcal{D}$	denominator in the expression for α_1^{appx}
T	T^* / T_1^*	$\mathcal{E}_{mn}$	mn^{th} component of coefficient matrix $\mathcal{E}$
		$\mathcal{F}$	quintic polynomial defined in the far field analysis
		$\mathcal{I}$	a binary integer variable taking value 1 or 0
		$\mathcal{L}$	ratio of shock-thickness to the upstream mean-free-path

$\mathcal{M}$	relative magnitude of the sum of higher order terms to the first order term of quintic polynomial, $\mathcal{F}$	κ	function used in the normal mode equations
		Λ^*	second coefficient of viscosity (N.s.m ⁻²)
		Λ	Λ^*/μ_1^*
$\mathcal{N}$	numerator in the expression for α_1^{appx}	λ	mean-free-path based on variable hard sphere molecular model (m)
$\mathcal{P}$	vector of flow quantities $\mathcal{P} = (\rho, u_x, u_y, T)^T$	λ_{max}	maximum mean-free-path in the base flow (m)
$\mathcal{R}$	Ratio of $\bar{T}_x - \bar{T}_n / (\bar{T}_x - \bar{T}_n)_{\text{max}}$ in the upstream to downstream	μ^*	dynamic gas viscosity (N.s.m ⁻²)
$\mathcal{S}$	septic polynomial defined in the far field analysis	μ	μ^*/μ_1^*
$\mathcal{T}$	quadratic polynomial defined in the far field analysis	$\xi_a, \xi_b, \xi_c, \xi_d, \xi_e, \xi_f, \xi_g, \xi_h$	nondimensional functions in the normal mode energy equation
Greek symbols			
α_n	n th characteristic value in the general form of amplitude function in the far field analysis	Π^*	function relating viscous stress tensor in the ACE formulation with the strain rate tensor (N.s.m ⁻²)
β	wavenumber in the y-direction perpendicular to shock propagation	ρ^*	mass density (kg.m ⁻³)
		ρ	ρ^*/ρ_1^*
β_{ulim}	maximum possible limit of β	Σ^*	function relating viscous stress tensor in the ACE formulation with the divergence of velocity vector (N.s.m ⁻²)
Γ	gamma function	σ_T	total collision cross section (m ²)
γ	specific heat ratio	τ^*	viscous stress tensor (Pa)
δ	Kronecker's delta function	τ	nondimensional stress tensor $\tau^* L_s^* / (\mu_1^* u_{x,1}^*)$
ϵ	a small value used in linear decomposition	ϕ	nondimensional function in the normal mode momentum equations
ζ	function appearing in the real part of characteristic values α_6 and α_7	χ	coefficients in a fifth order polynomial defined in the far field analysis
η	function appearing in the imaginary part of characteristic value α_6 and α_7	ψ	nondimensional function in the normal mode momentum equations
θ	function defined in a solution of a characteristic value		

Ω	complex eigenvalue	ulim	upper limit
ω	viscosity index of a gas in Variable Hard Sphere model	max	maximum
		min	maximum
Operators		i	imaginary part of a complex function or a number
$\bar{w}(x)$	a flow or transport quantity in a base flow	r	real part of a complex function or a number
$\hat{w}(x)$	amplitude function of flow or transport quantity $w(x, y, t)$	ref	reference value
$ w $	absolute value of quantity w	x, y, z	with respect to Cartesian directions
$\Delta[Q^*]$		Superscripts	
collision integral of molecular function Q^*		appx	approximate value or expression
$\langle Q^* \rangle_f$	moment of molecular function Q^* with the velocity distribution function f	DB	defined in the analysis of Duck and Balakumar
$\nabla \cdot \mathbf{w}$	divergence of a vector $\mathbf{w}$	GP	obtained from the method of Gilbarg and Paolucci
Subscripts		m	pertaining to Mott-Smith based constitutive model
1	upstream value	n	pertaining to Navier-Stokes-Fourier constitutive model
2	downstream value		
k	subscript taking values of 1 or 2 for upstream and downstream quantities, respectively	'	derivative with respect to x
llim	lower limit	*	dimensional macroscopic flow or transport parameters

6.1 Introduction

The design of hypersonic vehicles depends heavily on computational predictive capabilities for laminar to turbulent flow transition [50], dynamics of shock-wave/boundary-layer interactions (SBLIs) [21, 156, 179], and active flow control [221]. Vast majority of research in improving these capabilities focuses on understanding the stability of boundary-layers [40, 48–50, 128, 130, 222, 223], laminar separation bubbles [31, 45, 47, 122, 123], and shear layers [126, 224–226], while either completely excluding shocks from the analysis or modeling them as discontinuous jumps or without accurately resolving their internal structure. Using high-fidelity kinetic simulations, our past work has shown that these phenomena could be intimately related to shocks, for example, the internal shock structure exhibits low-frequency molecular fluctuations that may alter the frequencies of upstream perturbations before they interact with the boundary-layer [210, 227]. In hypersonic SBLIs, we have shown that shocks are strongly coupled with the separated region [30], can experience synchronized oscillations with the perturbations in the shear layer [23] or excited boundary-layer [228], and even exhibit three-dimensional linear instabilities in their internal structure in synchronization with the laminar separation bubble [31, 203]. These findings warrant a methodical investigation of instabilities in isolated shocks. In the middle of the last century, substantial research was conducted to understand the interactions of external disturbances with stand-alone shocks, which include investigation of how acoustic, vorticity and entropy waves amplify, reflect, or transmit through an inviscid shock treated as a discontinuous jump [58–61, 170, 229]. However, little attention has been given to understanding the intrinsic stability of finite-thickness (viscous) steady shock layers in terms of characterizing the potential asymptotic and transient growth of perturbations imposed on the shock. Such analyses for isolated one-dimensional, finite-thickness shock layers can be good stepping-stones for a comprehensive understanding of more complicated flow systems involving shocks.

The study of potentially self-excited perturbations in a finite-thickness steady normal shock was attempted three decades ago by Duck and Balakumar [1] to the best of the authors' knowledge. They imposed small-amplitude, harmonic perturbations to the macroscopic solution of a nominally one-dimensional shock layer (see Fig. 6.4), governed by Navier-Stokes equations obtained using the method of Gilbarg and Paolucci [7], and studied the temporal stability problem, which, in a nutshell, assumes that the spatial structure of the harmonic perturbations remains unchanged while their amplitude may grow or decay in time. These authors did not find any discrete eigenmodes in their numerically obtained eigenspectra, but only the modes that are a part of stable continuous branches referred to as 'continuum modes' based on the terminology used by Grosch and Salwen [224]. Stable continuous branches have been found for problems involving a mean flow in an unbounded or infinite domain which approaches a constant velocity in the far field, such as a shear layer, wake, jet, or a boundary layer developed on external surfaces [224, 230, 231]. Grosch and Salwen [224] also discussed mechanisms through which lightly-damped continuum modes can lead to transition, such

as quasi-steady distortion of the mean flow or non-parallel effects. In the context of the stability of the shock layer, non-parallel effects may be important in a shock formed over a blunt body whose strength changes along the plane of the shock. Therefore, there is merit in understanding the continuous branches obtained from the temporal analysis of shocks.

In this regard, the analysis of Duck and Balakumar [1] was incomplete and required further investigation. For example, in their analysis, the characteristics of the continuous branches were not discussed, including questions such as whether the presented continuous branches are always stable or are only stable for their chosen conditions, what parameters govern the temporal decay rates of continuum modes, and what is the spatial decay behavior of their continuum eigenfunctions. Also, they did not present any continuum eigenfunctions, rendering it inconclusive whether the numerically obtained continuous branches are physically possible, *i.e.* whether the eigenfunctions decay to zero in the far field up and downstream of the shock. Answers to these questions can be found through the analytical solution of amplitude functions in the far field, which was indeed attempted by Duck and Balakumar [1]; however, the resulting seventh order characteristic equation was deemed too difficult to solve. In this work, we revisit the temporal stability problem for a finite-thickness one-dimensional shock layer subjected to small-amplitude, harmonic perturbations and explore the above aspects. We also show two exact and one approximate root of the septic characteristic equation, the latter root governing the decay behavior of the least damped continuum modes having perturbation wavelength on the order of the maximum mean-free-path.

In terms of accurate modeling of the internal shock structure, it is well-known that the predictions of the transport flow quantities based on the Navier-Stokes-Fourier (NSF) constitutive equations used in the Navier-Stokes equations (NSE) increasingly deviate from those obtained from the kinetic theory [37, 62, 63] as the Mach number increases ($M > 1.4$). Bird [32] showed that the normal viscous stress components and the x -directional heat flux in the shock layer obtained from the kinetic Direct Simulation Monte Carlo (DSMC) method are poorly approximated by the NSF constitutive functions as the degree of translational nonequilibrium in the internal region of the shock increases with Mach number. Therefore, better constitutive equations are required to study the stability of shock layers obtained from DSMC at higher Mach numbers in the supersonic and hypersonic range. To that end, we have derived a set of constitutive equations based on the well-known bimodal approximation of Mott-Smith (MS) [68] for the velocity distribution function (VDF) in the shock layer, which, although not perfect, are better than the NSF equations in terms of approximating the DSMC transport quantities. Compressible equations based on these constitutive equations are termed here as the anisotropic conservation equations (ACE), which are expected to predict the same continuum modes as the NSE for shock layers obtained from DSMC at low Mach numbers but reveal increasing differences at higher Mach numbers. Through such comparisons, we would like to find out whether the translational nonequilibrium

in the shock layer makes the shock more or less stable. Among other existing compressible formulations, there are the Burnett [232, 233] and Super-Burnett equations [234], Grad's 13 and 21-moment equations [235–237], Myong's nonlinear coupled constitutive relations (NCCR) [238–240], and more recently derived, Onsager-13 moment [241] and Onsager-Burnett [242, 243] equations. A good summary of these approaches is provided in Ref. [244]. We have not explored these other formulations in this work, but such studies can be performed in the future.

The organization of this chapter is as follows: Sec. 6.2 describes the characteristics of a DSMC-derived 1-D shock layer, which includes DSMC input parameters and basic flow features of a 1-D shock layer in Sec. 6.2.1, the translational nonequilibrium in the internal shock structure and the motivation for the kinetic constitutive equations in Sec. 6.2.2. Section 6.3 is devoted to the formulation of linear stability analyses, the basic overview of which is provided in Sec. 6.3.1, and the summary of NSE and ACE formulations is discussed in Sec. 6.3.2, respectively. Section 6.3.3 describes the linearization of NSE and ACE and their decomposition into $O(0)$ base flow and $O(\epsilon)$ normal mode equations. Results are presented in Sec. 6.4, which includes Sec. 6.4.1 dedicated to the discussion of the least stable continuous branch in the eigenspectra obtained from the two formulations at $Ma = 1.2, 3$, and 5 and Sec. 6.4.2, describing eigenmodes on the more damped continuous branch. A summary of the main findings is offered in Sec. 6.5.

In the supplementary sections, Sec. 6.6.1 describes the derivations of MS constitutive equations for 1-D steady shock layers and some discussion regarding their extension to two-dimensions. The normal mode equations obtained from the two formulations are written in the form of elements of linear operators of the eigenvalue problem in Sec. 6.6.2. Section 6.6.3 shows comparison of eigenspectra obtained using the NSE formulation derived in this work with the results of Duck and Balakumar [1]. The test cases describing the variation in eigenspectra with number of grid points are presented in Sec. 6.6.4. Finally, the analytical solution of normal mode equations obtained using the NSE formulation in far fields of a shock layer is described in Sec. 6.6.5.

6.2 Characteristics of DSMC-derived, 1-D Argon Shock Layers

6.2.1 Input parameters and basic features of 1-D DSMC base flows

The base flow profiles of 1-D shock layers are obtained from the DSMC method [37] using the SUGAR solver [39], where the description of the DSMC simulation of 1-D shocks can be found in Chapter 1. In summary, a discontinuous 1-D shock propagating in the x^* direction is initialized using the Rankine-Hugoniot jump conditions [150] for the

x^* -directional bulk velocity, mass density, and translational temperature, r_u , $r_\rho = r_u^{-1}$, and r_t , respectively, defined as

$$\begin{aligned} r_u &= \frac{u_{x,2}^*}{u_{x,1}^*} = \frac{2 + (\gamma - 1)Ma^2}{(\gamma + 1)Ma^2} \\ r_\rho &= \frac{\rho_2^*}{\rho_1^*} = \frac{u_{x,1}^*}{u_{x,2}^*} \\ r_t &= \frac{T_2^*}{T_1^*} = \frac{u_{x,2}^*}{u_{x,1}^*} \left[1 + \frac{2\gamma(Ma^2 - 1)}{(\gamma + 1)} \right] \end{aligned} \quad (6.1)$$

at a specified upstream Mach number $Ma = u_{x,1}^* / \sqrt{\gamma R T_1^*}$, for argon gas species having mass $m = 6.63 \times 10^{-26}$ kg, reference molecular diameter $d_{\text{ref}} = 4.17 \times 10^{-10}$ m, gas constant $R = 208.24$ J.kg⁻¹.K⁻¹, and specific heat ratio $\gamma = 5/3$. Subscripts ‘1’ and ‘2’ refer to flow quantities in the far field upstream and downstream of the shock layer, while a star superscript denotes a dimensional quantity.¹ The dynamic viscosity and thermal conductivity, μ^* and k^* , are calculated using the variable hard sphere (VHS) molecular model [37] as

$$\mu^* = C(T^*)^\omega \quad (6.2)$$

$$k^* = \frac{15}{4} R \mu^* \quad (6.3)$$

In Eq. (6.2) C is a constant, defined as

$$C = \frac{(15/8)(\pi m k_b)^{1/2} (4k_b/m)^{\omega-0.5}}{\Gamma(4.5 - \omega) \sigma_{T,\text{ref}} (c_{r,\text{ref}})^{2(\omega-0.5)}} \quad (6.4)$$

where k_b is the Boltzmann constant, $\sigma_{T,\text{ref}} = \pi d_{\text{ref}}^2$ is the total collision cross-section, $c_{r,\text{ref}}$ is the average relative speed of molecules (Eq. (4.46) in [37]), and Γ is the gamma function. The viscosity index ω is assumed to be one for simplicity, *i.e.* the gas is assumed to be composed of Maxwell molecules.

The flow quantities for the DSMC and linear stability analyses of $Ma = 1.2, 3$, and 5 shocks that depend on the upstream Mach number are presented in Table 6.1, while other upstream flow quantities, $\rho_1^* = 6.63 \times 10^{-4}$ kg.m⁻³, $T_1^* = 300$ K, $\mu_1^* = 2.688 \times 10^{-5}$ N.s.m⁻², $k_1^* = 2.1 \times 10^{-2}$ W.m⁻¹.K⁻¹ are the same for all three cases. These Mach numbers were chosen to study the effect of increasing degree of translational nonequilibrium on the modal response of the shock. The steady-state, macroscopic base flow quantities obtained from DSMC are denoted with an overbar, *i.e.* $\bar{P}^* = \{\bar{\rho}^*, \bar{u}_x^*, \bar{T}^*\}$ is a set of such quantities depending on x^* alone. Here, $x^* = 0$ is set to the location where the magnitude of the bulk velocity gradient is a maximum, *i.e.* $|d\bar{u}_x^*/dx^*|_{\text{max}}$. The shock-thickness L_s^* , shown in Table 6.1,

¹The superscript is omitted for the dimensional gas properties of m , d_{ref} , R , and specific heat at constant volume, $c_v = R/(\gamma - 1)$.

is defined as the overall velocity change across the shock divided by the maximum velocity gradient,

$$L_s^* = \frac{u_{x,1}^* - u_{x,2}^*}{\left| \frac{d\bar{u}_x^*}{dx^*} \right|_{\max}} \quad (6.5)$$

while the upstream Reynolds number is defined based on this shock-thickness as

$$Re = \frac{\rho_1^* u_{x,1}^* L_s^*}{\mu_1^*} \quad (6.6)$$

In DSMC, the value of the Prandtl number, Pr , is not imposed a-priori but calculated based on gas properties, which for a monatomic gas, is equal to $Pr = 2\gamma/5$.

Ma	$u_{x,1}^* / (\text{m.s}^{-1})$	$L_s^* / (\text{m})$	Re	$L_s^* / \bar{\lambda}_{\max}^*$	β_{ulim}
1.2	387.01	0.00325	31.19	24.10	151.4
3.0	967.52	0.00114	26.35	6.93	43.5
5.0	1612.54	0.00152	60.16	6.34	39.8

Table 6.1: Flow quantities for three Mach number cases.

The DSMC-derived nondimensional base flow quantities $\bar{u}_x = \bar{u}_x^* / \bar{u}_{x,1}^*$ and $\bar{T} = \bar{T}^* / T_1^*$ are shown in Fig. 6.1(a) for $Ma = 1.2$, and Fig. 6.1(b) for $Ma = 3$ and 5. Profiles of nondimensional mass density, $\bar{\rho} = \bar{\rho}^* / \bar{\rho}_1^*$, are not shown but can be easily obtained as $\bar{\rho} = \bar{u}_x^{-1}$. At $Ma = 1.2$, the DSMC-derived base flow profiles agree with the solution of NSE for the shock layer obtained using the method of Gilbarg and Paolucci [7], denoted with a superscript ‘GP’, indicating that the NSE formulation can be used to study linear stability analysis of DSMC-derived base flow at this low Mach number. At higher Mach numbers, however, the NSE formulation is not adequate to represent the true translational nonequilibrium region in the shock layer, as will be shown in Sec. 6.2.2. Note that in this work we have used base flows obtained from DSMC for linear stability analyses and compared the modal response of shock layers obtained from two formulations: the NSE formulation based on NSF constitutive equations and the ACE formulation based on constitutive equations derived using the MS bimodal approximation [68].

Furthermore, in this work the stability characteristics of these base flows will be studied against small-amplitude, 2-D, harmonic perturbations with wavelengths smaller than the shock thickness along the direction normal to shock propagation (y^*). To assess the minimum possible perturbation wavelength of harmonic perturbations, estimation of the maximum local mean-free-path, $\bar{\lambda}_{\max}^*$, is needed, as will be explained in Sec. 6.3. To obtain this base flow

quantity, Fig. 6.2 shows the variation of the local mean-free-path, $\bar{\lambda}^*$, calculated for the VHS gas model (Eq. (4.65) in [37]), normalized by the upstream mean-free-path, $\bar{\lambda}_1^*$, for all Mach numbers studied. It is seen that at $Ma = 1.2$, $\bar{\lambda}_{\max}^*$ is in the upstream region, while at higher Mach numbers, it exists inside the shock layer and increases with increase in Mach number. This variation is related to relative changes in local number density, $\bar{n}^*$, and a function of temperature, $(\bar{T}^*)^{\omega-1/2}$, on which $\bar{\lambda}^*$ depends inversely and directly, respectively. For the same reason, the downstream mean-free-path is smaller at $Ma = 3$ compared to $Ma = 1.2$ but larger at $Ma = 5$ than $Ma = 3$. Table 6.1 also shows the ratio of L_s^* to $\bar{\lambda}_{\max}^*$, which is quite large at $Ma = 1.2$ but plateaus to ~ 6 at high Mach numbers.

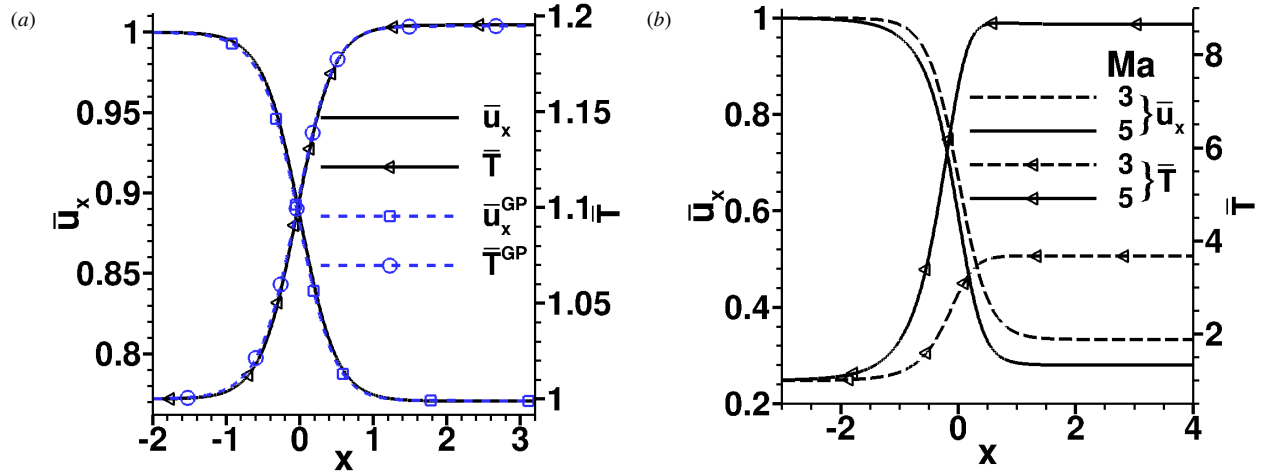


Figure 6.1: Base flows of argon shock layers showing spatial variation of flow quantities $\bar{u}_x$ and $\bar{T}$ for (a) $Ma = 1.2$ obtained from DSMC and using the method of Gilgarg and Paolucci [7] and for (b) $Ma = 3$ and 5 obtained from DSMC.

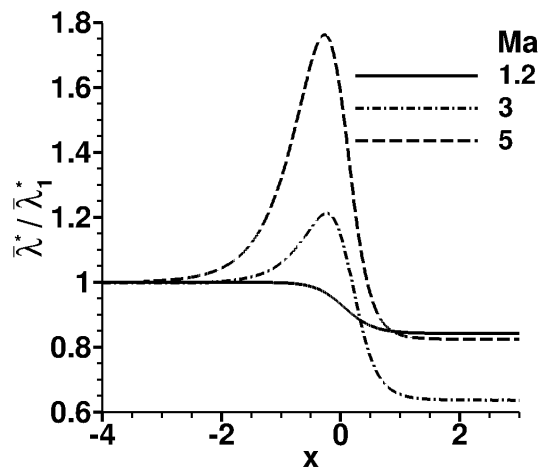


Figure 6.2: Ratio of local to upstream mean-free-paths, $\bar{\lambda}^* / \bar{\lambda}_1^*$ in Mach 1.2, 3 and 5.

6.2.2 Translational nonequilibrium in a 1-D shock layer and the Mott-Smith (MS) distribution functions

Since the focus of this work is on quantifying the non-continuum effects in a shock layer, a brief overview of these effects is summarized below. A shock layer in a monatomic gas is characterized by the region of translational nonequilibrium, where the distribution functions of particle velocities and energies are bimodal in contrast to their Maxwellian distributions in the equilibrium regions upstream and downstream of a shock [210]. Figure 6.3(a) shows typical velocity distribution functions (VDFs) of particles at $x^* = 0$ obtained from the DSMC simulation at $Ma = 5$, f_{v_x} and f_{v_y} , respectively, of the x^* - and y^* -directional molecular velocity components, v_x^* and v_y^* , normalized by upstream most-probable-speed $v_{m,1}^*$. The differences in the spread of the distributions result in differences in the x^* - and transverse-directional, and overall temperatures, $\bar{T}_x^*$ and $\bar{T}_y^* = \bar{T}_z^* = \bar{T}_n^*$, $\bar{T}^*$, respectively. The VDFs $f_{v_x}^m$ and $f_{v_y}^m$, shown in Fig. 6.3(a), are obtained from the bimodal approximation of MS and they will be defined shortly.

By defining the difference $(\bar{T}_x - \bar{T}_n)$ as the measure of the degree of translational nonequilibrium, plotted in Fig. 6.3(b), where temperatures are nondimensionalized by T_1^* , it is seen that at $Ma = 1.2$, the amount of nonequilibrium is negligible, while it increases substantially with Mach number. By normalizing $(\bar{T}_x - \bar{T}_n)$ by its maximum value, $(\bar{T}_x - \bar{T}_n)_{\max}$, we can define $\mathcal{R}$ as a ratio of the area under the curve of this quantity on the cold (upstream) to the hot (downstream) sides of a shock layer. At $Ma = 1.2$, $\mathcal{R} \sim 1$, indicating that the region of translational nonequilibrium is nearly symmetric about $x = 0$, while $\mathcal{R}$ increases to 1.18 and 1.89 for $Ma = 3$ and 5, indicating an increase in this region on the cold side. These observations are qualitatively consistent with the conclusion first put forward by Liepmann *et al.* [62] that noncontinuum effects are more prominent on the cold side of the shock layer than the hot side as the shock strength increases.

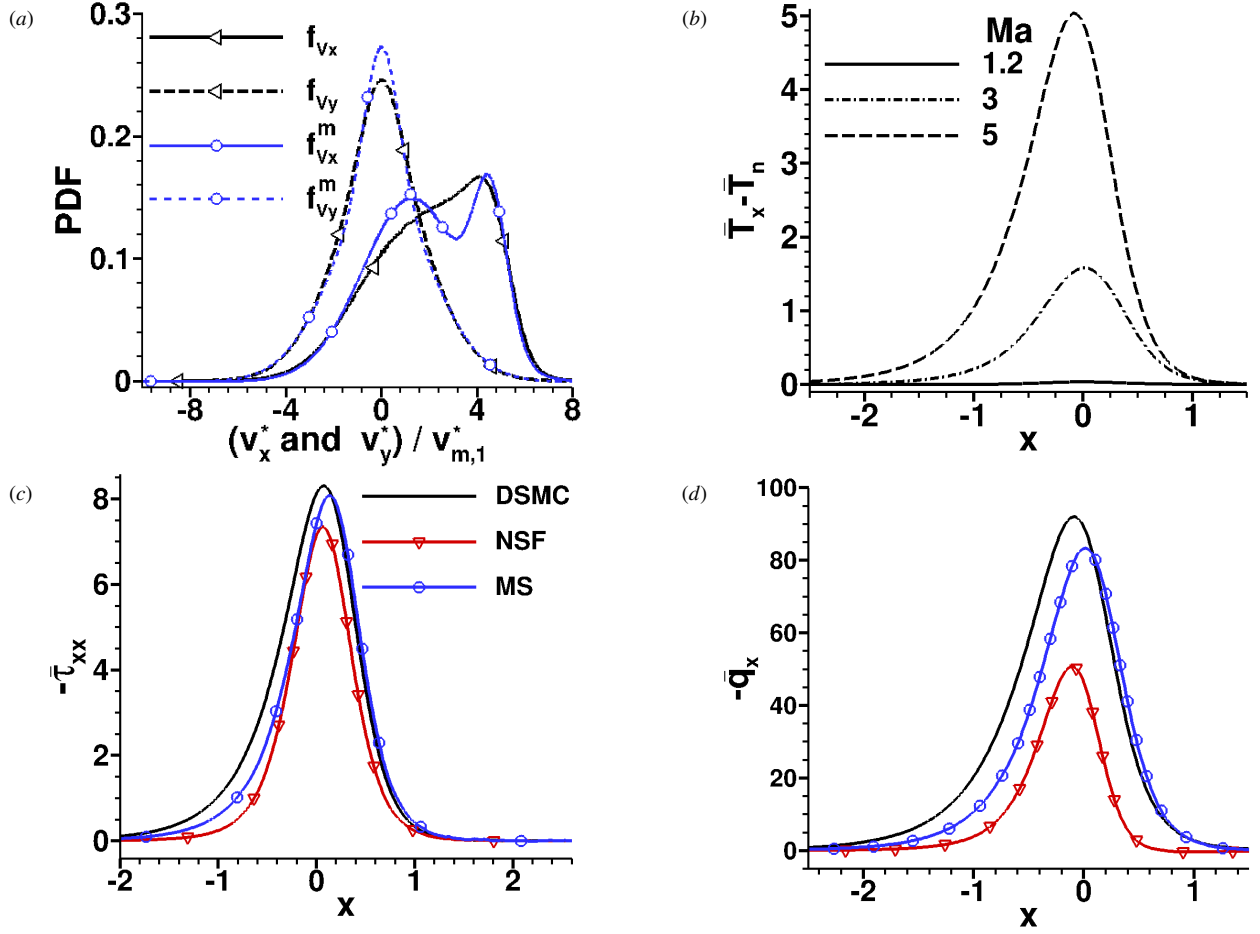


Figure 6.3: x^* - and y^* -directional VDFs at $Ma = 5$ and $x^* = 0$ obtained from DSMC and the MS bimodal approximation are compared in (a), the degree of translational nonequilibrium, $(\bar{T}_x - \bar{T}_n)$, at the three Mach numbers is shown in (b), and the comparisons of transport quantities $\bar{\tau}_{xx}$ and $\bar{q}_x$ obtained from DSMC, NSF and MS models at $Ma = 5$ are shown in (c) and (d), respectively.

