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BOOK OF ABSTRACTS

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R. Caflisch, "Accelerated Simulation Methods for Rarefied Gases and Plasmas"
**Session 1: DSMC Development**

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Development of the ARISTOTLE Webware for Cloud-Based Rarefied Gas Flow Modeling

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High vacuum environments are critical for many industrial processes, including manufacturing of micro- and nano-electronics, pharmaceuticals, and surface coatings [1]. Computational tools, such as the direct simulation Monte Carlo (DSMC) method [2], can help us better understand, analyze, and optimize these important physical processes. However, the complexity to install, test, and set-up typical DSMC implementations can create a barrier for effective use by non-DSMC experts. This paper reviews the recent development of A Rarefied Industrial gas Simulation Tool On The cLoud Environment (ARISTOTLE) webware that will enable cloud-based modeling of rarefied gas flows. ARISTOTLE [3] is built on the open-source SPARTA library [4,5], developed by our partners at Sandia National Laboratories. The goal is to allow users to log-in to the ARISTOTLE interface through a web browser, define the geometry and inflow parameters, and execute the simulation seamlessly on a scalable compute architecture. Post-processing can be performed on the cloud environment using available tools or the user can alternatively download the full simulation results file for off-site storage and further post-processing. This work leverages a workflow structure that enables a wide range of simulation scenarios that are highly customizable to predict both steady-state and transient gas flows that interact with arbitrary geometric features. Automated routines are used to confirm that DSMC cell-size and time-step requirements are met. In addition to a description of the architecture, this work will present selected analysis of transient flows that have been performed with the DSMC library. For example, Figure 1 (left) shows a snapshot from simulation of gas flow within a bell chamber and Figure 1 (middle) and (right) show snapshot a rarefied gas plume interacting with a substrate.

Fig.1: (left) Simulation of gas flow within a bell chamber. (middle) Snapshot of gas molecules rendered within a chamber with a plume-substrate interaction. (right) Quantitative prediction of the total gas number density and gas velocity streamlines for the plume-substrate interaction snapshot.

ACKNOWLEDGEMENTS

The authors graciously acknowledge funding provided by the US Department of Energy under award DE-SC0013088 and Spectral Sciences, Inc. under IR&D award 6186-001.

REFERENCES

The ability of SPARTA [1], a parallel DSMC code to deliver improved computational efficiency while maintaining the unprecedented accuracy of the DSMC method, in dealing with complicated gas flows is examined. To this end, SPARTA is validated against complex flows in two and three dimensions, where experimental results are available. The benchmark cases examined for this purpose include two and three dimensional ones, such as the 25/55 deg biconic geometry proposed by the NATO Research Technology Organization [2], [3] and the 70 deg. spherically blunted cone by Allègre and et al. [4]. The flow around these configurations is characterized by strong shock-shock, shock-boundary layer interactions, and large separation areas. Thus, these cases contain high-speed low-density regions, low-speed high-density regions, laminar expanding regions, and laminar recirculation zones. These features are sensitive to the temporal and spatial discretization of the simulations, so a DSMC simulation of these situations exercises the full spectrum of spatial and temporal conditions, making them particularly useful as validation cases. Figure 1, presents the results for the 25/55 deg. biconic, featuring an Edney Type-V shock-shock interaction.

![Figure 1. Total velocity plot – 2D axisymmetric simulation.](image)

REFERENCES


ACKNOWLEDGEMENTS

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.
Implementation of the real gas effects models in SMILE-GPU DSMC numerical tool

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The Direct Simulation Monte Carlo (DSMC) [1] method is the major numerical technique for solving problems of the high-altitude aerothermodynamics of space vehicles. For the altitudes lower than 85 km (in the near-continuum flow regime) the applicability of methods of continuum CFD is still questionable, yet 3D DSMC computations may require tremendous computational resources. One of the promising areas of high-performance computations is the employment of the Graphics Processing Units (GPUs). The high-performance DSMC computational tool SMILE-GPU for 3D computations on hybrid GPU/CPU-based supercomputers has been developed at ITAM (Novosibirsk) and applied to different non-reacting rarefied flows with significant degree of thermal non-equilibrium [2-3].

At altitudes below 85 km, the aerothermodynamic properties of reentry vehicles are substantially affected by dissociation and exchange chemical reactions. Spacecraft reentry of Martian or Lunar missions occurs at rather high velocities, and ionization processes and plasma effects should be taken into account as well. For near-continuum flow regime surface chemical processes can have substantial effects on aerothermodynamics. The present work is aimed at further development of SMILE-GPU tool in order to make it applicable to non-equilibrium chemically reacting ionized flows about space vehicles with catalytic recombination on the surface [4].

Parallel computations on GPUs are performed in accordance with the Single Instruction Multiple Data (SIMD) technology: one instruction is simultaneously performed by all cores to the set of data corresponding to these cores. Efficient implementation of the real gas effects models on GPUs requires taking into account specific features of the GPU architecture. For example, to increase the computation efficiency, the procedure of chemical collisions is taken outside of the collision cycle. If a chosen pair of particles is expected to react in a collision, this pair is stored in a special list. After the collision cycle is finished, these reactions are performed. As all reactions are implemented in the same manner and each thread models one reaction, this procedure is extremely efficient for the SIMD technology.

The following gas-phase and surface chemical processes have been implemented at the current stage:
- dissociation and exchange chemical reactions;
- associative and electron-impact ionisation as well as dissociative recombination reactions and surface neutralisation;

Detailed verification of the new version of the SMILE-GPU tool and its application to problems of spacecraft aerothermodynamics will be presented in the full-length paper.

REFERENCES

Extension of the Viscous Collision Limiting Direct Simulation Monte Carlo Technique to Multiple Species

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There are many flows of interest that span a wide range of length scales where regions of both rarefied and continuum flow exist and neither DSMC nor CFD are appropriate everywhere. One such flow problem is the low-to-intermediate altitude (below roughly 80 km) hypersonic flow around a lifting re-entry vehicle where large gradient-based Kn values are expected within the bow shock, in the shock layer around sharp leading edges, in shock wave boundary layer interaction regions, and in near-wake regions involving rapid expansion and/or comparatively low density. For flows such as these, hybrid one or two-way coupled CFD-DSMC techniques have been developed [1-3] that can provide both high accuracy and high efficiency, but tend to suffer from considerable code complexity and/or a “person in the loop” requirement which limits automation and increases the time required to generate results. In an effort to overcome these limitations, efforts have also been devoted to the efficient extension of DSMC to very low Kn regimes [4, 5] where code complexity is greatly reduced and there remains consistency in models for various gas phenomena.

More recently, a new viscous collision limiter (VCL) DSMC technique [6, 7] has been proposed to incorporate effects of physical diffusion into collision limiter calculations. It used local time step adaptation to equate numerical and physical transport coefficients, and employed a temperature-based viscosity model as an alternative to collision dynamics models traditionally used for diffusive transport modeling in DSMC. The original work was derived for a single species gas and a representative blunt-body flow is presented in Fig.1 as a comparison of translational temperature between VCL-DSMC and DSMC.

The current work extends the VCL-DSMC technique to gases with multiple species. Similar arguments are used to equate numerical and physical transport coefficients. However, a more rigorous treatment of determining the mixture viscosity was required. To do this, the work of Stephani et. al. [8, 9] is referred to where they develop a consistent treatment of transport properties for DSMC/CFD applications. In particular, they derive a mixture viscosity from the VHS/VSS cross section models determined from the first-order Chapman-Enskog approximation of the mixture viscosity. VCL-DSMC simulations are to be performed with efficiency and accuracy comparisons to traditional DSMC and CFD solutions.

REFERENCES

Session 2: Moment Equations I

(INVITED) Torrilhon, "Modeling Rarefied Gas Flow Based on Moment Equations"

Mohammadzadeh, Struchtrup, "Modeling Thermal Transport over Micron Distances in a Silicon Membrane"

Tensuda, Groth, McDonald, "Multi-Dimensional Validation of a Maximum-Entropy-Based Interpolative Moment Closure"
Modeling Rarefied Gas Flow Based on Moment Equations

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It is generally accepted that kinetic theory based on a statistical description of the gas provides a valid framework to describe processes in a rarefied regime or at small scales. However, in many applications this detailed statistical approach yields a far too complex description of the gas. It turns out to be desirable to have a continuum model based on partial differential equations for the fluid mechanical field variables, like density, velocity and temperature. This model should accurately approximate the multi-scale phenomena present in kinetic gas theory in a stable and compact system of field equations.

For small Knudsen numbers the classical laws of Navier-Stokes and Fourier are very successfully applied. In the transition regime at intermediate Knudsen numbers a fluid description is still possible, although a larger set of field variables or higher derivatives may be needed. The limit for continuum models is currently somewhere between \( Kn=0.5 \) and 1, depending on the process. The aim of the research field is to establish continuum models and push their limit further. This talk will review the achievements of moment equations and, in particular, regularized moment equations, as presented in [1] and recently discussed in [2], applied to flows in the transition regime. These models have been further developed in the last years and are available for a number for various physical applications, like mixtures [3] and polyatomic gases [4].

One of the main advantages of continuum models is typically the potential computational efficiency. However, there is another interesting fact that is often underestimated. Nonequilibrium flows exhibit behavior that contrasts with the intuition of fluid dynamics and is difficult to understand. The simulations of Boltzmann and DSMC may give accurate predictions of this behavior, but it is important to realize that their results actually do not easily provide a detailed physical understanding of the process. The reason is that our understanding of physical phenomena is often based on the structure and qualitative behavior of mathematical equations and their solutions. Our intuition about these phenomena arises from analytical solutions for small models that display how the coupling of the mathematical terms influences the behavior of the solution. The mere simulation result does not allow this kind of understanding. The advantage of continuum equations is that they come with manageable partial differential equations that allow one to identify physical effects and coupling phenomena that occur in nonequilibrium flows. Hence, we will discuss some exemplary analytical solutions for model situations that provide physical insight into the intriguing flow patterns and help us understand rarefaction effects.

We will also present results for nonlinear extensions of moment equations based on maximum-entropy closures [5]. This approach requires to use modern hardware acceleration techniques but may provide a efficient CFD tool in particular for hypersonic rarefied gases and plasmas.

REFERENCES

Modeling Thermal Transport over Micron Distances in a Silicon Membrane

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Johnson et al [1] used the thermal grating method to experimentally study the heat transport in a silicon wafer. Their measurements demonstrate that the diffusion equation fails to predict the transport of heat already at micron level. They studied the thermal decay in a silicon wafer and reported that low frequency phonons, that cannot be captured by the classical heat equation, play an important role when the length scale of the flow becomes less than 5 μm. Moreover, by changing the width of the Silicon wafers, they studied the effect of boundaries on heat transport, and observed that due to the boundary drag, less heat is transported when the wafer becomes narrower.

Recently, we proposed a system of moment equations [2] to describe phonon transport in crystal lattices. The underlying kinetic equation employs frequency dependent relaxation times to distinguish between low and high frequency phonons in phonon-phonon collision processes. Moreover, we considered a finite size for the Brillouin zone, which depends on the working temperature of the system. In this system of equations macroscopic moments are based on powers of frequency and wave vector to properly capture all microscopic properties of phonons.

Using Grad's closure [3], we derived a closed system of macroscopic moment equations, and its corresponding set of boundary conditions that can capture the heat transport in crystal lattice at small scales. We used this system to model a simple one dimensional steady state heat transfer problem in a very long silicon wafer, and demonstrated that the heat transfer in the wafer deviates from the Fourier's law well below the classical threshold for the diffusion equation.

In the current study we employ this system of moment equations to model the thermal grating experiment reported by Johnson et al. [1]. For this means, we use eigenvalue-eigenvector analysis to analytically solve the two dimensional Poiseuille flow of phonons in a Silicon wafer. Our results show a good agreement with the reported experimental data, and demonstrate the importance of considering low and high frequency phonons at micro scale and beyond.

ACKNOWLEDGEMENTS

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Multi-Dimensional Validation of a Maximum-Entropy-Based Interpolative Moment Closure

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and

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The method of moment closures offers an alternative modelling technique for transition-regime non-equilibrium flows with the potential for reduced computational cost relative to traditional methods, such as direct simulation Monte Carlo (DSMC). Recently, a new, interpolative-type, maximum-entropy-based, 14-moment closure, which considers heat transfer, has been proposed [1]. Unlike the maximum-entropy closure on which it is based [2], the interpolative closure provides closed-form expressions for the closing fluxes. While still presenting singular solutions in regions of realizable moment space, the interpolative closure proves to have a large region of hyperbolicity while remaining tractable. Furthermore, its singular nature is deemed advantageous for practical simulations, such as the computation of shocks with large Mach numbers [1].

This study presents a further numerical and mathematical investigation of this new moment closure. A mathematical dispersion analysis of the governing moment transport equations is performed, which verifies the system’s stability as well as demonstrating its potential to be applied to high-Mach-number flows. The applicability of the 14-moment interpolative closure to multi-dimensional flows is examined by solving several two-dimensional canonical flow problems, including Couette flow, conduction between heated flat plates, subsonic flow past a circular cylinder, and lid-driven cavity flow, in both the continuum and transition regimes. As such, this study represents one of the first applications of this novel closure to multi-dimensional flows. In order to obtain solutions to the governing equation system, a finite-volume numeric solver and corresponding solid-wall half-Maxwellian boundary conditions have been developed. Both an implicit and semi-implicit time-marching method have been considered, and it is found that the fully-implicit method leads to significant computational gains, including up to a factor of 15 reduction in CPU time.

The two-dimensional results are compared to analytic solutions; Navier-Stokes solutions; other moment closures, such as the 10-moment Gaussian and regularized Gaussian closures [3]; DSMC results; and experiment. The Couette flow and heat transfer between flat plates cases were found to be in good agreement with trusted analytical solutions, and correctly predicted the non-equilibrium phenomena of velocity slip and temperature jump. The results for subsonic flow around a circular cylinder showed expected behaviours such as velocity slip and an increase in boundary-layer thickness with increasing Knudsen number. These results also showed an improved prediction of drag coefficient for high-Knudsen-number flows, relative to the 10-moment Gaussian closure, when compared to experimental results. The lid-driven cavity results were successful in predicting the presence of regions of expansion cooling and viscous heating, as well as a counter-gradient heat flux, which was also seen in the DSMC results.

ACKNOWLEDGEMENTS

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Session 3: Micro-channel Flow

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Submillimeter-sized channels are present in many medical and industrial tools such as microfilters used to detect biological and chemical entities. In order to describe the gas flows in these microchannels, the DSMC methods are frequently used but a large computation time is usually required to obtain the solutions [1,2]. Consequently, it is of main interest to develop asymptotic models to describe these flows.

In this contribution, our purpose is to model the flow of a mixture of two compressible gases in circular microchannels. The temperature of the channel wall depends on the longitudinal space variable \( z \). We are interested in flows at low Mach numbers and at low to moderate Knudsen numbers that corresponds to the slip-flow regime. Consequently, the movement equations are the usual macroscopic balance laws of mass, momentum and energy (Navier-Stokes-Fourier equations) with additional coupling terms in the momentum and energy equations [3,4,5]. At the walls, first order jump boundary conditions for the velocity and the temperature are set [6].

The flow is assumed to be axisymmetric and steady. For each gas, the balance equations are written with dimensional and dimensionless quantities. A small parameter \( \varepsilon \) related to the geometry of the micro pipe is built from the longitudinal and transversal characteristic length scales. We introduce, for each gas, the Mach number and the Reynolds number built with the longitudinal length scale. The Knudsen number can be expressed in terms of these two dimensionless numbers. The characteristic velocities in each direction are identical for the two gases. In order to investigate the significant degeneracies [7], we assume that the Reynolds number and that the Mach number are small or of order unity. The analysis of the magnitudes of the terms in the balance laws leads to a Mach number of order \( \varepsilon \) and to a Reynolds number of order unity.

The solution at the first order is investigated. At this approximation order, we obtain a set of eight equations. The coupling terms in the momentum and energy equations are conserved. The radial momentum equations lead to pressures depending only on \( z \). From the energy equations and the temperature boundary conditions, we obtain gas temperatures equal to the wall temperature. The longitudinal momentum equations are solved to obtain the longitudinal velocities. These velocities are solutions of modified Bessel equations and can be explicitly given in terms of the pressures and their first order derivatives. The radial momentum equations lead to pressures depending only on \( z \). From the energy equations and the temperature boundary conditions, we obtain gas temperatures equal to the wall temperature. The longitudinal momentum equations are solved to obtain the longitudinal velocities. These velocities are solutions of modified Bessel equations and can be explicitly given in terms of the pressures and their first order derivatives.

As a consequence of the mass balance equations, the pressures are given by a set of two coupled ordinary differential equations. These two equations are linear in term of the longitudinal pressure gradients but strongly non linear in \( z \). They are solved with MATLAB for given values of the inlet pressures and of the mass flow rates. The pressures are nonlinear in \( z \) and this even in the absence of slip. The results of this asymptotical modeling are compared to DSMC simulations in the same configuration.

REFFERENCES

Asymptotic modeling of flows of a mixture of two monoatomic gases in a coplanar microchannel

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Gas mixtures are often present in micrometric devices, such as heat exchangers, propulsion systems... The Direct Simulation Monte Carlo (DSMC) methods are relevant to describe gas flows in microsystems, but they are computationally expensive [1,2,3]. So, it is interesting to introduce asymptotic models [4].

Here, our purpose is to study the steady flow of a mixture of two monatomic gases in a coplanar microchannel. The channel walls are at rest and they have the same temperature depending on the longitudinal variable x only. The gas flows are assumed assumed to be at low Mach numbers and low to moderate Knudsen numbers. Consequently, the flows are described by the Navier-Stokes-Fourier equations with coupling terms, and with first order jump boundary conditions for velocity and temperature on the walls. Additionally, a small parameter equal to the ratio of the transversal and longitudinal lengths is introduced. An asymptotic modeling of the gas flows of this gas mixture in the microchannel was built and presented in the last International Symposium on Rarefied Gas Dynamics [4]. At the first order, a set of eight differential equations for mass, momentum and energy, has been written. It should be noted that the coupling terms in momentum and energy equations are kept.

This equation set is studied. A well as Poiseuille flows, the transverse momentum equations lead to pressures depending only on the longitudinal variable x. From the two energy equations and the temperature jumps on the walls, we prove that the gas temperatures are equal to the wall temperature; so the two gas temperatures are known and they depend on the variable x only. Then, the longitudinal momentum equations give the longitudinal velocities in terms of the pressures and their gradients. Finally, as a consequence of the mass balance equations, the pressures of each gas are given by a set of two coupled ordinary differential equations. These equations are linear in terms of the pressure derivatives, but they are strongly nonlinear in x. They are solved with Matlab software for given values of the pressures at the microchannel inlet, of the mass flow rates, and of the given wall temperatures. For argon-neon mixture, the longitudinal profiles for pressures, concentrations and longitudinal velocities are obtained and discussed, as well as the transversal profiles for the longitudinal velocities. The increase in the wall temperature between the inlet and the outlet of the microchannel is a significant factor in the pressure increase. The thermal creep effect is discussed.

Other binary gas mixtures are considered. For fixed value of the variable x, we note that the longitudinal velocity of the gas with the higher molecular mass is higher than those of the gas with the smaller molecular mass.

The results of this asymptotic modeling are compared to some DSMC simulations in the same configuration. There is a reasonable agreement. We finish with some conclusions and comments on this modeling

REFERENCES

Onsager’s Cross Coupling Effects in Gas Flows Confined to Micro-channels

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In rarefied gases, mass and heat transport processes interfere with each other, leading to the mechano-caloric effect and thermo-osmotic effect, which are of interest to both theoretical study and practical applications. We employ the unified gas-kinetic scheme \cite{1} to investigate these cross coupling effects in gas flows in micro-channels. Our numerical simulations cover channels of planar surfaces and also channels of ratchet surfaces, with Onsager’s reciprocal relation \cite{2} verified for both cases, as shown in Fig.1 and Fig.2.

For channels of planar surfaces, simulations are performed in a wide range of Knudsen number and our numerical results show good agreement with the literature results, see Fig.1. For channels of ratchet surfaces, simulations are performed for both the slip and transition regimes. In the slip regime, the data fitting of our numerical results gives $L_{MQ}=0.0483Kn^{0.562}$, which confirms the theoretical prediction $L_{MQ}\propto Kn^{0.571}$\cite{3}. We also show that the off-diagonal kinetic coefficients for cross coupling effects are maximized at a Knudsen number in the transition regime, see Fig.2. Finally, a preliminary optimization study is carried out for the geometry of Knudsen pump based on channels of ratchet surfaces.

\begin{figure}[h]
\centering
\includegraphics[width=0.45\textwidth]{fig1}
\caption{Channel of planar surfaces: normalized off-diagonal coefficients versus the Knudsen number. The reference is the S-model solution based on the variational method by Chernyak et al. \cite{4}}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=0.45\textwidth]{fig2}
\caption{Channel of ratchet surfaces: normalized off-diagonal coefficients versus the Knudsen number. Both coefficients exhibit their maxima at Kn \approx 0.28.}
\end{figure}

ACKNOWLEDGEMENTS

This work is supported by Hong Kong RGC Grants No. HKUST604013 and C6004-14G.

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Study of rarified gas flow in suddenly expanded microchannel

Abhimanyu Gavasane, Upendra Bhandarkar, Amit Agrawal, A.M. Pradeep

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The gas flow through a microfluidic device may encounter different flow conditions such as change in direction, change in cross sectional area and change in wall heat flux. These different circumstances alter the fluid flow and thermal characteristics of a micro fluidic system. Gas flow through a micron sized device becomes rarefied and compressible on account of the small characteristic dimension. The Knudsen number (Kn) of such flow is typically greater than 0.001. Conventional computational fluid dynamics (CFD) methods fail to predict the flow behavior in a microchannel accurately due to slipping of the flow at the wall, while experimental techniques have their own limitations in measuring the local flow properties due micron sized channels. The Direct Simulation Monte Carlo (DSMC) [1] method is a good alternative to study high Knudsen number microchannel flows. The flow through a straight microchannel has been studied rigourously in the past by using DSMC. However, very little attention was given to flows undergoing sudden changes in the cross sectional area.

The formation of a secondary flow in the corner region of an expanded microchannel modifies the flow characteristics as observed in the DSMC simulation of a nano step [2]. However, formation of secondary flow was not found in experimental study of rarefied gas flow in conventional tubes [3] and numerical study using Lattice Boltzmann Method in a microchannel flow [4]. For rarefied microchannel gas flows, Reynolds number (Re) as well as Knudsen number, together determine the flow characteristics. The effect of only the Knudsen number was studied in past for nano step geometry [2]. The objectives of this paper are: (a) to study secondary flow in a suddenly expanded microchannel for different Knudsen numbers and Reynolds numbers, (b) to study effect of the individual parameters on the reattachment of flow, and (c) to identify critical combination Kn and Re (if any) where secondary flow disappears. An in-house MPI parallelized DSMC code is developed to study the flow in a nano step geometry. Figure 1 shows formation of secondary flow in the nano step geometry for inlet Kn of 0.05 and 0.5. The junction Re numbers are 5.57 and 0.3. It is seen that with increase in the Knudsen number, secondary flow disappears. However Reynolds number of the flow is also seen to decrease. These detailed results will be presented and discussed in the conference.

fig.1: Secondary flow in a microchannel for different Kn and Re.

REFERENCES
S. Succi, "Lattice Boltzmann Beyond Navier-Stokes Hydrodynamics: Where Do We Stand?"
Historically, the Lattice Boltzmann (LB) method was designed to provide an efficient computational alternative to the numerical discretization of the Navier-Stokes equations of continuum fluid mechanics [1,2]. Over the years, however, it has become apparent that, with due extensions, LB can describe a broad variety of complex non-equilibrium flows across a broad range of scales, from fully-developed turbulence, to multiphase dense and rarefied micro flows, all the way down to biopolymer translocation in nanopores [3,4]. Lately, the method has also shown promising potential for the simulation of quantum-relativistic flows, such as quark-gluon plasmas, electron transport in graphene and relativistic magnetohydrodynamics [5]. Many of these applications involve strong non-equilibrium effects similar to those met in the study of rarefied gas dynamics.

In this Graeme Bird's lecture, we shall briefly survey the basic ideas behind the LB method and discuss its recent extensions to non-hydrodynamic regimes. Finally, prospects for future multiscale applications, including recent coupling to Bird's Direct Simulation Monte Carlo will also be touched upon [6].

**ACKNOWLEDGEMENTS**

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**REFERENCES**

Session 5: DSMC Applications I

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<td>&quot;Recent Developments of DSMC within the Reactive Plasma Flow Solver PICLas&quot;</td>
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Direct Simulation Monte Carlo Investigation of Hydrodynamic Instabilities in Gases

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The Rayleigh-Taylor instability (RTI) [1,2] and the Richtmyer-Meshkov instability [3,4] are investigated using Bird’s Direct Simulation Monte Carlo (DSMC) [5] method of molecular gas dynamics. The DSMC method has been demonstrated to provide accurate solutions to the Boltzmann equation under the assumption of molecular chaos. Due to the inherent statistical noise and the significant computational requirements, DSMC is hardly ever applied to hydrodynamic flows. Here, DSMC simulations are performed to quantify the growth of a single-mode perturbation on the interface between two atmospheric-pressure monatomic gases as a function of the Atwood number and the gravitational acceleration for the RTI and of the shock Mach number for the RMI. The DSMC results reproduce all of the qualitative features of these instabilities and are in reasonable quantitative agreement with existing theoretical and empirical models. Consistent with previous work, the DSMC simulations indicate that the growth rates of these instabilities follow universal behaviors. In simulations with wide domains, the resulting numbers of bubbles and spikes are in agreement with the most unstable wavelength.

Figure 1. DSMC simulations of the Rayleigh-Taylor (left) and Richtmyer-Meshkov (right) instabilities in gases.

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On the Inverse Magnus Effect for Flow Past a Rotating Cylinder

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The Magnus effect [1], whereby a rotating solid body experiences a transverse aerodynamic lift force has been studied both experimentally and numerically by various researchers and has many practical applications [2]. Of particular interest is the lift force under free-molecular conditions which is in the opposite direction to that associated with conventional Magnus effects. This change in lift force direction which occurs with increase in flow rarefaction is often referred to as the inverse Magnus effect [3]. The authors [4, 5] have recently studied numerically, the onset of inverse Magnus effect for a cylinder with various degrees of flow rarefaction under very high speed flow conditions. It was shown that there is a subtle interplay between the Mach number and Knudsen number for the occurrence of the inverse Magnus effect. In this work, we aim to consider different cylinder rotation rates and extend the study to moderate subsonic flow conditions. The numerical study is carried out using the direct simulation Monte Carlo (DSMC) method with the aid of dsmcFoam software [6]. The impact of Reynolds number and Knudsen number on the onset of inverse Magnus effect will be studied. A sensitivity study of cylinder wall temperature on lift and drag forces as well as the inversion point at which the lift inversion takes place will also be carried out.

ACKNOWLEDGEMENTS

This work was supported through the United Kingdom Engineering and Physical Sciences Research Council (EPSRC) under grants EP/N016602/1 and EP/K038427/1. The authors would also like to thank Tom Scanlon of the University of Strathclyde for providing an updated version of the dsmcFoam code.

REFERENCES

Heat Transfer Simulation of Rarefied Laminar Flow Past a Circular Cylinder

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The flow past a circular cylinder is a classical fluid dynamics problem and, despite its simple geometry, its analysis is complicated. This is due to the fact that a number of different complex flow regimes may exist (such as steady attached flow, steady recirculated flow, vortex shedding, turbulence) depending on the flow conditions.

For the simulation of these flows, many research efforts have concentrated on the use of incompressible Navier-Stokes equations with no-slip boundary conditions. It is only recently that some research work has been done to assess the rarefaction effects on these flows. For example, the slip on hydrophobic surfaces is studied by performing incompressible flow calculations and replacing the no-slip boundary conditions by the slip boundary conditions [1]. Direct numerical simulations are also performed for rarefied laminar flows past a circular cylinder to determine the aerodynamic forces [2].

The present study is a continuation of the work presented in [2] and focuses on the heat transfer effects when the cylinder is heated. These calculations are performed by modifying a two-dimensional direct simulation Monte Carlo program (G2) of G.A. Bird [3]. In the simulations, different Mach numbers are considered with varying rarefaction (i.e. Knudsen numbers, Kn, of 0.02 and higher). The results are in agreement with what is observed in experiments. Normalized number density contours at a Knudsen number of 0.02 and Reynolds number of 24.63 are presented in Fig. 1 for two different cylinder temperatures. In the figure, cylinder is between x/D= 0 and 1 (where D is the diameter) and only upper half of the domain is shown due to symmetry. For the present subsonic flows, the outflow boundary condition model proposed in [4] is adopted. In this model, the incoming molecules at the outflow boundaries are determined by adjusting the outflow boundary conditions according to the local rarefaction using an exponential bridging formula between the continuum and the free-molecule limits. The effects of domain size and the bridging formula are also checked.

Fig.1: n/n∞ contours for Kn=0.02, Re=24.63

REFERENCES

Recent Developments of DSMC within the Reactive Plasma Flow Solver PICLas

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In order to enable the numerical simulation of rarefied plasma flows in thermal and chemical non-equilibrium, electromagnetic interactions as well as particle collisions have to be considered. A common approach is to use particle-based methods. The Particle-in-Cell (PIC) method simulates charged collisionless gas flows by solving the Vlasov-Maxwell equation system [1] while particle collisions in neutral reactive flows are treated by the Direct Simulation Monte Carlo (DSMC) method [2]. Therefore, PICLas is being developed, a coupled simulation code that enables three-dimensional particle-based simulations combining high-order PIC and DSMC schemes for the simulation of reactive, rarefied plasma flows. PICLas enables time-accurate simulations on unstructured hexahedral meshes and is parallelized for high-performance computing [3]. Additionally to an overview of PICLas, the current development status of the DSMC module will be presented. This includes the relaxation of polyatomic gases [4], the extension of the chemical modelling to gas-surface interactions, and the implementation of steady-state detection routines.

REFERENCES

Session 6: Moment Equations II

| (INVITED) McDonald, "Approximate Maximum-Entropy Moment Closures for Gas Dynamics"
| Laplante, Groth, "Comparison of Maximum Entropy and Quadrature-Based Moment Closures for Shock Transitions Prediction in One-Dimensional Gaskinetic Theory"
| Collyer, Lockerby, "Derivation and Application of Fundamental Solutions to Grad’s Linearised Moment Equations" |
Approximate Maximum-Entropy Moment Closures for Gas Dynamics

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Traditional gas-dynamic models rest on a continuum assumption and retain no information regarding the microscopic, particle nature of a gas. These methods have been extremely successful in the prediction of flows that remain in local thermodynamic equilibrium. Methods that seek to maintain a description of gas-particle evolution, such as the Direct Simulation Monte Carlo method [1] or direct discretizations of the Boltzmann equation [2], are theoretically applicable to all flows, however they bring added computational expense. The added expense of these particle methods becomes more and more prohibitive as the traditional, equilibrium regime is approached.

The method of moment closures of the Boltzmann equation, pioneered by Grad [3], holds the promise of new models that have complexity that is comparable to traditional methods, while extending the region of physical validity to non-equilibrium, transition-regime flow situations. The original closures of Grad take the form of first-order balance laws. Unfortunately, though these closure appear to have the structure of hyperbolic equations, hyperbolicity can be lost and the equations can become ill-posed for moderate deviations from local equilibrium. Regularizations of these closure exist that supplement these balance laws with terms containing higher-order derivatives [4]. The resulting equations have been successful in predicting many transition-regime flows. However, the supplemented models no longer take the form of first-order balance laws. Such first-order models have many physically and mathematically desirable properties, which are lost through regularization.

An alternative closure technique, based on the local maximization of the entropy of the presumed distribution function, has also been proposed [5, 6]. Members of this alternate hierarchy of closures are first-order balance laws with a guarantee of hyperbolicity whenever the underlying entropy-maximization problem is solvable. Unfortunately, for all but the lowest-order members of the theory, the assumed form of the distribution function cannot be integrated in closed form. The result is that closing fluxes cannot be easily expressed as a function on known moments. Also, it has been shown that there exist physically realizable states for which a corresponding maximum-entropy distribution does not exist [7]. In these regions, closing fluxes become singular.

Recently, an interpolation technique for the missing closing fluxes of the fourteen-moment closure of the maximum-entropy hierarchy has been developed [8, 9]. The result is a closed-form first-order hyperbolic system for the prediction of viscous heat-conducting gas flows both in the continuum and transition regime. This talk demonstrates the derivation of this approximate maximum-entropy closure. A new improvement on the original model is also shown. A coupled space-time discontinuous Galerkin scheme for the efficient solution of the resulting governing equations is shown. Practical advantages of the purely first-order hyperbolic nature of the governing equations are demonstrated. Comparisons are made between numerical results obtained using the new closure, traditional continuum models, and particle-based methods.

REFERENCES

Comparison of Maximum Entropy and Quadrature-Based Moment Closures for Shock Transitions Prediction in One-Dimensional Gaskinetic Theory

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In computational fluid dynamics, the Navier-Stokes-Fourier (NSF) equations and direct simulation Monte Carlo (DSMC) are traditionally used to model continuum and non-equilibrium flows respectively. However, there exists a transitional non-equilibrium regime in which the NSF equations fall short due to the assumption of continuity. Though DSMC remains valid, it becomes computationally expensive in this regime. An alternative avenue thus consists in using moment closure methods to evaluate this category of flows.

In this study, the hyperbolic 5-moment system examined in [1,2], in which a closure approximation is required for the fifth random velocity moment, $s$, will be reconsidered. Three different moment closures are considered based on the following lower order moments: $\rho, u, p, q$ and $r$. The first of these is an interpolative closure based on maximization of thermodynamic entropy as proposed by McDonald et al. [1,2]. Additionally, two quadrature-based closure techniques will be considered. The first is based on the representation of the distribution function in terms of a combination of Dirac delta functions having weights $w$ and abscissa $\xi$, as originally considered by McGraw [3] in the context of aerosol dynamics. The quadrature weights and points are determined such that the approximate distribution function reproduces the lower order moments exactly. Here, three quadrature points are used, the first being centered at zero since the first order moment is always null. The second method, described by Chalons et al. [4], extends the Dirac delta representation by assuming a bi-Gaussian distribution function of standard deviation $\sigma$. The result is a combination of two weighted Maxwell-Boltzmann distributions shifted in velocity space. In both cases, the higher order moment is subsequently obtained by integrating the reconstructed distribution function over velocity space.

The paper will consider the application of the aforementioned closures to the prediction of stationary shock structures and the solution of Riemann problems. The moment equation solutions to these problems are computed using a standard finite-volume technique. As a basis for comparison, solutions to the problems are determined by directly solving the underlying kinetic equation for which the BGK approximation is used to represent collisional processes. The discrete velocity method of Mieussens [5] is used for the latter. Additionally, the moment closure results are compared to the equivalent near-equilibrium NSF results.

REFERENCES

Derivation and Application of Fundamental Solutions to Grad’s Linearised Moment Equations

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Creeping flow (also known as Stokes flow) is flow at vanishingly small Reynolds number. This classic topic has many applications, particularly in micro- and nano-flow technology, owing to both the small scale and the low speeds encountered. In these conditions the inertia of the fluid can be neglected, and (for vanishingly small Knudsen numbers) the momentum and continuity equation reduce to the Stokes equations. A common mathematical tool for the analysis of creeping flows is a fundamental singularity solution to the Stokes equations, known as the Stokeslet (so-called in 1953 [1] but first derived by Lorentz in 1897 [2]). This fundamental solution – in essence a Green’s function for the Stokes equations – is the flow response to a Dirac delta forcing term applied to the momentum equation.

In the most straightforward use, a flow field is represented by a superposition of Stokeslets (positioned outside of the domain) that are given a combination of strengths chosen to satisfy the same number of conditions at nodes on the boundary. This approach is described briefly in Sherman’s textbook on viscous flow [3], and is known as the method of fundamental solutions or the superposition method [4,5]. Another use of the Stokeslet (and its variants, e.g. the Blakelet and Rotlet) is within the related, but more-established, boundary integral method [6]. Both approaches have the advantage of having a flow domain that is meshless, and a dimensionality that is reduced in order by one (the boundary is discretized rather than the volume). The Stokeslet is also in itself of interest, as a fundamental solution to the Stokes equations, and can be used to conveniently derive certain analytical results.

As is commonly known, in flows departed far from local thermodynamic equilibrium (i.e. at non negligible Knudsen numbers) the Stokes constitutive law becomes invalid/inaccurate. As such, the Stokeslet has limited applicability in the analysis of creeping gas flows at the micro/nano scale. However, constitutive closures exist that extend the applicability of the continuum treatment to higher Knudsen numbers. Notably, Grad’s family of moment equations [7] (and particularly their ‘regularised’ counterparts [8,9]) have attracted significant attention in recent years.

In this paper, for the first time, we derive fundamental solutions to these equations for very low Reynolds number flows; equivalent to the Stokeslet, but applicable to higher Knudsen numbers. We first present the “Gradlet” (a fundamental solution to the linearised form of Grad’ s 13 moment equations) and second the “R13let” (a fundamental solution to the linearised form of the Regularised 13 moment equations). The veracity of these solutions is demonstrated.

A simple numerical implementation of the method of fundamental solutions (employing a superposition of Gradlets) is presented for some three-dimensional creeping flows. Simulation results for low-speed flow around a sphere are compared to published analytical results (for Grad’s linearised 13 moment equations), kinetic theory, and experiment.

REFERENCES

## Session 7: Flows Though Porous Media

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Modeling of Pressure-driven Gas Transport through Micro-/Nanoscale porous media

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Gas flow in porous media is used in various industrial processes such as dissociation reaction, desiccation, adsorption and reduction reaction. It is important to understand flow phenomena in porous media for improvement of performance of devices including such processes. In porous media with pores as small as a mean free path of gas molecules, i.e., micro-/nanoscale pores, the gas flow cannot be treated as a continuum and is governed by the Boltzmann equation because the Knudsen number is in the order of unity. Therefore, the direct simulation Monte Carlo (DSMC) method [1], which is the stochastic solution of the Boltzmann equation, is used for numerical simulations in the present study.

Figure 1 shows the computational domain used in the present study. The inside structure of porous media is imitated by randomly arranging solid spherical particles which interpenetrate each other. Gas flows in porous media driven by the pressure gradient in the y direction are studied. In our previous work, we investigated the factor which governs gas flow in porous media by performing the DSMC simulations [2]. In this work, using the results obtained in the DSMC simulations, we propose the model to estimate the gas transport in porous media. Figure 2 shows the comparison between the flow velocity estimated by the proposed model and that obtained in the DSMC simulations for various conditions. The flow velocity estimated by the proposed model agrees well with that obtained in the simulations. We can say that the proposed model can provide a reliable prediction.

REFERENCES
Thermal Protection System (TPS) materials are designed to protect the space vehicle and its crew from the aerothermodynamic heating during re-entry into the Earth’s atmosphere. Candidate TPS materials such as Phenolic Impregnated Carbon Fibers (PICA) form a complex network of carbon fibers at the micrometer scale through which the gases diffuse. Modeling and predicting the heat transfer and material response to the chemically reacting flow is important to establish the performance of the TPS and required tolerances for manned flight. Since the Knudsen number of these flows is high, Direct Simulation Monte Carlo (DSMC) [2] is employed.

The irregular network of the fibrous microstructure, shown in Fig.1, is modeled using 1.5 million surface triangles and the flow domain has nearly 30 million argon gas particles. To model such large scale problems efficiently, we have developed a Cuda-based Hybrid Approach for Octree Simulations (CHAOS) DSMC [2] solver that uses a hybrid MPI-CUDA paradigm. Morton Z-curves are employed to construct forest of linear octrees to group nearest neighbor particles into leaf nodes (analogous to cells in a grid based approach) such that binary collisions are performed between them. A volume of fluid [3] method is implemented to compute the exact volume of the gas portion of the leaf nodes that are intersected by the immersed body. Accurate volume calculation is important to compute collision frequencies that drives the physics of the DSMC calculations. Figure 1 shows the velocity streamlines of argon gas through the porous microstructure and the variation of surface heat flux on the material. The permeability of the porous material will be calculated from these simulations and we will also analyse the effect of a wall at the exit that may result in a backflow of gas particles.

ACKNOWLEDGEMENTS

We would like to thank Prof. Wen Mei Hwu for providing us with access to GPUs on the GEM cluster and for his valuable suggestions. Thank you to Dr. Arnaud Borner for the microstructure and useful discussions. This research is part of the Blue Waters sustained-petascale computing project, which is supported by the National Science Foundation (awards OCI-0725070 and ACI-1238993) and the state of Illinois. Blue Waters is a joint effort of the University of Illinois at Urbana-Champaign and its National Center for Supercomputing Applications.

REFERENCES

Gas Separation by the Molecular Exchange Flow through Micropores of the Membrane

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The present work is devoted to the fabrication of a gas separator system that makes use of the molecular exchange flow in the Knudsen pump [1-3]. Figure 1 is the schematic of the Knudsen pump used in the present work. A porous polymeric membrane (mixed cellulose ester, pore size ~ 0.1 µm, thickness ~ 100 µm, 3 x 3 cm in size) separates two channels H and C. The temperature and pressure in H are higher than those in channel C. Since the pore size is close to the mean free path of gas molecules around 1 atm, the thermal transpiration flow of the rarefied gas is induced in the direction of C→H. This flow is canceled by the Poiseuille flow (H→C) by the pressure difference. In the case of mixture, however, species fluxes cannot be simultaneously canceled out by a pressure difference alone. Theory and experiment show that the light gas flows from C to H, while the heavy gas flows from H to C (molecular exchange flow) [1, 2].

The system diagram of the present gas separator is shown in Fig. 2. The system comprises two Knudsen pumps, KNP1 and 2, and a diaphragm pump (E. M. P. Co. Ltd, DM-360ST). The Knudsen pumps are used to induce the molecular exchange flow, and the diaphragm pump is used to supply a circulating flow in the system. Its direction is indicated by thick arrows in Fig. 2. The mass flow controller (MFC) sets the speed of the circulating flow much faster than that of molecular exchange flow. In this case, the gases from micropores in KNP1 and 2 flow downstream in each channels by the convection effect of the fluid dynamics. As a result, light and heavy gases are concentrated at, respectively, point S and P in Fig. 2. These gases can be produced from S and P if we supply the feed mixture from point F.

In our previous work [2], a different system where the diaphragm pump and KNP1 in Fig. 2 are replaced by a larger Knudsen pump, which requires around 100 K temperature difference. In the present system, the temperature differences in the Knudsen pumps are much small; it is 34 K for KNP1 and 17 K for KNP2 although the system obtain a similar gas separation performance as in [2]. The difference of mole percentage between two gases at S and P is around 6 % when the volume flow rate of the feed mixture is 1 cm³ (STP)/min. In this preliminary experiment, 50 %v/v helium-neon mixture is used for the feed gas mixture and the pressure of the gas in the system is around 1.5 atm.

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Direct Simulation of Gas Transport in Porous Media

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Unconventional gas resources, including tight-sand gas, coalbed methane, and shale gas, are becoming important energy sources as conventional gas production is declining. These hydrogen-rich gases are “cleaner” replacements to carbon-rich and air-polluting coals. However, their extraction poses a new research challenge: understanding and quantifying the gas flow physics in exceptionally low permeability porous media with pore spaces as small as a few nano-meters across. The empirical Klinkenberg model considers gas-slip at pore surfaces, which extends the validity of Darcy’s law to the slip regime. Some models have also been proposed to take into account the Knudsen diffusion effects. However, in the transition regime, the nonlinear Knudsen layers (thin gas layers at bounding surfaces, with a thickness of the order of a molecular mean free path) are important, but have not yet been properly considered [1]. Even worse, all of these models are only heuristically extended from phenomenological models (see [2] for example) for pores with simple geometries. A pre-condition for applying these models is to simplify pore space so that the flow paths in porous media instead consist of a bundle of tortuous connected simple passages. This makes a heuristic extension of phenomenological models even more arbitrary and becomes impossible to validate the models. The reported agreements between model predictions and experimental data are due to the use of a few tuneable parameters in the models, including the tangential momentum accommodation coefficient [1].

To uncover the gas transport physics and to predict flow properties of porous media, we utilise the recent rapid advances in high-resolution imaging technologies which can resolve the pore structures of ultra-tight porous media. We have systematically performed pore-scale study by directly solving the kinetic model equations on the porous media samples. Our findings may transform the commonly-used heuristic approaches and provide a rational scaled-up model at the Darcy scale. For example, our simulation results shown in Fig. 1 clearly contradict the currently-accepted concept of importance of so-called Knudsen diffusion to gas transport in ultra-tight porous media.

ACKNOWLEDGEMENTS
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**Session 8: Fokker-Planck Equation**

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Time Dependent Solution a Fokker-Planck Equation with Equilibrium Bistable States; Eigenvalue Spectrum and the Approach to Equilibrium

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There are many systems such as isomeric reactive systems [1,2], laser systems [3] and climate models that have been modeled with a Fokker-Planck or Smoluchowski equation with bistable states at equilibrium [4]. The Fokker-Planck equation (FPE) of interest in this paper is of the form

$$\frac{\partial P(x,t)}{\partial t} = \frac{\partial P(x,t)}{\partial x} \left[ A(x) + B(x) \frac{\partial P(x,t)}{\partial x} \right] = LP,$$

(1)

where \(A(x)\) and \(B(x)\) are the drift and diffusion coefficients. An often used model are the choices \(A(x) = x^3 - x\) and \(B(x) = \epsilon\) [5]. Here we choose \(A(x) = x^5 - x\) and the equilibrium distribution for this system, defined by \(\frac{\partial P(x,t)}{\partial t} = 0\) is given by

$$P_{eq}(x) = \exp \left[ -\frac{1}{\epsilon} \left( \frac{x^6}{6} - \frac{x^2}{2} \right) \right],$$

(2)

with two maxima sharply distributed about \(x = \pm 1\) with decreasing \(\epsilon\). We seek a solution in terms of the eigenfunctions and eigenvalues of the linear operator, \(L\), defined by the right hand side of Eq. (1) [6]. The FPE can be transformed to a Schrödinger equation isospectral with the Fokker-Planck operator and the potential belongs to the class of potentials in supersymmetric quantum mechanics [7,8]. For small \(\epsilon\), the dependence of the first excited state, \(\lambda_1\) almost degenerate with \(\lambda_0 = 0\) versus \(\epsilon\) is compared with the theory by Kramers [1].

References

Collision Frequency Closure for Fokker-Planck Model of Hard Sphere Gases

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It has been shown recently that the Fokker-Planck kinetic model can be employed as an approximation of the Boltzmann equation for rarefied gas flow simulations [1]. Similar to the direct simulation Monte-Carlo (DSMC), the Fokker-Planck solution algorithm is based on the particle Monte-Carlo representation of the distribution function. Yet opposed to DSMC, here the particles evolve along independent stochastic paths where no collisions need to be resolved. That leads to significant computational advantages over DSMC, considering small Knudsen numbers [2].

The original Fokker-Planck model (FP) for rarefied gas flow simulations was devised according to the Maxwell type pseudo-molecules [3]. More realistic molecular models such as hard spheres require special attentions because now the collision frequency becomes a function of the molecular velocity. That imposes yet another challenge for kinetic models, due to the fact that molecular velocity dependency of the collision frequency has to be accounted for [4]. Therefore, an appropriate collision frequency model has to be employed for accurate simulations of hard sphere gases.

In this talk, we derive collision frequency closures for the Fokker-Planck description of hard sphere gases (ν-FP). The closures are constructed upon the generalisation of Green-Kubo relations for non-equilibrium distribution functions. These model frequencies characterise auto-correlation functions of the molecular velocity fluctuations, whereas they result in the self diffusion, viscosity and heat conductivity coefficients close to the equilibrium. Therefore, the newly introduced collision frequencies provide relaxation time scales for the Fokker-Planck approximation of hard sphere gases. Note that the closures are consistent in a sense that the original FP model is obtained in the limit of Maxwell interactions. For assessment of the model, validation studies are performed for planar Couette flows, Sod shock tube and high Mach flow around a vertical plate using both v-FP and DSMC simulations. Compared to the regular FP simulations, significant improvements are achieved especially at high Mach flows (see Fig. 1). This is interesting, since while the accuracy of the v-FP model is comparable to DSMC, its computational cost remains similar to the regular FP; hence much more efficient than DSMC at low Knudsen numbers.

REFFERENCES


Fig.1 : Mach 5 flow of hard sphere argon around a vertical plate at Knudsen 0.1. Top to bottom: temperature contours calculated by FP, ν-FP and DSMC.
A Fokker-Planck model of the Boltzmann equation with correct Prandtl number

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Abstract:

We propose an extension of the Fokker-Planck model of the Boltzmann equation to get a correct Prandtl number in the Compressible Navier-Stokes asymptotics. This is obtained by replacing the diffusion coefficient (which is the equilibrium temperature) by a non diagonal temperature tensor, like the Ellipsoidal-Statistical model (ES) is obtained from the Bathnagar-Gross-Krook model (BGK) of the Boltzmann equation. Our model is proved to satisfy the properties of conservation and a H-theorem. A Chapman-Enskog analysis and two numerical tests show that a correct Prandtl number of 2/3 can be obtained.

ACKNOWLEDGEMENTS

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REFERENCES

A Multi-scale Method for Rarefied and Continuum Gas Flows Based on Fokker-Planck Model

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Multi-scale flows are widely existed in the micro-electro-mechanical system (MEMS) and aerospace engineering [1], such as flow fields inside a micro-nozzle or surrounding a re-entry vehicle. To accurately and efficiently simulate these flows is challenging, since both the rarefied and continuum regimes should be simulated in the computational domain at the same time. The DSMC-CFD hybrid approach is a commonly used numerical scheme to deal with these problems. However, with two fundamentally different types of solvers, it suffers from difficulties regarding to their amalgamation [2]. Therefore, it is benefit to calculate the multi-scale flows by a kinetic scheme uniformly, where the rarefied and continuum solvers can be adaptively implemented according to the spatial and temporal scales. One typical and successful kinetic scheme is the UGKS method proposed by Xu [3]. However, as the UGKS is performed with discrete velocities, it is inefficient for the 3D simulation. In the current paper, a particle numerical method based on the Fokker-Planck model has been developed.

The Fokker-Planck equation, which can be considered as an approximation for the Boltzmann equation, simplifies the binary collision model by a continuum stochastic process. Therefore, the related particle numerical schemes are more efficient than the DSMC method, e.g. the Fokker-Planck model (FPM) method [4] for the rarefied gas flows and the diffusive information preservation (D-IP) [5] method for the continuum flows. In both FPM and D-IP methods, molecular motions are computed by explicit solutions of the Langevin equation, which results in non-uniform transport properties with different time steps; therefore, their time steps are restricted. To address this difficulty, we propose a unified discrete Fokker-Planck model (UD-FPM) method, which corrects the transport properties in terms of the time step by using the analytical solutions for viscosity, thermal conductivity and pressure of the Langevin model. Therefore, exact transport processes can be satisfied for any temporal discretization. To validate this method, several benchmark problems have been calculated at a wide range of spatial and temporal scales, such as the heat flux of thermal Couette flow with different spatial and temporal discretization in figure 1. The results show that the UD-FPM method is accurate and efficient in both rarefied and continuum flow regimes.

ACKNOWLEDGEMENTS

The supports of National Natural Science Foundation of China under Grant Nos. 51506063 & 51276076 and China Postdoctoral Science Foundation under No. 2014M562019 are gratefully acknowledged. This work is also supported by the Special Program for Applied Research on Super Computation of the NSFC-Guangdong Joint Fund (the second phase).

