DIRECT SIMULATION MONTE CARLO 2019: THEORY, METHODS, AND APPLICATIONS

SEPTEMBER 22-25, 2019

SANTA FE, NEW MEXICO, USA

CONFERENCE CO-CHAIRS

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VENUE

The conference hotel is the site for all
technical sessions and meals, except the banquet.

CONFERENCE AGENDA

Sunday, September 22, 2019

11:00 am	7:00 pm	Registration Desk
1:00 pm	5:00 pm	Short Course
5:30 pm	8:30 pm	Reception

Monday, September 23, 2019

7:00 am	1:00 pm	Registration Desk
7:00 am	8:00 am	Breakfast
8:00 am	8:30 am	Meet and Greet
8:30 am	9:00 am	Welcome
9:00 am	9:40 am	Technical Presentations
9:40 am	10:00 am	Break
10:00 am	11:40 am	Technical Presentations
11:40 am	1:00 pm	Lunch
1:00 pm	3:00 pm	Technical Presentations
3:00 pm	3:20 pm	Break
3:20 pm	5:00 pm	Technical Presentations
5:00 pm	6:00 pm	SPARTA Users Meeting

Tuesday, September 24, 2019

7:00 am	1:00 pm	Registration Desk
7:00 am	8:00 am	Breakfast
8:00 am	9:00 am	Keynote Lecture
9:00 am	10:00 am	Technical Presentations
10:00 am	10:20 am	Break
10:20 am	11:40 am	Technical Presentations
11:40 am	1:00 pm	Lunch
1:00 pm	3:00 pm	Technical Presentations
3:00 pm	3:20 pm	Break
3:20 pm	5:00 pm	Roundtable Discussion
6:30 pm	9:00 pm	Banquet

Wednesday, September 25, 2019

7:00 am	1:00 pm	Registration Desk
7:00 am	8:00 am	Breakfast
8:00 am	10:00 am	Technical Presentations
10:00 am	10:20 am	Break
10:20 am	11:40 am	Technical Presentations
11:40 am	1:00 pm	Lunch

GENERAL CONFERENCE INFORMATION

Registration Desk

The registration desk is located near the presentation room and will be open during these hours.

11:00 am -	7:00 pm	Sunday
7:00 am -	1:00 pm	Monday
7:00 am -	1:00 pm	Tuesday
7:00 am -	1:00 pm	Wednesday

The standard registration fee covers all technical sessions, the welcome reception, all breakfasts, lunches, and breaks, and the banquet. An additional fee is required to attend the short course. Additional tickets for the reception and the banquet may be purchased at the registration desk.

Presentation Format

All presentations are organized in a single track given in one room: there are no parallel sessions. The keynote lecture is allotted 60 minutes, the invited presentations are allotted 40 minutes each, and the contributed presentations are allotted 20 minutes each. Please be sure allow ample time for questions within these periods.

Audiovisual Services

The meeting room is equipped with a laptop computer connected to a projector. Individuals may preload their presentations onto this computer, or they may connect their laptops to the projector to show their presentation. In the latter situation, any time lost due to computer difficulties will be subtracted from the speaker's allotted time. The times before and after technical sessions provide good opportunities to preload presentations onto the provided laptop computer.

CONFERENCE HOTEL

Drury Plaza Hotel in Santa Fe

Located in the heart of downtown Santa Fe, the Drury Plaza Hotel in Santa Fe sits adjacent to St. Francis Cathedral, built by Archbishop Jean Baptiste Lamy between 1869 and 1886. Lamy arrived in Santa Fe and first built a rectory, which was later expanded and became known as the Old Seminary. In 1865, Lamy sold the building to the Sisters of Charity, who had come to New Mexico to help treat the sick by opening area hospitals. The first hospital they opened was in the Old Seminary, and they continued to run hospitals in the area until the mid-1900s.

By the 1950s, the Sisters of Charity had run out of room and needed to build a new hospital. That structure served as St. Vincent's Hospital for 20 years and is now the main building at the hotel. The hospital occupied the building until 1977, when the structure became the home to the New Mexico Department of Cultural Affairs. The site was also used for movie sets, as well as serving as the location of the New Mexico Film Commission.

Drury Hotels bought the property in 2007 and began researching the history. The property had been in disrepair, and the community was eager for the beloved building to be restored. Archeologists were hired before any excavation or building occurred. In fact, foundations of the Sisters of Charity buildings were uncovered. The hotel preserved the history and the original architecture while adding a restaurant, Eloisa, and parking space.

A historic renovation, the Drury Plaza Hotel in Santa Fe is LEED® Certified by the U.S. Green Building Council for energy efficiency in the design. The hotel is within walking distance of the Plaza in Downtown Santa Fe and the Georgia O'Keeffe Museum. Palace Avenue Arts selected the artwork for the interior from the most creative artists of a wide array of art markets.