In addition, more the degree of translational nonequilibrium, larger the values of normal components of the viscous stress tensor $\bar{\tau}^*$ denoted as $\bar{\tau}_{xx}^*$ and $\bar{\tau}_{yy}^*$, and x^* -directional component of heat flux vector $\bar{q}_x^*$. Note that the shear stress components, $\bar{\tau}_{xy} = \bar{\tau}_{yx}$, and the y^* -directional heat flux, $\bar{q}_y$, are zero in a 1-D shock layer [91]. Figures 6.3(c) and 6.3(d) show the nondimensional x -directional normal stress and heat flux, $\bar{\tau}_{xx} = \bar{\tau}_{xx}^* L_s / \mu_1^* u_{x,1}^*$ and $\bar{q}_x = \bar{q}_x^* L_s / k_1^* T_1^*$, respectively, in a $Ma = 5$ shock layer.

The DSMC-derived transport quantities in a 1-D shock layer $\bar{\tau}^*$ and $\bar{q}^*$ can be compared with quantities $\bar{\tau}^{n*}$ and $\bar{q}^{n*}$ obtained from the NSF constitutive equations using the DSMC macroscopic flow quantities, *i.e.* $\bar{\tau}^{n*} = s^n(\bar{P}^*, \bar{\mu}^*)$ and $\bar{q}^{n*} = h^n(\bar{P}^*, \bar{k}^*)$, where s^n and h^n are NSF constitutive functions that will be given in Sec. 6.3.2. It is well-known that at low Mach numbers ($M \leq 1.4$), the NSF constitutive models predict the DSMC-derived transport quantities fairly

well because the degree of translational nonequilibrium is low, however, the inadequacies of these models become apparent at high Mach numbers. Figures 6.3(c) and 6.3(d) clearly show that $\bar{\tau}_{xx}^n$ and $\bar{q}_x^n$ at $Ma = 5$ are significantly underpredicted in the entire shock layer, while the NSF models correctly predict zero $\bar{\tau}_{xy}^n$, $\bar{\tau}_{yx}^n$, and $\bar{q}_y^n$ (not shown). In summary, the limitations of NSF constitutive equations in predicting DSMC-derived transport quantities arise from the strong bimodal distributions of particles in the shock layer.

To obtain better constitutive equations than those used in the NSF equations, we have used the well-known MS bimodal approximation [68] to construct distributions in the shock layer assuming a linear combination of up and downstream Maxwellian distributions,

$$\bar{n}^{m*} f^m = N_1 f_1 + N_2 f_2 \quad (6.7)$$

where $\bar{n}^{m*}$ is the local number density and f_1 , f_2 are the Maxwellian distributions in the up and downstreams, respectively, given as

$$f_k = \frac{1}{(v_{m,k}^*)^3 \pi^{3/2}} \exp \left[-\frac{(v_x^*)^2 - (u_{x,k}^*)^2 + (v_y^*)^2 + (v_z^*)^2}{(v_{m,k}^*)^2} \right] \quad k \in 1, 2 \quad (6.8)$$

In Eq. (6.8), $v_{m,1}^*$ and $v_{m,2}^*$ are the most-probable-speeds in the up and downstream regions, respectively, $u_{x,1}$ and $u_{x,2}$ are up and downstream bulk velocities, respectively, and $\mathbf{v}^* = [v_x^*, v_y^*, v_z^*]^T$ is a vector of instantaneous molecular velocity components. Fractions N_1 and N_2 vary along x^* but can typically be obtained using only the up and downstream quantities, while successive moments of Eq. (6.7) are taken to obtain macroscopic flow quantities $\bar{n}^{m*}$, $\bar{u}_x^{m*}$, and $\bar{T}^{m*}$ in the shock layer. These flow quantities compare within small differences with the respective DSMC-derived quantities, $\bar{n}^*$, $\bar{u}_x^*$, and $\bar{T}^*$ (see Ref. [210]). Figure 6.3(a) shows the comparison of x^* and y^* -directional MS distributions, $f_{v_x}^m$ and $f_{v_y}^m$, respectively, with the DSMC-derived distributions at $Ma = 5$. These directional MS distributions can be obtained from f^m by integrating differential probability $f^m dv_x^* dv_y^* dv_z^*$ over its remaining components. The MS model gives a qualitatively better approximation in terms of bimodality of the PDF, although it slightly overestimates the contribution of the upstream high velocity particles and shows a distinct second dominant peak.

In this work we make use of the known DSMC-derived base flow quantities, $\bar{n}^*$ and $\bar{u}_x^*$, to predict functions N_1 and N_2 and derive equations for viscous stress tensor and heat fluxes vector, that is, $\bar{\tau}^{m*} = s^m(\bar{P}^*, \bar{\mu}^*)$ and $\bar{q}^{m*} = h^m(\bar{P}^*, \bar{k}^*)$, respectively, where s^m and h^m are MS constitutive functions for stress and heat flux, respectively. These constitutive functions are summarized in Sec. 6.3.2, while their derivation is given in Appendix 6.6.1. Figures 6.3(c) and 6.3(d) respectively show that the nondimensional x -directional stress $\bar{\tau}_{xx}^m$ and heat flux $\bar{q}_x^m$, predicted from the MS model,

compare well with the respective DSMC-derived quantities in the hot side of the shock layer but not as well on the cold side. However, these predictions are much better than the NSF models across the entire shock layer.

6.3 Formulation of Linear Stability Analysis based on Temporal Amplification Theory

6.3.1 Overview of temporal analysis of 1-D shock layers

The general 2-D, compressible equations are derived by taking moments of the Boltzmann equation [91] and written as,

$$\frac{D\rho}{Dt} = -\rho (\nabla \cdot \mathbf{u}) \quad (6.9)$$

$$\rho \frac{Du_x}{Dt} = -\frac{1}{\gamma Ma^2} \frac{\partial(\rho T)}{\partial x} + \frac{1}{Re} \left(\frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{xy}}{\partial y} \right) \quad (6.10)$$

$$\rho \frac{Du_y}{Dt} = -\frac{1}{\gamma Ma^2} \frac{\partial(\rho T)}{\partial y} + \frac{1}{Re} \left(\frac{\partial \tau_{yx}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y} \right) \quad (6.11)$$

$$\begin{aligned} \rho \frac{DT}{Dt} = & -(\gamma - 1)\rho T (\nabla \cdot \mathbf{u}) + \frac{Ec\gamma}{Re} \left(\tau_{xx} \frac{\partial u_x}{\partial x} + \tau_{yx} \frac{\partial u_x}{\partial y} + \tau_{xy} \frac{\partial u_y}{\partial x} + \tau_{yy} \frac{\partial u_y}{\partial y} \right) \\ & - \frac{\gamma}{PrRe} \left(\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} \right) \end{aligned} \quad (6.12)$$

where t is the nondimensional time, D/Dt is the material derivative, ∇ is the 2-D divergence operator in Cartesian coordinates, and $\mathbf{u} = [u_x, u_y]^T$ is the bulk velocity vector. Note that equations are nondimensionalized using $t = t^* u_{x,1}^* / L_s^*$, $x = x^* / L_s^*$, $y = y^* / L_s^*$, $\rho = \rho^* / \rho_1^*$, $\mathbf{u} = \mathbf{u}^* / u_{x,1}^*$, $T = T^* / T_1^*$, $\mu = \mu^* / \mu_1^*$, $k = k^* / k_1^*$, $\boldsymbol{\tau} = \boldsymbol{\tau}^* L_s^* / (\mu_1^* u_{x,1}^*)$, $\mathbf{q} = \mathbf{q}^* L_s^* / (k_1^* T_1^*)$. Also, the Eckert and Prandtl numbers, Ec and Pr , respectively, may be written as,

$$\begin{aligned} Ec = (\gamma - 1) Ma^2 &= \frac{(u_{x,1}^*)^2}{c_v \gamma T_1^*} \\ Pr &= \frac{c_v \gamma \mu_1^*}{k_1^*} \end{aligned} \quad (6.13)$$

It is easy to check that for a monatomic gas, the above formula for Pr gives the same value as $2\gamma/5$ defined earlier in Sec. 6.2.1. Closure of Eqs. (6.9)–(6.12) is obtained using constitutive relationships, $\boldsymbol{\tau} = s(P, \mu)$ and $\mathbf{q} = h(P, k)$, where $P = \{\rho, u_x, u_y, T\}$ is a set of flow quantities depending on x, y, t . Equations (6.9)–(6.12) along with the

constitutive equations are linearized by decomposing the flow quantity vector $\mathcal{P} = [\rho, u_x, u_y, T]^T$ as

$$\mathcal{P}(x, y, t) = \bar{\mathcal{P}}(x) + \epsilon \hat{\mathcal{P}}(x) \exp[i(\beta y - \Omega t)] + c.c. \quad (6.14)$$

where the assumption of $\epsilon \ll 1$ is made, $\bar{\mathcal{P}} = [\bar{\rho}, \bar{u}_x, \bar{u}_y = 0, \bar{T}]^T$ and $\hat{\mathcal{P}} = [\hat{\rho}, \hat{u}_x, \hat{u}_y, \hat{T}]^T$ are the known and unknown vectors of nondimensional 1-D base flow quantities and perturbation amplitude functions, respectively, $\beta = 2\pi/L_y$ is a specified wavenumber in the y -direction where $L_y = L_y^*/L_s^*$ is the nondimensional wavelength of harmonic perturbations, $\Omega = \Omega_r + i\Omega_i$ are the unknown eigenvalues, normalized by $u_{x,1}^*/L_s^*$, whose real part indicates frequency and the imaginary part is the temporal growth rate, and $c.c.$ indicates complex conjugation so that $\hat{\mathcal{P}}$ is real. The nondimensional transport coefficients μ and k that appear in constitutive functions $\tau = f(P, \mu)$ and $q = g(P, k)$ are decomposed as

$$\begin{aligned} \mu &= \bar{\mu} + \epsilon \frac{d\bar{\mu}}{d\bar{T}} \hat{T}(x) \exp[i(\beta y - \Omega t)] + c.c. \\ k &= \bar{k} + \epsilon \frac{d\bar{k}}{d\bar{T}} \hat{T}(x) \exp[i(\beta y - \Omega t)] + c.c. \end{aligned} \quad (6.15)$$

where

$$\begin{aligned} \bar{\mu} &= \bar{T}^\omega \\ \frac{d\bar{\mu}}{d\bar{T}} &= \omega \bar{T}^{(\omega-1)} \\ \bar{k} &= \bar{\mu} \end{aligned}$$

A sketch describing a nominally 1-D shock layer subjected to harmonic perturbations is shown in Fig. 6.4.

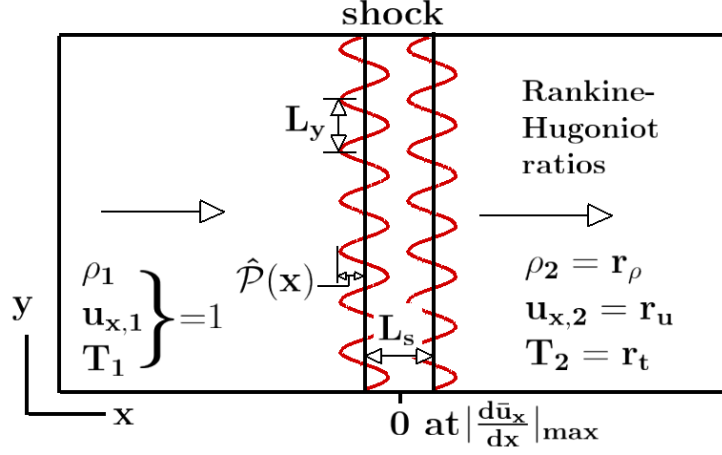


Figure 6.4: A sketch describing nominally 1-D shock imposed with 2-D harmonic perturbations (not drawn to scale). Quantities shown are nondimensional.

With these definitions, the $O(0)$ base flow and $O(\epsilon)$ perturbation terms are separated, the latter leading to the set of normal mode equations written in the form of an eigenvalue problem as

$$\mathcal{A}\hat{\mathcal{P}} = \Omega\mathcal{B}\hat{\mathcal{P}} \quad (6.16)$$

or,

$$\begin{pmatrix} \mathcal{A}_{11} & \mathcal{A}_{12} & \mathcal{A}_{13} & \mathcal{A}_{14} \\ \mathcal{A}_{21} & \mathcal{A}_{22} & \mathcal{A}_{23} & \mathcal{A}_{24} \\ \mathcal{A}_{31} & \mathcal{A}_{32} & \mathcal{A}_{33} & \mathcal{A}_{34} \\ \mathcal{A}_{41} & \mathcal{A}_{42} & \mathcal{A}_{43} & \mathcal{A}_{44} \end{pmatrix} \begin{pmatrix} \hat{\rho} \\ \hat{u}_x \\ \hat{u}_y \\ \hat{T} \end{pmatrix} = \Omega \begin{pmatrix} \mathcal{B}_{11} & 0 & 0 & 0 \\ 0 & \mathcal{B}_{22} & 0 & 0 \\ 0 & 0 & \mathcal{B}_{33} & 0 \\ 0 & 0 & 0 & \mathcal{B}_{44} \end{pmatrix} \begin{pmatrix} \hat{\rho} \\ \hat{u}_x \\ \hat{u}_y \\ \hat{T} \end{pmatrix} \quad (6.17)$$

We have used the Chebyshev spectral method [245] to discretize the eigenvalue problem defined in Eq. (6.16) at $(N + 1)$ Gauss-Lobatto collocation points, where N is the degree of Chebyshev polynomial. For all cases discussed in this work, we use a domain length of $-120 \leq x \leq 120$, unless specified otherwise. Dirichlet boundary conditions are imposed in the far fields up and downstream of the shock layer where perturbations are assumed to go to zero as $x \rightarrow \pm\infty$. In summary, in the linear stability analysis a value of the perturbation wavenumber, β , is specified and a corresponding spectrum of eigenmodes, plotted as Ω_r versus Ω_i , is obtained as a solution.

Now we define the maximum physically acceptable value of β , β_{ulim} , which corresponds to the smallest physically relevant perturbation wavelength, $L_{y,\min}^* = L_{y,\min} L_s^*$. For perturbations of macroscopic flow quantities to exist, the smallest perturbation wavelength must be greater than the maximum mean-free-path, that is $L_{y,\min}^* \geq \bar{\lambda}_{\max}^*$. This criterion ensures that perturbation wavelength is greater than the local values of $\bar{\lambda}$ in the entire base flow, and allows

us define β_{ulim} as

$$\beta_{\text{ulim}} = \frac{2\pi}{L_{y,\min}} = 2\pi \frac{L_s^*}{\bar{\lambda}_{\max}^*} \quad (6.18)$$

The variation of $\bar{\lambda}$ in the base flow was shown earlier in Fig. 6.2, while the values of $L_s^*/\bar{\lambda}_{\max}^*$ and β_{ulim} at three Mach number cases studied in this work are listed in Table 6.1. As the Mach number increases $\bar{\lambda}_{\max}^*$ increases resulting in the decrease in β_{ulim} , as seen from β_{ulim} of 151.4, 43.5, and 39.8 for $Ma = 1.2, 3$, and 5 , respectively. It must be noted that, by limiting our criterion that $L_{y,\min}^* = \bar{\lambda}_{\max}^*$, we ignore the perturbations having wavelengths smaller than $\bar{\lambda}_{\max}^*$ that might exist partially in the regions upstream and downstream of the location where $\bar{\lambda}^* = \bar{\lambda}_{\max}^*$ in our linear stability analyses. Such analysis would require performing linear stability analyses on partial domains of the shock layer, which is out of the scope of the present work.

6.3.2 The Navier-Stokes-Fourier (NSF) and Mott-Smith (MS) constitutive equations

In the NSF models, the constitutive equation for the viscous stress tensor $\tau^{n*} = f^n(P^*, \mu^*)$ is defined by assuming a linear relationship of the stress tensor with the strain rate tensor, S^* , an isotropic medium, and symmetry of the stress tensor, as

$$\tau_{ij}^{n*} = 2\mu^* S_{ij}^* + \Lambda^* (\nabla^* \cdot \mathbf{u}^*) \delta_{ij} \quad (6.19)$$

where δ_{ij} is the Kronecker's delta function, and $\Lambda^* = -2\mu^*/3$ is the second coefficient of viscosity, and the strain rate tensor is defined as

$$S_{ij}^* = \frac{1}{2} \left(\frac{\partial u_i^*}{\partial x_j^*} + \frac{\partial u_j^*}{\partial x_i^*} \right) \quad (6.20)$$

Using the Fourier's law of heat conduction, the heat flux vector, $\mathbf{q}^{n*}$, is given as,

$$q_i^{n*} = -k^* \frac{\partial T^*}{\partial x_i^*} \quad (6.21)$$

When the bimodal MS approximation is used, however, the constitutive equations for the 1-D base flow quantities,

$\bar{\tau}^{m*} = s^m(\bar{P}^*, \bar{\mu}^*)$ and $\bar{q}^{m*} = h^m(\bar{P}^*, \bar{k}^*)$, can be written as

$$\begin{aligned}\bar{\tau}_{xx}^{m*} &= A_a \frac{T_1^*}{\bar{T}^*} \frac{\bar{\rho}^*}{\rho_1^*} \bar{\mu}^* \frac{d\bar{u}_x^*}{dx^*} \\ \bar{\tau}_{yy}^{m*} &= A_b \frac{T_1^*}{\bar{T}^*} \frac{\bar{\rho}^*}{\rho_1^*} \bar{\mu}^* \frac{d\bar{u}_x^*}{dx^*} \\ \bar{\tau}_{xy}^{m*} &= \bar{\tau}_{yx}^{m*} = 0\end{aligned}\tag{6.22}$$

and

$$\begin{aligned}\bar{q}_x^{m*} &= -\bar{k}^* B_a \left(\frac{T_1^*}{\bar{T}^*} \right) \left(\frac{T_1^*}{\bar{\rho}^*} \right) \frac{d\bar{\rho}^*}{dx^*} + \frac{2}{5} \frac{\bar{k}^* \bar{\tau}_{xx}^{m*}}{\bar{\mu}^* R} \bar{u}_x^* + \frac{2}{5} \frac{\bar{k}^* \bar{\tau}_{xy}^{m*}}{\bar{\mu}^* R} \bar{u}_y^* \\ \bar{q}_y^{m*} &= 0\end{aligned}\tag{6.23}$$

where A_a , A_b , and B_a are constants that depend on the Rankine-Hugoniot ratios as

$$A_a = \frac{2}{5} \gamma M a^2 (r_u + r_u^2)\tag{6.24}$$

$$A_b = \left(r_u \frac{1 - r_t}{1 - r_u} \right)\tag{6.25}$$

$$B_a = r_t^2 - \frac{1}{5} \left((\gamma M a^2)^2 (1 - r_u^3) + 8 \gamma M a^2 (1 - r_u r_t) + 5(1 - r_t^2) \right) \frac{r_u}{1 - r_u}\tag{6.26}$$

The full derivation is provided in the supplementary Sec. 6.6.1.

The MS constitutive relationships can be extended to 2-D, *i.e.* $\tau^{m*}(x, y, t) = s^m(P^*, \mu^*)$ and $q^{m*}(x, y, t) = h(P^*, k^*)$, as follows, which are then substituted in Eqs. (6.9)–(6.12) to obtain the anisotropic conservation equations (ACE). Starting with the viscous stress tensor, we assume its general form to depend on the strain rate tensor and divergence of the bulk velocity vector, similar to Eq. (6.19), as

$$\tau_{ij}^{m*} = \Pi^* S_{ij}^* + \Sigma^* (\nabla^* \cdot \mathbf{u}^*) \delta_{ij}\tag{6.27}$$

where the forms of functions Π^* and Σ^* must be

$$\begin{aligned}\Pi^* &= (A_a - A_b) \frac{T_1^*}{\bar{T}^*} \frac{\rho^*}{\rho_1^*} \mu^* \\ \Sigma^* &= A_b \frac{T_1^*}{\bar{T}^*} \frac{\rho^*}{\rho_1^*} \mu^*\end{aligned}\tag{6.28}$$

for the linear stress-strain relationship of Newtonian fluids to hold, as proved in supplementary Sec. 6.6.1.

For the heat flux, the 2-D x^* -directional component, q_x^{m*} is assumed to have the same form as $\bar{q}_x^{m*}$ in Eq. (6.23), *i.e.*

$$q_x^{m*} = -k^* B_a \left(\frac{T_1^*}{T^*} \right) \left(\frac{T_1^*}{\rho^*} \right) \frac{d\rho^*}{dx^*} + \frac{2}{5} \frac{k^* \tau_{xx}^{m*}}{\mu^* R} u_x^* + \frac{2}{5} \frac{k^* \tau_{xy}^{m*}}{\mu^* R} u_y^* \quad (6.29)$$

and to be consistent with the stress formulation, the 2-D forms of τ_{xx}^{m*} and τ_{xy}^{m*} , obtained from Eq. (6.27), are substituted in Eq. (6.29) to obtain

$$\begin{aligned} q_x^{m*} = & -k^* B_a \frac{T_1^*}{T^*} \frac{T_1^*}{\rho^*} \frac{d\rho^*}{dx^*} + \frac{2}{5} \frac{k^*}{R} u_x^* \frac{T_1^*}{T^*} \frac{\rho^*}{\rho_1^*} \left(A_a \frac{\partial u_x^*}{\partial x^*} + A_b \frac{\partial u_y^*}{\partial y^*} \right) \\ & + \frac{2}{5} \frac{k^*}{R} u_y^* \frac{T_1^*}{T^*} \frac{\rho^*}{\rho_1^*} \frac{(A_a - A_b)}{2} \left(\frac{\partial u_x^*}{\partial y^*} + \frac{\partial u_y^*}{\partial x^*} \right) \end{aligned} \quad (6.30)$$

For the y^* -directional component, q_y^{m*} , we assume the same Fourier's law of heat conduction used in the compressible NSE, *i.e.* $q_y^{m*} = q_y^{n*}$, which is justified because both DSMC and Fourier's law predict zero heat flux in a 1-D shock layer at all Mach numbers. This assumption implies that the presence of strong bimodality in the x^* -direction is assumed to not affect substantially the $O(\epsilon)$ perturbations in the heat flux in the y^* -direction.

A comparison of the constitutive equation for the stress tensor, Eq. (6.27), with Eq. (6.19), obtained from the NSF equations, shows that the values of A_a and A_b are $4/3$ and $-2/3$, respectively, in the NSE formulation, whereas in the kinetic formulation, they vary with the strength of the shock. Figure 6.5(a) shows that the kinetically-obtained values increase significantly with Mach number, while a closer look at the variation at low Mach numbers ($1.1 < Ma < 1.6$) in Fig. 6.5(b) shows that they do not approach monotonically to $4/3$ and $-2/3$, respectively, but become slightly smaller in magnitude at $Ma = 1.16$. The kinetically-derived equation also includes an extra factor of $T_1^* \rho^* / (T^* \rho_1^*)$, which varies in the entire shock layer. Turning to the heat flux formulation, Eq. (6.30) for q_x^{m*} is very different from the Fourier's law used in the NSE formulation. Figure 6.5(c) shows that the constant B_a , defined in Eq. (6.26), increase monotonically with Mach number and changes sign at $Ma = 2.46$, because the term r_t^2 dominates over the second term in the equation. Table 6.2 lists the values of these constants at the three Mach numbers that will be considered in Sec. 6.4.

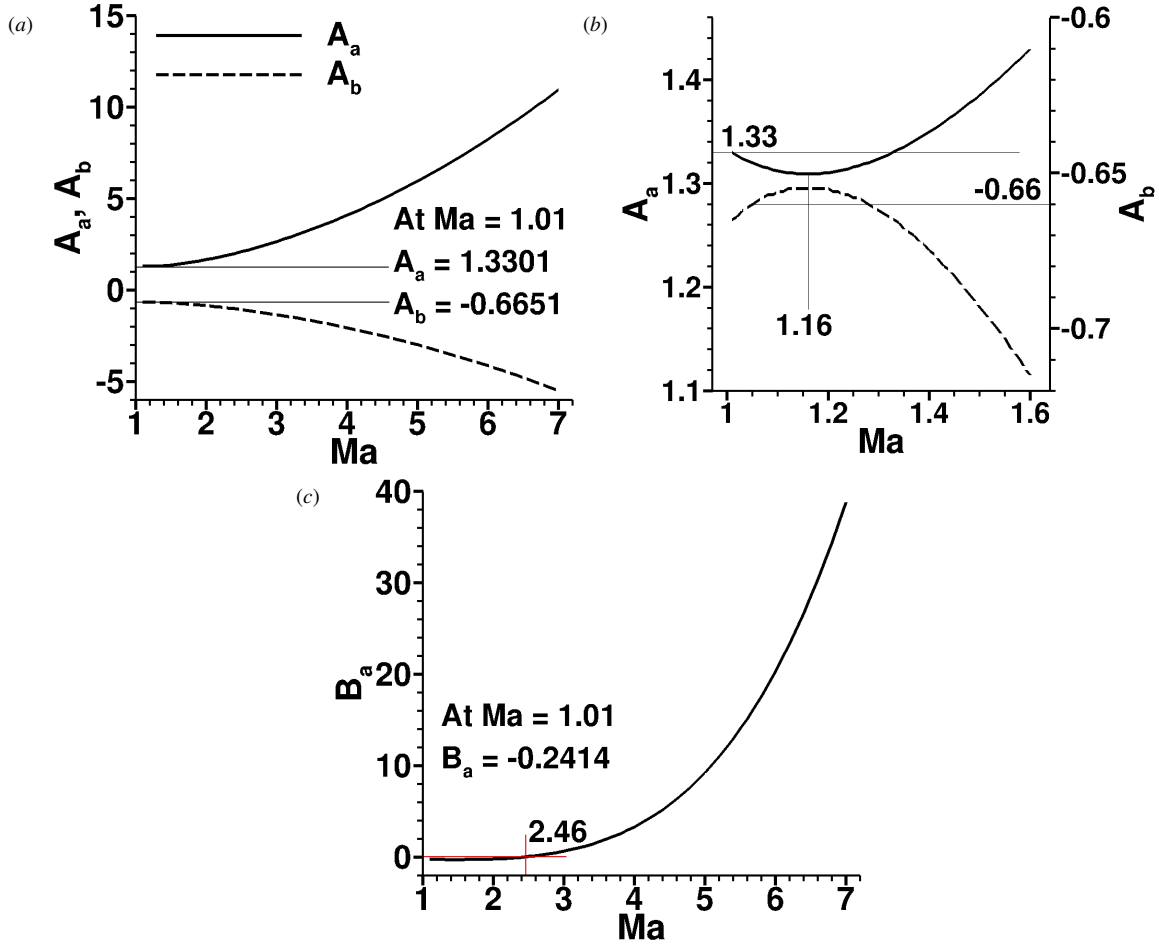


Figure 6.5: (a) and (b) show the variation of constants A_a , A_b in the kinetic constitutive equations with Mach number, where the latter shows variation within $1.1 < Ma < 1.6$. (c) shows the variation of constant B_a .

Ma	A_a	A_b	B_a
1.2	1.3104	-0.6552	-0.2551
3.0	2.6670	-1.3330	0.6669
5.0	5.9730	-2.9869	9.2709

Table 6.2: Constants A_a , A_b , and B_a used in the kinetic constitutive equations for ACE.