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Session 9: Jets and Plumes

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Impact of Nozzle Separation on the Plumes of two Parallel Thrusters

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Two identical, interacting plumes emanating from model thrusters with parallel axes separated from 50 to 150 throat diameters are studied numerically. The nozzle throat Reynolds number is set to nearly 15,000 to match that of a small bi-propellant attitude control thruster, but the simulated gas is nitrogen with a stagnation temperature of 300K. The near-isentropic, dense plume core is computed with the DLR Navier-Stokes solver TAU [1] and the conditions at a suitably defined interface are then used on the inflow boundary of a separately conducted DSMC simulation [2]. The results are shown to agree favorably with particle flux measurements on a similar configuration in the DLR high-vacuum plume test facility STG [3]. Varying the nozzle separation distance alters the degree of rarefaction in the interaction plane, and by tagging DSMC particles according to their origin, the effect on the individual plume may be investigated. The impact of nozzle axis separation on mass- and momentum flux along the line formed by the intersecting planes of symmetry is quantified with respect to the linear superposition of non-interfering plumes, expanding on previously presented work [4].

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Fig.1: Patterson probe signal X along a circular arc at r/δ=10. Symbols: from experiment [3], line: DSMC computation.
Fast Computation of High Energy Elastic Collision Scattering Angle for Electric Propulsion Plume Simulation

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In the plumes of Hall effect thrusters and ion thrusters, ions electrostatically accelerated to high energy can experience elastic collisions with the slow neutral atoms exiting the thrusters. During the collisional process, the high energy ions exchange momentum with their collision partners, and some fraction of the population is deflected at angles greater than the plume divergence. Meanwhile, the elastic collision may involve an exchange of one or more electrons, leading to a slow CEX ion and a high energy atom after each charge-exchange (CEX) process. Proper modeling of these collisions is particularly important in accurately determining the plume current profile and assessing the integration of spacecraft components as well as the thruster life and long duration performance; the slow CEX ions are prone to electric fields that direct the ions toward the spacecraft and thruster components, resulting in contamination through sputtering and deposition after gaining significant energies.

The elastic collision between high energy ions and slow atoms has been approximated by a few different methods. In a particle-in-cell (PIC) model developed by Oh [1], simple models were employed; the elastic collision was treated as isotropic scattering whereas the CEX collision was handled without any exchange of momentum. More recently, the elastic collision has been calculated by a detailed model that solves the classical scattering equation with a precise interatomic potential [2, 3, 4]. This method provides much more accurate scattering characteristics necessary for plume simulations. However, the numerical integration of classical scattering equation is computationally expensive such that the collision calculation can be a bottleneck to a massive particle simulation. An alternative method is to use a curve-fit representative of a center-of-mass (CM) differential cross section to determine post-collision particle velocities [5, 6]. This method is much faster than the direct numerical integration. However, it is limited to the energy that the differential cross-section is provided at; therefore, the method cannot handle multiple collisions since the differential cross-section is no longer applicable to a particle that has experienced a single elastic collision event.

The objective of this research is to develop a fast and accurate method to compute the scattering angle for an elastic collision between high energy ions and slow atoms. Instead of using the experimentally determined differential cross-section, the CM differential cross-section can be numerically computed from the classical theory at any incident ion energy. By tabulating or finding fitting coefficients for applicable range of impact parameters and energies, a fast and accurate determination of the elastic scattering becomes possible. These methods will be discussed and compared by their performance in this paper.

REFERENCES


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Column Number Density Expressions Through $M = 0$ and $M = 1$ Point Source Plumes Along Any Straight Path

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Providers of payloads carried aboard the International Space Station must conduct analyses to demonstrate that any planned gaseous venting events generate no more than a certain level of material that may interfere with optical measurements from other experiments or payloads located nearby. This requirement is expressed in terms of a maximum column number density (CND). Depending on the level of rarefaction, such venting may be characterized by effusion for low flow rates, or by a sonic distribution at higher levels. Since the relative locations of other sensitive payloads are often unknown because they may refer to future projects, this requirement becomes a search for the maximum CND along any path.

In another application, certain astronomical observations make use of CND to estimate light attenuation from a distant star through gaseous plumes, such as the “Fermi Bubbles” emanating from the vicinity of the black hole at the center of our Milky Way galaxy, in order to infer the amount of material being expelled via those plumes.

This paper presents analytical CND expressions developed for general straight paths based upon a free molecule point source model for steady effusive flow and for a distribution fitted to model flows from a sonic orifice. Among other things, in this Mach number range it is demonstrated that the maximum CND from a distant location occurs along the path parallel to the source plane that intersects the plume axis at a right angle. For effusive flows this value is exactly twice the CND found along the ray originating from that point of intersection and extending to infinity along the plume’s axis. For sonic plumes this ratio is reduced to about $4/3$. 
Non-Equilibrium Processes by a Gas Phase Synthesis of Diamond

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In this work the gas-dynamic phenomena by gas phase synthesis of diamond, based on thermal activation on the extended surface in a cylindrical channel, discussed in [1, 2], are considered. The modeling by Direct Simulation Monte Carlo method includes:
a) processes by thermal activation of hydrogen and methane molecules in a tungsten cylindrical channel and flow in it;
b) subsonic or supersonic flow of mixture behind the channel exit;
c) mixing of activated flow with flow of particles from stagnation surface (just reflected or reflected with a transformation). Challenge of calculations is the lack of data on constants of interactions molecules and their fragments with hot surfaces. In some cases these constants can be determined in results of modeling of flows [3] in experiments at high vacuum [4]. Just for the illustration results of calculation of hydrogen flow in the cylindrical channel are given in fig 1. The typical atmosphere near the surface of deposition contains the mixture of fragments H, CH₃, CH₂, CH, C, C₂ with molecules H₂ and CH₄ in a transition state with Knudsen numbers of order of 0.2 and below. This region is difficult for analysis. All processes be considered are interesting from point of view of physical phenomena. Main practical use can be extracted from data of gas atmosphere computation near the surface: translational velocity and internal energy distribution functions for particles, colliding with surface of deposition. These data can be calculated only by knowledge of transformation of energy particles in result of interaction with solid surface.

ACKNOWLEDGEMENTS

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Fig.1: Two-dimensional flow distribution and stream lines of atomic hydrogen. Distances are given in meters.
**Session 10: Micro Scale Flows and Devices I**

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Microdevices Enabled by Rarefied Flow Phenomena

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We review emerging applications of rarefied gas dynamics for microscale sensing, actuation, power generation and thermal management. The performance of conventional fluidic devices such as pumps, combustors and heat engines decreases at the microscale due to greater viscous and heat transfer losses. However, the close coupling between non-equilibrium gas, liquid and solid-state transport and electromagnetic phenomena enables unconventional micro/nanodevices. We consider three distinct examples of devices with non-equilibrium gas-phase transport based on i) very large thermal gradients; ii) increased capillary forces; iii) high electric fields – all of which are generated by scaling down device size. The first example is thermostress convection [1] which permits actuation and control of gas-phase transport by temperature gradients and offers novel methods for gas sensing, pumping, and species separation. In macroscale systems, the operating temperatures necessary to generate significant flow actuation by thermostress convection are prohibitively high. For N/MEMS devices however, thermal gradients on the order of tens of millions of Kelvin per meter could be achieved, allowing these effects to be exploited. The Microscale In-Plane Knudsen Radiometric Actuator (MIKRA) shown in Fig. 1 applies thermally-driven rarefied flow for gas sensing in vacuum environments [2]. The second example is the Film Evaporation MEMS Tunable Array (FEMTA), a novel thermal valve for vapor flow control at low pressures. Small-scale effects of surface tension, hydrophobicity, and film boiling are utilized to create a temperature-dependent containment mechanism for polar liquids against a vacuum. When thin-film heating increases the meniscus temperature past a critical point determined by geometry and contact angle, vacuum boiling is initiated and continues as long as power is applied. This creates a rarefied plume that generates thrust in the micro-Newton range with high repeatability and at a low input power (< 1 Watt). FEMTA microthrusters[3] designed, microfabricated and tested at Purdue Birck Nanotechnology Center involve submicron heaters embedded in a nozzle with less than 10 micron throat and use water as propellant. Finally, quantum tunneling of electrons from metals occurs at extremely high electric fields achievable by a moderate voltage bias applied across micron-sized gaps. The field emission dielectric barrier discharge (FE-DBD) creates a highly positive space charge and leads to non-equilibrium microplasma as the operational frequency (MHz – GHz) exceeds the frequency of electron energy relaxation. The plasma imparts momentum and energy to the neutral gas without any moving parts, which can be utilized in microchannels where the flow is dominated by high viscous losses or to sustain combustion at reduced temperatures in microreactors. For devices described above we discuss the challenges and further research needs for rarefied flow modeling and experimental studies.

ACKNOWLEDGEMENTS

The work on MIKRA has been supported by NSF CAREER award 1055453 and NSF AIR-TT award 1602061. The research on FE-DBD has been supported by NSF ECCS award 1202095. The FEMTA development is supported by NASA Smallsat partnership program through grants NNX13AR02 and NNX15AW40A. I.B. Sebastiao was supported by the Brazilian National Council for Scientific and Technological Development (CNPq-Brazil) under grant GDE/201444/2012-7.

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Prediction of Rarefied Micro-Nozzle Flows using the SPARTA Software

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Predicting the performance characteristics and designing optimal configurations of micro-propulsion systems is vital for the growth of smaller, more cost-effective satellites. The geometric constraints on the system can restrict nozzle exit diameters to be smaller than a millimeter. The small size limits the characteristic length scales of the flowfield to be on the order of the mean free path within the nozzle and the gas interaction with the surface forms a relatively large boundary layer that can affect the thrust. In addition, limitations in conventional manufacturing can result in wavy walls that may have an effect on the thruster performance [1]. Conventional nozzle design codes use the continuum and inviscid approximations, which are inappropriate for micro-nozzle design and analysis. Recent works [2-4] have demonstrated the direct simulation Monte Carlo (DSMC) method to accurately predict the flow in micro-nozzles under steady-state conditions. However, for some applications, the micro-thruster may be required to operate with pulsed conditions where the unsteady portions of the thrust time may be important. Development of the SPARTA library [5] has enabled exploration of unsteady flow features using the DSMC method in a highly flexible manner [6]. This paper will present recent work that utilizes the SPARTA library to understand the time-scales required for development of the important flow features, such as the thick boundary layers, and its effect on the thrust profile for micro-propulsion nozzles. This work will also explore the effect of the wall waviness due to manufacturing limitations. The baseline geometry for the nozzle, shown in Figure 1 (top), is taken from [3,4] and will allow comparison with future measured results, while Figure 1 (bottom) shows a snapshot of the particle locations at the nozzle startup.

Fig.1: (top) Schematic of nozzle geometry used in DSMC simulations and (bottom) snapshot of DSMC simulation during the unsteady startup.

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REFERENCES

Selection of DSMC Parameters for Reducing Computational Expense in Simulation of 3D Microchannel Flows

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Direct Simulation Monte Carlo (DSMC) technique has proven to be a successful method to simulate rarefied gas flows in micro-channels. A majority of DSMC simulations are carried out for two dimensional domains due to the domain geometry and also because a 3D simulation is computationally expensive. Computational time can be reduced by proper selection of the number of cells (or cell size), particles per cell, and initial distribution of particles. Generally cell size is selected to be one third of the mean free path of the gas [1]. However the gradient of velocity in the flow direction is lesser than that in the direction normal to the flow. This ensures that even if the cell size in the flow direction is equal to the mean free path (or slightly higher), it will not affect the computational results [2]. There also exist studies that suggest a minimum number of simulated molecules per cell [3] without mentioning the corresponding statistical error. Decreasing the number of simulated molecules per cell leads to faster simulations; however, the number of time steps required for reducing the statistical noise increases. Besides this, the simulated particles are distributed in the cells initially according to the specified inlet pressure, outlet pressure or linear pressure variation in the domain. These initial conditions affect the total simulation time. Thus there is a need to identify appropriate cell size, number of particles per cell and initial simulation condition to reduce the computational expense of 3D simulations.

Fig. 1: Variation of stream velocity along flow direction

A 3D MPI based parallelized in-house DSMC code is developed and validated for micro-channel gas flow simulation. Simulations are carried out for Argon gas flow in a straight micro-channel with an inlet Knudsen number 0.1, cell size equal to $\lambda/3$, $2\lambda/3$, $\lambda$, $2\lambda$, $4\lambda$ and $8\lambda$. The centreline velocity along the flow direction for these cell sizes are compared in figure 1. It is observed from figure 1, that the centreline velocity does not vary significantly even when the cell size is twice the mean free path. Similar results are obtained for centreline pressure and temperature variations along the flow direction. Similarly, streamwise velocity, pressure and temperature in cells located adjacent to the walls do not vary significantly when cell size is twice the mean free path. In the present study, selection of appropriate cell size, particle number per cell and initial condition to reduce 3D simulation time for various operating and geometric parameters has been conducted. These results will be presented at the conference.

REFERENCES
On the Accuracy of the SBT Collision Algorithm in Nanoflows and Hypersonic Regime

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This paper presents a review of the accuracy of the Simplified Bernoulli Trial (SBT) algorithm and its invariants, i.e., SBT-TAS (transient adaptive subcells) and ISBT (intelligence SBT) in the simulation of a wide spectrum of rarefied flow problems, ranging from collision frequency ratio evaluation in the equilibrium condition, comparison of the Sonine-polynomial coefficients prediction in the Couette flow with the theoretical prediction of the Chapman-Enskog expansion, accurate wall heat flux solution for the Fourier flow in the slip regime, rarefied flow over NACA0012 airfoil, flow inside micro/nano nozzles and divergent channels, and hypersonic flows over cylinder and biconic geometries [1-6]. We summarize advantages and requirements that utilization of the SBT collision algorithm brings to a typical DSMC solver.

Fig. 1: SBT solution for different test cases

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Session 11: DSMC in Hypersonic Flows

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Aerodynamic Characterization of the Jet of an Arc Wind Tunnel

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The arc wind tunnel is a facility for the simulation of the heat flux experienced by space vehicles in high altitude, hypersonic atmospheric re-entry. Tests in such a kind of facility are aimed at the design of the Thermal Protection System (TPS). It is well known that, due to very aggressive environment and to rather high rarefaction level of the jet, the measurement of fluid-dynamic quantities is difficult. For this reason, the evaluation of the jet aerodynamic parameters (velocity, temperature, gas composition, etc.) relies also on computer codes, simulating the tunnel operation by input data such as mass flow rate of the test gas, voltage and current to the heater, etc.. The arc wind tunnel at the Department of Industrial Engineering in Naples (Italy) [1], [2], named Small Planetary Entry Simulator (SPES), was designed also for the measurement of aerodynamic forces and for carrying out basic research in the field of material catalycity. SPES is provided with a water-cooled Pitot tube (for the measurement of the jet total pressure) and with static pressure taps along the tunnel wall to be used in conjunction with the computing analysis.

The simulation of the flow field in SPES relies on two codes working in tandem or the output from the first one is the input to the second one: 1) one-dimensional, inviscid code simulating the flow field in the heater, in the mix-chamber and in the nozzle up to the continuum breakdown position along the nozzle axis. This position is identified by the condition that the Bird’s continuum breakdown parameter $P \geq 0.02$ [3]. 2) Direct Simulation Monte Carlo code DS2V-64 bits [4] simulating the flow field in the remaining part of the nozzle and in the test chamber. The thermo-fluid-dynamic parameters at the exit section of the nozzle are considered as the jet or the “free stream” parameters.

An interesting problem, considered in this paper by means of the present computing procedure, has been the simulation of the flow field around the Pitot tube and of the measurement of the total pressure. As reported by Stephenson [5] and Kokin [6], the measure of the total pressure, in rarefied flow, may be even four times the theoretical value. Therefore, a substantial correction must be applied to the measured data. In the present paper a correction factor is proposed for the total pressure measured in SPES. The correction factor has been evaluated by the comparison of the measured total pressures with that computed by the present procedure.

Twelve tests have been made using nitrogen as test gas: mass flow rate ($m_{N_2}$) of 0.3 and 0.5 g/s, electric power to the heater in the range 10-22 kW. Figure 1 shows the profiles of pressure measured by the Pitot tube and computed by the present procedure both made not-dimensional by the theoretical stagnation pressure behind a normal shock wave ($p_{02}$). According to the suggestions by Stephenson [5] and Kokin [6], the measured and the computed pressures are correlated in concise form by means of the Reynolds number behind a normal shock wave ($R_{2D}$, $D$ is the outer diameter of the Pitot tube).

**REFERENCES**

DSMC Computations of Hypersonic Flow Separation and Re-attachment in the Transition to Continuum Regime

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The characteristics of high-enthalpy, low-density flow separation over an expansion-compression configuration (the so called ‘Tick’ model) are investigated using the Direct Simulation Monte Carlo method. The chosen configuration exemplifies generic flows of planetary entry vehicles with a minimal influence of pre-existing boundary layer on the separation characteristics. Another salient flow feature of the present configuration is the onset of separation after a strong expansion at the sharp leading edge, where the slip effects counter-act the pressure build-up instigated by the downstream compression surface.

The computations are performed using the code SPARTA, but as an attempt towards code verification, the results are compared with Bird’s code, DS2V. An extensive convergence study, based on both spatial and temporal aspects of the flow, is performed to attain a grid-independent solution and also to ascertain the time required to achieve steady-state flow-field solutions. The computational predictions are evaluated in terms of surface parameters such as pressure, heat flux, shear stress and velocity slip. A typical heat flux distribution over the model surface, for varying grid sizes, is shown in Fig 1. In a previous paper by the same authors [1], it has been suggested that, under incipient separation conditions, the velocity slip can be a better indicator of separation region rather than the usually studied shear stress behaviour. This is investigated further in this paper.

An examination of the local, gradient-based, Knudsen number distribution over the flow domain indicates that the flow regime extends from continuum to rarefied. This makes the present geometry a very suitable example for fundamental studies on hypersonic flow separation, in contrast to the extensively studied geometries such as cylinder/flare, bi-conics [2], compression corners [3] etc. It also assists in analysing the efficiency of molecular simulation methods to predict the flow behaviour in the transitional regime. The computational studies are supplemented with experiments currently being conducted at the T-ADFA free-piston shock tunnel at UNSW Canberra, Australia.

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This study forms part of the Australian Research Council Grant, DP-140100842, and this support is gratefully acknowledged. Our sincere thanks are due to Michael A. Gallis and Steve Plimpton, who are the developers of SPARTA code at Sandia National Laboratories, for the useful discussions and comments. Thanks are also due to Dr. Melrose Brown, at UNSW Canberra, for his generous help in debugging many of the installation issues as well as helpful practical advice.

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Uniform rovibrational collisional $N_2$ bin model for DSMC with application to atmospheric entry flows

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In previous work [1], a state-to-state model for internal energy exchange and molecular dissociation in nitrogen was implemented in a flow solver based on the direct simulation Monte Carlo (DSMC) method [2]. The elementary reaction cross sections for the $N_2 (v,J) + N$ system were extracted from a quantum-chemical database compiled at NASA Ames Research Center [3]. Due to the high computational cost of simulating the full range of inelastic collision processes of this system (approx. 23 million reactions), a coarse-grain model [4] (Uniform RoVibrational Collisional bin model) was used instead. This allowed to reduce the original 9390 rovibrational levels of $N_2$ to between 10-100 energy bins. The DSMC implementation was verified by comparing simulations of an adiabatic heat bath with those of the equivalent system of master equations.

In the present work, the dependence of the gas thermodynamic properties and the inelastic cross sections on the binning strategy is examined further. A compromise between a small number of bins and the best reproduction of the behavior of the full system is sought by introducing bins of variable energy width. The model is then applied to studying internal energy excitation and dissociation of $N_2$ as the gas is compressed across a normal shock wave. In this case the effects of inelastic collisions on the shock structure are of special interest (e.g. the incubation length for dissociation of $N_2$ and the overall shock thickness).

In a third step, the reduced model is used to simulate 2D and 3D flow configurations which more closely reproduce the conditions of high-speed entry into Earth's atmosphere. For this purpose, the URVC bin model has to be adapted to be integrated with a separate high-performance DSMC code [5], capable of handling complex geometries and parallel computations.

REFFERENCES

Numerical Analysis of Thermal and Chemical Nonequilibrium in Dissociating Oxygen Shock Waves

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Development and application of physically realistic models for thermally and chemically non-equilibrium gas flows is hindered by the lack of reliable and detailed data for model validation. This issue is most apparent for flows with significant degree of non-equilibrium, in the flow regimes where a kinetic approach needs to be used, where there are very few datasets available. One of the more recent and reliable experiments is [1] where a UV light absorption detection was used to measure the vibrational temperature profiles in high enthalpy oxygen shock waves. First attempts to validate kinetic models of energy transfer and chemical reactions [2] using the direct simulation Monte Carlo (DSMC) method have led to the realization that neither popular empirical DSMC models, nor more sophisticated and arguably better models based on quasiclassical results, can provide acceptable agreement with experimental data [1]. More recently [3], significant differences were observed between [1] and advanced coupled vibration-dissociation models.

To better understand possible reasons for the disagreement, the authors examine the interaction between the thermal and chemical non-equilibrium at microscopic level, the nonelastic and chemical rates, and the gas properties, in high temperature thermal relaxation for flow conditions of experiments [1]. The DSMC method is used in all computations. The collision models range from empirical Larsen-Borgnakke to quasiclassical (QC) state-to-state for the internal energy transfer, and Bird's total collision energy to Koura's weak vibrational bias (WVB) extended to include rotational modes [4] for the dissociation. The baseline collision model is VSS-QC-WVB, with parameters for the energy transfer and dissociation models obtained through detailed comparison of energy-dependent cross sections and temperature dependent rates with available theoretical results for pairs O₂-O₂ and O₂-O, as well as N₂-N₂ and N₂-N. An example of such a comparison is shown in Fig. 1 (top), where the WVB model with different vibrational favouring parameters is compared with [5]. An illustration of vibrational nonequilibrium in a heated front behind the shock for different models is given in Fig. 1, bottom. Note that such a nonequilibrium results in several times lower dissociation rate. The full paper will consider the impact of macroscopic rates on vibrational populations and flow parameters, the strength of the vibration-dissociation coupling, the adiabatic vibration-vibration energy transfer, collision diameter increasing with vibrational level, and non-equilibrium chemical reaction rates.

ACKNOWLEDGEMENTS

The work was supported in part by the Air Force Office of Scientific Research (Program Officer Dr. Ivett Leyva).

REFERENCES

The hypersonic flow of nitrogen gas over a double wedge was simulated by the DSMC method using two dimensional and three dimensional geometries. The numerical results were compared with experiments conducted in the HET facility for a high-enthalpy pure nitrogen flow corresponding to a free stream Mach number of approximately seven [1]. Since the conditions for the double wedge case are near-continuum and surface heat flux and size of the separation are sensitive to DSMC numerical parameters [2], special attention was paid to the convergence of these parameters for both geometries. The 2-D simulation were performed using more than 1.1 billion simulated particles whereas, for the 3-D case, the number of simulated particles and collision cells used were about 19 billion and 4 billion, respectively. At the beginning of the simulation, the separation zone was predicted to be small and the heat flux values for the 2-D model were comparable with the experimental data. However, for increasing time, it was observed that the heat flux values and shock profile strongly deviated from the experiment. Investigation of a three-dimensional model showed that the flow is truly three-dimensional and the side edge pressure relief provides good agreement between simulations and experiments. It was found that the simulated translational temperature contours are non-uniform in the z-direction shown in Fig.1 and the separation zone predicted by the three-dimensional calculations was found to be smaller compared to that of a two-dimensional geometry and had a significant effect on the flow stability. This paper also shows a certain amount of slip velocity which has significant effect on the size of the separation zone and flow steadiness [3]. Therefore, the zero slip assumption is an obvious shortcoming of Navier-Stokes solutions of this problem.

ACKNOWLEDGEMENTS

The research is supported by the Air Force Office of Scientific Research through AFOSR Grant No. FA9550-11-1-0129 with a subcontract award number 2010-06171-01 to UIUC. This research is also a part of the Blue Waters sustained-petascale computing project, which is supported by the National Science Foundation and the state of Illinois.

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<td>Mirza, Nizenkov, Fasoulas</td>
<td>Simulation of flow around a 70-degree blunted cone using two particle methods in a wide Knudsen number range.</td>
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The Boltzmann equation is often used to model rarefied gas flows in the transition or kinetic regimes for moderate to large Knudsen numbers. However, standard moment methods like Grad's approach [1] lack hyperbolicity of the equations. We give examples for failure of Grad’s method and overcome the deficiencies with the help of the new hyperbolic moment models QBME and HME, derived by an operator projection framework in [2]. The new model equations are in partially-conservative form meaning that a subset of the equations cannot be written in conservative form due to some changes in these equations. This leads to additional numerical difficulties. The influence of the partially-conservative terms on the solution is analyzed and we present a numerical study to compare several numerical schemes for the solution of the partially-conservative PDE systems, including the PRICE-C scheme by Canestrelli [3] and the wave propagation scheme by LeVeque [4]. Furthermore, the accuracy of the different hyperbolic moment models is compared to a discrete velocity reference solution together with a convergence study for increasing number of moments. Unless extreme flow conditions are considered first results show that the methods give accurate results despite the fact that the model equations cannot fully be written in conservative form.

REFERENCES
Shock wave and fluid instability simulations at different Knudsen numbers with a kinetic particle approach

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We present and discuss results for two and three dimensional shock wave and fluid instability simulations with a Monte Carlo particle kinetic code. The simulations are performed for a large range of Knudsen numbers to study the impact of kinetic effects on the structure and dynamics of shock waves and fluid instabilities. Performed studies include the Sod, Noh, and Sedov shock tests in two and three dimensions and two-dimensional Rayleigh-Taylor and Kelvin-Helmholtz simulations [1,2]. For simulations that are close to the continuum limit (i.e. for small Knudsen numbers) we compare our results to analytic predictions and hydrodynamic simulations.

Our aim is to develop a Monte Carlo code that can capture flows for a wide range of Knudsen numbers and large physical systems. For future applications of the code, our focus lies on core-collapse supernova (CCSN) and inertial confinement fusion (ICF) capsule implosion studies. The dynamics of both systems is predominantly shaped by shock waves, fluid instabilities and flows with large Knudsen numbers in form of neutrinos and deuterium/tritium ions for CCSN and ICF capsule implosion, respectively. In addition to the above standard shock and fluid instability tests, which serve as validation and benchmark problems for our code, we also present simulations that are more directed towards CCSN [3] and ICF studies, namely implosion and gravitational collapse simulations.

ACKNOWLEDGEMENTS

This work used the Extreme Science and Engineering Discovery Environment, which is supported by the National Science Foundation Grant No. OCI-1053575. I.S. acknowledges the support of the High Performance Computer Center at the Institute for Cyber-Enabled Research at Michigan State University. This research was supported in part by Lilly Endowment, Inc., through its support for the Indiana University Pervasive Technology Institute, and in part by the Indiana METACyt Initiative. The Indiana METACyt Initiative at Indiana University is also supported in part by the Lilly Endowment, Inc.

REFERENCES

Local velocity grids for deterministic simulations of rarefied flows in two dimensions

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In most of deterministic numerical methods for rarefied gas dynamics, the kinetic equation is discretized with a finite set of discrete velocities. This set is generally a global Cartesian grid, which is the same grid for every point in the physical domain, and for every time. The advantages of this approach is its simplicity, and the fact that the discrete model satisfies many strong properties of the continuous one (stability, positivity, for instance). This is due to the fact that all the distribution functions are discretized with the same grid. However, for some practical problems with strong variations of macroscopic temperature and velocity fields, like in atmospheric re-entry hypersonic flows, this approach is very expensive. Indeed, some distributions are very large (in zones where the temperature is large, like in the shock wave), while other distributions are very narrow (in zones where the temperature is small, like in the upstream flow, or close to a solid isothermal boundary). This requires that the discrete velocity grid must be very large and very dense in order to capture all the different distribution functions. Another problem, in particular for unsteady flows, is that it is sometimes very hard to know \textit{a priori} what grid has to be used for a correct computation: the strong temperature variations may indeed occur after some transient phase.

In [1], we have proposed a method that uses a discretization of the kinetic equation on local velocity grids: these grids dynamically adapt in time and space to the variations of the width of the distribution functions. Contrary to other recent works [2,3], even the bounds of each local grids can vary in time and space. However, this work was restricted to 1D problems, both in space and velocity.

In this talk, an extension of [1] to two-dimensional problems will be presented: the additional cost of the 2D aspect requires to modify different elements of our method. The properties of this new method will be illustrated with several test cases.

ACKNOWLEDGEMENTS

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REFERENCES

Discrete Velocity Models for Multicomponent Mixtures and Polyatomic Molecules without Nonphysical Collision Invariants and Shock Profiles

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An important aspect of constructing discrete velocity models (DVMs) for the Boltzmann equation [1,2] is to obtain the right number of collision invariants [1,3]. It is a well-known fact that, in difference to in the continuous case, DVMs can have extra collision invariants, so called spurious collision invariants, in plus to the physical ones. A DVM with only physical collision invariants, and so without spurious ones, is called normal. The constructions of such normal DVMs has been studied a lot in the literature for single species as well as for binary mixtures, e.g. see [3-5]. For binary mixtures also the concept of supernormal DVMs has been introduced in [3]. Supernormal DVMs are defined as normal DVMs such that both restrictions to the different species are normal as DVMs for single species.

In this presentation we extend the concept of supernormal DVMs to the case of multicomponent mixtures and introduce it for polyatomic molecules. By polyatomic molecules we mean here that each molecule has one of a finite number of different internal energies, which can change, or not, during a collision. We will present some general algorithms for constructing such models, but also give some concrete examples of such constructions.

The two different approaches above can be combined to obtain multicomponent mixtures with a finite number of different internal energies, and then be extended in a natural way to chemical reactions.

The DVMs are constructed in such a way that we for the shock-wave problem [6,7] obtain similar structures as for the classical discrete Boltzmann equation (DBE) for one species [8], and therefore will be able to apply previously obtained results for the DBE in [8]. In fact the DBE becomes a system of ordinary differential equations (dynamical system) and the shock profiles can be seen as heteroclinic orbits connecting two singular points (Maxwellians). Our previous results in [8] then give us the existence of shock profiles for shock speeds close to a typical speed, corresponding to the sound speed in the continuous case. For binary mixtures this extension was already treated in [9].

REFERENCES

Flow Simulation around a 70-Degree Blunted Cone with Two Particle Methods in a Wide Knudsen Number Range

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Gas flows that are of interest to the field of aerospace engineering can span over multiple orders of magnitude in density. For example, the gas in front of a re-entry vehicle can be treated as a continuum whereas the flow is highly rarefied in the wake of the heat shield. Such a large density gradient poses a significant challenge to numerical simulation tools, where a compromise has to be made between accuracy and performance.

Two particle-based methods, the established Direct Simulation Monte Carlo (DSMC) method [1] and the novel Low Diffusion (LD) method [2] are compared in terms of accuracy and performance. While DSMC enables the physically accurate simulation of rarefied gas flows, LD enables the efficient simulation of dense flows under continuum assumption.

In the framework of PICLas [3], both methods have been utilized to simulate the gas flow around a 70° blunted cone in a wide range of Knudsen numbers from 0.001 to 10. On the one hand the simulation of this test case suits well to demonstrate the performance limitation of the DSMC method. On the other hand the advantage of using the LD implementation in dense flow regions, where the computational effort can be reduced substantially, becomes evident. Additionally, both methods are validated by comparison to existing experimental heat flux measurements [4]. The benefit of applying a novel particle-based method to simulate continuum flows instead of using a Navier Stokes solver is that LD can be easily coupled with DSMC [5]. The research towards a coupled application of both methods to enable the efficient and physically accurate simulation of flows with large density gradients is addressed in this work.

ACKNOWLEDGMENTS

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Session 13: Plasma Applications

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Ionized gas plasmas near room temperature are used in a remarkable number of technological applications mainly because they are extraordinarily efficient at exploiting electrical power for useful chemical and material transformations near room temperature. For example, plasma-assisted thin film deposition and etching applications in integrated circuit manufacture have evolved into technologies that allow control of features at the nanometer scale in commercial processes.

One of the newest area of low temperature ionized gas plasmas - or cold atmospheric plasma (CAP) - is the use of CAP for biomedical applications. In this case, the temperature-sensitive material is living tissue. [1]

CAP research directed towards biomedical applications such as sterilization, surgery, wound healing and anti-cancer therapy has seen remarkable growth in the last 3-5 years, but the mechanisms responsible for the biomedical effects have remained mysterious. It is known that CAP readily create reactive oxygen species (ROS) and reactive nitrogen species (RNS). ROS and RNS (or RONS), in addition to a suite of other radical and non-radical reactive species, are essential actors in an important sub-field of aerobic biology termed ‘redox’ (or oxidation-reduction) biology. The evidence suggesting that RONS generated by plasmas are responsible for their observed therapeutic effects is now fairly extensive. [2,3] In addition, evidence shows that electric fields and photons can play significant biomedical roles under some conditions. The mechanisms responsible for interactions between the active plasma and living matter are still a matter of debate and active research. [4]

REFERENCES

Crossed Contributions to Electron and Heavy Particle Transport Fluxes for Magnetized Plasmas in the Continuum Regime

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An accurate modeling of dissipative effects in magnetized plasmas is crucial to many applications. A particular focus is placed on solar physics and electric propulsion applications. We propose to calculate the crossed contributions to the mass and energy transport fluxes coupling the electrons and heavy particles, such as atoms and ions, in multicomponent plasmas in translational thermal nonequilibrium. This effect was first introduced by Kolesnikov [1]. To derive asymptotic solutions for multicomponent plasmas based on kinetic theory, it is essential to solve the distribution functions in the Enskog expansion up to second-order for electrons and up to first-order for heavy particles [2]. However, the second-order electron transport fluxes should not be confused with Burnett fluxes. The heavy-particle diffusion velocities and heat flux are proportional to an average electron force expressed in terms of the electron diffusion driving force and temperature gradient. Conversely, the electron diffusion velocity and heat flux are proportional to the heavy-particle diffusion driving forces and temperature gradient. The magnetic field induces anisotropic transport fluxes when the electron collision frequency is lower than the electron cyclotron frequency of gyration around the magnetic lines. The explicit expressions for the transport coefficients are obtained by means of a Galerkin spectral method [3].

After the complete plasma description of [2] is given, practical expressions for the full transport systems necessary to compute the transport coefficients for thermal nonequilibrium plasmas are presented. The expressions are valid for both partially and fully ionized plasmas. In addition, the multi-temperature formulation for strongly magnetized plasmas is shown to be consistent with the weakly magnetized expressions in the limit of low magnetic fields. This was previously shown by Giovangigli [4] for the thermal equilibrium case. To the authors’ knowledge, this is the first time these expressions are computed based on the correct scaling of the Boltzmann equation obtained from a dimensional analysis accounting for the electron to heavy particle mass ratio and Hall parameter. The relative importance of the Kolesnikov effect is then studied through comparisons with the classical mass and energy transport modes.

REFERENCES

Hybrid Kinetic/Fluid Modeling of Silicon Nanoparticles Dynamics in Silane Plasma Discharges

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Plasma Enhanced Chemical Vapor Deposition (PECVD) using parallel plate capacitively coupled radio frequency (RF) glow discharge systems has become the mainstream technology for large area deposition of silicon thin films for electronic applications. It is known that the deposition rate increases, associated with PECVD process running at higher pressure or RF power, will lead to the formation of clusters, nanoparticles and eventually powders [1]. This is a strong motivation for deriving a detailed model from the kinetic theory coupled with a kinetic model for the dust particles.

A complete derivation of fluid plasma equations from the kinetic theory has been performed, accounting for inelastic collisions, internal degrees of freedom, thermal non-equilibrium between electrons and heavy particles, and influence of the electric field. Following the Chapman-Enskog’s method [2-3], we have obtained the zeroth-order Euler equations, and first-order Navier-Stokes and drift-diffusion equations. On the other hand, the nanoparticles are handled with a discrete sectional model accounting for both size and charge distribution [4-5]. This sectional model accounts for nucleation, surface growth, and coagulation, but also transport properties and drag forces exerted on nanoparticles.

The resulting equations for a self-similar flow have been solved numerically. The RF frequency was fixed at 13.56MHz, the pressure set at 2Torr, RF voltage amplitude was set at 100V, and the gas temperature at 500K. The inlet partial pressure of silane was varied from 5 to 20% of the total gas pressure of the SiH₄/H₂ inlet mixture. The electrode separation distance was 2cm. We investigate the charging mechanism in the first steps of nanoparticles nucleation and growth, when the size of the particles does not exceed a few nanometers. This regime is of particular importance since there are few experimental data for this size range, and since it is believed to be the optimal regime with regard to thin-film deposition [1].

ACKNOWLEDGEMENTS

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REFERENCES

The Preserving Neutron Flux Properties Discrete Scheme for Multi-media Time-dependent Neutron Transport Equations

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There exist numerical solution oscillation and negative flux for typical discrete scheme when solving multi-group multi-media sophisticated time-dependent neutron transport equations which brings difficulty for mathematics and physics analysis. In this paper, the numerical solution oscillation for sophisticated problem is investigated. The influence of time discrete scheme and space discrete scheme on this oscillating phenomenon is analyzed for neutron transport equations. In addition, the preserving positive neutron transport scheme (PPLD) is studied. The new scheme can take 0 order moment and 1 order moment of the neutron transport equation. Numerical experiments show that second-order time evolution scheme and linear discontinuous finite element method yield more accurate results and provide very smooth physical quantity curves. Based on the non-oscillation scheme, the positive scheme gives the non-negative neutron angular flux. These preserving physical properties neutron transport schemes maintain the smooth of neutron multiplication constant and positivity of neutron flux.

Fig.1: J for mutigroup problem

Fig.2: flux for PPLD method (the maximal value is 102.732, the minimal value is 0)

REFERENCES

Session 14: 12th Lloyd Thomas Lecture

T. Minton, "Dynamics of Energetic Gas Surface Collisions"
Dynamics of Energetic Gas Surface Collisions

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Energetic gas-surface collisions, where incident atoms or molecules have translational energies that are one or two orders of magnitude higher than thermal energies at room temperature, exhibit interesting and potentially useful scattering phenomena. The dynamics of such collisions involve pathways that are unusual and often difficult to predict – for example, the surmounting of reaction barriers that are typically unreachable and subsequent formation of uncommon or unknown products, reaction trajectories that deviate significantly from the minimum energy path and lead to unexpected product angular or internal energy distributions, penetration or diffusion into surfaces, highly localized and non-thermal scattering on surfaces, and production of surfaces or materials through non-equilibrium routes.

These high-energy gas-surface interactions might seem to be exotic, but there are numerous situations where such extreme interactions influence the outcome of practical endeavors, such as the analytical probing of liquid surfaces [1], spacecraft degradation in low-Earth orbit [2], energy accommodation during aerobraking in planetary atmospheres [3], heat shield ablation during atmospheric entry [4], materials growth under non-equilibrium conditions [5], and thin-film sputtering [6]. One can imagine many additional technological applications where the knowledge of energetic gas-surface collision dynamics would be important. Studies of these dynamics can reveal the rich details of the chemical and physical processes whenever a surface is subjected to a gas at high collision energies or temperatures, thus providing a foundation upon which to build predictive models.

This lecture will highlight the fundamental aspects of energetic gas-surface scattering dynamics in the context of their applications to liquid surface probes and spacecraft-environment interactions. The relative importance of non-thermal (often referred to as “direct” or “impulsive”) scattering events versus thermal desorption is an important characteristic of energetic gas-surface collisions. The non-thermal interactions are localized on the surface and are reminiscent of gas-phase collisions. Like gas-phase collision, the dynamics of non-thermal gas-surface collisions report unique aspects of the interaction potential, revealing detailed information about the structure and reactivity of a surface.

ACKNOWLEDGEMENTS


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Kihara, Kotsubo, Yoshimoto, Kinefuchi, Takagi, "Incident Energy Dependence of Scattering Behavior of Water Molecules on Si (100) and Graphite Surfaces"

Mehta, Levin, Murray, Minton, "Study of Non-Reactive Scattering from Graphene Using Beam Experiments and Molecular Dynamics"

Nakauchi, Mabuchi, Kinefuchi, Takeuchi, Tokumasu, "Scattering Dynamics of Oxygen Molecules of Nafion Membrane"

Aoki, Giovangigli, Hattori, "A Kinetic Model of Adsorption on Solid Surfaces"
Incident Energy Dependence of Scattering Behavior of Water Molecules on Si (100) and Graphite Surfaces

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Gas flows in carbon- or silicon-based nanostructures are of great interest due to their potential application in various devices such as polymer electrolyte fuel cells [1] and permeation membranes [2]. Since the interactions between gas molecules and solid surface greatly affect nanoscale gas flow [3], it is important to understand the scattering behavior of gas molecules on solid surface. In this study, we conducted the molecular beam scattering experiments of water molecules on silicon and graphite surfaces to reveal the impacts of incident energy and surface property on their scattering dynamics. We used a highly-oriented pyrolytic graphite surface and a Si (100) surface terminated with hydrogens and hydroxyl groups. The incident energy of water molecules was varied from 35 to 370 meV, covering their thermal energy distribution at room temperature. The angular distributions of scattering intensity and mean translational energy were measured using the time-of-flight method.

The experimental results indicate that scattering distributions greatly change according to the surface kind and the incident energy. The in-plane scattering angle distributions on the graphite surface [4] are shown in Fig.1 (a). The angular distribution for the lower incident energy (35 meV) is less directive, showing that water molecules with lower incident energy are more likely to accommodate with the graphite surface. This seems to be typical scattering behavior on an atomically flat surface. On the other hand, as shown in Fig.1 (b), the in-plane scattering angle distribution on the Si (100) surface is more directive for the lower incident energy (35 meV), while the angular distribution for the higher incident energy (65 meV) exhibits an almost cosine-like scattering. Performing the molecular dynamics simulation, we have revealed that this characteristic scattering behavior on the Si (100) surface is originating from the atomic corrugation of the surface. Detailed discussion will be presented in a subsequent full paper.

REFERENCES


Fig.1: In-plane scattering angle distributions of water molecules on a graphite surface (a) and a Si (100) surface (b). The incident translational energies are 35 and 65 meV. The surface temperature and the incident angle are 300 K and 40°, respectively.
Study of Non-Reactive Scattering from Graphene Using Beam Experiments and Molecular Dynamics

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Gas Surface Interactions (GSI) are an integral part in the transfer of energy from the fluid to surface. Heat transfer, boundary layer formation, and surface chemistry are some of the important aspects covered under GSI. The focus of this work is to use beam experiments and molecular dynamics (MD) to understand the causes and mechanisms of GSI at an atomistic level. Non-reactive collisions can be analyzed purely in terms of incidence and reflection properties. To understand GSIs, trajectory simulations in MD are performed on a graphene (HOPG) surface using nitrogen and argon gas at incidence speeds and angle used for the beam experiments. We have used graphene as the surface because it has a planar topology at an atomic level representing a ‘clean’ engineering surface.

It was determined from MD that GSIs can be classified into three categories, namely single collision, multiple collisions with escape, and multiple collision without escape [1]. The statistics of gas molecules performing either of the three categories of collision depends on the incidence speed and angle of the gas molecule. The reflection angle probability distributions from MD are compared with those observed by the beam experiments [2] and as shown in Fig.1, the MD results were able to replicate the lobular distribution. Parallel momentum conservation (PMC) [3] predicts that if the gas molecule scatters closer to the surface normal, it gains energy from the surface, even if the gas is at a higher temperature that the surface. For the distributions shown in Fig.1, trajectories with scattering angle less than their respective incidence angle represent collisions where the gas molecule gained energy from the cold surface. This phenomenon was observed from both the beam experiments as well as MD simulations. We will also present our findings on the effect of van der Waal’s interaction potential well-depth on the post-reflection angle and kinetic energies of the gas. Similar MD simulations will be performed using argon to understand the effect of diatomic versus monoatomic gas on GSIs.

ACKNOWLEDGEMENTS

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Scattering Dynamics of Oxygen Molecules on Nafion Membrane

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Mass transport in polymer electrolyte fuel cells (PEFCs) significantly affects its reaction efficiency. In particular, the oxygen transport in catalyst layers (CLs) is one of the dominant factors of power losses in PEFCs [1]. In CLs, the oxygen transport depends greatly on the nanoscale characteristics of the scattering and diffusion of oxygen molecules on ionomer surface, which is composed of perfluorosulfonic acid membranes as typified by Nafion. Kinefuchi et al. have investigated the oxygen diffusion resistance in CLs using direct simulation Monte Carlo method, and reported that the simulation does not well reproduce the experimental results [2]. This disagreement is due to the inaccurate interaction model between oxygen molecules and ionomer surface. An interaction model, which can reproduce the scattering and diffusion phenomena on ionomer surface, is required for more accurate analysis of the oxygen transport in CLs. The construction of the model needs the detailed understanding of the gas–surface interaction.

In this study, we have analyzed the dynamics of oxygen scattering on ionomer surface using molecular dynamics simulation. It was found that oxygen molecules with high incident energy tend to lose their translational energy when they reflect on the ionomer surface. Scattering angle distributions show that the scattering behaviors are not sensitive to the incident angle and energy.

ACKNOWLEDGEMENTS

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REFERENCES

A Kinetic Model of Adsorption on Solid Surfaces

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The interaction of gases with solid surfaces is relevant in scientific and engineering applications like hypersonic reentry, ablation phenomena or chemical deposition reactors [1, 2]. This is a strong motivation for investigating kinetic models of adsorption processes—at a scale intermediate between molecular simulation [3] and fluid models [4]—and deriving rigorously kinetic as well as fluid reactive surface boundary conditions using the Chapman-Enskog method.

Kinetic models assuming chemical equilibrium at the solid boundary only differ from Maxwell boundary conditions by the values of equilibrium partial densities. More detailed kinetic models involve Boltzmann equations taking into account the interaction of gas particles with an average surface potential as well as phonons near the surface boundary [5, 6, 7, 8, 9]. Monte Carlo Direct Numerical simulations [7], particle trapping, homogenization along the surface [8], and kinetic boundary conditions [9] have notably been investigated. Only gas particles interacting with the surface have been considered in these models, that is, physisorption phenomena. However, chemical bonds may also be formed between particles and the surface leading to chemisorption and it is natural to consider the chemisorbed species as another type of molecule compared to its parent gas phase. A kinetic model describing both physisorption and chemisorption is presented in this study for a single monatomic gas, the situation of multicomponent mixtures or polyatomic gases lying out of the scope of the present work.

A single kinetic equation is used to describe both gas particles and physisorbed particles interacting with wall phonons. The phonons are assumed to be in equilibrium [5] although a kinetic equation for phonons may also be considered [10, 11]. The gas plus physisorbate kinetic equation is coupled to a kinetic equation describing localized chemisorbed species analog to the kinetic equations for lattice gases described by Bogdanov at al. [6]. The transition between physisorbed particles and chemisorbed particles is described by a chemistry term in the kinetic equations. A modified kinetic entropy is introduced for the coupled systems and a H theorem is established.

The Chapman-Enskog expansion is then introduced with a fluid scaling of the kinetic equations. A multiscale asymptotic analysis is performed in the gas, the physisorbate and the chemisorbate. Zeroth order distributions are investigated as well as overall mass conservation through the adsorbate layer, and the asymptotic analysis requires to consider a small convective Stefan flow velocity. The fluid adsorption boundary conditions formally associated with the adsorption surface reaction

\[ B(s) + A(p) \leftrightarrow B(b) + A(s) \]

are investigated where A(p) denotes the gas/physisorbate particle, A(s) the chemisorbed particle, B(s) the surface layer crystal particle and B(b) the bulk crystal particle. The fluid boundary conditions are derived and only involves the dynamics of the chemisorbate, that of the physisorbate playing no role. The gas flux from the adsorbate layer dynamics is mostly due to the gas/physisorbate particle production by desorption of the chemisorbate.

REFERENCES

### Session 16: Numerical Methods II

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An Efficient Collision Limiter Monte Carlo Simulation for Hypersonic Near Continuum Flows

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The direct simulation Monte Carlo (DSMC) method can solve flows in any regime from continuum to free molecular, but due to its computational efficiency the method is mostly used to solve transitional to rarefied flows. In order to reduce the expensive collision part in simulating hypersonic flow near continuum, a modified DSMC method with collision limiter scheme is implemented in the regions of high density flow in thermal equilibrium. The continuum breakdown parameters based on gradient-length local Knudsen number are characterized different regions of the flow. The breakdown regions of nonequilibrium are computed using the standard DSMC method while the equilibrium regions are computed using the collision-limited DSMC method with a larger time step and cell size. Local density gradient-based dynamic adaptation of collision and sampling cells refinement is employed in the high gradient regions including strong shocks and boundary layer near surface. A varied time step scheme is adopted to make sure a more uniform distribution of model particles per collision cell throughout the computational domain. To give a constant ratio of local time step interval to particle weights can avoid particles cloned or destroyed when they cross interface from cell to cell. The collision limiter DSMC method means that the total number of collisions per cell per time step is limited on average to two per molecule. In high density equilibrium regions, the velocity distribution function may tend to Maxwellian equilibrium distribution with little amount of collision numbers, and the cost of computational time can be greatly reduced. This is an all-particle hybrid method and its main advantage is that only small changes of standard DSMC code can greatly enhance computational efficiency. Another way to speed-up the simulation has been to use a MPI parallel implementation of DSMC code. The aerodynamic characteristics of a wave rider shape with sharp leading edge are simulated in the test state for hypersonic near continuum. The test has been finished in hypersonic low density wind tunnel of China Aerodynamics Research and Development Center (CARDC). The test conditions are as follows: Mach number twelve, angles of attack range from 0 to 15 degrees, Knudsen number 8.2e-5. The computed axial force and normal force and pitching moment coefficients varying with angles of attack have good agreements with the experimental data. And this shows that the hybrid collision limiter DSMC method with adaptive mesh refinement and varied time step can efficiently simulate hypersonic near continuum flows.

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Fokker-Planck-DSMC Algorithm for Simulations of Rarefied Gas Flows: Parallel Implementation and 3D Simulations

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In the Direct Simulation Monte Carlo (DSMC) method, the collision operator of the Boltzmann equation is approximated via the explicit calculation of binary collision events. When the Knudsen number (Kn) becomes low, the large number of collisions per time interval makes DSMC computationally expensive. In the Fokker-Planck (FP) based particle Monte Carlo scheme introduced in [1], and further developed in [2] and [3], however, independent continuous stochastic processes for the phase space evolution of each particle are integrated in time. The computational cost of the FP method is thus independent of Kn. Furthermore, it allows for time step and grid cell sizes larger than the respective collisional scales required by DSMC. Finally, the FP-DSMC scheme [4] combines FP and DSMC via an adaptive collision operator and is both accurate and efficient in the whole Kn range.

So far, FP-DSMC was successfully applied to flows in and around relatively simple geometry. In this contribution, we present a general purpose parallel implementation of FP-DSMC capable of simulations containing arbitrary, complex geometry. The implementation supports different collision operators (DSMC, FP, FP-DSMC), different molecular collision models, as well as monatomic and diatomic species. In the latter case, vibrational and rotational degrees of freedom are treated according to [3]. Parallelism in the overall simulation algorithm is exploited on a coarse grain level via domain decomposition and message passing, and further on the a fine grain level via shared memory parallel processing of per-cell and per-particle instructions.

We present three-dimensional test cases for assessment: firstly, results of the simulation of supersonic argon flow past a sphere are compared to pure DSMC for various grid resolutions, demonstrating accuracy and efficiency of the FP-DSMC algorithm; secondly, treatment of arbitrary geometry is demonstrated by the simulation of molecular nitrogen flow past a highly porous body representative of a Draconids meteoroid at atmospheric entry conditions.