Hotel Location, Phone, and Website

Drury Plaza Hotel in Santa Fe
6828 Paseo de Peralta; Santa Fe, New Mexico 87501 USA; 1-505-424-2175
https://www.druryhotels.com/locations/santa-fe-nm/Drury-Plaza-Hotel-in-Santa-Fe

CONFERENCE BANQUET

Rio Chama Steakhouse

Tuesday's banquet will be held at the Rio Chama Steakhouse, which is just a short walk from the conference hotel. Cocktails will be available for purchase beginning at 6:30 PM, and dinner will be served at 7:00 PM. Rio Chama is located in the oldest neighborhood in Santa Fe, the Barrio de Analco, which means "neighborhood on the other side of the river."

In 2001, Rio Chama opened its doors to the public. The original restaurant included the bar and the dining room and, open in the summer, the courtyard and patio. In 2005, they acquired an additional building to accommodate larger groups. They have affectionately named this space the Baca House in honor of a long-time employee whose grandparents had owned the house. In 2006, Rio Chama renovated the room next to the Baca House to add the Humidor–the only public cigarette and cigar bar in Santa Fe. In 2007, Rio Chama completed construction of two new spaces in the main facility: the President's Room and the Abiquiú Room. The President's Room is a banquet room with seating for 120 people that has hosted many prestigious guests, including Bill Richardson and Mikhail Gorbachev. The Abiquiú Room is a private 36-seat wine cellar that features a collection of Georgia O'Keefe photos done by her personal photographer.

BACKGROUND AND SCOPE

"Direct Simulation Monte Carlo 2019: Theory, Methods and Applications" will be held in Santa Fe, New Mexico, USA on September 22-25, 2019.

The goal of this meeting is to bring together developers and practitioners of the Direct Simulation Monte Carlo (DSMC) method. Talks will cover all types of DSMC-related work: theoretical foundations, verification and validation, convergence, computational efficiency, hydrodynamic fluctuations, flow instabilities, algorithm development, aerospace, hypersonics, microscale flows, nanoscale flows, plasmas, transport properties, collisional energy exchange, gas-phase chemical reactions and ionization, gas-surface interactions, planetary atmospheres, dense gases, liquids, granular flow, and experiments relevant to DSMC.

The conference goals are similar to the prior DSMC conferences in Milan, Italy, in 2003, in Santa Fe in 2005, 2007, 2009, 2011, 2013, and 2017, and in Hawaii in 2015. These successful conferences provided unique opportunities for participants to assess the current state of the art and the future directions of the DSMC method. By bringing together participants whose work spans a wide spectrum of DSMC-related research, development, and applications, these conferences promoted significant interactions among key innovators in the DSMC community. We hope to continue the successes of these past conferences at the present one.

On Sunday afternoon, Professor Kelly A. Stephani, University of Illinois at Urbana-Champaign, Illinois, USA, will present a four-hour short course: "From Shock Layer to Surface: DSMC Thermochemical Models for Hypersonics and High-Temperature Aerothermodynamics."

On Tuesday morning, Professor Alina A. Alexeenko, Purdue University, West Lafayette, Indiana, USA, will present the Graeme A. Bird Keynote Lecture. Her talk is entitled "Taming Fire: Molecular Simulations of Combustion." Professor Alexeenko is internationally recognized for her research on simulations and experiments of nonequilibrium gas dynamics.

Michael A. Gallis and Alejandro L. Garcia
Conference Co-Chairs

KEYNOTE SPEAKER

On Tuesday morning, Professor Alina A. Alexeenko will present the Graeme A. Bird Keynote Lecture. Previous Keynote Lecturers were Graeme A. Bird (2005), Berni Alder (2007), Andres Santos (2009), E. Phillip Muntz (2011), Kazuo Aoki (2013), Alejandro L. Garcia (2015), and Iain D. Boyd (2017). Her lecture is entitled "Taming Fire: Molecular Simulations of Combustion."