6.3.3 The linearization of the 2-D Compressible Navier-Stokes Equations (NSE) and Anisotropic Conservation Equations (ACE)

To obtain the 2-D nondimensional NSE, the transport quantities τ^{n*} and q^{n*} , given by Eqs. (6.19) and (6.21), respectively, are nondimensionalized and substituting in Eqs. (6.9)–(6.12). The final set of continuity, x-momentum, y-momentum, and energy equations in the NSE formulation is written as

$$\frac{D\rho}{Dt} = -\rho (\nabla \cdot \mathbf{u}) \quad (6.31)$$

$$\rho \frac{Du_x}{Dt} = -\frac{1}{\gamma Ma^2} \frac{\partial(\rho T)}{\partial x} + \frac{1}{Re} \frac{\partial}{\partial x} \left(2\mu \frac{\partial u_x}{\partial x} + \Lambda (\nabla \cdot \mathbf{u}) \right) + \frac{1}{Re} \frac{\partial}{\partial y} \left(\mu \left(\frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x} \right) \right) \quad (6.32)$$

$$\rho \frac{Du_y}{Dt} = -\frac{1}{\gamma Ma^2} \frac{\partial(\rho T)}{\partial y} + \frac{1}{Re} \frac{\partial}{\partial x} \left(\mu \left(\frac{\partial u_y}{\partial x} + \frac{\partial u_x}{\partial y} \right) \right) + \frac{1}{Re} \frac{\partial}{\partial y} \left(2\mu \frac{\partial u_y}{\partial y} + \Lambda (\nabla \cdot \mathbf{u}) \right) \quad (6.33)$$

$$\begin{aligned} \rho \frac{DT}{Dt} = & -(\gamma - 1)\rho T (\nabla \cdot \mathbf{u}) + \frac{Ec\gamma}{Re} \Lambda \left(\frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} \right)^2 + \frac{Ec\gamma}{Re} \mu \left[2 \left(\frac{\partial u_x}{\partial x} \right)^2 + 2 \left(\frac{\partial u_y}{\partial y} \right)^2 \right. \\ & \left. + \left(\frac{\partial u_y}{\partial x} + \frac{\partial u_x}{\partial y} \right)^2 \right] + \frac{\gamma}{PrRe} \frac{\partial}{\partial x} \left(k \frac{\partial T}{\partial x} \right) + \frac{\gamma}{PrRe} \frac{\partial}{\partial y} \left(k \frac{\partial T}{\partial y} \right) \end{aligned} \quad (6.34)$$

To obtain the 2-D kinetic nondimensional ACE, we use the transport quantities τ^{m*} , q_x^{m*} , and q_y^{m*} , given by Eqs. (6.27), (6.30), and (6.21), respectively, nondimensionalize them, and substitute them into Eqs. (6.9)–(6.12), as well. The final set of continuity, x-momentum, y-momentum, and energy equations in the ACE formulation is written as

$$\frac{D\rho}{Dt} = -\rho (\nabla \cdot \mathbf{u}) \quad (6.35)$$

$$\rho \frac{Du_x}{Dt} = -\frac{1}{\gamma Ma^2} \frac{\partial(\rho T)}{\partial x} + \frac{1}{Re} \frac{\partial}{\partial x} \left[\mu \frac{\rho}{T} \left((A_a - A_b) \frac{\partial u_x}{\partial x} + A_b (\nabla \cdot \mathbf{u}) \right) \right] + \frac{1}{Re} \frac{\partial}{\partial y} \left(\mu \left(\frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x} \right) \right) \quad (6.36)$$

$$\rho \frac{Du_y}{Dt} = -\frac{1}{\gamma Ma^2} \frac{\partial(\rho T)}{\partial y} + \frac{1}{Re} \frac{\partial}{\partial x} \left(\mu \left(\frac{\partial u_y}{\partial x} + \frac{\partial u_x}{\partial y} \right) \right) + \frac{1}{Re} \frac{\partial}{\partial y} \left[\mu \frac{\rho}{T} \left((A_a - A_b) \frac{\partial u_x}{\partial y} + A_b (\nabla \cdot \mathbf{u}) \right) \right] \quad (6.37)$$

$$\begin{aligned}
\rho \frac{DT}{Dt} = & -(\gamma - 1)\rho T(\nabla \cdot \mathbf{u}) + \frac{Ec\gamma}{Re} A_b \mu \frac{\rho}{T} \left(\frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} \right)^2 \\
& + \frac{Ec\gamma}{Re} (A_a - A_b) \mu \frac{\rho}{T} \left[\left(\frac{\partial u_x}{\partial x} \right)^2 + \left(\frac{\partial u_y}{\partial y} \right)^2 + \frac{1}{2} \left(\frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} \right)^2 \right] - \frac{\gamma}{PrRe} \frac{\partial}{\partial x} \left[-k B_a \frac{1}{T\rho} \frac{\partial \rho}{\partial x} \right. \\
& \left. + B_b k u_x \frac{\rho}{T} \left(A_a \frac{\partial u_x}{\partial x} + A_b \frac{\partial u_y}{\partial y} \right) + B_b k u_y \frac{\rho}{T} \frac{(A_a - A_b)}{2} \left(\frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x} \right) \right] + \frac{\gamma}{PrRe} \frac{\partial}{\partial y} \left(k \frac{\partial T}{\partial y} \right) \quad (6.38)
\end{aligned}$$

where

$$B_b = \frac{2}{5} \gamma Ma^2 \quad (6.39)$$

By using the linear decomposition for ρ , u_x , u_y , T , μ , and k described in Eqs. (7.1) and (6.15) in the 2-D, compressible NSE (Eqs. (6.31)–(6.34)), and in the 2-D, compressible ACE (Eqs. (6.35)–(6.38)), the $O(0)$ base flow and $O(\epsilon)$ perturbation terms are separated to obtain the nondimensional 1-D, steady, base flow equations and the normal mode equations, respectively, for each formulation, as presented below. In the following equations, a prime denotes a derivative in the x -direction.

The $O(0)$ base flow continuity, x -momentum, and energy equations are respectively written for the NSE formulation as

$$\bar{\rho} \bar{u}'_x + \bar{u}_x \bar{\rho}' = 0 \quad (6.40)$$

$$\bar{\rho} \bar{u}_x \bar{u}'_x + \frac{1}{\gamma Ma^2} (\bar{\rho} \bar{T})' - \frac{1}{Re} \left((2\bar{\mu} + \bar{\Lambda}) \bar{u}'_x \right)' = 0 \quad (6.41)$$

$$\bar{\rho} \left(\bar{u}_x \bar{T}' + (\gamma - 1) \bar{T} \bar{u}'_x \right) - \frac{Ec\gamma}{Re} (2\bar{\mu} + \bar{\Lambda}) (\bar{u}'_x)^2 - \frac{\gamma}{PrRe} \left(\bar{k} \bar{T}' \right)' = 0 \quad (6.42)$$

and the ACE formulation as

$$\bar{\rho} \bar{u}'_x + \bar{u}_x \bar{\rho}' = 0 \quad (6.43)$$

$$\bar{\rho} \bar{u}_x \bar{u}'_x + \frac{1}{\gamma Ma^2} (\bar{\rho} \bar{T})' + \frac{A_a}{Re} \left(\frac{\bar{\rho}}{\bar{T}} \bar{\mu} \bar{u}'_x \right)' = 0 \quad (6.44)$$

$$\bar{\rho} \left(\bar{u}_x \bar{T}' + (\gamma - 1) \bar{T} \bar{u}'_x \right) + A_a \frac{Ec\gamma \bar{\rho} \bar{\mu} (\bar{u}'_x)^2}{Re \bar{T}} + \frac{\gamma \bar{k}}{PrRe} \left(-B_a \frac{\bar{\rho}'}{\bar{T} \bar{\rho}} + A_a B_b \bar{u}_x \frac{\bar{\rho}}{\bar{T}} \bar{u}'_x \right)' = 0 \quad (6.45)$$

The $O(\epsilon)$ normal mode continuity, x -momentum, y -momentum, and energy equations for both formulations can be written together as follows, where terms indicated with an overbrace and underbrace indicate terms that are zero in the ACE and NSE formulations, respectively. The terms are also color coded such that those in red have a different

functional form depending on the formulation used, those in olive-green only appear in the NSE formulation because of Fourier's law of heat conduction used for q_x , while those in blue only appear in the ACE formulation because of MS constitutive equation used for q_x . Some of the red terms drop out in the NSE formulation because the partial derivatives of those terms are zero.

Continuity:

$$\bar{u}'_x \hat{\rho} + \bar{u}_x \hat{\rho}' + \bar{\rho}' \hat{u}_x + \bar{\rho} \hat{u}'_x + i\beta \bar{\rho} \hat{u}_y = i\Omega \hat{\rho} \quad (6.46)$$

x -momentum:

$$\begin{aligned} & \left(\frac{1}{\gamma Ma^2} \bar{T}' + \bar{u}_x \bar{u}'_x \right) \hat{\rho} + \frac{1}{\gamma Ma^2} \bar{T} \hat{\rho}' + \left(\beta^2 \frac{\bar{\psi} - \bar{\phi}}{2} + \bar{\rho} \bar{u}'_x \right) \hat{u}_x \\ & + (\bar{\phi}' + \bar{u}_x \bar{\rho}) \hat{u}'_x + \bar{\phi} \bar{u}''_x + i\beta \bar{\psi}' \hat{u}_y - i\beta \left[\frac{\bar{\psi} - \bar{\phi}}{2} - \bar{\psi} \right] \hat{u}'_y \\ & + \left(\frac{\partial^2 \bar{\phi}}{\partial \bar{T}^2} \bar{T}' \bar{u}'_x + \frac{\partial \bar{\phi}}{\partial \bar{T}} \bar{u}''_x + \frac{\bar{\rho}'}{\gamma Ma^2} \right) \hat{T} + \left(\frac{\partial \bar{\phi}}{\partial \bar{T}} \bar{u}'_x + \frac{\bar{\rho}}{\gamma Ma^2} \right) \hat{T}' \\ & + \underbrace{\left(\frac{1}{\bar{\rho}} \frac{\partial \bar{\phi}}{\partial \bar{T}} \bar{T}' \bar{u}'_x + \frac{\partial \bar{\phi}}{\partial \bar{\rho}} \bar{u}''_x \right) \hat{\rho} + \frac{\partial \bar{\phi}}{\partial \bar{\rho}} \bar{u}'_x \hat{\rho}' + \frac{1}{\bar{\rho}} \frac{\partial \bar{\phi}}{\partial \bar{T}} \bar{\rho}' \bar{u}'_x \hat{T}}_{\text{zero in NSE}} = i\Omega \bar{\rho} \hat{u}_x \end{aligned} \quad (6.47)$$

y -momentum:

$$\begin{aligned} & i\beta \frac{\bar{T}}{\gamma Ma^2} \hat{\rho} - i\beta \frac{\bar{\psi}' - \bar{\phi}'}{2} \hat{u}_x + i\beta \left(\bar{\psi} - \frac{\bar{\psi} - \bar{\phi}}{2} \right) \hat{u}'_x - \beta^2 \bar{\phi} \hat{u}_y \\ & + \left(\bar{u}_x \bar{\rho} - \frac{\bar{\psi}' - \bar{\phi}'}{2} \right) \hat{u}'_y - \frac{\bar{\psi} - \bar{\phi}}{2} \hat{u}''_y + \left[i\beta \left(\frac{\bar{\rho}}{\gamma Ma^2} + \frac{\partial \bar{\psi}}{\partial \bar{T}} \bar{u}'_x \right) \right] \hat{T} + \underbrace{i\beta \frac{\partial \bar{\psi}}{\partial \bar{\rho}} \bar{u}'_x \hat{\rho}}_{\text{zero in NSE}} = i\Omega \bar{\rho} \hat{u}_y \end{aligned} \quad (6.48)$$

Energy:

$$\begin{aligned}
& (\bar{u}_x \bar{T}' + (\gamma - 1) \bar{T} \bar{u}_x') \hat{\rho} + \bar{\rho} \bar{T}' \hat{u}_x + \left(2Ec\gamma \bar{\phi} \bar{u}_x' + (\gamma - 1) \bar{\rho} \bar{T} \right) \hat{u}_x' \\
& + i\beta \left(2Ec\gamma \bar{\psi} \bar{u}_x' + (\gamma - 1) \bar{\rho} \bar{T} \right) \hat{u}_y + \left(\beta^2 \bar{\kappa} + Ec\gamma \frac{\partial \bar{\phi}}{\partial \bar{T}} \bar{u}_x'^2 + (\gamma - 1) \bar{\rho} \bar{u}_x' \right) \hat{T} + \bar{u}_x \bar{\rho} \hat{T}' \\
& \quad \underbrace{- (\bar{\kappa})'' \hat{T} - 2(\bar{\kappa})' \hat{T}' - \bar{\kappa} \hat{T}''}_{\text{do not appear in ACE}} \\
& + \underbrace{\left[(\bar{\xi}_b)' + (\bar{\xi}_h)' \right] \hat{\rho} + \left(\bar{\xi}_b - (\bar{\xi}_a)' + \bar{\xi}_h \right) \hat{\rho}' - \bar{\xi}_a \hat{\rho}'' + (\bar{\xi}_g)' \hat{u}_x + \left((\bar{\xi}_d)' + \bar{\xi}_g \right) \hat{u}_x'}_{\text{do not appear in NSE}} \\
& \quad \underbrace{+ \bar{\xi}_d \hat{u}_x'' + i\beta (\bar{\xi}_e)' + (i\beta \bar{\xi}_e) \hat{u}_y' + \left[(\bar{\xi}_c)' + (\bar{\xi}_f)' \right] \hat{T} + \left(\bar{\xi}_c + \bar{\xi}_f \right) \hat{T}'}_{\text{do not appear in NSE}} = i\Omega \bar{\rho} \hat{T}
\end{aligned} \tag{6.49}$$

where functions $\bar{\phi}$, $\bar{\psi}$ and their derivatives (red terms) for both formulations are defined in Table 6.3, functions $\bar{\xi}_j$ for $j = a$ to h and their derivatives (blue terms) that appear in the normal mode energy equation (6.49) for the ACE formulation are listed in Table 6.4.

Function	NSE	ACE
$\bar{\phi}$	$-\frac{1}{Re} (2\bar{\mu} + \bar{\Lambda})$	$-\frac{A_a}{Re} \frac{\bar{\mu}}{\bar{T}}$
$\bar{\psi}$	$-\frac{\bar{\Lambda}}{Re}$	$-\frac{A_b}{Re} \frac{\bar{\rho}}{\bar{T}} \bar{\mu}$
$\bar{\phi}'$	$\frac{d\bar{\phi}}{d\bar{T}} \bar{T}'$	$\frac{\partial \bar{\phi}}{\partial \bar{\rho}} \bar{\rho}' + \frac{\partial \bar{\phi}}{\partial \bar{T}} \bar{T}'$
$\bar{\psi}'$	$\frac{d\bar{\psi}}{d\bar{T}} \bar{T}'$	$\frac{\partial \bar{\psi}}{\partial \bar{\rho}} \bar{\rho}' + \frac{\partial \bar{\psi}}{\partial \bar{T}} \bar{T}'$
$\frac{\partial \bar{\phi}}{\partial \bar{T}}$	$-\frac{1}{Re} \left(2 \frac{d\bar{\mu}}{d\bar{T}} + \frac{d\bar{\Lambda}}{d\bar{T}} \right)$	$-\frac{A_a}{Re} \frac{\bar{\rho}}{\bar{T}} \frac{d\bar{\mu}}{d\bar{T}} - \frac{\bar{\phi}}{\bar{T}}$
$\frac{\partial \bar{\phi}}{\partial \bar{\rho}}$	0	$-\frac{A_a}{Re} \frac{\bar{\mu}}{\bar{T}}$
$\frac{\partial^2 \bar{\phi}}{\partial \bar{T}^2}$	$-\frac{1}{Re} \left(2 \frac{d^2 \bar{\mu}}{d\bar{T}^2} + \frac{d^2 \bar{\Lambda}}{d\bar{T}^2} \right)$	$-\frac{A_a}{Re} \frac{\bar{\rho}}{\bar{T}} \frac{d^2 \bar{\mu}}{d\bar{T}^2} - \frac{2}{\bar{T}} \frac{\partial \bar{\phi}}{\partial \bar{T}}$
$\frac{\partial \bar{\psi}}{\partial \bar{T}}$	$-\frac{1}{Re} \frac{d\bar{\Lambda}}{d\bar{T}} = -\frac{1}{2} \frac{d\bar{\phi}}{d\bar{T}}$	$-\frac{A_b}{Re} \frac{\bar{\rho}}{\bar{T}} \frac{d\bar{\mu}}{d\bar{T}} - \frac{\bar{\psi}}{\bar{T}}$
$\frac{\partial \bar{\psi}}{\partial \bar{\rho}}$	0	$-\frac{A_b}{Re} \frac{\bar{\mu}}{\bar{T}}$

Table 6.3: Definitions of functions $\bar{\phi}$, $\bar{\psi}$ for both formulations.

The derivatives of $\bar{\mu}$ that appear in Table 6.3 are written as

$$\begin{aligned}\frac{d\bar{\mu}}{d\bar{T}} &= \omega \bar{T}^{\omega-1} \\ \frac{d^2\bar{\mu}}{d\bar{T}^2} &= \omega(\omega-1)\bar{T}^{\omega-2}\end{aligned}\tag{6.50}$$

and $\bar{\kappa}$ and its derivatives are written as

$$\begin{aligned}\bar{\kappa} &= \frac{\gamma \bar{k}}{PrRe} \\ \bar{\kappa}' &= \frac{\gamma}{PrRe} \frac{d\bar{k}}{d\bar{T}} \bar{T}' \\ \bar{\kappa}'' &= \frac{\gamma}{PrRe} \left(\frac{d^2\bar{k}}{d\bar{T}^2} \bar{T}'^2 + \frac{d\bar{k}}{d\bar{T}} \bar{T}'' \right)\end{aligned}\tag{6.51}$$

Section 6.6.2 provides the equations that relate the elements of linear operators $\mathcal{A}$ and $\mathcal{B}$, defined in Eq. 6.17, for both formalisms, with Eqs. 6.46–6.49.

j	$\bar{\xi}_j$	$\bar{\xi}'_j$
a	$B_a \frac{\gamma}{PrRe} \frac{1}{\bar{T}\bar{\rho}} \bar{k}$	$B_a \frac{\gamma}{PrRe} \frac{1}{\bar{T}\bar{\rho}} \left[\frac{d\bar{k}}{d\bar{T}} \bar{T}' - \frac{\bar{k}\bar{T}'}{\bar{T}} - \frac{\bar{k}\bar{\rho}'}{\bar{\rho}} \right]$
b	$\bar{\xi}_a \frac{\bar{\rho}'}{\bar{\rho}}$	$B_a \frac{\gamma}{PrRe} \frac{1}{\bar{T}\bar{\rho}} \left[\frac{\bar{T}'\bar{\rho}'}{\bar{\rho}} \frac{d\bar{k}}{d\bar{T}} + \frac{\bar{\rho}''\bar{k}}{\bar{\rho}} - \frac{\bar{T}'\bar{\rho}'\bar{k}}{\bar{T}\bar{\rho}} - \frac{2(\bar{\rho}')^2\bar{k}}{\bar{\rho}^2} \right]$
c	$\bar{\xi}_a \frac{\bar{\rho}'}{\bar{T}}$ $-B_a \frac{\gamma}{PrRe} \frac{1}{\bar{T}\bar{\rho}} \bar{\rho}' \frac{d\bar{k}}{d\bar{T}}$	$B_a \frac{\gamma}{PrRe} \frac{1}{\bar{T}\bar{\rho}} \left[\frac{\bar{\rho}'\bar{k}}{\bar{T}} + \frac{2\bar{T}'\bar{\rho}'}{\bar{T}} \frac{d\bar{k}}{d\bar{T}} - \frac{2\bar{T}'\bar{\rho}'\bar{k}}{\bar{T}^2} \right.$ $\left. - \frac{(\bar{\rho}')^2\bar{k}}{\bar{\rho}\bar{T}} - \bar{\rho}'' \frac{d\bar{k}}{d\bar{T}} + \frac{(\bar{\rho}')^2}{\bar{\rho}} \frac{d\bar{k}}{d\bar{T}} - \bar{\rho}'\bar{T}' \frac{d^2\bar{k}}{d\bar{T}^2} \right]$
d	$A_a B_b \frac{\gamma}{PrRe} \frac{\bar{\rho}\bar{u}_x}{\bar{T}} \bar{k}$	$A_a B_b \frac{\gamma}{PrRe} \left[\frac{\bar{\rho}'\bar{k}\bar{u}_x}{\bar{T}} + \frac{\bar{\rho}\bar{k}'\bar{u}_x}{\bar{T}} + \frac{\bar{\rho}\bar{k}\bar{u}_x'}{\bar{T}} - \frac{\bar{\rho}\bar{k}\bar{u}_x}{\bar{T}^2} \bar{T}' \right]$
e	$\frac{A_b}{A_a} \bar{\xi}_d$	$\frac{A_b}{A_a} \bar{\xi}'_d$
f	$A_a B_b \frac{\gamma}{PrRe} \bar{u}_x' \frac{d\bar{k}}{d\bar{T}} \frac{\bar{u}_x\bar{\rho}}{\bar{T}}$ $-\frac{\bar{u}_x'}{\bar{T}} \bar{\xi}_d$	$A_a B_b \frac{\gamma}{PrRe} \left[\frac{\bar{u}_x'\bar{\rho}'\bar{u}_x}{\bar{T}} \frac{d\bar{k}}{d\bar{T}} - \frac{\bar{u}_x'\bar{\rho}'\bar{k}\bar{u}_x}{\bar{T}^2} + \frac{\bar{T}'\bar{u}_x'\bar{u}\bar{\rho}}{\bar{T}} \frac{d^2\bar{k}}{d\bar{T}^2} \right.$ $\left. + \frac{\bar{u}_x''\bar{u}_x\bar{\rho}}{\bar{T}} \frac{d\bar{k}}{d\bar{T}} - \frac{2\bar{T}'\bar{u}_x'\bar{u}_x\bar{\rho}}{\bar{T}^2} \frac{d\bar{k}}{d\bar{T}} - \frac{\bar{u}_x''\bar{k}\bar{u}_x\bar{\rho}}{\bar{T}^2} \right.$ $\left. + \frac{2\bar{T}'\bar{u}_x'\bar{k}\bar{u}_x\bar{\rho}}{\bar{T}^3} + \frac{(\bar{u}_x')^2\bar{\rho}}{\bar{T}} \frac{d\bar{k}}{d\bar{T}} - \frac{(\bar{u}_x')^2\bar{k}\bar{\rho}}{\bar{T}^2} \right]$
g	$A_a B_b \frac{\gamma}{PrRe} \frac{\bar{u}_x'\bar{k}\bar{\rho}}{\bar{T}}$	$A_a B_b \frac{\gamma}{PrRe} \left[\frac{\bar{u}_x'\bar{k}\bar{\rho}}{\bar{T}} + \frac{\bar{u}_x'\bar{k}'\bar{\rho}}{\bar{T}} + \frac{\bar{u}_x'\bar{k}\bar{\rho}'}{\bar{T}} - \frac{\bar{u}_x'\bar{k}\bar{\rho}}{\bar{T}^2} \bar{T}' \right]$
h	$A_a B_b \frac{\gamma}{PrRe} \frac{\bar{u}_x'\bar{k}\bar{u}_x}{\bar{T}}$	$A_a B_b \frac{\gamma}{PrRe} \left[\frac{\bar{u}_x''\bar{k}\bar{u}_x}{\bar{T}} + \frac{\bar{u}_x'\bar{k}'\bar{u}_x}{\bar{T}} + \frac{(\bar{u}_x')^2\bar{k}}{\bar{T}} - \frac{\bar{u}_x'\bar{k}\bar{u}_x}{\bar{T}^2} \bar{T}' \right]$

Table 6.4: Definitions of functions $\bar{\xi}_j$ and $\bar{\xi}'_j$ for $j = a$ to h .

6.4 Comparison of Eigenspectra from the Two Formulations at $Ma = 1.2, 3$ and 5

In this section, we discuss the results from the linear stability analyses of the Mach numbers 1.2, 3 and 5 DSMC shock layers by solving the normal mode equations obtained from the NSE and ACE formulations, *i.e.* Eqs. (6.46)–(6.49) presented in Sec. 6.3.3. It will be shown that the eigenspectra reveal eigenmodes that are a part of continuous branches, consistent with the observations of Duck and Balakumar [1]. Sections 6.4.1 and 6.4.2 are dedicated to the discussion of the first and the second least damped continuous branches, respectively. Also, the comparison of our NSE formulation with the eigenspectra obtained from Duck and Balakumar [1] for shock layer profiles obtained using the method of Gilbarg and Paolucci [7] is provided in the supplementary Sec. 6.6.3.

6.4.1 Comparison of the least stable continuous branch ‘u’

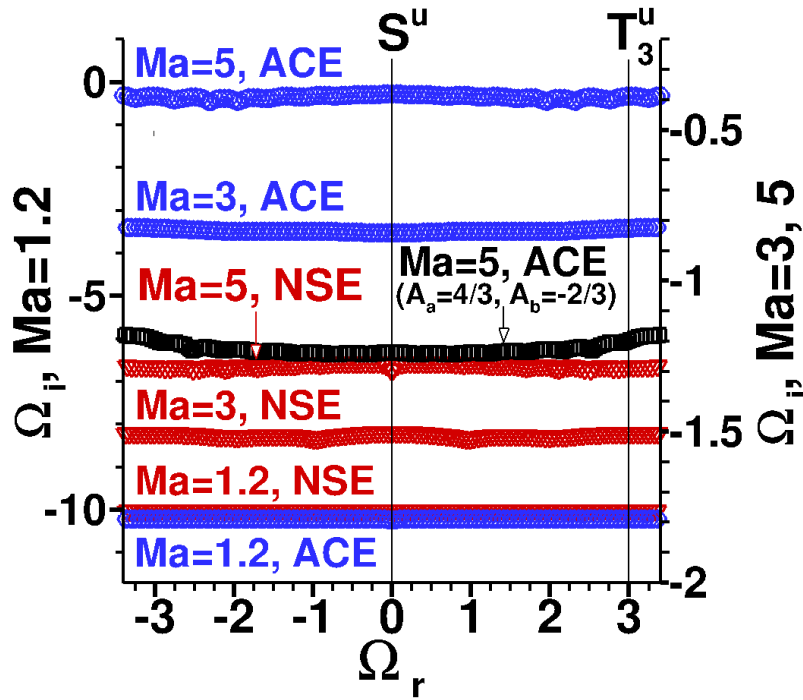


Figure 6.6: Comparison of the least stable continuous branch u in the eigenspectra obtained from the ACE and NSE formulations at $\beta = \beta_{ulim}$ and $Ma = 1.2, 3$, and 5. Eigenmodes S^u and T_3^u are indicated with vertical lines at $\Omega_r = 0$ and 3, respectively.

The least stable continuous branches, denoted as ‘ u ’, obtained from both formulations at the three Mach numbers are shown in Fig. 6.6. It must be noted that a continuous branch represents a continuum of modes, and therefore, cannot

Ma	S''		T_3''	
	ACE	NSE	ACE	NSE
1.2	-10.23	-10.04	-10.21	-10.03
3	-0.82	-1.50	-0.83	-1.51
5	-0.38	-1.25	-0.39	-1.29

Table 6.5: Decay rate, Ω_i , for stationary traveling continuum modes S'' and T_3'' on branch u obtained from the ACE and NSE formulations.

be fully resolved by a finite number of Chebyshev points used in our eigenvalue solver for obtaining eigenspectra, numerically. Therefore, the continuous lines seen in Fig. 6.6 are actually composed of closely spaced points, referred to as continuum modes [224], that represent the continuous branch. In this work 2000 grid points are used and it is checked that the decay rates of continuum modes do not vary by more than 0.2% when grid points are varied from 2000 to 2400, where the latter limit requires highest wall-clock time of 48 hours on available supercomputers to run our serial linear stability code. This small variation in continuous with changes in grid points is shown in the supplementary Sec. 6.6.4.

The stationary ($\Omega_r = 0$) and traveling continuum modes on these branches are denoted with capital letters $S^{(\text{label})}$ and $T_{\Omega_r}^{(\text{label})}$, respectively, where subscript Ω_r indicates the nondimensional frequency of the traveling mode and superscript ‘(label)’ denotes the branch label. For example, a traveling continuum mode T_3'' , indicated in the figure, represents a mode located closest to the vertical line at $\Omega_r = 3$ on branch u. Also, the continuous branches are sufficiently resolve such that the stationary continuum mode S'' has a zero frequency up to four decimals ($\Omega_r < 10^{-4}$).