All test cases are run on a hybrid distributed-shared memory parallel system, which provides the capability for the implementation to handle simulations on the order of $10^8$ computational particles.

REFERENCES


An Open Source Hybrid CFD-DSMC Solver for
High-Speed Flows

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A hybrid solver to simulate high-speed, non-equilibrium flows has been developed within the free, open source software OpenFOAM [1]. The solver uses Computational Fluid Dynamics (CFD) in regions where the flow can be considered continuum and Direct Simulation Monte Carlo (DSMC) in regions where the continuum assumptions break down and non-equilibrium appears. The algorithm reduces the computational expense from a pure DSMC simulation by using a locally calculated breakdown parameter to distinguish between the continuum region, which will be simulated using the less expensive compressible solver rhoCentralFoam [2], and the rarefied region, simulated using the particle-based solver dsmcFoam [3]. The information is exchanged between the two different solvers using state-base coupling. Comparisons are made for a heat transfer problem for argon for Knudsen numbers 0.005, 0.01, 0.05, 0.1, 0.2, and 0.4 using pure CFD, pure DSMC, the hybrid CFD-DSMC, and an analytical continuum solution. For the hybrid, the CFD and DSMC domains were fixed, with the DSMC domain being 30% of the full domain. At Knudsen 0.005 close agreement exist between all the results, with a small discrepancy occurring near the walls between the continuum solutions and the DSMC and hybrid solver. Increasing the Knudsen number increases this discrepancy between the CFD and DSMC solutions to the point of having a maximum difference of 7% of the initial temperature difference. Despite the CFD solver presenting this temperature difference, the CFD-DSMC hybrid and the DSMC results agree quite well up to Knudsen 0.1. Increasing the Knudsen number more than that increases the error, as the DSMC domain should extend to a higher percentage, or even all, of the domain. These results show that an open source CFD-DSMC hybrid solver has been correctly implemented for a heat transfer problem. The future work will focus on increasing the number of test cases validated using the hybrid, as well as enabling the automatic determination of DSMC and CFD subdomains.

REFERENCES

Kinetic Approach for Describing Biological Systems

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We consider a biosystem as an open nonequilibrium system the properties of which can be described on the basis of kinetic approach with the help of appropriate kinetic equations. According to this method we attempt to evaluate sizes and periods of the bio-organism’s lifespan connecting these values with the inner characteristics of the processes. The obtained results can be compared with numerous empirical data, see [1-2].

Biosystems are modeled with the use of the nonuniform relaxation problems (NRP) [3, 4] and some general properties of such systems are considered. The size $L$ of the region of the spatial nonuniformity associated with the biological system can be evaluated as $L \sim u \tau$, where $u$ is the characteristic velocity of the flow in the biology structure (the blood in mammals or the water in green leaves) and $\tau$ is the average time of the biochemical reaction. This evaluation based on the kinetic description of the nonequilibrium open system can be made more precise taking into account properties of a fractal structure of the vascular system, see [5, 6]. The problem of the lifespan of a biological system is also studied. There are many theories of aging (see e.g. [7]) describing the degradation mechanisms, but from the kinetic point of view these approaches do not possess sufficient generality. The kinetic method allows us to simulate degradation in time using different relaxation problems for closed and open systems. In the case of a closed system the local distribution tends to the equilibrium state (the “thermal death”) in a period of the order of $\tau$. The main idea consists in considering an open system as a close system in the other time scale $T \gg \tau$. This analogy is related to the structure: for the closed system the degradation is realized between the same molecules, for the open system the degradation takes a place for the molecules changed due to metabolism, so our previous kinetic description has been based on the “structural distribution function” [8]. In the present study aging of the open system is described by means of two distributions in two time scales (that is related to description by means of the "structural distribution function"). The ratio $T/\tau$ of two relaxation times corresponds to the known dimensionless value, see [1, 2]. One can consider a steady processes without degradation by the kinetic equation for a hypothetical metabolic transport for large time scales to maintain this system in a stationary state.

A special attention is paid to the behavior of the nonequilibrium entropy, the NRP model describes the increases of entropy from input to output according to the ideas by Schrödinger. In this way we treat a living system as a structure with the entropy less than that in the non-living system of the same mass. The traditional approach to the notion on entropy, which does not take into account the correlation of the parts in the nonequilibrium flow system, leads to the conclusion that the entropies of these two structures are equal, see e.g. [9]. Besides the problem of the NRP type with the “fast flow”, the analogous problems with the nonequilibrium “slow flows” are posed. The formulations of the problems with the boundary conditions of the membrane type, which intend to simulate processes in a living cell, are discussed.

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### Session 17: Plasma Flows and Processes

**Invited** Boeuf, "Negative Ion Production and Extraction for the Neutral Beam Injection System of ITER"

Pfeiffer, **Binder**, Fasoulas, Copplestone, Munz, "Comparison of Plasma Plume Expansion Simulations Using Fully Kinetic Electron Treatment and an Electron Fluid Model"

Foleto, **Pitchford**, Puech, Fontane, Joly, "Visualization of a Helium Jet in Open Air, With and Without Ignition of a Plasma"
Negative Ion Production and Extraction for the Neutral Beam Injection System of ITER

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A large part of the 50 MW plasma heating necessary to get the 500 MW of fusion power in the international fusion experiment ITER will be obtained by injection of fast neutral deuterium atoms in the tokamak [1]. The fast atoms will heat the plasma by ionization and charge exchange collisions. The two, 17 MW power neutral beam injectors of ITER will each deliver a 1 MeV beam energy for 1 hour. The neutral beam will be generated by the neutralization of ions extracted from a low temperature plasma source and accelerated at 1 MeV. Since the neutralization efficiency of positive ions by collisions is very small at this high energy, the neutral beam injection (NBI) system will be based on the neutralization of negative ions of deuterium (hydrogen in the preliminary experiments and tests). Due to the limited efficiency of neutralization and to other losses in the accelerator, the negative ion source must deliver 40 A of D- (H-) to reach the required power of 17 MW of the neutral beam.

The negative ion source for the ITER NBI system is based on RF inductively coupled plasmas (ICP) where the plasma generated by ICP drivers expands in a diffusion chamber separated from the extraction region by a magnetic filter. Several prototypes with one to four ICP drivers are being designed and studied at the Max Planck Institute for Plasma Physics (IPP) in Garching, Germany [2] and the full size negative ion source for the ITER NBI system, consisting in eight ICP drivers (about 100 kW each) will be constructed by Consorzio RFX in Padova, Italy [1].

In this lecture, after an introduction on the characteristics of the NBI system, we will focus on the physics of the negative ion source and of the negative ion extraction from the plasma. In order to reduce the stripping losses (collisional detachment in the source and in the accelerator), the negative ion source must operate at a sufficiently low gas density, below 0.3 Pa. At this low pressure, volume production of negative ion by dissociative attachment on vibrationally excited hydrogen or deuterium molecules is not sufficient to provide the required negative ion current. In order to increase the negative ion current, the plasma grid surface is covered with a caesium layer. Due to the low work function of caesium, hydrogen or deuterium atoms hitting the surface can pick up an electron from the surface by an Auger process, leading to negative ion emission from the surface.

In order to understand and optimize the operation of the negative ion source important efforts have been devoted to the modeling and simulation of the negative ion source and negative ion extraction [3], [4], [5]. This includes a description of the plasma physico-chemistry (fluid models, [3]), with a strong coupling between the plasma and the gas kinetics (neutral depletion due to ionization, non-Maxwellian distributions of gas atoms and molecules that can be described by DSMC methods), as well as a description of the complex charged particle transport in the magnetized plasma, through the magnetic filter and in the extraction region (kinetic simulations [5]). An important issue of negative ion extraction is to limit the current of co-extracted electrons. This implies the use of magnets to generate a magnetic barrier in front of each aperture of the plasma grid, leading to a complex extraction physics. The lecture will present an overview of the different aspects of the physics and modeling of the negative ion source and negative ion extraction.

REFERENCES

Comparison of plasma plume expansion simulations using fully kinetic electron treatment and an electron fluid model

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The expansion of the plasma plume resulting from laser ablation plays an important role in a large number of applications, e.g. material processing, medical laser applications or novel propulsion concepts. Here, a high-order three dimensional Particle-In-Cell code is used to simulate such a plasma plume expansion, shown in Fig. 1 on the right-hand side. A big challenge in this kind of simulation is the handling of the electrons due to their low inertia and following high acceleration. Therefore, two different treatments for the electron modelling are compared. On the one hand, the electrons are simulated as a normal particle species in a kinetic manner, which strongly decreases the time step size and therefore increases the computational effort. On the other hand, the electrons are simulated using an electron fluid model that reduces the computational cost but is less accurate [1,2]. Additionally, the different results of both methods will be compared regarding chemical reactions, e.g. ionization and ion recombination. The electron potential is solved using a high-order highly parallel Hybrid Discontinuous Galerkin (HDG) method [3]. This method also allows the simulation of computationally expensive three-dimensional setups.

Fig. 1: Plasma plume expansion. The slice shows the electrostatic potential, the ions are the red-colored particles and the velocity magnitude of the electrons is shown with the white-blue color scale.

REFERENCES

Visualization of a Helium Jet in Open Air, with and without Ignition of a Plasma

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It is now well-established that stable non-equilibrium plasmas can be generated in a helium jet surrounded by open air. Such plasmas can be initiated by applying high voltage pulses (positive pulses, nominally 5 kV, 10 kHz) to an electrode embedded inside a dielectric tube of small diameter (some mm's or less), through which there is a flow of helium. After application of the voltage, the plasma is generated near the electrode, then spreads along the inner surface of the dielectric tube and continues to propagate in the helium jet past the exit plane of the tube at speeds in excess of 10 km/s for centimeters or more. The reduced electric field strength, $E/N$, the ratio of the electric field strength to the neutral density is highest at the edges of the plasma column (i.e., at the interfaces between the conductive plasma and the nonconducting air) and is sufficient to maintain the gas phase ionization required for propagation in helium. $E/N$ is also high at the radial boundaries of the plasma and sufficient to create reactive species but not high enough to cause ionization of the surrounding air. Thus the plasma is confined to the volume of the helium jet and continues to propagate as long as $E/N$ (or the applied voltage) is sufficient [1]. The possibility of generating reactive species at atmospheric pressure and at positions far removed from the plasma source is of interest in many technical areas and for biomedical applications in particular [2]. In this communication, we will present Schlieren images showing the influence of the generation of a plasma on the helium jet. For reasons not yet clear, the laminar to turbulent transition point appears closer to the exit plane of the tube when the plasma is initiated. The details depend on the Reynolds number and the applied voltage amplitude and frequency [3].

Proposed mechanisms for this influence include an increase in the gas temperature or momentum transfer from the ions to the neutrals, analogous to the "ion wind" phenomenon studied for application in plasma actuators, but neither proposition can yet account for the observations.

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## Session 18: Gas Surface Interactions II

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Measurement of Energy Accommodation Coefficient for Binary Gas Mixtures of Noble Gases

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The gas-surface interaction plays an important role in the heat transfer in the high Knudsen number flow. To describe the gas-surface interaction by a single parameter, the energy accommodation coefficient has been used [1, 2], which is also called the thermal accommodation coefficient. This accommodation coefficient represents the mean efficiency or probability of energy transfer between gas molecules and a solid surface. It has been studied for long time experimentally, theoretically and numerically [1, 2]. Since the accommodation coefficient varies with the gas species and the surface conditions (material, structure, cleanliness, etc.), many gas-surface pairs have been studied; however, reports on a measurement of the energy accommodation coefficient for a gas mixture are still limited.

In this study, we investigated the effect of the mole fraction of gas mixtures on the energy accommodation coefficient. The measurement system is explained elsewhere [3]. The heat flux from heated sample surfaces was measured in a vacuum environment. In a very low pressure condition like the free-molecular flow regime, the heat flux is proportional to the pressure and energy accommodation coefficient; therefore, the accommodation coefficient can be obtained by measuring the heat flux as a function of pressure, which is called the low-pressure method [2]. In our system, we employed an empirical relation [4] to represent the heat flux in the transitional flow regime to increase measurement points. A glass surface was employed as a surface sample. As test gases, binary mixtures of helium and argon with molar ratios of 0:100, 25:75 50:50, 75:25 and 100:0 were employed. We can conclude that the measured accommodation coefficients are well reproduced by a linear function of the molar ratio.

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REFERENCES
Material Exposure Effects in a Simulated Low-Earth Orbit Environment

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Spacecraft operating in low-Earth orbit (LEO) are subjected to a number of hazardous environmental constituents that can lead to decreased system performance and reduced operational lifetimes. Due to their thermal, optical, and mechanical properties, polymers are used extensively in space systems; however they are particularly susceptible to material erosion and degradation as a result of exposure to the LEO environment [1, 2]. The focus of this research is to examine the material erosion and mass loss experienced by Kapton and similar polymers due to exposure in a simulated LEO environment. In addition to the polymer samples, silver and gold specimens will be examined to measure the rate of oxidation and as a control specimen, respectively. A magnetically filtered oxygen plasma source has been developed and characterized for the purpose of simulating the low Earth orbit environment [3]. The plasma source can be operated at a variety of discharge currents and gas flow rates, of which the plasma parameters downstream of the source are dependent. The characteristics of the generated plasma were examined as a function of these operating parameters to optimize the production of O⁺ ions with energy relevant to LEO applications, where the ram energy of the ions due to the motion of the satellite relative to the LEO plasma is high (e.g. 7800 m/s, which corresponds to approximately 5 eV of kinetic energy for O⁺ ions). The plasma downstream of the source consists of streaming ions with energy of approximately 5 eV and an ion species fraction that is approximately 90% O⁺.

REFERENCES

Analytic Model of the Effect of Poly-Gaussian Roughness on Rarefied Gas Flow near the Surface

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Applying different models of surface roughness in statistical simulation of rarefied gas molecular flow at high Knudsen numbers we investigate asymptotically and numerically the dependence of the macro-parameters of the flow on surface roughness of the walls and on geometrical shape of the surface. Our approach is based on simulating surface roughness on micro-level by a wide class of poly-Gaussian (with probability density as the mixture of Gaussian densities [1]) or Gaussian random processes [2]. The results of rarefied gas flow Monte-Carlo simulation for both models of roughness are compared. Substantial difference is detected, as well in asymptotical expressions [3], as in numerical results. At the same time the results are substantially different from the calculations using more simple models applied by other researchers [4]. The properties of poly-Gaussian model are studied allowing a better coincidence of its statistical parameters with the parameters of real polished surfaces, or rough surfaces processed by extrusion, pressing and other technologies. Analytic expansion of the roughness operator $\hat{S}$, being fully determined by geometrical shape of roughness and by the trajectory of reflected gas atom (see [5]), is obtained from the representation of scattering function $V$ on rough surface in the form $V = \hat{S} V_0$. Physical and chemical parameters of the gas and of the surface are accounted by the local scattering function $V_0$. Main advantage of the model is based on relative simple relations between the parameters of the model and the basic statistical characteristics of random field. Considered statistical approach permits to apply not only diffuse-specular model of the local scattering function $V_0$ of reflected gas atoms, but also Cercignani-Lampis scattering kernel or phenomenological models of scattering function.

Obtained results allow us to make following conclusion. The comparison between poly-Gaussian and Gaussian models shows more significant effect of roughness in aerodynamic values for poly-Gaussian model as well in asymptotic as in numerical calculations. The restrictions on correlation and weighted functions (being the main parameters of the poly-Gaussian process) must be taken into account by simulating real rough surface to ensure that the model satisfies the basic necessary properties. The main properties of poly-Gaussian random processes and fields are similar to corresponding properties of Gaussian processes and fields. However the asymptotic of the number of level-crossings (if Gaussian component in the spectrum is absent) is substantially different; therefore the influence of surface roughness on momentum and energy exchange coefficients increases noticeably for poly-Gaussian model compared to Gaussian one.

REFERENCES

Molecular Simulation of Evaporation Mass Flux during Net Evaporation/condensation

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Heat and mass transfer caused by nonequilibrium phase change (net evaporation or condensation) plays an important role in the vapor-liquid two-phase flows. The vapor-liquid two-phase flow during net evaporation or condensation is essentially nonequilibrium because these mass fluxes originate from molecular motions, e.g., evaporation, reflection, and condensation of molecules, in the vicinity of the interface. Hence, a conventional continuum description such as the fluid-dynamics-based approach is inappropriate, and a molecular-gas-dynamics-based description is required.

The Boltzmann equation that is a governing equation of molecular gas dynamics describes the spatio-temporal development of a molecular velocity distribution function in whole vapor phase. Once the velocity distribution function is obtained as the solution of the Boltzmann equation, macroscopic variables in vapor and fluxes through the interface are obtained as its moments [1]. In the analysis of the Boltzmann equation, we have to impose the appropriate velocity distribution function leaving from the interface as the kinetic boundary condition (KBC).

The proper specification of the KBC is most important issue to analysis the vapor-liquid two-phase flows based on the Boltzmann equation. Some models have been proposed for the KBC [2]-[4]. We follow a widely-used model as the KBC including evaporation and condensation coefficient [4]. According to this KBC, the evaporation and condensation coefficients are defined by the molecular mass flux at the vapor-liquid interface.

In our recent study [5][6], we proposed a determination method of the evaporation and condensation coefficients during net evaporation or condensation, and determine these coefficients over a wide range of degree of nonequilibrium and liquid temperature. However, in this method, we assumed a concept of spontaneous evaporation [4] in order to determine the evaporation coefficient. In addition, some other studies [4][7] have adopted this concept. According to this concept, the evaporation coefficient depends only on liquid temperature and is independent of the degree of nonequilibrium.

The aim of this study is to verify the concept of spontaneous evaporation during net evaporation or condensation in consideration of the dependence of liquid temperature. In this study, we estimate the evaporation coefficient using interphase boundary [8][9] by a molecular simulation based on mean-field kinetic theory [10]; we set two boundaries (vapor boundary and liquid boundary), and then we estimate each molecular mass flux by counting the number of evaporation, reflection, and condensation molecules through these boundaries. Note that the evaporation coefficient is related to the evaporation mass flux [4]. Thus, we can examine a relation between the evaporation coefficient and the degree of nonequilibrium by estimating the evaporation mass flux during net evaporation or condensation.

The result of this study showed that the evaporation mass flux is independent of the degree of nonequilibrium, indicating that the evaporation coefficient during net evaporation or condensation can be assumed as the function of liquid temperature. Furthermore, the estimated evaporation coefficient is almost equal to that estimated by assuming the concept of spontaneous evaporation. We conclude that the concept of spontaneous evaporation can be adopted the vapor-liquid two-phase flow during net evaporation and condensation.

REFERENCES

POISEUILLE CHANNEL FLOW BY DOUBLING

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The flow of a rarefied gas between two plates, commonly called Poiseuille flow, has been studied extensively in the BGK approximation [1-6]. In particular, in Ref. 6, the Analytical Discrete Ordinates (ADO) method was developed to determine the velocity profile and flow rate “very efficiently” as well as accurate [6]. Here, we provide an equally efficient and accurate solution using the methods of doubling, which however is arguably a simpler and a more straightforward approach. Specifically, we consider the following reduced BGK model of Poiseuille flow [6]

\[
\left( \mu \frac{\partial}{\partial \tau} + 1 \right) Y(\tau, \mu) = \int_{-\infty}^{\infty} du \frac{e^{-u^2}}{\sqrt{\pi}} Y(\tau, u); \quad \mu \in (-\infty, \infty), \quad \tau \in (0, a) \tag{1a,b,c}
\]

where symmetry about the flow centerline has been assumed. \(\alpha\) is the accommodation coefficient for a channel of full width 2a. The approach is first to map the \(\mu\)-variable into \([-1,1]\) with a convenient continuous function and subsequently discretize the mapped “directions” \([-1,0]\) and \([0,1]\) with zeros of half-range Legendre polynomials of degree \(N\). The resulting equations are a coupled set of first order ODEs in \(\tau\) to be resolved over a representative spatial interval \(h\) of uniform material properties. After approximating the matrix exponential of the solution as a Padé approximant, one recasts the result in the form of a response matrix giving the distribution exiting the interval in terms of that entering. We find the response over the channel from centerline to wall by continuously doubling the single interval response over the channel half width. Thus, from the incoming boundary conditions of Eqs(1b,c) and the channel response, the distribution at the channel wall (and centerline) is most conveniently solved for. At this point, we have the desired solution at the wall for a single discretization \(N\). To achieve high precision efficiently, the entire numerical procedure is wrapped in several Wynn-epsilon convergence accelerations [7] in \(h\) and \(N\), where a sequence of solutions is converged to approximate its limit. The accompanying table for the velocity at the wall of a channel of width 1 is included as an initial verification of the doubling method. All values, with two additional digits of precision, on rounding agree with those of Ref. 6. It is emphasized that the doubling approach is an entirely discretized solution in space and “direction” and is decidedly less mathematically involved than the ADO method since no eigenvalues and ad-hoc adjustments are necessary. In addition, we find all responses independently from the surface sources. Finally, doubling is applied to a fixed uniform interval to give the necessary responses to obtain interior quantities at desired edits. In this way, one can routinely achieve 9-place

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**Session 19: DSMC Applications II**

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<td>&quot;Investigation of Velocity-Space Coupling Approach in DSMC for Tail-Driven Processes&quot;</td>
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<td>&quot;Modeling of Near-Continuum Laminar Boundary Layer Shocks Using DSMC&quot;</td>
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DSMC simulation of Rayleigh-Brillouin scattering in binary mixtures

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Rayleigh-Brillouin scattering in gases is of interest for the interpretation of light scattering experiments aimed at remote sensing of the atmosphere [1,2]. These experiments probe the kinetic regime where solutions of the linearized Boltzmann equation must be sought to obtain the fluid fluctuations spectra. Owing to the well known mathematical difficulties connected with the Boltzmann equation, most of the theoretical analysis of experimental spectra has been based on kinetic model equations [3,4,5,6]. However, the accuracy and, to some extent, the availability of kinetic models becomes increasingly problematic when considering complex gases like mixtures of polyatomic species. Since, however, DSMC provides a solution of the full Boltzmann equation with no additional assumptions beyond the adopted molecular collision model, it is interesting to investigate whether it can provide an interpretation of light scattering experiments based on first principles molecular properties only. The method has been recently applied to the simulation of RBS spectra in molecular Oxygen demonstrating excellent agreement with experiments [7]. In this work, we use DSMC to simulate RBS experiments in mixtures of noble gases and compare the results to the experimentally measured spectra [6]. Comparisons are also made with the results of the kinetic model proposed in [5] and used in Ref. [6] to study RBS experiments with mixtures of noble gases. Different models for the description of the interactions among the mixture species are tested and recommendations on the application of the method to mixtures of molecular gases, of interest for the applications, are drawn.

REFERENCES

State-specific catalytic recombination boundary condition for DSMC methods in aerospace applications

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Accurate characterization of the hypersonic flow around a vehicle during its atmospheric entry is important for a precise quantification of heat flux margins, which need to be considered at the moment of designing the craft's thermal protection system (TPS). Coupled physical phenomena occurring in the gas, e.g., strong departure from thermal and chemical equilibrium, radiative heating and complex gas-surface interactions, make the prediction of these flows a challenging task. A related application, where the heat loads due to aerodynamic heating are a major concern, is the development of prediction tools for space debris demise and risk assessment. Debris from launcher stages and satellites at end-of-life is increasingly becoming a threat to satellites and other space systems while still in orbit, but may also be a direct threat for humans when remains, that have not fully disintegrated during descent, impact Earth's surface. While a conservative approach can be applied in the first case by overestimating the heat flux during the heat shield design, the minimum heat flux must be carefully estimated in the second case to predict destruction (or not) of the material.

In both cases, exothermic reactions promoted by the catalytic properties of the surface material, may be a major contributor to the overall heat flux. Therefore, it is important for numerical flow solvers, to take these phenomena into account. At high altitudes the continuum description based on the Navier-Stokes equations fails. For these conditions a kinetic description based on the Boltzmann equation is required and an appropriate numerical method, such as the Direct Simulation Monte Carlo [1] (DSMC) method, must be used.

This work describes the development and implementation of a wall boundary condition for catalytic recombination of atomic into molecular nitrogen within the framework of a DSMC code developed at the von Karman Institute [2]. In this code, gas-phase internal energy exchange and dissociation are treated using state-specific reaction cross sections derived from the detailed quantum-chemical database for the $N_2 (\nu, J) + N$ system generated at NASA Ames Research Center [3]. A coarse-grain model [4] is used to reduce the number of internal states and state-specific reactions to a manageable level.

The catalytic boundary condition is based on an approach inspired by [5]. However, in the present case the state-specific surface recombination probabilities can be imposed by the user. This represents an important aspect in modeling catalysis, since experiments and molecular dynamics highlight that only part of the chemical energy is absorbed by the wall, with the formed molecules leaving the surface in an excited state. The implementation is verified in a simplified geometrical configuration by comparing the numerical results with an analytical solution, developed for a 1D-diffusion problem in a binary mixture. In the following step, the effect of catalysis in a hypersonic flow around a blunt body (2D infinite cylinder in cross-flow) is studied. Preliminary results show that, although high temperatures are reached in the bow shock region in front of the body, very little dissociation occurs at the chosen Knudsen numbers ($Kn = 0.2$). For this reason, the influence of exothermic recombination on wall heat flux appears to be very low in the rarefied regime.

REFERENCES

Investigation of Velocity-Space Coupling Approach in DSMC for Tail-Driven Processes

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Direct simulation Monte Carlo (DSMC) method has been widely used on solving non-equilibrium problems because of its efficiency and simplicity compared with direct numerical solutions of the Boltzmann equation. However, a significant challenge is posed in DSMC for modeling a process which is dominated by the collisions of high-energy particles in the distribution tail, as shown in Figure 1. The tail region is represented by a small number of particles and collision events are rare, which leads to poor statistics and poor resolution of tail-driven processes. Therefore, an improvement for DSMC is required to correctly model the tail-driven processes, such as thermo-chemical reaction processes.

In this study, a velocity-space coupling approach is investigated to improve the resolution and poor statistics of tail distributions in DSMC. The velocity space is regarded as bulk and tail regions according to the location of a velocity space interface, $E_b$. The bulk distribution, $f_{DSMC}$, is evolved in DSMC where there are sufficient particles and low stochastic noise. The distribution tail, $f_{BE}$, is computed through the solution of the Boltzmann equation (BE) solver in a reduced region of velocity space, which is regarded as kinetic correction of tail for DSMC. Figure 2 shows the velocity distribution function of the equilibrium state of a bimodal-relaxation example problem using the coupled DSMC/BE approach. Based on the same number of particles used in the simulations, this velocity-space coupling approach provides an improved solution in the distribution tail, and enables selective particle weighting in velocity space. The quantitative arguments will be provided to determine the location of interface of two approaches in velocity space. An appropriate criterion for combining two distributions will also be discussed. This coupling approach offers the significant improvement to reduce the statistical noise in the tail-driven processes and also provides higher resolution for velocity distribution function in DSMC.

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REFERENCES

Computational Investigation of Free-Molecular Gas Flows Using DSMC and CFD

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The high transitional and free-molecular regimes in which the mean free path is much larger than the characteristic length of the body immersed in gas flows can be described by the direct Simulation Monte Carlo method [1] or through the use of an appropriate collisionless Boltzmann equation [2]. Application of these methods for studying free-molecular gas flows requires knowledge of the details of the molecular interaction with the body surface and the range of applicability of the collisionless approximation [3]. While intermolecular collisions can be ignored in convex geometry, gas particle-surface interaction remains important in describing the essential flow behavior. However, in complex geometries with concave section in which several gas molecules may be found simultaneously, intermolecular collision may not be ignored [2], casting serious doubt on the use of the collisionless Boltzmann equation.

In this study, the flow behavior and molecular distribution function of the gas flows near free-molecular limit are investigated for several complex geometries. In addition, the accuracy of the collisionless Boltzmann equation is examined by comparing important flow properties with DSMC. Further, together with results of the pressure and viscous stresses on the surface, effects of gas-surface interaction models on the accuracy of the DSMC and collisionless model in free-molecular regime are analyzed for various complex geometries.

Lastly, we will report the validity range of the conventional Navier-Stokes-Fourier models, which are based on the physical conservation laws of mass, momentum, and energy in conjunction with the first-order linear constitutive relations, in high transitional and free-molecular regimes. We also hope to report the first results of the second-order mesoscale theory derived exactly from the kinetic Boltzmann equation through the method of moments and the balanced closure [4], which was found to guarantee the correct asymptotic free-molecular limit.

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REFERENCES

Modeling of near-continuum laminar boundary layer shocks using DSMC

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The Direct Simulation Monte Carlo [1] method has been used to model laminar shock wave boundary interactions of hypersonic flow over a 30/55-deg double-wedge configuration studied in the Hypervelocity Expansion Tube facility [2]. The impact of thermochemical effects on these interactions by changing the chemical composition from nitrogen to air for a stagnation enthalpy of 8.0 MJ/kg flow are investigated using the 2-D wedge model. As shown in Fig.1, the simulations are found to reproduce many of the classic features related to Edney Type V strong shock interactions that include the attached, oblique shock formed over the first wedge, the detached bow shock from the second wedge, the separation zone, and the separation and reattachment shocks that cause complex features such as the triple point for both cases. However, results of a reacting air flow case indicate that the size of the separation length, the time required to reach steady state, and the movement of the triple point toward the leading edge is much less than the nitrogen case. In contrast to 2-D nitrogen case, the measured and computed heat flux values were found to be in good agreement at both the aft and front part of the wedge. Chemical reactions were found to increase the peak heat transfer rate which is consistent with calculations performed by Ballaro et al [3]. Additionally, the derived NO vibrational temperature based on the measured post-shock emission spectroscopy was compared with the simulation.

ACKNOWLEDGEMENTS

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Fig.1: Shock structure and Mach numbers in the shock interaction region at 100µs using the 2-D wedge geometry.
### Session 20: Numerical Methods in Plasmas

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Symmetric Pseudo-Spectral Velocity Discretization Schemes for Kinetic Equations with Energy Diffusion in Plasma Physics

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A promising idea for reducing the cost of continuum kinetic calculations modeling Fokker-Planck collisions in plasma physics is to represent the radial velocity using non-standard orthogonal polynomials [1]. However, direct pseudo-spectral discretizations in this basis lead to nonsymmetric operators and, often, unstable time-stepping schemes. We find that these difficulties disappear when the pseudo-spectral scheme is derived from a proper Galerkin framework. This leads to dramatic improvements in efficiency and accuracy over finite differences.

To quantify the correctness of the projected dynamics in finite dimensional spaces of orthogonal polynomials, we have developed a new algorithm for computing the spectral density function of singular Sturm-Liouville boundary value problems with a continuous spectrum [2]. This leads to a generalized Fourier transform in which the solution of the PDE is represented at each time as a continuous superposition of (non-normalizable) eigenfunctions. We compute the eigenfunctions using an arbitrary order collocation-based implicit Runge-Kutta method in double or quadruple precision arithmetic. The spectral density function is computed by complexifying the spectral parameter $\lambda$ and taking the limit of the Titchmarsh-Weyl $m$-function as the imaginary part of $\lambda$ goes to zero. In this way, even for singular initial conditions, we are able to compute exact solutions (to 30 digits) of a model PDE that retains the highest order terms in the radial velocity variable. This serves as an excellent independent test of the accuracy of the Galerkin approach, which is carried out in detail in [3].

The goal of the present work is to develop faster pseudo-spectral discretizations derived from the Galerkin framework of [3] to preserve the self-adjoint structure of the discretized singular Sturm-Liouville operator, and to develop hybrid hp-discretizations that combine the high order accuracy of the orthogonal polynomial approach with the banded structure of finite-difference methods. We also explore the connection between the eigenfunctions of the discrete operator and the non-normalizable eigenfunctions of the continuous operator, as well as the effects of domain truncation, which also causes the continuous spectrum to become discrete.

REFERENCES
Effect of Electronic Excitation on High-Temperature Flows of Ionized Nitrogen and Oxygen Mixtures behind Strong Shock Waves

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In the present study strongly non-equilibrium one-dimensional steady-state flow behind the plane shock wave is studied taking into account electronic degrees of freedom of both neutral and ionized species. High-temperature chemically reacting five-component ionized mixtures of nitrogen (N/\textsubscript{2}/N/\textsuperscript{2}/N/N/\textsuperscript{+}/e) and oxygen (O/\textsubscript{2}/O/\textsuperscript{2}/O/O/\textsuperscript{+}/e) are considered. The quantity of electronic energy levels which is taken into account for nitrogen mixture are 170 and 625 electronic energy levels for N and N\textsuperscript{+}, and 5 and 7 electronic terms for N\textsubscript{2} and N\textsuperscript{2+} respectively (rotational-vibrational modes are also included into consideration). For ionized oxygen mixture 204 and 625 electronic energy levels for O and O\textsuperscript{+}, and 7 electronic terms for both O\textsubscript{2} and O\textsubscript{2+} are accounted, improving the model developed in [1-3]. Kinetic scheme includes non-equilibrium reactions of ionization, dissociation, recombination and charge-transfer. The system of governing equations is based on the assumption that translation and internal energy relaxation is fast whereas chemical reactions and ionization proceed on the macroscopic gas-dynamics time-scale.

The developed model is applied to simulate the flow behind a plane shock wave under initial conditions characteristic for the spacecraft re-entry from an interplanetary flight (Hermes and Fire II experiments [4]). Fluid-dynamic parameters behind the shock wave as well as transport coefficients and the heat flux are calculated. The effect of electronic excitation on kinetics, dynamics and heat transfer is analyzed for both nitrogen and oxygen mixtures. The results for two mixtures are compared between each other, and the differences are shown.

ACKNOWLEDGEMENTS

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REFFERENCES

The kinetic foundations of non-dissipative transport theory of single component charged gases, in the presence of an electromagnetic field, are presented within the five dimensional formalism first proposed by Kaluza back in 1919 [1]. This formalism includes the electric charge-mass ratio as the fifth component of the particle velocity, and makes use of the so-called cylindrical condition, in which all the partial derivatives with respect to the fifth coordinate are made equal to zero. It is well-known that the Lorentz force and the Maxwell equations are obtained from this approach using the mathematical framework of general relativity. Since the effect of the fields is viewed as a consequence of the space-time curvature inherent to the extra dimension, several transport effects can be predicted using basic techniques already applied successfully in the treatment of the 4D relativistic Boltzmann equation [2].

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Statistical foundations of Kaluza’s magnetohydrodynamics II: Navier-Stokes regime.

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The first order in the gradients Chapman-Enskog solution method for the Boltzmann Equation (BE) is applied to the analysis of the transport properties of a dilute charged single component gas in the presence of an external electromagnetic field. The BGK model for the collision kernel is used to show that, in the non-relativistic treatment, the contribution of the field to the first order in the gradients correction to the distribution function vanishes unless a steady state approximation of the BE is assumed. In order to surpass this drawback two relativistic alternatives are applied to the analysis of the problem. Firstly, special relativistic kinetic theory using the Lorentz force is applied [1]; secondly a general relativistic-type approach introducing a fifth spatial dimension is considered in the treatment of the BE [2]. It is shown that in the latter treatment the effect of the fields is preserved even in the low temperature, non-relativistic regime. It is concluded that the 5D approach can consistently describe most of the known transport processes present in simple charged dilute gases.

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**REFERENCES**

Relativistic transport coefficients for a single component charged gas in the presence of an electromagnetic field: kinetic theory approach within a BGK-type model.

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It is well known that the transport properties of dilute gases are significantly modified as their temperature increases. Moreover, purely relativistic effects have been predicted in such systems by taking into account the relativistic nature of individual particle's dynamics in Boltzmann's equation. In particular, relativistic kinetic theory yields a heat flux which can be driven by fields other than the temperature gradient even for single component fluids [1-3]. These purely relativistic effects have no non-relativistic counterparts and even though their structure resembles the cross-effects, the latter are only present for mixtures. These relativistic couplings are additional to the cross-effects when a multiple component system is considered.

In the present work the relativistic Boltzmann equation is solved for a single species charged fluid in the presence of an electromagnetic field as a generalization of the electrostatic case presented in Ref. [3]. The relaxation time approximation within Marle's model is used to address both the weak and strong magnetic field cases. Euler's equations in an arbitrary laboratory frame are introduced within the Chapman-Enskog solution in order to assure its existence. The distribution function obtained within such formalism in the Navier-Stokes regime is shown to depend on the electromagnetic field. This coupling leads to a non-vanishing thermoelectromagnetic effect in the weak field limit for a single component fluid. This contribution to dissipation is strictly relativistic and vanishes in the non-relativistic limit, in which cross-effects are only present for mixtures, as pointed out above.

The calculation is carried out in an arbitrary inertial reference frame and the co-moving frame is considered to be the one moving with the fluid's hydrodynamic velocity. This representation corresponds to the so-called Eckart's frame and is here compared to previous works where other representations have been considered. The implications of these results in the mathematical structure of the entropy production of the system will also be discussed [4].

ACKNOWLEDGEMENTS

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### Session 21: RGD in Planetary Science

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DSMC Simulation of Io’s Unsteady Tvashtar Plume


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Jupiter’s moon Io supports its rarefied atmosphere with tidally-driven episodic volcanism: its many plumes emit volatile gases that contribute directly to the local atmospheric column, and that condense to the surface in frost deposits to be sublimated under diurnal insolation or sputtered by incident plasma. The largest volcanic plumes exhibit violent and intricate structure, with canopies rising to hundreds of km above the Ionian surface. In early 2007, the NASA New Horizons (NH) spacecraft captured the active Tvashtar plume in a time sequence of panchromatic images at high spatial resolution and observed both discrete “filamentary” patterns in descending particulate structure, and a massive traveling canopy wave. These are transient and asymmetric features, indicative of Tvashtar’s unresolved and complex vent processes. In this work, we introduce a methodology for identifying vent spatial and temporal scales in this rarefied plume with a ballistic model and algorithmic processing of NH imagery. These parameters are then applied in three-dimensional and unsteady DSMC simulations of Tvashtar’s plume with comprehensive physical modeling that aim to reproduce the observed canopy structures, providing insight into the dynamics of transient extra-terrestrial volcanic plumes.

Constraints on the length and frequency scales of the eruption process at the vent can be deduced by analyzing the evolution of the plume in the time-sequenced Tvashtar images. Estimates of eddy size and structure from NH observation are coupled with steady DSMC simulation of plume streamlines. Applying Taylor’s hypothesis that such eddies are perturbations traveling with mean flow enables the tracing of eddies back to their origin at the vent, yielding length scales that constrain vent size and morphology. A simple ballistic model for the system is demonstrated that exhibits similar dynamic phenomena to those noted in the Tvashtar plume, and an image processing algorithm is developed to connect scale observations to conditions at the vent. After this technique is tested and refined on the ballistic model, it is applied to New Horizons imagery, further informing parameter selection in the DSMC. DSMC simulation of the Tvashtar plume begins with axisymmetric plumes (Fig.1). Unsteadiness at the unresolved vent is simulated as on/off pulses with two periods, exciting whole-plume dynamics like the traveling wave and localized particulate structure. Vent parameters are varied between a generic fire fountain and lava lake, with length scales constrained by the ballistic model, as parameter space is explored in pursuit of the critical spatial and temporal frequencies that qualitatively reproduce the dynamical phenomena of Tvashtar's plume. Vent asymmetry may be introduced as sloshing magma waves in an elongated vent, or a varied particulate density around the vent perimeter. The Tvashtar model is an outgrowth of our established planetary atmospheric and plume-dynamic DSMC code, modified to address the transient-vent application. Updates add capability, e.g. physical processes like plume-plasma interaction and Coriolis forcing (significant at Tvashtar’s high latitude), and improve computational efficiency. Dynamic load balancing schemes in latitude and longitude, and an adaptive cell distribution scheme in altitude, allow regions of interest within the canopy structure to be resolved more finely than bulk atmospheric flow, enabling the evolution of traveling waves and periodic filament structure.

ACKNOWLEDGEMENTS

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HCN Production from Impact Ejecta on the Early Earth

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Major impact events have drastically altered the evolution of life on Earth\textsuperscript{1}. They are responsible for several mass-extinctions, including the Chicxulub event that ended the dinosaur era\textsuperscript{2}, and are proposed as a mechanism for HCN production during the Late Heavy Bombardment (LHB). These large impacts vaporize a large volume of silica, which nucleates into milli-scale spherules that re-entry globally. These spherules compress and heat the upper atmosphere, producing high speed winds and a thermal radiation pulse that reaches Earth’s surface. The reactions initiated by the re-entry of these spherules produce chemical species that diffuse to the Earth’s surface, altering the environment on a global scale. In the case of the Chicxulub impact, the spherules produced \(1.5 \times 10^{14}\) moles of NO\textsuperscript{3}, which is sufficient to trigger global algal blooms in the upper ocean\textsuperscript{4}. A similar mechanism may produce HCN in a primordial Earth atmosphere\textsuperscript{5}, and could play a role in the origin of life. Therefore, it is of great interest to the scientific community to precisely determine the net production of these synthesized chemical species.

With typical diameters on the order of 1 mm\textsuperscript{6}, the spherules deposit most of their energy around 100 km in altitude\textsuperscript{3}. Due to the atmospheric compression, this falls within the regime of thermochemical nonequilibrium. Consequently, most existing scientific estimates incorrectly predict dissociation and recombination rates\textsuperscript{7} for key reaction pathways involved in these ejecta calculations. Our approach employs the direct simulation Monte Carlo (DSMC) method to more accurately determine the initial production rate of HCN precursors in the flow around re-entering spherules. We use the Statistical Modeling in Low-Density Environment (SMILE) code, which utilizes the Total Collisional Energy (TCE) model for reactions. The collisions are described by the Variable Soft Sphere (VSS) and Larsen-Borgnakke (LB) models. Using the aforementioned production rates, we form a response surface and propagate spherule trajectories to obtain the net HCN production. We follow this with a turbulent diffusion transport model developed for trace species. This provides improved, time-accurate predictions of HCN surface column density.

ACKNOWLEDGEMENTS

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Development of a melting model for meteors

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During the atmospheric entry of meteoroids, evaporation and melting take place triggering the phenomenon known as meteor. Ablation products interact with the ionized gas of the shock layer and are driven to the wake, inducing a signature that can be detected by radars. Recent efforts have been made by the Belgian Institute for Space Aeronomy to estimate the velocity and trajectory of meteors, by means of an innovative technique based on radio waves. The Belgian Radio Meteor Stations (BRAMS) [1] experiment consists of a series of receivers spread all over Belgium to study the meteor atmospheric entry, collect, and standardize meteor observation data. The estimation of meteoroid mass flux is particularly difficult to quantify from radar observations alone, and it is necessary to augment observation data with numerical modeling to have a reasonable estimate of the meteoroid material deposition in the atmosphere. In this work, we propose to study the meteor ablation with a numerical approach similar to those used in the aerospace community to model the gas-surface interaction over thermal protection system materials [2].

We apply a strategy based on an aerospace-engineering-derived approach (i.e., steady-state CFD with surface ablation model). The flow governing equations are solved through a 1D Stagnation-line CFD solver coupled with the Mutation++ [3] library where state-of-the-art thermodynamic and transport properties of the flow field are included. A boundary condition, based on an open-system multi-phase chemical equilibrium problem (i.e., gas-solid), is developed to describe the interaction between the atmosphere and objects with a complex elemental composition. The boundary procedure consists in solving a surface mass balance and a surface energy balance to retrieve the surface temperature and the mass loss flux. The melting of the material is modeled by solving a Stefan problem through an implicit coupling of a 1D unsteady material code with the flow solver. By this means it is possible to track the fusion front and to estimate the amount of mass that is removed by mechanical erosion.

We will analyze the ablation of meteors at altitudes at lower than 70 km with low entry velocities in the continuum regime. Stagnation-line simulations for meteors of different sizes will be performed accounting for the physical phenomena described above. The solution of the material solver will be compared with the steady-state governing equations for liquid layers shown by [4].

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REFERENCES

The RZC model for prediction of the gas environment of the PHILAE probe during its 2014 descent to the nucleus of the comet 67P

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One of the objectives of the ESA “ROSETTA” mission to the comet 67P was to insert, in August 2014, an orbiter probe around the nucleus of the comet, and to deposit the “PHILAE” lander at the surface of the nucleus in November 2014. The selection of the landing site and the definition of the release point and initial descent velocity vector were made in the period August – November 2014 on the basis of physical simulations of the descent trajectory. This requested an assessment of the gravitational and aerodynamic forces on PHILAE. We here describe the so-called RZC model developed to predict the gas environment of 67P in November 2014 and compute the aerodynamic force. We first outline the unusual difficulties resulting from (1) the extreme complexity of the nucleus surface on all scales, (2) the absence of direct measurements of the gas flux at the surface itself, (3) the time-dependence of the gas production induced by the fast nucleus rotation, (4) the need to perform the whole program within three months. Then we outline the physical approach adopted to overcome these difficulties, and describe the RZC model which included two differing tools: (1) a set of gasdynamic/gaskinetic codes to compute the vacuum outflow of a rarefied gas mixture from a central, highly anisotropic and rotating source; (2) a specially developed code to derive the central source parameters from data on the nucleus provided by the first observations from the orbiter probe. The satisfactory operation of the RZC code in the weeks preceding the November 2014 PHILAE descent is shown, and the forecasted aerodynamic force during the PHILAE descent is compared to the gravitational force.
Comparison of hydrodynamic and kinetic models of thermal escape from planetary atmospheres

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Thermal escape is the process of mass loss of a planetary atmosphere by gas molecules who leave the atmosphere with translational energies exceeding the gravitational binding energy. To date, the majority of theoretical studies of thermal escape employ hydrodynamic models of gas flows, which have their roots in the Navier-Stokes equations. The nature of the thermal escape problem, however, hampers the straightforward application of the full Navier-Stokes equations, because they require to some extent artificial boundary conditions that should be posed in the exosphere, where flow is highly rarefied and strongly non-equilibrium, and the continuum equations, which are derived from the Boltzmann equation assuming small deviations from local equilibrium, are invalid. The kinetic models based on the Boltzmann equation, on the contrary, naturally account for non-equilibrium of gas flow in the exosphere and, thus, can be used to predict the transition of the atmospheric flow from continuum flow below the exobase to nearly free molecular flow in the exosphere. The goal of the present paper is to perform comprehensive theoretical and numerical study of properties of the hydrodynamic model of atmospheric escape and to establish the domain of its validity by means of systematic comparison of results of hydrodynamic and kinetic simulations performed under identical conditions. The consideration is limited by the so-called Parker’s model of thermal escape, which was first developed for stellar winds [1] and implies the search of solutions of one-dimensional hydrodynamic equations for an inviscid but thermally conducting gas with a critical point and vanishing temperature far from the source. The properties of solutions of Parker’s model are studied for neutral mon- and diatomic gases with the viscosity index varying from 1/2 to 1. The domains of existence and uniqueness of solutions in terms of the source Jeans escape parameter and Knudsen number are established. The solutions are found to exist only in a narrow range of the critical point Jeans parameter. The lower and upper limits of this range correspond to solutions that are dominated by either heat conduction or adiabatic expansion. Thermal escape described by Parker’s model is found occurs in two asymptotic regimes: the low-density (LD) regime, when escape is dominated by heat conduction, and the high-density (HD) regime, when escape is dominated by adiabatic expansion. Expressions for the mass and energy escape rates in these regimes are found theoretically. The kinetic simulation are performed with the Direct Simulation Monte Carlo method for mon- and diatomic gases based on the Variable Hard Sphere molecular model, where the energy exchange between translational and rotational degrees of freedom of gas molecules is accounted for with the Larsen-Borgnakke model. The comparison of results of hydrodynamic and kinetic simulations performed in identical conditions shows that Parker’s model is capable of describing thermal escape only in the HD regime, providing decent agreement with the kinetic model in terms of the atmospheric structure below the exobase and the mass and energy escape rates [2,3]. In the LD regime, Parker’s model predicts much faster drop in atmospheric temperature and less extended atmospheres, and can both over- and underestimate the escape rates in orders of magnitude. Based on this finding, a criterion of validity of Parker’s model for atmospheric escape is developed in terms of the source Knudsen number and Jeans escape parameter.

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Due to the numerous applications of granular materials in industry as well as its relevance in nature, researchers are extensively studying the microscopic and macroscopic properties of granular materials under different physical conditions [1, 2]. A rapid granular flow resembles the classical picture of a molecular gas and therefore the fluidized state of granules is termed as granular gas [3]. The main difference between molecular and granular gases is that the dissipation of kinetic energy of granules through inelastic collisions which is characterized by the restitution coefficient $\alpha$ with $0 \leq \alpha \leq 1$. The most important feature of rapid granular flows is that they can be supersonic [4] and shock waves form even under normal conditions. A plane shock wave is generated when a supersonic gas flows into a subsonic gas; mathematically, this is nothing but a discontinuity across which the hydrodynamic fields undergo discontinuous jumps. Here we present a detailed analysis of the Riemann problem of planar shock waves for a dilute granular gas by solving Navier-Stokes-order hydrodynamic equations numerically using relaxation type numerical scheme [5, 6]. We found that the maxima of granular density and temperature occurring within the shock-layer and these profiles are found to be asymmetric [7, 8]. The granular temperature at the upstream and downstream ends of the shock decay according to Haff's law $[\theta(t) \sim t^2]$. The Haff's law seems to hold with-in the shock-layer up-to a certain time for weak shocks, but deviations occur for strong shocks. The effect of Mach number (Ma) and inelasticity ($\alpha$) on all hydrodynamic field profiles are discussed (see for example Fig. 1).

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Coarse-grained Monte Carlo simulation of excitation and ionization collisions

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Simulation of partially ionized plasmas can be very challenging due to a wide range of both elastic and inelastic collisional processes occurring at different spatial and temporal scales. In the limit of small Knudsen number, the plasma can be described by fluid-like equations, and the kinetics can be modeled by constructing a set of rate equations for the corresponding moment variables of the distribution function (density, momentum, energy). For finite Knudsen number, individual particle interactions become significant and the full distribution function needs to be resolved either by means of particle representation or a continuum fluid in phase-space.

We present a Monte Carlo (MC) collision method to model excitation and ionization collisions in a partially ionized plasma. [1] Due to the large number of the atomic states included in the simulation, the collision rates can span several orders of magnitude making the MC sampling algorithm very inefficient. In order to overcome this difficulty, we propose a complexity reduction method based on atomic level grouping. High order of accuracy of the reduction method is achieved by imposing an internal distribution within each group. [2] The stiffness induced by the collisional kinetics can be significantly relieved with minimal loss in accuracy. This is illustrated in figure 1, which shows the time evolution of the electron energy distribution function (EEDF) in a relaxation test using the proposed complexity reduction method (dashed) and comparison with the reference solution (solid).

Fig.1: Heating test with 10 atomic levels (3 discrete levels and 1 Boltzmann group): reduced (solid) vs. full (dashed). For the EEDF, 100,000 samples were used and $T_e = 4.3$ eV initially.

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REFERENCES

Improvement of simple models for state-to-state and multi-temperature reaction rate coefficients

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In theoretical modeling of highly non-equilibrium processes a variety of models and approaches are used, which differ by the level of sophistication of the described processes. Among the most common approaches we can distinguish the state-to-state and multi-temperature descriptions. The state-to-state model was originally used for simple one-dimensional and two-dimensional flows due to its computational complexity. With the development of modern computer technologies, implementation of this approach for simulations of more complex flows becomes possible. For this purpose knowledge about dissociation and exchange reaction rate coefficients for all energy states is required.