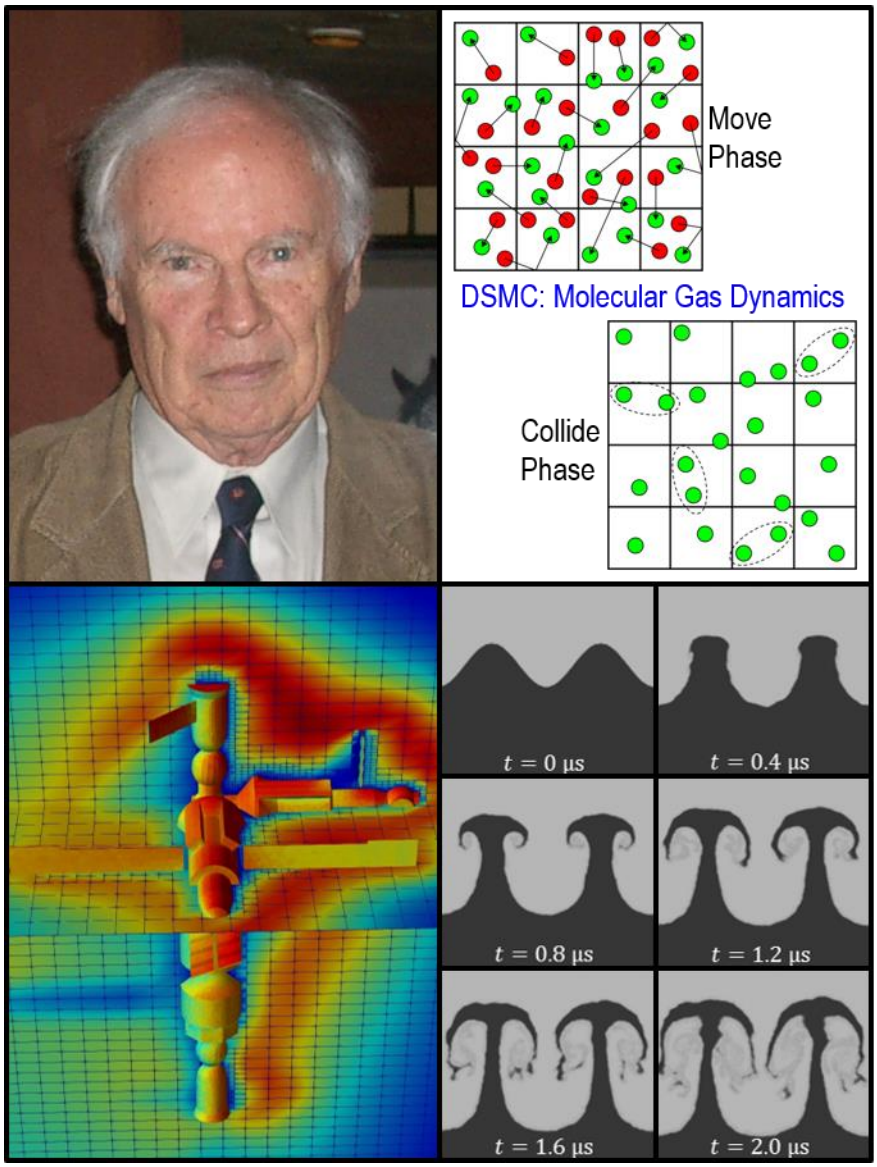
Professor Alexeenko is internationally recognized for her research involving computational and experimental studies of rarefied gas flow phenomena occurring in both high-altitude flight, such as smallsat propulsion, spacecraft contamination, plume interactions, high-altitude aerothermodynamics, in emerging technologies, such as micro-electro-mechanical systems for space communications and micropropulsion, and in vacuum manufacturing processes. Broadening applications of rarefied gas dynamics is one of her long-term research goals. Alexeenko's group at Purdue has developed fast computational algorithms and solvers for the deterministic solution of rarefied flow problems. Such new techniques are especially useful in studying low-speed and/or unsteady flows and have allowed her group to address several challenging problems, such as aerodynamic damping in MEMS devices and shock wave propagation in microscale geometries. Additionally, her research has led to novel microdevice concepts that exploit unique microscale, rarefied flow physics for gas sensing and smallsat propulsion.

Professor Alexeenko received a B.S. in Mathematics from Novosibirsk State University in 1997, an M.S. in Applied Mathematics from Novosibirsk State University in 1999, and a Ph.D. in Aerospace Engineering from Pennsylvania State University in 2003. During 2004-2006, she was a research consultant for the Air Force Research Laboratory at Edwards Air Force Base and a postdoctoral scholar in the Aerospace and Mechanical Engineering Department at the University of Southern California. Professor Alexeenko became Assistant Professor of Aeronautical and Astronautical Engineering at Purdue University in 2006 and was promoted to Associate Professor in 2012 and Full Professor in 2016. In 2014, she founded the Advanced Lyophilization Technology Consortium (LyoHUB). Professor Alexeenko has served on the International Advisory Committee of the Rarefied Gas Dynamics Symposium since 2016 and served as Chair of the AIAA Thermophysics Technical Committee during 2016-2018. Professor Alexeenko has authored 80+ journal articles, 110+ conference papers, 3 book chapters, and 5 patent applications.

GRAEME A. BIRD COMMEMORATIVE ISSUE

Physics of Fluids, Volume DSMC2019, Issue 1, November 2019
Guest Editor: M. A. Gallis

Since its introduction, Direct Simulation Monte Carlo (DSMC) has revolutionized the field of rarefied gas dynamics. Physics of Fluids has played a major role in the advancement of DSMC, with the first paper on the topic, by Professor Graeme A. Bird, publishing in Physics of Fluids in 1963 (https://doi.org/10.1063/1.1710976). This Special Topic Collection is dedicated to the memory of Professor Bird and aims to elucidate the past and illuminate the future of DSMC.