At $Ma = 1.2$, Fig. 6.6 shows that both formulations predict highly damped modes with similar decay rates. Table 6.5 lists the decay rates of continuum mode S'' obtained from both formulations at the three Mach numbers, where it can be seen that at $Ma = 1.2$, the difference between the two formulations is only a 2%, which can be attributed to small differences in the constitutive equations. Specifically, the constitutive equation for τ^m in the ACE formulation includes an extra factor of $\rho^* T_1^* / (\rho_1^* T^*)$ and parameters $A_a = 1.3104$ and $A_b = -0.6552$ compared to the constitutive equation in the NSE formulation, which uses $A_a = 1.3333$ and $A_b = -0.6666$, respectively. Also, the model for q_x^m used in ACE (Eq. 6.30) is different from the Fourier’s law used for q_x^n in the NSE, as discussed in Sec. 6.3.2.

In contrast, the comparison of branch u at higher Mach numbers reveals a number of notable differences. An immediate observation from Fig. 6.6 and Table 6.5 is that both formulations predict significantly less damped eigenmodes with increase in Mach number, indicating *longer decay of harmonic perturbations to stronger shocks*. This behavior is related to the increasing degree of translational nonequilibrium with Mach number (Fig. 6.3(b)), as discussed next.

Table 6.5 shows that ACE predicts ~ 45 and $\sim 70\%$ smaller magnitudes of decay rates (slower decay) than NSE at $Ma = 3$ and 5, respectively. This increasing difference is a consequence of the capability of ACE in resolving the

increasingly larger regions of translational nonequilibrium in stronger shocks, as shown in Fig. 6.3(d) by the difference in transport flow quantities at $Ma = 5$. This capability of ACE can be mainly attributed to increasing magnitudes of constants A_a and A_b used in the constitutive equation of τ^m . For example, Table 6.2 shows that the values of these constants used in ACE are 5.973 and 2.9869, respectively, at $Ma = 5$, as opposed to 1.3333 and 0.6666, used in NSE. In fact, when we repeat the analysis with ACE at $Ma = 5$ and $\beta = \beta_{ulim}$ by artificially imposing the latter (NSE) values for these constants, we obtain an interesting result that branch u becomes almost as stable as that predicted by NSE, as shown in Fig. 6.6. This calculation increases the decay rate of S'' predicted by ACE from -0.38 to -1.24 , the latter value is only 0.8% larger than the decay rate of -1.25 predicted by NSE. This finding shows that a better resolution of noncontinuum effects in a shock layer leads to lower magnitudes of decay rates, that is, slower decay of perturbations, and supports our claim that the decay time is directly proportional to the amount of translational nonequilibrium in a shock layer.

Returning to the comparison of decay rates at $Ma = 1.2$, the reason that ACE predicts 2% larger magnitude of decay rate than NSE is due to a slightly lower magnitudes of constants A_a and A_b used in the ACE than NSE (see Table 6.2). Furthermore, it also becomes clear as to why when we increase the Mach number from 3 to 5, the magnitude of decay rate of S'' predicted by ACE decreases by $\sim 54\%$, compared to only $\sim 17\%$ predicted by NSE, as seen from Table 6.5. This larger difference in ACE is again due to a better resolution of the increasingly larger region of translational nonequilibrium with Mach number by ACE than NSE. In summary, the above numerical observations show that increase in the degree of translational nonequilibrium with Mach number and the better constitutive functions lead to the prediction of slower decay of perturbations.

Next, we study the shape of eigenfunction of mass density, $\hat{\rho}_r$, obtained from the NSE formulation at $Ma = 1.2$ and $\beta = \beta_{ulim}$ in Figs. 6.7(a) and 6.7(b) for stationary and traveling continuum modes S'' and T_3'' , respectively. It is seen that both eigenfunctions decay gradually over a much larger distance ($\sim 25L_s$) upstream of the shock layer compared to the downstream ($\sim 5L_s$), while the decay behavior of the S'' is monotonic whereas that of T_3'' is sinusoidal.

To understand this asymptotic variation of eigenfunctions, *i.e.* as $x \rightarrow \pm\infty$, we simplify the normal mode equations in the far field of the shock layer, as discussed in the supplementary Sec. 6.6.5, and solve analytically for the amplitude functions $\hat{\mathcal{P}} = [\hat{\rho}, \hat{u}_x, \hat{u}_y, \hat{T}]^T$ in terms of Ω_r , Ω_i , γ , Ma , Re , β , and far field flow quantities ρ_k , $u_{x,k}$, and T_k , where $k = 1$ and 2 refer to upstream and downstream flow quantities. A solution proportional to $\exp(\alpha x)$ is assumed [see Eq. (6.97)], where α_n are characteristic values governing the far field behavior of the amplitude functions. This procedure results in a characteristic equation of seventh order in α_n , denoted as $\mathcal{S} = 0$ [see Eq. (6.102)], having seven characteristic solutions α_1 to α_7 , governing the asymptotic variation eigenfunctions. However, only those characteristic values for which the eigenfunctions decay to zero as $x \rightarrow \pm\infty$ are physical. This implies that the real part of α_n ,

denoted as $\alpha_{n,r}$, must be positive for upstream conditions and negative for downstream conditions [see Eqs. (6.98) and (6.99)]. Also, if the imaginary part $\alpha_{n,i}$ is nonzero then the eigenfunction exhibits sinusoidal spatial oscillations.

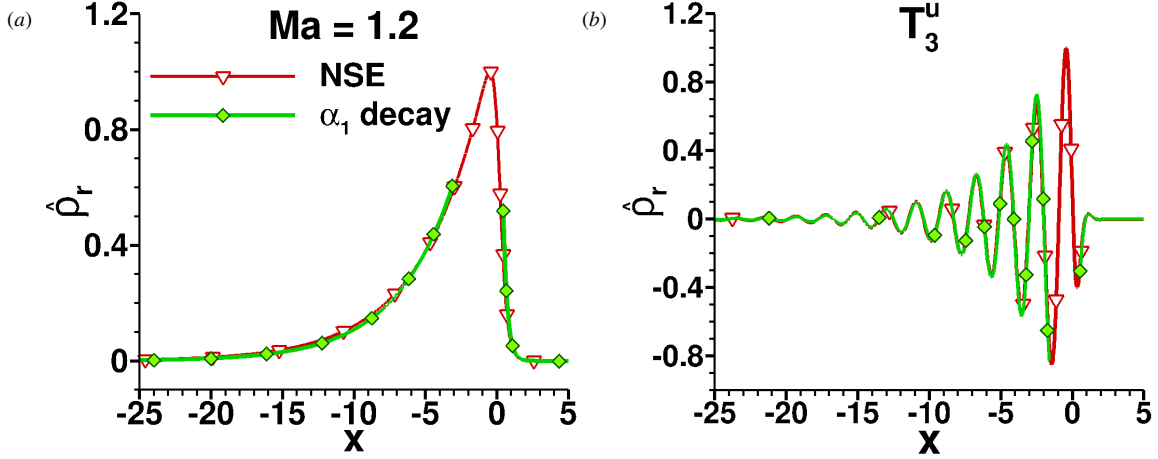


Figure 6.7: At $Ma = 1.2$ and $\beta = \beta_{ulim}$, comparison of $\hat{\rho}_r$ obtained from the NSE normal mode equations with the far field decay solution governed by the α_1 characteristic value for continuum eigenmodes S'' in (a) and T_3^u in (b).

The seven characteristic values for continuum modes S'' and T_3^u at $Ma = 1.2$ and $\beta = \beta_{ulim}$ are listed in Table 6.6, where boldened entries indicate physically possible values of α_n . Interestingly, only α_1 is acceptable in both the streams, while other characteristic values fail to satisfy the condition that the eigenfunction decays in both far fields. Similar behavior was observed at other Mach numbers, as seen from Table 6.7 for $Ma = 5$ and $\beta = \beta_{ulim}$. Using the value of α_1 , the far field behavior of the real part of amplitude functions, $\hat{\rho}_r$, can be predicted as

$$\hat{\rho}_r = \exp[\alpha_{1,r}(x - x_{ref})] \left\{ \hat{\rho}_{r,ref} \cos[\alpha_{1,i}(x - x_{ref})] + \hat{\rho}_{i,ref} \sin[\alpha_{1,i}(x - x_{ref})] \right\} \quad (6.52)$$

where $\hat{\rho}_{r,ref}$ and $\hat{\rho}_{i,ref}$ are the reference values obtained from the solution of normal mode equations at any location x_{ref} in the far field of the shock layer. Figure 6.7 shows excellent comparison of $\hat{\rho}_r$ obtained from the linear stability analysis at $Ma = 1.2$ and $\beta = \beta_{ulim}$ with the far field solution, labeled as ' α_1 decay', indicating that the shape of these eigenfunctions is indeed governed by the only physical characteristic value α_1 , which exhibits decay on either sides of the shock layer. Good comparisons were also found for other Mach numbers and eigenfunctions (not shown).

From this analysis, we can now see from Table 6.6 that the real part $\alpha_{1,r}$ is an order of magnitude lower in the upstream for both continuum modes S'' and T_3^u , and therefore, in Fig. 6.7, we see a gradual spatial decay of eigenfunctions in the upstream direction than the downstream. Also, since the imaginary part $\alpha_{1,i}$ is zero for S'' , its eigenfunction decays monotonically. On the other hand, Tables 6.6 and 6.7 show that the α_1 characteristic value for the traveling continuum mode T_3^u exhibits an imaginary part $\alpha_{1,i}$ equal to $\Omega_r = 3$ in the upstream. As a result, the far field

behavior of amplitude functions of T_3^u is sinusoidal, and it agrees exactly with the predictions of linear stability analysis, as shown in Fig. 6.7(b) for $Ma = 1.2$ and $\beta = \beta_{ulim}$. It can be seen that $\alpha_{1,i} = \Omega_r$ in the upstream for $Ma = 1.2$ as well as 5, which indicates an interesting fact that with increase in the frequency (Ω_r) of a traveling continuum mode $T_{\Omega_r}^u$, the spatial wavelength of sinusoidal oscillations of eigenfunctions would decrease. This behavior is indeed found to be true, as described in Sec. 6.6.4, which makes it harder to resolve the structure of higher frequency traveling modes, and as a result, branch u eventually splits into two branches, $u+$ and $u-$.

α_n	S^u		T_3^u	
	upstream	downstream	upstream	downstream
α_1	0.250	-3.495	0.240 + i 3.000	-3.508 + i 3.894
α_2	159.5	157.5	159.5 - i 0.187	157.5 - i 0.198
α_3	163.7	161.8	163.8 - i 0.238	161.8 - i 0.263
α_4	-140.2 + i 1.742	-141.7 + i 2.083	-140.2 + i 1.955	-141.7 + i 2.314
α_5	-140.2 - i 1.742	-141.7 - i 2.083	-140.2 - i 1.530	-141.6 - i 1.852
α_6	-135.6	-137.8	-135.6 + i 0.309	-137.8 + i 0.337
α_7	166.7	163.9	166.8 - i 0.309	163.9 - i 0.337

Table 6.6: For continuum modes S^u and T_3^u at $Ma = 1.2$ and $\beta = \beta_{ulim}$, seven characteristic values of α_n governing the decay of eigenfunctions in far fields of a shock layer.

α_n	S^u		T_3^u	
	upstream	downstream	upstream	downstream
α_1	0.133	-10.07	0.173 + i 3.000	-9.90 + i 10.81
α_2	40.86	39.91	40.86 - i 0.082	39.91 - i 0.034
α_3	67.17	41.55	67.18 - i 1.516	41.53 - i 0.663
α_4	-38.69	-39.66	-38.70 + i 0.082	-39.67 + i 0.034
α_5	-22.02	-35.63	-22.04 - i 1.516	-35.69 - i 0.570
α_6	-19.05	-36.10	-19.06 + i 1.834	-36.10 + i 0.939
α_7	79.20	43.03	79.22 - i 1.836	43.03 - i 0.939

Table 6.7: For continuum modes S^u and T_3^u at $Ma = 5$ and $\beta = \beta_{ulim}$, seven characteristic values of α_n governing the decay of eigenfunctions in far fields of a shock layer.

Turning to the discussion of how we obtained the solution of characteristic values presented in Tables 6.6 and 6.7, note that it is possible to obtain general solutions for only two of the seven roots, α_6 and α_7 , as shown in Eqs. (6.110) and (6.111) of Sec. 6.6.5, by separating a quadratic factor $\mathcal{T}$ of the septic polynomial $\mathcal{S} = 0$ (see Eq. (6.103)). The remaining quintic polynomial $\mathcal{F}$ (Eq. 6.104) was found to be too difficult to factorize, and therefore, was solved numerically to obtain α_1 to α_5 for specified values of γ , Re , Ma , β , Ω_r , Ω_i , and the far field flow quantities for the two continuum modes discussed. More importantly, it is also shown in Eq. (6.108) of supplementary Sec. 6.6.5 that it is possible to obtain an approximate solution α_1^{appx} of $\mathcal{F} = 0$, if we ignore the higher order terms of the polynomial

Ma	Parameter	S''		T_3''	
		upstream	downstream	upstream	downstream
1.2	α_1	0.250	-3.495	0.240 + i 3.000	-3.508 + i 3.894
	α_1^{appx}	0.250	-3.462	0.223 + i 3.003	-3.499 + i 3.849
	$\mathcal{M}$	0.047%	0.546%	0.037% + i 0.569%	0.559% + 0.601%
5	α_1	0.133	-10.07	0.173 + i 3.000	-9.90 + i 10.81
	α_1^{appx}	0.133	-9.662	-0.112 + i 2.981	-9.879 + i 9.968
	$\mathcal{M}$	0.427%	3.387%	2.086% - i 9.293%	5.019% - 2.562%

Table 6.8: Comparison of the approximate solution α_1^{appx} with numerically computed value of α_1 and the relative magnitude $\mathcal{M}$, defined in Eq. (6.108), for continuum modes S'' and T_3'' at $\beta = \beta_{\text{ulim}}$ and $Ma = 1.2, 5$. Boldened entries indicate physically possible values of α_n .

$O(\chi_l(\alpha_n)^l)$ for $l \geq 2$, *i.e.* if the condition in Eq. (6.106) is met, where coefficients χ_l are defined in Eq. (6.105). This solution is shown in Table 6.8 for both continuum modes S'' and T_3'' at $Ma = 1.2, 5$ and $\beta = \beta_{\text{ulim}}$, and is compared with the numerical solution of α_1 .

We see that for the stationary continuum mode, α_1^{appx} is an excellent approximation to α_1 , as it predicts the same value in the upstream for both Mach numbers and is about 0.94 and 4% different in the downstream for $Ma = 1.2$ and 5, respectively. The slightly larger difference of 4% at $Ma = 5$ in the downstream can be understood by looking at the ratio $\mathcal{M}$ of the sum of higher order terms with the first order term of $\mathcal{F}$, as defined in Eq. (6.108) and shown in Table 6.8. For S'' , this ratio is ~ 0.05 and 0.5% for the up and downstream conditions at $Ma = 1.2$, respectively, and $\sim 0.4\%$ for the upstream conditions at $Ma = 5$. However, for the downstream conditions at $Ma = 5$, $\mathcal{M}$ is $\sim 3.4\%$, suggesting that we obtain larger difference in the numerical and approximate solutions when $\mathcal{M}$ is larger. For T_3'' at $Ma = 1.2$, the predictions of the approximate solution are still acceptable, however, at $Ma = 5$ the approximate solution does not predict a decaying solution for the upstream conditions. This is mainly because the sum of the imaginary parts of higher order terms that were ignored in the approximation is 9% of the imaginary part of the first order term in $\mathcal{F}$, suggesting that our assumption is no longer valid. Based on these comparisons, we can state with certainty that when $\mathcal{M}$ is lower than 1%, the approximate solution α_1^{appx} is an excellent approximation to α_1 .

Since for the stationary continuum mode, α_1^{appx} was found to be an excellent approximation to α_1 , we can plot its variation with Ω_i for up and downstream conditions to determine the possible values of Ω_i for which α_1^{appx} is physically acceptable. Answering this question may hold clues to the primary question that was raised in this section, *i.e.* how does Ω_i vary with Ma , Re , β , γ , and far field flow quantities. Variation of α_1^{appx} with Ω_i is shown for $\beta = \beta_{\text{ulim}}$ and $Ma = 1.2$ and 5 in Figs. 6.8(a) and 6.8(b), respectively. It is seen that for specified values of γ , Ma , Re , and β , we should expect a physically acceptable solution of eigenfunctions for a *range* of Ω_i values, such that $\alpha_{1,r}^{\text{appx}}$ is positive in

the upstream and negative in the downstream allowing spatial decay of perturbations in both far fields. This range is $-12.7 < \Omega_i < -9.7$ and $-4.1 < \Omega_i < -1.13$ for $Ma = 1.2$ and 5, respectively. Indicating on these plots, the decay rate of the least stable continuum mode S^u of -10.04 and -1.25 for $Ma = 1.2$ and 5, respectively (see Table 6.5), we see that the linear stability solver predicts a least damped decay rate in the vicinity of the maximum possible value of Ω_i . It is also seen that both up and downstream solutions have a negative slope and as Ω_i decreases, the magnitude of α_1^{appx} increases in the upstream and decreases in the downstream based on Eq. (6.108), which means eigenfunctions will decay faster in the upstream and slower in the downstream direction for more stable continuum modes. It will be shown in Sec. 6.4.2 that the linear stability analysis also predicts a lower branch, 'l', having a stationary continuum mode S^l , whose decay rate is closer to the lower physically possible limit of Ω_i .

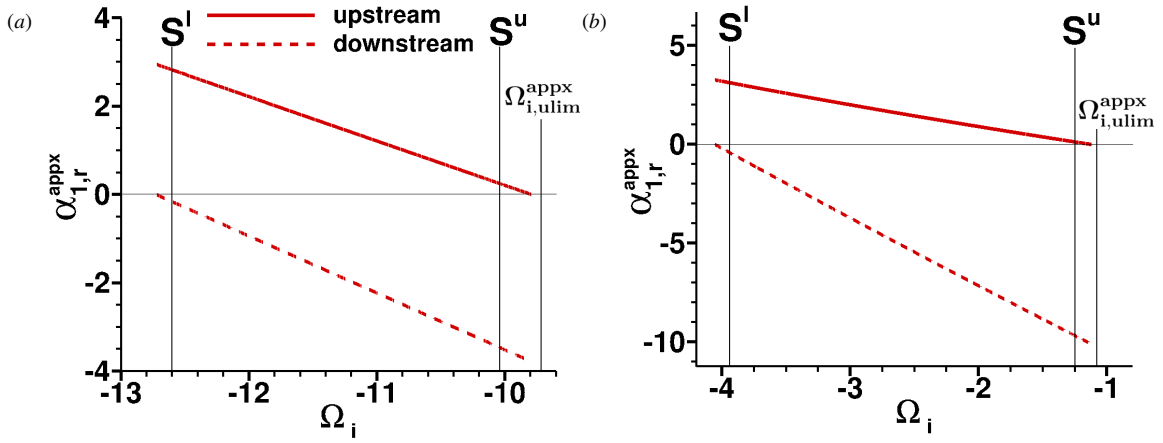


Figure 6.8: Variation of $\alpha_{1,r}^{\text{appx}}$ as a function of decay rate Ω_i at $\beta = \beta_{\text{ulim}}$ and $Ma = 1.2$ in (a) and $Ma = 5$ in (b).

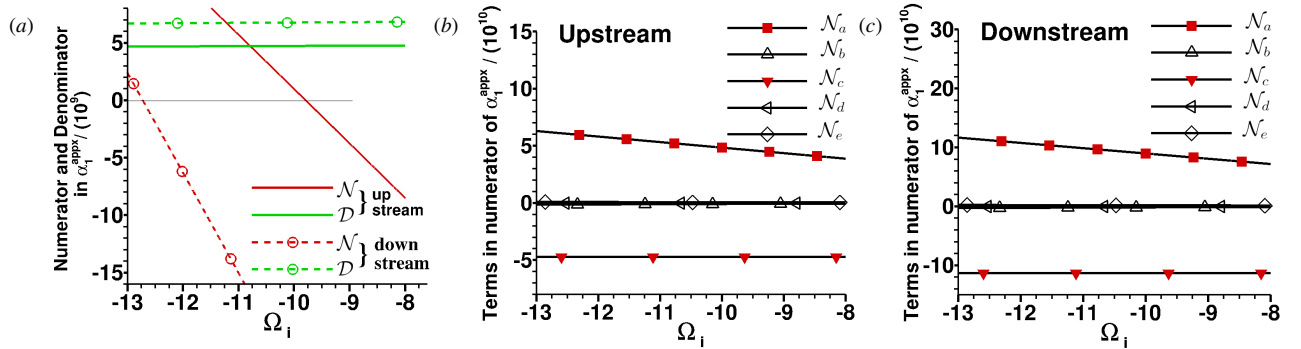


Figure 6.9: At $Ma = 1.2$ and $\beta = \beta_{\text{ulim}}$, comparisons of the numerator $\mathcal{N}$ and denominator $\mathcal{D}$ in the expression of $\alpha_{1,r}^{\text{appx}}$ in the up and downstreams are shown in (a). Comparison of individual terms $\mathcal{N}_a$ to $\mathcal{N}_e$ for the up and downstreams are shown in (a) and (b), respectively.

Since the range of Ω_i observed in Fig. 6.8 varies significantly from $Ma = 1.2$ to 5, we may ask what parameters

such as γ, Re, Ma, β and far field flow quantities, do the limits of this range depend on? Since continuum mode S'' obtained from linear stability analysis is in the proximity of the upper limit of Ω_i , by answering the above question, we will, in turn, be able to understand how does the least stable decay rate vary with the governing parameters of the problem. Here we only find approximate expression for the limits of range Ω_i . The lower and upper limits are denoted as $\Omega_{i, \text{llim}}^{\text{appx}}$ and $\Omega_{i, \text{ulim}}^{\text{appx}}$, respectively. Figure 6.9(a) shows the numerator and denominators, $\mathcal{N}$ and $\mathcal{D}$, respectively, defined in Eq. (6.108) in the expression for α_1^{appx} , for both stream conditions at $Ma = 1.2$ and $\beta = \beta_{\text{ulim}}$. It is seen that the denominator is positive for all values Ω_i shown, while only the numerator changes sign, resulting in the sign change of α_1^{appx} . This is true for $Ma = 5$ as well (not shown). We can now compare the individual terms of the numerator, *i.e.* $\mathcal{N}_j$ for $j = a$ to e , defined in Eq. (6.109), for up and downstream conditions, as shown in Figs. 6.9(b) and 6.9(c), respectively. For both streams, terms $\mathcal{N}_a$ and $\mathcal{N}_c$ have a comparable magnitude, but they are higher by at least an order than the other terms, $\mathcal{N}_b, \mathcal{N}_d$, and $\mathcal{N}_e$. This is found to be true even for $Ma = 5$ (not shown). If we ignore these small terms and set α_1^{appx} equal to zero, *i.e.* $\mathcal{N}_a + \mathcal{N}_b \approx 0$, we obtain

$$-Ma^2\beta^4(\gamma - 1)(4Ma^2\gamma\Omega_{i, \text{ulim}}^{\text{appx}} + 3Re) = 0, \quad k = 1 \text{ (upstream)} \quad (6.53)$$

$$-r_\rho Ma^2\beta^4(\gamma - 1)r_t^{2\omega}(4Ma^2\gamma\Omega_{i, \text{llim}}^{\text{appx}} + 3Re r_t^{1-\omega}r_\rho) = 0, \quad k = 2 \text{ (downstream)} \quad (6.54)$$

Solving these equations, we obtain a first order approximation to the limits of Ω_i as

$$\Omega_{i, \text{ulim}}^{\text{appx}} = -\frac{3Re}{4Ma^2\gamma} \quad (6.55)$$

$$\Omega_{i, \text{llim}}^{\text{appx}} = -\frac{3Re r_t^{1-\omega}r_\rho}{4Ma^2\gamma} \quad (6.56)$$

The simple equation for the upper limit give us valuable insights into the decay rate of S'' . First, it shows that the stationary continuum mode will always decay. Next, the Ma^2 in the denominator shows that the higher the Mach number, the slower the decay of perturbation. This clarifies our earlier observation of the continuous branch u becoming less stable with increase in Mach number, as seen in Table 6.2. Also, the Reynolds number, Re , in the numerator shows that increase in the viscosity would lead to the longer decay of perturbations. However, it must be noted that for the 1-D shock layer, Reynolds number varies with Mach number and we cannot change Reynolds number by keeping the Mach number constant. To understand this relationship, Reynolds number can be written as

$$Re = \frac{\rho_1^* u_{x,1}^* L_s^*}{\mu_1^*} = \frac{\rho_1^* Ma \sqrt{\gamma R T_1^*} L_s^*}{C (T_1^*)^\omega} = \frac{Ma \sqrt{\gamma R}}{C} \frac{\rho_1^* L_s^*}{(T_1^*)^{\omega-0.5}} \quad (6.57)$$

where we have expressed the upstream velocity in terms of the Mach number and used the definition of dynamic

viscosity from Eq. (6.2). Next we note that the ratio $\mathcal{L}$ of shock-thickness L_s^* to the upstream mean-free-path,

$$\lambda_1^* = \frac{m(T_1^*)^{\omega-0.5}}{\sqrt{2}\pi d_{\text{ref}}^2 \rho_1^* (T_{\text{ref}}^*)^{\omega-0.5}} \quad (6.58)$$

varies with Mach number, as shown in Fig. 6.10, and write Eq. (6.57) as

$$Re = Ma \mathcal{L} \frac{\sqrt{\gamma R}}{C} \frac{\rho_1^*}{(T_1^*)^{\omega-0.5}} \lambda_1^* = Ma \mathcal{L} \frac{m \sqrt{\gamma R}}{C \sqrt{2}\pi d_{\text{ref}}^2 (T_{\text{ref}}^*)^{\omega-0.5}} \quad (6.59)$$

This equation shows that $Re \propto Ma \mathcal{L}$, and therefore, Re cannot be varied by keeping Ma constant. Furthermore, if we make a crude piecewise linear approximation and express $\mathcal{L} = a + bMa$, where the y-intercept a and slope b are indicated in Fig. 6.10 for $Ma = 1.2$ to 2 , 2 to 3 , and 3 to 7 , we can write $Re \propto aMa + bMa^2$ and see that $\Omega_{i,\text{ulim}}^{\text{appx}}$ remains inversely proportional to Ma .

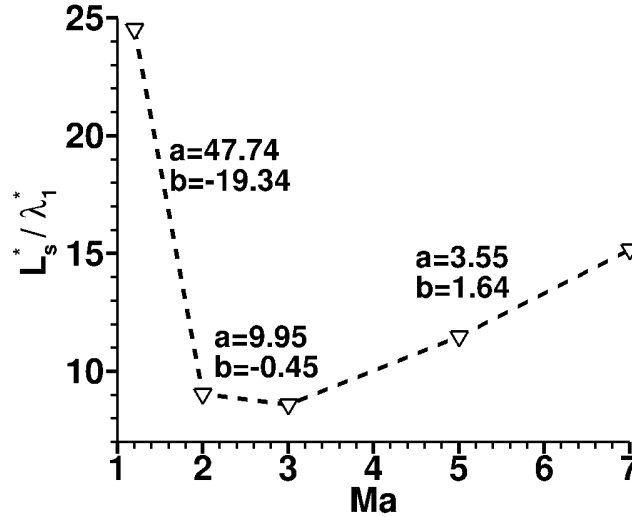


Figure 6.10: Variation of $\mathcal{L} = L_s^*/\lambda_1^*$ with upstream Mach number for argon shocks simulated with DSMC for $\omega = 1$.