Modern methods of molecular dynamics allow obtaining very accurate data for the state-specific rate coefficients [1-3]. But this data cannot be directly used in the computational fluid dynamics (CFD) due to the lack of data for all energy states and a limited applicability range for existing data approximations. Moreover these approximations are closely associated with the used oscillator model and cannot be transferred to other models of vibrational spectrum.

On the other hand, for the description of state-to-state and multi-temperature dissociation rate coefficients there is a fairly simple semi-empirical model based on the Treanor-Marrone model [4,5]. It involves an adjustable parameter \( U \) obtained by fitting the fluid-dynamic variables to experimental data for some specific flow conditions. The disadvantage of commonly used parameter values like \( D/6k \) or \( 3T \) (\( D \) is the dissociation energy, \( k \) is the Boltzmann constant, \( T \) is the temperature) is that they cannot provide a good accuracy of rate coefficients in the whole range of temperatures and vibrational states [5,6]. The main idea of this study is to improve the simple Treanor-Marrone model defining its parameter \( U \) as a function of temperature and vibrational energy. To derive this function we compare our results with those obtained by trajectory calculations [1,2]. As a result, piecewise functions \( U(\varepsilon, T) \), depending on the temperature and the vibrational energy \( \varepsilon \) were obtained, providing a high accuracy for the dissociation rate coefficients of nitrogen and oxygen.

The proposed state-to-state model is then used to calculate two-temperature dissociation rate coefficients as functions of translational-rotational and vibrational temperatures. For this purpose, the state-specific rate coefficients are averaged with different vibrational distributions for both harmonic and anharmonic oscillators; we use Boltzmann, Treanor and Gordiets distributions in our study. The rate coefficients and non-equilibrium factors are compared to those calculated with commonly used values of the parameter \( U \), with widely known Park model [7] as well as with recent experimental data [8]. The effects of strong vibrational excitation and anharmonicity on the two-temperature dissociation rate coefficients are evaluated.

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REFERENCES

Coarse-graining of N₂-N Relaxation Collisions using 2-D bins

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A high fidelity, coarse-grained internal energy relaxation model for the N₂-N system is proposed with an emphasis on efficient implementations in the direct simulation Monte Carlo (DSMC) method. A novel two-dimensional binning approach with various bin energy resolutions in the rotational and vibrational modes is developed for treating the internal mode of N₂. Both bin-to-bin and state-specific relaxation cross sections are obtained using the Molecular Dynamics (MD/QCT) method with various Potential Energy Surfaces (PESs) as well as using the state-specific database of Jaffe [1]. Good agreement between the bin-to-bin and state-specific relaxation cross sections is achieved with the use of a 99 bin model. A Variable Soft Sphere (VSS) form of total cross sections for use in DSMC is also derived from MD/QCT which is found to better capture the forward-preferential scattering behavior in collisions at hypersonic conditions. The 99 bin model is used in homogeneous DSMC relaxation simulations which recover the state-specific master equation results of Panesi [2] when the Jaffe [1] state-specific cross sections are used. Comparing between results using the state specific cross sections based on the ReaxFF PES [3] and using the master equations, the rotational relaxation times are in general agreement while there are larger differences between the vibrational relaxation times. However, these differences become smaller as the translational temperature increases because the difference in the energy barrier between the Jaffe and ReaxFF PESs becomes less important.

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Nonequilibrium Dissociation from Ab-Initio Calculations

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A new dissociation model, suitable for use in direct simulation Monte Carlo (DSMC) and computational fluid dynamics (CFD) calculations is presented. The model accounts for coupling between internal energy and dissociation, explicitly accounting for non-Boltzmann vibrational energy ($v$) distribution functions. For shock-heated flows, the model captures over-population of high $v$-levels at early times, as well as the depletion of high $v$-levels during quasi-steady-state (QSS) dissociation, compared to Boltzmann vibrational energy distributions (times $t_1$, $t_2$, and $t_3$ in Figs. 1 and 2). These non-Boltzmann effects are then coupled to the dissociation probability (used in DSMC) or dissociation rate (used in CFD). The model is parameterized using ab-initio data, obtained using Direct Molecular Simulation (DMS) [1,2,4]. The DMS method replaces stochastic collision algorithms in DSMC with trajectory calculations performed on ab-initio potential energy surfaces (PESs) [3]. DMS calculations directly simulate rovibrational excitation and dissociation processes with no assumptions regarding internal energy distributions, or the decoupling of rotation and vibration. A number of discoveries regarding nitrogen rovibrational excitation and dissociation have been made through DMS calculations [4], and the data has been used to construct a new model, which is described in the current paper.

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Comparison Between Phenomenological and Ab-Initio Reaction and Relaxation Models in DSMC

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High-fidelity collision models are needed to describe highly nonequilibrium flows, such as shocks and hypersonic boundary layers [1]. Accurate state-to-state internal energy exchange and reaction cross-sections can be obtained from quasi-classical trajectory (QCT) calculations with ab-initio potential energy surfaces [2]. However, there are over $10^{16}$ state-to-state cross sections even for simple air species. Due to computational memory limitations, such large cross-section databases cannot be used in full flowfield solvers for each collision-pair combination. Recently, Kulakhmetov et al. [3] have proposed compact relaxation and dissociation models based on Maximum Entropy (ME) considerations that can be calibrated to ab-initio calculations with a reduced set of parameters. The ME-QCT-VT relaxation model describes the complete set of $O_2$+$O$ vibrational-translation (VT) transition cross-sections with just 11 parameters and reproduces QCT-calculated state-to-state relaxation rates in the 2,500 – 20,000 K temperature range within 30%. Likewise, the dissociation model captures state-specific and equilibrium dissociation rates in the same temperature range within 25%.

Here we implement the new models in a direct simulation Monte Carlo (DSMC) solver [4] and compare their predictions to the established Larsen-Borgnakke (LB) and total collision energy (TCE) phenomenological models. For consistency, both the LB and TCE models are calibrated to QCT-calculated $O_2$+$O$ rates [5]. The model comparison test cases include 0-D thermochemical relaxation under isothermal (constant trans-rotational temperature and variable vibrational temperature) and adiabatic conditions. The final manuscript will show that both the ME-QCT-VT and LB models can reproduce vibrational relaxation accurately but the TCE model is unable to reproduce nonequilibrium rates even when it is calibrated to accurate equilibrium rates. The new reaction model does capture QCT-calculated nonequilibrium rates. Figure 1 illustrates how the calibrated phenomenological LB-TCE and the ab-initio models predict different relaxation behavior of a vibrationally cold ($T_v < T_r = T_k$) $O_2$+$O$ reacting mixture. We explain the prediction differences based on the new model features in all studied cases.

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Calculation of State-Resolved Cross-Sections for the $\text{N}_2(X^1\Sigma_g^+) + \text{O}(3\text{P}) \rightarrow \text{N}(4\text{S}) + \text{NO}(X^2\Pi)$ Zeldovich Reaction

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Nitric oxide formed under nonequilibrium conditions through the Zeldovich reactions is important in high enthalpy air flows. NO formation affects aerothermal loads and emissions of hypersonic vehicles [1] and $\text{H}_2 + \text{O}_2$ mixture ignition in scramjets [2]. Additionally, recent calculations by Parkos et al. [3] shows that nonequilibrium effects increase amount of NO formed by the asteroid impact ejecta. For Chixculub impact increased NO influx is sufficient for causing an end-Cretaceous algal bloom, and it is now a viable marine extension mechanism. Flows with significant nonequilibrium are typically modeled in direct simulation Monte Carlo (DSMC) calculations using phenomenological models that are calibrated to equilibrium experiments. However, these models become inaccurate when they are extrapolated to highly nonequilibrium conditions. The aim of this work is to calculate state-resolved cross-sections for the $\text{N}_2(X'\Sigma) + \text{O}(3\text{P}) \rightarrow \text{N}(4\text{S}) + \text{NO}(X^2\Pi)$ Zeldovich reaction and to build a preliminary compact model.

In this work, we study the dynamics of $\text{N}_2 + \text{O}$ collisions in the 0.1 to 19 eV energy range. Dissociation and exchange cross-sections are produced using the quasi-classical trajectory (QCT) method with an ab-initio surface calculated by Gamallo et al. [4]. Rates, based on these cross sections, match those previously reported in literature [5]. A sample of dissociation and exchange cross sections are shown in Figs. 1 and 2. The cross-sections exhibit strong vibrational favoring. The exchange cross-sections at first increase with total collisional energy until there is enough energy to dissociate molecules. This trend is not predicted by TCE model, shown by solid lines. The vibrational distributions of product NO molecules are shown in Fig 3. In contrast to the Larsen-Borgnakke (LB) model predictions, QCT calculations show that created NO molecules favor intermediate vibrational levels rather than the ground level. The favored levels increase when the pre-collision vibrational level of $\text{N}_2$ is increased but they are not significantly affected by the pre-collision translational and rotational energy. The final manuscript will also present cross sections for nonreacting collisions and an extended set of dissociation and exchange cross sections. The calculate cross sections will be used to create compact models based on ME-QCT model by Kulakhmetov et al [6].

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Studies of a Thermostress Convection-Based Actuator

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Thermostress convection encompasses a series of rarefied gas phenomena which manifest in highly non-isothermal transitional flows[1]. These non-equilibrium effects have been investigated theoretically since the 19th century, however, due to constraints imposed on ambient pressure and device temperature, their experimental measurements and practical implementation at macroscale are challenging and scarce [2]. For micro/nanoscale geometries, the small characteristic length scales make such non-equilibrium conditions easier to achieve, giving thermostress convection novel applications in actuation, gas sensing and separation, as well as thermal management. This work aims to quantify the behavior of these effects in a macroscale actuator and, through non-dimensionalization, use the results to estimate the performance of a microscale implementation. The setup consists of a series of interdigitated aluminum vanes having alternating high and low temperatures. A schematic representation is provided in Figure 1. The cool vanes are stationary and attached to a µNewton torsional balance, allowing the magnitude of the thermal stresses to be quantified. The heated vanes are moving and regulated at a user-defined temperature setpoint. Engaging the heating elements develops a strong thermal gradient (~50 K/mm) within the hot-cold vane gap, resulting in a thermostress convection flow. Due to the proximity of the cold moving vanes the thermal gradient at the embedded edge of the heated stationary vane is stronger than at its external free edge, leading to a bulk flow from the former to latter. This flow, in turn, induces a shear stress on the heated vanes that is measured by the torsional balance.

In addition to experimental measurements, simulations were carried out using the SPARTA DSMC[3] software in an effort to understand detailed flow field structures and the mechanisms of force production. The results are provided in Figure 2 for a vane temperature difference of 30 K and engagement of 30%. The data demonstrate a monotonic decrease in shear stress towards higher Knudsen numbers, a result which is consistent with similar studies on thermostress convection[4]. This result stems from the higher velocity near the embedded edge at elevated pressures, leading to an increased flow rate towards the free edge.

REFERENCES
Developing Experiments with Nanomechanical Resonators to Probe Rarefied Gas Dynamics

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Originating in the interest to understand how sensitive instruments based on micro/nanomechanical (MEMS/NEMS) resonators could be affected by gas damping [1], experimental methods based on nanoresonators are now emerging to study the transition and free molecular flow regimes of Rarefied Gas Dynamics (RGD).

Nanomechanical resonators in their simplest form, are cantilevered or doubly-clamped nanowires, nanotubes or nanobeams, controllably set into vibration around one of their selected resonance frequencies. The width of the spectra at high vacuum and in chosen gas at selected pressure and temperature, are used to calculate the quality factors and evaluate the gas damping on the structure. We seek to measure and understand gas damping behaviour as a function of rarefaction (Kn) and unsteadiness (resonant frequency in relation to relaxation time) [2].

Some of the experimental challenges to be overcome [3] are the availability of materials with a range of stiffness (resonance frequencies) and low intrinsic damping; fabrication methods allowing devices with low distortion or intrinsic stress; control of clamp rigidity and device isolation; removal of artifacts arising from the driving/detection schemes of nanowire vibration. Nanoresonators made by a field-directed assembly technique (Fig. 1), allow large numbers of nanoresonators with a broad range of materials to be made in arrays over large areas [4,5] and have been shown [4] to address many of these challenges. We will review a few recent experimental studies: the first showing the use of high-frequency cantilevered resonators made from single-crystal diamond [6] that yield data to enable scaling studies of rarefaction and unsteadiness, as well as accommodation coefficients for this material in different gases; second, experiments performed in 4He at 4.2K, in near ideal-gas conditions, which cover a range of rarefaction extending to continuum flow [7], and address the uncertainty [2] in the cross-over region; and finally, a recent scaling theory, allowing gas damping of a nanoscale resonator to be evaluated from measurements made for larger devices, which shows promise when tested against experimental data [8].

ACKNOWLEDGEMENTS

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REFERENCES

Comparison Of Density-Sensitive and Fluorescence Visualization in Low-Density Separated Flow


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Visualization of hypersonic rarefied flow can prove to be very challenging, as the relatively small number of particles means signals are intrinsically low; and the fact that the flows are highly luminous means that interference intensity is relatively significant when compared to signal intensity. This paper compares the effectiveness, in terms of flowfield visualization, of two techniques used to visualize the hypersonic leading-edge separation around a ‘tick’-shaped model [1]: resonantly enhanced shearing interferometry (RESI) [2] and nitric oxide planar laser-induced fluorescence (NO PLIF) [3].

RESI is a density-sensitive flow visualization method based upon the method of shearing interferometry, but using a light source tuned close to a resonant transition in lithium atoms seeded into the nozzle plenum of the T-ADFA free-piston shock tunnel. At the relatively high total specific enthalpy (11 MJ/kg) investigated in this study, the lithium is vaporized and enhances the refractivity of the gas, making the variations in the flowfield more apparent. A powerful broadband laser source is passed through the optical system, and an image results in which the intensity of the light is proportional to the spatial derivative in the density, much like a standard Schlieren image. The technique is amenable to being used with high-speed cameras, allowing for highly time-resolved video to be obtained. The paper outlines the effects of seeding with atomic lithium and a lithium salt, as well as a comparison between narrowband and broadband laser sources.

RESI, like all similar visualization techniques, has the limitation of being integrated across the line of sight of the light ray passing through the flow. NO PLIF is a sheet-based method that excites fluorescence using UV light at 226 nm to excite transitions in naturally occurring nitric oxide within the flow. The fluorescence is detected using an intensified CCD camera. As the fluorescence is only generated in the sheet, the technique is capable of visualizing flow with high spatial resolution, but without being able to make measurements at the high rates accessible with RESI. The intensity of the fluorescence is affected by the temperature, composition, pressure and speed of the molecules in the flow, and a typical visualization image is shown in Fig. 1. By exciting different NO transitions, the contrast in the image can be manipulated, and the ratio of images obtained using different transitions can also be used for temperature measurements.

The paper outlines the complementary nature of the two techniques, and compares the images obtained using each to show how each method captures the important flow features of the separated flow. The NO PLIF images will also be used to measure rotational temperature in the freestream, which will be compared with computations of the expected nozzle exit temperature.

ACKNOWLEDGEMENTS

Funding for this experimental investigation was provided by the US Air Force through the Asian Office of Aerospace Research and Development grant 134013, and by the Australian Research Council Discovery Projects Scheme DP 140100842 . We also acknowledge Dr James Moss for his insights into the fluid dynamics of the leading-edge separation.

REFERENCES

Microgravity Experiments in Rarefied Gas Dynamics

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The use of microgravity provides profound advantages and sometimes the only possibility of investigating various rarified gas dynamic phenomena. Suffice it to mention measurement of phoretic transport coefficients [1], simulation of astrophysical processes and particularly of protoplanetary dust agglomeration [2], vast research in complex (dusty) plasma [3], etc. One of the goals of the current work is to assess the microgravity-oriented instrumentation and experimental procedures that may have interest in ground research and applications. Particularly, we present the Cloud Manipulation System [4] that appeared to be by far more efficient than the traditional electrodynamic balance (Paul trap) in manipulation of dust cloud consisting of millions of particles. It is based on the use the thermophoresis and thermal creep induced gas flows. The system allows creating big fractal-type agglomerates of up to 1 mm in size from a cloud of micrometre-size grains, in situ investigation of the morphology, mobility, mechanical and optical properties of the free-floating agglomerates, including the two-phase flow phenomena in heavy-loaded clouds.

Quantitative description of a vast variety of kinetic properties requires higher accuracy. The coefficients are often known in a limited region of parameters, sometimes described by the contradictory models, not sufficiently well verified experimentally. It is true even for the most extensively investigated transport phenomena – thermophoresis and photophoresis, not to say about diffusiophoresis, gravito-photophoresis, and various other types of particle motion driven by physicochemical transformation and accommodation peculiarities on the particle-gas interface. In most cases, the accuracy and sometimes the entire possibility of the measurement is limited by the presence of gravity. Floating particles have the density considerably different from that of the gas. They sediment, often with gliding and tumbling, that perturbs the motion trajectory, local hydrodynamic environment around particles, all together complicating definition of the response. Measurements at very high or very low Knudsen numbers are of particular difficulty. Experiments assume creating a well-defined force, i.e. certain potential gradient. Most often, it results in the gas density non-uniformity and thus in perturbations from gravitational convection on the Earth.

The advantages of microgravity in measurements of kinetic properties are well admitted since long ago. There is a set of performed experiments in this area, mostly, on thermophoresis but also on photophoresis, diffusiophoresis, and thermal creep. In the coming years, we anticipate a genuine break-through in high-quality particle transport measurements resulting in substantial advancement in aerosol microphysics and rarefied gas dynamics.

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REFERENCES

Characterization of a seeded pulsed molecular beam using the Velocity Map Imaging technique

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An experimental study coupled with modeling and numerical simulation has been led to characterize the time dependent density and velocity distribution in a pulsed molecular beam generated by a pulsed valve associated to an oven placed downstream the nozzle [1,2]. The Velocity Map Imaging technique (VMI) has been used to characterize simultaneously the density of photoions (number of impacts on the detector) and their velocity distribution (positions of impacts on the detector) as a function of time. In the pulsed operating mode, the flow oscillates between the effusive and the supersonic regime, via the transition one, as the pressure and consequently the Knudsen number, changes inside the oven: The density and velocity distribution vary consequently (see the left panels of Figure 1). A simple model using a combination of a statistical model and a hydrodynamic one allows expressing the molecular density and velocity distribution at any point of the molecular beam along the jet axis. It reproduces adequately the experimental data (see right panels of Figure 1).

REFERENCES

Investigation into the anomalous Nusselt number in the Slip Flow Regime

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This paper presents the experimental study of heat transfer in slip flow in a circular tube with a constant wall temperature boundary condition. An earlier experimental investigation [1] had reported anomalously low values of Nusselt number (Nu) in the slip flow regime for constant wall temperature boundary condition. The present study is an extension of [1] which was aimed at obtaining the first ever heat transfer measurements in the slip flow regime. Those results were completely new and the Nusselt numbers were in disagreement (by 2-3 orders of magnitude) with the computational and theoretical Nu reported in the literature under similar heat transfer and fluid flow conditions. Further cross experiments with different tube material and working fluid confirmed the low Nusselt numbers.

In a technical note by [2], the authors had critically reviewed some of the ‘new results’ in micro-fluidics and had claimed that most of the results in micro-fluidics that do not follow the predictions of classical fluid mechanics are a result of neglecting certain assumptions that are not applicable for micro-domains. As an example, they considered the determination of Nu based on temperature values at the inlet and outlet and compared it with Nu based on local temperatures. They showed that the axial wall conduction is non-negligible in case of micro-geometries which could lead to misleading values of Nu. In light of these arguments, to reaffirm the experimental Nu, it was decided to attempt local temperature measurements which could shed more light on the actual axial temperature variation of the fluid.

The experimental set up consists of a circular tube with a water jacket that maintains a constant wall temperature boundary condition. A detailed description of the experimental arrangement can be found in [1]. In addition to the inlet and exit temperature ports used in the earlier test section, the present test section includes two extra ports which are used to insert two more thermocouples at different axial locations along the center of the circular tube.

Figure 1 shows the variation of Nusselt number with Knudsen number (Kn). It is seen that the Nu obtained from temperature measurements at the inlet and outlet are indeed misleading, with Nusselt numbers that are at least 2 order of magnitude less than that obtained in the present experiments. The analytical solutions of [3] and [4] for rarefied gas flow in microtube with constant wall temperature boundary conditions are also included in Figure 1. It is seen that, although the Nusselt numbers in the present experiments are significantly higher than those reported in [1], they are nevertheless an order of magnitude less than the analytical predictions. As per our knowledge, these are the first local temperature measurements made in rarefied gas flow in tubes and no other experimental data is available for comparison. Further temperature measurements resolving the radial temperature distribution in the tube may help explain the discrepancy in the analytical and experimental observations.

ACKNOWLEDGEMENTS

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Ion Velocity Distributions in Ionospheres

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Owing to infrequent collisions with the background neutral atmosphere, the ion velocity distribution of an ionosphere can differ significantly from a Maxwellian shape. This is particularly true when the ions are accelerated by the ambient electric and magnetic fields that can combine to produce ExB drifts that are supersonic with respect to the neutral gas with which they collide. It is important to know the distribution functions because the interpretation of satellite and radar data depends on their knowledge.

Transport properties like vertical drifts and heat flows along the geomagnetic field are also intimately related to the velocity distributions. Many situations have been envisaged over the years. The simplest is one for which the electric field is uniform and the mean free path sufficiently short that the problem can be solved locally and with relatively few complications [1]. A more complicated problem is one for which the electric field changes linearly with space either in a cartesian geometry or in a cylindrical situation centered about a magnetic field tube, this makes the problem nonlocal even if the mean free path is relatively small (Fig. 1) [2,3].

A more complex situation still is one for which the mean free path becomes so large that the distributions functions have to be determined through boundary conditions. This problem has been so far partially tackled through a boundary layer approximation [4] and numerically [5]. Interesting distribution functions can emerge from this situation (Fig. 2) if strong electric fields are temporarily imposed along a magnetic field tube. In this case important transients need to be taken in consideration when dealing with densities, fluxes and temperatures, with again strong implications for satellite and radar observations. Time permitting, some relevant examples of radar and satellite observations will be presented.

REFERENCES

Hot Oxygen Geo-corona in the Topside Ionosphere

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The distribution of hot oxygen geo-corona in the topside ionosphere resulting from the production of energetic oxygen atoms is modeled using an isotropic Boltzmann equation that includes gravity. Yee et al. [1] first reported the experimental evidence of a hot oxygen geo-corona in the F-region ionosphere. The production of translational energetic atomic oxygen and the resulting corona was the subject of several theoretical studies, in which the dissociative recombination of $O_2^+$ and $NO^+$ was identified as the primary sources of hot oxygen in the F-region [2], and the Boltzmann equation was sometimes used to model the interactions between the thermal and non-thermal oxygen atoms [3]. In the topside ionosphere above the F-region, the production of oxygen geo-corona was previously thought to be insignificant, due to the negligibly small molecular ion densities in ionospheric models such as the International Reference Ionosphere (IRI) [4]. However, new in-situ ion composition observations from the Enhanced Polar Outflow Probe (e-POP) [5] reveal the frequent presence of molecular ions in the topside ionosphere in the auroral region, at densities that are more than an order of magnitude larger than IRI model values. We present the solution of the Boltzmann equations based on these new ion composition data, which suggests a significant contribution from the dissociative recombination of the molecular ions to the production of observed non-thermal oxygen atoms and the escape of these non-thermal atoms near the exobase.

REFERENCES

Fluctuation dynamics and structure formation in a dissipative relativistic dilute gas: the static background case.

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Dissipation in dilute gases is enhanced when the thermal energy of the system becomes comparable to the rest energy of its constituents [1]. Firstly, as is well known, the bulk viscosity does not vanish for relativistic gases and the shear viscosity is significantly modified [1,2]. Also, the heat flux in such scenario is coupled not only with the temperature gradient but also to the number density gradient and with the gravitational field [3, 4]. Moreover, the relativistic Boltzmann equation leads to an extra source of momentum in the transport equations due to the heat flux. These modifications can alter significantly the dynamics of the gas.

In this work, the case of a self-gravitating dilute relativistic fluid is addressed. The system of relativistic transport equations is linearized using first order fluctuation theory and the corresponding dispersion relation is analyzed. It is shown that, while in the non-relativistic case the Jeans mass is not altered by neither thermal nor viscous dissipation [5,6], such parameter is modified by thermal dissipation for relativistic systems. The correction to this criterion depends on the ratio of microscopic and gravitational characteristic times and vanishes for low temperatures systems. In both the relativistic and non-relativistic cases it is shown that viscous dissipation only affects the dynamics of decaying modes and the purely oscillatory behavior is not present in the formalism.

The dependence of the correction to Jeans mass and wave number with the microscopic collision time will be studied as well as the modifications to the Rayleigh-Brillouin spectrum for decaying modes. The impact of thermal dissipation due to the gravitational field is also briefly discussed.

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The search for structure formation from gas clouds is an old subject that goes back to 1902 when Jeans [1] used the system of phenomenological equations of mass and momentum densities together with the Poisson equation and showed that small perturbations in the mass density, pressure, velocity and gravitational potential in a static background with wavenumber smaller than the Jeans wavenumber could evolve with time. In terms of balance of forces the fluctuations can grow in time if the inwards directed gravitational force is larger than the outwards directed internal pressure of the gas.

Jeans theory describes the gravitational instability of self-gravitating systems by searching for conditions that small perturbations can grow and lead to a collapse of the system. It was formulated before the knowledge of the Universe expansion and one has to take into account the Jeans "swindle", which imposes that the Poisson equation is valid only for the perturbations, since the background solution of constant mass density, pressure, gravitational potential and vanishing velocity satisfy the balance equations of mass and momentum densities, but not the Poisson equation.

Here the dynamics of self-gravitating fluids is analyzed within the framework of a collisionless Boltzmann equation [2,3,4,5] in the presence of gravitational fields and Poisson equation. The equilibrium distribution function takes into account the expansion of the Universe and a pressureless fluid in the matter dominated Universe. Without invoking Jeans "swindle" a dispersion relation is obtained by considering small perturbations of the equilibrium values of the distribution function and gravitational potential. The collapse criterion, which happens in an unstable region where the solution grows exponentially with time, is determined from the dispersion relation.

The collapse criterion in a static Universe occurs when the wavenumber \(k\) is smaller than the Jeans wavenumber \(k_J\), which was the solution found by Jeans. For an expanding Universe it is shown that this criterion is \(k \leq \sqrt{(7/6)} \ k_J\). As a consequence the ratio of the mass contained in a sphere of diameter equal to the wavelength \(\lambda = 2\pi/k\) to the Jeans mass in an expanding Universe is smaller than the one in a static Universe. This implies that in an expanding Universe a smaller mass ratio is needed to initiate the collapse.

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REFERENCES

Kinetic Models for Space Plasmas: Recent Progress for the Solar Wind and the Earth’s Magnetosphere

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Recent models for the solar wind and the inner magnetosphere have been developed using the kinetic approach. The solution of the evolution equation is used to determine the velocity distribution function of the particles and their moments. The solutions depend on the approximations and assumptions made in the development of the models. Effects of suprathermal particles often observed in space plasmas are taken into account to show their influence on the characteristics of the plasma, with specific applications for coronal heating and solar wind acceleration. We describe in particular the results obtained with the collisionless exospheric approximation based on the Lorentzian velocity distribution function for the electrons and its recent progress in three dimensions [1].

The effects of Coulomb collisions obtained by using a Fokker-Planck term in the evolution equation were also investigated, as well as effects of wave turbulence for the electrons [2] and of kinetic Alfven waves for the protons [3].

For solar wind especially, modelling efforts with both magnetohydrodynamic and kinetic treatments have been compared and combined for improvement of the predictions at the vicinity of the Earth. Photospheric magnetograms serve as observational input in semi-empirical coronal models used for estimating the plasma characteristics up to coronal heliocentric distances taken as boundary conditions in solar wind models.

The solar wind fluctuations influence the perturbations of the space environment of the Earth and generate geomagnetic storms. In the magnetosphere of the Earth, the trajectories of the particles are simulated to study the plasmasphere, the extension of the ionosphere along closed magnetic field lines and to better understand the physical mechanisms involved in the radiation belts dynamics [4].

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Numerical and Experimental Capabilities for Studying Rocket Plume-Regolith Interactions

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For future space missions in which soft landings on extra-terrestrial bodies will be required, e.g. [1], it is important to understand the interaction of the propulsion system with the surface of the body. During the landing phase, the surface regolith can become contaminated with the chemicals presents inside the rocket plume. For a sample return mission, it is necessary to minimise the degree of contamination in the collected soil so that it can be analysed reliably upon return. The body’s surface topography will also be altered by the presence of the rocket plume through an erosion process, which could have implications for the physical process of collecting soil samples.

Finally, the interaction of the nozzle plume and the surface regolith will lead to the generation of a dust cloud that could lower the effectiveness of the spacecraft’s soft landing navigation equipment and influence the forces and torques acting on the spacecraft.

In Europe, there are currently no experimental facilities designed specifically to provide measurements for the interaction of a rocket plume with a regolith. A new vacuum facility that is under development for performing these measurements will be discussed.

Simultaneously, numerical and analytical techniques for performing complimentary simulations of these rocket plume-regolith interactions are being developed. Results for hybrid computational fluid dynamics (CFD) and direct simulation Monte Carlo (DSMC) simulations of plumes from rocket nozzles expanding in near vacuum conditions and impinging on flat plates will be presented, showing how the surface pressure and shear stress change with nozzle height above the surface. Fig. 1 is an example of the annular shaped shear stress distribution that is characteristic of a plume impinging normally on a flat plate. The CFD code used is Fluid Gravity Engineering’s Thermochemical Implicit Non-Equilibrium Algorithm (TINA); an inhouse version of dsmcFoam [4] is used for the DSMC calculations. The development of a DSMC adsorption/desorption boundary condition for predicting regolith contamination will also be presented.

REFERENCES

Lift Acting on a Spinning Sphere in a Slow Flow of a Rarefied Gas

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Slow uniform flow past a sphere is not only a classical problem in fluid dynamics, but also one of the most fundamental problems in rarefied gas dynamics (e.g., [1, 2]). When a sphere is rotating in a flow, it experiences the lift in addition to the drag. In the case of a free molecular gas, the lift was shown to be expressed as $F_L = -(2/3) \rho_\infty L^3 (\hat{\mathbf{v}}_\infty \times \hat{\mathbf{v}}_\infty)$, where $\rho_\infty$ is the density of the uniform stream, $\mathbf{v}_\infty$ its velocity, $\Omega$ the angular velocity of the sphere, and $L$ the sphere radius (e.g., [3, 4]). Therefore, the direction of the lift is apparently opposite to what one would expect in a continuum flow (see, for example, [5]). This inversion of the lift, peculiar to highly rarefied gases, was later termed as the inverse Magnus effect [4].

To clarify the transition of the lift in terms of the degree of gas rarefaction, we need to investigate a flow past a spinning sphere for a wide range of Knudsen numbers. Recently, an asymptotic theory of a flow past a sphere at low Mach numbers was developed in the case of a non-rotating sphere [6]. The purpose of the present study is to extend the previous analysis to the case of a rotating sphere, and derive a general form of the lift.

We therefore consider a sphere (radius $L$), rotating around the $x_1$-axis at constant angular velocity $\Omega = (\Omega, 0, 0)$, held in a uniform flow with velocity $\mathbf{v}_\infty$, pressure $p_\infty$, and temperature $T_\infty$, as shown in Fig. 1. The vector $\mathbf{v}_\infty$ lies in the ($x_1, x_2$) plane and is deflected from the $x_1$-axis by angle $\alpha$. The temperature of the sphere is assumed to be uniform and is the same as that of the uniform flow. We investigate the steady flow around the sphere on the basis of the Boltzmann equation and the diffuse reflection condition on the boundary, under the following conditions: (i) the Mach number is small ($|\mathbf{v}_\infty|/(\sqrt{T_\infty} \sqrt{\rho_\infty})^2 \ll 1$; $R$ is the gas constant); (ii) the spin parameter is finite ($S = L[\Omega/|\mathbf{v}_\infty|] = O(1)$); (iii) the Knudsen number is finite ($Kn = \ell_\infty/L = O(1)$). Here, $\ell_\infty$ is the mean free path of the gas molecules in the reference equilibrium state at rest.

Let us introduce the following dimensionless quantities: $\hat{\mathbf{v}}_\infty = \mathbf{v}_\infty/(2R\sqrt{T_\infty})^{1/2}$, $\hat{\Omega} = L\Omega/(2RT_\infty)^{1/2}$, and $k = (\sqrt{\pi}/2)Kn$. We also introduce a small parameter $\epsilon = |\hat{\mathbf{v}}_\infty| \ll 1$. Then, the drag and lift on the sphere are expressed, up to the second order of the Mach number, as

$$\frac{F_D}{p_\infty L^2} = \hat{h}_D(k) + O(\epsilon^2), \quad \frac{F_L}{p_\infty L^2} = (\hat{\mathbf{v}}_\infty \times \hat{\Omega})h_L(k) + O(\epsilon^2),$$

where $\gamma_1$ is a constant such that $\mu = (\sqrt{\pi}/2)\gamma_1\rho_\infty(2RT_\infty)^{-1/2}$ is the viscosity of the gas at the reference state, and $h_D(k)$, $c_1(k)$, and $h_L(k)$ are functions depending only on $k$ (or the Knudsen number). The values of $h_D$ and $c_1$ for the BGK model are given in [6] (see also [2] for $h_D$ for a hard-sphere gas). $h_L(k)$ is to be determined numerically.

Thus, the inversion of the lift, if it takes place at some Knudsen number, does not depend on the angle between $\hat{\mathbf{v}}_\infty$ and the axis of revolution of the sphere, but is solely determined by the Knudsen number.

REFERENCES

Numerical Investigation of the Aerodynamics of the REX-Free Flyer in the Rarefied Gas Regime

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The REX-Free Flyer is a concept study by the German Aerospace Center (DLR) in an effort to develop an orbital experimental platform to fill the gap between short duration experiments such as drop towers/sounding rockets and long-term missions at the International Space Station (ISS). The envisioned reusable vehicle, shown in Fig. 1, shall enable day- and week-long experiments in high-quality weightlessness [1]. The unique sharp-edged geometry promises improved aerodynamic properties and a less complex heat flux environment. A soft and controlled re-entry shall guarantee a recovery of the experimental setup.

The Direct Simulation Monte Carlo (DSMC) method [2] is used to simulate a Mach 20 nitrogen flow around a scaled-down model of REX in the rarefied gas regime. The DSMC module of PICLas, a coupled Particle-in-Cell (PIC) and DSMC code [3], is utilized. The code is developed cooperatively by the Institute of Aerodynamics and Gas Dynamics (IAG) and the Institute of Space Systems (IRS) at the University of Stuttgart.

First, a brief overview of the implemented numerical and phenomenological models is given. Simulation parameters ensuring physical simulation results are presented. Consequently, the code is used to investigate the lift, drag, and pitching moment coefficients at three different angles of attack: 0°, 14°, and 52°. To verify the simulation results, coefficients are compared to an approximate method, where acceptable agreement can be found considering the underlying assumptions, and to dsmcFoam, where excellent agreement between the different DSMC implementations is found. Furthermore, the complex three-dimensional flow environment is investigated and presented in more detail. The paper is concluded with an overview of the required computational resources.

REFERENCES

Air-Breathing Electric Propulsion systems (ABEP) are currently investigated to utilize the residual atmosphere as propellant for drag-compensating thrusters on spacecraft in (very) low Earth orbits [1, 2, 3]. The key concept for an efficient intake of such a system is to feed a large fraction of the incoming flow to the thruster section by a high transmission probability $\Theta$ for the inflow while the backflow should be as low as possible. This is the case for rarefied flows through tube-like structures of arbitrary cross section when assuming diffuse wall reflections inside and after the tubes, and macroscopic velocities $u$ larger than the thermal velocity $v_{th} \propto \sqrt{k_B T / m}$ [1].

The theory of transmission (Knudsen diffusion) of free molecular flow through cylinders is well known for $u = 0$ [4], but only very few research results are available for $u > 0$ [5]. In addition, no detailed data about the velocity distribution functions (VDF) of the flow is available, which is necessary for a realistic modelling of the inflow condition in kinetic simulations starting directly at the end of the transmitting structures.

Therefore, the desired theoretical characteristics of intakes for ABEP are pointed out here and the results of a sensitivity analysis by Monte Carlo simulations concerning $\Theta$ and the VDF of free molecular flows through tube-like structures are presented. Based on simple algebraic relations, an intake can be optimized in terms of collection efficiency, which is directly related to the thrust-to-drag ratio. It is shown that $\Theta$ can be separated into parts of direct and indirect transmission and depends only on non-dimensional values of the tube geometry combined with $v_{th}$ and $u$. Additionally, simulation results of a complete exemplary ABEP configuration are shown illustrating the influence of modelling quality of the VDF and inter-particle collisions.

REFERENCES

Charged Aerodynamics of a Low Earth Orbit Cylinder

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Abstract.
All bodies orbiting Earth interact with plasma in some manner. These interactions are complex, rich in physical phenomena and for spacecraft, potentially hazardous. In Low Earth Orbit (LEO), some of these interactions include; high surface charging in polar orbits, body ram and wake flows, arcing phenomena, self-induced noise and the anomalous ionisation of out-gassed neutrals [1][2]. In general, study of the LEO plasma-body interaction has not been concerned with the force exerted on the structure. The aerodynamic interaction of LEO orbiting bodies with the neutral environment constitutes the largest non-conservative force on the body. The work presented here demonstrates that under certain conditions the plasma-body interaction may comprise a measurable proportion of the total atmospheric force vector experienced by an orbiting body compared to neutrals.

This work uses a hybrid Particle-in-Cell (PIC) - Direct Simulation Monte Carlo (DSMC) code called pdFoam. The self-consistent electrostatic flowfield about a charged cylinder in a mesosonic plasma flow representative of conditions experienced by a polar orbiting LEO body is modelled. The electron distribution function is represented by a non-linear Boltzmann electron fluid and ion gas-surface interactions are assumed to be that of a neutralising, conducting, thermally accommodating solid wall with diffuse reflections. The variation of aerodynamic properties with surface potential given fixed flow conditions is investigated.

An example of major variations in flow structure with surface potential is shown in Figure 1. Ion density contours shown in Figure 1 a) and b) demonstrate the variation of ion absorption radius about a 0.3m radius cylinder with uniform surface potentials $\phi_s$ of $-1V$ and $-50V$ respectively. The source of the density peak in the ram flow in Figure 1 b) and effect of ion absorption radius on aerodynamic properties are presented in the full paper. Relative contributions of charged and neutral species to the aerodynamic properties of the cylinder provide insights into the atmospheric forces experienced by a LEO orbiting body, and yield conditions of interest for further study where the contribution of charged species to the atmospheric force vector are significant.

ACKNOWLEDGEMENTS
The Authors gratefully acknowledge the insights of Dr Tom Scanlon and Prof Richard Brown at the James Weir Fluid Laboratory and for the use of their DSMC code, dsmcFoamStrath, as the basis for the development of the PIC-DSMC code, pdFoam, used herein.

REFERENCES
A Green-Kubo Approach to Reduce Collision Separation Error in the Direct Simulation Monte Carlo Method

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One major distinguishing feature of the direct simulation Monte Carlo (DSMC) method is an allowance for unphysically large separation distances between colliding particles. This approximation contributes to enormous efficiency gains relative to deterministic molecular dynamics procedures, while potentially becoming a dominant source of numerical error in any DSMC fluid transport calculation. It has been extensively documented both empirically and theoretically that DSMC simulation accuracy depends strongly on the prevention of collision separation distances which are large in comparison to the local mean free path [1]. As a consequence, the ratio of mean collision separation to mean free path is commonly used as a metric for DSMC numerical accuracy [2], and considerable research efforts have been directed toward the efficient reduction or minimization of collision separation for a fixed particle population [3]. Despite the known importance of collision separation as an error source, algorithm modifications to reduce this error have focused almost exclusively on collision partner selection, and other error reduction strategies have been largely overlooked. In this work, we consider one alternate strategy to reduce collision separation error independent of collision partner selection.

As a starting point in the present work, we consider DSMC transport coefficient expressions of Alexander et al. [4] and Hadjiconstantinou [5], derived for a monatomic hard sphere simple (one species) gas as a function of the unidirectional mean-squared collision separation and/or time step interval. These expressions follow from the Green-Kubo viscosity derivation of Wainwright [6] using the hard sphere stress tensor autocorrelation function. We introduce a cell-based factor for the collision cross section, which eliminates the collision separation contribution to thermal conductivity by equating Green-Kubo and Enskog thermal conductivity expressions; this leads to a significant reduction in the theoretical collision separation error in viscosity. By adjusting post-collision particle locations as suggested by Hadjiconstantinou [5], we are able to simultaneously correct for the influences of collision separation and time discretization error through the use of an effective mean-squared collision separation $\langle \delta^2 \rangle$ averaged over the time step interval. Substantial error reductions in transport coefficients are predicted over a wide range of $\langle \delta \rangle$ values.

A hypersonic cylinder flow is used to quantitatively assess accuracy improvements in flowfield and surface flux quantities for a canonical flow problem. A further assessment is then performed through comparison with both standard DSMC and Navier-Stokes simulation results for a very low Knudsen number test case, in order to demonstrate the potential applicability of the modified collision routines to flow regimes for which current DSMC procedures may be prohibitively expensive. Although the proposed algorithm modification is currently formulated only for the unrealistic case of a simple hard sphere gas, it is hoped that the underlying principles behind this modification can be extended as a general means to substantially reduce collision separation error in DSMC and to make DSMC more suitable for simulation of very low Knudsen number flows.

REFERENCES

### Session 26: Molecular Dynamic Simulations

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Simulations of condensation flows induced by reflection of weak shocks from liquid surfaces

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The condensation of a vapor onto a liquid film, induced by the reflection of a shock wave, provides both a useful experimental technique [1] and theoretical test problem to investigate interfacial transport phenomena. In this work, the flow properties are studied by three computational tools. The first one is based on Molecular Dynamics simulations [2] of the Lennard-Jones fluid [3] which provide the most fundamental description and the reference flow properties. The second one is based on a Diffuse Interface Model (DIM) [4] which, in principle, can describe both the liquid and vapor phase by a single PDE’s set. The third one consists of a hybrid model (HM) in which the liquid is described by a simple hydrodynamic model and the vapor by the Boltzmann equation. The two phases are coupled by kinetic boundary conditions [5, 1]. Previous applications [6, 7] of the three models to evaporation flows has shown that DIM fails to predict the correct evaporation rate and the jumps of macroscopic quantities across the Knudsen layer, whereas HM computed evaporation rates and macroscopic quantities profiles agrees very well with MD reference data. Condensation flow simulations discussed in the present work confirm the good performance of HM and indicate that the deviations of DIM solutions from MD results is smaller than in the case of evaporation flows where a thicker kinetic layer is present. Examples of the obtained results are shown In Figure 1, showing a snapshot of the flowfield generated by a shock wave impinging on a thin liquid film, initially at reduced temperature $T^*_{l} = 0.8$.


REFERENCES

Molecular Dynamics Simulation on Kinetic Boundary Conditions of Gas-Vapor Binary Mixture

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With progression of advanced technologies using net evaporation/condensation, heat and mass transfer between liquid and gas phases has become very important in recent years from the viewpoints of molecular and micro-scale mass transfer. In general, the gas phase adjacent to the liquid interface is composed of multicomponent gas mixture, e.g., vapor (condensable gas) and gas (noncondensable gas). Hence, the influence of gas molecules for evaporation and condensation of vapor molecules or dissolution of gas molecules in the bulk liquid phase (Henry's law) gets much attention in the physical process with heat and mass transfer at a gas-liquid interface: for example, cavitation bubble collapse, molecular distillation with evaporation and condensation, and dissolution of oxygen molecules into a thin water layer in porous media of a fuel cell.

Since evaporation and condensation are originated from the molecules outgoing from and colliding onto an interface, the molecular gas dynamics is capable of treating vapor flows near the interface. The kinetic boundary condition (KBC) at the interface plays an essential role in the nonequilibrium region near the interface [1]. The key physical processes of molecules at the interface are evaporation and reflection because the KBC is composed of the molecules outgoing from the interface to vapor phase. The aim of this study is to propose the KBCs for gas mixture in gas-liquid equilibrium state by using our proposed method [2]. In this study, we use Ar as vapor molecules, and Ne as gas molecules.

The schematic of the simulation model is shown in Fig. 1. By using the two boundaries (Gas-vapor and liquid boundaries), several mass fluxes (evaporation, condensation, dissolution, degassing and reflection) can be counted. Also, from this study, we discuss the characteristic behaviors of gas and vapor molecules and velocity distribution functions of KBC for gas and vapor molecules.

![Fig.1: Schematic of molecular dynamics simulation](image-url)

REFERENCES

Molecular Dynamics Study of Force Acting on a Model Nano Particle Immersed in Fluid with Temperature Gradient: Effect of Interaction Potential

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Mass transport under temperature gradient in fluid is known as Soret effect. In particular, when micro particles in a fluid such as aerosols in a gas or colloids in a liquid are concerned, the phenomenon is called thermophoresis. The velocity $v_T$ of the micro particle is assumed to be proportional to a temperature gradient: $v_T = -D_S T \nabla T$, where $D$, $S_T$, and $T$ are, respectively, the diffusion coefficient, the Soret coefficient, and the temperature of surrounding media. Since $D$ is positive, the direction of thermophoresis is characterized by $S_T$, namely, micro particles move to the colder (or hotter) region of the fluid in the cases with a positive (or negative) $S_T$. Recently, thermophoresis in a micro-scale device has drawn attention as a new particle manipulation technique in micro/nano engineering [1] and bioengineering [2]. Therefore, it is important to establish a method to predict $S_T$ of a target particle theoretically. In many cases, $S_T$ is positive at room temperature, but negative $S_T$ may be preferred in applications since heating a solution is easier than cooling it. Thus, it is also important to clarify dominant factors that determine the sign of $S_T$.

In the case of a gas, the mechanism of thermophoresis is well explained by the use of kinetic theory of gases (see, e.g., [3]), and negative $S_T$ can be realized for large value of $\lambda_p/\lambda_g$, where $\lambda_p$ and $\lambda_g$ are, respectively, thermal conductivities of the particle and the gas. However, in the case of liquid, even the sign of $S_T$ is hard to predict with the present theoretical framework. Difficulties arise from the fact that $S_T$ depends not only on particle bulk characteristics but also its surface property, which is dependent on a solution under consideration. Therefore, microscopic description is necessary to clarify the nature of $S_T$. Using molecular dynamics (MD) simulation, some basic properties of thermophoresis in Lennard-Jones (LJ) fluid are investigated for various values of mass, size, and thermal conductivity of the particle, viscosity of a solvent, and wetting property [4]. However, the sign of $S_T$ obtained in [4] is positive for all cases in spite of the fact that $S_T$ can take both signs. In this study, the effect of interaction potential between surrounding fluid molecules and the target particle is investigated using MD simulation, with particular interest on the sign change of $S_T$ due to the different interaction potential.

A model particle is immersed in a rectangular box filled with LJ molecules with diameter $\sigma$. The center of mass of the particle is connected to the center of the box via a harmonic potential, thereby the particle stays close to the origin during the simulation. The model particle has larger diameter $\sigma_0 (\approx 5\sigma)$ than surrounding LJ molecules. The LJ fluid is either in a gas phase or liquid phase. In the $x$ and $y$ directions, we employ periodic boundary conditions. On the other hand, a wall with purely repulsive potential is placed at each end of the box in the $z$ direction. In order to produce a temperature gradient in the box, temperature-controlled regions of thickness $4\sigma$ are prepared adjacent to the repulsive walls. The linear dimension of the box in the $x$ and $y$ directions and the $z$ direction are more than, respectively, $18\sigma$ and $38\sigma$, and these values are chosen so that the size of the box yields minor effect. The interaction between the model particle and surrounding LJ molecules is described by either LJ potential or purely repulsive potential. In order to evaluate thermophoresis of the model particle, we quantify a force acting on the particle in the $z$ direction. It is shown that, in the case of liquid, $S_T$ evaluated from the force is positive (or negative) when the interaction is LJ potential (or purely repulsive potential). The results indicate that the effect of the interaction between the model particle and surrounding LJ molecules is significant enough to affect the sign of $S_T$.

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REFERENCES

Molecular Dynamics Investigation of Energy Redistribution During Gas-Surface Collisions

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For a variety of industrial applications ranging from the aerospace technology to gas separation devices, accurate modeling of gas-surface interaction is crucial for an appropriate analysis of the problem at hand. In general, gas-surface interaction involves a range of complex physical phenomena, such as particle adsorption, surface diffusion, non-Maxwellian desorption, surface reactions and non-equilibrium polarization of the reflected molecules. While ballistic scattering of monatomic molecules can be well approximated with existing scattering kernels, little work has been done so far regarding the analysis of more complex scenarios involving polyatomic molecules. With this in mind, the aim of the present investigation is as follows.

First, a comprehensive molecular dynamics (MD) study of $O_2$ and $N_2$ molecules scattering from a graphite surface has been conducted. Of particular interest is the rate of energy transfer between different molecular modes and the solid surface during the collision and its potential effect on the scattering process. MD data has been collected for a wide energy spectrum of the impinging molecules and the specific surface temperatures, with particular focus on the case of high thermal non-equilibrium between translational and rotational kinetic modes. The obtained results are compared with the numerical, theoretical and experimental data already reported in the open literature. Second, in an attempt to define suitable boundary conditions, the obtained MD results have been used to tune the scattering kernel proposed by Gorji and Jenny [2]. Unlike the Maxwell and CL kernels, the resulting kernel allows for the coupling of translational and rotational degrees of freedom, which provides a more realistic description of the scattering process. Furthermore, the possibility to generalize the new kernel for both Maxwellian and non-Maxwellian desorption has been investigated. In conclusion, it is shown how strong thermal non-equilibrium states can be exploited for effective separation of gas mixtures, for which the details of gas-surface interaction are decisive.

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REFERENCES

Scattering Properties of Gas molecules on Self-Assembled Monolayers using Molecular Dynamics Simulation

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Self-assembled monolayers (SAMs), which are highly ordered structures of long-chain molecules on a metallic surface by self-organization, have been used in the surface modification of the MEMS/NEMS [1][2]. In order to investigate the gas flow of high Knudsen number, it is necessary to specify the boundary condition for the reflected gas molecules at a solid surface. Therefore, it is interesting to study the scattering behavior of the reflected gas molecules on SAMs interface and investigate the effect of surface functionalization with SAMs on the momentum and energy transfer at the interface. The present author has studied the scattering properties of monoatomic and diatomic gases on various solid surfaces based on the molecular dynamics (MD) method and proposed the boundary condition of reflected gas molecule as in previous papers [3]-[6]. The objective of this study is to provide data for better understanding of characteristics of reflected gas molecules on SAMs interface.

In the present study, the scattering properties of argon (Ar) gas molecules on the SAM surface which consists of C\textsubscript{3}H\textsubscript{7}SH molecules chemically adsorbed on the gold (Au) surface are investigated by using MD simulation. Figure 1 shows the SAM surface model in the MD simulation. The trapping probability, the angular distribution and the angular scattering distribution for the reflected gas molecule are analyzed for various incident energies and angles. It is shown that the trapping probability is higher at low incident energy. The energy accommodation coefficient and the tangential momentum accommodation coefficient of argon molecules on the SAM surface are also obtained. It is found that the angular scattering distribution for small incident angle is almost close to the distribution of diffuse reflection. The results will be presented at the Symposium.

ACKNOWLEDGEMENTS

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REFERENCES

**Session 27: Boltzmann and Related Equations**

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Fast numerical methods for rarefied gas dynamics simulations

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In particular, we focus on the development of fast methods for the solution of the collisional Boltzmann equation for rarefied gases by coupling this new semi-Lagrangian approach which handles the transport part with a fast spectral approach for solving the collisional operator.