Sunday, September 22, 2019

Session 1: Short Course

Chair: M. A. Gallis

1:00-5:00	**From Shock Layer to Surface: DSMC Thermochemical Models for Hypersonics and High-Temperature Aerothermodynamics** K. A. Stephani
5:30-8:30	**Reception**

From Shock Layer to Surface: DSMC Thermochemical Models for Hypersonics and High-Temperature Aerothermodynamics

K. A. Stephani

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The DSMC short course will provide an overview of recent advances in the modeling of hypersonic and high-temperature aerothermodynamic flows. Our discussion will focus on thermophysical processes relevant for the shock layer and gas-surface interactions. Models outlined will include the following.

(i) A state-based dissociation and recombination model constructed from ab initio potential energy surface (PES).
(ii) State-based transport model computed from scattering analysis of the O3 PES.
(iii) Surface-energetic and gas-surface interactions described from the surface phonon density of states.

All of these models will be described in the context of the DSMC framework [1], and their implementations and examples will be provided to show their utility for hypersonics applications.

[1] G. A. Bird, *Molecular Gas Dynamics and the Direct Simulation of Gas Flows*, Oxford University Press, Oxford, UK (1994).

Monday, September 23, 2019

Session 2: New Frontiers

Chair: M. A. Gallis, A. L. Garcia

8:30-9:00	**Welcome** J. S. Lash
9:00-9:40	**Invited:** **The International Space Station from a Former DSMC Practitioner's Perspective** G. J. LeBeau
9:40-10:00	**Break**

The International Space Station from a Former DSMC Practitioner's Perspective

G. J. LeBeau

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What has a wingspan as large as an American football field, weighs in at 900,000 pounds, is powered by an acre of solar panels, and travels continuously at over 17,000 miles per hour? If you guessed the International Space Station, you would be correct. By its name alone, you may already have some appreciation of the international partnership of countries from around the world that have come together to provide a continuous human presence in low Earth orbit for over 18 years. But have you ever wondered what it took to assemble this monumental engineering feat and what it takes to maintain its operations? Or maybe more importantly, what are its capabilities, and what is its role going forward? This and other aspects of the International Space Station will be addressed.

Gerald J. "Jay" LeBeau is the Deputy Manager of the Mission Integration and Operations Office in the International Space Station Program at NASA's Johnson Space Center (JSC) in Houston, Texas. Prior to this role, he served 25 years in JSC's Engineering Directorate as an aerosciences analyst and manager supporting various NASA programs, including the Space Shuttle, International Space Station, Orion, Commercial Cargo, and Commercial Crew programs. Much of his technical work involved the application of Direct Simulation Monte Carlo tools to these and other applications. He is also the primary original author of NASA's DSMC Analysis Code (DAC) software, which is used within NASA, industry, and academia to analyze rarefied-gas-dynamics environments.

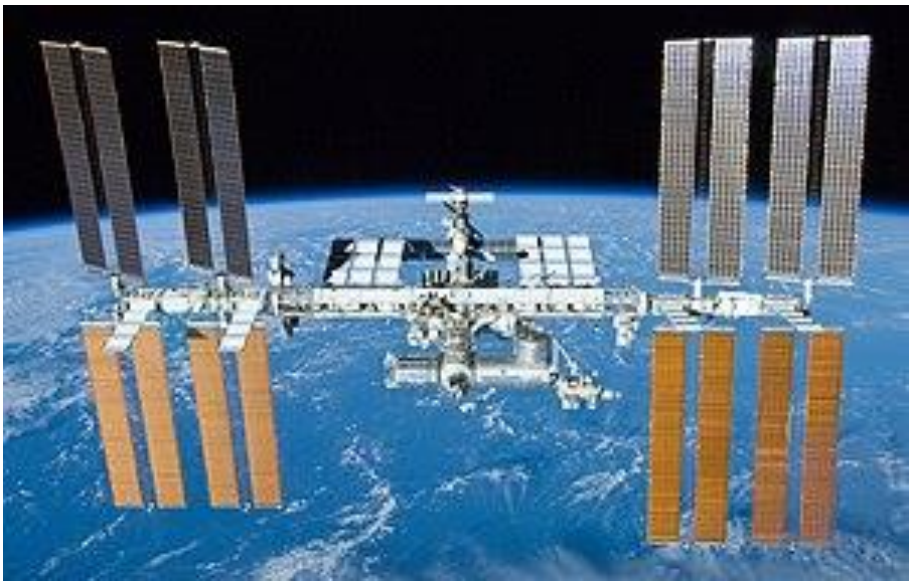

Image credit: Wikipedia.

Monday, September 23, 2019

Session 3: Gas-Surface Interactions

Chair: D. B. Goldstein

10:00-10:20	**Implicit Surface Models in the SPARTA DSMC Code** S. J. Plimpton, A. Borner
10:20-10:40	**Data-Based Modeling of Gas-Surface Interactions in Rarefied Gas Flow Simulations** N. Andric, P. Jenny
10:40-11:00	**Multiscale Method Using Moving DSMC Domain for Unsteady Nonlinear Acoustics** E. Jun, C. White, M. Borg
11:00-11:20	**Monte Carlo Methods for Nanoscale Oscillatory Flows** D. R. Ladiges, J. E. Sader
11:20-11:40	**DSMC Simulations of Vortex Shedding from a Circular Cylinder** J. R. Torczynski, M. A. Gallis
11:40-1:00	**Lunch**

Implicit Surface Models in the SPARTA DSMC Code

S. J. Plimpton

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Triangulated surfaces are often used in DSMC simulations to represent the surfaces of objects in a gas flow. Many codes, including SPARTA [1], allow a list of triangles to be explicitly defined in an input file. The DSMC grid overlays or conforms to the triangulated object, and individual triangles may span many grid cells.