Interestingly, we also see a factor of $4/3$ in the denominator of the above equations, which appears because the value of the function ϕ in the normal mode equations obtained from the NSE formulation (see Table 6.3) is equal to $\phi_1 = -4/(3Re)$ in the upstream far field (see Eq. (6.90)). If we had used the general constitutive equation for stress tensor of the ACE formulation (see Eq. (6.27)), we would have obtained the factor A_a in place of $4/3$, as seen from the definition of function ϕ for ACE in Table 6.3. Furthermore, it was shown in Fig. 6.5(a) that A_a reduces to $4/3$ at $M \leq 1.4$, but increases substantially at higher Mach numbers. Therefore, having A_a in the denominator of Eq. (6.55) instead of $4/3$ would mean that as the Mach number increases with the degree of translational nonequilibrium, we will obtain a slower decay of perturbations. This is also consistent with the results seen earlier in Table 6.3 that shows that

ACE predicts a less stable continuum mode than NSE. It must be noted that the above approximation where $\mathcal{N}_b$, $\mathcal{N}_d$, and $\mathcal{N}_e$ terms are neglected is only valid for large values of β , and that $\Omega_{i,\text{ulim}}^{\text{appx}}$, and consequently S'' , varies with β as well when β is substantially smaller than β_{ulim} , as discussed at the end of this section. In this case, the equation for $\Omega_{i,\text{ulim}}^{\text{appx}}$ will be more complicated.

Next, we look at the comparison of the real parts of eigenfunctions of mass density $\hat{\rho}_r$, x - and y -directional bulk velocities, $\hat{u}_{x,r}$ and $\hat{u}_{y,r}$, respectively, and temperature T_r of S'' obtained from the two formulations shown respectively in Figs. 6.11(a)–6.11(d) for $Ma = 1.2$, Figs. 6.11(e)–6.11(h) for $Ma = 3$, and Figs. 6.11(i)–6.11(l) at $Ma = 5$. The imaginary parts of these eigenfunctions are qualitatively similar, and hence, are not shown here. The eigenfunctions obtained from ACE and NSE formulations agree well at $Ma = 1.2$, as expected from the low degree of translational nonequilibrium, shown earlier in Fig. 6.3(b). On the other hand, with increase in Mach number, the differences between the two formulations increase, not only in the shock layer but also in the far field. These differences are a direct consequence of increasing difference in the transport flow quantities predicted by the two formulations, as shown in Fig. 6.3(d).

Turning to the traveling continuum mode T_3'' , we saw in Fig. 6.7(b) that the slower decay of eigenfunction on the upstream side was due to the real part of characteristic value, $\alpha_{1,r}$, being an order of magnitude lower in the upstream than the downstream. Now we show the comparison of a sample eigenfunction $\hat{u}_{y,r}$ for T_3'' obtained from the two formulations in Figs. 6.12(a), 6.12(b), and 6.12(c) for $Ma = 1.2$, 3, and 5, respectively. At $Ma = 1.2$, the eigenfunctions predicted by both formulations have the same spatial dependence in their amplitude, phase and wavelength of sinusoidal oscillations, however, with increase in Mach number, differences are seen in the amplitude and phase predicted by the two formulations, while their wavelengths are found to be the same. The similarity of wavelength indicates that characteristic value $\alpha_{1,i}$ must be the same for both of the formulations, while the differences in amplitude and phase could originate from inside the shock layer ($-1 \leq x \leq 1$). In terms of the qualitative differences in amplitude, ACE predictions are larger for $\hat{\rho}_r$ and $\hat{T}_r$ and smaller for $\hat{u}_{x,r}$, $\hat{u}_{y,r}$ than NSE, while the differences between the two formulations increase with Mach number (here, only shown for $\hat{\rho}_r$).

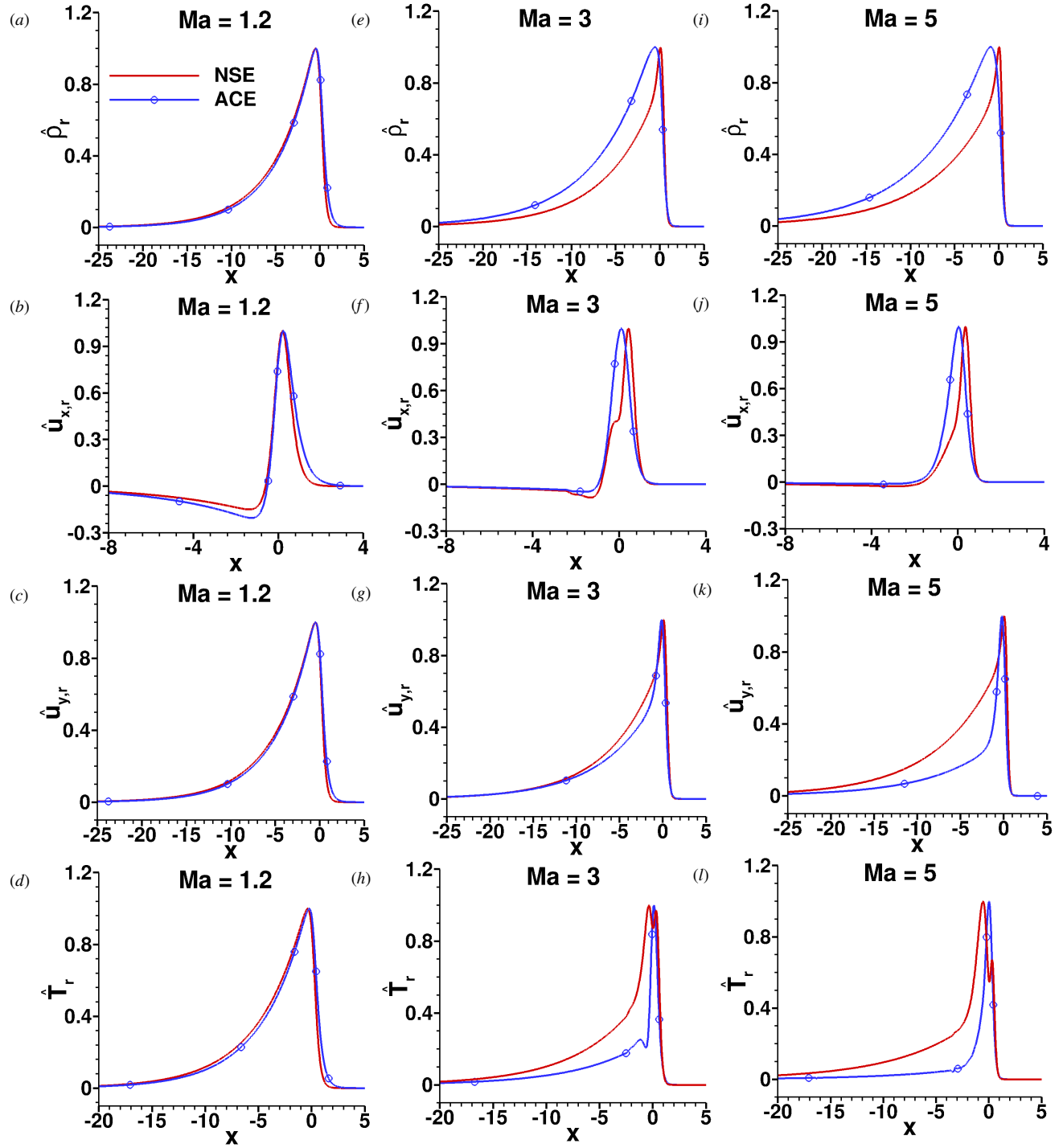


Figure 6.11: For continuum mode S^u , comparison of real parts of eigenfunctions obtained from the NSE and ACE formulations. $\hat{\rho}_r$, $\hat{u}_{x,r}$, $\hat{u}_{y,r}$, and $\hat{T}_r$ are shown in (a)–(d) for $Ma = 1.2$, (e)–(h) for $Ma = 3$, and (i)–(l) for $Ma = 5$.

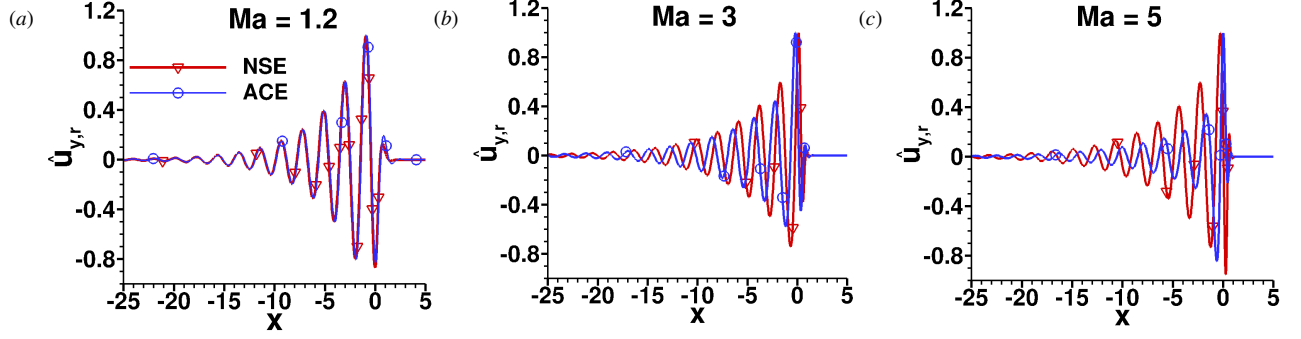


Figure 6.12: For T_3^u , comparison of real parts of eigenfunctions obtained from the NSE and ACE formulations. $\hat{u}_{y,r}$ is shown for $Ma = 1.2$ in (a), $Ma = 3$ in (b), and $Ma = 5$ in (c).

Finally, we look at the variation in decay rates of S'' obtained from linear stability analyses performed at β lower than β_{ulim} , that is, perturbation wavelength L_y^* larger than $\bar{\lambda}_{\text{max}}^*$, such that the ratio $L_y^*/\bar{\lambda}_{\text{max}}^*$ is increased from 1 to ~ 4 . The variations in decay rates at $Ma = 1.2$ are shown in Fig. 6.13(a), while those at $Ma = 3$ and 5 are shown Fig. 6.13(b). At $Ma = 1.2$, as $L_y^*/\bar{\lambda}_{\text{max}}^*$ increases, *i.e.* β decreases, continuum modes become slightly more stable, and the variation in Ω_i increases. This could be understood as follows. We showed in Eq. (6.55) that our first order approximation for the upper limit of Ω_i , *i.e.* $\Omega_{i,\text{ulim}}^{\text{appx}}$, and as a result the decay rate of S'' , does not depend on β . We had made this approximation by ignoring terms $\mathcal{N}_b$, $\mathcal{N}_d$ and $\mathcal{N}_e$ in comparison to terms $\mathcal{N}_a$ and $\mathcal{N}_b$ in Eq. (6.108) for α_1^{appx} . However, this assumption breaks down for lower β values, and it was found that except for $\mathcal{N}_d$, all terms have a comparable magnitude, which causes a dependence of Ω_i on β . Furthermore, the comparison of the two formulations shows that the ACE formulation remains 2% lower than NSE, as was observed at $L_y^* = \bar{\lambda}_{\text{max}}^*$.

At higher Mach numbers, the ACE formulation predicts nearly similar decay rates for all perturbation wavelengths studied, while the NSE formulation predicts that the continuum modes become more stable with increase in L_y^* . As a result, the difference between the two formulations increases with increase in $L_y^*/\bar{\lambda}_{\text{max}}^*$. Furthermore, the eigenfunctions at lower β values have similar shapes as at $\beta = \beta_{\text{ulim}}$, meaning that they belong to the same family of continuum modes. This is shown in Fig. 6.13(c) for S'' obtained from ACE at $Ma = 5$. A similar behavior is observed for traveling continuum modes in the proximity of S'' .

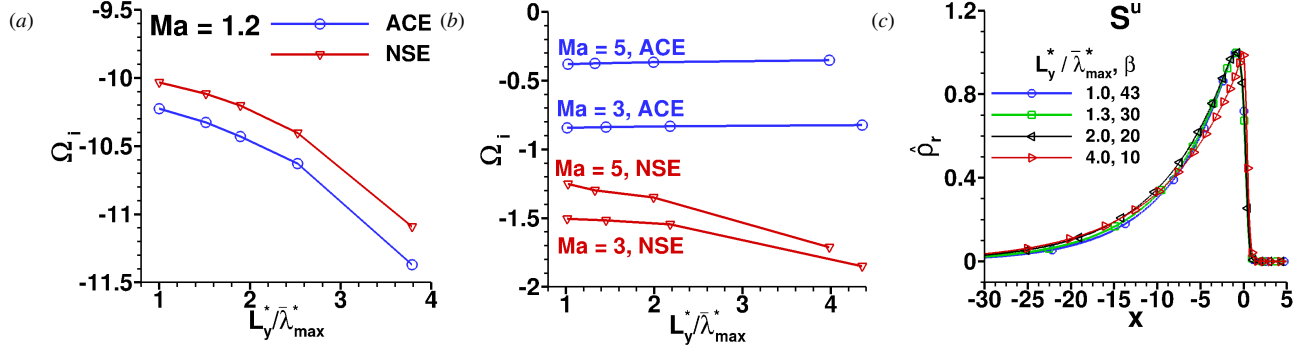


Figure 6.13: The variation of decay rates of S'' , obtained from the ACE and NSE formulations as a function of perturbation wavelength L_y^* , normalized by maximum mean-free-path $\bar{\lambda}_{\max}^*$, for $Ma = 1.2$ in (a) and $Ma = 3$ and 5 in (b) Comparison of eigenfunctions for S'' at $Ma = 5$ for different β values is shown in (c).

6.4.2 Comparison of continuum modes of the damped continuous branch 'l'

Until now we looked at eigenfunctions of the least damped branch u , which decay gradually upstream of the shock layer rather than the downstream. Now we show that there exists a branch 'l', more damped than branch u , whose eigenfunctions decay gradually downstream of the shock layer and rapidly upstream of it. Continuous l-branches obtained from both formulations at the three Mach numbers and $\beta = \beta_{\text{ulim}}$ are shown in Fig. 6.14, marking the locations of the stationary and traveling continuum modes S^l and T_3^l , respectively. The decay rates of these modes are listed in Table 6.9 and their eigenfunctions $\hat{\rho}_r$, obtained from the NSE formulation, are shown in Fig. 6.15, where S^l and T_3^l are seen to exhibit spatial decay behavior that is monotonic and sinusoidal, respectively.

It turns out that the spatial decay behaviors of these continuum modes are also governed by the α_1 characteristic value out of the seven solutions of the far field septic polynomial, listed in Table 6.10. The good comparison of the analytical solution obtained using α_1 characteristic value in Eq. (6.52) and the solution obtained from linear stability analysis using the NSE formulation is shown in Figs. 6.15(a) and 6.15(b) for the stationary and traveling modes, respectively. For continuum modes S^l and T_3^l , $\alpha_{1,r}$ is an order of magnitude larger upstream than the downstream, which explains their gradual decay downstream, while $\alpha_{1,i}$ is zero for S^l and nonzero for T_3^l , which explains the monotonic and sinusoidal decay behavior of these eigenfunctions, respectively.

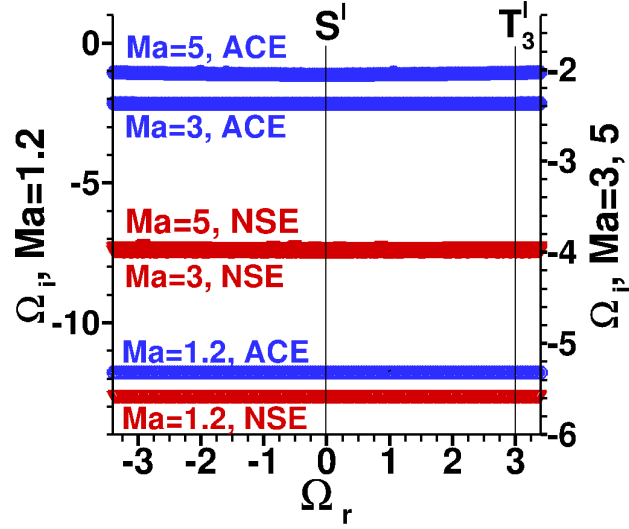


Figure 6.14: Comparison of continuous branch I in the eigenspectra obtained from the ACE and NSE formulations at $\beta = \beta_{ulim}$ and $Ma = 1.2, 3$, and 5 .

Ma	S^I		T_3^I	
	ACE	NSE	ACE	NSE
1.2	-11.78	-12.60	-11.77	-12.59
3	-2.38	-3.99	-2.37	-3.98
5	-2.05	-3.94	-2.03	-3.94

Table 6.9: Decay rate, Ω_i , for S^I and T_3^I on branch I obtained from the ACE and NSE formulations.

Furthermore, the approximate solution α_1^{appx} , obtained using Eq. (6.108) is also a good approximation to α_1 for both stationary and traveling continuum modes, as shown in Table 6.11. Earlier in Fig. 6.8, the variation of α_1^{appx} with Ω_i was shown, where a range of Ω_i was established for which α_1^{appx} exhibits values that are physically acceptable in both streams. In this figure, it is also seen that the growth rate of S^I is very close to the lower limit, $\Omega_{i,lim}^{appx}$ (Eq. (6.56)), as shown earlier in Fig. 6.8. At this lower limit, since α_1^{appx} in the upstream is an order of magnitude larger than the downstream, we see slower spatial decay in the downstream. A first order approximation for this lowest limit of Ω_i can be obtained using Eq. (6.56), which shows that it varies directly with Re and the density ratio across the shock r_ρ , inversely with the square of Ma and exhibits a factor of $4/3$ in the denominator which comes from the constitutive equation for the NSF equations in the NSE formulation.

α_n	S^l		T_3^l	
	upstream	downstream	upstream	downstream
α_1	2.810	-0.161	2.810 + i 3.000	-0.161 + i 3.892
α_2	159.4	157.4	159.4 - i 0.187	157.4 - i 0.197
α_3	163.6	161.6	163.6 - i 0.238	161.6 - i 0.265
α_4	-140.0 + i 1.752	-141.5 + i 2.100	-140.0 + i 1.965	-141.5 + i 2.331
α_5	-140.0 - i 1.752	-141.5 - i 2.100	-140.0 - i 1.539	-141.4 - i 1.869
α_6	-135.3	-137.5	-135.3 + i 0.310	-137.5 + i 0.337
α_7	166.5	163.6	166.5 - i 0.310	163.6 - i 0.337

Table 6.10: For S^l and T_3^l at $Ma = 1.2$ and $\beta = \beta_{ulim}$, seven characteristic values of α_n governing the decay of eigenfunctions in far fields of a shock layer.

Ma	Parameter	S^l		T_3^l	
		upstream	downstream	upstream	downstream
1.2	α_1	2.810	-0.161	2.810 + i 3.000	-0.161 + i 3.892
	α_1^{appx}	2.825	-0.161	2.797 + i 3.032	-0.198 + i 3.890
	$\mathcal{M}$	0.538%	0.026%	0.529% - i 0.581%	0.037% - 0.619%

Table 6.11: Comparison of the approximate solution, α_1^{appx} , with numerically computed value of α_1 and the relative magnitude $\mathcal{M}$, defined by Eq. (6.108), for S^l and T_3^l at $\beta = \beta_{ulim}$ and $Ma = 1.2$.

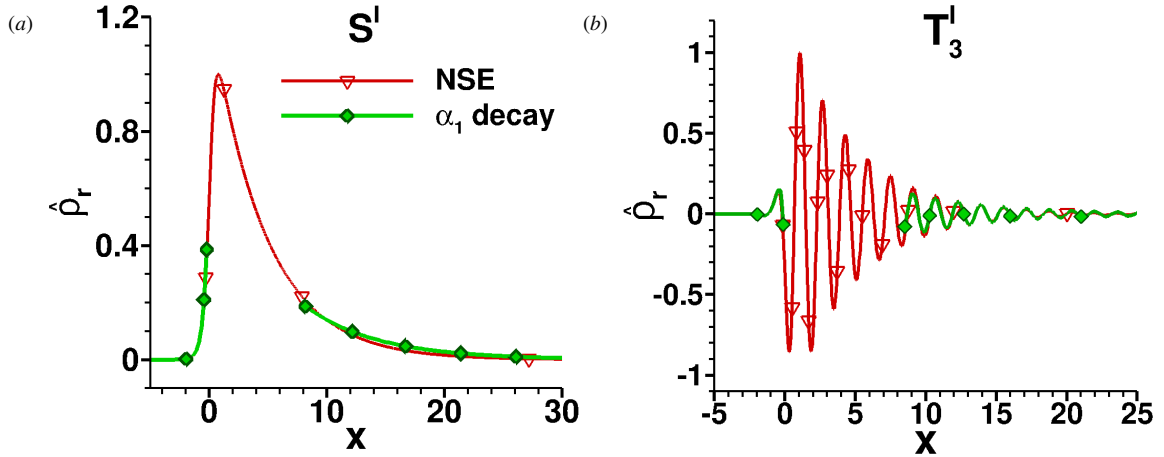


Figure 6.15: At $Ma = 1.2$ and $\beta = \beta_{ulim}$, comparison of $\hat{p}_r$ obtained from NSE normal mode equations with the far field decay solution governed by α_1 characteristic value for continuum modes S^l in (a) and T_3^l in (b).

The slow spatial downstream decay of eigenfunctions on branch l suggests that there might be a symmetry between the eigenfunctions of branch l and u about $x = 0$. Comparison of eigenfunctions of S^l with S^u are shown in the array of Fig. 6.16, that is Figs. 6.16(a)-6.16(f), plotted as a function of the absolute x -coordinate, $|x|$. The first, second, and third columns of the figure show the comparisons of eigenfunctions at $Ma = 1.2, 3$ and 5 , respectively, while the

top and bottom rows of the figure correspond to comparisons of eigenfunctions $\hat{u}_{y,r}$ from the ACE and $\hat{T}_r$ from the NSE formulations, respectively. At $Ma = 1.2$, eigenfunctions of both continuum modes look symmetric about $x = 0$ for either of the formulations and this is true for eigenfunctions of any macroscopic flow parameters. However, as the Mach number increases, the difference between the eigenfunctions of the two continuum modes increases indicating an asymmetry between their shapes. This increasing asymmetry with Mach number can be explained by comparing the variation of α_1^{appx} with Ω_i for up and downstream conditions, as shown in Figs. 6.8(a) and 6.8(b) for $Ma = 1.2$ and 5, respectively. It is seen that at $Ma = 1.2$, the slopes of solution for up and downstreams are nearly the same, such that the magnitude $|\alpha_1^{\text{appx}}|$ of 0.25 in the upstream for S^u is close to 0.16 in the downstream for S^l . However, at $Ma = 5$, the slopes of solutions for up and downstreams are significantly different, as a result, $|\alpha_1^{\text{appx}}|$ for S^u in the upstream is very different (0.13) from that for S^l in the downstream (0.40), which results in the asymmetry.

Turning to T_3^l , we first see the good comparison of its eigenfunction, $\hat{T}_r$, obtained from both formulations at $Ma = 1.2$ and $\beta = \beta_{\text{ulim}}$ in Fig. 6.17(a). Eigenfunctions compared well at $Ma = 3$ as well (not shown), however at $Ma = 5$, the spatial wavelength of sinusoidal variation was found to be too small to accurately resolve the eigenfunctions. Furthermore, unlike the symmetry between the stationary continuum modes, T_3^l and T_3^u were not found to be asymmetric about $x = 0$ even at $Ma = 1.2$, as shown in Fig. 6.17(b). It is seen that the spatial decay of the amplitude functions of these two continuum modes is similar, however, a clear difference is observed in their spatial sinusoidal wavelength. This difference can be explained by the differences in $\alpha_{1,i}$ for these continuum modes which is equal to 3.0 in the upstream for T_3^u , whereas it is 3.892 in the downstream for T_3^l .

Finally, in terms of the importance of these more damped continuum modes, it must be noted that although the present analysis is of a planar normal shock rather than a curved bow shock, it is not a bad approximation along the stagnation line of highly blunt bodies to make the following qualitative observation. The spatial decay of eigenfunctions on branch I continues on the downstream side for about 25 shock layer thicknesses, a distance comparable to the shock-stand off distances on typical blunt bodies such as reentry vehicles. This implies that shock forming on such bodies must interact with the boundary layers forming on these bodies and such interactions may be important in terms of the receptivity of the boundary layer.

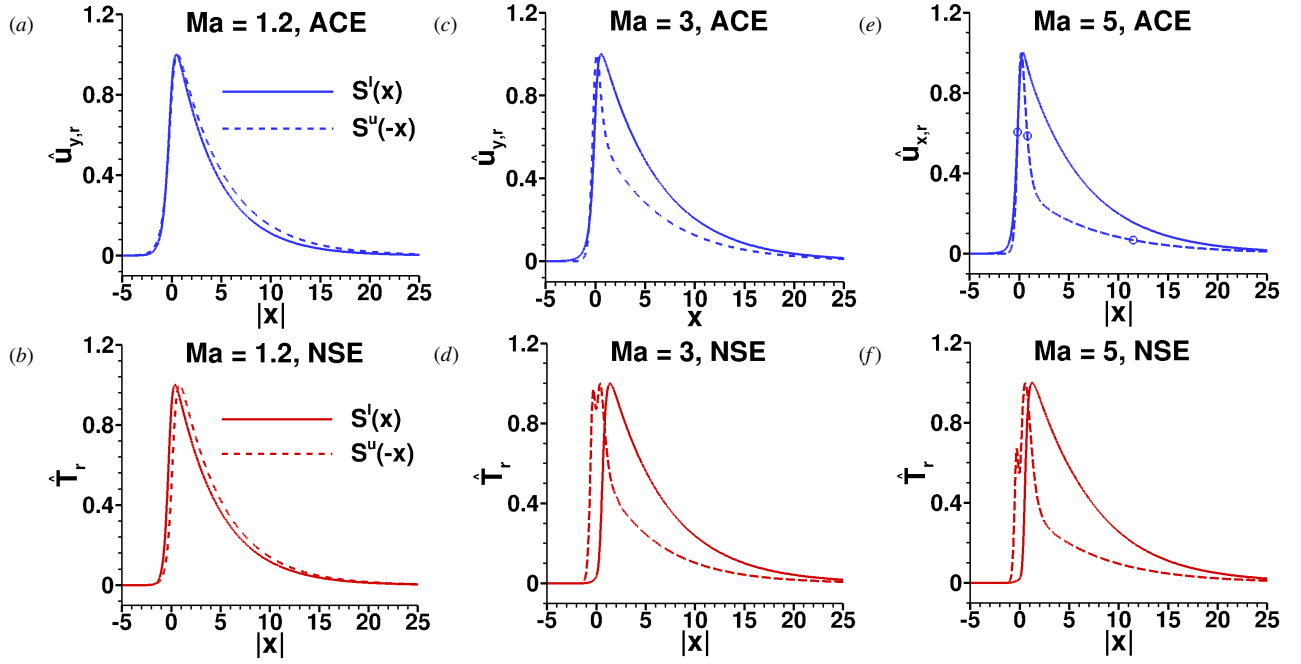


Figure 6.16: Comparison of eigenfunctions of S^u and S^l as a function of $|x|$ at $\beta = \beta_{\text{ulim}}$. Specifically, $\hat{u}_{y,r}$ obtained from ACE is shown at $Ma = 1.2$ in (a), $Ma = 3$ in (c), and $Ma = 5$ in (e), while $\hat{T}_r$ from NSE is shown at $Ma = 1.2$ in (b), $Ma = 3$ in (d), and $Ma = 5$ in (f).

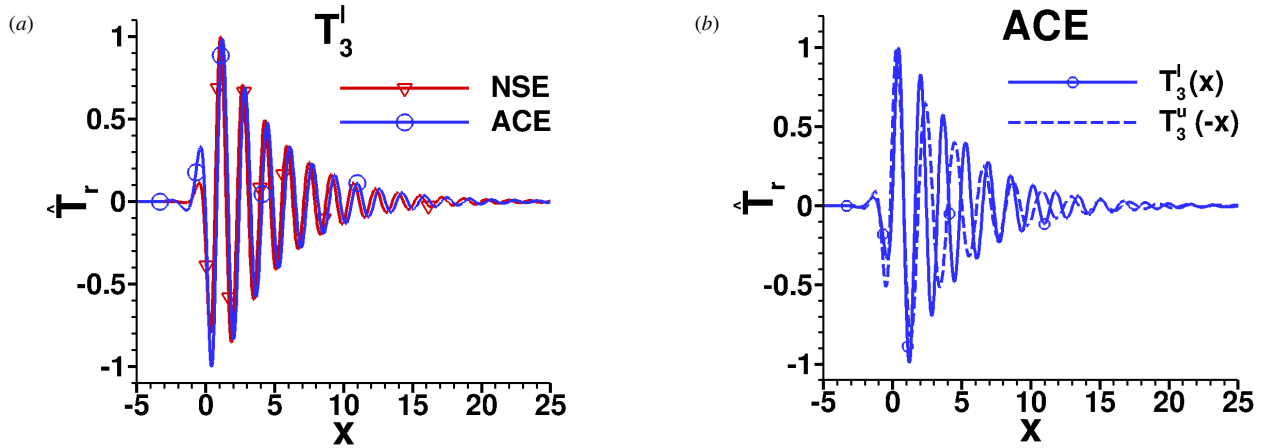


Figure 6.17: At $Ma = 1.2$ and $\beta = \beta_{\text{ulim}}$, (a) shows the comparison of eigenfunction $\hat{T}_r$ of T_3^l , indicated in Fig. 6.14, obtained from the NSE and ACE formulations, while (b) shows the comparison of $\hat{T}_r$ for T_3^l and T_3^u , plotted as a function of $|x|$.