We start discussing a first order method which is based on the solution of the collision part on a grid and on the exact solution of the transport part by following the characteristics backward in time. This method on the contrary to classical semi-Lagrangian schemes does not need to reconstruct the distribution function at each time step. This allows to tremendously reduce the computational cost and to perform efficient numerical simulations of simple kinetic equations up to the six dimensional case on a single processor laptop machine.

We then extend this approach to high order reconstruction of the distribution function. In this situation, the idea consists in updating at each time step the extreme points of the distribution function for each velocity of the lattice instead of updating the solution in the cell centers, these extremes points being located at different positions for any fixed velocity of the lattice. The result is a class of scheme which permits to preserve the structure of the solution over very long times compared to existing methods from the literature.

We finally demonstrate the capability of this class of schemes to deal with parallel architectures by introducing the specifics treatments and algorithms which should be developed for an OpenMP and CUDA parallelizations. The goal is to prove that the schemes are well adapted to these types of parallelizations, that the gain in CPU time is substantial on nowadays affordable computers and that their very good scalability makes this approach a real competitor with respect existing schemes for the solution of multi dimensional kinetic models.

REFERENCES

In this talk, I will present joint work with C. Hauck (ORNL) and M. Murillo (LANL) on a new multi-species BGK model for dense plasmas. This model conserves mass, momentum, and kinetic energy and allows for a more clear connection to the underlying cross sections and inter-species collision rates. We study the transport properties of the model and apply the method to an interface problem, comparing diffusion coefficients with theory and molecular dynamics results.
On Deterministic Evaluation of the Boltzmann Collision Operator on Octrees in $O(N^2)$ Operations

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Fully deterministic evaluation of the Boltzmann collision integral for gases remains difficult in multidimensional applications. Solvers based on the Fourier-Galerkin approach require only $O(N^2)$ operations, see e.g., [1,2], and were successfully applied to simulation of one-dimensional flows including flows with thermal non-equilibrium. Computational costs of the Fourier-Galerkin method can be lowered to $O(MN \log N)$, see, e.g., [3,4], to allow its use in multidimensional simulations with simple geometries and flow conditions. A limitation of the existing techniques is that they use uniform partitions in the velocity variable and are not adaptive. Discontinuous Galerkin (DG) discretizations of the Boltzmann collision operator in the velocity variable on octrees can provide an alternative to the Fourier-Galerkin approach. A key component of the method is the affine convolution form of the Galerkin projection of the collision integral

$$I(\tilde{\xi}, k) = \frac{2^{k/2}}{\omega \Delta \tilde{\nu}} \int_{\mathbb{R}^3} \left( f(2^{-k} \tilde{\nu} + \tilde{\xi}) f(2^{-k} \tilde{\mu} + \tilde{\xi}) A(\tilde{\nu}, \tilde{\mu}, \phi) d\tilde{\nu} d\tilde{\mu} \right)$$

where the pre-computed kernel $A(\tilde{\nu}, \tilde{\mu}, \phi)$ contains information about the collision process and is defined by (see [5,6])

$$A(\tilde{\nu}, \tilde{\mu}, \phi) = \frac{1}{2} \int_0^{2\pi} \int_0^\pi \left( \phi(\tilde{\nu}) + \phi(\tilde{\mu}) - \phi(\tilde{\nu}) - \phi(\tilde{\mu}) \right) b dB d\tilde{\theta}.$$

Here $\tilde{\nu}$ and $\tilde{\mu}$ are the pre-collision and $\tilde{\nu}'$ and $\tilde{\mu}'$ are the post-collision velocities of a pair of particles, $\tilde{\xi} = \tilde{\nu} - \tilde{\mu}$, and $b$ and $\tilde{\xi}$ are the collision impact parameters; $\omega \Delta \tilde{\nu}$ is the proportional to the volume of the support of the basis function $\phi(\tilde{\nu})$ and $\tilde{\xi}$ is a vector and $k$ is an integer. A special case of (1), corresponding to $k=0$, was used in [5,6] to design methods to evaluate the Boltzmann collision integral on uniform velocity meshes. DG basis functions on octrees are obtained from a single set of basis functions $\phi(\tilde{\nu})$ by affine transforms, $\phi^{j,k}(\tilde{\nu}) = 2^{k/2} \phi(2^k(\tilde{\nu} - \tilde{\xi},k))$. Invariance properties of kernel $A(\tilde{\nu}, \tilde{\mu}, \phi)$ with respect to affine transforms (see e.g., [5,6]) imply that the Galerkin projection of the collision operator $I_{\phi,k}$ on the DG octree basis function $\phi^{j,k}(\tilde{\nu})$ can be recovered from (1) as $I_{\phi,k} = I(\tilde{\xi}, k)$. The pre-computed kernel $A(\tilde{\nu}, \tilde{\mu}, \phi)$ requires $O(N^{5/3})$ units of storage where $N$ is the total number of the velocity discretization points [5]. The convolution form (1) can be computed in $O(N^2 \log N)$ operations using known fast techniques. An application of the Fourier transform to (1) leads to an $O(N^2)$ algorithms for computing the Boltzmann collision operator on octrees with $O(N^{5/3})$ units of storage requirement for the pre-computed kernels in the case of spherically symmetric interaction potentials. Overall, affine convolution formulation (1) allows the design of adaptive deterministic algorithms with practical computational time and memory requirements and has the potential to make the deterministic Boltzmann equation solution accessible in multidimensional applications.

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REFERENCES

Numerical Simulation of Flow around Rectangular Cylinders Using Boltzmann Equation

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Flow around square and rectangular cylinders frequently occur in engineering applications. For example, buildings, monuments, and towers are permanently exposed to wind. Similarly, piers, bridge pillars, and legs of offshore platforms are continuously submitted to the load produced by maritime or fluvial streams [1]. It is known that the flow around a rectangular cylinder can exhibit an unsteady behaviour: the shear layer separated from windward corner, reattachment characteristics of the flow and vortices shedding into the wake are dependent on the cylinder’s aspect ratio (width to height, \(A/H\)). Therefore, accurate prediction of aerodynamics of rectangular cylinders, due to their common use in bridge and building industry, have received particular interest from both practical and academic standpoints.

Nowadays, the flow around square cylinders has been widely investigated both experimentally [2-4] and numerically [1, 4-6]. Experimental works have been conducted in wind tunnels or water channels to determine aerodynamics loads on cylinders of different cross sections and vortex shedding frequency in its wakes [2-4]. Despite the geometrical simplicity of the problem, the numerical simulation of such a flow is not a trivial task, due to several factors: presence of adverse pressure gradients, separation and reattachment zones, recirculating regions, highly curved streamlines, and eddy interactions. It should be noticed that the most part of papers deals with Navier-Stokes equations, or with large-eddy simulation (LES), using the classical sub-grid Smagorinsky model.

In the present work unsteady incompressible flow around rectangular cylinder with aspect ratio varying from 1 to 8 has been numerically analyzed by the Boltzmann kinetic equation. The direct numerical method for solving the Boltzmann equation, (see [7]) is applied and optimized using MPI (Message Passing Interface) for computations on MVS-100K. The flow patterns and the wake periodic features are numerically examined at \(Re \geq 300\). Important physical mechanisms determining vortex shedding frequency are studied. It was found that flow configurations over rectangular cylinders are strongly dependent on the aspect ratio. Global quantities such as the Strouhal number, the recirculation length and the surface pressure coefficient are computed and compared with the available wind tunnel test results proposed in the literature. Streamlines and vorticity magnitude isosurface are also presented. The obtained results showed good agreement with available numerical and experimental data from other works.

ACKNOWLEDGEMENTS

This work was supported by the Russian Science Foundation, Project 14-11-00870.

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## Session 28: Slip Flow Regime

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Slip/Jump Coefficients and Knudsen-Layer Corrections for the ES Model in the Generalized Slip-Flow Theory

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Recent development of micro device technologies enhances the research activity on gas flows in the slip-flow regime, namely gas flows for small Knudsen numbers, both numerically and experimentally. A systematic asymptotic theory which describes the behavior of the gas for small Knudsen numbers has been established with a firm foundation in the 1960s and 1970s on the basis of the BGK model [1, 2] and later on the basis of the original Boltzmann equation [3]. In the linear case of this theory (we call it the generalized slip-flow theory here), the fluid-dynamic-type equations and their appropriate slip/jump boundary conditions which describe the overall behavior of the gas and formulas of the Knudsen-layer correction to the overall solution are given up to the second order in the Knudsen number expansion. In this case, the resulting system is diffusion-dominant [4, 5], because the linearized setting implies the flows with small Reynolds number.

In order to apply the resulting system to specific problems, the values of the slip/jump coefficients appearing in the boundary condition and the data of the Knudsen-layer correction are required. They are obtained by solving the elemental one-dimensional half-space problems of the linearized Boltzmann equation. Currently, a complete set of them is available only for the BGK model [1, 2, 4] and very recently for a hard-sphere gas [6, 7].

In the meantime, as is well-known, the celebrated BGK model cannot reproduce the correct value of the Prandtl number of a gas, though it is widely accepted and has been used for the analyses of rarefied gas flows. The ES model [8] has often been used recently as the displacement of the BGK model, because it satisfies the requirements of the correct Prandtl number and the H theorem.

In the present work, we have obtained a complete set of numerical values of the slip/jump coefficients and the data of the Knudsen-layer corrections up to the second order for the ES model for a monatomic gas under the diffuse reflection boundary condition, assuming the Prandtl number of the gas is 2/3. In the numerical computation, we have used a reliable numerical method based on the integral form of the Boltzmann equation which was developed recently in Refs. [6, 7] for the computation for a hard-sphere gas. The values of slip/jump coefficients are also obtained from the information about the first-order Knudsen layer by applying the theory of symmetry relation [9, 5]. The values obtained from two different approaches agree within the accuracy of computation, which strongly supports the validity of the set of the obtained data.

REFERENCES

Unstable Rarefied Gas Flow Conditions in a Channel

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Nonlinear dynamic system corresponding to rarefied gas flow in a channel is investigated based on iterative equations like

\[ x_{m+1} = \tan \left[ \psi \left( l_m, \arctan \frac{2x_m - \tau(1 + x_m^2)}{p(1 + x_m^2) - 2} \right) \right] \tag{1} \]

Here the function \( \psi \) and the variable \( l_m \) are determined by the geometrical shape of the channel, \( x_m \) and \( x_{m+1} \) are successive values describing the trajectory of a gas particle in the channel, and \( p \) and \( \tau \) are the momentum exchange coefficients. Under certain conditions iterative equations of the type (1) may have unstable solutions in some regions of the values of gas-surface interaction parameters [1]. Numerical calculations have demonstrated that a negligible change of one of the parameters of scattering function (less than 1%) near the bifurcation points causes the substantial difference in gas flow in a channel. As non-random solutions as well random solutions can be observed on bifurcation diagrams. Some of obtained solutions have a physical meaning of locking the channel, i.e. its conductivity reduces significantly. The scattering function is supposed to be close to ray-diffuse model, where the ray model, as well as the specular model, determines only one velocity of reflected gas atoms by given incident velocity. The ray-diffuse model has better experimental confirmation in comparison with the specular-diffuse model widely applied in practical DSMC calculations. However, the problem of the empirical confirmation of the obtained numerically effect is still difficult, because the scattering conditions of this type are hardly reproducible experimentally. To verify the bifurcations of simulated type experimentally all considered physical values in the flows are to be set exactly to the same values as detected in our calculations. Adding the extra parameter of scattering function allows us extending the region where considered dynamic system (related to rarefied gas flow) is unstable in the parametric space. Simulated unstable states of the system are close to physical situations observed in experiments. Obtained connection between the parameters of nonlinear dynamic system and momentum exchange coefficients (or accommodation coefficients) makes it possible to express analytic evaluations in terms of aerodynamic characteristics including Knudsen and Mach numbers, temperature factor etc.

REFERENCES

Microproduction Inaccuracy Analysis using Knudsen Number Depending Correction Functions

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The pressure drop of a transonic Laval nozzle depends on the rarefaction degree of the gas flow. Therefore relative deviations of the numerical data can be used for describing the influence of the rarefaction of the gas flow. This deviation can be predicted by using a second-order modelling approximation for the Knudsen number depending correction function in the slip-flow regime (e.g. Dongari et al. [1]). With the usage of experimental data the correction function can be calibrated eliminating the error resulting from the accuracy. The investigated case is a micronozzle flow with Knudsen numbers in the slip-flow regime near the nozzle throat in vacuum environment. Compared gases are neon, argon, krypton and xenon. Figure 1 (left) shows both the experimental and the numerical results for the absolute pressure in the ionization chamber $p_{ch}$ of the arc-jet thruster inside a small-scale vacuum chamber for all studied gases and mass flow rates (e.g. Alexeenko et al. [2]). The numerical, dimensionless pressure drop $S$ is corrected by using the coefficients $C_1$ and $C_2$:

$$S_{corr} = S_{sim} \left[ 1 + \frac{Kn_{sim}}{C_1} \left( 1 + C_2 Kn_{sim} \right) \right]; \quad S = \frac{\Delta p D^4}{\rho \mu L} = \frac{\Delta p D^4}{m \mu L} \frac{p}{\rho M} T.$$  \hspace{1cm} (1)

The corrected absolute pressure in the ionization chamber of the nozzle can be calculated based on $S_{corr}$. The pressure drop corresponding to its dimensionless form $S$ is replaced by the difference between the pressure in the ionization and the vacuum chamber $\Delta p = p_{ch} - p_{vac}$. A further transformation of the equation gives a second degree polynomial with $p_{ch}^{corr}$ as a function of $S_{corr}$. The results for the experimental and the corrected absolute pressure are shown in Fig. 1 (right) for all studied noble gases as a function of the mass flow rate. The results from the proposed approach show very good agreement with the experimental results for studied gases at all mass flow rates.

FIGURE 1. left: Experimental and numerical pressure in the ionization chamber vs. mass flow rate, right: Experimental and corrected pressure in the ionization chamber for the studied gases.

REFERENCES

Solid-state Heat Transfer in the Slip and Early Transition regime. An Asymptotic Theory

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We use a Hilbert procedure [1] to obtain asymptotic solutions to the Boltzmann equation modeling phonon transport in crystalline materials under the relaxation-time approximation. This procedure yields the continuum equations and boundary conditions governing phonon-mediated heat transfer in the limit of a small but finite mean-free path.

Specifically, we show [2] that the traditional heat conduction equation featuring Fourier’s law as a constitutive relation is valid in the bulk at least up to second order in the Knudsen number for time-independent problems and first order for time-dependent problems. As expected, Fourier’s law does not hold within distances on the order of a few mean-free paths from the boundary; this breakdown is a result of kinetic effects that are always present close to the boundary and require solution of a Boltzmann boundary layer problem to be determined. However, because boundary effects appear at the order of Knudsen number or higher, they are negligible in the macroscopic limit of vanishing Knudsen number where the traditional no-jump and no-flux boundary conditions are recovered for prescribed temperature and diffusely reflecting boundaries, respectively.

At first order in Knudsen number or higher, the asymptotic solution requires that the inner, boundary layer solution be matched to the outer, bulk solution; this process yields boundary conditions for the Fourier description as well as additive corrections in the form of universal kinetic boundary layers. The boundary conditions for both prescribed temperature and diffusely reflecting boundaries are shown to be of the jump type, in direct analogy to slip boundary conditions obtained in the rarefied gas case. The associated jump coefficients as well as corrective boundary layers are parametrized by the material model and the phonon-boundary interaction model (Boltzmann boundary condition).

We also show that the asymptotic solution procedure can be used to solve the Kapitza resistance problem associated with an interface between two materials (within the Boltzmann equation approximation). The well-known temperature jump at the interface [3] is shown to be a result of the incompatibility between the distribution functions in the two materials, requiring a two-sided boundary layer matching procedure.

All results are validated via comparisons with low-variance deviational Monte Carlo simulations [4-6] for a variety of material models.

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The authors would like to thank T. R. Akylas for many helpful comments and discussions. N.G.H. would also like to thank K. Aoki and S. Takata for many useful comments and discussions. This work was supported, in part, by the Singapore-MIT Alliance and in part by the Solid-State Solar-Thermal Energy Conversion Center (S3TEC), an Energy Frontier Research Center funded by the US Department of Energy, Office of Science, Basic Energy Sciences, under Awards No. DE-SC0001299 and No. DE-FG02-09ER46577.

REFERENCES

Molecular kinetic approach to acoustic waves in compressible boundary layer flow

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We have been studying various problems that are difficult to solve with ordinary formulae of hydrodynamics using the kinetic theory of gas. We use the Boltzmann equation with the collision term in the BGK model and diffuse reflection is used as the boundary condition on the wall surface.

Here we are concerned with the problem of shock-boundary layer interaction ([1] for example) and consider the problem in the title as a start.

First we produce a steady compressible boundary layer flow by uniform flow on a half-flat plate. We will then investigate the propagation of the acoustic wave generated near the wall surface.

Calculation conditions are: Knudsen number Kn=0.0001, time step Δt=0.00001, physical space 0<x<4, 0<z<1, and the molecular each velocity component will be calculated within the range of -6 to 6, where velocity is made non-dimensional at the maximum probability velocity and distance at the representative length in mean free path/Kn.

The number of grid points is set to 400×100×18×18 and the initial temperature set to 300(K). Density and velocity U are initially assumed to be uniform. We could obtain the resulting steady boundary layer flow after about 300 thousand steps, which can be compared with Blasius solution for incompressible flow [2].

An example of the results is shown in Fig. 1. The figure at the top depicts the distribution of the velocity vector to the initial uniform flow velocity U=0.1. Point sound sources is inserted at location (2, 0.1) at t=0 into a steady solution that was obtained. The figure at the bottom depicts the distribution of x direction components of velocity by color.

In comparing the figure top and bottom, the boundary layer can be observed to meander considerably due to the influence of the sound source accompanying its expansion at the same time in the upstream of the point sound source and it becomes narrower again downstream of the point sound source.

REFERENCES


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On Boundary Conditions for Regularized Burnett Equations

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In dimensionless units the stationary and linearized Burnett equations take the form

\[ \nabla \cdot u = 0, \quad \nabla \rho + \nabla \mathcal{T} = \epsilon \mu \Delta u + \epsilon^2 G \mathcal{V} \Delta \rho, \quad \Delta T = 0. \]

\( \mu \) is the dimensionless viscosity, \( G \) a positive Burnett parameter of the order of 1 and \( \epsilon \) is essentially the Knudsen number. The Hybrid Burnett equations [1] as well as the Generalized Burnett equations [2] due to Bobylev take the same form.

We choose a half-space problem. The unit of length is chosen as a characteristic length of the boundary values. We assume that the fields are proportional to \( \exp(ikx) \) so that the relevant \( k \)-values are of the order of 1 and take the region to be \( y > 0 \).

Taking the divergence of the second equation above we find

\[ \Delta \rho = \epsilon^2 G \Delta^2 \rho. \]

The solutions tending to zero at \( y = \infty \) are \( \rho = \exp(-ky) \) and \( \rho = \exp(-\sqrt{(2\epsilon^2G)^{-1} + k^2y}) \). The second solution has a length scale of order mean free path and has to be discarded as it is outside of the range of validity of the Burnett equations. This solution is given in Struchtrup [3]. We show that also for the general 3-dimensional case such an unphysical solution is eliminated by imposing the boundary condition \( \Delta \rho = 0 \). Further, we show that \( \Delta \rho \) vanishes in the whole region so that the Burnett term in the momentum equation vanishes and the equations reduce to the well-known fluid dynamics equation. This is consistent with the results given in Takata et al [4].

The solutions can now be written

\[ u_x = [A-(A+iB)ky] \exp(ikx-ky), \quad u_y = [B-i(A+iB)ky] \exp(ikx-ky), \quad T = C \exp(ikx-ky). \]

We apply the second order boundary conditions derived by Sone, Takata and others, see [4]. We now use as unit of length the length scale of the boundary values. This gives a linear system for \( A, B, C \). Its determinant \( D(z) \) is a polynomial of 6th degree in \( z = \epsilon k \). Using the values of the coefficients for hard spheres given in [4] we find the coefficient of \( z^6 \) to be -0.08886 whereas the coefficient of \( z^6 \) is 1. It is clear that the determinant changes sign and thus has a zero. This means that this problem is not well-posed. A small variation of the Fourier amplitude of boundary values around the zero will give rise to a large change of the solution.

It is, however, possible to regularize the boundary conditions by the change of variables

\[ u_y = \tilde{u}_y + \epsilon^2 \beta \partial_y \tilde{u}_y, \quad T = \tilde{T} + \epsilon^2 \partial_y \tilde{T}; \quad u_x = u_y - \epsilon^2 \beta \partial_y u_y, \quad \tilde{T} = T - \epsilon^2 \partial_y T. \]

We then obtain a boundary problem of the same kind but with a different determinant \( \tilde{D}(z) \). Choosing \( \beta, \delta \) suitably \( \tilde{D}(z) \) is shown to have no zeros so that the linearized boundary value problem for a half-space is well-posed.

REFERENCES

A three-dimensional finite volume method for conservation laws in conjunction with modified solution for nonlinear coupled constitutive relations

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It is believed that non-equilibrium effects play a vital role in high-speed and rarefied gas flows and the accurate simulation of these flow regimes are far beyond the capability of Navier-Stokes-Fourier equations which are based on small deviation from local thermodynamic equilibrium. To solve this problem, Eu provided another way which was different from Grad’s 13 moment method and Burnett equation and proposed generalized hydrodynamic equations which are consistent with the laws of irreversible thermodynamics[1]. Based on Eu’s generalized hydrodynamics equations, a computation model, namely the nonlinear coupled constitutive relations (NCCR), was developed by R.S.Myong and applied successfully to one-dimensional shock wave structure and two-dimensional rarefied flows[2-4].

While the NCCR model has been developed and shown its advantages, more numerical methods should be investigated and employed to make it more practical. In this paper, finite volume schemes including LU-SGS time advance scheme, MUSCL interpolation and AUSMPW+ scheme, are firstly adopted to investigate NCCR model’s validity and potential in three-dimensional complex hypersonic rarefied gas flows. Moreover, in order to solve the computational stability problems in 3D complex flows, a modified solution is developed for the NCCR model.

Finally, the modified solution is tested for a slip complex flow over a 3D hollow cylinder-flare configuration. The heat flux coefficient distribution on the surface of a hollow cylinder-flare configuration is presented in Fig.1 and more results will be analyzed in the full paper. The numerical results show that the NCCR model by the modified solution yields good solutions in better agreement with the DSMC results and experimental data than NSF equations, and imply NCCR model’s great potential capability in further application.

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REFERENCES

Calculus and design of Discrete Velocity Models using computer algebra

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In [1,2], a framework for a calculus with Discrete Velocity Models (DVM) has been derived. The rotational symmetry of the discrete velocities can be modelled algebraically by the action of the cyclic group $C_4$. Taking this point of view, the linearized collision operator can be represented in a compact form as a matrix of elements in the group algebra. Or in other words, by choosing a special numbering it exhibits a certain block structure which lets it appear as a matrix with entries in a certain polynomial ring. A convenient way for approaching such a structure is the use of a computer algebra system able to treat these algebraic structures.

This kind of representation provides a deeper understanding of the collision operator and allows the structured design of collision models. Such a design has to meet two types of requirements: the desired asymptotic behaviour in the hydrodynamic limit (expressed in terms of the flow parameters), and sufficient degrees of freedom for the modeling of rarefied features like boundary and interface layers, creep flows etc.

In the talk we demonstrate the use of the computer algebra system FriCAS/AXIOM [3,4] for the generation of the velocity and the collision sets and for the analysis of the structure of the collision operator. Concerning the fluid dynamic limit, the system provides the characterization of sets of collisions and their contribution to the flow parameters. It allows the design of rotationally invariant symmetric models for prescribed Prandtl numbers.

The talk illustrates the use of FriCAS/AXIOM with a number of examples of growing complexity.

REFERENCES


Solving the Enskog Equation by the Fast Spectral Method

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(Use the Microsoft Word template style: Paper Author)

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Abstract. The Boltzmann equation is the fundamental equation describing the collective motion of gas molecules from the continuum-fluid to the free-molecular flow regimes, when the molecular mean free path is much larger than the effective molecular diameter. However, when the gas is compressed to high densities that the mean free path is comparable to the molecular diameter, the Boltzmann equation must be modified. Here, the Enskog equation is introduced and solved by the fast spectral method. Several typical dense gas flows (such as Fourier flow, Couette flow, and Poiseuille flow) are simulated. These flows are ‘rarefied’, albeit dense, since the molecular mean free path could be comparable to the channel width. Some novel flow dynamics as a consequence of the competition between the mean free path, channel width, and molecular diameter are found and analysed.
A Discontinuous Finite Element Method For Neutron Transport Equations on 3-D Unstructured Grids

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Time-dependent neutron transport equation is a kind of important hyperbolic partial differential equation in nuclear science and engineering applications. High dimension neutron transport calculation include computing of space grid, angle direction, energy group and time step, is very complex and huge scale scientific calculation problem. Discontinuous finite element discrete ordinates (DFE-Sn) method is very efficient for solution of such equations especially while concerned with complicated physics including multimedia, larger grid distortion, complex initial and boundary conditions.

In this paper, the discrete scheme of Sn discrete ordinate and discontinuous finite method 3-D unstructured tetrahedral meshes are presented. We developed a serial solver with DFE-Sn method to solve time-dependent neutron transport equations on unstructured tetrahedral grids. Domain decomposition scheme, parallel Sn sweep algorithm and multi level Parallel Algorithm on unstructured grids are adopted to improve the efficiency, the parallel computation for the scheme is realized on MPI systems. Numerical experiments demonstrate the accuracy and efficiency of these methods.

Key words: discontinuous finite element method, transport equations, unstructured meshes, domain decomposition, sweep algorithm

REFERENCES

Session 30: 14th Harold Grad Lecture

R. Caflisch, "Accelerated Simulation Methods for Rarefied Gases and Plasmas"
Collisional kinetics is a multiscale phenomenon due to the disparity between the continuum (fluid) and the collisional (particle) length scales. This talk will describe a class of simulation methods for gases and plasmas, and acceleration techniques for improving their speed and accuracy. Starting from the Boltzmann equation for rarefied gases or the Landau-Fokker-Planck equation for plasmas, the focus will be on a binary collision model [1] that is solved using a Direct Simulation Monte Carlo (DSMC) method. Acceleration of this method is achieved by coupling the particle method to a continuum fluid description. The velocity distribution function $f(v,x,t)$ is represented as a combination of a Maxwellian $M(v, \rho, u, T)$ (the thermal component) and a set of discrete particles $k(v,x,t) = \sum \delta(v-v_i) \delta(x-x_i)$ (the kinetic component), in which $(\rho, u, T) = (\rho(x,t), u(x,t), T(x,t))$, $(v_i, x_i) = (v_i(t), x_i(t))$ and $i$ varies from 1 to $N$. For systems that are close to (local) equilibrium, this reduces the number $N$ of simulated particles that are required to represent $f$ for a given level of accuracy. Collisions between particles in $M$ can be ignored, since $M$ is an equilibrium, and collisions between particles in $k$ are handled as in DSMC. Collisions between $M$ and $k$ are simulated by sampling a particle from $M$, selecting a particle from $k$, and simulating their collision as in DSMC. Equilibration of particles in $k$, as well as disequilibrium of particles from $M$, due to the collision process, is represented by a thermalization/dethermalization step that employs an entropy criterion [2]. In particular, the entropy of a particle in $k$ is computed by attaching additional variables to the particle, which is similar to the method of [3] and related works. Spatial transport is simulated by decomposing the transport terms into a Maxwellian component which contributes to the evolution of $(\rho, u, T)$, and a remainder which contributes to the evolution of $k$. Efficiency of the representation is greatly increased by inclusion of particles with negative weights. As discussed in [4], this significantly complicates the simulation, but we recently developed a more tractable approach [5, 6]. The accelerated simulation method will be compared with standard DSMC for both spatially homogeneous problems such as a bump-on-tail (figure 1) and inhomogeneous problems such as nonlinear Landau damping (figure 2).

**ACKNOWLEDGEMENTS**

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**Session 31: Numerical Methods III**

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A Hybrid Solver for Rarefied-Continuum Flows Using Discrete Velocities and Lattice Boltzmann Methods

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Over the last decades, several hybrid solvers have been developed for mixed rarefied-continuum flows. These solvers utilize kinetic models in the rarefied regions and fluid models in the continuum regions, see [1]. The kinetic models are either based on the direct numerical solution of the Boltzmann (or model) kinetic equations or use particle-based (DSMC) methods. For the continuum zones, a variety of schemes for solving fluid (moment’s) equations have been used. Here, we propose a new hybrid scheme based on discrete velocities for both kinetic and fluid zones. A variant of such a hybrid scheme has already been considered in [2] where the same set of discrete velocities have been used in both rarefied and continuum regions, with a Maxwellization procedure applied in the continuum region to approximate the Euler equations. To further advance this approach, it is naturally to assume that a small number of the discrete velocities can be used in the fluid region. For example, the Lattice Boltzmann Method (LBM) operates with a minimal set of discrete velocities to simulate flows close to equilibrium (for example D3Q19), see e.g. [3-4]. In [5], the principal possibility of coupling LBM with Boltzmann solvers in a unified framework was mentioned. Generally, in the continuum region, the number of the moments can be equal the number of the discrete velocities. For practical implementation, we have to either continuously adapt the velocity lattice (grid) or match the two solutions at an interface between the two regions. For the discrete velocity method, this problem is partially resolved by using adaptive meshes in velocity space, as discussed in [5-9].

Thus, our new hybrid solver select velocity lattice (grid) based on local (in space) flow properties. The local gradient of the macroscopic flow parameters determine criteria for selecting discrete velocity set. We consider a possibility of either a continuous adaptation of the velocity grid or a sharp transition between the lattice and discrete velocity grid at interfaces between kinetic and fluid domains. Different models for the collision term, which already exist in our Unified Flow Solver (UFS), are used for constructing a hybrid scheme based on this algorithm.

For testing, validation and demonstration of the new concept, we first consider the classical problem of heat transfer between solid surfaces with different temperatures. More complicated problems involve low speed flows in microsystems and porous media with large variations of gas density.

ACKNOWLEDGEMENTS

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REFERENCES

A BGK-type Model with Enforced Relaxation of Moments for Non-Continuum Flows

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Accurate modeling of time dependent non-continuum flows requires highly efficient kinetic solvers. Model kinetic equations, e.g., the Bhatnagar-Gross-Crook (BGK), ellipsoidal-statistical BGK, and Shakhov models, can be used in time-dependent multidimensional simulations, however, these models lack physical accuracy in regions of strong deviation from equilibrium. At the same time, the use of more physically realistic models, such as those given by the Boltzmann collision integral, is often prohibitively expensive. In [1], the BGK model was extended by introducing a velocity-dependent collision frequency that is a linear combination of given functions $\psi_i(\vec{u})$, $i = 0, \ldots, k$,

$$\nu(\vec{u}) = \sum_{i=0}^{k} c_i(t)\psi_i(\vec{u}).$$

The coefficients $c_i(t)$, $i = 1, \ldots, k$ are determined from the condition that moments $f^M_{\nu}(t)$ of the solution relax with the prescribed relaxation frequencies $\nu^\nu$. At each time step, $c_i(t)$ are determined by solving

$$(\nu_{\nu}(t) - \nu_{\text{BGK}})(f^M - f_{\nu}) = \sum_{i=0}^{k} c_i(t) \int_{R^3} \psi_i(\vec{u})(f^M(t, \vec{u}) - f(t, \vec{u}))\varphi(\vec{u}) d\vec{u}.$$

The relaxation frequencies $\nu_{\nu}$ are determined by evaluating the full Boltzmann collision operator (e.g., using method of [2]) and applying the formula

$$\nu_{\nu}(t) = \frac{\hat{I}_{\nu}}{f^M - f_{\nu}(t)},$$

where $\hat{I}_{\nu}$ are the corresponding moments of the Boltzmann collision operator. The approach was implemented as a part of a collection of subroutines, DGVlib, for the development of discontinuous Galerkin discretizations in the velocity variable and for the evaluation of the collision operator using different collision models. The approach was applied to the solution of 1D and 2D supersonic flows. Numerical modeling, illustrated in Fig. 1, shows that the enforcement of the relaxation rate for directional temperatures allows for significant accuracy improvement as compared to solutions of classical model equations. Computational overhead due to the enforcement of moments is moderate to high depending on the number of enforced moments.

ACKNOWLEDGEMENTS

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REFERENCES

Recovering the full Navier Stokes equations with lattice Boltzmann schemes

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We wish to use the lattice Boltzmann schemes with mutiresolution relaxation times \cite{4} to the approximation of the full compressible Navier Stokes equations. Preliminary results have been obtained in \cite{6, 7} when using a single particle distribution. A popular idea proposed in \cite{1, 8} is the use of several particle distributions. One particle distribution is devoted to the conservation of mass and momentum and an other one to the conservation of energy. With this framework, remarkable numerical results have been obtained in the context of the Boussinesq approximation \cite{9}.

When we adapt the Taylor expansion method \cite{2} to this situation with two particle distributions, we have observed that the nonlinear dissipation term of energy due to the fluid viscosity cannot be captured asymptotically. This defect has its origin in precise algebraic properties of standard lattice Boltzmann schemes and associated momenta. This difficulty has also been considered in the context of Bhatnagar Gross Krook approximation \cite{3, 5}. In consequence, the initial framework of mutiresolution relaxation times must be adapted. In particular, source terms must be added to a pure "collide-stream" algorithm in order to capture this nonlinear dissipation term.

We will present at the conference our analysis and various tentatives to overcome this difficulty. First for a linearized one-dimensional context. Then for nonlinear situations at one and two space dimensions.

References

Direct Modeling for Computational Fluid Dynamics

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Fluid dynamic equations are valid in their respective modeling scales, such as the particle mean free path scale of the Boltzmann equation and the hydrodynamic scale of the Navier-Stokes (NS) equations. With a variation of the modeling scales, theoretically there should have a continuous spectrum of fluid dynamic equations. Even though the Boltzmann equation is claimed to be valid in all scales, many Boltzmann solvers, including direct simulation Monte Carlo method, require the cell resolution to the order of particle mean free path scale. Therefore, they are still single scale methods. In order to study multiscale flow evolution efficiently, the dynamics in the computational fluid has to be changed with the scales. A direct modeling of flow physics with a changeable scale may become an appropriate approach [1]. The unified gas-kinetic scheme (UGKS) is a direct modeling method in the mesh size scale, and its underlying flow physics depends on the resolution of the cell size relative to the particle mean free path. The cell size used in UGKS is not limited by the particle mean free path. With the variation of the ratio between the numerical cell size and local particle mean free path, the UGKS recovers the flow dynamics from the particle transport and collision in the kinetic scale to the wave propagation in the hydrodynamic scale. The central ingredient of the UGKS is the coupled treatment of particle transport and collision in the flux evaluation across a cell interface, where a continuous variation of flow physics is modeled. The UGKS has the asymptotic preserving (AP) property of recovering the NS solutions in the continuum flow regime, and the full Boltzmann solution in the rarefied regime. In the mostly unexplored transition regime, the UGKS itself provides a valuable tool for the non-equilibrium flow study.

The traditional theoretical fluid dynamic research is mostly based on the partial differential equations, such as the Navier-Stokes and the Boltzmann equation. All these equations are the modeling of flow physics in different scales. One difficulty to get the fluid dynamic equations in the transition regime is due to the lack of a valid modeling scale to identify the physics in such a regime. Theoretically, there should have a continuous change of scale in the modeling from the scale of macroscopic flow variation to the particle mean free path. Second difficulty in modeling the transition regime is due to the variation of variables. Physically, the modeling must be able to cope with a few degrees of freedom (macroscopic variables) in the NS equations to the infinite number of particle movement in the kinetic description. Any fixed number of degree of freedom cannot work properly. The third difficulty is about the unification of the underlying physical picture in the modeling. For the NS equations, the isolated fluid element is used for the modeling with the implementation of equation of state and the constitutive relationships. For the kinetic modeling, the particle can freely transport and collide with others, and there is no closed fluid element concept at all. The UGKS overcomes all these difficulties through the adaptation of the cell size and time step as the modeling scales, and the use of both macroscopic flow variables and gas distribution function as the flow variables. Therefore, the UGKS not only provides a numerical scheme for the flow study in all flow regimes, but also constructs valid governing equations for the recovery of a continuous spectrum of flow physics.

At the current stage, the UGKS can present accurate solutions in all flow regimes for monatomic and diatomic gases. At the same time, the multiple scale modeling mechanism can be extended to develop numerical schemes for other transport processes, such as the radiative transfer and the plasma simulation. In this paper, we are going to discuss the modeling issue in UGKS, its applications, and possible direction for its future development.

ACKNOWLEDGEMENTS

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Session 32: Plasma Flows and Processing

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Effective Potential Kinetic Theory for Strongly Coupled Plasmas

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Strongly coupled plasmas are highly charged, dense, or cold ionized matter in which the Coulomb potential energy at the average interparticle spacing exceeds the average kinetic energy of particles. Standard Boltzmann-based theories break down in this situation because many-body correlations strongly influence particle dynamics. The effective potential theory provides a method for extending plasma theory into the strongly coupled regime by relaxing the assumptions underlying the Boltzmann equation: binary scattering and molecular chaos. The binary collision approximation is relaxed by treating particle interactions via the potential of mean force, rather than the bare Coulomb potential [1]. The potential of mean force is obtained by taking two scattering particles at fixed positions and averaging over the positions of all other particles. It is related to the radial density distribution function. The theory relaxes the molecular chaos assumption by treating the excluded volume (or Coulomb hole) in repulsive interactions using a modified version of Enskog’s kinetic equation for hard spheres [2]. Calculated transport coefficients are compared with molecular dynamics simulations and measurements from ultracold plasma experiments. These reveal that the theory is accurate well into the strongly coupled regime, breaking down when the system exhibits liquid-like behaviors (see figure 1). A number of properties are considered, including diffusion, viscosity and thermal conductivity.

Recently, the effective potential theory was also applied to determine ionic transport properties in dense plasmas, including the warm dense matter regime characterized by densities near those of solids and temperatures from several to hundreds of electron volts [3]. This was achieved by applying a recent quantum hypernetted chain approximation [4] to determine the effective potential, including novel dense plasma effects such as electron degeneracy and pressure ionization.

ACKNOWLEDGEMENTS

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REFERENCES

A Unified Gas Kinetic Scheme for Plasma Simulation

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In this work, we extend the unified gas kinetic scheme (UGKS) [1] to the multi-component plasma simulation. Our scheme is a finite volume scheme constructed based on the Vlasov-Boltzmann-Maxwell equations. For the fluid part, the numerical flux is calculated from the integral solution of Vlasov-Boltzmann equations at cell interface, which includes particle transport, collision, and electromagnetic acceleration. The numerical flux is critical in the determination of the multiscale property of the scheme, which provides the flow dynamics from the particle free transport to the equilibrium state formation. For the electromagnetic fields, the perfectly hyperbolic forms of the Maxwell equations [2] are solved for divergence free preservation of the magnetic field. At the same time, the fluid parts are implicitly coupled with the electromagnetic source terms. The UGKS is a physically reliable multiscale method which is able to simulate plasma from the kinetic Vlasov regime to the continuum hydrodynamic regime. When the spatial scale is comparable to the skin depth, our scheme can capture the two-fluid effects [3]. As the skin depth approaches zero, our scheme can automatically present the magneto-hydrodynamics (MHD) solutions. For the first time, the plasma physics in the whole flow regimes can be calculated by the same UGKS.

In the kinetic scale, our scheme can capture the nonlinear Landau damping, as shown in Fig. 1. In the continuum regime, we apply the same plasma UGKS to one dimensional Brio-Wu shock tube problem. Fig. 2 shows that the MHD solution from the UGKS when the normalized Larmor radius is small.

In conclusion, the UGKS has been successfully extended to the plasma simulation in all regimes.

REFERENCES

Fig. 1: Time evolution of electric field in $L_2$ norm in nonlinear Landau damping.

Fig. 2: Density profile of Brio-Wu shock tube with $r_L = 3 \times 10^{-3}$. 
Deterministic Conservative Solver for the Inhomogeneous Fokker-Planck-Landau Equation Coupled with Poisson Equation

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In this article, we propose a deterministic conservative solver for the inhomogeneous Fokker-Planck-Landau equation coupled with Poisson equation. The evolution of the probability distribution function \( f(x, v, t) \) obeys the following nonlinear partial integrodifferential equation, which writes, for \( v \in \mathbb{R}^3, x \in \Omega_x \subseteq \mathbb{R}^3 \),

\[
\begin{align*}
\partial_t f + v \cdot \nabla_x f - \mathbf{E}(t, x) \cdot \nabla_v f &= Q_{FPL}(f, f), \\
\mathbf{E}(t, x) &= -\nabla_x \Phi(t, x), \\
-\Delta_x \Phi(t, x) &= 1 - \int_{\mathbb{R}^3} g(t, x, v) dv, \\
\Phi(t, x) &= \Phi_B(t, x) \quad x \in \partial \Omega_x .
\end{align*}
\]

where the collision kernel \( Q_{FPL} \) writes

\[
Q_{FPL}(f, f) = \nabla_v \cdot \int_{\mathbb{R}^3} S(v - v_\ast)(f(v_\ast)\nabla_v f(v) - f(v)\nabla_v f(v_\ast)) dv_\ast ,
\]

\[
S(u) = |u|^{-1}(\mathbf{I}_d - \frac{u \otimes u}{|u|^2}) ,
\]

with \( \mathbf{I}_d \) being the \( d \times d \) identity matrix;

This is a rather realistic and primary model for collisional plasma. Through time-splitting scheme, a Vlasov-Poisson problem and a homogeneous Landau problem are obtained. These two subproblems can be treated separately. In our solver, Runge-Kutta Discontinuous Galerkin (RK-DG) method and conservative spectral method are adopted to the two subproblems, respectively. Since two completely different numerical schemes are applied separately, our challenge is to link two different meshes, in a conservative way. Therefore, we have designed a new conservation correction process such that, after projecting the conservative spectral solution onto the DG mesh, the conserved moments are transferred to the DG solution as well. To verify our solver, numerical experiments on linear Landau damping are provided.
**Session 33: Non-Equilibrium Flows I**

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<td>&quot;Problems for Kinetic Equation with Nonequilibrium Boundary Conditions and Possible Tests&quot;</td>
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Continuum modelling of shock waves through granular gases and the role of statistical fluctuations

N. Sirmas and M. I. Radulescu

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Shock waves driven through granular media have been shown to become unstable. For example, experiments have identified unstable formations of finger-like jets in granular media dispersed by shock waves driven through air. Similar formations are observed for granular media that is subjected to a vertically oscillating bed. The complex dynamics involved in these past configurations have prevented the authors to clearly identify the mechanisms controlling the instability. This problem was previously addressed by developing a Molecular Dynamics (MD) model to look at the classical problem of a piston propagated shock wave into a system of 2D particles [1]. Particles were assumed to be smooth disks that collide inelastically if the impact velocity of binary collisions exceeded some threshold, which is a simple treatment for viscoelastic collisions. By allowing for finite dissipation within the shock wave, instabilities were found in the form of distinctive high density non-uniformities and convective rolls within the shock structure. The present study looks to recover such a shock structure and evolution at the continuum level. This is done by modelling the problem via the Euler and Navier-Stokes (N-S) equations for a granular gas, and introducing perturbations in the flow field to account for statistical fluctuations. The model involves a piston propagating into a system of disks, with an initial packing fraction $\eta$, at velocity $u_p$. Smooth discs collide inelastically with a constant coefficient of restitution $\varepsilon$ if the impact velocity of two colliding disks exceeds some threshold $u^*$. We solve the N-S and Euler equations for a 2D granular gas [2] with the software package MG. The transport coefficients from Jenkins and Richman [3] are used and the energy sink term accounting for inelastic collisions, present in both the Euler and N-S descriptions, has been modified to include the activation threshold. A parametric study is completed to compare the evolution of the 1D structure obtained from Euler and N-S simulations with those from MD. Results are in good agreement for varying $u_p$, $u^*$, $\varepsilon$ and $\eta$. The 2D structure is obtained from Euler and N-S simulations with incoming density perturbed in accordance with the statistics seen in MD. Figure 1 shows the morphology of density obtained from N-S and MD, for the case where $u_p/u^*=2.0$, $\varepsilon=0.95$ and $\eta=0.012$. For this case, the N-S results are in good agreement with the overall structure seen in MD, recovering the same wavelength and amplitude of pattern formations at the piston face. The inviscid solution yields a chaotic structure extending from the piston, however the bulk spacing of features is similar to what we see from MD and N-S. Similar results are also observed for varying $u_p$, $u^*$ and $\eta$. In comparing with the 1D structure, the spacing of these patterns is found to be on the same order as the relaxation length scale behind the shock structure.

ACKNOWLEDGEMENTS

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REFERENCES

Sensitivity of Heat Fluxes in Hypersonic CO$_2$ Flows to the State-to-state Kinetic Schemes

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Mars exploration programs, the interest in which was almost lost after several unsuccessful missions, are currently experiencing a revival. Recently, the hypersonic boundary layer of a vehicle entering the Mars atmosphere has been investigated by means of a state-to-state vibrational kinetics model [1-3]. The peculiarity of the model applied in those studies, with respect to simplified ones used in low-temperature plasma applications [4], is that the different vibrational modes of the CO$_2$ molecule are assumed to be strongly coupled. Moreover, it is possible to include in the kinetic scheme all kinds of state-to-state vibrational transitions like vibrational-translational VT$_1$, VT$_2$ and VT$_3$ transitions in symmetric, bending and asymmetric modes, inter-mode energy exchanges within CO$_2$ molecule VV$_{1,2}$, VV$_{2,3}$, VV$_{1,2,3}$, inter-mode energy exchanges between molecules of different chemical species, as well as dissociation/recombination reactions; the total number of transitions is about tens thousands. One should confess that flow simulations based on such a detailed model, while accurate, are extremely time and resource consuming.

In recent works [4], a CO$_2$ molecule is modeled using a few symmetric stretching and bending vibrational levels but the whole asymmetric stretching ladder CO$_2$(0,0,v3); the modes are assumed independent which reduces considerably the possible number of vibrational states; the kinetic scheme includes several selected vibrational transitions and, at the same time, detailed electron-heavy particle collision kinetics. Another way to simplify the problem is to use multi-temperature models for a CO$_2$ flow description [3].

The objective of the present work is to check the limits of applicability for simplified models and assess the sensitivity of fluid dynamic variables, mass and energy fluxes to the collisional processes included into the model. First, we focus on kinetic processes not yet considered in our previous studies, such as VT$_1$, VT$_3$ and VV$_{1,2}$ transitions and review the scarce available data on their rate coefficients. Then we add successively different kinds of energy exchanges into the source terms of the 1-D Boundary Layer equation system and solve it numerically. Thanks to a state-to-state transport model [5-6] based on the modified Chapman-Enskog theory, the heat conductivity, viscosity, diffusion and thermal diffusion coefficients as well as heat and diffusion fluxes are calculated. Peculiarities of heat and mass transfer in CO$_2$ are discussed.

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REFERENCES

Influence of state-to-state vibrational distributions on transport coefficients of a single gas

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The state-to-state models of non-equilibrium flows are based on the assumption that the rates of vibrational relaxation and chemical reactions are comparable with the rate of fluid dynamic parameters variation whereas translational and rotational relaxations terminate much faster [1]. The main advantage of this approach is that it does not postulate the existence of some quasi-stationary molecular distributions over vibrational states. The state-to-state transport models developed in the literature have a serious limitation since, to derive the final expressions for collision integrals, it is assumed that the elastic collision cross sections do not depend on the vibrational state of colliding molecules. However, it is known that the size of molecules varies considerably for different excited states thus affecting the collision cross sections. Hirschfelder in 1957 [2] noted that electronically excited atoms become huge and therefore applying commonly used expressions for collision integrals are questionable. The effect of atomic diameters on transport properties of equilibrium plasmas was discussed in [3] and in [4] it was studied the heat conductivity of electronically excited atoms and molecules under non-equilibrium conditions. It was found that at high temperature the size of atoms influences significantly the collision integrals. For this reason, one can expect a similar effect in high-temperature vibrationally excited gases. The diameters of rotationally and vibrationally excited molecules were studied in [5, 6] and in these papers it was shown that for high vibrational states, the size of oscillators is significantly larger compared to that of the ground state. The objective of the present work is to evaluate the effect of the diameter of rotationally and vibrationally excited diatomic molecules on the collision integrals which are required for the calculations of state-to-state transport coefficients. We consider five diatomic species, N₂, O₂, NO, H₂ and Cl₂ and calculate the size of these molecules for different excited states [7]. It is shown that under conditions of local thermal equilibrium, the effect of vibrational excitation on the shear viscosity and thermal conductivity coefficients is found to be negligible for temperatures below 5000 K, except for the case of Cl₂ molecule, while for temperatures greater than 10 000 K the contribution of excited states becomes important.

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REFERENCES

Problems for Kinetic Equation with Nonequilibrium Boundary Conditions and Possible Tests

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New formulations of the problems with the nonequilibrium distribution functions in the boundaries are generalizations of Nonuniform Relaxation Problems (NRP), see [1-2]. Possible anomalous momentum and heat transfers are studied. We consider the nonequilibrium boundary conditions both for supersonic and subsonic regimes for 1D NRP. Calculations based on the direct solution of the Boltzmann equation show different localization of anomalous transport for supersonic and subsonic flows. In Fig. 1 profiles of the temperature and heat flux are shown for the supersonic condition on the flow inlet \((x=0)\) and two variants (supersonic and subsonic) of boundary conditions downstream.

Besides NRP with the characteristic Knudsen number \(Kn\sim1\) a problem of heat transfer and also the Couette problems with nonequilibrium boundary conditions are formulated and solved. Temperature profiles for 1D heat transfer problem are demonstrated in Fig. 2. The boundary condition on the left boundary (for outgoing molecules) is set to be a Maxwellian with non-zero velocity along the flow. The number density is determined from the condition of zero mass flux in the boundary and this leads to nonequilibrium near the boundary. In the right boundary the ordinary condition for the heat transfer problem is posed. In this case the heat flux is negative for all Knudsen numbers, and there are large regions of anomalous heat transfer. Other types of nonequilibrium boundary conditions are also considered. The presence and localization of anomalous transport zones depend on the temperatures of walls and Knudsen number.

Several experimental tests can be proposed to consider the mentioned effects, e.g. by means of the optic lattices [3] of the magnetic trap [4] or of the oscillating plate [5]. The latter problem can be considered as a quasi-stationary if a period of the oscillation are significantly greater than the characteristic process of the spatial relaxation. These simulations allow us to present a new possibilities for applications, in particular to rule the distributions downstream in the nonequilibrium convection, cooling a gas in the beam downstream without “the opposite parasite” fluxes.

ACKNOWLEDGEMENTS

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### Session 34: Boltzmann and Related Equations II

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Lid-Driven Cavity Flow using a Discrete Velocity Method for Solving the Boltzmann Equation

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We extend a one dimensional discrete velocity method [1] for solving the Boltzmann equation to two spatial dimensions. The collision integral is solved by discretizing velocity space and computing collisions between velocity classes selected randomly using a Monte Carlo method. Arbitrary post-collision velocities are mapped back onto the grid using a projection scheme which conserves mass, momentum, and energy [2]. In addition, a variance reduction scheme [3,4] is implemented to decrease noise and further reduce computational effort. The convection part of the equation is computed using upwind finite differences. Previous work has successfully applied this method to the homogeneous BKW relaxation and 1D shock problems [4,5]. Additionally, the method has been applied to problems involving multiple species and rotational and vibrational energy [5,6]. We apply this discrete velocity scheme to the 2D lid-driven square cavity flow problem. Results are obtained for a range of Knudsen numbers and lid speeds. Convergence with respect to grids in physical and velocity space is investigated and quantities such as heat flux rates, separation points, and vortex location are compared to benchmark results [7] computed using other schemes such as DSMC and Navier-Stokes solvers.