We have developed an alternate surface model in which integer values are defined on the corner points of a regular DSMC grid. For example, the values can be read from an experimental 3D image file of a complex porous material. A Marching Cubes (MC) algorithm [2] is used with a specified threshold value to implicitly define triangles, each of which is wholly contained in a single grid cell. In aggregate, the triangles represent the material surface as a collection of watertight objects so that gas can flow through it in the usual DSMC manner. The figure shows an example of millions of implicit triangles created in this way.

We discuss how implicit surfaces are implemented in SPARTA and give performance data for how they can be used in parallel to run models with billions of triangles on thousands of compute nodes. An advantage of the implicit surface representation is that the corner-point values can evolve in time as gas particles collide and react with the surface. The triangulation can then be updated periodically to reflect the new corner-point values. We present preliminary results for a simple ablation model to illustrate how this works, in a similar fashion to [3].

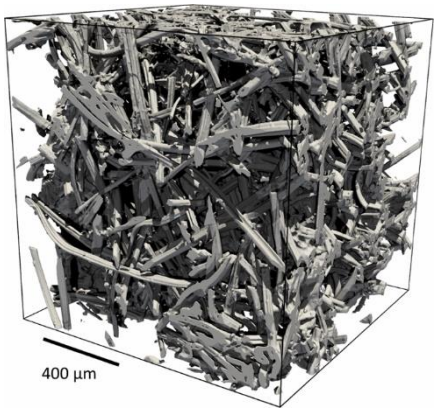

Figure 1. A ParaView visualization of triangulated surfaces generated from a micro-tomographic image of a FiberForm™ sample. The original 3D image was from a 0.52-mm^3 cube of material with 0.65-µm voxel edge size; the volume fraction of material is 14.4 %. To create this image, the MC algorithm mapped the voxels to (800)^3 grid cells and produced 57.4 million triangles to represent the surface of the material.

[1] S. J. Plimpton and M. A Gallis, "SPARTA Direct Simulation Monte Carlo (DSMC) Simulator," Sandia National Laboratories, https://sparta.sandia.gov/ (2019).

[2] L. Custodio, T. Etiene, S. Pesco, and C. T Silva, "Practical Considerations on Marching Cubes 33 Topological Correctness," *Computers & Graphics*, **37** (7), 840-850 (2013).

[3] J. C. Ferguson, F. Panerai, A. Borner, and N. N. Mansour, "PuMA: The Porous Microstructure Analysis Software," *SoftwareX*, **7**, 81-87 (2018).

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525. This paper describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the paper do not necessarily represent the views of the U.S. Department of Energy or the United States Government. A. B. would like to acknowledge funding from the NASA Entry Systems Modeling project.

Data-Based Modeling of Gas-Surface Interactions in Rarefied Gas Flow Simulations

N. Andric, P. Jenny

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In this work, a novel data-driven approach to gas-surface interaction modeling based on a recently introduced Distribution Element Tree (DET) method [1] is presented. The DET method is a computational technique that allows efficient probability density estimation with the possibility of conditional and unconditional random number sampling from the constructed distribution [2]. The input data are obtained by running an extensive set of molecular dynamics (MD) simulations of nitrogen-molecule scattering from a graphite surface [3]. By combining the obtained MD database with the DET method, a generalized kernel of gas-surface interaction can be constructed. The major benefit of this approach lies in the sampling of a post-scattered molecular state directly from the data itself and thus conserving all the relevant physics without the need for an accommodation-coefficient formulation and calibration. A direct comparison between the DET-based kernel and a classical scattering kernel is performed using the available numerical and experimental data. Furthermore, the implementation of the DET-based kernel inside a DSMC code and some obtained results are presented. The suitability of the proposed approach for modeling the scattering of diatomic molecules is particularly discussed. Additionally, satisfaction of the detailed-balance relation by the DET-based kernel is demonstrated.