6.5 Summary

A framework for studying linear stability of 1-D shock layers against 2-D harmonic perturbations has been developed, to solve the normal mode equations obtained from the traditional NSE formulation as well as the newly developed ACE formulation. The fully-resolved, steady base flows of 1-D shock layers at $Ma = 1.2, 3$, and 5 were computed using the particle-based DSMC method, which allowed for accurate solutions of regions of translational nonequilibrium in the interior of the shock. The constitutive equations used in the ACE formulation were first derived for a 1-D, steady shock layer using the MS bimodal VDF for a gas of Maxwell molecules ($\omega = 1$) and then extended to two-dimensions so that it could be used to study 2-D harmonic perturbations to 1-D shock layers. The motivation for using the ACE formulation stemmed from the fact that its constitutive equations are substantially better than the traditional NSF constitutive equations at approximating the DSMC-derived normal viscous stresses and the x -directional heat flux at high Mach numbers ($M > 1.2$). As a result, the comparison of these two formulations for linear stability analyses of DSMC-derived shock layers allows for quantifying the effects of translational nonequilibrium on the stability of shock layers.

Modal analyses were carried out assuming small-amplitude, 2-D, harmonic perturbations having wavelength, L_y^* , on the order of maximum mean-free-path in the entire base flow, $\bar{\lambda}_{\max}^*$. For $L_y^* = \bar{\lambda}_{\max}^*$, eigenspectra obtained from the two formulations exhibit eigenmodes that belong to only continuous branches, where the least stable continuous branch u consists of both stationary and traveling continuum modes. At $Ma = 1.2$, the decay rates of continuum modes on branch u predicted by the ACE formulation compared within only 2% difference with the NSE formulation, as expected from the small degree of translational nonequilibrium in the shock layer. More importantly, the comparison of the two formulations at high Mach numbers highlighted that the noncontinuum effects lead to a less stable branch, and that the prediction of decay rates strongly depends on how well the constitutive relations resolve the true translational nonequilibrium region in the shock layer.

The eigenfunctions of the stationary and traveling continuum modes of the least stable branch u were found to decay monotonically and sinusoidally in the far field, respectively, while the spatial decay rate was an order of magnitude lower in the upstream than the downstream. This spatial decay of eigenfunctions was shown to be governed by only one physically possible characteristic value of out seven, predicted by a septic characteristic equation obtained by simplifying the normal mode equations in the far field of the shock layer. This characteristic value α_1 was numerically shown to be the root of a quintic polynomial, factorized from the septic polynomial, while an approximate equation, α_1^{appx} , was obtained, which is in excellent agreement with α_1 , as long as the sum of the higher order terms in the quintic polynomial that were ignored for obtaining the approximate solution is lower than 4% of the first order term. This holds for all three Mach numbers studied in this work.

By analyzing the equation for α_1^{appx} , which depends on γ , Ma , Re , β and far field flow quantities, it was shown that there exists a range of decay rates Ω_i for which physically acceptable values of α_1^{appx} are possible in both far fields. Linear stability analysis predicts a least stable continuous branch having decay rates close to the maximum limit of this range. By studying the dependence of the limits of this range on governing parameters, it was shown that this family of continuum modes is always stable, but it becomes less stable by increase in Ma , decrease in γ , and increase in the magnitude of normal stresses, *i.e.* increase in the degree of translational nonequilibrium. It was also shown that the ACE formulation, which uses a general constitutive equation of stress tensor, must predict a less stable decay rate than the NSE formulation, consistent with the observations of linear stability analysis. This is because the ACE coefficients A_a and A_b , derived using Mott-Smith's bimodality assumption, are proportional to Mach number, rather than constants $4/3$ and $-2/3$ assumed in the traditional NSF constitutive equations. Furthermore, Ω_i was found to be nearly independent of the spanwise wavenumber, β , when β is close to β_{lim} , while Ω_i changes nonlinearly with β for lower values of β . The linear stability analyses conducted at lower β values, that is at higher ratio of perturbation wavelengths to the maximum mean-free-path, $L_y^*/\bar{\lambda}_{\text{max}}^*$, showed that the continuous branch becomes more stable by decreasing β .

Comparison of eigenfunctions obtained from the two formulations showed that both stationary and traveling continuum modes compared very well at $Ma = 1.2$, but with the increase in Mach number, differences were observed between the two formulations in both the shock layer as well as the far field. These differences were attributed to the better capability of the ACE in approximating the increasing region of translational nonequilibrium at higher Mach numbers.

Continuum modes on the second less stable branch I were also analyzed, which exhibit eigenfunctions having a very gradual decay downstream of the shock layer compared to upstream in contrast to continuum modes on branch u. This lower branch was found to be in the proximity of the lower limit of the range of Ω_i for which physically acceptable values of α_1^{appx} exist. The slower spatial decay rate on the downstream side rather than the upstream was shown to be a consequence of the negative slope of the variation of α_1^{appx} with Ω_i . The importance of these more damped continuum modes on branch I can be argued based on the gradual decay of their eigenfunctions on the downstream side of the shock layer, which suggests that they may interact with a boundary layer formed on a blunt body and could cause potential excitation of the boundary layer.

6.6 Supplemental Information

6.6.1 Derivation of Mott-Smith Constitutive Functions in 1-D and Deduction of Functions

Π^{m*} and Σ^{m*}

To derive the constitutive relations for a 1-D, DSMC-derived, steady shock layer, we start with the 1-D Boltzmann moment equation

$$\frac{d[\bar{n}^* \langle v_x^* Q^* \rangle]}{dx^*} = \Delta[Q^*] \quad (6.60)$$

where Q^* is any function of molecular velocity components, $\bar{n}^*$ is the local number density obtained from DSMC, $\langle v_x^* Q^* \rangle$ is a moment of the molecular function $v_x^* Q^*$ with respect to the velocity distribution function in a shock layer, and $\Delta[Q^*]$ is the collision integral [37] (see Eq. 3.26(e)). Equation (6.60) will be used by assuming $Q^* = (v_x^*)^2$, $(v_y^*)^2$, and $v_x^* (v^*)^2$, where v^* is the molecular speed, to obtain constitutive equations for $\bar{\tau}_{xx}^{m*}$, $\bar{\tau}_{yy}^{m*}$, and $\bar{q}_x^{m*}$, respectively; the choice of these functions which will be clear shortly.

In this work, the moment in Eq. (6.60) is calculated with respect to the MS bimodal distribution function, f^m , in the shock layer, *i.e.* $\langle v_x^* Q^* \rangle \approx \langle v_x^* Q^* \rangle_{f^m}$, which can be written as

$$\bar{n}^* \langle v_x^* Q^* \rangle_{f^m} = N_1^* \langle v_x^* Q^* \rangle_{f_1} + N_2^* \langle v_x^* Q^* \rangle_{f_2} \quad (6.61)$$

where functions N_1^* and N_2^* can be calculated from DSMC flow quantities $\bar{u}_x^*$ and $\bar{n}^*$ as (see pg. 419 of Ref. [91])

$$N_1^* = \frac{n_1^* u_{x,1}^*}{u_{x,1}^* - u_{x,2}^*} \left(1 - \frac{u_{x,2}^*}{\bar{u}_x^*} \right) \quad (6.62)$$

$$N_2^* = N_1^* - \bar{n}^* \quad (6.63)$$

and $\langle v_x^* Q^* \rangle_{f_1}$ and $\langle v_x^* Q^* \rangle_{f_2}$ are moments with respect to up and downstream Maxwellian velocity distribution functions, obtained from Eq. 6.8.

Next, the collision integral, $\Delta[Q^*]$, can be analytically derived for Maxwell molecules (see pg. 364 of Ref. [91]), which is written for $Q^* = v_i^* v_j^*$ as

$$\Delta[v_i^* v_j^*] = \frac{\bar{p}^* \bar{\tau}_{ij}^{m*}}{m \bar{\mu}^*} \quad (6.64)$$

and for $Q^* = v_i^* (v^*)^2$ as

$$\Delta[v_i^* (v^*)^2] = 2 \frac{\bar{p}^* \bar{\tau}_{ij}^{m*}}{m \bar{\mu}^*} \bar{u}_j^* - \frac{5 \bar{p}^* R \bar{q}_i^{m*}}{m \bar{k}^*} \quad (6.65)$$

where $\bar{p}^*$ is the pressure.

Using the above collision integrals in Eq. (6.60) and evaluating the moment using Eq. (6.61) for a specific choice of Q^* , we can obtain constitutive equations for stress tensor and heat flux components. The key steps in the derivations of $\bar{\tau}_{xx}^{m*}$ and $\bar{q}_x^{m*}$ are described next, while $\bar{\tau}_{yy}^{m*}$ can be easily obtained using a similar procedure for $\bar{\tau}_{xx}^{m*}$.

For $\bar{\tau}_{xx}^{m*}$, we choose $Q^* = (v_x^*)^2$ and use Eq. (6.64) to write Eq. (6.60) as

$$\frac{d\langle \bar{n}^* (v_x^*)^3 \rangle_{fm}}{dx^*} = \frac{\bar{p}^* \bar{\tau}_{xx}^{m*}}{m \bar{\mu}^*} \quad (6.66)$$

The evaluation of the moment $\langle \bar{n}^* (v_x^*)^3 \rangle_{fm}$ and its derivative with respect to x^* , written as

$$\frac{d\langle \bar{n}^* (v_x^*)^3 \rangle}{dx^*} = \frac{2}{5} u_{x,1}^* [(u_{x,1}^*)^2 - (u_{x,2}^*)^2] \frac{dN_1^*}{dx^*} \quad (6.67)$$

is described in Ref. [37] (see Eq. (8.34)). From Eq. (6.62), the derivative

$$\frac{dN_1^*}{dx^*} = \frac{\bar{n}^* u_{x,2}^*}{\bar{u}_x^* (u_{x,1}^* - u_{x,2}^*)} \frac{d\bar{u}_x^*}{dx^*} \quad (6.68)$$

where the mass conservation equation

$$n_1^* u_{x,1}^* = \bar{n}^* \bar{u}_x^* \quad (6.69)$$

is used for simplification. From Eqs. (6.68), (6.67) and (6.66), we write

$$\bar{\tau}_{xx}^{m*} = \frac{m \bar{\mu}^*}{\bar{p}^*} \frac{2}{5} u_{x,1}^* (u_{x,1}^* + u_{x,2}^*) \frac{\bar{n}^* u_{x,2}^*}{\bar{u}_x^*} \frac{d\bar{u}_x^*}{dx^*} \quad (6.70)$$

which can be simplified using Eq. (6.69) and the Rankine-Hugoniot ratios, r_ρ , r_u , and r_t , defined in Sec. 6.2.1 to obtain the final equation of $\bar{\tau}_{xx}^{m*}$, shown in Eq. (6.22).

Next, for $\bar{q}_x^{m*}$, we choose $Q^* = v_x^* (v^*)^2$ and use Eq. (6.65) to write Eq. (6.60) as

$$\frac{d\langle \bar{n}^* (v_x^* v^*)^2 \rangle_{fm}}{dx^*} = 2 \frac{\bar{p}^* \bar{\tau}_{xx}^{m*}}{m \bar{\mu}^*} \bar{u}_x^* - \frac{5 \bar{p}^* R \bar{q}_x^{m*}}{m \bar{k}^*} + \underbrace{2 \frac{\bar{p}^* \bar{\tau}_{xy}^{m*}}{m \bar{\mu}^*} \bar{u}_y^*}_0 \quad (6.71)$$

The third term on the right hand side is zero in 1-D, however, it is retained here because it may be nonzero in a 2-D equation, which is derived based on the 1-D equation, as described in Sec. 6.3.2. The moment $\langle \bar{n}^* (v_x^* v^*)^2 \rangle_{f^m}$ can be simplified as

$$\begin{aligned} \langle \bar{n}^* (v_x^* v^*)^2 \rangle_{f^m} &= \langle \bar{n}^* (c_x^* + u_x^*)^2 [(c_x^* + u_x^*)^2 + 2(c_y^*)^2]^2 \rangle_{f^m} \\ &= \bar{n}^* \langle (u_{x,1}^*)^4 + (c_x^*)^4 + 6(u_{x,1}^* c_x^*)^2 + 2(u_{x,1}^* c_y^*)^2 + 2(c_x^* c_y^*)^2 \rangle_{f^m} \end{aligned} \quad (6.72)$$

and evaluated using Eq. (6.61) to obtain

$$\begin{aligned} \langle (\bar{n}^* v_x^* v^*)^2 \rangle_{f^m} &= \left[N_1^* 5R^2 (T_1^*)^2 + N_2^* 5R^2 (T_2^*)^2 \right] \\ &\quad + \left[N_1^* ((u_{x,1}^*)^4 + 8(u_{x,1}^*)^2 RT_1^*) + N_2^* ((u_{x,2}^*)^4 + 8(u_{x,2}^*)^2 RT_2^*) \right] \end{aligned} \quad (6.73)$$

In this equation, N_2^* can be eliminated from the second right side term using Eq. (6.63), and from the fifth right side term using the first moment of the MS distribution

$$\bar{n}^* \bar{u}_x^* = N_1^* u_{x,1}^* + N_2^* u_{x,2}^* \quad (6.74)$$

and the mass conservation Eq. (6.69), to write

$$\begin{aligned} \bar{n}^* \langle (v_x^*)^2 (v^*)^2 \rangle_{f^m} &= N_1^* 5R^2 \left[(T_1^*)^2 - (T_2^*)^2 \right] + \bar{n}^* 5R^2 (T_2^*)^2 + n_1^* u_{x,1}^* \left[(u_{x,2}^*)^3 + 8u_{x,2}^* RT_2^* \right] \\ &\quad + N_1^* \left[(u_{x,1}^*)^4 + 8(u_{x,1}^*)^2 RT_1^* - u_{x,1}^* (u_{x,2}^*)^3 - 8u_{x,1}^* u_{x,2}^* RT_2^* \right] \end{aligned} \quad (6.75)$$

By substituting Eq. (6.75) into Eq. (6.71) and using Eq. (6.68) and the Rankine-Hugoniot ratios, Eq. (6.71) may be written as

$$\begin{aligned} \bar{q}_x^{m*} &= \bar{k}^* \frac{T_1^* T_1^*}{\bar{T}^* \bar{\rho}^*} \frac{r_u}{5(1-r_u)} \frac{d\bar{\rho}^*}{dx^*} \left[(\gamma M a^2)^2 (1-r_u^3) + 8\gamma M a^2 (1-r_u r_t) + 5(1-r_t^2) \right] \\ &\quad - \bar{k}^* r_t^2 \frac{T_1^* T_1^*}{\bar{\rho}^* \bar{T}^*} \frac{d\bar{\rho}^*}{dx^*} + \frac{2}{5} \frac{\bar{k}^* \bar{\tau}_{xx}^{m*}}{\bar{\mu}^* R} \bar{u}_x^* + \underbrace{\frac{2}{5} \frac{\bar{k}^* \bar{\tau}_{xy}^{m*}}{\bar{\mu}^* R} \bar{u}_y^*}_0 \end{aligned} \quad (6.76)$$

which can be rearranged into the final form of $\bar{q}_x^{m*}$, given in Eq. (6.23).

Next, to prove that $\Pi^*(x, y, t)$ and $\Sigma^*(x, y, t)$ are given by Eq. (6.28), we first show that their $O(0)$ base flow parts

$\bar{\Pi}^*(x)$ and $\bar{\Sigma}^*(x)$ are written as

$$\begin{aligned}\bar{\Pi}^* &= (A_a - A_b) \frac{T_1^*}{\bar{T}^*} \frac{\bar{\rho}^*}{\rho_1^*} \bar{\mu}^* \\ \bar{\Sigma}^* &= A_b \frac{T_1^*}{\bar{T}^*} \frac{\bar{\rho}^*}{\rho_1^*} \bar{\mu}^*\end{aligned}\tag{6.77}$$

as follows. Equation (6.27) for the 2-D stress tensor $\tau_{ij}(x, y, t)$ is linearized by substituting

$$\begin{aligned}\mathbf{u}^*(x, y, t) &= \bar{\mathbf{u}}_x^*(x) + O(\epsilon) \\ \boldsymbol{\tau}^{m*}(x, y, t) &= \bar{\boldsymbol{\tau}}^{m*}(x) + O(\epsilon) \\ \Pi^*(x, y, t) &= \bar{\Pi}^*(x) + O(\epsilon) \\ \Sigma^*(x, y, t) &= \bar{\Sigma}^*(x) + O(\epsilon)\end{aligned}\tag{6.78}$$

where $\bar{\boldsymbol{\tau}}^{m*}$, $\bar{\Pi}^*$, and $\bar{\Sigma}^*$ are $O(0)$ base flow quantities, while the form of $O(\epsilon)$ terms is not specified as it is not required here for the discussion. Then, by collecting the $O(0)$ terms, we obtain

$$\begin{aligned}\bar{\tau}_{xx}^{m*} &= (\bar{\Pi}^* + \bar{\Sigma}^*) \frac{d\bar{u}_x^*}{dx^*} \\ \bar{\tau}_{yy}^{m*} &= \bar{\Sigma}^* \frac{d\bar{u}_x^*}{dx^*} \\ \bar{\tau}_{xy}^{m*} &= \bar{\tau}_{yx}^{m*} = 0\end{aligned}\tag{6.79}$$

By comparing Eq. (6.79) with Eq. (6.22), obtained from the MS theory, we see that $\bar{\Pi}^*$ and $\bar{\Sigma}^*$ are indeed given by Eq. (6.77).

Now based on Eq. (6.77), we prove that the form of $\Pi^*(x, y, t)$ and $\Sigma^*(x, y, t)$ must be given by Eq. (6.28) for the assumption of linear stress-strain relationship of Newtonian fluids to be valid. It is easy to check that by substituting the linear decomposition for Π^* and Σ^* and

$$\begin{aligned}\rho^*(x, y, t) &= \bar{\rho}^*(x) + O(\epsilon) \\ T^*(x, y, t) &= \bar{T}^*(x) + O(\epsilon) \\ \mu^*(x, y, t) &= \bar{\mu}^*(x) + O(\epsilon)\end{aligned}\tag{6.80}$$

in Eq. (6.28), and collecting $O(0)$ terms, we obtain Eq. (6.77), proving the “sufficiency” condition that $\bar{\Pi}^*$ and $\bar{\Sigma}^*$ are indeed $O(0)$ base flow quantities of Π^* and Σ^* . It can be further argued that Π^* and Σ^* must be uniquely defined as written in Eq. (6.28) by noticing that if there were additional terms present, then their $O(0)$ base flow parts would have

to be zero and such additional terms must include u_y^* or its gradients, because it is the only macroscopic flow quantity that is zero in the base flow. The presence of such additional terms would violate the assumption of linear stress-strain relationship.

6.6.2 Elements of Linear Operators in an Eigenvalue Problem

The elements of linear operators $\mathcal{A}$ and $\mathcal{B}$, defined in Eq. 6.17, can be written for the two formulations using a binary integer variable $\mathcal{I}$, which acts as a switch to enable one of the formulations, that is,

$$\mathcal{I} = \begin{cases} 0 & \text{ACE} \\ 1 & \text{NSE} \end{cases}$$

Elements of matrix $\mathcal{A}$:

$$\begin{aligned} \mathcal{A}_{11} &= (\bar{u}'_x) + \bar{u}_x \frac{d}{dx} \\ \mathcal{A}_{12} &= \bar{\rho}' + \bar{\rho} \frac{d}{dx} \\ \mathcal{A}_{13} &= i\beta\bar{\rho} \\ \mathcal{A}_{14} &= 0 \\ \mathcal{A}_{21} &= \left[\frac{1}{\gamma Ma^2} \bar{T}' + \bar{u}_x \bar{u}'_x + (1 - \mathcal{I}) \left(\frac{1}{\bar{\rho}} \frac{\partial \bar{\phi}}{\partial \bar{T}} \bar{T}' \bar{u}'_x + \frac{\partial \bar{\phi}}{\partial \bar{\rho}} \bar{u}''_x \right) \right] \\ &\quad + \left[\frac{\bar{T}}{\gamma Ma^2} + (1 - \mathcal{I}) \frac{\partial \bar{\phi}}{\partial \bar{\rho}} \bar{u}'_x \right] \frac{d}{dx} \\ \mathcal{A}_{22} &= \left(\frac{\beta^2 \bar{\mu}}{Re} + \bar{\rho} \bar{u}'_x \right) + (\bar{\phi}' + \bar{u}_x \bar{\rho}) \frac{d}{dx} + \bar{\phi} \frac{d^2}{dx^2} \\ \mathcal{A}_{23} &= i\beta \bar{\psi}' - i\beta \left[\frac{\bar{\mu}}{Re} - \bar{\psi} \right] \frac{d}{dx} \\ \mathcal{A}_{24} &= \left(\frac{\partial^2 \bar{\phi}}{\partial \bar{T}^2} \bar{T}' \bar{u}'_x + \frac{\partial \bar{\phi}}{\partial \bar{T}} \bar{u}''_x + (1 - \mathcal{I}) \frac{1}{\bar{\rho}} \frac{\partial \bar{\phi}}{\partial \bar{T}} \bar{\rho}' \bar{u}'_x + \frac{\bar{\rho}'}{\gamma Ma^2} \right) + \left(\frac{\partial \bar{\phi}}{\partial \bar{T}} \bar{u}'_x + \frac{\bar{\rho}}{\gamma Ma^2} \right) \frac{d}{dx} \end{aligned} \tag{6.81}$$

$$\begin{aligned}
\mathcal{A}_{31} &= \mathrm{i} \frac{\beta \bar{T}}{\gamma M a^2} + (1 - \mathcal{I}) \frac{\partial \bar{\psi}}{\partial \bar{\rho}} \bar{u}'_x \\
\mathcal{A}_{32} &= -\mathrm{i} \frac{\beta \bar{\mu}'}{Re} + \mathrm{i} \beta \left(\bar{\psi} - \frac{\bar{\mu}}{Re} \right) \frac{d}{dx} \\
\mathcal{A}_{33} &= \left[-\beta^2 \bar{\phi} \right] + \left(\bar{u}_x \bar{\rho} - \frac{\bar{\mu}'}{Re} \right) \frac{d}{dx} - \frac{\bar{\mu}}{Re} \frac{d^2}{dx^2} \\
\mathcal{A}_{34} &= \left[\mathrm{i} \beta \left(\frac{\bar{\rho}}{\gamma M a^2} + \frac{\partial \bar{\psi}}{\partial \bar{T}} \bar{u}'_x \right) \right] \\
\mathcal{A}_{41} &= \left[(1 - \mathcal{I}) [(\bar{\xi}_b^m)' + (\bar{\xi}_h^m)'] + (\gamma - 1) \bar{T} \bar{u}'_x + \bar{u}_x \bar{T}' \right] + (1 - \mathcal{I}) \left[\left(\bar{\xi}_b^m - (\bar{\xi}_a^m)' + \bar{\xi}_h^m \right) \frac{d}{dx} - \bar{\xi}_a^m \frac{d^2}{dx^2} \right] \\
\mathcal{A}_{42} &= (1 - \mathcal{I}) (\bar{\xi}_g^m)' + \bar{\rho} \bar{T}' + \left((1 - \mathcal{I}) [(\bar{\xi}_d^m)' + \bar{\xi}_g^m] + 2Ec\gamma \bar{\phi} \bar{u}'_x + (\gamma - 1) \bar{\rho} \bar{T} \right) \frac{d}{dx} \\
&\quad + (1 - \mathcal{I}) \bar{\xi}_d^m \frac{d^2}{dx^2} \\
\mathcal{A}_{43} &= \mathrm{i} \beta \left((1 - \mathcal{I}) (\bar{\xi}_e^m)' + 2Ec\gamma \bar{\psi} \bar{u}'_x + (\gamma - 1) \bar{\rho} \bar{T} \right) + \left[(1 - \mathcal{I}) \mathrm{i} \beta \bar{\xi}_e^m \right] \frac{d}{dx} \\
\mathcal{A}_{44} &= \left[\left[(1 - \mathcal{I}) [(\bar{\xi}_c^m)' + (\bar{\xi}_f^m)'] - (\bar{\kappa}^n)'' \mathcal{I} + \beta^2 \bar{\kappa}^n + Ec\gamma \frac{\partial \bar{\phi}}{\partial \bar{T}} \bar{u}_x'^2 + (\gamma - 1) \bar{\rho} \bar{u}'_x \right] \right. \\
&\quad \left. + \left(\bar{u}_x \bar{\rho} - 2(\bar{\kappa}^n)' \mathcal{I} + (1 - \mathcal{I}) (\bar{\xi}_c^m + \bar{\xi}_f^m) \right) \frac{d}{dx} - \bar{\kappa}^n \mathcal{I} \frac{d^2}{dx^2} \right]
\end{aligned} \tag{6.82}$$

where appropriate functions $\bar{\phi}$, $\bar{\psi}$ must be chosen based on the formulation used, as shown in Table 6.3, functions $\bar{\xi}_j$ and $\bar{\xi}_j'$ for $j = a$ to h are obtained from Table 6.4, and derivatives of $\bar{\mu}$ and $\bar{\kappa}$ are obtained from Eqs. (6.50) and (6.51), respectively.

Elements of matrix $\mathcal{B}$:

$$\begin{aligned}
\mathcal{B}_{11} &= \mathrm{i} \\
\mathcal{B}_{22} &= \mathrm{i} \bar{\rho} \\
\mathcal{B}_{33} &= \mathrm{i} \bar{\rho} \\
\mathcal{B}_{44} &= \mathrm{i} \bar{\rho}
\end{aligned} \tag{6.83}$$

6.6.3 Comparison of Eigenspectra with Duck and Balakumar

In this section, we have validated our NSE formulation by reproducing eigenspectra of shock layers shown by Duck and Balakumar [1] using base flows generated from the method of Gilbarg and Paolucci [7].

Duck and Balakumar performed linear stability analyses of $Ma = 2$ and 5 shock layers, assuming $Pr = 0.72$, $\gamma = 1.4^2$, the Sutherland's law for dynamic viscosity, and Reynolds number Re^{DB} of unity, defined based on the length scale of inverse unit Reynolds number, $L^{DB} = \mu_1^*/\rho_1^*u_{x,1}^*$. The nondimensional base flow profiles of $\bar{\rho}^{GP}$ and $\bar{T}^{GP}$ obtained from the method of Gilbarg and Paolucci at $Ma = 2$ are shown in Fig. 6.18(a). Using this length scale, they defined perturbation wavenumber β^{DB} and the complex nondimensional eigenvalue Ω as

$$\beta^{DB} = \frac{2\pi}{L_y^*} L^{DB*} \quad (6.84)$$

$$\Omega^{DB} = \frac{\Omega^{DB*} L^{DB*}}{u_{x,1}^*} \quad (6.85)$$

and presented eigenspectra for $\beta^{DB} = 0.5, 1$, and 5 for $Ma = 2$ and 5.

Figures 6.18(b), 6.18(c), and 6.18(d) show a comparison of their eigenspectra using $\beta^{DB} = 0.5$ and 1 at $Ma = 2$, and $\beta^{DB} = 5$ at $Ma = 5$, respectively, with eigenspectra obtained using our NSE formulation. At $Ma = 2$, $\beta^{DB} = 0.5$ and $Ma = 5$, $\beta^{DB} = 5$ the least stable branches in eigenspectra obtained from the NSE formulation compare very well with that of [1] and are within the expected error in digitization, while the comparison at $Ma = 2$ and $\beta^{DB} = 1$ is only qualitatively similar and does not agree well. This difference could possibly be because of smaller domain length or the lack of grid resolution, however these details are not provided by Duck and Balakumar. We have used the Chebyshev spectral method to discretize the eigenvalue problem at $(N + 1)$ Gauss-Lobatto collocation points [245], where N is the degree of Chebyshev polynomial, used a domain extent of $-120 \leq x \leq 120$, and specified Dirichlet boundary conditions.