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Implicit GKUA for Computable Modeling of Boltzmann Equation and Multi-Body Flows in Various Flow Regimes

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The Boltzmann equation can describe the gas transport phenomena for the full spectrum of flow regimes and act as the main foundation for the study of complex gas dynamics including spacecraft re-entering Earth’s atmosphere. However, the difficulties encountered in solving the full Boltzmann equation are mainly associated with the nonlinear multidimensional integral nature of the collision term, and an exact solution of the Boltzmann equation is impractical for the analysis of practical complex flows. Numerical statistical or relaxation kinetic model equations resembling various order of moments of the original Boltzmann equation have been put forward. In this work, instead of solving the full Boltzmann equation, it can be indicated that a unified computational modeling based on the colliding relaxation evolution of the Boltzmann equation has been presented in describing flow transport phenomena around complex bodies in various flow regimes, and the theory and computational techniques of a gas-kinetic unified algorithm (GKUA) have been presented in past decades \cite{1-3} and used to simulate the re-entering aerodynamics from highly rarefied free-molecular flow to continuum regimes with the development of massive parallel implementation.

Based on the previous GKUA, a new implicit scheme of cell-centered finite volume is presented for directly solving the unified Boltzmann model equation covering various flow regimes, and a multi-block docking grid generation method is designed for complex irregular body. Then, the GKUA with the implicit scheme and multi-block docking grid has been firstly established and used to solve the flow problems around the multi-bodies covering various flow regimes with the whole range of Knudsen numbers from 10 to 0.0001. It is shown that the present algorithm and model possess much higher computational efficiency and faster converging properties. The flow problems including two and three side-by-side cylinders are simulated from highly rarefied to near-continuum flow, and the computed results are found in good agreement with the DSMC simulation and theoretical solutions, which verify the good accuracy and reliability of the present method. It is observed that in the near-continuum transitional flow regime, the spacing of multi-body increases to six times of the diameter of the single-body, the interference effects of multi-bodies tend to be negligible, see Fig.1, and it is feasible for the present method to combine with the gas-kinetic scheme \cite{4} to simulate irregular multi-body flows around disintegrating debris of uncontrolled spacecraft in near-space flying surroundings.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig1.png}
\caption{Hypersonic large-scale and multi-body flows covering various flow regimes for spacecraft falling disintegration}
\end{figure}

ACKNOWLEDGEMENTS
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REFERENCES
Deterministic-Stochastic Approach to Evaluate the Boltzmann Collision Operator in $O(MN)$ Operations

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Deterministic evaluation of the Boltzmann collision operator in multi-dimensional applications continues to be challenging. We propose an approach that can, in principle, lead to a fast deterministic-stochastic evaluation of the collision integral. The new algorithm uses a convolution form of the Galerkin projection of the collision operator:

$$I(\xi) = \frac{8}{\omega^N} \int_{\mathbb{R}^N} \int_{\mathbb{R}^N} f(\vec{\xi}) A(\vec{u}, \vec{u}; \phi) f(\vec{u}) d\vec{u} d\vec{v}$$

where the pe-computed kernel $A(\vec{u}, \vec{u}; \phi)$ carries information about collisions (see, e.g., [1,2]). In the case of uniform discontinuous Galerkin discretizations, all basis functions $\phi^j(\vec{u})$ are obtained from a set of functions $\phi^i(\vec{u})$ defined on a single cell by a shift, i.e., $\phi^j(\vec{u}) = \phi(\vec{u} + \vec{\xi}_j)$. In this case, projections of the collision operator on these basis functions are given by $I_j^i = I(\vec{\xi}_j)$. The new algorithm is obtained by performing the SVD decomposition of the discretized collision kernel $A_{ij} = A(\vec{u}_i, \vec{u}_j; \phi)$, determining its $M$ largest eigenvalues $\lambda_k$ and the corresponding eigenvectors $\varphi_k$, and by constructing an SVD compression of $A(\vec{u}, \vec{u}; \phi)$. The final step consists of approximating the unknown solution by a sum of a small number of homogeneous Gaussian densities $f^G_k(\vec{u})$ resulting in the following scheme

$$I(\vec{\xi}) = \frac{8}{\omega^N} \sum_{k=1}^M \sum_{j=1}^{\hat{M}} \lambda_k \left( \int_{\mathbb{R}^N} f^G_k(\vec{u} - \vec{\xi}) \varphi_k(\vec{u}) \right) \left( \int_{\mathbb{R}^N} f^G_k(\vec{u} - \vec{\xi}) \varphi_k(\vec{u}) \right) .$$

Stochastic maximization of the logarithm of the likelihood function [3] is used to determine the macroparameters of the approximating densities. The algorithm was applied to the solution of the problem of spatially homogeneous relaxation and solutions were compared to solutions obtained by a full Boltzmann solver [1]. The method achieves more than ten fold speedup in comparison to the fully deterministic method of [1,2].

ACKNOWLEDGEMENTS

The authors were supported by the HPTi PETTT Project PP-SAS-KY06-001, by the Interdisciplinary Research Institute for the Sciences at SCUN, by the Oak Ridge Institute for Science and Education and by AFOSR Grant No.F4FGA04296J003. Computer resources were provided by the XSEDE supported by National Science Foundation Grant No. OCI-1053575, by the DOD HPC Defense Shared Resource Center at AFRL, WPAFB and by the Rosen Center for Advanced Computing at Purdue University.

REFERENCES

Shock Wave Structure in Polyatomic Gases: Numerical Analysis using a Model Boltzmann Equation

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According to the old experiments [1] and the recent theoretical work [2] based on extended thermodynamics, a shock wave in a polyatomic gas may have a unique structure, which cannot be seen in a monoatomic gas. While the upstream Mach number $M$ is slightly larger than 1, profiles of the physical quantities inside the shock wave are smooth (type A in [2]). However, a doubly layered structure appears for larger $M$ (type C in [2]); it is composed of a thin layer (with the thickness comparable to the mean free path), where the profiles change steeply from their upstream equilibrium values, and a successive thick layer (with the thickness several orders larger than the mean free path), where the profiles slowly approach their downstream equilibrium values. Such a thick layer appears due to the slow relaxation of the internal modes.

The aim of the present study is to confirm the occurrence of the above mentioned transition of the shock wave structure in polyatomic gases on the basis of kinetic theory. We employ the ellipsoidal statistical (ES) model of the Boltzmann equation for polyatomic gases [3], and carry out a numerical analysis by means of a finite-difference method.

Figure 1 shows profiles of the density $\tilde{\rho}$, temperature $\tilde{T}$, and flow velocity $\tilde{v}$, normalized in the conventional manner, for $M = 5$. The ratio of the specific heats $\gamma$, the Prandtl number $Pr$, and the ratio of the bulk viscosity $\mu_b$ to the shear viscosity $\mu_s$ are set as $(\gamma, Pr, \mu_b/\mu) = (1.4, 0.787, 0.736)$ in panel (a) for $N_2$ gas. Those in panels (b) and (c) for pseudo-CO$_2$ gas are set as $(4/3, 0.767, 10)$ and $(4/3, 0.767, 100)$, respectively; we add ‘pseudo-’ because the realistic value of $\mu_b/\mu$ for CO$_2$ is $O(10^3)$ [4]. The profiles for $N_2$ are qualitatively similar to results for monoatomic gases. The profiles for pseudo-CO$_2$ with large $\mu_b/\mu$ show the doubly layered structure (corresponding to type C in [2]). The thickness of the shock wave for pseudo-CO$_2$ increases with increasing $\mu_b/\mu$. Thus a large computational domain will be required for real CO$_2$, which is the reason for the use of small $\mu_b/\mu$’s in the present computation.

![Profiles of the normalized density $\tilde{\rho}$, temperature $\tilde{T}$, and flow velocity $\tilde{v}$ for the upstream Mach number $M = 5$. (a) $N_2$, (b) Pseudo-CO$_2$ with $\mu_b/\mu = 10$, and (c) Pseudo-CO$_2$ with $\mu_b/\mu = 100$. Here $l_0$ is the mean free path in the upstream equilibrium.](image)

REFERENCES


Slip and Jump Boundary conditions for the compressible Navier-Stokes equations based on an asymptotic analysis of the Boltzmann Equation

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It is known from Maxwell that the standard boundary conditions of the Navier-Stokes equation need to be modified to be valid in the slip regime. Based on a simple assumption for normal momentum flux across the Knudsen layer, Maxwell proposed to modify the no-slip boundary conditions by adding a slip velocity, with a coefficient that depends on the Knudsen number. Later, the same method was applied by Smoluchowski to add a temperature jump to the boundary condition on the temperature (see [1]). Various authors tried to modify these boundary conditions (see [2], for instance) to improve their accuracy in more complex problems (curved boundaries, moving boundaries, etc.).

However, there is a more rigorous way to derive these boundary conditions, that can, in principle, give a correct result for very general problems. The idea is to make an asymptotic analysis of the Boltzmann equation, coupled to a boundary layer analysis in the Knudsen layer. This was done by Sone [3,4] based on a Hilbert expansion, and by Coron [5] based on the Chapman-Enskog expansion. While the work of [3,4] has been largely used for linear to slightly non linear problems, it seems to be seldom used for compressible (finite Mach number and large Reynolds number) flows. Similarly, the work of [5] seems to be unknown from the community of hypersonic flows for instance.

In this paper, we want to revisit the work of [5] to show the wide potential applications of this approach to derive correct boundary conditions for the Navier-Stokes equations in the slip regime. First, we will show how to obtain these boundary conditions for general time-dependent problems with moving boundaries. Second, we will explicitly derive the conditions for a steady supersonic flow around a solid body of arbitrary shape, when the solid-wall interaction is modeled by a reflection with partial accommodation.

ACKNOWLEDGEMENTS

The work of G. Martalò has been carried out with financial support from the French State, managed by the French National Research Agency (ANR) in the frame of the “Investments for the future” Programme IdEx Bordeaux-CPU (ANR-10-IDEX-03-02).

REFERENCES

Numerical computation and validation of extended boundary conditions for Navier-Stokes equations

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The simulation of the gas flow around a space shuttle is of great interest in order to design such vehicles. During its re-entry, the shuttle crosses different layers and the physical models, used in the simulations, strictly depend on the altitude. At low altitudes, the air is a continuous medium and the flow can be described by the compressible Navier-Stokes equations. At high altitudes, the flow is in the rarefied regime and the kinetic equations are more appropriate to describe it. In the middle layers, both models can be used and they should give the same macroscopic solution, since the Chapman-Enskog theory shows that the Navier-Stokes equations can be seen as the asymptotic approximation of the kinetic ones for small values of the mean free path.

The possibility of using both models at middle-low altitudes is the basic idea of the approach proposed in [1] in order to compute a suitable set of extended boundary conditions for the macroscopic equations and to describe the interaction between gas and surface.

The boundary analysis suggests that the correct boundary conditions to be imposed are a slip condition for the velocity and a jump condition for the temperature. Such conditions are already known in the frame of aerodynamic simulations as a suitable modification of the Maxwell-Smoluchowski conditions [2], but their coefficients are often deduced by means of empirical considerations. However, by following the approach in [1], one can obtain the coefficients in a more rigorous way by solving suitable half space problems.

In particular, one has to determine the asymptotic states of the solutions of such problems and, by revisiting [3], their numerical computation can be done directly and efficiently by means of a spectral method, by avoiding the computation in the whole half space and hence by reducing the computational cost. The approach has been proposed initially in order to deal with the diffuse reflection condition at the solid wall at microscopic level. We shall present an extension of the method also to situations involving more realistic conditions, like the non complete accommodation case. The numerical approximation of the coefficients will be given in both cases.

The last part will be devoted to the validation of such boundary conditions for the Navier-Stokes description. We shall compare the results from the simulations of the continuum model with those obtained by solving BGK equations. The accuracy of these boundary conditions will be investigated, as compared to the reference kinetic solution, for the most significant macroscopic quantities (like the heat flux at the solid wall). The difference with more standard Maxwell-Smoluchowski boundary conditions will also be shown.

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Atmospheric entries of meteors

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Meteoroids are small planetary bodies entering into planetary atmosphere at velocities up to 72 km/s. Such formidable velocities cause melting and evaporation of the meteor material in the transitional flow regime [1]. The meteor phenomenon has been mainly studied by geophysicists to answer science questions such as: what is the mass input of cosmic metals into atmospheres [2]? Engineers ignored meteors for a long time, at the exception perhaps of the design phase of the Apollo capsule, where observations of meteorites determined the use of ablative materials for heat shields [3]. Today, massive meteors are subjects of intensive study by space agencies, as possible threats to mankind. In this paper, we focus instead on falling stars, which range in size from small meteoroids to unnoticed atmospheric dust (from 1 m across down to micron-size grains).

Owing to their large entry speed, modeling meteors enhances tremendously the simulation challenges encountered in aerospace technology applications, such for instance space debris and electric propulsion. Indeed, understanding melting of meteor material can help engineers to predict the degradation of debris of satellites at end of life. These man-made space debris constitute a danger when, not fully destroyed during reentry, they impact the Earth. Another example is the study of the complex electron chemistry in meteor trails. A similar chemistry problem is the prediction of electron populations in the plume exhausting electric propulsion thrusters, driving their performance.

Meteors are natural flight experiments at zero cost: roughly 50 tons of small meteor material enters into the Earth atmosphere every day. They can be observed based on a network of radio wave receiving stations, optical emission spectroscopy cameras, as well as collected on ground as meteorites. For instance, the BRAMS [4] network observation data rely on forward scattering of radio waves emitted by a beacon off the ionized meteor trail [5].

In this paper, we will first introduce the meteor phenomenon and emphasize similarities with some aerospace engineering technology applications. Then, we will show some preliminary experimental results obtained in the VKI high-enthalpy Plasmatron facility with the aim of studying the melting and vaporization of meteor material, following a methodology developed to characterize thermal protection materials [6]. We will review some physico-chemical models and computational methods that can be used to study the meteor phenomenon, by highlighting the complexity of the problem due to its intense multiphysics and multiscale nature [7-10]. Finally, we will propose some improved solution methods to estimate the mass of meteor material from observation data: for instance, stochastic techniques proved to be useful when rebuilding free stream conditions in atmospheric reentry flows of spacecraft by providing indications about the impact of physico-chemical model and measurement uncertainties on the rebuilt quantities.

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REFERENCES

Modeling, numerical method and validation for the simulation of rarefied flows for reentry

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During re-entry of space shuttle, various kind of atmospheric layers are encountered at high speed. To develop such shuttles, one has to compute parietal flux and aerodynamic coefficients on such objects and so to simulate precisely air flows around them. In the upper layers of the atmosphere, the air is in a rarefied state (the mean free path of the particles of air is not too small with respect to the size of the shuttle) and the use of the kinetic theory of gas via the Boltzmann equation is needed (the Navier-Stokes equations are no longer valid in this regime). More precisely, the air is in transitional regime and the classical BGK model is used here: the complex collision term of the Boltzmann equation is replace by a relaxation toward equilibrium. This model is simpler than Boltzmann equation but keep the same conservation properties. However, it deals with simple modelling of the gas (monoatomic for example).
The BGK model is approximate with a discrete velocity method and a deterministic solver. A finite volume scheme is used to achieve stationary computations (see [1]). The use of an AMR velocity grid ([2]) was a significate improvement in term of computational cost and 3D realistic computations were made.
In this talk, we will present the evolutions of the BGK model for more complex gas (polyatomic, with small Prandtl number, with chemical reactions). We also present the numerical method of order 2 used to achieve simulation in 2D and 3D. We will pay attention to the numerical order of the method, by computing the correct boundary conditions with respect to the scheme. We will also detail the validation of the code by comparison with experimental data.

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A DSMC Surface Chemistry Model for Carbon-Based Ablators

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A detailed molecular surface chemistry model for the DSMC method is proposed and implemented into the SPARTA DSMC solver [1], verified, and validated. Molchanova et al. [2] constructed a molecular model for surface recombination in DSMC that includes different surface processes (adsorption, desorption, Eley-Rideal and Langmuir-Hinshelwood). The macroscopic model of Deutschmann et al. [3], in which a detailed mechanism of heterogeneous catalytic reactions in dissociated air is proposed, is used as a starting point. All surface processes can be divided into two groups: surface mechanisms, which involve only the particle adsorbed by the surface (desorption and Langmuir-Hinshelwood), and impact mechanisms, which also involve gas-phase particles (adsorption, Eley-Rideal). These surface reactions have been implemented in SPARTA and show excellent agreement with results from Ref. [2]. Using a similar approach, the 14-reaction kinetic model of oxygen-carbon interaction suggested by Zhlukhtov and Abe [4] is implemented in SPARTA, and verified. First, a closed box containing molecular oxygen at 1 atm is initialized, with one of the walls modelled as reactive carbon. The final system composition is tracked for different temperatures and compared with $O_2-C_{(s)}$ equilibrium compositions obtained from the CEA software [5], and the results are shown in Fig.1. It can be seen that the new DSMC model shows good agreement with the CEA equilibrium composition. A non-equilibrium case was also investigated in which a graphite rod was placed inside a cylindrical pressure-driven channel flow of $O_2$, with a pressure of 250Pa. The oxidation rate was computed and compared with experimental results. Finally, we will model the oxidation of flat and rough carbon surfaces due to a hyperthermal beam of $O/O_2$ and compare with the results of Murray et al. [6].

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REFERENCES

Assessment of Rarefaction Effects on the SARA Capsule

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Reentry vehicles which typically operate in rarefied gas environments are subject to extremes of velocity and altitude during the reentry phase. Hence, it is of extreme importance that the aerodynamic and thermal loads are properly characterized and accurately assessed for the development of a light-weighted and efficient thermal protection system. The vehicle may also encounter gas-side chemical reactions that can have a significant influence on aerodynamic performance and vehicle surface heat flux [1]. Numerical models which fail to incorporate such reacting flows miss out an essential part of the flow physics surrounding the vehicle. According to the Brazilian Program for Space Activities [2], it is of great importance the development of a suborbital platform in order to conduct scientific and technological experiments in low gravity environment. This suborbital platform, named SARA (acronym for Satélite Recuperável Atmosférico), has been developed by Instituto de Aeronáutica e Espaço (IAE) at Departamento de Ciência e Tecnologia Aeroespacial (DCTA) and it can carry 55 kg of scientific equipment, stay in orbit during the execution of the experiments, and return to Earth after the accomplishment of the tasks. In order to guarantee a safe return of the capsule and experiments inside of it, the precise determination of the aerodynamic performance, heating rates, and pressure loads acting on the capsule surface during the reentry becomes necessary. Figure 1 show the influence of chemical reactions on the shock wave and wake temperature for the SARA capsule at 95 km altitude. In this way, the purpose of this investigation is to assess the rarefaction effects on the flowfield structure during different phases of the SARA reentry trajectory using the DSMC technique [3]. In addition, hypersonic rarefied gas flow simulations are performed in a full 3-D geometry and using the “Quantum-Kinetic” (Q-K) chemistry model [4].

REFERENCES

State-to-State Kinetics and Transport Properties of Electronically Excited N and O atoms

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During the last decade electronic degrees of freedom have received a lot attention in the transport kinetic theory [1-3]. It was shown that in high-temperature flows, neglecting electronic excitation may lead to underestimation in the convective heat flux and aerodynamic forces. The objective of the present paper is to improve our previous studies on kinetic and transport properties of non-equilibrium high-temperature reacting flows of neutral atoms [3-5] taking into account state-to-state electronic energy kinetics and state-specific transport coefficients, and to implement the developed model to simulations of diffusion and heat transfer in flows after strong hypersonic shock waves.

A theoretical state-to-state model for a non-equilibrium high-temperature reacting flow of neutral atomic mixtures of nitrogen (N(4S), N(2D), N(2P)) and oxygen (O(3P), O(1D), O(1S)), taking into account three lowest electronic energy levels, is developed. Ionization is not discussed in the paper since its objective is to study the pure effect of electronic excitation on the transport properties in state-to-state approach.

The model is developed on the basis of the modified Chapman-Enskog method [6]. A closed set of governing equations is derived from the kinetic equations for the distribution functions. The transport terms are written in the first-order approximation of the method, and the algorithm for the calculation of transport coefficients is proposed. The contribution of electronic degrees of freedom into the heat and mass transfer is evaluated. The results obtained in the frame of one temperature and state-to-state models are compared.

The results obtained in this study will be implemented for simulation of the flow behind a plane shock wave under initial conditions characteristic for the spacecraft re-entry from an interplanetary flight (Hermes and Fire II experiments [7]), where electronic excitation is of importance.

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**Session 36: Evaporation and Condensation**

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Half-space Problem of unsteady evaporation and condensation of polyatomic gas

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Half-space problems for steady gas flows with evaporation and condensation have been studied analytically and numerically [1, 2, 3]. In the half-space problems, evaporation or condensation can take place only when macroscopic variables at infinity and on the condensed phase satisfy certain relations. It is practically important that the relations are used as boundary conditions for fluid-dynamic equations at the vapor-liquid interface for small Knudsen numbers. These studies [1, 2, 3] however have not examined the case where the evaporation and condensation at the interface take place periodically in time. Therefore, there remains a question about an effect of time-periodic evaporation and condensation flows.

In the present study, we consider time-periodic polyatomic gas (methanol, water, etc.) flows on the basis of linearized polyatomic version of the ellipsoidal-statistical Bhatnager-Gross-Krook (ES-BGK) model Boltzmann equation [4] in a semi-infinite expanse of an initially equilibrium polyatomic gas bounded by its planar condensed phase (Figure 1). The kinetic boundary condition $f_\infty$ at infinity is the local Maxwellian with periodically time-varying macroscopic variables: pressure $p_\infty$, temperature $T_\infty$, and velocity $v_\infty$, and the boundary condition on the condensed phase is the complete condensation condition [5, 6]. The time scale of variation of macroscopic variables, e.g., the inverse of angular frequency of sound wave, is assumed to be much larger than the mean free time of gas molecules, and the variations of those from a reference state are assumed to be sufficiently small. Therefore, weak evaporation and condensation take place periodically in time at the surface of condensed phase. We numerically investigate thus formulated half-space problem for the linearized polyatomic version of ES-BGK model equation with the finite difference method, and will discuss about relations between macroscopic variables at infinity and on the condensed phase.

**Fig.1:** Half-space problem.

**REFERENCES**

Evaporation/Condensation Boundary Conditions for the Regularized 13 Moment Equations

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The regularized 13 moment equations (R13) are a set of macroscopic equations that describe rarefied gas flows in the transition regime, with Knudsen numbers below unity [1-4]. The R13 equations and their boundary conditions are derived from the Boltzmann equation and its boundary conditions, and—with within their range of applicability—they provide an accurate and fast tool for the simulation of rarefied gas flows [1-4]. Here, we extend the applicability of the R13 equations by presenting their boundary conditions for evaporating/condensating interaction with the liquid phase. The boundary conditions are derived from the Maxwell model with evaporation from the boundary conditions for the Boltzmann equation, following the same method as the derivation for standard walls [3].

The model has two adjustable parameters that describe the interaction of an incident vapor particle with the liquid: the condensation probability $\vartheta$, and the accommodation coefficient $\chi$, which is the probability that a non-condensing particle is diffusely reflected.

To evaluate the capabilities of the model, we consider analytical solutions for two simple 1D problems, namely Ytrehus’ half-space evaporation problem [5], and heat and mass transfer through a vapor confined by two liquid layers at different temperature [6]. The results show that the R13 equations provide sufficient accuracy, including Knudsen layers (see Fig. 1), and the well-known inverted temperature profile in the vapor phase (Fig. 2). DSMC and BGK simulations will be used for comparison and fine tuning of the R13 boundary conditions, similar to the method employed for no-evaporating surfaces [7].

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Discrete Velocity Models: Bifurcations, hydrodynamic limits and application to an evaporation condensation problem

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Within the framework of Discrete Velocity Models (DVM) we discuss the following aspect concerning the hydrodynamic limit. It is a well-known fact that steady transport operators based on the Boltzmann collision operator and linearized around a Maxwellian at zero bulk velocity exhibit a typical structure concerning the null space (see e.g. [1]). Introducing a small bulk velocity breaks up this structure and gives rise to a certain bifurcation phenomenon which can be described explicitly in terms of the characteristic quantities of the collision model. Combined with an appropriate scaling which has proven useful in a number of models for diffusion phenomena (e.g. [2]), this approach provides explicit formulas which may serve as closure relations for the moment hierarchy in the macroscopic limit.

As an example, the same principle can be readily applied to an evaporation condensation problem for a binary gas mixture which was discussed in the literature [3,4] and which under the classical asymptotic analysis approach leads to a “ghost effect” which is hard to interpret. The method at hand, however, resolves this seeming paradox.

REFERENCES

A coupling simulation for the radiative transfer problem based on the domain decomposition method

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Radiation multigroup diffusion equation and radiation heat conduction equation are usually used in transport theory research and numerical simulation. Although one can solve the radiation diffusion equation in the entire domain, to reduce the computational cost, it is more advocated to use a domain decomposition method.

In this paper we present an approach to simulate the coupling model of multigroup radiation diffusion and heat conduction. Typically a domain decomposition is done by an iteration procedure at each time step, in which the multigroup diffusion and the heat conduction equation are solved through an interface condition which provides the boundary conditions for each subdomain, alternately until convergence of the successive approximation is reached. The two different interface conditions are obtained seperately based on the flux or temperature continuousness across the interface. The numerical results of the transfer tube problem demonstrate the effect of the coupling simulation on the computing efficiency as well as accuracy. Figure 1 indicates that the numerical solution by the coupling model seems to be the same accuracy as well as the 20 multi-group diffusion model. Tab.1 shows the computing time by the coupling equations are much more efficiency to solve than the multi-groups diffusion. Also The effect of the coupling simulation by the different interface conditions are discussed.

![Fig.1: Radial profiles comparison of radiative temperature at z=350um by different modeling.](image)

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Motionless Heat Pump – A New Application of Thermal Transpiration

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Thermal transpiration [1], which is a phenomenon unique to rarefied gases, is a one-way flow induced by a thermal gradient on a wall. This flow can occur in the pressure range from 100 Pa to 100 kPa by use of porous materials with nanoscale pores [2-5].

A motionless heat pump system proposed here uses the thermal transpiration pump, which is called a Knudsen pump, and a phase change of water. This heat pump is expected to be used as an air-conditioner in a car or factory driven by exhaust heat. The device configuration is shown in Fig.1. Two chambers, which are called an evaporator and a condenser, are filled with water and vapor. The pressure inside the evaporator \( P_E \) and that inside the condenser \( P_C \) are the saturated vapor pressures at respective chamber temperatures \( T_E \) and \( T_C \). They are connected by two channels. One channel is with Knudsen pumps in cascade in a vapor phase and the other is with a valve in a water phase. The Knudsen pump unit consists of a glass fiber filter and two passages in which a coolant with temperature \( T_L \) or an exhaust heat carrier with temperature \( T_H \) flows (\( T_L < T_H \)). The average pore size of the glass fiber filter is 0.7 µm and the thickness of the filter is 380 µm.

When Knudsen pump is operated, the vapor flows from the evaporator to the condenser. In the evaporator, the pressure drop encourages water to evaporate and absorb heat, then the temperature \( T_E \) falls corresponding to \( P_E \) drop. On the contrary, in the condenser, the pressure rise encourages vapor to condensate and generate heat, then \( T_C \) goes up corresponding to \( P_C \) rise. These mean that the temperature difference obtained in this heat pump system depends on the pressure difference attained by the Knudsen pumps. The power output \( W \) depends on the mass flow rate of the vapor \( Q_T \). By the latent heat of phase change of water \( L \), \( W \) is calculated by \( W = L Q_T \).

The delivery capacity of the vapor of the above Knudsen pump has been measured by the volumetric method [6] at 1.7 kPa, which is the saturated vapor pressure at 288 K. In this experiment, two chambers are filled with only vapor. The results are shown in Fig.2. \( \Delta T \) is the temperature difference between the coolant and the exhaust heat carrier. \( \Delta P \) is the pressure difference of two chambers and \( Q \) is the mass flow rate of vapor per unit area. \( \Delta P_{\text{MAX}} \) is the pressure difference at \( Q = 0 \) and \( Q_{\text{MAX}} \) is the flow rate at \( \Delta P = 0 \). Figure 2(a) plots \( \Delta P_{\text{MAX}} \) corresponding to \( \Delta T \) and Figure 2(b) plots \( Q_{\text{MAX}} \). \( \Delta P_{\text{MAX}} \) and \( Q_{\text{MAX}} \) are almost in proportion to \( \Delta T \). \( \Delta P_{\text{MAX}} \) is 57.6 Pa and \( Q_{\text{MAX}} \) is 0.0484 mg/sec/cm\(^2\) at \( \Delta T = 120 \) K. The heat pump performance becomes practical by amplifying \( \Delta P \) with a cascade connection of the Knudsen pumps.

REFERENCES

Numerical analysis of thermal creep flow induced around ratchet structure

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Linke et al. [1] reported that after a droplet dropped on a highly heated surface with ratchet structure, a droplet moves in the definite direction in such a way as to clamber up a ratchet wall. Not only a droplet but also a disk of solid carbon dioxide on a hot ratchet moves in the same direction [2]. This experiment indicates that the characteristic properties of liquid droplet such as nonuniform Laplace pressure and Marangoni forces are not the main cause for this phenomenon. Thus, we consider that gas film between surfaces plays an important role for this phenomenon. Würger [3] proposed the hypothesis that thermal creep flow induced around the ratchet structure may transport a droplet. Since thermal creep flow cannot be captured by the Navier-Stokes equations but is governed by the Boltzmann equation, in this study we use the direct simulation Monte Carlo (DSMC) method [4], which is the stochastic solution of the Boltzmann equation.

The computational domain is shown in Fig. 1. The upper surface imitates the bottom of a water droplet having the low temperature $T_{\text{drop}}$. The lower surface represents the heated ratchet with high temperature $T_{\text{wall}}$. Gas is water vapor of 1 atm. Figure 2 shows temperature and velocity distributions obtained in the DSMC simulation. The nonuniform temperature distribution is induced by large temperature difference between the two surfaces. Thermal creep flows are induced by temperature gradients in the vicinity of ratchet surface and vortexes appear in the groove. In order to move a droplet in the same direction as the experiment, the upper surface must be exerted the rightward shear stress. In the present simulation, the rightward shear stress on the upper surface was obtained as a whole.

**Fig. 1:** Computational domain.

**Fig. 2:** Temperature and velocity distributions. ($T_{\text{drop}}=373$ K, $T_{\text{ini}}=423$ K, $T_{\text{wall}}=473$ K, $h=1.0$ µm, $d=0.5$ µm, $L=2.0$ µm)

REFERENCES

On the Radiometric Flow in a Ratchet-Channel Nano-Pump

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We present a detailed description of the characteristics of a ratchet-type small-scale gas-pump suggested by Donkov et al. [1]. The pump consists of a ratchet channel with the temperature gradient applied between the opposing walls, see Fig. 1-a. Here, we report the physical mechanism of flow induction within the pump and show that the combination of reflection properties, geometric configuration and boundary temperature of this pump induces a directed radiometric-type flow (Fig. 1-b). Benefiting from DSMC simulations, we suggest the optimum working condition and geometry of the pump. An illustrative example of the velocity contour in the pump is shown in Fig. 1-c. Comparison of DSMC simulation with analytical relations is reported, where appropriate, see Fig. 1-d.

REFERENCE

Spatially accurate vacuum sensors with low-power requirements are needed for emerging applications such as small satellites and in-vacuum manufacturing processes. These challenges can be addressed with Micro-ElectroMechanical Systems (MEMS) based technologies that exploit rarefied flow effects. A novel sensor – Microscale In-plane Knudsen Radiometric Actuator (MIKRA) – has been developed to ultimately measure both pressure and gas composition [1]. This sensor relies on the development of Knudsen thermal forces, which are thermally driven forces generated within rarefied flows [2-3]. Because thermal gradients on the order of $10^6$ K/m can be feasibly obtained in MEMS-based devices, the use of Knudsen forces can be efficiently exploited in MIKRA. The MIKRA sensor mainly consists of sets of stationary heater and moveable shuttle arms separated by a small gap. The Knudsen forces on the shuttle arm can be measured, and correlate to the local pressure and gas composition around this sensor. In the current configuration, the gap and temperature difference between the heater and shuttle arms are around 20 microns and 30 K, respectively. While the net force and heat transfer occurring in the heater-shuttle system can be measured experimentally, an accurate velocity and gas temperature mapping is beyond the resolution of currently available sensors. In order to better understand the rarefied flow structure occurring in MIKRA, the direct simulation Monte Carlo (DSMC) method has been employed to model a single heater-shuttle pair. Using the SPARTA solver [4], we showed that the DSMC calculations for N$_2$ flows agree with our experimental data [5]. Figure 1 illustrates the pure N$_2$ flow structure obtained with SPARTA for Kn=1.8. In this work, our main goal is to extend our previous investigations to cover pressure and temperature conditions typically observed in lyophilization chambers. In particular, we want to quantify how the concentration of water vapor affects the Knudsen force production and heat transfer. Additionally, we investigate the effects of thermal gradient and Knudsen number on species diffusion and separation.

ACKNOWLEDGEMENTS

This work was supported by NSF CBET grant #1055453 “CAREER: Quantifying and Exploiting Knudsen Thermal Forces in Nano/Microsystems”. The second author is supported by the Brazilian National Council for Scientific and Technological Development (CNPq-Brazil) under grant GDE/201444/2012-7.

REFERENCES

A Study of Transport of a Microscale Object due to the Knudsen Force

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Recently, Nabeth et al. [1] reported that when a uniformly heated microbeam is immersed in a cold gas and is located in the vicinity of the cold substrate, the microbeam moves to the opposite side of the cold substrate. Similarly Li et al. [2] reported that when a uniformly heated microbeam located in the vicinity of the horizontal cold chamber wall is oriented from the horizontal axis, it receives a torque to make the microbeam return back to its horizontal orientation. These motions of the uniformly heated microbeams can be understood by considering the momentum transfer between the isothermal microbeam and gas molecules colliding with it in a nonuniform temperature field. Such kind of force and torque due to a temperature gradient with a characteristic length as much as the molecular mean free path of ambient gas molecules are called “Knudsen force” and “Knudsen torque”, respectively.

On the other hand, Linke et al. [3] reported that when a water droplet drops on a highly heated surface with ratchet structure, it is levitated by the Leidenfrost effect and moves in the definite direction in such a way as to clamber up the vertical wall of the ratchet structure. Würger [4] proposed the hypothesis that a thermal creep flow is induced around the ratchet structure and transports a droplet. We investigated this phenomenon by performing DSMC simulations and pointed out that the Knudsen force enough to move the droplet is exerted on it [5].

In the present study, we investigate how to levitate and transport a microscale object by the Knudsen force.

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### Session 38: Hypersonics

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Pitot Pressure Analyses in CO$_2$ Condensing Rarefied Hypersonic Flows

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In order to improve the accuracy of rarefied aerodynamic prediction, a hypersonic rarefied wind tunnel (HRWT) [1,2] has been developed at Japan Aerospace Exploration Agency (JAXA). While this wind tunnel has been limited for inert gases, such as nitrogen or argon, we lately plan to extend the capability of HRWT to CO$_2$ hypersonic flows for several Mars missions [3]. One of the objectives on Mars missions is life detection exploration on Mars [4], and the accuracy of a landing site is crucial from the viewpoint of mission scope and planetary protection. In order to improve the prediction accuracy of the flight path and the landing site for the mission, rarefied aerodynamic prediction is important since its flight duration in rarefied flow regime is relatively long in the Martian atmosphere.

Figure 1 shows flow conditions of CO$_2$ nozzle flows in a HRWT test section, and direct simulation Monte Carlo (DSMC)[5] results at 0.12 g/s are compared with extended saturated vapor pressure curves of Giauque [6] and an extended isentropic line from the triple point. The flow conditions in the HRWT test section were obtained for stagnation temperature between 298 K and 1,600 K. Although degree of super-saturation decreases with increasing the stagnation temperature, the HRWT conditions are between the isentropic and vapor lines. Thus, for CO$_2$ rarefied aerodynamic measurements, condensation effect may not be negligible. Namely, the understanding of CO$_2$ condensing rarefied hypersonic flows is crucial to improve the accuracy of aerodynamic measurements [7].

In this study, we first develop numerical schemes for CO$_2$ condensing flows. Second, we estimate hypersonic nozzle flow conditions with CO$_2$ condensation in the HRWT test section. Third, we numerically analyze condensation effect on pitot tube measurements, and finally we evaluate the degree of super-saturation in HRWT by comparing measured pitot pressure values with estimated ones.

ACKNOWLEDGEMENTS

The research performed at JAXA was partly supported by the Grant-in-Aid for Scientific Research (C), No. 15K06611 from Japan Society for the Promotion of Science (JSPS) whose support is gratefully acknowledged.

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Analysis of Steady Hydrogen-Air Detonation Waves with Vibrational Nonequilibrium

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In high-speed atmospheric flows, strong shocks create vibrationally underpopulated (i.e., vibrationally cool) gas mixtures, which may decrease the reaction rate efficiency for chain reactions (e.g., \( \text{H} + \text{O}_2 \rightarrow \text{O} + \text{OH} \) and \( \text{O} + \text{H}_2 \rightarrow \text{H} + \text{OH} \) in hydrogen-air mixtures). For instance, Fiévet et al. have shown that including vibrational nonequilibrium in scramjet combustor CFD simulations decreased the ignition length by approximately 50% compared to the standard model that assumes thermal equilibrium [1]. We look to extend this analysis to rotating detonation engines (RDEs), which also operate at high speeds and near-atmospheric pressure. Our goal is to quantify the effect of vibrational nonequilibrium on the ignition length and combustion processes in an RDE. To this end, this work will simulate one-dimensional steady detonation waves under RDE operating conditions.

The initial work to assess the effect of vibrational nonequilibrium on a steady detonation wave was to implement the model and simulate a canonical test problem. Alongside the one-dimensional, inviscid, steady Navier-Stokes equations, a vibrational nonequilibrium transport equation was derived, which tracked the vibrational energy of each polyatomic species. Each species was characterized by a unique vibrational temperature \((T_{v,i})\) and a shared translational-rotational temperature \((T_r)\). A coupled vibration-chemistry-vibration (CVCV) model was implemented and modified by the nonequilibrium rates calculated by Voelkel et al. [2,3]. Given an initial state, a shocked state was calculated by solving for the roots of the transport equations holding species mass fraction constant. Then, the ordinary differential equations described the evolution of the vibrational energy and species mass fraction were numerically solved. Fig. 1 shows the translational temperature and vibrational temperature of \(\text{H}_2\), \(\text{O}_2\), and \(\text{N}_2\) for a piston-driven detonation wave initialized at 1 atm, 300 K, and 200 m/s. Compared to the equilibrium case, immediately after the shock, \(T_r\) is higher because the vibrational energy is frozen through the shock. However, vibration-translation energy relaxation decreases \(T_r\) by approximately 100 K before the detonation wave. Continuation of this work will use RDE operating conditions as the initial conditions, analyze the steady-state solution, and assess the effect of the vibrational nonequilibrium on the ignition length and combustion processes.

ACKNOWLEDGEMENTS

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Hypersonic Reacting Flow Simulations using the hy2Foam Open-Source Two-Temperature CFD Solver

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The newly coded open-source two-temperature computational fluid dynamics (CFD) solver hy2Foam has been developed to tackle the highly complex flow physics of the hypersonic Earth atmospheric re-entry [1]. Implemented within the OpenFOAM framework [2], the code has the capability to model physical phenomena relative to the high-speed chemically-reacting environment surrounding a spacecraft. The non-equilibrium conditions are treated by making the distinction between the trans-rotational and multiple vibrational-electronic energy pools. This allows the modelling of energy exchanges between the pools and the introduction a chemistry-vibration source term into the Navier-Stokes-Fourier equations. Species thermal properties follow the Blottner and Eucken formulas while mixture properties are recovered using either Wilke’s or Gupta’s mixing rules. hy2Foam has been extensively validated for a 5-species air using fundamental zero-dimensional benchmark cases. Validation for a one-dimensional shock tube and a two-dimensional cylinder at Mach 6.5 has also been carried out and has been compared with previously published data. The aim of this study is to perform a comparison between hy2Foam and the open-source direct simulation Monte-Carlo (DSMC) code dsmcFoam [3] for challenging Mach 20 flows past a circular cylinder. Emphasis will be made on the importance of considering chemical reactions and the inclusion of the electronic mode to correctly estimate the aerothermal loads.

ACKNOWLEDGEMENTS

The CFD results were obtained using the EPSRC funded ARCHIE-WeSt High Performance Computer (www.archie-west.ac.uk/). EPSRC grant no. EP/K000586/1. This work has also been awarded an ARCHER Resource Allocation Panel (RAP) grant.

REFERENCES

Sensitivity Analysis of DSMC Parameters for a Radiating 11-Species Air Hypersonic Flow

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This research investigates the influence of input parameters on the simulation of a hypersonic flow scenario using the direct simulation Monte Carlo (DSMC) method. Using our DSMC code, a hypersonic shock tube experiment in rarefied air is simulated which acts as our baseline for the subsequent sensitivity analysis. The results of this DSMC simulation are compared to experimental data such as the recent NASA Electric Arc Shock Tube (EAST) results [1]. For the considered hypersonic simulations, high enough temperatures are experienced that the modeling of ionization is necessary and an 11-species air model is required. In a previous work, our DSMC code which included these high temperature physics was used to simulate a similar hypersonic shock tube flow [2]. Although comparable in scope, the DSMC simulation used in [2] did not include certain models that are now deemed critical to accurately comparing to experimental data. For example, it was determined that the representation of electronic excitation is necessary to the computation of the emission spectra. In order to remedy this, electronic excitation is included in the current research following the model detailed by Liechty in Ref. [3].

After improving the DSMC code and choosing a nominal simulation scenario from the EAST data, a sensitivity analysis is performed by varying the computational DSMC and physical model input parameter values. Due to the extreme conditions of these hypersonic flows, experimental results are limited to obtaining quantities such as the post-shock emission spectra. The sensitivity analysis in [2] was only performed for quantities of interest (QoIs) that could not be directly compared to the EAST data because radiation was not modeled in our DSMC code. In order to directly compare to the EAST spectra, our DSMC results are post processed by the NEQAIR line-by-line radiative solver [4]. Once NEQAIR is linked with the DSMC code, a QoI for the sensitivity analysis is chosen from the radiative results, such as the spectrally integrated emission intensity. The sensitivity analysis is then performed by selecting the input parameters from a prior distribution and performing the full simulation. The sensitivity of the QoI to each input parameter is computed from the Pearson correlation coefficient and the mutual information which will be used to rank the input parameters by sensitivity. In the future, this ranking will be used to decide which input parameters will be investigated in an uncertainty quantification study and calibration to experimental data. The results of the present sensitivity analysis allows for the reduction in the parameter space of an uncertainty quantification and can guide future investigations into obtaining more accurate input parameters or models for hypersonic simulations.

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Investigation on Critical Pressure Ratio of Hypersonic Low-density Wind tunnel Vacuum System

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Abstract: Once the flow field is established, the pressure in vacuum container increases continuously for an intermittent type wind tunnel. When the pressure rises up to certain extent, the static pressure in test section would be unstable, and the flow field is destroyed at the same time. The vacuum pressure at the unstable time point is called critical pressure. The Mach number is usually high in hypersonic low density wind tunnel, which means the needed pressure ratio is also high. Since the requirement for vacuum system is rigorous, and the cost of vacuum system is expensive, the exact critical pressure ratio is important for designers. To study the critical pressure ratio, the experiment is carried out in Φ0.3m hypersonic low density wind tunnel, where the Mach number is over than 10. The pressure in the test section, pitot tube, diffuser and vacuum container have been measured (Fig.1). The critical pressure ratio of M10 and 12 and 16 are given in Fig.2. The influence factors are also analyzed.

Key words: hypersonic; vacuum system; critical pressure ratio

Fig.1 sketch of measurement point in low density wind tunnel

Fig.2 critical pressure ratio of high mach number flow field

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Conservative Bin-to-Bin Fractional Collisions

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Stochastic methods such as direct simulation Monte Carlo (DSMC) and particle in cell (PIC) have been the workhorse tools for rarefied gas and plasma dynamics for decades. The computational cost of suppressing statistical noise in these methods has long been a hindrance for flows with high dynamic range in densities and in length-scales such as ionizing breakdown, chemical reactions with trace species, and spacecraft plume interaction models. The noise is further exacerbated by unsteady flows where time averaging is inappropriate and in cases where fluctuations can non-linearly feed back through the system as in the case of evaluating electron mobility in hybrid Fluid/PIC models used for modeling Hall Effect thrusters[1]. To address the issue of poor statistical power, models that relax the constraint on uniform physical to computational particle ratio have been developed. The addition of conservative local dynamic phase space reconstruction using these weighted particles enables direct control over the number of particles per cell, a key parameter influencing statistical noise, while simultaneously preserving velocity distribution shape so that numerical thermalization and artificial entropy growth are inhibited [2,3].

The development of robust phase space reconstruction has also opened the door to a new class of collision models for particle codes based on fractional rather than Monte Carlo techniques. This change enables much more direct control over the statistical noise due to collisions through a finer stochastic sampling of the collision integral than was previously possible. Such fractional collision methods replacing MCC ionization as well as DSMC elastic collisional relaxation have been demonstrated in conjunction with phase space reconstruction methods in References [3,4] among others. For the DSMC replacement, fractional collision methods are particularly critical because the standard “all-or-nothing” collision of the DSMC method is inherently incompatible with variable computational weight particles. Even compensating for the dynamic range of relatively simple axi-symmetric flows can cause significant on-axis issues related to variable radial weighting procedures that simply use cell averaged weights in the collision routines [4]. Most other prior attempts to account for variable weights without global phase space reconstruction have relied on merging fractional pre- and post-collision fragments within the collision step. Merging these pieces is a particularly poor choice because it necessarily violates energy conservation, merges particles far apart in velocity space causing artificial thermalization, directly violates detailed balance, and fails to converge to the physical solution even with refinement of increased particle count.

Though these fractional collision methods have been demonstrated to reproduce results based off the original fixed weight methods, in this work, the idea of combining the fractional collision and the reconstruction process into a single step is explored as a means of reducing the memory overhead from storing extra fractional collision particle information only for it to be destroyed in the subsequent conservative merging reconstruction process. The combined collision process then becomes conservative non-local fluxes of mass, momentum, and energy between phase space bins used to update the quantities required for generation of the reconstructed particles. In addition to the octree-based bins used in the authors’ prior phase space reconstructions, other velocity space decomposition strategies will also be investigated that avoid holes in the distribution to support improved implicit collision processes. Direct comparison of cost and error to standard multi-dimensional DSMC results such as supersonic flow over a sphere will also be explored.

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Distribution A: Approved for public release; distribution unlimited. AFTC/PA clearance No. 16123.
Implementation of the DSMC decomposition into ballistic and collision parts to some classical rarefied flows

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Rarefied gas flows are characterized by long mean free paths, compared to the problem characteristic length, leading to moderate and high Knudsen numbers associated to very interesting non-equilibrium transport phenomena appearing at such flows. Moreover due to the long mean free paths at each point of the flow domain, even far from the boundaries, the particle distribution is composed of particles arriving directly from the boundaries without interacting with other particles and of particles arriving after an arbitrary number of collisions. Decomposing the distribution into those two parts namely the ballistic and collision parts and computing the corresponding parts of the solution can provide physical information and help interpret complex phenomena. The decomposition is based on the DSMC method, introducing a tag on each particle indicating whether it belongs to the ballistic or collision part and adjusting accordingly the sampling procedure.

Recently this DSMC distribution decomposition technique has been applied to investigate two thermally driven flows in cavities. In the first configuration, the bottom and top walls were kept at constant and different temperatures while a linear temperature distribution between the top and bottom temperatures was applied to the lateral walls [1]. It was observed that a flow near the lateral boundaries was formed, having a velocity from hot-to-cold regions, contrary to the thermal creep flow. In the second configuration, three walls of the cavity were kept at a constant low temperature and the other at a higher temperature [2]. An interesting finding was that the heat flux departing from the hot wall, for some given Knudsen number, had a non-monotonic behaviour with respect to the temperature ratio and a maximum heat flux appeared at some intermediate ratio. In both configurations the decomposition technique provided solid physical explanation of the observed unexpected non-equilibrium phenomena. Furthermore, the same DSMC decomposition has been applied to provide a quantitative explanation to the classical Knudsen minimum, observed in fully developed flows through long capillaries of various cross sections [3].

In the present work the DSMC decomposition methodology is briefly described and its implementation to the above flow setups is briefly reviewed. In addition this methodology is also applied to the typical rarefied gas flow between two concentric cylinders, with the inner one rotating at a constant speed and the outer one being stationary. As it is well-known at some small values of the tangential momentum accommodation coefficient of the outer cylinder and of gas rarefaction an inverted velocity profile is observed. This non-equilibrium phenomenon is also investigated using the decomposition technique and some useful insight in addition to the available prediction is provided.

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REFFERENCES

A Framework for Direct, Normal, High Order Approximations of Boltzmann's Collision Operator

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The discretization of the right-hand side of the Boltzmann equation (aka the collision operator) on uniform grids generally suffers from some well known problems prohibiting the construction of direct (deterministic) high order approximations which exactly sustain the basic properties of the collision operator. These problems mainly relate to problems arising from the discretization of spheres on uniform grids and the necessity that the discretization must possess some symmetry properties in order to provide the discrete versions of properties stemming from the continuous collision operator. The properties we are interested in are the number of collision invariants, avoidance of artificial collision invariants, type of equilibrium solutions and the H-Theorem. We present a scheme to construct discretizations in 2 and 3 dimensions using arbitrary classical 1D (and thus simple) quadrature formulas on uniform grids. Applying two simple adjustments to these simple approximations provides us with an approximation that possesses the correct properties and the convergence orders of the used schemes simply (divided by a constant factor) translate into the convergence order of the whole approximation. The talk will finish with an example (based on simple Newton-Cotes formulas), a look at the real numerical error and the numerical complexity.

Our approach is comparable to the approach by Rogier and Schneider [1], the subsequent works by Michel and Schneider as well as Panferov and Heintz [2, 3] who used Farey sequences for the discretization. Moreover we use results obtained by Bobylev in [4] in order to derive one of our adjustments. The theoretical considerations necessary are presented in the context of DVMs.

REFERENCES

Inverse Laplace Transform as a Tool for Calculation of State-specific Cross Sections of Inelastic Collisions

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Reliable data on state-specific cross sections of physical-chemical processes are required for DSMC rarefied flow simulations as well as in the transport kinetic theory for the calculation of reaction and relaxation rates in viscous non-equilibrium flows. Data obtained by means of molecular dynamics are often not suitable for implementation, and therefore derivation of analytical expressions for the cross sections is of vital interest for applications.

In the present study we utilize the state-to-state dissociation rate coefficients and those of VV and VT transitions obtained in [1-4] using quasi-classical trajectory calculations (QST) in order to derive analytical formulas for the cross sections of corresponding collisions depending on molecular vibrational states. For this purpose, we first obtain approximate expressions for the state-specific rate coefficients suitable for applying the inverse Laplace transform in the analytical form. The accuracy of proposed approximations is within 3-5% for vibrational energy transitions; for dissociation rate coefficients the discrepancy does not exceed an order of magnitude in the whole range of considered vibrational levels and temperatures.