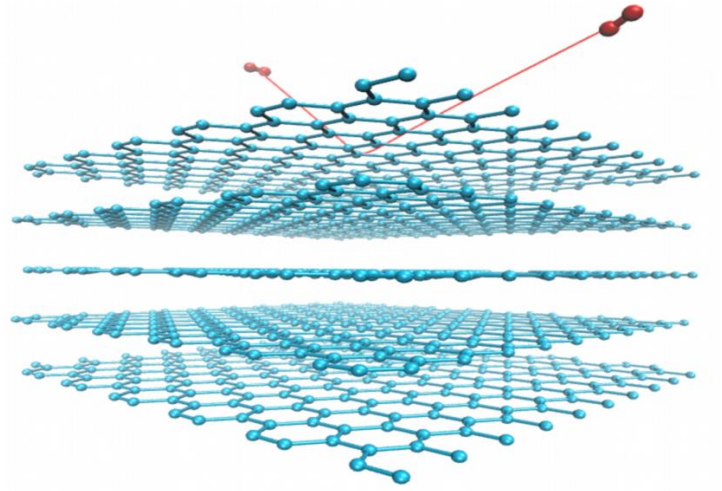

Figure 1: Schematic view of a nitrogen molecule scattering from a graphite surface in the MD simulation.

[1] D. W. Meyer, "Density Estimation with Distribution Element Trees," *Statistics and Computing*, **28**, 609-632 (2018).
[2] D. W. Meyer, "(Un)Conditional Sample Generation Based on Distribution Element Trees," *Journal of Computational and Graphical Statistics*, **27**, 940-946 (2018).
[3] N. Andric and P. Jenny, "Molecular Dynamics Investigation of Energy Transfer During Gas-Surface Collisions," *Physics of Fluids*, **30**, 077104 (2018).
[4] N. Andric, D. W. Meyer, and P. Jenny, "Data-Based Modeling of Gas-Surface Interaction in Rarefied Gas Flow Simulations," *Physics of Fluids*, **31** (06), 067109 (2019).

Funding for this research was provided by the Swiss National Science Foundation under the grant number 153116.

Multiscale Method Using Moving DSMC Domain for Unsteady Nonlinear Acoustics

E. Jun [1], C. White [2], M. Borg [1]

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DSMC can capture physical properties of nonlinear problems such as non-equilibrium, attenuation, and dispersion of acoustic waves [1]. However, time-dependent DSMC computations need a very large amount of computation particles and long time-scales to reduce the statistical noise. In this talk, we develop a multiscale method that uses moving domain decomposition, with the aim of modeling local disturbances in the moving wave only, with the rest of gas ignored from the computation. As a result, we reduce the overall computational cost that would otherwise require a full DSMC solution. Figure 1 shows the propagation of one-dimensional sinusoidal pulse. At the beginning of the simulation, the pulse is generated at the center of simulation domain. The pulse disperses, gets attenuated, expands, and detaches in time. The challenge in our multiscale method is to model the pulse only as it moves through the domain using DSMC, while ignoring the rest of uninteresting physics happening elsewhere.

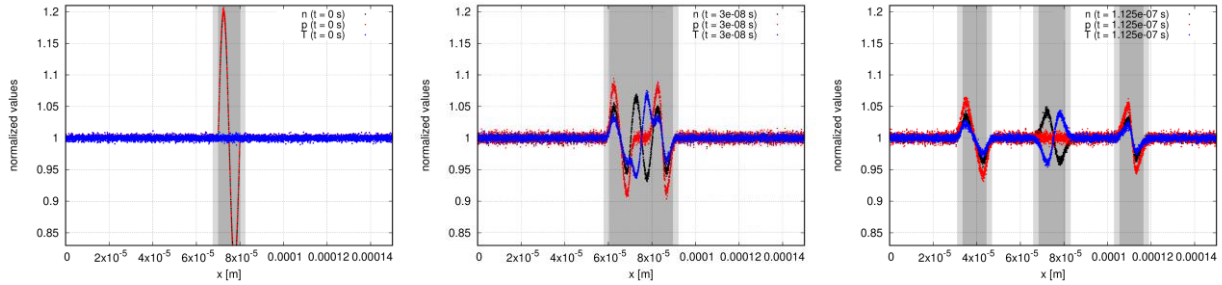

Figure 1. Sinusoidal pulse propagation in stationary domain for full DSMC simulation. (n = number density, p = pressure, T = temperature).

We apply a moving domain decomposition scheme to simulate only regions where the acoustic pulse exists. At the beginning of the simulation, the size of the computation domain is the width of the initial pulse plus a small buffer on either side. As the pulse moves, it spreads out, and so the domain expands according to the local growth of the pulse. Figure 2 shows the results with the moving domain scheme. It successfully captures the expanding and moving acoustic pulse. The computation speed up obtained from our method scales as L/w, where L is the length of the domain, and w is the width of the pulse. As the pulse travels at the speed of sound, the length it travels can be much larger than L. As future steps, a detailed analysis is presented based on the Knudsen number, Kn, which is defined as the mean free path over domain width. Also, we find discrepancies with Euler results, which strengthens the need for this multiscale method.