Although, Duck and Balakumar do not show any eigenfunctions, we calculated the eigenfunctions of the least damped continuum modes for the three conditions discussed above using our linear stability solver based on the NSE formulation. Starting with $Ma = 2$ and $\beta^{DB} = 0.5$, Fig. 6.18(b) shows that there is a least damped a traveling continuum mode with frequency $\Omega_r^{DB} = 0.28$, indicated as $T_{0.28}^P$. An eigenfunction $\hat{\rho}_r$ of this continuum mode is shown in Fig. 6.19(a), which can be observed to not die away to zero as $x \rightarrow \pm\infty$, a required criterion for eigenfunctions to be physically acceptable. Instead, it grows in the far fields of the shock layer, and at the domain boundaries, is equal to zero only because of the imposition of Dirichlet boundary conditions. Dirichlet boundary conditions also cause

² $\gamma = 1.4$ means a diatomic gas, however the formulation of Duck and Balakumar does not specify a rotational temperature. For a monatomic gas, Pr must be $2/3$. Because of this inconsistency, these profiles cannot be compared with a monatomic shock layer obtained from DSMC.

pointwise oscillations where the value of eigenfunction alternates between two values, which is clearly seen on the downstream side of the shock layer.

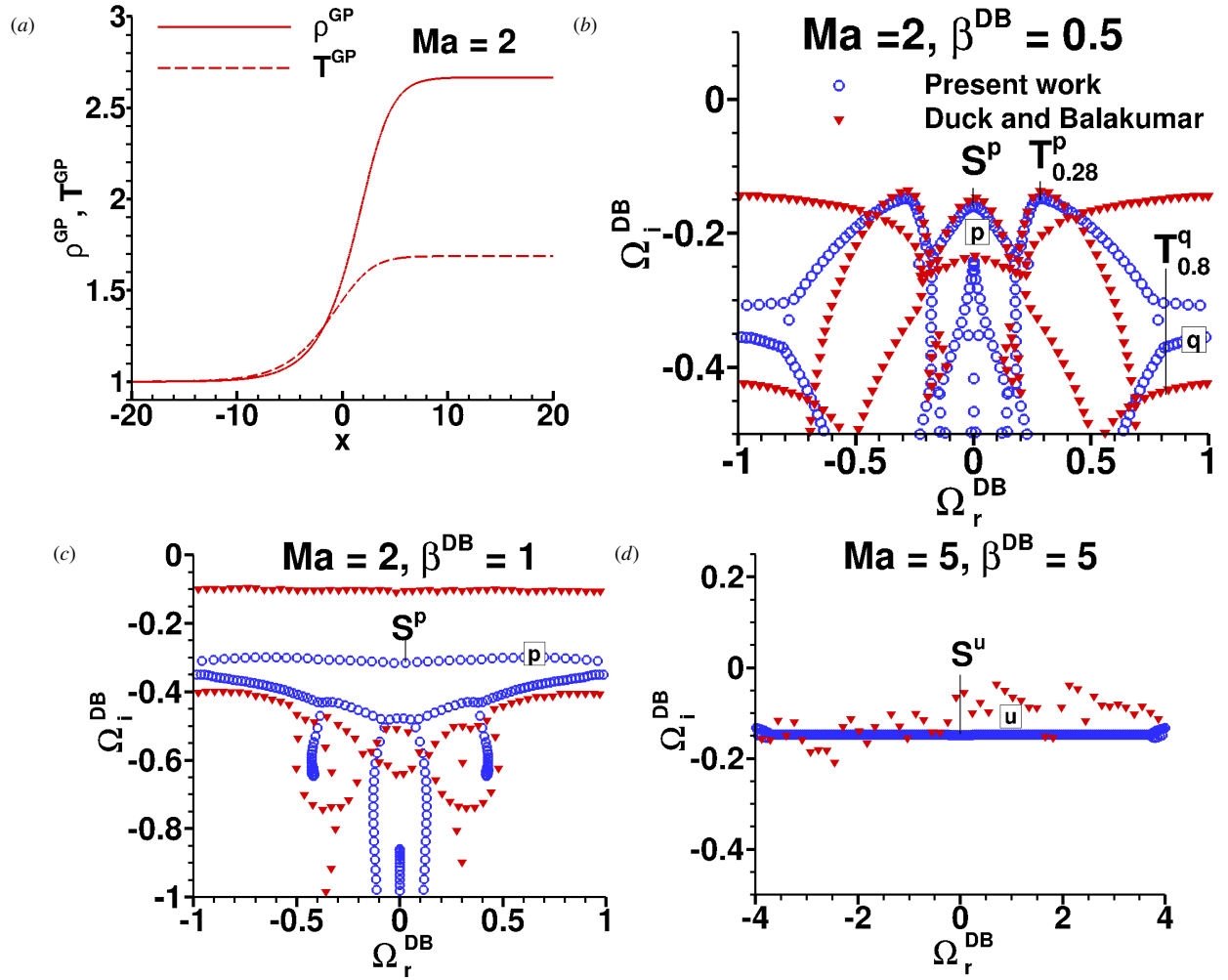


Figure 6.18: The nondimensional base flow profiles obtained from the method of Gilbarg and Paolucci at $Ma = 2$, $Re^{DB} = 1$, $Pr = 0.72$, and $\gamma = 1.4$ are shown in (a). Comparison of eigenspectra obtained from the NSE formulation presented in this work with eigenspectra obtained from the work of Duck and Balakumar for $\beta^{DB} = 0.5$ and 1 at $Ma = 2$ in (b) and (c), respectively, and $\beta^{DB} = 5$ at $Ma = 5$ in (d).

To ensure that the far field growth of the eigenfunction was not induced by our imposition of Dirichlet boundaries, three additional cases were run by imposing Neumann boundary conditions on both ends of the domain. For these cases the domain length was 40, 80, and 160, while the number of grid points were 400, 800, and 1600, respectively, such that the grid resolution remained the same. A comparison of the eigenfunctions for these cases is shown in Fig. 6.19(b), where it can be seen that all eigenfunctions exhibit sinusoidal and monotonic growth on the up and downstream sides

of the shock layer, indicating that the far field growth seen in Fig. 6.19(a) was not caused by Dirichlet boundaries and the continuum mode $T_{0.28}^P$ is indeed physically unrealistic. Similarly, the second dominant stationary continuum mode S^P , indicated in Fig. 6.18(b), was also found to be physically unrealistic (eigenfunctions not shown). Only on branch q , were physically acceptable continuum modes found that decay to zero in the far field. A sample traveling continuum mode having frequency, $\Omega^{DB} = 0.8$, denoted as $T_{0.8}^q$, is indicated in Fig. 6.18(b), and its eigenfunction is shown in Fig. 6.19(c). This eigenfunction exhibits a sinusoidal spatial decay on both sides of the shock layer, while the decay is more gradual on the downstream side than the upstream.

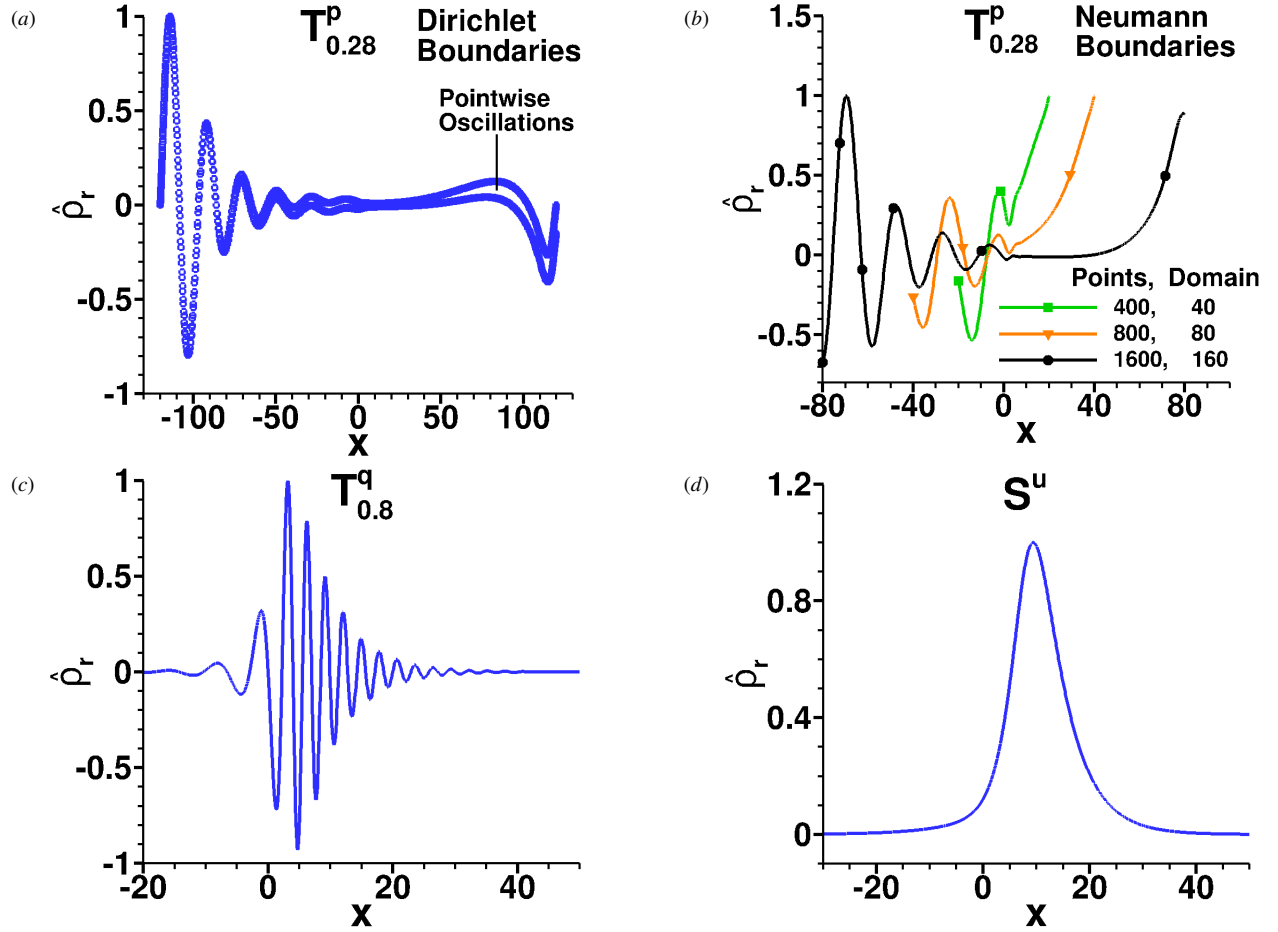


Figure 6.19: (a)–(c) show eigenfunction $\hat{\rho}_r$ of continuum modes at $Ma = 2$ and $\beta^{DB} = 0.5$, indicated in Fig. 6.18(b), obtained from our NSE formulation. Eigenfunctions of the least damped, traveling continuum mode $T_{0.28}^P$ obtained using Dirichlet and Neumann boundary conditions are shown in (a) and (b), respectively, and that of continuum mode $T_{0.8}^q$ obtained using Dirichlet boundary conditions is shown in (c). $\hat{\rho}_r$ of continuum mode S^u at $Ma = 5$ and $\beta^{DB} = 1$, indicated in Fig. 6.18(d), is shown in (d).

For the other two eigenspectra, shown in Fig. 6.18(c) for $Ma = 2$, $\beta^{DB} = 1$ and 6.18(d) for $Ma = 5$, $\beta^{DB} = 5$, the continuum modes on the least stable branches p and u decay to zero in the far fields. The stationary continuum mode S'' on branch u for $Ma = 5$ and $\beta = 5$ is shown in Fig. 6.19(d), where it can be seen that it decays monotonically on either sides of the shock layer. However, it looks different from the eigenfunction S'' obtained using DSMC base flows for monatomic argon shocks discussed in Sec. 6.4. The change in shape may be attributed to inconsistencies in the input conditions in terms of Pr and γ or the Sutherland's law of dynamic viscosity used by Duck and Balakumar.

6.6.4 Variation in Eigenspectra with Number of Grid Points at $Ma = 1.2$

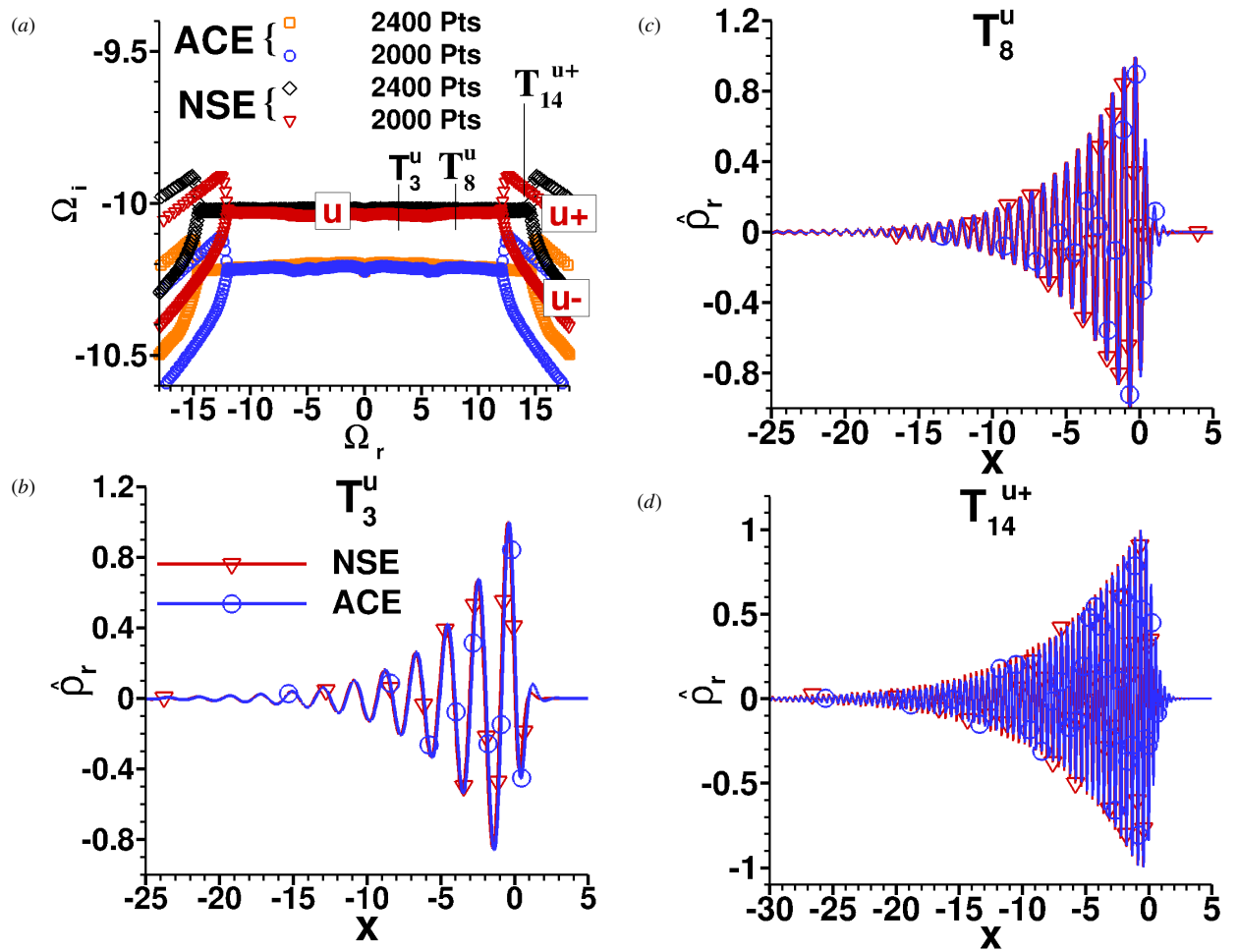


Figure 6.20: At $Ma = 1.2$ and $\beta = \beta_{ulim}$, the variation of eigenspectra for 2000 and 2400 grid points obtained from the ACE and NSE formulations and branches u , u^+ and u^- for the NSE solution with 2000 grid points are shown in (a), and the comparisons of $\hat{\rho}_r$ are shown for traveling continuum modes T_3^u in (a), T_8^u in (b), and T_{14}^{u+} in (c).

In this section, the variation in eigenspectra obtained at $Ma = 1.2$ and $\beta = \beta_{\text{ulim}}$ using the ACE and NSE formulations with change in number of grid points is shown in Fig. 6.20(a). For both formulations, the continuum modes having lower frequencies, $0 \leq |\Omega_r| \leq 10$, have approximately the same decay rate, while with increase in the number of grid points, the frequency at which the least stable branch u splits into a higher and lower branch, denoted as ' $u+$ ' and ' $u-$ ', respectively, increases. This branch splitting occurs because the number of grid points become insufficient to fully resolve the eigenfunctions of continuum modes as Ω_r increases. This can be understood from Figs. 6.20(b) and 6.20(c), which show eigenfunctions of traveling continuum modes T_3^u and T_8^u on branch u having frequencies $\Omega_r = 3$ and 8, respectively, obtained using 2000 grid points. With increase in Ω_r , the spatial wavelength of the sinusoidally decaying portion of eigenfunction decreases, requiring more number of grid points for smoothly capturing their spatial variation. Eigenfunction T_{14}^{u+} on branch $u+$ having $\Omega_r = 14$, shown in Fig. 6.20(d), reveals that it has a similar qualitative shape as eigenfunction on branch u , where it decays sinusoidally and gradually on the upstream side of the shock layer, however, its spatial wavelength is extremely small, and therefore, poorly resolved.

6.6.5 Solution of Navier-Stokes normal mode equations in the two far fields of the shock

In this section, the equations governing the characteristic spatial decay of eigenfunctions in the far fields of a shock layer are derived. By substituting the derivatives of base flow quantities $\bar{\mathcal{P}}' = \bar{\mathcal{P}}'' = 0$ in the normal mode Eqs. (6.46)–(6.49) specific to NSE and replacing $[\bar{\rho}, \bar{u}_x, \bar{T}, \bar{\phi}, \bar{\psi}, \bar{\kappa}]^T = [\rho_k, u_{x,k}, T_k, \phi_k, \psi_k, \kappa_k]^T$, where $k = 1$ and 2 stands for fields up and downstream of a shock layer, respectively, we obtain simplified continuity, x -momentum, y -momentum, and energy equation, written as

$$u_{x,k} \hat{\rho}' - i\Omega \hat{\rho} + \rho_k \hat{u}'_x + i\beta \rho_k \hat{u}_y = 0 \quad (6.86)$$

$$\begin{aligned} \frac{T_k}{\gamma Ma^2} \hat{\rho}' + \left(\beta^2 \frac{\psi_k - \phi_k}{2} - i\Omega \rho_k \right) \hat{u}_x + u_{x,k} \rho_k \hat{u}'_x + \phi_k \hat{u}''_x \\ - i\beta \left[\frac{\psi_k - \phi_k}{2} - \psi_k \right] \hat{u}'_y + \frac{\rho_k}{\gamma Ma^2} \hat{T}' = 0 \end{aligned} \quad (6.87)$$

$$\begin{aligned} i \frac{\beta T_k}{\gamma Ma^2} \hat{\rho} + i\beta \left(\psi_k - \frac{\psi_k - \phi_k}{2} \right) \hat{u}'_x - \left(\beta^2 \phi_k + i\Omega \rho_k \right) \hat{u}_y \\ + u_{x,k} \rho_k \hat{u}'_y - \frac{\psi_k - \phi_k}{2} \hat{u}''_y + i\beta \frac{\rho_k}{\gamma Ma^2} \hat{T} = 0 \end{aligned} \quad (6.88)$$

$$(\gamma - 1) T_k \rho_k \hat{u}'_x + i\beta (\gamma - 1) T_k \rho_k \hat{u}_y + (\beta^2 \kappa_k - i\Omega \rho_k) \hat{T} + u_{x,k} \rho_k \hat{T}' - \kappa_k \hat{T}'' = 0 \quad (6.89)$$

$$\text{where } \{\rho_k, u_{x,k}, T_k, \phi_k, \psi_k, \kappa_k\} = \begin{cases} \{1, 1, 1, \frac{-4}{3Re}, \frac{2}{3Re}, \frac{\gamma}{PrRe}\} & k=1 \text{ (upstream)} \\ \{r_\rho, r_\rho^{-1}, r_t, \frac{-4r_t^\omega}{3Re}, \frac{2r_t^\omega}{3Re}, \frac{\gamma r_t^\omega}{PrRe}\} & k=2 \text{ (downstream)} \end{cases} \quad (6.90)$$

These are a set of four complex ordinary differential equations having four unknowns $\hat{\mathcal{P}} = [\hat{\rho}, \hat{u}_x, \hat{u}_y, \hat{T}]^T$, whose solution is sought in terms of γ , Ma , Re , Pr , β , Ω_r , and Ω_i , in both far fields. They can be further written as four second order equations

$$\begin{aligned} \hat{\rho}'' &= \left(\frac{i\Omega}{u_{x,k}} + \frac{\rho_k T_k}{\gamma Ma^2 u_{x,k} \phi_k} \right) \hat{\rho}' + \frac{\rho_k}{u_{x,k} \phi_k} \left(\beta^2 \frac{\psi_k - \phi_k}{2} - i\Omega \rho_k \right) \hat{u}_x + \frac{\rho_k^2}{\phi_k} \hat{u}_x' \\ &\quad - \left(\frac{i\beta \rho_k}{u_{x,k}} + i \frac{\beta \rho_k}{\phi_k u_{x,k}} \left[\frac{\psi_k - \phi_k}{2} - \psi_k \right] \right) \hat{u}_y' + \frac{\rho_k^2}{\gamma Ma^2 u_{x,k} \phi_k} \hat{T}' \end{aligned} \quad (6.91)$$

$$\begin{aligned} \hat{u}_x'' &= -\frac{T_k}{\gamma Ma^2 \phi_k} \hat{\rho}' - \frac{1}{\phi_k} \left(\beta^2 \frac{\psi_k - \phi_k}{2} - i\Omega \rho_k \right) \hat{u}_x - \frac{u_{x,k} \rho_k}{\phi_k} \hat{u}_x' + i \frac{\beta}{\phi_k} \left[\frac{\psi_k - \phi_k}{2} - \psi_k \right] \hat{u}_y' \\ &\quad - \frac{\rho_k}{\gamma Ma^2 \phi_k} \hat{T}' \end{aligned} \quad (6.92)$$

$$\begin{aligned} \hat{u}_y'' &= \frac{i2\beta T_k}{\gamma Ma^2 (\psi_k - \phi_k)} \hat{\rho} + i\beta \left(\frac{2\psi_k}{(\psi_k - \phi_k)} - 1 \right) \hat{u}_x' - \left(\beta^2 \frac{2\phi_k}{(\psi_k - \phi_k)} + \frac{i2\Omega \rho_k}{(\psi_k - \phi_k)} \right) \hat{u}_y \\ &\quad + \frac{u_{x,k} \rho_k 2}{(\psi_k - \phi_k)} \hat{u}_y' + \frac{i\beta \rho_k 2}{\gamma Ma^2 (\psi_k - \phi_k)} \hat{T} \end{aligned} \quad (6.93)$$

$$\hat{T}'' = \frac{i(\gamma - 1)T_k \Omega}{\kappa_k} \hat{\rho} - \frac{(\gamma - 1)T_k u_{x,k}}{\kappa_k} \hat{\rho}' + \frac{(\beta^2 \kappa_k - i\Omega \rho_k)}{\kappa_k} \hat{T} + \frac{u_{x,k} \rho_k}{\kappa_k} \hat{T}' \quad (6.94)$$

where the equation for $\hat{\rho}''$ is obtained by taking the derivative of Eq. (6.86) and substituting for $\hat{u}_x''$, shown in Eq. (6.92), which in turn is obtained by rearranging Eq. (6.87). Equation for $\hat{u}_y''$ can be obtained by rearranging Eq. (6.88), while that for $\hat{T}''$ can be obtained by simplifying Eq. (6.89) using Eq. (6.86). It will be shown that this rearrangement of the system of equations makes it easier to calculate its characteristic determinant.

By defining $e_1 = \hat{\rho}$, $e_2 = \hat{u}_x$, $e_3 = \hat{u}_y$, and $e_4 = \hat{T}$, Eqs. (6.91)–(6.94) can be written in the form

$$e_m'' = \sum_{n=1}^{n=4} (C_{mn} e_m + \mathcal{E}_{mn} e_m') \quad \text{for } m = 1, 2, 3, 4 \quad (6.95)$$

and expressed in a matrix form as

$$\begin{pmatrix} e_1'' \\ e_2'' \\ e_3'' \\ e_4'' \end{pmatrix} = \begin{pmatrix} 0 & C_{12} & 0 & 0 \\ 0 & C_{22} & 0 & 0 \\ C_{31} & 0 & C_{33} & C_{34} \\ C_{41} & 0 & 0 & C_{44} \end{pmatrix} \begin{pmatrix} e_1 \\ e_2 \\ e_3 \\ e_4 \end{pmatrix} + \begin{pmatrix} \mathcal{E}_{11} & \mathcal{E}_{12} & \mathcal{E}_{13} & \mathcal{E}_{14} \\ \mathcal{E}_{21} & \mathcal{E}_{22} & \mathcal{E}_{23} & \mathcal{E}_{24} \\ 0 & \mathcal{E}_{32} & \mathcal{E}_{33} & 0 \\ \mathcal{E}_{41} & 0 & 0 & \mathcal{E}_{44} \end{pmatrix} \begin{pmatrix} e_1' \\ e_2' \\ e_3' \\ e_4' \end{pmatrix} \quad (6.96)$$

where C_{mn} and $\mathcal{E}_{mn}$ are 16 components of coefficient matrices C and $\mathcal{E}$, respectively. Following the similar procedure as Mack [48] for boundary layer equations, the solutions of Eq. (6.95) are assumed to have the general form

$$e_m = \sum_{n=1}^{n=8} D_n b_m^{(n)} \exp(\alpha_n x) \quad \text{for } m = 1, 2, 3, 4 \quad (6.97)$$

where α_n are eight complex characteristic values, $b_m^{(n)}$ are 64 components of eight characteristic vectors $\mathbf{b}^{(n)}$, and D_n are eight arbitrary constants of integration.