Then, applying the inverse Laplace transform we derive analytical expressions for the cross sections of the following reactions: VV transitions in \( \text{N}_2 \) and \( \text{O}_2 \); VT transitions in \( \text{N}_2 \) and \( \text{O}_2 \) in collisions with atoms \( \text{N} \) and \( \text{O} \) respectively; dissociation of \( \text{N}_2 \) and \( \text{O}_2 \) molecules from any vibrational state during collisions with corresponding atoms. The results are analyzed in a wide range of particle relative velocities and vibrational levels. Comparisons are made with the cross sections of vibrational energy exchanges predicted by the forced harmonic oscillator (FHO) model [5], the dissociation cross sections are compared to those calculated with a simple model based on the rigid spheres interaction potential accounting for vibrational energies of the dissociating molecules. It is shown that cross sections of VV transitions increase almost linearly with the energy of colliding particles. VT-exchanges and dissociation reaction manifest threshold behavior, and their cross sections are non-monotonic. The dissociation threshold is considerably shifted towards the low energy region for high vibrational states.

The analytical expressions for the state-dependent cross sections of collisional processes proposed in this study can be easily implemented in DSMC flow solvers.

ACKNOWLEDGEMENTS

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**Session 40: Kinetic Approaches**

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The High Performance Parallel Algorithm for Unified Gas-Kinetic Scheme

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The numerical mechanism of Unified Gas-kinetic Scheme (UGKS) is consistent with the underlying physical model that the particle transport is coupled with collision. It releases UGKS from the constraint that time step should be less than particle collision time or the cell size less than the mean free path. This property, which is called asymptotic preserving property, guarantees the high efficiency and accuracy of UGKS especially for flows in a broad range of Knudsen numbers [1]. Despite the existing work in typical but simple flows, UGKS is extended to model three-dimensional flows internal and external on complicated grid system for aircrafts. Two different parallel algorithms are adopted, the spatial multi-block grids technique and the decomposition of molecular velocity domain into blocks. To improve communication efficiency among neighboring processors, the spatial domain and velocity domain are divided into different communicators and distributed according to a two-dimensional Cartesian topology applied in phase space. This structure works with intra-communicators in spatial domain for data exchange and other intra-communicators in velocity domain for sum reduction to moment integral. The extension algorithm is validated by some well-studied three-dimensional cases, including cavity flow and flow past a sphere. For three-dimensional cavity flow (Kn=0.1), the predicted temperature fields agree well with the results of Huang et al. [2]. In supersonic flow past a sphere (Kn=0.236, Ma=5), the calculated density and temperature profiles are in good agreement with the results of Mieussens [3]. To illustrate the capability of the algorithm, flow past a spacecraft is also computed. To test the scalability of the algorithm especially for large-scale problems, the speed-up ratio is shown in the figure. The total degrees are 17.4 billion. Calculations are run on 729 to 5832 processors. It can be seen that the speed-up is near linear and thus the efficiency is around 1, which reveals the good scalability of the present algorithm.

ACKNOWLEDGEMENTS

The authors would like to thank K. Xu at Hong Kong University of Science and Technology and P. Yu at Zhejiang Institute of Hydraulics & Estuary. This work is supported by National Key Basic Research and Development Program (2014CB744100), National Natural Science Foundation of China (91330203) and Special Program for Applied Research on Super Computation of the NSFC-Guangdong Joint Fund (the second phase). Part of computation is done in National Supercomputing Center in Liling (Tianhe-2), Changsha (Tianhe) and Jiangnan Institute of Computing Technology.

REFERENCES

Quasiparticle Pairs in Kinetic Theory

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Pair collisions are the main interaction process in the Boltzmann gas dynamics. To account this interaction in the statistical description of the gas systems one need to possess a two-particle distribution function. As is well known, Ludwig Boltzmann presented it by the product of two one-particle functions and wrote his famous kinetic equation (for one-particle distribution function) with the collision integral in its right part.

The report is based on the kinetic equation[3] for two-particle distribution function, which was obtained by making use of exactly the same physical assumptions as Ludwig Boltzmann has done. Instead of the collision integral, there are the linear scattering operator and the chaos projector in the right part of the two-particle equation. The Boltzmann equation then follows from this equation without any additional assumptions by performing a simple integration. Because of the scattering operator is simpler then Boltzmann collision integral this equation opens new opportunities for mathematical description of the Boltzmann gas dynamics. In particular, using renormalized form of the scattering operator obtained in [2], we can present this two-particle equation in the form of Liouville equation in the 9-D phase space.

It follows from this equation that to describe statistically the dynamics of gas systems we can replace the pairs of molecules with pairs of quasiparticles, whose distribution function coincides with the distribution function of the real molecules. Quasiparticles and real molecules have quite different dynamics. Real molecules are moving chaotically due to collisions but quasiparticle pairs do not collide and are moving along smooth trajectories in the 9-D phase space, slowly rotating (accounting effect of collisions).

The use of quasiparticle pairs is more convenient for simulation then the single quasiparticles introduced on the base of renormalized Boltzmann equation [1,2], because the energy of the system of quasiparticle pairs is conserving automatically in the course of simulation and it is possible to contruct the algorithm for which there is no need for energy corrections[4,5].

In the report there are also presented possible simplifications of the algorithm and results of numerical simulations of classical rarefied gas problems utilizing quasiparticles pairs.

REFERENCES

Moment Equations for a Reactive Quaternary Gaseous Mixture

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Kinetic modelling of chemically reacting mixtures has gained importance in the scientific literature in the past decades. In [1], an initial attempt was made towards understanding the influence of chemical reactions upon the perturbation of the Maxwell’s distribution function. The existence of a unique equilibrium and its stability for a reactive quaternary gaseous mixture has been proved in [2]. Moreover in [3], the Grad’s-13 moment system has been derived for a reactive gaseous mixture. Moving in the same direction as the previous work, we will firstly discuss the collision dynamics of smooth reactive hard sphere model. The drawbacks, which arise by the description of chemical reactions while using the classical smooth inelastic hard sphere model, have been discussed in detail. A new model which does not suffer from these drawbacks has been proposed using which certain useful velocity transformations have been derived. These velocity transformations have been found to converge to the single gas and the binary mixture case for appropriate physical parameters.

Using the fourteen moment model discussed in [4] as a motivation, we will derive the Grad’s-14 moment system for a reactive quaternary mixture. The influence of various physical parameters and the initial conditions upon the relaxation behaviour of the proposed moment system has been studied. To understand the influence of the fourteenth moment upon the relaxation of the system, the results obtained from the Grad’s-14 moment system have been compared to those obtained from Grad’s-13 moment system and the Euler equations. Similar to [4], the fourteenth moment has been found to have a profound influence upon the relaxation properties of the system which, similar to the granular gases, is a result of the presence of inelastic scattering in the system.

REFERENCES

An Asymptotic Preserving Implicit Unified Gas Kinetic Scheme for frequency-dependent Radiative Transfer Equations

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In this talk, an asymptotic preserving implicit unified gas kinetic scheme (IUGKS) is constructed for frequency-dependent radiative transfer equations. Different from the original asymptotic preserving unified gas kinetic scheme which uses the explicit initial value of radiation intensity in boundary fluxes' construction as in the previous works (Sun et al., J. Comput. Phys. 285(2015), pp. 265-279 [1] and J. Comput. Phys. 302(2015), pp. 222-238 [2]). Here the boundary fluxes we constructed is implicit depending on the radiation intensity, thus the time step constraint by the Courant-Friedrichs-Lewy (CFL) condition is not needed anymore, and the asymptotic preserving property holds uniform with the small Knudsen parameter. The numerical results show that this implicit method can use large time step and save computational time greatly.

ACKNOWLEDGEMENTS

The current research was supported by the Science and Technology Development foundation of China Academy of Engineering Physics (Grant No.2015B0202041, 2015B0202040) and NSFC (Grant No. 11371068) for Sun; by the National Basic Research Program under Grant 2011CB309705 and NSFC (Grant Nos. 11229101, 11371065) for Jiang; by Hong Kong research grant council (620813,16211014), HKUST SBI14SC11, and NSFC-91330203 for Xu.

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### Session 41: Vacuum Gas Dynamics

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Transmission Probability and Active Pumping Ability of the Channel with Moving Partition Plane

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The gas flow in a vacuum system can be free molecular, transitional, or viscous flows depending on the Knudsen number Kn, the ratio of the mean free path of the molecules to the typical size of a vacuum system. When Kn>10, the inter-molecular collision of gas molecules is negligible and the gas flow is mainly determined by the interaction of the gas particles with the walls of the vacuum system. In such a case, the Test Particle Monte Carlo (TPMC) simulation method is an appropriate approach for designing the vacuum system. One typical application is the simulation of the transmission probability of a vacuum channel, which is very important in the vacuum system design, being used to calculate the conductance, estimate the effective pumping speed and choose adequate vacuum pumps.

On the other hand, the vacuum channel itself can be pumping when its walls are coated with active pumping materials such as Non Evaporable Getter (NEG) or argon frost [1-3]. The active pumping ability of the channel, which is different from its transmission probability, is characterized by the ratio of the number of molecules absorbed by the channel to the number of molecules flowing into the channel.

In this paper we will present the TPMC simulations of the transmission probability and the active pumping ability of a rectangular channel of different physical parameters [4]. The novel feature of the channel is that it has a partition plane in the middle which is moving up and down, and so it is a dynamical system. The system was simulated by our developed TPMC code ProVac3D with a new subroutine considering the moving partition plane. In order to obtain precise simulation results, at least $10^{11}$ test molecules were simulated in parallel on the supercomputer Helios in Japan. It is found that the amplitude and the frequency of the movement will affect both transmission probability and the active pumping ability of the channel. Moreover, it is also found that both transmission probability and the active pumping ability of the channel with the moving partition plane are no longer independent of the mass of the gas molecule.

ACKNOWLEDGEMENTS

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Study on a Gas Transport System based on Thermal Induced Flow

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Thermal induced flows are one of the peculiar phenomena in the rarefied gas dynamics and have been investigated in previous study [1]. These flows are applied to the gas separators [2] and gas transport systems including pumps [3] and compressor [4]. In this study, a gas transport system which is driven by the thermal edge flow is investigated experimentally. The experimental equipment is consisted of two vacuum chambers, a glass tube that connected these chambers, an auxiliary vacuum pump to attain the low gas pressures needed to enable thermal edge flow, vacuum gauges, and a set of thin plates with slits that were colored such that the front and back surfaces had different heat absorption characteristics, as shown in Fig.1. Thermal edge flow was induced near the edge of the slits of thin plates by irradiating the infrared lamp.

Figure 2 shows the pressure ratio of the two chambers \( p_A/p_B \) depend on \( p_A \) for different interval s between plates with slit width \( W=5\text{ mm} \), and slit interval \( H=5\text{ mm} \). The temperatures of the black and white sides of the plates were 100 and 140 °C, respectively. The pressure ratio \( p_A/p_B \) decreased with \( p_A \) reached a minimum around \( p_A=1-1.5 \text{ Pa} \), and then increased with increasing pressure in chamber A regardless of the plate interval (\( s=2.5, 7.5, \) or \( 12.5 \text{ mm} \)). The pumping effect was observed to be most significant when \( p_A/p_B \) was the smallest and observed to be reached a maximum when the plate interval was \( s=12.5 \text{ mm} \) and the pressure ratio \( p_A/p_B \) was around 0.96. We also investigated the effect of the slit width \( W \), slit spacing \( H \), and shape of the slit on the pressure ratio \( p_A/p_B \).

REFERENCES

Measurement of Gas Viscosity using Photonic Crystal Fiber

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A new measurement technique for gas viscosity coefficient is designed and demonstrated using the technique of diode laser absorption spectroscopy. Gas flow is driven under a pressure gradient between two gas cells, through a photonic crystal fiber (PCF) surrounded by a furnace for temperature adjustment, as depicted in Fig. 1. PCF with 20-micron diameter enables gas flow to be investigated under different flow regimes from rarefied to continuum. Infrared radiation from a diode laser is coupled into the fiber to be guided through the gas, and the light attenuation due to absorption from the molecular absorbing species is measured by a photodetector placed at the exit of gas cell B. An analytical relationship between gas concentration, velocity profile and viscosity coefficient in the unsteady flow from gas cell A to gas cell B after gas is impulsively introduced into gas cell A is derived using the Navier-Stokes equations and applied for the determination of gas viscosity as a function of temperature, based on the mass flux of gas measured by the absorption of the laser light, using the Beer-Lambert law. The advantage of this technique is that the system has no moving parts and can be used to obtain measurements of viscosity at high temperatures, which will provide practical data for modelling gas motion. Because these correlations are usually derived using measured data at low to moderate pressures and temperatures\textsuperscript{1}, the validity of this extrapolation approach needs to be determined by experiments over a range of temperatures. Although the experiments presented here will use a short 1-m fiber for these proof-of-concept viscosity measurements, the system also has the potential advantage of being able to be used at higher Knudsen numbers, because long hollow-core fibers can be used to maximise absorption, with potential applications in validating viscosity models that include the effect of slip.

The information that is directly obtained from absorption spectroscopy is the gas concentration inside the capillary as a function of time, whose second derivative relates to the flow velocity as a function of time. The derivative terms of velocity with respect to space in the flow direction are zero after the flow reaches a fully-developed state. Because the velocity profile can be directly related to the mass flux measured through the absorption, and the pressure distribution is assumed to be linearly distributed along the fiber length at a given time, the viscosity coefficient of the gas can be determined in the unsteady state while the gas moves from cell A to cell B, based on momentum conservation.

![Experimental arrangement](image)

**Fig.1: Experimental arrangement**

REFERENCES

Molecular Contamination Modeling with CTSP

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This paper reports on a recently developed simulation tool for modeling transport of molecular and particulate contaminants. Contamination modeling is of great importance to spacecraft designers, as even few monolayers deposited on a sensitive optical instrument or a high voltage detector can severely impact its performance [1]. Historically, contamination has been modeled using ray tracing methods [2]. CTSP (Contamination Transport Simulation Program) was developed to address several shortcomings of such tools. CTSP follows approach similar to Particle in Cell (PIC) or Direct Simulation Monte Carlo (DSMC) and concurrently traces many simulation macroparticles [3]. This allows the code to compute not only the surface flux, but also the number density and partial pressure of contaminants. Particles are advanced using the Leapfrog method. The code can thus consider forces acting on the molecules, including electrostatic attraction, or in the case of larger particulates, aerodynamic drag, gravity and orbital motion. But unlike PIC or DSMC codes, CTSP does not require a volume mesh. Octree is used to efficiently select surface elements to test for particle impacts. The code includes a detailed outgassing model that lets structures consist of a mixture of trapped gases and a multi-component surface layer of adsorbed contaminants. Diffusion rates and molecular residence times are computed considering surface temperature and activation energies. This allows CTSP to naturally consider the effect of surface temperature on deposition rates. Figure 1a) compares the partial pressure of water inside a vacuum chamber with a warm (left) and a cold shroud (right). A shroud below the water condensation temperature leads to water molecules “sticking” to the shroud, which also leads to an overall decrease in water partial pressure. If the temperature of the shroud increased to model thermal transition, the adsorbed water would automatically release once the shroud crossed the condensation temperature. Such “dumps” of water are common in thermal vacuum testing and can lead to significant pressure spikes [4]. Figure 1b) shows another application for modeling the environment near a satellite. Here the density of contaminants released by spacecraft vents is plotted along with surface deposition rates. Coupling such a simulation with a decay rate model for the outgassed fluxes can provide operators with an insight on when it is safe to open instrument doors. These two cases are considered in detail in the paper. The paper begins by describing the numerical approach used by CTSP, along with the particle push, octree implementation, and the surface model. Spatial variation in partial pressures in a vacuum chamber is then considered. Virtual QCM and pressure gauge are implemented. Molecular environment near a generic spacecraft is considered next. Here we present recent work to model electrostatic return using Green’s functions. The paper is concluded with few remarks on a recent effort to parallelize the code and speed up the performance by utilizing GPUs.

Figure 1. a) Comparison of the effect of shroud temperature on water vapor partial pressure in a vacuum chamber. b) Molecular deposition rate due to outgassing and venting, and number density of vented contaminants

REFERENCES

Drag Acting on a Spherical Particle: Numerical Analysis of a Fundamental Problem and Its Application

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The study of a flow of a rarefied gas past a sphere (spherical particle) is one of the most fundamental problems in rarefied gas dynamics [1, 2]. The information on the drag plays an important role in aerosol science. The problem has been investigated by many authors (e.g., [3, 4]) on the basis of the linearized Boltzmann equation or its kinetic models. Recently, the analysis was extended to a weakly non-linear case, and the correction to the linear drag due to the small but finite flow speed was obtained, by means of an asymptotic analysis of the Boltzmann equation for small Mach numbers [5]. According to [5], the drag up to the second order of the Mach numbers is expressed as follows:

\[
F_D = \frac{p_\infty L^2}{\rho_0} \left( 1 - \frac{c_1(k) \epsilon}{2 \gamma_1} \right) h_0(k),
\]

where \(F_D\) is the drag, \(v_\infty\) is the velocity of the uniform flow at infinity, \(T_\infty\) its temperature, \(p_\infty\) its pressure, \(L\) the radius of the sphere, \(R\) the (specific) gas constant, \(\gamma_1\) the constant related to the viscosity \(\mu_\infty\) at the reference equilibrium state by \(\mu_\infty = (\sqrt{\gamma_1/2}) \gamma_1 p_\infty (2RT_\infty)^{-1/2} \ell_\infty\) (\(\ell_\infty\) is the molecular mean free path), and \(k = (\sqrt{\gamma_1/2}) \kappa\) with \(\kappa = \ell_\infty / L\) being the Knudsen number. \(\epsilon\) is a small parameter defined by \(\epsilon = \vert v_\infty \vert / (2RT_\infty)^{1/2} = (5/6)^{1/2} M_a\), where \(M_a = \vert v_\infty \vert / (5R T_\infty/3)^{1/2}\) is the Mach number of the flow. The numerical functions \(h_0(k)\) and \(c_1(k)\), which essentially depend on the Knudsen number (or \(k\)), represent the linearized drag and its nonlinear correction, respectively. It should be stressed that the correction \(c_1(k)\) is obtained through the analysis of the linearized problem (without solving the second-order problem).

The accurate numerical values of \(h_0(k)\) are known for a hard-sphere gas as well as for the BGK model, and can be found in [4]. However, as for \(c_1\), only preliminary results were obtained in [5] for the BGK model. In this study, we first revisit the classical problem of a flow past a sphere and obtain \(c_1\) (and \(h_0\)) on the basis of the ellipsoidal-statistical (ES) model (with the Prandtl number \(Pr = 2/3\)) under the diffuse reflection boundary condition. Then, we compute the drag from the formula (1) with the aid of the obtained \(h_0\) and \(c_1\). A comparison of the drag between the different models is also made.

Figure 2 shows the drag \(F_D(= |F_D|)\) obtained from (1) as a function of the Mach number \(M_a\) in the case of \(Kn = 1\). The solid (dashed) line represents the result for the BGK (ES) model. The open symbol represents the result of the DSMC computation by Volkov [6] for a slowly rotating sphere. The overall agreement is quite good both for the BGK and ES models.

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### Session 42: Non-Equilibrium Flows II

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Vibration-dissociation coupling in multi-temperature viscous gas flows

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Correct modeling of non-equilibrium process rates remains an important question in the study of high-temperature viscous gas flows. A number of models have been developed to account for cross-coupling between various slow processes which occurs in non-equilibrium flows, including semi-empirical models [1,2] and more rigorous ones [3,4], some of which also take into consideration anharmonicity of vibrational spectra [4], but most of these models do not account for viscous effects. A few comparisons to strict self-consistent models for vibrational and chemical relaxation rates have been performed in [5,6]. However, the influence of different factors, such as the degree of vibrational non-equilibrium, velocity divergence and mixture composition on these rates in viscous flows remains poorly studied, and the applicability of various simple and semi-empirical models, such as the Treanor–Marrone model and the Landau–Teller equation has not been assessed properly for strongly non-equilibrium flows.

In the present study we use a self-consistent kinetic theory approach to model vibrational and chemical relaxation in viscous binary mixture flows, accounting for cross-coupling effects between these processes. Expressions for first-order corrections to the rate coefficients are obtained and compared with other models (the FHO model [7] for vibrational energy transitions, the Park [8] and Treanor–Marrone [1] models for dissociation reactions). Vibrational relaxation rates are compared to the widely used Landau–Teller model and its modifications [6, 9]. Vibration-dissociation coupling terms are also compared to those given by other models [1].

The proposed self-consistent models are applied for simulations of flows behind strong shock waves and in nozzles to estimate the influence of various degrees of thermal and vibrational non-equilibrium on vibrational and chemical relaxation rates. Vibrational relaxation times are also computed for these flows based on a kinetic theory definition [6, 9], and compared to the widely used Millikan–White [10] model and Park’s correction [2], to assess the influence of various flow conditions on vibrational relaxation rates and study the applicability of the Landau–Teller formula.

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Non-Equilibrium Heat Transfer in a Cavity Flow in Rarefied Regime

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Recent development in micro- and nanoelectromechanical systems (MEMS/NEMS) has generated extensive interests in studying gaseous flows in these systems. Gas flows at these scales involve complex processes due to rarefaction. It is well accepted that standard continuum methods like the Navier-Stokes-Fourier are inadequate to describe gas flows in the transition and slip flow regimes. Molecular based methods are usually adopted to simulate such flows. Among the molecular based methods is the Direct Simulation Monte Carlo method (DSMC). It solves the Boltzmann equation and is currently the dominant numerical technique for simulating gas flows in transition regime. However, the computational cost of this method is high in comparison with continuum methods. Volume diffusion (bi-velocity) continuum model offers an alternative continuum method for simulating rarefied gas flows [1]. According to this model, at higher Knudsen numbers the contribution of molecular spatial stochasticity increases. Previous works have shown that results from volume diffusion model improves Navier-Stokes-Fourier predictions [2]. In the present study, we simulate a nano-cavity heat transfer problem as it provides an excellent test for a new continuum flow method. Simulations are carried out for Knudsen numbers within the slip and higher transition flow regimes where non-local-equilibrium and rarefaction effects dominate. We contrast predictions by a Navier-Stokes-Fourier model corrected by volume diffusion flux in its constitutive equations to that of the direct simulation Monte Carlo (DSMC) method and the standard Navier-Stokes-Fourier model.

Fig. 1. Energetic heat flux (a) lines overlaid on the temperature contour for Kn = 1 in comparison with DSMC heatflux (b)

The results confirm existence of the unconventional cold-to-hot heat transfer for large Knudsen numbers (Fig.1). Strong non-equilibrium features are captured by the volume diffusion model. Some agreements with DSMC are observed. The new model also allows description of Knudsen boundary layer in the temperature and velocity fields.

REFERENCES


Non-equilibrium Reaction Rates in Air Flows Behind Shock Waves. State-to-state and Three-temperature Description

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In this paper non-equilibrium rates of dissociation and Zeldovich exchange reactions in shock heated air flows are studied in the frame of state-to-state and three-temperature flow description. Prediction of non-equilibrium reaction rates in high-temperature air flows is very important for gas dynamic problems and was considered in many papers for various conditions using different kinetic theory approaches (see Refs. in [1]). The influence of non-equilibrium vibrational kinetics on reaction rates behind shock waves [2] and in nozzle flows [3] was studied for dissociation in binary mixtures N$_2$/N, O$_2$/O and for exchange reactions N$_2$(i)+O=NO+N, O$_2$(i)+N=NO+O in the five-component shock heated air flows [1].

In the present paper we apply the method developed in [2], [3], [1] for study the rates of dissociation and exchange reactions in the flows of air mixture N$_2$(i)/O$_2$(i)/NO/N/O behind shock waves by averaging state-dependent reaction rate coefficients with vibrational distributions obtained in different approaches. Firstly, governing equations for macroscopic air flow parameters in the relaxation zone behind a shock have been solved numerically in the state-to-state, three-temperature and one-temperature kinetic theory approximations for different free stream conditions. Then state-dependent rate coefficients for N$_2$ and O$_2$ dissociation and exchange reactions were averaged with 1) state-to-state distributions, 2) two-temperature Treanor distributions, 3) one-temperature non-equilibrium Boltzmann distributions depending on vibrational temperatures and 4) thermal equilibrium distributions. State-dependent rate coefficients are calculated using the Treanor-Marrone model [4] for dissociation and expressions proposed by Warnatz et al. for exchange reactions [5].

Variation of global reaction rate coefficients obtained in different approaches along the relaxation zone is studied and numerical estimates for differences between reaction rate coefficients found in the frame of the most accurate state-to-state approach and using more simple two-temperature and one-temperature distributions are obtained for various distances from the shock front.

ACKNOWLEDGEMENTS

This study is supported by Saint Petersburg State University (grant 6.50.2522.2013) and Russian Fund of Basic Research (project 15-01-02373).

REFERENCES

Heat Transfer in Nonequilibrium Boundary Layer Flow past a Partly Catalytic Wall

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Surface catalysis has huge influence on the aeroheating performance of hypersonic vehicles. In the reentry flow problem of a traditional blunt vehicle, it is reasonable to assume a frozen boundary layer surrounding the vehicles’ nose, and atoms can only recombine and release heat on the catalytic wall. As a result, the heat conducted across the boundary layer to the wall surface could be decoupled with the heat transfer due to the atoms diffusion. However, it is shown at present that when considering a hypersonic cruise vehicle flying in the medium-density air space, the boundary layer flow around its sharp leading-edge is likely to be nonequilibrium rather than frozen due to rarefied gas effects. The atoms that leave a partly catalytic wall surface could also recombine into molecules and release heat in the near-wall flow field, which will alter the heat conduction across the boundary layer and may even lead to significant influence on the total heating characteristics. This new feature results from the coupling of the rarefied nonequilibrium near-wall flow field and the partly catalytic wall surface and is beyond the scope of classical aeroheating prediction theories.

In this paper, the theoretical modeling and the direct simulation Monte Carlo (DSMC) method are employed to study the corresponding mesoscopic flow, reaction and heat transfer phenomena near the leading edge of the near space hypersonic vehicles. Since the recombination reaction involves triple collision of atoms (or molecules), its reaction rate is proportional to the square of gas density. Therefore, even for the same rarefaction degree, the boundary layer flow around a re-entry vehicle at a high altitude can be considered as frozen, but in the corresponding flow around a sharpened nose flying at a relatively low altitude, the gaseous recombination effects could not be directly ignored and the boundary layer is likely to be chemical nonequilibrium[1]. The binary collision law becomes invalid to model the rarefied nonequilibrium flow when the triple collision (leading to exothermic recombination reaction) and the binary collision (leading to endothermic dissociation reaction) are both important, and thus the physical mechanism should be clearly discussed and the flow similarity (if it still exists) should be revisited in the current flow problem. Based on a theoretical analysis and DSMC simulation of various flow cases considering ranging density, nose radius, velocity and catalysis properties, the coupling effects between the nonequilibrium boundary layer and the partly catalytic wall are quantitatively discussed and evaluated.

REFERENCES

Microscopic Analysis of the Combustion Induction Period in Auto-Ignition at Low Temperature

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Combustion is a complex problem involving multi-scale physical processes and multi-stage chemical reactions. Physical processes at different length scales affect overall or local combustion behaviours, even for homogeneous premixed combustions. For instance, the auto-ignition at low temperature may become non-homogeneous as localized ignition spots will appear randomly in the physical space [1]. Localized ignition has been studied in the literature. It is generally believed that the chain reactions at those spots are accelerated by various physical effects, including temperature or pressure fluctuation and surface reactions. But the region where ignition starts is not fully studied and the microscopic characteristics of local ignition are not well understood.

The ignition process can be divided into two stages, the induction period and thermal explosion period. During the induction period, a small part of fuel and oxygen will convert to radicals (such as H, O, OH) at a rather low rate. The rate to generate radicals depends strongly on the temperature. At low temperature, the radicals are generated from time to time and are distributed randomly in the space, which is resulted from random molecular collisions subjected to thermal fluctuation.

The typical ignition delay time is plotted in Fig. 1, which shows that low temperature ignition has long ignition delay time. Accurate prediction of the ignition delay time, however, has to be related to the understanding of microscopic combustion processes.

In this work, we employ kinetic theory and DSMC method to analyze the microscopic behaviour of auto-ignition in a hydrogen-oxygen mixture. It can be shown that the average ignition delay time depends on the volume of the considered system (Fig. 2). We argue that randomness is the reason to account for the difference of the ignition delay time between a tiny system and a big system. Namely, there is a tiny spot in a big system that will generate radicals in a much fast pace than other locations, and this tiny spot sparks the reactions in other locations. The location of this spot and time for the initial appearance of radicals in this spot is randomly though. We find that the randomness exists in different step of chemical reactions and their influence on the ignition delay time behaves quite differently, which will be detailed in the full paper. The effects of discrete nature of particles and thermal movement will be also addressed.

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Session 43: Heat and Mass Transport

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An investigation of a mixed convection in a rarefied gas

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Natural convection is found in various engineering applications such as cooling nano- or microelectronic devices, petroleum reservoirs or solar energy collectors. Heat transfer in flows in which there is a combination of forced and natural convection are referred to as mixed convection and are complex phenomena due to interaction of different forces [1]. Flows in such applications can be in the transition or slip flow regimes where Navier-Stokes-Fourier loses their validity while molecular based methods such as Direct Simulation Monte Carlo method become computationally expensive.

A new approach to the continuum description of a fluid accounting for its non-continuum aspect has been recently introduced [2]. This theory was first proposed based on the observation in thermophoresis experiments [3]. The underlying principle is the existence of two independent velocities in any continuum fluid; the volume velocity and the mass velocity. The resulting equations are completed in a thermo-mechanically consistent continuum flow equations [4].

In the current study we simulate a mixed convection (natural convection in a lid-driven cavity) problem of a rarefied gas. We carried out simulations in a wide range of Knudsen number. We compare volume diffusion model in a modified solver under OpenFOAM with standard Navier-Stokes-Fourier.

![Temperature distribution and heat fluxes at Kn = 1 for the (a) energetic heat flux \( J_u \), (b) entropic heat flux \( q_{ve} \) and (c) heat flux for the conventional NSF \( q_{NSF} \).](image)

Volume diffusion model shows slip at the walls for Kn > 0.5. For higher Knudsen numbers volume-diffusion model captures non-local equilibrium effects in corners of the cavity and an unconventional cold-to-hot heat transfer (Figure 1).

We show that adding volume diffusion correction to the Navier-Stokes equation allow to describe non-local equilibrium phenomena at micro/nano scale in this configuration.

REFERENCES


Convective Heat Transfer to a Flat Plate in Rarefied High Mach Number Flow

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Aerodynamic heating in high-speed gas dynamics presents one of the most serious challenges in the design of super- and hypersonic vehicles and propulsion systems [1]. Rarefied high-Mach-number gas flow past a sharp flat plate in the slip-flow regime (0.001 ≲ Kn ≲ 0.1) provides the fundamental knowledge of how wall heat transfer and skin friction scale with the key dimensionless flow parameters.

Of special interest in high-speed convection heat transfer is the recovery temperature $T_r$ [2, 3, 4], which is the temperature of wall reaching thermal equilibrium with the gas flow. $T_r$ is usually represented by the dimensionless recovery factor $r_c$. Theoretical work by Pohlhausen [5] and van Driest [6] provided solutions to the laminar compressible boundary-layer equations for a flat plate in the continuum-flow regime (Kn < 0.001). The famous relation $r_c \approx \sqrt{Pr}$ for a flat plate in the continuum-flow regime has been derived analytically [5], validated experimentally [7] and verified by van Driest’s similarity solutions. But validity of this important relation has been mistakenly extended into the slip-flow regime without justification for decades till this day. This paper will focus on seeking solutions from the Illingworth (also called Lees-Dorodnitsyn) similarity equations and full Navier-Stokes-Fourier equations (modified with slip and jump boundary conditions in both approaches). $r_c$, the Nusselt number Nu and skin friction coefficient $C_f$ for a flat plate are presented as a function of Re, Ma and Kn in the slip-flow regime. The case for using the correct recovery temperature for defining convection heat transfer coefficient is also presented.

References


Polyatomic Gases; Macroscopic Boundary Conditions and Heat Conduction Analysis

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A high-order macroscopic model for the accurate description of rarefied polyatomic gas flows is introduced based on a new proposed kinetic model [1]. The different energy exchange processes are accounted for with a two term collision model. The proposed kinetic model, which is an extension of the S-model, predicts correct relaxation of 4 higher moments and delivers the accurate Prandtl (Pr) number. Also, the model has a proven H-theorem.

The order of magnitude method [2,3] is applied to the primary moment equations to acquire the optimized moment definitions and the final scaled set of Grad's 36 moment equations for polyatomic gases. At the first order, a modification of the Navier-Stokes-Fourier (NSF) equations is obtained, which shows considerable extended range of validity in comparison to the classical NSF equations in modeling sound waves. At third order of accuracy, a set of 19 regularized PDEs (R19) is obtained. Furthermore, the terms associated with the internal degrees of freedom yield various intermediate orders of accuracy, a total of 13 different orders.

Thereafter, boundary conditions for the proposed macroscopic model are introduced. The unsteady heat conduction of a gas at rest is studied numerically and analytically as examples of boundary value problem. The results for different gases are given and effects of Knudsen numbers, degrees of freedom, accommodation coefficients and temperature dependent properties are investigated. For some cases, the higher order effects are very dominant and the widely used first order set of the Navier Stokes Fourier equations fails to accurately capture the gas behavior and should be replaced by the proposed higher order set of equations.

ACKNOWLEDGEMENTS

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REFERENCES

Adjoint Formulations for Accelerating Monte Carlo Simulations

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We discuss adjoint formulations of the linearized Boltzmann equation as a means of providing computational benefits in the simulation of practical problems of interest. Although this talk will focus on phonon transport following the extensive description in [1], adjoint formulations are relevant to a variety of fields, including rarefied gas dynamics [2]. We first derive the adjoint formulation for the linearized Boltzmann equation describing phonon transport under the relaxation-time approximation. We then discuss the computational implications of this formulation resulting from the connection it provides between the forward problem of interest and the adjoint problem defined below. The duality between these two problems is facilitated by generalizing the role of initial and boundary conditions to those of particle emitters and the role of ensemble averaging to that of a particle detector. Under this generalization, moments of the distribution function in the forward (original) problem, can be calculated, with no approximation, by considering a backward problem in which computational particles are emitted by the original problem detectors, travel backward in time, and are collected by the emitters of the original problem. By switching emitters and detectors, this approach makes large computational savings possible; provided the original source is larger than the original detector, using the original source as the detector increases the number of particles that contribute to the signal and thus reduces the statistical uncertainty associated with the averaging process. The computational speedup scales with the relative size of the source and detector and can be quite large in problems where very high resolution is required in small regions of phase space (including spectral resolution). We note that the adjoint formulation and the associated benefits are not limited to Monte Carlo methods relying on deviational formulations [3-5]; we expect similar benefits when applied to other types of Monte Carlo techniques such as DSMC.

We also show that the proposed adjoint-based methods are particularly well suited to problems involving a wide range of length scales (e.g., nanometers to hundreds of microns) and lead to computational methods that can calculate quantities of interest with a cost that is independent of the system characteristic length scale, thus removing the traditional stiffness of kinetic descriptions.

ACKNOWLEDGEMENTS

This work was supported, in part, by the Singapore-MIT Alliance and in part by the Solid-State Solar-Thermal Energy Conversion Center (S3TEC), an Energy Frontier Research Center funded by the US Department of Energy, Office of Science, Basic Energy Sciences, under Awards No. DE-SC0001299 and No. DE-FG02-09ER46577.

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Session 44: Moment Equations III

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The Analysis of Different Variants of R13 Equations Applied to the Shock-Wave Structure

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This study is devoted to the investigation of linear and four nonlinear variants of regularized thirteen moment set of equations (R13) obtained for Maxwell molecules [1]. The difference between the sets of R13 equations is in definition of higher order moments. The work continues the analysis [2-4] of the R13 equations based on numerical results for shock-wave structure problem for monatomic Maxwell gas. The goal of the present study is to get the answer to assess the boundaries of the applicability of the R13 variants to numerical modelling of supersonic nonequilibrium flows in terms of the shock-wave Mach number and the local Knudsen number defined in several different ways. In this work the local Knudsen number is based on gradients of density, temperature, heat flux and stress tensor components ([5]). R13 numerical results have been compared and analyzed with DSMC results obtained with SMILE software system [6]. The shock-wave structure has been obtained in a wide Mach number range (from M=1.0 to M=10.0). The detailed analysis of gas macro-parameters’ profiles inside the shock will be presented in the full-length paper.

ACKNOWLEDGEMENTS

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M1 for rarefied gas dynamics

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This paper is devoted to the derivation and the implementation of an angular moment model from a BGK model. The motivation of deriving such models is to get intermediate descriptions between fluid and kinetic ones. Indeed, they are a good compromise between the precision of kinetic models and the cheap cost of fluid models. They are derived by extracting angular moments from the kinetic equation and by specifying a closure on the distribution function. This closure guarantees in particular that the moment system that is written is closed. In the present case, the closure is constructed by solving an entropy minimisation problem ([1], [2], [3]). These models have been mainly developed in the context of radiative transfer and plasma physics. But in the present work we apply them to a rarefied gas dynamics context. Moreover, these models are not in general Galilean invariant ([4], [5]). One solution is to consider the moving frame associated to the gas flow and to extract the moments with respect to this frame. Hence, applying this approach to a BGK model, we are able to construct a moment model that satisfies to Galilean invariance. Finally, we implement and validate the model on some test cases.

REFERENCES

The use of moment closures for the numerical prediction of gaseous flows, in both general nonequilibrium and near-equilibrium continuum regimes, provides several immediate advantages. The closures lead to transport equations for an extended set of macroscopic quantities or moments that provide descriptions of gaseous flow behaviour that are potentially valid from the continuum limit, through the transition regime, up to and approaching the near-collisionless or free-molecular flow limit. This is in contrast to traditional fluid-mechanic descriptions, such as the Euler and Navier-Stokes equations, which are only valid in or near local equilibrium and are therefore inappropriate for situations with significant deviations from equilibrium. Large deviations from equilibrium are common for micro-scale flows, highly rarefied flows, and flows with extreme gradients, such as those encountered in shock waves.

In addition to the modelling advantages, moment closures present many numerical advantages. The moment approaches are much less expensive than particle simulation techniques commonly used to described non-equilibrium gaseous flows (e.g., direct-simulation Monte Carlo (DSMC) methods), particularly for near-continuum and low-speed flows. Moreover, the generally first-order nature of moment equations allows for the prediction of viscous or heat-transfer effects without the need for the evaluation of second derivatives (this is in direct contrast to the Navier-Stokes equations). Numerical solutions to first-order hyperbolic equations are less sensitive to grid irregularities that often result from adaptive-mesh-refinement or embedded-boundary techniques. Removing the requirement for the discretization of higher than first-order derivatives also means that numerical solution schemes can gain an extra order of spatial accuracy for the same reconstruction stencil when compared to descriptions requiring the discretization of second-order derivatives. Accurate numerical schemes have been devised which are well-suited to the solutions of hyperbolic partial-differential equations, including upwind Godunov-type finite-volume and discontinuous-Galerkin schemes, and which can exploit the computational advantages offered by adaptive mesh refinement (AMR). While accurate solution methods have also been developed for equations have an elliptic and/or parabolic nature, the development of effective schemes with AMR that handle conservation equations of mixed type with equal elegance has proven to be significantly more of a challenge.

The accurate and efficient numerical solution of moment closures for describing viscous and heat-conducting phenomena of continuum-limit and non-equilibrium gaseous flows in three space dimensions is considered. In particular, a fully-implicit finite-volume scheme with a scalable block-based AMR strategy is described for on three-dimensional, multi-block, body-fitted hexahedral computational meshes is discussed and applied to the solution of hyperbolic and regularized moment closures based on maximum-entropy formulations. The application of the moment closures to a range of canonical near-equilibrium and non-equilibrium flows, including channel flows and flow past cylinders and spheres, is examined and the potential computational benefits of the moment techniques are explored.
Session 45: Non-Equilibrium Flows III

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Vibrational Specific Simulation of Nonequilibrium Radiation from Shock-Heated Air

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During a hypersonic reentry into a planetary atmosphere, a massive amount of the free stream kinetic energy is converted, across a strong bow shock wave through inelastic collisions, into internal energy of the gas. After the shock, in the relaxing flow, the competition between various collisional and radiative processes occurring at different time scales rules the distribution of the energy in the dissociating, ionizing and radiating flow. When the time scale of collisional processes of internal levels and the chemical time scale is comparable with the aerodynamic one, internal levels of heavy species are not populated according to the Maxwell-Boltzmann distribution. Particularly sensitive, in this respect, is the population density of internal energy level of NO which is governed by complex channel of NO formation following on a strong coupling between chemical kinetics to the vibrational kinetics. Standard multi-temperature (MT) models [1] describe the coupling with a phenomenological and somewhat *ad hoc* approach. Since, however, vibrationally specific rate coefficients from *ab initio* methods are becoming available to describe vibrational relaxation and reactive processes, it is interesting to study the nonequilibrium radiation from shock-heated air with a vibrationally specific, or state-to-state (StS) approach [2].

In this study, shock waves in air are simulated with a StS approach, making use of recent QCT results for the Zeldovich exchange reactions of NO formation on theoretically calculated Potential Energy Surfaces (PES) [3-4]. Fig.1 shows the formation of NO in a typical case. The radiative signature is determined on the basis of the spectroscopic database HTGR [5] tabulating exhaustive radiative properties validated at high temperature for NO and N$_2$ radiative systems. Simulated spectra are compared to shock tube measurements performed in Moscow [6] in conditions representative of Earth entries (v ~ 4-8 km/s).

REFERENCES

Similarity Criteria in Vibrationally and Electronically Excited Gases

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Fluid dynamic equations written in the dimensionless form depend on well known similarity criteria like Reynolds (Re), Mach (M), Prandtl (Pr), Schmidt (Sc) or Lewis (Le) numbers. The common practice in computational fluid dynamics is to assume the numbers associated with heat transfer and diffusion, i.e. Pr, Sc and Le to be constant. While in local equilibrium or under conditions of weak deviations from equilibrium this assumption does not considerably affect the accuracy of predicted flow-field and heat fluxes, its validity for strongly non-equilibrium flows has not been thoroughly assessed up to now, except a few works [1,2].

In the present study, we consider two types of strongly non-equilibrium flows. The first case is related to one-temperature chemically non-equilibrium flows of gases with electronically excited atoms and molecules. As is shown in [1,3,4], for high temperatures the internal heat conductivity coefficient of atoms (which is basically zero if electronic excitation is neglected) exceeds significantly that of molecules. On the basis of data for viscosity, thermal conductivity and diffusion coefficients obtained using kinetic theory algorithms, the behavior of Prandtl, Schmidt and Lewis numbers for N2/N and O2/O gas mixture flows is studied. For monatomic gases the Prandtl number is commonly assumed to be equal 2/3. However, taking into account excitation of electronic degrees of freedom yields a non-constant Prandtl number which becomes a non-monotonic function of temperature. The behaviour of Lewis number is inverse to Prandtl number (since Schmidt number monotonically decrease). The effect of mixture composition on the Pr, Sc and Le numbers is also evaluated in a wide temperature range.

Another type of a strongly non-equilibrium flow considered in this paper is the binary mixture flow with completely coupled VV, VT relaxation and dissociation behind a shock wave. We apply the state-to-state transport theory algorithm developed in [5] to calculate heat conductivity, shear viscosity and diffusion coefficients and corresponding dimensionless numbers as functions of the distance from the shock front for different initial conditions considered in [6]. In the state-to-state approach, Sc and Le numbers depend not only on the chemical species but also on the vibrational state. The influence of initial Mach number and initially non-equilibrium vibrational distributions on the dimensionless numbers behind the shock front is evaluated.

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Approximating the M2 Method for Radiative Transfer in Slab Geometry

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We consider moment closure for radiative transfer equation in slab geometry. The standard spectral method known as the \( P_n \) equation suffer from the drawback that their solution does not remain realizable [4]. The Mn method, where the energy density is reconstructed by solving a constrained strictly convex optimization problem, has all the desired qualities. They are hyperbolic equations in conservative form, all moments evolve in the realizable set, and they satisfy an entropy dissipation law [3]. However, Mn moment equations are expensive and difficult to implement because in general the defining optimization problem must be solved numerically and can be ill-posed [1]. We look at the simplest member of the hierarchy of the extended quadrature method of moments (EQMOM) studied in [5], which gives equations for the zeroth-, first-, and second-order moments of the energy density of photons in the radiative transfer equations in slab geometry. First we show that the equations are well-defined for all moment vectors consistent with a non-negative underlying distribution, and that the reconstruction is explicit and therefore computationally inexpensive. Second, we show that the resulting moment equations are hyperbolic. These two properties make this moment method quite similar to the attractive but far more expensive M2 method. We confirm through numerical solutions to several benchmark problems that the methods give qualitatively similar results.

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## Session P1: Space Vehicle Aerodynamics

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Thermal Lift Generation and Drag Reduction in Rarefied Aerodynamics

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In the aerodynamic design of new technologies in low ambient pressures such as Hyperloop and Mars exploration helicopter, the quantifying the effect of rarefied atmosphere become crucial for not only understanding the flow dynamics in continuum breakdown regions but also finding the areas of potential application of new physics. For example, an effect which is only be effective in non-continuum regime such as thermal transpiration can be exploited to control the flow separation and create lift using the excess heat generated in these applications. In this aspect, main goals of this study is to investigate the feasibility of using the temperature gradient for lift generation and drag control for airfoils slip regime. As an initial study, a NACA 0012 airfoil is studied with a high temperature surface on the bottom for the lift creation for different Knudsen numbers. Lift coefficients for different Knudsen numbers can be seen in Figure 1 (a) with the solution of Ellipsoidal statistical Bhatnagar-Gross-Krook (ES-BGK) Boltzmann equation (solid lines) and Continuum Ansys Fluent solver (dashed lines). It was seen that for lower velocities, continuum solver under predicts the lift generation when the Knudsen number is 0.00129 due to local velocity gradients reaching slip regime although lift coefficient is higher with the Boltzmann ES-BGK solutions as shown in Figure 1 (b).

Similarly, the feasibility of using thermal transpiration for drag reduction is studied. Initial study in drag reduction includes an application of a thermal gradient at the upper surface of a NACA 0012 airfoil near trailing edge at a 12-degree angle of attack and 5 Pa pressure. It was seen that the thermal gradient makes streamlines closer at the separation location due to transfer of momentum. Furthermore, the drag is reduced by 4% when the thermal gradient was applied in this pressure. The final paper will include the effect of length and strength of the thermal gradient on the drag reduction and lift generation.

Figure1: (a) Lift coefficient versus Mach number for different Knudsen numbers with ES-BGK (solid line) and NS (dashed line) solvers. (b) Local Knudsen number contours based on temperature gradients for Kn=0.00129. (c) A thermal gradient application on NACA 0012 airfoil for drag reduction and streamlines

References

DSMC Simulation for Effects of Angles of Attack on Rarefied Hypersonic Cavity Flows

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The thermal protections system is a crucial element in atmospheric re-entry missions of aerospace vehicles. Usually, in the thermal load calculations, the analysis assumes that the vehicles has a smooth surface. However, discontinuities or cavities between the thermal protection plates have to be expected due to sensor installation, fabrication tolerance, and different expansion rates of no-similar materials. Such surfaces discontinuities may constitute a potential source of enhanced heat flux to the vehicle surface, or even cause a premature transition from laminar to turbulent flow [1]. To operate safely, it is necessary to predict the flow field structure and these consequently undesired thermal loads. Quantities of theoretical, experimental, and numerical studies have been conducted for the purpose of investigating the effect of cavities present on the vehicles' surface on the aerodynamic properties. However, the majority of studies in the literature have focused on solely on hypersonic flows over cavities in the continuum regime. As a matter of fact, very little information has been available on these problems in the rarefied regime, except that several researchers [2-5] have studied rarefied hypersonic cavity flows by employing the direct simulation Monte Carlo (DSMC) technique, with the emphasis on investigating the effects of the length-to-depth of the cavity on the flow field structure and aerodynamic surface quantities. The present work extends the aforementioned previous studies by investigating two-dimensional rarefied hypersonic flows over a flat plate with a cavity (Fig. 1) by employing the DSMC method, focusing on the effect of angle of attack on aerodynamic properties. The primary goal is to assess the flow field structure and aerodynamic surface quantities, including heat transfer and pressure coefficients for a family of angles of attack (AOAs) at 80 km altitude in a re-entry environment. The density ratio \( \rho/\rho_\infty \) contours with streamline traces inside the cavity for two angles of attack, \( \alpha = 0^\circ \) and \( 30^\circ \) are presented in Fig. 2. It is apparent that the flows inside the cavities are characterized by a recirculation structure and a "dead-water" region. For the case of \( \alpha = 0^\circ \), the streamline pattern shows a primary vortex system filled in the upper-half region and a dead-water region in the remainder of the cavity. For the case of \( \alpha = 30^\circ \), a different flow structure is observed; a second vortex is formed just beneath the primary vortex, and the area of the "dead-water" region shrinks. As a result of the growing AOAs, the separated shear layer is able to penetrate deeper into the cavity and attach itself to the cavity walls, enhancing momentum and energy transfer to cavity walls. So, both the peak pressure and heat transfer coefficients increase with the AOAs, as Fig. 3 shows.

REFFERENCES

Fast and Accurate Prediction for Aerodynamic Forces Acted on Satellites Flying in Low-Earth Orbit

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A fundamental prerequisite for satellites operating in a Low-Earth Orbit (LEO) is the availability of fast and accurate prediction of non-gravitational aerodynamic forces [1], which is characterized by the free-molecular flow regime. Computational methods like the analytical integral method and direct simulation Monte Carlo (DSMC) technique are important tools in accurately computing aerodynamic forces. However, the former can’t deal with multiple reflections caused by complex or concave geometries, and the latter is computationally expensive and cannot be employed real time. Relatively speaking, the test particle Monte Carlo (TPMC) method [2] can reduce a large amount of storage capacity and computer time, and could simulate different gas surface interaction models for energy and momentum exchange [3]. What’s more, it can also model the effects of flow shadowing and multiple reflections caused by complex concave geometries [4].

This work has developed a general computer program for the accurate calculation of aerodynamic properties in the free-molecular flow regime using the TPMC method, and then aerodynamic forces acted on a satellite with two solar panels (Fig. 1), flying in a LEO at an altitude of 250 km, are calculated for different gas-surface interaction models by the computer program, with the effects of flow shadowing and multiple reflections quantitatively researched and analyzed.

Numerical calculations have been carried out for flows past a flat plate, and a comparison of drag coefficients between TPMC results and free-molecular flow theoretical formulas [5] is presented in Fig. 2. Obviously for three freestream speed ratios ($s = 1, 5, 10$), all TPMC results and analytical expressions match very well, proving that the method used here is valid. Having the computational method validated, aerodynamic drags acting on the satellite with two solar panels using the TPMC method are plotted in Fig. 3, with a comparison with results from the DSMC. It is evident that drag coefficients of this satellite increase with angles of attack, and both results are in good agreement.

However, according to Table 1, the expense of the TPMC is much less than that of the DSMC, showing its advantage over the DSMC in processing speed and consuming memory storage when dealing with aerodynamic properties of satellites flying in a LEO.