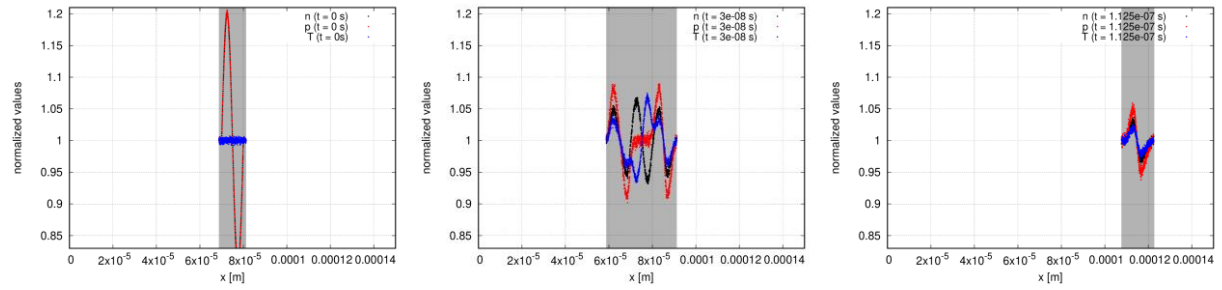

Figure 2. Sinusoidal pulse propagation with moving domain scheme.

[1] A. L. Danforth and L. N. Long, "Nonlinear Acoustic Simulation Using Direct Simulation Monte Carlo," *Journal of the Acoustical Society of America*, **116**, 1948 (2004).

Monte Carlo Methods for Nanoscale Oscillatory Flows

D. R. Ladiges

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Gas flows generated by resonating nanoscale devices typically occur in the non-continuum, low Mach number regime. Numerical simulation of such flows presents a significant challenge to traditional Direct Simulation Monte Carlo (DSMC), which has motivated the development of several Monte Carlo methods for low Mach number flows (Eg. [1,2]). Extending this approach, we present a frequency-domain Monte Carlo method [3,4] for oscillatory low Mach number gas flows, based on the linearized Boltzmann equation. This circumvents the need for temporal simulations, providing direct access to both amplitude and phase information using a pseudo-steady algorithm. The proposed method is demonstrated with several examples, and good agreement is found with both existing time-domain Monte Carlo methods and accurate numerical solutions of the Boltzmann-BGK equation. Additionally, we demonstrate that the frequency-domain method provides a significant improvement in statistical convergence compared to existing time-domain Monte Carlo approaches.

[1] S. Ramanathan and D. L. Koch, "An Efficient Direct Simulation Monte Carlo Method for Low Mach Number Noncontinuum Gas Flows Based on the Bhatnagar-Gross-Krook Model," *Physics of Fluids*, **21** (3), 033103 (2009).

[2] T. M. M. Homolle, N. G. Hadjiconstantinou, "Low Variance Deviational Simulation Monte Carlo," *Physics of Fluids*, **19** (4), 041701 (2007).

[3] D. R. Ladiges and J. E. Sader, "Frequency-Domain Monte Carlo Method for Linear Oscillatory Gas Flows," *Journal of Computational Physics*, **284**, 351-366 (2015).

[4] D. R. Ladiges and J. E. Sader, "Frequency-Domain Deviational Monte Carlo Method for Linear Oscillatory Gas Flows," *Physics of Fluids*, **27** (10), 102002 (2015).

DSMC Simulations of Vortex Shedding from a Circular Cylinder

J. R. Torczynski, M. A. Gallis

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The Direct Simulation Monte Carlo (DSMC) method [1] is used to simulate flow past a circular cylinder. The gas is hard-sphere argon at 273.15 K, which has a sound speed of 307.9 m/s and a viscosity of 2.117×10^{-5} Pa·s. The freestream is at 6.876×10^{-5} kg/m^3, 3.91 Pa, and 30.79 m/s. The cylinder diameter is 1 m, with unity accommodation at 273.15 K. These values yield a Reynolds number of 100, a Mach number of 0.1 (essentially incompressible), and a Knudsen number of 0.00162 (essentially continuum). Sandia's DSMC code SPARTA [2] is used to simulate this system. The two-dimensional computational domain is rectangular and extends 5 diameters upstream, 10 diameters downstream, and 5 diameters laterally on both sides. This domain is meshed with 0.72 billion square cells whose side length is 1/4 mean free path. Each cell contains ~100 particles, yielding a total of 72 billion particles in the domain. The time step is 1.4824 μs, which is 1/3 of the mean collision time. Simulations are run on Sequoia, an IBM Blue Gene/Q petascale supercomputer at Lawrence Livermore National Laboratory [3]. The figure shows the streamwise velocity component at 8 equally spaced times over one shedding cycle. The lateral force on the cylinder is periodic at 5.4 Hz, which yields a Strouhal number of 0.175. A COMSOL [4] simulation of the same flow problem yields the same value, which is about 6% larger than the corresponding value for an infinitely wide domain [5].