We would like to find α_n values that satisfy

$$e_m \rightarrow 0 \quad \text{as} \quad \begin{cases} x \rightarrow \infty & \text{when } k = 1 \text{ (upstream)} \\ x \rightarrow -\infty & \text{when } k = 2 \text{ (downstream)} \end{cases} \quad \text{for } m = 1, 2, 3, 4 \quad (6.98)$$

meaning that the real part of a characteristic value, denoted as $\alpha_{n,r}$, must satisfy

$$\alpha_{n,r} \begin{cases} > 0 & \text{when } k=1 \\ < 0 & \text{when } k=2 \end{cases} \quad (6.99)$$

Substitution of an individual term of the summation in Eq. (6.97) in Eq. (6.95) yields

$$\begin{bmatrix} \alpha_n \mathcal{E}_{11} - \alpha_n^2 & C_{12} + \alpha_n \mathcal{E}_{12} & \alpha_n \mathcal{E}_{13} & \alpha_n \mathcal{E}_{14} \\ \alpha_n \mathcal{E}_{21} & C_{22} + \alpha_n \mathcal{E}_{22} - \alpha_n^2 & \alpha_n \mathcal{E}_{23} & \alpha_n \mathcal{E}_{24} \\ C_{31} & \alpha_n \mathcal{E}_{32} & C_{33} + \alpha_n \mathcal{E}_{33} - \alpha_n^2 & C_{34} \\ C_{41} + \alpha_n \mathcal{E}_{41} & 0 & 0 & C_{44} + \alpha_n \mathcal{E}_{44} - \alpha_n^2 \end{bmatrix} \begin{bmatrix} b_1^{(n)} \\ b_2^{(n)} \\ b_3^{(n)} \\ b_4^{(n)} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \quad (6.100)$$

By setting the determinant of the characteristic matrix equal to zero, we obtain

$$\begin{aligned}
& -(C_{41} + \alpha_n \mathcal{E}_{41}) \begin{vmatrix} C_{12} + \alpha_n \mathcal{E}_{12} & \alpha_n \mathcal{E}_{13} & \alpha_n \mathcal{E}_{14} \\ C_{22} + \alpha_n \mathcal{E}_{22} - \alpha_n^2 & \alpha_n \mathcal{E}_{23} & \alpha_n \mathcal{E}_{24} \\ \alpha_n \mathcal{E}_{32} & \mathcal{E}_{33} + \alpha_n \mathcal{E}_{33} - \alpha_n^2 & C_{34} \end{vmatrix} \\
& + (C_{44} + \alpha_n \mathcal{E}_{44} - \alpha_n^2) \begin{vmatrix} \alpha_n \mathcal{E}_{11} - \alpha_n^2 & C_{12} + \alpha_n \mathcal{E}_{12} & \alpha_n \mathcal{E}_{13} \\ \alpha_n \mathcal{E}_{21} & C_{22} + \alpha_n \mathcal{E}_{22} - \alpha_n^2 & \alpha_n \mathcal{E}_{23} \\ C_{31} & \alpha_n \mathcal{E}_{32} & C_{33} + \alpha_n \mathcal{E}_{33} - \alpha_n^2 \end{vmatrix} = 0
\end{aligned} \tag{6.101}$$

Equation (6.101) forms an octic characteristic equation, $\alpha_n \mathcal{S} = 0$, having a trivial solution $\alpha_8 = 0$, where $\mathcal{S}$ is a septic polynomial having nontrivial roots, α_1 to α_7 . Solving equation $\mathcal{S} = 0$ is difficult, however it was found using the Mathematica software [246] that the individual determinants in Eq. (6.101) exhibit a common quadratic factor $\mathcal{T}$, which allows us to write $\mathcal{S}$ as

$$\mathcal{S} = \mathcal{T} \mathcal{F} = 0 \tag{6.102}$$

where

$$\mathcal{T} = (\alpha_n^2 T_k^\omega - Re \alpha_n - \beta^2 T_k^\omega - Re \Omega_i \rho_k + i Re \Omega_r \rho_k) \tag{6.103}$$

$$\mathcal{F} = \sum_{l=1}^{l=5} \chi_l (\alpha_n)^l + \chi_0 \tag{6.104}$$

The latter polynomial is quintic and has coefficients

$$\begin{aligned}
\chi_5 &= T_k^{-\omega} \\
\chi_4 &= \frac{T_k^{-2\omega}}{4Ma^2\gamma(\gamma-1)} \left[\rho_k(\gamma-1)(4Ma^2\gamma(\Omega_i - i\Omega_r)T_k^\omega + 3ReT_k\rho_k) - Re(4 + 3Ma^2\gamma(\gamma-1)) \right] \\
\chi_3 &= \frac{T_k^{-3\omega}}{4Ma^4\gamma(\gamma-1)} \left[3Re^2(Ma^2 - T_k\rho_k^2) - 8Ma^4\beta^2(\gamma-1)\gamma T_k^{2\omega} \right. \\
&\quad \left. - 2Ma^2Re(4 + 3Ma^2\gamma(\gamma-1))(\Omega_i - i\Omega_r)T_k^\omega\rho_k \right] \\
\chi_2 &= \frac{T_k^{-3\omega}}{4Ma^4\gamma(\gamma-1)} \left[9Ma^2Re^2\rho_k(\Omega_i - i\Omega_r) - 8Ma^4\beta^2T_k^{2\omega}\rho_k\gamma(\gamma-1)(\Omega_i - i\Omega_r) \right. \\
&\quad \left. - 6Ma^2Re\beta^2(\gamma-1)T_k^{1+\omega}\rho_k^2 - 3Re^2T_k\rho_k^3(\Omega_i - i\Omega_r) \right. \\
&\quad \left. + Ma^2ReT_k^\omega(4 + 3Ma^2\gamma(\gamma-1))(\beta^2 - (\Omega_i - i\Omega_r)^2\rho_k^2) \right] \\
\chi_1 &= \frac{T_k^{-3\omega}}{4Ma^2\gamma(\gamma-1)} \left[4Ma^4\beta^4(\gamma-1)\gamma T_k^{2\omega} + 2Ma^2Re\beta^2(4 + 3Ma^2\gamma(\gamma-1))(\Omega_i - i\Omega_r)T_k^\omega\rho_k \right. \\
&\quad \left. + 9Ma^2Re^2(\Omega_i - i\Omega_r)^2\rho_k^2 + 3Re^2\beta^2T_k\rho_k^2 \right] \\
\chi_0 &= \frac{T_k^{-3\omega}\rho_k}{4Ma^4\gamma(\gamma-1)} \left[4Ma^4\beta^4\gamma(\gamma-1)(\Omega_i - i\Omega_r)T_k^{2\omega} \right. \\
&\quad \left. + Ma^2Re\beta^2(4 + 3Ma^2\gamma(\gamma-1))(\Omega_i - i\Omega_r)^2T_k^\omega\rho_k + 3Ma^2Re\beta^4(\gamma-1)T_k^{1-\omega}\rho_k \right. \\
&\quad \left. + 3Ma^2Re^2(\Omega_i - i\Omega_r)^3\rho_k^2 + 3Re^2\beta^2(\Omega_i - i\Omega_r)T_k\rho_k^2 \right]
\end{aligned} \tag{6.105}$$

Further factorization of $\mathcal{F}$ was found to be difficult, and therefore, in this work, the solution to $\mathcal{F} = 0$ is obtained numerically to obtain five solutions α_1 to α_5 using specified values of γ , Ma , Re , β , Ω_i , Ω_r , and far field flow quantities given in Eq. (6.90) for $k = 1$ and 2 , *i.e.* up and downstreams, respectively.

It is possible to obtain an approximate solution for one of the five characteristic values, denoted as α_1^{appx} , if the sum of the terms of the order $O(\alpha_n^l)$ for $l \geq 2$ is smaller in comparison to the term $O(\alpha_n)$, *i.e.* the relative magnitude defined by the ratio

$$\mathcal{M} = \left| \frac{\sum_{l=2}^5 \chi_l \left(\alpha_1^{\text{appx}} \right)^l}{\chi_1 \alpha_1^{\text{appx}}} \right| \ll 1 \tag{6.106}$$

Then the approximate solution can be written as

$$\alpha_1 \approx \alpha_1^{\text{appx}} = -\frac{\chi_0}{\chi_1} \quad (6.107)$$

By simplifying Eq. (6.107), we can write

$$\alpha_1^{\text{appx}} = \frac{\mathcal{N}}{\mathcal{D}} = \frac{\mathcal{N}_a + \mathcal{N}_b + \mathcal{N}_c + \mathcal{N}_d + \mathcal{N}_e}{\mathcal{D}_a + \mathcal{D}_b + \mathcal{D}_c + \mathcal{D}_d} \quad (6.108)$$

where

$$\begin{aligned} \mathcal{N}_a &= -\rho_k 4Ma^4 \beta^4 \gamma (\gamma - 1) (\Omega_i - i\Omega_r) T_k^{2\omega} \\ \mathcal{N}_b &= -\rho_k Ma^2 Re \beta^2 \left(4 + 3Ma^2 \gamma (\gamma - 1) \right) (\Omega_i - i\Omega_r)^2 T_k^\omega \rho_k \\ \mathcal{N}_c &= -\rho_k 3Ma^2 Re \beta^4 (\gamma - 1) T_k^{1+\omega} \rho_k \\ \mathcal{N}_d &= -\rho_k 3Ma^2 Re^2 (\Omega_i - i\Omega_r)^3 \rho_k^2 \\ \mathcal{N}_e &= -\rho_k 3Re^2 \beta^2 (\Omega_i - i\Omega_r) T_k \rho_k^2 \\ \mathcal{D}_a &= 4Ma^4 \beta^4 \gamma (\gamma - 1) T_k^{2\omega} \\ \mathcal{D}_b &= 2Ma^2 Re \beta^2 \left(4 + 3Ma^2 \gamma (\gamma - 1) \right) (\Omega_i - i\Omega_r) T_k^\omega \rho_k \\ \mathcal{D}_c &= 9Ma^2 Re^2 \rho_k^2 (\Omega_i - i\Omega_r)^2 \\ \mathcal{D}_d &= 3Re^2 \beta^2 T_k \rho_k^2 \end{aligned} \quad (6.109)$$

It turns out that α_1 governs the decay behavior of the first and second least stable stationary and traveling eigenmodes for the conditions studied in this work and α_1^{appx} is a good approximation for α_1 when $\mathcal{M}$ is less than 1%, as discussed in Sec. 6.4.1.

On the other hand, $\mathcal{T} = 0$ can be solved exactly to obtain two roots

$$\alpha_6 = T_k^{-\omega} \left(\frac{Re}{2} + \zeta + i\eta \right) \quad (6.110)$$

$$\alpha_7 = T_k^{-\omega} \left(\frac{Re}{2} - \zeta - i\eta \right) \quad (6.111)$$

where

$$\begin{aligned}
\zeta &= \frac{1}{\sqrt{2}} \sqrt{\sqrt{\theta^2 + Re^2 \Omega_r^2 T_k^{2\omega} \rho_k^2} + \theta} \\
\eta &= -\frac{1}{\sqrt{2}} \frac{\Omega_r}{|\Omega_r|} \sqrt{\sqrt{\theta^2 + Re^2 \Omega_r^2 T_k^{2\omega} \rho_k^2} - \theta} \\
\theta &= \frac{Re^2}{4} + \beta^2 T_k^{2\omega} + Re \Omega_i T_k^\omega \rho_k
\end{aligned} \tag{6.112}$$

Since $\zeta \geq 0$, it is easy to see the conditions on the real parts of α_1 and α_2 , written as

$$\alpha_{6,r} > 0 \quad \forall \quad \Omega_i, \Omega_r \in \mathbb{R} \tag{6.113}$$

$$\alpha_{7,r} \begin{cases} > 0 & \text{if } \zeta < \frac{Re}{2} \\ < 0 & \text{if } \zeta > \frac{Re}{2} \end{cases} \tag{6.114}$$

Therefore, it is seen from Eq. (6.113) that $\alpha_{6,r}$ satisfies a condition in Eq. (6.99) only in the upstream but not in the downstream, hence it is not a physically possible characteristic value. $\alpha_{7,r}$, on the other hand, may satisfy both conditions in Eq. (6.99), if the first and second conditions in Eq. (6.114) are met in the up and downstreams, respectively. Requirement of both of these conditions lead to the following inequality

$$-\frac{\Omega_r^2 + \beta^2}{Re} > \Omega_i > r_i^\omega r_\rho \left(-\frac{\Omega_r^2 + \beta^2}{Re} + \frac{\beta^2}{Re} (1 - r_\rho^{-2}) \right) \tag{6.115}$$

At conditions of $Ma = 1.2$ shock layer studied in this work, for a stationary continuum mode ($\Omega_r = 0$), the above equation leads to $-735 > \Omega_i > 677$ showing that spatial decay of eigenfunctions of type α_7 exists for substantially more damped continuum modes than the least damped continuum mode discussed in Sec. 6.4.

Chapter 7

Conclusion and Future Work

The major findings of this work are summarized in this chapter with some considerations for future research directions.

7.1 Conclusions

A new efficient DSMC framework based on AMR/octree unstructured grids has been demonstrated for the modeling of near-continuum, strong shocks in hypersonic flows. The SUGAR code is able to capture the different length scales in such flows through the use of a linearized representation of the unstructured grid using the Morton-based space filling curve for efficient access of collision cells or leaves. This problem is challenging for DSMC solvers using unstructured grids because the high gradients of macroscopic flow quantities in the shock layer create unbalanced root-to-leaf cell structures. Comparison with a two-level Cartesian grid DSMC solver on a single processor showed that for an unstructured approach to be competitive, particle mapping must be performed on a linearized octree structure, and close attention must be paid to the particle data structure. It was shown that the use of a linked-list-based approach, although responsive to the dynamic variation of particle number densities throughout the simulation domain, can lead to large time penalties when accessing memory cache. If these two general factors are considered, the AMR/octree approach is competitive timewise with multi-level Cartesian grid or patch approaches and offers much more flexibility for flows with embedded geometries and flows that have both compression and expansion regions.

With an efficient single processor version of the code, strategies were developed to achieve a strong scaling of nearly ideal speed-up on 4096 processors and 87% weak scaling efficiency for 8192 processors for a strong shock created by flow over a hemisphere. To achieve these very good scalings, algorithms were developed to weight the computational work of a processor by the use of profiled run-time data, create maps to optimize processor point-to-point communications, and efficiently generate new DSMC particles every time step. In addition, for computing temperature-dependent rotational and vibrational relaxation rates in the thermal nonequilibrium models required in high Mach number flows, accurate modeling of local collision temperatures is carried out on a sampling grid designed to be compatible with the Morton-based space-filling-curve usage of leaf cells.

An important goal of our code development was to enable DSMC simulations in the continuum regime. Because such simulations require many billions of computational particles and cells, additional optimizations were made for reducing the run-time memory usage of processors. Our approach was demonstrated in the modeling of the SBLIs in a hypersonic flow at Mach 7, unit Reynolds number $Re = 5.2 \times 10^4 \text{ m}^{-1}$, and Knudsen number $Kn = 3.4 \times 10^{-3}$ over a double-wedge configuration having $30^\circ - 55^\circ$ cross-sectional profile and a half-span of 50.8 mm. The simulation reproduced the complex hypersonic SBLIs, captured three-dimensional surface rarefaction effects such as velocity and temperature jump, and showed that the pressure relief effects affect the size of the separation bubble, which in turn influences gas-surface measurements such as pressure and heat flux over the span. The flow was found to be unsteady, which led us on a new path to explore the reason for unsteadiness by eliminating the effect of pressure-relief, *i.e.* to conduct spanwise-periodic simulations to investigate the stability of the 2-D base flow against self-excited, small-amplitude, spanwise-periodic perturbations.

The fully-resolved spanwise-periodic DSMC simulations revealed a self-excited linear instability mechanism that causes the 2-D base flow to become unstable. The kinetic approach permitted space- and time-accurate modeling of the internal structure of shocks, surface rarefaction effects, thermal nonequilibrium, as well as, for the first time, time-accurate description of small-amplitude three-dimensional self-excited perturbations that arise from the interaction of the shock system with the three-dimensional LSB both inside the separation and detached shock layers and in the LSB. In line with the findings of Tumuklu *et al.* [23] for Mach 16 flow over an axisymmetric double cone, and Tumuklu *et al.* [30] for the two-dimensional counterpart of the present double wedge flow, the LSB was found to be strongly coupled with the separation and detached shock system. The origin of linear instability was traced in the vicinity of primary separation, *i.e.* the flow region of interaction of the separation shock and the bubble. This finding clearly points out that the observed mechanism is one of self-excitation and not the result of amplification of incoming upstream disturbances, a result which generalizes the concept of *oscillator*, introduced in an incompressible context either in weakly-nonparallel [124, 126] or in fully nonparallel flow [125], to include the interaction of the entire separation and detached shock system with the three-dimensional LSB.

The presence of amplified linear instability leads to the formation of spanwise-periodic flow structures in three-dimensional perturbations of macroscopic flow quantities inside the LSB, corresponding to the well-known striation wall pattern. More importantly, the present study showed that spanwise-periodic linear instability also exists in the internal structure of the separation and detached shock layers and in the vicinity of contact surfaces downstream of triple points; this shock-layer instability, which takes the form of cats-eyes patterns, is seen for the first time in the present work. Linear instability in the shock layer and the LSB are synchronized, with the spanwise-periodicity length of the structures forming inside the bubble and in the shock system being identical, and their amplitude growing with

the same average, linear temporal growth rate, $\Omega_i = 5.0 \text{ kHz} \pm 0.16\%$ at the conditions examined. The slow linear growth and long time-scale of low-frequency unsteadiness suggest that experimental test times must be sufficiently long if differences between the various experimental and numerical results are to be reconciled. Furthermore, the long time simulation of the flow revealed that, past the stage of linear instability growth, low-frequency unsteadiness of the triple point and consequently of the separation bubble sets in, having a time period of oscillation of $46T$, which corresponds to a Strouhal number of $St \sim 0.028$, consistent with the existing literature on turbulent SBLI. The long-time spatio-temporal evolution of the flow at the triple point T_2 revealed the presence of spanwise corrugation of the shock as well as sinusoidal oscillations in time.

The need for understanding the role of the internal structure of a shock in the stability of high-speed flows motivated the study of molecular fluctuations in an isolated one-dimensional shock. The investigation of macroscopic fluctuations in a DSMC-computed argon shock layer revealed two orders of magnitude lower dominant frequencies of fluctuations than found in the freestream, where they are on the order of inverse mean-collision-time. These disparities were attributed to the differences in particle distribution functions in the nonequilibrium zone of shock versus the equilibrium regime upstream. The investigation of correlation of the bimodal PDF of x -directional normalized particle energies with the overall stress in the shock inspired a Lotka-Volterra type two-energy-bin model, which accounted for the interaction of particles in the low and high energy bins of the PDF through intermolecular collisions and particle fluxes from neighboring computational cells. The model showed that the low frequencies in the shock correspond to timescales of relaxation of high-energy particles coming from upstream in the background of low-energy particles that have collided with particles downstream. In the freestream, the model predicted faster decay of fluctuations, $O(\text{MHz})$, and more importantly, an absence of low-frequency fluctuations consistent with the DSMC spectral analysis. Finally, a Strouhal number was defined based on the upstream bulk velocity and the density-gradient based shock-thickness to nondimensionalize the low-frequencies and was found to range from 0.007 to 0.011 with ± 1 standard deviation between 0.001 and 0.02 across a wide range of Mach numbers from 2 to 10. The range of Strouhal numbers was found to hold approximately for a Mach 7.2 shock simulated with different upstream temperatures and number density and explain qualitatively the frequencies inside a shock observed in the work of Chynoweth *et al.* [212].

Furthermore, a simple, more-accurate approach was devised to estimate the low-frequency fluctuations in a 1-D shock structure of argon, using analytically-derived PDFs of particle energies. The analytical PDFs in the up and downstream equilibrium regions of the shock compared very well with PDFs obtained from DSMC, and they were shown to have the form of noncentral Chi-squared PDFs. Using an approach similar to the bimodal approximation of Mott-Smith [68], the bimodal NCCS PDFs inside shock layers were constructed as a linear combination of the equilibrium upstream and downstream PDFs. By correlating the bimodal NCCS PDFs in shocks with the low-

frequencies of molecular fluctuations previously obtained from DSMC for the Mach number range from 3 to 5, it was found that the average low-frequency is directly proportional to the location of the high energy peak in the PDF generated by the contribution of particles from the upstream. For cases where the Mach number and upstream number density is constant, but upstream temperature is varied, the low-frequencies are found to be proportional to the most-probable-speed at the location of maximum velocity-gradient magnitude in the shock obtained from the Mott-Smith velocity PDF. Using these linear functions, it is demonstrated that one can estimate the low-frequency of fluctuations at an upstream number density of 10^{22} m^{-3} for a wide range of upstream temperatures and Mach numbers not explicitly simulated in our previous DSMC simulations. In the future, a similar approach can be used at other upstream number densities, and for other gases of practical importance, where the DSMC-derived low-frequencies can be obtained for a few selected input conditions, and using those, a broader database of low-frequencies can be generated through established correlations.

The presence of low-frequency fluctuations in shock layers suggests that they may play a key role in the receptivity process of transition in hypersonic flows and SBLIs, especially when the shock-thickness is comparable to other important length scales in the flow. Our work implies that the leading-edge shock interactions with freestream disturbances, such as tunnel-induced noise, may result in selective amplification of disturbances in the low-frequency range and consequent excitation of the downstream boundary-layer. Future numerical investigations focused on understanding the effect of freestream disturbances on transition should not ignore shock-induced perturbations in the boundary-layer within the range of Strouhal numbers established in this work. The estimates provided for low-frequency molecular fluctuations in the shock can be used as boundary conditions in the receptivity analyses to construct simplified models that account for the interaction of leading-edge shock with the boundary layer or to aid understanding of the changes in the spectrum of freestream noise after it interacts with the shock prior to excitation of the boundary-layer.

Finally, a framework for studying modal analysis of 1-D shock layers was developed, which solves the normal mode equations obtained from the traditional NSE formulation as well as the newly developed ACE formulation, which is derived based on the well-known Mott-Smith's assumption of bimodality of particle distribution functions for gas of Maxwell molecules ($\omega = 1$). The motivation for using the latter stemmed from the fact that its constitutive equations are substantially better than the traditional NSF equations at approximating the DSMC-derived normal viscous stresses and the x -directional heat flux at high Mach numbers ($M > 1.2$). Temporal analysis for $Ma = 1.2$, 3, and 5 one-dimensional shock layers was carried out assuming perturbation wavelengths on the order of maximum mean-free-path in the shock and using both formulations, which allowed for monitoring the effects of increasing degree translational nonequilibrium on the stability of shock layers. At $Ma = 1.2$, the decay rates of modes on the least stable branch predicted by the ACE formulation compared very well with the NSE formulation, as expected from the small

degree of translational nonequilibrium in the shock layer. At high Mach numbers, the comparison highlighted that the non-continuum effects lead to a less stable branch and that the prediction of decay rates strongly depends on how well the constitutive relations resolve the true translational nonequilibrium region in the shock layer.

The eigenfunctions of the stationary and traveling modes of the least stable branch u were found to decay monotonically and sinusoidally in far fields, respectively, while the spatial decay rate was an order of magnitude lower in the upstream than the downstream. This spatial decay of eigenfunctions was shown to be governed by only one physically possible characteristic value of out seven, predicted by a septic characteristic equation obtained by simplifying normal mode equations in far fields of a shock layer. This characteristic value α_1 was numerically shown to be the root of the quintic polynomial, $\mathcal{F}$, factorized from the septic polynomial, $\mathcal{S}$, while an approximate equation, α_1^{appx} , was obtained, which is in excellent agreement with α_1 , as long as the sum of the higher-order terms in the quintic polynomial that were ignored for obtaining the approximate solution is lower than 4% of the first-order term. By analyzing the equation for α_1^{appx} , which depends on γ , Ma , Re , β and far field flow quantities, it was shown that there exists a range of decay rates Ω_i for which physically acceptable values of α_1^{appx} are possible in both far fields. Linear stability analysis predicts a least stable continuous branch having decay rates close to the maximum limit of this range. By studying the dependence of the limits of this range on governing parameters, it was shown that this family of modes is always stable, which becomes less stable by the decrease in Re , increase in Ma , decrease in γ , and increase in the degree of translational nonequilibrium. It was also shown that the ACE formulation, which uses a general, better constitutive equation for stress tensor than used in the NSE, must predict a less stable decay rate than the NSE formulation, consistent with the observations of linear stability analysis.

The decay rate Ω_i was found to be nearly independent of the spanwise wavenumber, β , when β is close to β_{lim} , while Ω_i changes nonlinearly with β for lower values of β . The linear stability analyses conducted at lower β values, *i.e.* at higher ratio of perturbation wavelengths to the maximum mean-free-path, $L_y^*/\bar{\lambda}_{\max}^*$, showed that the continuous branch becomes more stable by decreasing β . Comparison of eigenfunctions obtained from the two formulations showed that both stationary and traveling modes compared very well at $Ma = 1.2$, while with the increase in Mach number, differences were observed between the two formulations in both the shock layer as well as far fields. These differences were attributed to the better capability of the ACE than NSE in approximating the increasing region of translational nonequilibrium at higher Mach numbers. Furthermore, eigenmodes on the second less stable branch l exhibit eigenfunctions having a very gradual decay downstream of the shock layer compared to upstream in contrast to modes on branch u and this spatial behavior was also found to be governed by the analytical solution of α_1^{appx} . The gradual decay of these eigenfunctions on the downstream side suggests that these modes, although less stable, may be important as they may interact with a boundary layer formed on a blunt body.

7.2 Suggestions for Future Work

7.2.1 Effects of nonequilibrium thermochemical reactions on shock-laminar separation bubble instabilities

Our study of self-excited linear instabilities in spanwise-periodic simulations over a double-wedge only involved molecular nitrogen species. However, Tumuklu *et al.* [30] had also investigated 2-D flows over the same configuration using non-reacting air species consisting of molecular nitrogen and oxygen and reacting air species where oxygen dissociation and $N_2 + O$ exchange reaction was modeled. Nonequilibrium thermochemical effects were found to affect shock structure, size of the separation bubble, and the time required to reach a steady state. These effects may also influence the linear instabilities observed in our work, and therefore, it would be instructive to study spanwise-periodic flow simulations of these flows.

To perform such simulations, the SUGAR code must be extended to include chemical reactions. Specifically, particle-data structures must account for the modification of species identity of post-collisional products, their sorting, and the creation of new product species. The existing data structure keeps track of species ID; however, implementation of algorithms such as the total collision energy (TCE) model [247], a general user interface to specify chemical reactions, and a rigorous validation study is required.

7.2.2 Interactions of low-frequency fluctuations in shock layers on external disturbances

We have shown that the internal structure of shocks exhibits two orders of magnitude lower fluctuations than the equilibrium region in the upstream. The next step is to introduce small-amplitude, random disturbances in various frequency ranges upstream of the shock and investigating their interactions with a shock. It is expected that the low-frequencies with Strouhal number $St \sim O(0.01)$ will be amplified more than the higher frequencies. It is problematic to study this problem in a 1-D setup for a normal shock because of issues related to boundary conditions discussed in Chapter 4. Therefore, an almost-normal bow shock over a blunt body with specular walls will be an easier case. Furthermore, similar studies on oblique shocks can test if the boundary-layers can be indirectly excited through such interactions.

7.2.3 Investigations of stability analysis of shocks

The temporal analysis of 1-D shocks against two-dimensional harmonic perturbations revealed a family of modes having eigenfunctions whose spatial decay rate is governed by the approximate solution α_1^{appx} of a quintic polynomial, $\mathcal{F}$. This solution showed that these modes always decay, *i.e.* physically acceptable values of α_1^{appx} exist in both far

fields for $\Omega_i < 0$. The exact solution of five roots of $\mathcal{F}$ is found to be very difficult; however, such investigation may help us better understand if other roots exhibit physically acceptable solutions in both far fields for some parametric values of $\gamma, Ma, Re, \beta, \Omega$ and far field flow quantities, and whether such acceptable solutions exist for $\Omega_i > 0$, *i.e.* when a shock is unstable. Our temporal analysis can be further extended to include bow shocks and oblique shocks, where the latter case would require a simultaneous analysis of shock and boundary-layer. Furthermore, the ansatz used in our temporal analysis (Eq. 7.1) assumed that harmonic perturbations evolve exponentially in time while retaining the shape of amplitude functions. However, we also need to investigate non-modal effects assuming ansatz

$$\mathcal{P}(x, y, t) = \bar{\mathcal{P}}(x) + \epsilon \hat{\mathcal{P}}(x, t) \exp[i\beta y] + c.c. \quad (7.1)$$

which allows for investigation of transient algebraic growth of perturbations [248].

7.2.4 Effect of material environment interactions on flow stability

From the historical example of the X-15 flight described in Chapter 1, we learned that the intense heat from the impinging shock burnt the ablative material coating on the aircraft's surface. Such interactions must, in turn, alter the features of SBLIs. Spacecrafts for exploratory space missions also experience extreme thermal conditions during reentry, and to reduce the heat load, their heat shields are equipped with an ablative thermal protection system (TPS). A major advantage of this class of TPS materials is the porous microstructure that makes them lightweight with the capability to reduce heat loads on the space capsule by thermal depolymerization, also known as the process of pyrolysis [249–252]. These materials may interact chemically with species in the high-temperature environment surrounding the spacecraft, which are known as material environment interactions. Understanding the effect of these interactions on the stability of the flow, SBLIs, and bow shocks over space capsules re-entering the Earth's atmosphere is a relatively unexplored topic [253].

In the course of author's Ph.D., he has developed stochastic approaches to study thermal response modeling of microstructures of ablative heatshield materials [252, 254]. Since these works do not investigate flow instabilities in the external flow environment, they are somewhat unrelated to the main topic of this work and hence are not included in this dissertation. However, future students may find them useful, especially the analysis of timescales of thermal response, for investigating flow instabilities in the presence of ablative materials.

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