![Fig. 1: Schematic of a satellite with two solar panels.](image)

![Fig. 2: Drag coefficients of a flat plate with free-molecular flow over itself.](image)

![Fig. 3: Drag coefficients of a satellite with two solar panels at 250 km.](image)

| Table 1: The computational expenses of the TPMC and DSMC method in the case of the satellite with two solar panels flying at 250 km. |
| --- | --- | --- |
| Number of CPUs | TPMC | DSMC |
| Physical Memory (MB) | 4.52 | 72 × 34 |
| Time (second) | 500 | 69544 |

REFERENCES

Impact of Martian Atmosphere Parameters Uncertainties on Entry Vehicles Aerodynamics for Hypersonic Rarefied Conditions

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Martian exploration become more and more important in the future planetary mission. However, Martian climate condition is more complex comparing with earth’s. Its density is lower than earth’s, which results in that rarefaction effect appears at lower altitude for entry capsules. Existing experience about that gas properties is very limited. Uncertainties impact of gas properties on aerodynamics has to be considered in vehicles designing. In this paper, attempt has been made to analyze impact of Martian atmosphere parameters uncertainties on entry vehicles aerodynamics for hypersonic rarefied conditions with DSMC code, which has been validated by comparing Viking vehicles flight data with present computational results. Then, by simulating flows around Mars Science Laboratory (MSL), impact error of free stream parameters uncertainties on aerodynamics is investigated. The 20% amplitude variation of atmosphere parameters is considered. The results show that the present numerical results shows a good agreement with the Viking flight data. Fig.1 shows pressure contours around MSL in different density, and Fig.2 shows aerodynamics under different free stream gas parameter. Gas species influence aerodynamics much by comparing CO\textsubscript{2} for Mars with air model for Earth, gas species difference brings on 0.8\degree trim angle difference, so it is also necessary for hypersonic rarefied conditions that CO\textsubscript{2} correction should be made while the aerodynamic data is predicted by air model, which conclusion is consistent with continuum one. Uncertainties of free stream density and velocity also influence aerodynamics and pitching moment a little. Axial force coefficient and normal force coefficient decrease as increasing density. Trim angle of attack change about 0.5\degree when free stream density and velocity change about 20%. Aerodynamics can be little influenced by free stream temperature, which the maximum error is below 0.5%. Pressure center position is not sensitive to free stream parameters. Pressure center position predicted by CO\textsubscript{2} gas model is more closer to center of gravity than by air model.

References


Aerodynamic Characteristics of the Upper Stages of a Launch Vehicle in Low-Density Regime

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Aerodynamic characteristics of the orbital block (configuration after separation of nose fairing of the launch vehicle) and the upper stage (configuration after separation of lower stage) of the launch vehicle (KSLV-II, Korea Space Launch Vehicle) at high altitude of low-density regime are analyzed by SMILE code which is based on DSMC (Direct Simulation Monte-Carlo) method [1]. For validations of the DSMC code, aerodynamic coefficients of Apollo capsule are also calculated and the results agree very well with the data predicted by others [2]. For the additional validations and applications of the DSMC code, aerodynamics of simple shapes of plate, wedge, and cone-cylinder in low-density regime are also analyzed and compared with others [3]. Aerodynamic characteristics in low-density regime differ from those of continuum regime. Although the predicted aerodynamic forces of the upper stage of a launch vehicle are very small since the dynamic pressure is extremely low in low-density regime, the forces may affect motion of the upper stage and the orbital block of launch vehicle. Therefore, aerodynamic coefficients of the upper stage and the orbital block of the launch vehicle in low-density regime are analyzed as a function of Mach numbers and altitudes. The predicted axial force coefficients of the orbital block and the upper stage of the launch vehicle are very high compared to those in continuum regime. In case of the orbital block which flies at very high altitude (higher than 250km), all aerodynamic coefficients are more dependent on velocity variations than altitude variations. In case of the upper stage which flies at high altitude (80km ∼ 150km), all aerodynamic coefficients except coefficient of axial force are more dependent on Mach number variations than altitude variations.

REFFERENCES

Investigation of Bridging Method to Predict Rarefied Aerodynamics of Mars Entry Capsules

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Martian gas density is lower than earth’s, which results in that rarefaction effect appears at lower altitude for entry capsules. Entry capsules will suffer a long time rarefaction effect while descending. Aerodynamic predictions in the transitional regime between free molecular and continuum flows become important for mission studies of entry vehicles, which provides accurate analysis of trajectory dynamics. Bridging method is frequently used to predict aerodynamics in this regime, given that is much more efficient. However, this method includes much empirical parameters, which can be derived from experimental, flight or computational data. To improve this method accuracy much more, in this paper, attempt has been made to analyze applicability of different bridging relations based on the Mars Pathfinder data (Fig.1). The difference of aerodynamics predicted by seventeen gas/surface interaction models is investigated (Fig.2). Free molecular limit Kn effect on aerodynamics is analyzed lastly (Fig.3). The result show that bridging relations, gas/surface interaction models and free molecular limit Kn number influence aerodynamics much more. Present data predicted by erf-log bridging relation shows a good agreement with computational data predicted by Direct Simulation Monte Carlo (DSMC) method than others. However, this relation has to take much more time. Sin-squared bridging relation is more efficient than erf-log one with some accuracy loss which can be avoided most by adjusting free molecular limit Kn number. Data predicted by gas-surface interaction model 3 and 13 labeled by reference [4] is more consistent with flight data, the axial force coefficient difference predicted by both models is below 5%, and the normal force coefficient is below 1%. Aerodynamics data keep an excellent agreement with computational data when free molecular limit Kn number is about 50 for sin-squared bridging relations. Erf-log bridging relations is not sensitive to free molecular limit Kn number, but that Kn number value should be above 50 to keep the accuracy in free molecular regime.

Fig.1 Axial force coefficient predicted by different bridge method (MPF)

Fig.2 Viking flight data comparison with different gas/surface interaction model

Fig.3 Aerodynamics predicted by different free molecular limit Kn

References


Session P2: DSMC Applications and Development

Morozov, Plotnikov, **Rebrov**, Yudin, "DSMC Study of Hydrogen and Methane Flows in a Hot Tube"

Molchanova, Kustova, Kashkovsky, **Bondar**, "DSMC Modelling of CO₂ Vibrational and Dissociation Kinetics"
DSMC study of hydrogen and methane flows in a hot tube


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The method of Hot-Wire Chemical Vapor Deposition (HWCVD) is widely used for thin film deposition from an activated precursor gas. The thermal activation can be realized in a hot cylinder, which provides considerable molecular dissociation at internal surfaces. Of course, it is necessary to consider the possibility of the reverse reaction, i.e. recombination. The present work is dedicated to elaboration of algorithm of the direct simulation Monte Carlo (DSMC) method [1] and numerical study of rarefied flows of hydrogen and methane through a hot tungsten cylinder, taking into consideration the dissociation and recombination at its surface. Choice of hydrogen and methane is conditioned by their wide using under deposition of diamond-like films [2].

To describe the process of particle interaction with the surface, the model of specular-diffuse reflection [1] is used. It is supposed that a particle is reflected diffusely from the surface with complete accommodation of momentum and energy with the probability \( \alpha \) or specularly with the probability \( 1 - \alpha \). To describe dissociation and recombination, the coefficients \( \alpha_d \) and \( \alpha_r \) are used. A molecule at collision with the surface splits into two particles with complete accommodation of momentum and energy with the probability \( \alpha_d \) or remains invariant with the probability \( 1 - \alpha_d \). Similarly two particles recombine into one molecule, which is reflected from the surface with complete accommodation of momentum and energy with the probability \( \alpha_r \), or do not recombine with the probability \( 1 - \alpha_r \).

It should be noted that the gas flow in a cylindrical channel was studied in a considerable number of theoretical, numerical, and experimental works (see, e.g. the works [3, 4]). However, the vast majority of researchers considered gas flow regardless of possible influence of heterogeneous processes on the surface. The closest to the subject is work [5], where the flow of hydrogen in a high-temperature cylindrical tungsten channel is used to show the importance of considering the processes of dissociation and recombination in the analysis of gas dynamics of the flow in the tube.

The DSMC method is used as a numerical tool. The variable soft sphere (VSS) molecular model [1] was adopted for simulation of molecular hydrogen, atomic hydrogen, methane, and methyl. Experimental results from works [6, 7] were used for correction of dissociation and recombination coefficients. The elaborated algorithm was used to study the effect of heterogeneous processes of dissociation and recombination on the dissociation degree of hydrogen during outflow from the cylindrical tube.

The obtained results may be useful for optimization of gas-dynamic sources of activated gas.

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REFERENCES

DSMC Modelling of CO2 Vibrational and Dissociation Kinetics

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The detailed knowledge of physics of the flow at different flight altitudes is crucial for predicting aerothermodynamics of space vehicles entering the CO2/N2 Martian atmosphere. Numerical modeling is currently the main tool for studying high-enthalpy non-equilibrium flows especially for high altitudes because the use of ground-based facilities for such flow regimes is limited. The principal numerical technique for spacecraft high-altitude aerothermodynamics prediction is the direct simulation Monte Carlo (DSMC) method [1]. Since mid-90s, the method has extensively been used to calculate hypersonic flows for conditions of Martian entry (see Ref. [2-6]).

An accurate account for real gas effects, namely, the excitation of internal degrees of freedom and chemical reactions, was shown to be important for aerothermodynamics of various bodies in the Earth atmosphere. Similarly, it is important for the Martian atmosphere as well. The DSMC simulation of energy transfer between different molecular modes and chemical reactions is complicated for the Martian atmosphere. This is because CO2 is a triatomic molecular system with no existing comprehensive DSMC collision model. In the previous works rather simple phenomenological models have been applied for vibrational energy transfer and dissociation modelling. In particular, the vibration-vibration transfer process and vibrational favoring of dissociation reaction, both of which are of high importance for CO2 high-enthalpy flows (see e.g. [7]), have been ignored.

The present paper is aimed at developing DSMC collision models for vibration-vibration, vibration-translation and chemical reaction processes based on the best available theoretical and experimental data. In particular, the cross-sections of the energy transfer and chemical reaction processes are obtained by solving the ill-posed inverse problems using the inverse Laplace transform and the Tikhonov regularization method in the manner similar to [8] and [9], respectively. The full-length paper will contain the results of implementation of the models in SMILE++ DSMC code [10], their verification and examples of application to problems of high-altitude aerothermodynamics of Martian entry.

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### Session P3: Plumes and Jets

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<td>Ji, Sun</td>
<td>&quot;3D Kinetic Simulation of Near-Field Plume Flows from an Anode-Layer Hall Thruster&quot;</td>
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Gas adsorption is present in many natural, physical, biological, and chemical systems, and is widely used in industrial applications such as drying, capturing and using waste heat to provide cold water for air conditioning (adsorption chillers), water purification and in vacuum pumping (sorption pumps and cryopumps). In this process, the particle removal triggers a mass transfer towards the adsorbing surface, while the strong temperature difference between the gas flow and the adsorbing surface, ensures the presence of heat transfer. The modelling of such flow conditions in a rarefied environment can be tackled either by the solution of the Boltzmann equation or alternatively by the Direct Simulation Monte Carlo method [1]. Recent work on gas adsorption is presented in [2] and [3], but it is noted that the former investigation does not take into account the temperature difference between the adsorbing plate and the gas, while the second study is focused on one-dimensional single gas flow.

The aim of this paper is to extend further the study of the adsorption process by simulating the steady-state binary gas mixture flow impinging on a circular adsorbing disc by using the DSMC method. A 2D axisymmetric flow configuration is assumed and the temperature of the adsorption panel is kept constant and varies between 4.5K and 300K, while the temperature of the incoming gas is assumed at ambient conditions. The aim of this work is to perform a parametric analysis in order to study the influence of the gas-surface interaction, including the thermal accommodation coefficient and the sticking coefficient, on the overall flow quantities assuming relevant for cryogenic applications binary gas mixtures, as for instance helium-hydrogen and argon-helium mixtures. The numerical results consist of the calculation of quantities of practical interest, as for instance pressure, density and temperature in the vicinity of the adsorbing disk as well as the pumping speed of the panel. The presented results cover a wide range of the Knudsen number namely from the free molecular to viscous flow regime. Gas components separation and interaction have been investigated as well. The present theoretical/numerical investigation may provide a complete data base, which can be applied as a tool on the design and optimisation of any cryogenic pumping system.

REFERENCES

Simulation of Small Clusters Formation in Water Vapor Plumes

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Development of models for the water vapor nucleation is of prime importance for the Earth and comets atmosphere physics, aerospace- and nanotechnologies. This paper presents the model for water oligomer formation/decay and corresponding DSMC modeling results for the stationary plume expanding through the orifice into vacuum. Related Knudsen numbers calculated via the orifice radius correspond to the transition and near-continuum flow regimes. Within the proposed model water molecules dimerization is considered as purely collisional, when dimer formation is described via triple collision and the reverse process (dissociation) occurs via the monomer-dimer collision. Higher clusters are formed via monomer-cluster collisions, and decay via unimolecular reactions. The probabilities of all kinetic processes are functions of individual (relative) velocities of particles, their internal energy and the number of internal degrees of freedom. The relations between those probabilities and the macroscopic rate constants (being the functions of the temperature) of corresponding reactions are discussed. The rate constants of the forward and reverse reactions are connected by the corresponding equilibrium constants. Within DSMC method elastic collisions of water monomers are described by VHS-model, monomer-cluster collisions are described via HS-model.

The outflow of pure water vapor from the reservoir through the round orifice into vacuum is considered. DSMC simulations being performed correspond to the constant reservoir stagnation parameters (pressure and temperature) of the experiment described in [1]. The computational domain contains the part of the reservoir and the expanding plume zone. Calculations with and without allowance for clustering are performed. For the flows without water cluster formation the influence of the rarefaction on the flow pattern is discussed and comparison with the free-molecular case is carried out. For the flows with clusterization the cluster size and plume gas-dynamic distributions are analyzed. Comparison with the experimental data on the terminal dimer mole fraction and with the computational results obtained in [2, 3] is performed. The suitability of the abovementioned clusterization model for the water plumes simulation is discussed.

REFERENCES

3D Kinetic Simulation of Near-Field Plume Flows from an Anode-Layer Hall Thruster

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Plume impingement is an important issue regarding the integration of Hall thrusters onto spacecraft. The plume of a Hall thruster involves complex plasma processes among high-energy ions, charge-exchange ions, neutrals, and fast-moving electrons. Hybrid DSMC-PIC method has been the major numerical approach to understand the detailed plume behaviour. For the electron description, previous studies have shown that the detailed fluid electron model [1] has advantages over the Boltzmann relation when the plume from the D55 anode layer Hall thruster was simulated using an axial-symmetric configuration [2]. A recent study of plumes from a cluster of thrusters showed that there were complex three-dimensional structures in the near field of the plume flow [3]. In this work, we use the 3D DSMC-PIC method with the detailed fluid electron model to investigate the near-field plume flows from the D55 Hall thruster. Figure 1 shows our preliminary simulated results where the cathode neutralizer has local effects on the electron temperature. A comparison with previous measurement [4] and simulation [2] is shown in Fig. 2, where the ion current density is plotted along the radial direction at 10 mm from the thruster exit plane. The ion current near the symmetric line is found to be non-zero, which agrees with the measurement. Figure 3 shows the ion current density at z=0 plane when a plume shield is included in the simulation. The effects of plume shield and shield optimization will be discussed in the full paper.

Fig.1: Electron temperature (ev) in near field. Fig.2: Radial profiles of ion current density at 10 mm from the thruster exit plane. Fig.3: Profile of ion current density at z=0 plane with shield included.

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## Session P4: Non-Equilibrium Flows

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<td>Kunova, Kustova, Mekhonoshina, Shoev</td>
<td>&quot;Numerical Simulation of Coupled State-to-State Kinetics and Heat Transfer in Viscous Non-Equilibrium Flows&quot;</td>
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Abstract. The inner shock wave structure with nonequilibrium effect is difficult to be accurately simulated due to the great gradient of density and temperature inside shock waves. In this paper, simplified conventional Burnett (SCB) equations were formulated for the computations of hypersonic shock wave structure in continuum-transition regime. The conventional Burnett equations were derived from the second-order Chapman–Enskog expansion of the velocity distribution function of Boltzmann equation. By neglecting conventional Burnett terms which were inversely proportional to Mach number, the constitutive relations in SCB equations were simplified specifically for hypersonic flow. Meanwhile, rotational and vibrational energy balance equations were also introduced to study the nonequilibrium relaxation processes inside the shock waves. One-dimensional Nitrogen shock wave structures at different Mach numbers of 5, 10, and 15 were simulated by using SCB and NS equations respectively. Generalized Rankine–Hugoniot relations were established to obtain the post-shock flow parameters in nonequilibrium flow. The numerical methods for solving the governing equations included three-order Runge-Kutta time-splitting method and AUSMPW+ flux-difference splitting method with MUSCL scheme. The normalized densities computed by the SCB and NS equations were presented in Figs. 1-3. More results about the normalized rotational and vibrational temperatures would be analyzed in the full paper. Compared with NS results, SCB equations could capture the shock waves structures more precisely and the flow variables were in better agreement with DSMC results at high Mach numbers.
Equilibrium and non-equilibrium properties of a relativistic gas at the transition temperature

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The Jüttner distribution function for equilibrium relativistic fluids has two well-known limits, the non-relativistic limit at low temperatures and ultra-relativistic limit for high temperatures [1]. Recently, this transition in velocity space, from a gaussian to a bimodal distribution, was described by Mendoza et al., [2]. Physically, the gas transitions between a regime where the relativistic energy is dominated by kinetic to another where the rest energy dominates. It has been found that the critical temperature at which the relativistic corrections becomes relevant, depends just on the dimension of the system, which allows for a description in terms of the theory of critical points (Montakhab et al., [3]). In this contribution a review of the thermodynamic quantities that are only dependent on the ratio between temperature and critical temperature, and the dimension is made. The role of the transition in the modification of dissipative fluxes for non-equilibrium systems is also explored. In particular, the purely relativistic terms that are usually proportional to the number density gradient [4] are studied. Also, the transport coefficients are written in terms of the transition temperature, which allows us to identify the lowest order relativistic effects just in terms of the dimension of the system.

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General Reynolds Analogy on Curved Surfaces in Hypersonic Rarefied Gas Flows with Non-equilibrium chemical reacting

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Hypersonic chemical non-equilibrium gas flows around blunt nosed bodies have been investigated in order to study the Reynolds analogy relation on curved surfaces. In previous research, a linear relation between $C_f/C_h$ (ratio of skin friction coefficient to heat transfer coefficient) and the local wall slop angle $\theta$ along blunt nosed bodies has been found in calorically perfect gas flows [1]. The relation, named as general Reynolds analogy, extend the classical Reynolds analogy relation from flat plate to curved surfaces with streamwise pressure gradient.

In this paper, a diatomic molecular “ideal dissociating gas” model [2] is applied to describe the momentum and energy transfer properties through hypersonic boundary layers with non-equilibrium “dissociation-recombination” reacting as presented in Fig. 1. Distributions of skin friction and heat transfer are calculated downstream the stagnation point with both the theoretical modeling method and DSMC method. Calculating results indicate that dissociated atoms exist outside the boundary layer both near and downstream the stagnation point, which increase the analogy coefficient. However, inside the boundary layer near cold walls, atoms recombination decelerate downstream the stagnation point, thus results to a non-linear Reynolds analogy relation. Effects of chemical reactions on Reynolds analogy are presented in Fig. 2. Explicit equations have also been constructed to describe the variations.

Fig. 1: Boundary layer momentum and heat transfer model.

Fig. 2: Distributions of $C_f/C_h$ with chemical reaction along $\theta$.

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Numerical simulation of coupled state-to-state kinetics and heat transfer in viscous non-equilibrium flows

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The present paper is devoted to investigation of non-equilibrium kinetics, diffusion and heat transfer behind shock waves in hypersonic flows of binary mixtures N_2/N and O_2/O. The state-to-state kinetic theory approach [1] is used for calculation of vibrational distributions, gas dynamic parameters and transport properties in the relaxation zone behind the shock front for different flow conditions. The governing flow equations include the equations for vibrational level population, number densities of atoms, gas temperature and velocity, and take into account non-equilibrium processes of dissociation, recombination and VT (TV) exchanges between vibrational and translational energies. The calculation algorithm for state-dependent transport coefficients developed in the frame of the kinetic theory requires solution of transport linear systems for all vibrational states at each step of numerical solution for governing equations. This procedure is very complicated and resource consuming. A simplified algorithm for calculation of diffusion and energy transfer is developed in [2] and applied in our earlier works [3-4]. The simplified way is based on the task splitting procedure: first, modelling of the inviscid flow in the Euler approximation is carried out and, then, calculations of the total energy flux and diffusion fluxes using the post-processing of obtained data is performed. While providing a tool for qualitative estimates of the heat and mass transfer in strongly non-equilibrium flows, such an approach cannot be applied for accurate heat flux assessments. The objective of the present paper is to study self-consistently the effects of state-dependent transport phenomena in non-equilibrium flows on the basis of the state-to-state kinetic theory. Fully coupled equations of fluid mechanics and state-to-state kinetics will be numerically solved in commercial flow solver ANSYS Fluent. The numerical algorithm of the state-to-state kinetics and transport coefficients evaluation will be implemented through the user defined functions. The implemented algorithm will be fully compatible with the core code and the resulting numerical tool can be used for simulation of 2D and 3D flows with the use of serial and parallel computations. Such a procedure will provide better accuracy of the viscous flow simulations based on the state-to-state kinetic theory.

ACKNOWLEDGEMENTS

This study is supported by the Russian Science Foundation (project 15–19-30016). O. Kunova acknowledges that she is employed by Saint-Petersburg State University in the frame of post-doctoral fellowship 6.50.2522.2013.

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### Session P5: Experimental Methods

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| Bosworth, Ketsdever, "Determination of the Effect of Particle Thermal Conductivity on Thermophoretic Force" |
Measurement of Thermophoretic Force on Spheroids

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Thermophoresis is the migration of an object within a fluid as a response to a thermal gradient. Thermophoretic force is the force that the object experiences due to the thermal gradient. The thermophoresis phenomenon in gasses was first studied by Tyndall [1] in 1870 where it was observed as dust particles being pushed away from a heated surface. Today, thermophoresis is utilized in many applications. For example, thermophoresis has been found to be beneficial in the mitigation of contaminants in plasma deposition process, harmful in boiler systems by causing particle deposition on surfaces and reducing heat exchange properties, and capable of sorting large particles by size to create concentration gradients in mixtures. Thermophoresis is an important mechanism of micro-scale fluid transport and has found numerous applications in the field of aerosol technology.

The primary focus of analytic and experimental work on thermophoresis in recent years has been on spherical particles. Theoretical limits have been developed for both the continuum and free-molecular regimes by Epstein [2] and Waldmann [3], respectively. The expansion of the theoretical limits from spheres to spheroids is performed by Leong [4] for the continuum regime. For the free-molecular regime, the process for a sphere as described in Bird [5] is expanded for the non-constant radii of a spheroid. This work, which is a continuation of [6], aims to make initial thermophoretic force measurements on a variety of spheroid shapes from the oblate disk to a prolate needle shape as depicted in figure 1. Force measurements are performed for each of the five spheroids depicted in figure 1. The thermal gradient is established between two parallel 61x61 cm copper plates with a separation distance of 40 cm for a range of Knudsen numbers. The first plate is heated or cooled while the second is allowed to remain at ambient temperature which creates a temperature gradient which can be altered by changing either the driven plate temperature or changing the plate separation around the test particle. The force is measured through a nano-Newton Thrust Stand (nNTS) which suspends the particle directly between the plates. The working fluid on which the thermal gradient is imposed is chosen to be Argon.

REFERENCES

Determination of the Effect of Particle Thermal Conductivity on Thermophoretic Force

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The migration of an object within a fluid as a response to a thermal gradient is known as thermophoresis. Thermophoretic force is the force that the object experiences due to the thermal gradient. In gasses, the thermophoresis phenomenon was first studied by Tyndall [1] in 1870. Tyndall observed thermophoresis in the form of dust particles being pushed away from a heated surface. Today, thermophoresis is utilized in many applications. For example, thermophoresis has been found to be beneficial in the mitigation of contaminants in plasma deposition process, harmful in boiler systems by causing particle deposition on surfaces and reducing heat exchange properties, and capable of sorting large particles by size to create concentration gradients in mixtures. Thermophoresis is an important mechanism of micro-scale fluid transport and has found numerous applications in the field of aerosol technology.

Theoretical derivations of thermophoretic force commonly are a function of, among other factors, either impacted particle thermal conductivity or the ratio of particle to gas thermal conductivity. Higher particle thermal conductivities allow for thermal energy to distribute evenly throughout a particle volume.

This work, which is a continuation of [2], aims to make initial thermophoretic force measurements on 5.1x5.1 cm plate particles of different materials with a variety of thermal conductivities as depicted in figure 1. Force measurements are performed for each of the four plates depicted in figure 1 which are copper, aluminum, stainless steel, and Teflon. The thermal gradient is established between two parallel 61x61 cm copper walls with a separation distance of 40 cm for a range of Knudsen numbers. The first wall is heated or cooled while the second is allowed to remain at ambient temperature which creates a temperature gradient which can be altered by changing either the driven wall temperature or changing the wall separation around the test particle. The force is measured through a nano-Newton Thrust Stand (nNTS) which suspends the particle directly between the plates. The working fluid on which the thermal gradient is imposed is chosen to be Argon.

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Session P6: Numerical Methods

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Rarefied Gas Simulations Using Quasiparticle Pairs

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Recently, the Boltzmann collision integral was rewritten in a divergence form [1,2]. It allows us to consider a distribution function of molecules as a density of quasiparticles, which are moving along smooth trajectories in the phase space under the force. Some variants of the algorithms of Kinetic Force Method were presented in [3,4].

In paper [5], the set of equations was proposed for two-particle distribution functions for gas mixtures. The effect of collisions in the two-particle Boltzmann equation is taken into account by scattering operator. It enables [6,7] to simulate the quasiparticle pair dynamics by rotating their relative velocity with the angular velocity depending on the distribution function.

In the report details of the Kinetic Force Method to model rarefied gas flows are considered. The analysis is founded on the kinetic equation for auxiliary two-particle distribution function of quasiparticle pairs. Interaction in quasiparticle pairs conserves energy and momentum and we use the algorithm for numerical simulation, which provides conservation laws automatically. We present results of numerical simulations of classical rarefied gas problems utilizing quasiparticles pairs for modeling.

ACKNOWLEDGEMENTS

The work was supported by the collaborative research project at the Institute of Fluid Science, Tohoku University.

REFERENCES

Mesh-Based and Particle-Based Kinetic Solvers with Adaptive Cartesian Mesh

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We have developed several mesh-based and particle-based kinetic solvers in an Adaptive Mesh and Algorithm Refinement (AMAR) framework, which combines adaptive mesh refinement (AMR) with the ability to select fluid and kinetic solvers on a cell-by-cell basis (Figure 1). The AMAR methodology was first developed for gas flows in mixed rarefied-continuum regimes [1], later extended for hybrid simulations of radiation transport, and is currently being advanced for simulations of partially ionized plasmas [2]. In the present paper, we will compare the implementation and capabilities of mesh-based and particle-based kinetic solvers and show examples of simulations using these solvers.

The kinetic module in the AMAR framework (Figure 1) can solve Boltzmann, Vlasov, and Fokker-Planck kinetic equations using Discrete Velocity Method (DVM). The Adaptive Mesh in Phase Space (AMPS) technique can adapt mesh in both physical and velocity spaces. The mesoscopic Lattice Boltzmann Method (LBM) uses a minimal set of discrete velocities as a subset of the DVM kinetic solvers for simulations of near-continuum flows.

The Direct Simulation Monte Carlo (DSMC), Photon Monte Carlo (PMC), and the Particle-in-Cell (PIC) modules are based on particle algorithms. We use cell-based particle storage, i.e. each cell has a list of particles assigned to it.

Two methods are used for domain decomposition for parallel computing: a fine-grained method using Space Filling Curves (SFC) and a coarse-grained using Forest of Trees (FOT). Kinetic solvers have been adapted for GPU computing. For hybrid kinetic-fluid simulations, GPUs were applied for the kinetic cells whereas the fluid cells were computed on CPUs. This methodology has been successfully demonstrated for mixed rarefied-continuum flow over a hypersonic scramjet [3].

We will discuss key differences between computational load of cells in particle-based and mesh-based kinetic solvers. These differences are of principal importance for the development of parallel algorithms for adaptive kinetic-fluid solvers using particle- and mesh-based schemes.

Finally, we will describe the latest additions to the AMAR toolset: an electrostatic PIC module [4] and a Discontinuous Galerkin Time Domain Maxwell solver [5], and outline challenges associated with coupling kinetics and electromagnetics. The cell-based AMR technique provides a convenient adaptive particle management algorithm for problems with exponential multiplication of particles.

ACKNOWLEDGEMENTS

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REFERENCES

Extension of deterministic steady-state marching kinetic solvers to unstructured grids

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In rarefied gas dynamics, deterministic solvers based on the so-called discrete velocity (or ordinates) method, are constantly gaining lately more attention [1]. They are implemented more widely than before, mainly due to their upgrading by introducing various numerical advancements and to their efficient parallelization on high performance computers. As it is well known in discrete velocity algorithms the continuous spectrum of molecular velocities is replaced by a set of discrete velocities, the choice of which depends on the peculiarities and characteristics of each problem, although general rules can be developed. In the case of steady-state flows a typical iteration scheme between the solution of the kinetic equations and the computed moments of the distribution function is introduced, until convergence is reached. The values of the distribution function in each iteration, may be obtained either by solving a system of linear equations or alternatively using a marching scheme on the physical space for each discrete velocity. This latter methodology provides considerable computational benefits, compared to the former one, in both CPU time and memory requirements. However, it has been adopted so far only on structured grids where the proper marching from node to node may be easily defined in terms of the node indexation.

The extension of this methodology to unstructured grids is considered in the present work. On unstructured grids finding the proper node sequence to propagate the information in the direction of each molecular velocity is not trivial. Following an erroneous path will result to the collapse of the algorithm. Furthermore, on unstructured grids the proper path for each discrete molecular velocity may be different. Here, the calculation of the node sequence is achieved in two different ways. The first one is based on purely geometrical issues and the second one on graph theory. The former one is simpler and faster but not always conclusive, while the second is computationally more demanding but also more robust. In the present work, a hybrid approach is followed using the geometrical methodology in the general case and applying the graph theory approach only when the former one fails. In all cases the node sequence is decided a priori and it remains constant during the iterative solution. In order to illustrate and compare the efficiency and accuracy of the developed algorithm some typical 2D benchmark rarefied gas dynamics problems are solved.

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REFERENCES

Burnett Simulations of Micro-Couette Flow using Modified Slip Boundary Conditions

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Gas or liquid flow through small channels has become more and more popular due to the micro-electro-mechanical systems (MEMS) fabrication technologies e.g., micro-motors, electrostatic comb-drive, micro-chromatographs, micro-actuators, micro-turbines and micro-pumps, etc. The flow property in and around these systems is always in the continuum-transition regime. In this condition, the mean free path of gas molecules approaches the characteristic scale of the micro-devices itself, and due to the little collisions the heat and momentum can not equilibrate between the wall and fluids quickly. Numerous work have been done for investigation of the MEMS. But it is very difficult to get the solutions for complex engineering configurations. A possible way is to investigate the Couette flows, as well as shear-driven micro-cavities and micro-channels. In this paper, we concentrate on the steady-state Couette flows. Converged solutions for steady-state micro Couette flows are obtained by using Conventional Burnett equations with a set of modified slip boundary conditions\[1\]. Instead of using the physical variables at the wall, the modified slip conditions use the variables at the edge of the Knudsen layer\[2\]. This is a physically plausible assumption. Because the Knudsen layer has a thickness only in the order of a mean free path. Molecules are likely to travel without collision in this layer. Numerical results for non-dimensional wall shear stress and heat flux are compared with those of the DSMC solutions. There are not much improvement in the accuracy by using this modified slip conditions. But the modified conditions perform much better than the unmodified slip conditions for numerical stabilization. Pressure profiles are investigated for three cases\[3\], which are \(Ma = 3, Kn = 0.03; 0.26; 0.94\). As we can see from all the results, the set of conventional Burnett equations with second order modified conditions are shown to be an appropriate model for the micro-Couette flows applied in micro-electro-mechanical systems (MEMS) or nano-electro-mechanical (NEMS) systems. As for the Simplified Conventional Burnett equations\[4\], we found that it can not get right results for Couette flows, which is proved in the appendix.

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REFERENCES

Numerical simulation of coupled state-to-state kinetics and heat transfer in viscous non-equilibrium flows

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The present paper is devoted to investigation of non-equilibrium kinetics, diffusion and heat transfer behind shock waves in hypersonic flows of binary mixtures $N_2/i$ and $O_2/i$. The state-to-state kinetic theory approach [1] is used for calculation of vibrational distributions, gas dynamic parameters and transport properties in the relaxation zone behind the shock front for different flow conditions.

The governing flow equations include the equations for vibrational level population, number densities of atoms, gas temperature and velocity, and take into account non-equilibrium processes of dissociation, recombination and VT (TV) exchanges between vibrational and translational energies. The calculation algorithm for state-dependent transport coefficients developed in the frame of the kinetic theory requires solution of transport linear systems for all vibrational states at each step of numerical solution for governing equations. This procedure is very complicated and resource consuming. A simplified algorithm for calculation of diffusion and energy transfer is developed in [2] and applied in our earlier works [3-4]. The simplified way is based on the task splitting procedure: first, modelling of the inviscid flow in the Euler approximation is carried out and, then, calculations of the total energy flux and diffusion fluxes using the post-processing of obtained data is performed. While providing a tool for qualitative estimates of the heat and mass transfer in strongly non-equilibrium flows, such an approach cannot be applied for accurate heat flux assessments.

The objective of the present paper is to study self-consistently the effects of state-dependent transport phenomena in non-equilibrium flows on the basis of the state-to-state kinetic theory. Fully coupled equations of fluid mechanics and state-to-state kinetics will be numerically solved in commercial flow solver ANSYS Fluent. The numerical algorithm of the state-to-state kinetics and transport coefficients evaluation will be implemented through the user defined functions. The implemented algorithm will be fully compatible with the core code and the resulting numerical tool can be used for simulation of 2D and 3D flows with the use of serial and parallel computations. Such a procedure will provide better accuracy of the viscous flow simulations based on the state-to-state kinetic theory.

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REFERENCES

On the Unsteady-state Couette Problem in the Transitional Regime

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We investigate the unsteady-state Couette problem for the transitional regime of a flow using DSMC method. The unsteady-state Couette problem is closely associated with Rayleigh problem and the steady Couette problem. In fact, it coincides with the Rayleigh problem until the perturbation from one plate reaches the other. On the other hand, unsteady-state Couette flow tends to the steady Couette flow as time increases. Thus, rarefied effects that are inherent to Rayleigh flow [1] are also inherent to the unsteady-state Couette flow if Knudsen number $Kn$ is sufficiently small. The rarefied effects that are inherent to steady Couette flow [2-4] take place for the unsteady-state Couette flow too (at certain moments of time). However, it is more interestingly that the unsteady-state Couette problem has the property which is not inherent to the Rayleigh problem and to the steady Couette problem either. Namely, in the latter problems, as rarefaction decreases, the flux of energy transferred to the plate changes sign only once and only from plus to minus. Unlike these problems, in the unsteady-state Couette problem the energy flux can change its sign also from minus to plus. Moreover the energy flux can change its sign repeatedly. The time dependencies of the flux of the energy $E$ that is transferred to the plate are shown in Fig. 1. The flux is normalized to the corresponding free molecular value. Temperatures of the plates $T_1$ and $T_2$ are normalized to the temperature of undisturbed gas $T_\infty$. Velocities of the plates $U_1$ and $U_2$ are normalized to $c_\infty = \sqrt{2RT_\infty}$, time $t$ is normalized to $\lambda_\infty / c_\infty$ where $R$ is the gas constant and $\lambda_\infty$ is the mean free path of the molecules in the undisturbed gas.

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# Session P7: Heat and Mass Transport

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Heat and Mass Transfer in Reacting Mixtures: Molecular Dynamics and Kinetic Theory Approaches

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Studying the transport processes in non-equilibrium chemically reacting mixtures is of vital importance for aerospace applications, chemical reactor technology and plasma-chemical technologies. Linear irreversible thermodynamics establishes phenomenological relations for heat and mass fluxes in terms of generalized thermodynamic forces [1, 2] but cannot give expressions for the coefficients in these relations. On the other hand, kinetic theory (KT) of strongly non-equilibrium gases is an efficient tool which allows closing fluid dynamic equations of reacting flows and provides algorithms for the calculation of kinetic coefficients such as viscosity, heat conductivity, multi-component and thermal diffusion as functions of collision integrals [3-5]. However uncertainties in the available data for cross sections of internal energy transitions and chemical reactions are still rather high, and KT models for transport coefficients require validation. While experimental measurements of heat and mass fluxes under strongly non-equilibrium conditions are in general unfeasible, non-equilibrium molecular dynamics (MD) can give an opportunity to validate advanced kinetic models for transport phenomena.

In [6], a method for non-equilibrium MD simulations of heat and mass transfer in a dissociating H$_2$-H mixture under the action of temperature gradient is proposed. The steady state of the closed system was characterized by non-zero component fluxes driven by the thermal force. The results were compared to those obtained using the KT-algorithms developed for weakly non-equilibrium flows [7], and a discrepancy between the MD and KT-based simulations was found. The extraordinary large thermal diffusion in the reacting mixture was emphasized. It is worth noting that the comparison performed in [6] is not completely appropriate since the considered regime is far from equilibrium and requires therefore more thorough treatment.

The objective of the present study is to elaborate a consistent approach allowing for the correct interpretation of MD simulations and thus to develop a tool for the validation of KT results for the transport processes. First we identify the transport coefficients obtained by means of MD and find how they are related to the heat conductivity, diffusion and thermal diffusion coefficients derived in [4] in the one-temperature approach under strong chemical non-equilibrium. Then we perform comparisons of transport coefficients and heat of transfer in the frame of MD and KT approaches and finally discuss possible sources of discrepancies arising between the MD and KT results.

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REFERENCES

A Thermodynamic view of heat transfer in different transport regimes

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The nature of the heat transfer process changes substantially according to transport regime. A thermodynamic view of the heat transfer is considered to understand better this regime dependent change. T-s diagram of different transport regimes is presented in Fig.1. The \( dp = 0 \) and \( d(p/\sqrt{T}) = 0 \) lines represent the two limit cases in transport, hydrodynamic and free molecular flow limits, respectively. As a useful parameter the coefficient \( \gamma \), defined as \( \gamma = Q_T/Q_p \) in [1], is also shown in the figure which helps to visualize the heat transfer during the transport processes. The transport processes are expressed as a polytropic process according to their \( \gamma \) values. In hydrodynamic limit, \( \gamma \) goes to 0, which corresponds to constant pressure process \( (dp = 0) \) and the polytropic component, \( n \), is equal to 0. In free molecular limit, \( \gamma \) goes to 0.5 which corresponds to the Knudsen process, \( d(p/\sqrt{T}) = 0 \), and the polytropic component is calculated as \( n=1/3 \). In this study, polytropic component is written by depending on the \( \gamma \) coefficient and the relation between these two parameters is formalized.

The curvatures of the lines in T-s diagrams are proportional with the specific heat capacities. Therefore, the heat capacities should be also considered to understand exact thermodynamic behaviour of the processes. The constant pressure heat capacity \( c_p \) is very well known and useful parameter for thermodynamic calculations in hydrodynamic limit. Knudsen heat capacity \( c_{Kn} \) has been recently introduced in [2] for free molecular flow regime and a linear relation between \( c_p \) and \( c_{Kn} \) has been presented according to \( \gamma \). In this work, molecular dynamics simulation of the heat capacity in different Knudsen numbers are performed for He, Ne and Ar gases. The variation of heat capacities in mid-range Knudsen numbers are presented for Neon and Argon in Fig. 2a and 2b, respectively. The simulation results converge to \( c_p \) and \( c_{Kn} \) values of considered gas in low Knudsen and high Knudsen numbers, respectively. It is shown that a power law fit best describes the changes on heat capacity with Knudsen number. The simulation results are compared with the analytical calculations for ideal gases and deviation from the ideal gases are discussed. The details of thermodynamic behaviour of the transport processes are presented and T-s diagram in Fig. 1 is modified according to simulation results.

REFERENCES

Quantum Degeneracy Effect on Gas Diffusion

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The physics of continuum and Knudsen diffusions are quite different than each other. These differences arise due to the relation between the mean free path of the particles and the length scale of the system. The characteristics of the flow regime (hydrodynamic or free molecular) and the analyzing methods (continuum and statistical) can be determined based on Knudsen number. Diffusion process has two different asymptotic behaviors in hydrodynamic and free molecular transport regimes for macro and nano scales respectively. Therefore, two different diffusion coefficients are generally used to obtain the diffusion properties in these both limits. However, in the literature, a single diffusion coefficient has been generalized spanning from hydrodynamic to free molecular transport regimes for Maxwell gases (MB) [1]. Also, the diffusion coefficients of Fermi (FD) and Bose (BE) gases have been separately derived for hydrodynamic and free molecular transport regimes by considering quantum size effects [2]. Furthermore, the quantum degeneracy effects on diffusion becomes an important parameter for low temperature or high density gas conditions where the interparticular distance is comparable to the thermal de Broglie wave length of the particles. In this work, the self-diffusion coefficient of Fermi/Bose gases are derived for both hydrodynamic and free molecular transport regimes in a rectangular diffusion domain and the both diffusion coefficients are expressed in a single relation including Knudsen number and the quantum degeneracy. Also, this relation gives information about the transition behavior of the diffusion coefficient between the regimes. The variations of diffusion coefficients with quantum degeneracy and Knudsen number are analyzed for Fermi and Bose gases in Fig 1 and Fig 2 respectively. It is clearly seen from Fig 1 that diffusion coefficient increases/decreases due to degeneracy in Fermi/Bose gas.

![Fig.1: Effect of quantum degeneracy on normalized diffusion coefficient for different Knudsen numbers.](image1)

![Fig.2: Effect of Knudsen number on normalized diffusion coefficient for Fermi and Bose gases at different degeneracy levels.](image2)

REFERENCES

Thermal conductivity, shear and bulk viscosities for a relativistic binary mixture.

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One of the most important outcomes of the kinetic theory is to provide analytic expressions for the transport coefficients for diluted gases. Appealing to astrophysical scenarios where the aforesaid theory can be applied, it may concern to the interstellar cloud gases and particular conditions in the interior of stars. In those cases, diluted gases can lie under the presence of a gravitational potential and within relativistic (high temperatures) conditions [1,2]. In the present work, we deal with a binary mixture of diluted relativistic gases within the framework of the kinetic theory, i.e. the Boltzmann equation. We assume that the gas is under the influence of an isotropic Schwarzschild metric and the gas is composed of particles with speeds comparable with the light speed. Taking into account the constitutive equations for the laws of Fourier and Navier-Stokes [3], we obtain general expressions for the thermal conductivity, the shear, and bulk viscosities. Those expressions are general in the sense that no interaction potential amongst the particles is considered. To evaluate the integrals we assume two physical conditions, namely, a hard-sphere interaction along with non-disparate masses for the particles of each component. We show the analytic expressions that depend of the local thermodynamic variables and show the behavior for the transport coefficients with respect to the relativistic parameter which relates the ratio of the rest energy of the particles to the thermal energy of the gas. We also demonstrate that the corresponding one component limit is recovered by considering particles with equal masses, in accordance with the kinetic theory when a single fluid is studied [2].

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Study of a flow in a plane micro-channel using a discrete spatial model of gas

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The rapid expansion of the miniaturization of mechanical and energetic devices leads to the introduction of flows in micro-channels in various fields of technology through applications related to biological systems, process engineering, aerodynamic and heat transfer with or without reactive flows. The problems encountered in the study of gas flows in micro-channels are to a great extend similar to those of rarefied gas. Micro-pipes and nano-pipes were manufactured in which rarefaction phenomena such as dynamical and thermal slips have been observed. In an attempt to understand the transition of unsteady gas flow in micro-channels to steady states, we investigate the unsteady two dimensional flow of a gas in a plane channel with given width and height and an infinite depth connecting two open semi-infinite areas which are denoted respectively inlet and outlet tanks. In the transitional regime characteristic of micro-channels flows the resolution of the Boltzmann equation is needed. To avoid the complexity of this equation we use a ten velocity discrete model of gas \cite{1}. Two dimensionless numbers (Knudsen number Kn and channel aspect ratio $\epsilon$ i.e. the height to width ratio) govern the flow. The resolution of the initial and boundary values multidimensional problem is done numerically using a fractional steps method \cite{2}. In the present study, the gas is initially homogeneous and isothermal and the temperatures of the channel's walls are equal and constant during the process. The gas has initially the temperature of the channel’s walls. The flow is induced by a density difference kept constant between the inlet and outlet tanks. The goal of the study is to analyze the changes of the macroscopic variables (average density, longitudinal and transversal velocities, and kinetic temperature) of flows in micro-channels. It is observed that after a transient phase notably characterized by the interaction of waves evolving in opposite directions generated by the density gradient, it is established a steady flow characterized by the division of the flow domain in three areas: two thin dynamical and thermal unbalanced layers attached to the walls separated by the interior of the channel at thermal equilibrium. At the start of the process, the value of the kinetic temperature along the micro-channel-axis oscillates around the initial temperature; it is due to the friction of the different gas layers at the entrance of the channel. The average density decreases sharply at the entrance at the start of the process and has a monotonic profile decreasing from the entrance to the exit of the channel at the steady state. The kinetic temperature has near the channel, an overshoot and becomes greater than the initial temperature of the flow at the start. At the steady state, it has a jump near the entrance and a jump at the exit of the channel. It increases from the inlet to a maximum at the outlet. The value of this maximum depends on the parameters and can be greater than the initial temperature. The study of the transient period is interesting in that it brings to the fore the symmetric shear flow induced by the oblique fluxes of particles coming from the edges of the walls at the entrance and the exit of the channel and the flowing back phenomenon which vanish at the steady state. At the steady state we notice rarefaction effects such as velocity slip, temperature jumps on the channel's walls at the entrance and the exit of the channel and the increase and decrease of the kinetic temperature respectively at the exit and at the entrance of the channel \cite{1}.

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Computation of 1-D shock structure using nonlinear coupled constitutive relations and generalized hydrodynamic equations

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The moment methods in rarefied gas dynamics could be divided into generalized hydrodynamic equations (GHE) and extended hydrodynamic equations (EHE), e.g., Burnett equations, Grad equations and R-13 equations, theoretically. Eu [1] firstly developed the GHE based on a nonequilibrium canonical distribution function and demonstrated the thermodynamically consistent of this model. Subsequently, nonlinear coupled constitutive relations (NCCR) was proposed by Myong [2,3] by omitting the product of heat flux and velocity gradient in GHE to reduce the computational complexity. According to the successful application in 1-D shock wave structure and 2-D flat plate flow, the capability of NCCR has already been demonstrated successfully [3,4].

The motivation of this study was to investigate the different behavior of NCCR and GHE for monatomic and diatomic gases in one-dimensional shock structure problems. And it also shed additional light on the influence of high-order difference schemes on the nonlinear constitutive relationships as a step to develop reliable high-order computational models for rarefied flows. Therefore, argon and nitrogen shock structure was calculated using both GHE and NCCR model up to Ma=50. The 5th order WENO scheme for inviscid term and the 6th order central difference scheme for viscid scheme were employed to compare with the 3rd order MUSCL and the 2nd order central difference scheme. Finally, the present results including shock wave profile and its qualitative properties by NCCR and GHE are compared with that of DSMC and NS equations. The results showed that the GHE yield 1-D shock wave in much closer agreement with DSMC results than do the NCCR model without considering the computational complexity and efficiency and there was no significant difference between high-order scheme and the second order scheme in present cases.

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REFERENCES

Emission Spectroscopy with an Embedded Sensor for the Study of Metallic Contamination in the T-ADFA Free Piston Shock Tunnel

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Emission spectroscopy is a useful technique to study hypersonic rarefied flows, as the high total enthalpy (for this work, 11 MJ/kg) means that there is a large amount of emission from both molecular and atomic species. Typically, experiments are designed to target molecular species to better understand the non-equilibrium chemistry that occurs in the flowfield; however, there is often significant metallic contamination from the experimental facility. This paper gives details of the metallic contamination in the T-ADFA free-piston shock tunnel.

We have constructed an optical-fiber-based emission system embedded into the cylindrical test model. This technique is based on previous experiments in the visible wavelength region by Kurtz et al. [1] and by Schuck and O’Byrne [2].

Iron contamination of OH spectra was previously noted by Cruden et al. [3] on the Japan Aerospace Exploration Agency's High-Enthalpy Shock Tunnel (HIEST) facility: they developed a fitting procedure to account for the contribution of the metallic emission. We observe strong lines from both iron and copper in our facility. We will present a systematic study on the effect of the materials used in the T-ADFA facility to find the origin of the metallic emission, and to reduce its contribution to the measured spectra. An example set of experimental and theoretical emission spectra is shown in Figure 1.

We present results using both a commercially available intensified CCD camera (Princeton Instruments ICCD) and give details of a new intensified linear CMOS array that we have developed using a Hamamatsu S11639 linear CMOS sensor coupled with a Photonis 1450NW image intensifier. The linear array is capable of line scan rates up to 4.8 kHz: this will allow us to temporally resolve the emission of the metallic species.

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REFERENCES

Non-resonant Gas-Optical Lattice Interaction with Feedback from the Gas to the Laser Radiation

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This work is devoted to a study of non-resonant interaction of polarized gas molecules with optical lattices. The optical lattice is created by fields of two counter-propagating laser beams of equal or different intensities. Angular frequencies of lasers may be slightly different in order to form a moving optical interference pattern. The phase velocity of the pattern is given by \( \xi = (\omega_1 - \omega_2)/|\mathbf{k}_1 - \mathbf{k}_2| \), where \( \omega_{1,2} \) and \( \mathbf{k}_{1,2} \) are angular frequency and wave vectors, respectively, of corresponding laser beams. Gas-optical lattice interaction is induced by a gradient force \( F = -\nabla U = \frac{\alpha}{2}(\mathbf{E} \cdot \mathbf{E}) \), where \( \alpha \) is the polarizability of gas molecules [1]. The problem of gas behavior in the presence of periodic optical lattice has been well studied [2, 3]. It can be shown as gas mixture separation [4], gas acceleration and heating due to a non-zero phase velocity of the optical potential. Periodic inhomogeneity of the gas density due to the gradient force leads to a change in the gas permittivity. A self-consistent problem of the gas flow and propagation of laser beams in such gas media with periodic modulation of the gas density is considered. The goal of this work is to study the unsteady processes of gas particles optical trapping and wave propagation and refraction in the presence of the influence of gas density inhomogeneity on radiation. The numerical technique applied to the gas flow modeling is the direct simulation Monte Carlo (DSMC) method [5]. The computations are performed by the SMILE++ DSMC code [6]. The effect of optical lattice on the gas is taken into account through a gradient force, which alters the velocity of molecules every computational time step. To understand the change in the laser beam passing through the inhomogeneous gas the gas density in each collision cell is estimated through sampling the number of particles. Then it is assumed that the gas density, which is constant inside the cells, changes on the cell boundaries in a jump. Based on the relations for the electromagnetic field on optical density jumps, propagation and reflection of radiation from a single source in a layered medium is calculated [7]. The total field is calculated as a superposition of the fields from two sources of radiation. Thus, the process of reaching the steady-state solution of optical trapping with allowance for self-consistent interaction between optical lattice and the gas is demonstrated. The method will be useful for studying gas to laser field interaction by realistic experimental conditions.

REFERENCES