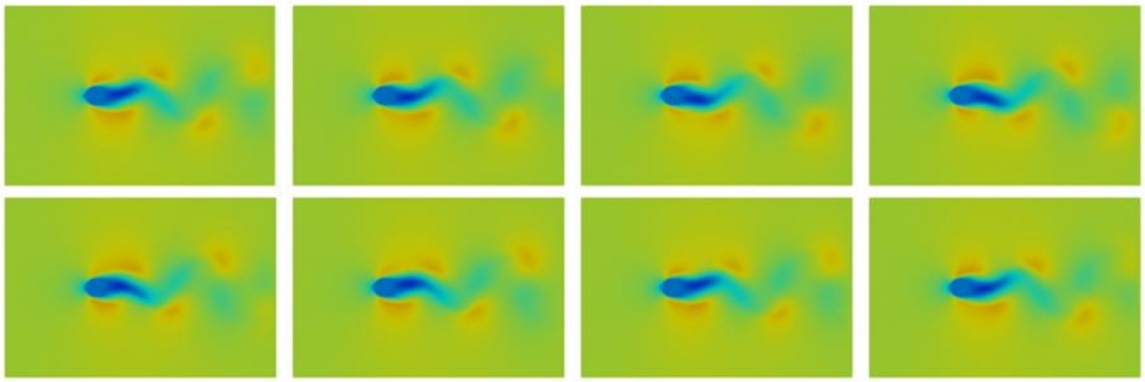

Figure 1. DSMC simulation of essentially incompressible flow past a circular cylinder at Re = 100. A single cycle of vortex shedding is shown. The Kármán vortex street [6] is clearly seen.

[1] G. A. Bird, *Molecular Gas Dynamics and the Direct Simulation of Gas Flows*, Oxford University Press, Oxford, UK (1994).
[2] S. J. Plimpton and M. A Gallis, "SPARTA Direct Simulation Monte Carlo (DSMC) Simulator," Sandia National Laboratories, https://sparta.sandia.gov/ (2019).
[3] Wikipedia, "Sequoia (supercomputer)," https://en.wikipedia.org/wiki/Sequoia_(supercomputer) (2019).
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Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525. This paper describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the paper do not necessarily represent the views of the U.S. Department of Energy or the United States Government.

Monday, September 23, 2019

Session 4: Hybrids

Chair: T. E. Schwartzentruber

1:00-1:20	**Analysis and Sensitivity Study of Nonequilibrium Hypersonic Flows Using DSMC and CFD** N. Adhikari, A. Chinnappan, A. A. Alexeenko
1:20-1:40	**Extension and Application of the Modular-Particle Continuum Method to Transient Flows** T. R. Deschenes, B. D. Smith, J. Quenneville, R. S. Taylor
1:40-2:00	**On-Average Error in Zero-Dimensional DSMC** W. J. McDoniel, C. H. Moore, G. A. Radtke, K. L. Cartwright, M. Bettencourt
2:00-2:20	**Potential Energy and Angular Momentum Conservation in Particle Merging and Collision Models** R. S. Martin
2:20-2:40	**Hybridizing DSMC and Discrete Velocity Methods in Velocity Space** G. P. Oblapenko, D. B. Goldstein, P. L. Varghese, C. H. Moore
2:40-3:00	**Accurate Particle Time Integration for Solving the Vlasov-Fokker-Planck Equation** P. Jenny, H. Gorji
3:00-3:20	**Break**

Analysis and Sensitivity Study of Nonequilibrium Hypersonic Flows using DSMC and CFD

N. Adhikari, A. Chinnappan, A. A. Alexeenko

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The complex coupling of nonequilibrium effects on the aerothermal load of a hypersonic spacecraft remains a challenging aspect of hypersonic flow modeling. The degree of nonequilibrium affects the chemical reactions which in turn affects the overall flow field. This work focuses on study of such nonequilibrium effects using Computational Fluid Dynamics (CFD) and DSMC techniques. Furthermore, the uncertainty associated with hypersonic flow modeling is assessed through sensitivity studies of a few important input parameters involved in such flow modeling.

In CFD, the nonequilibrium effects are modeled through internal energy relaxation equations with chemical-internal energy coupling models [1]. Recent developments and capabilities of CFD in solving hypersonic flows has been reviewed by Candler [2]. For this work, a commercial CFD solver, ANSYS Fluent, has been modified to solve nonequilibrium flows, similar to the work of Shoev et al. [3] with added improvements and capabilities.

Figure 1 shows a comparison of the bulk density field around a hypersonic cylinder with freestream Mach number of 6.13 in a partially dissociated nitrogen flow simulated in CFD and SPARTA DSMC [4]. The freestream Knudsen number based on the diameter of the cylinder is ~10^{-5}. This configuration represents the experiment by Hornung [5] and is often taken as a benchmark case for the validation of a nonequilibrium hypersonic CFD solution. Figure 2 shows the shock-wave stand-off distance in the CFD solution. The CFD method in this case uses Landau-Teller internal-energy relaxation model, Millikan-White relaxation-time correlation [6] with Park's non-preferential vibration-dissociation coupling model [1]. The species transport properties are calculated using the Hirschfelder model with LJ parameters in CFD while the VSS model has been used in DSMC. The flow fields obtained from CFD and DSMC are comparable to each other for most of the flow with the exception of the shock start position in DSMC. The DSMC result shows a slight irregularity in the shock profile and warrants further investigation.

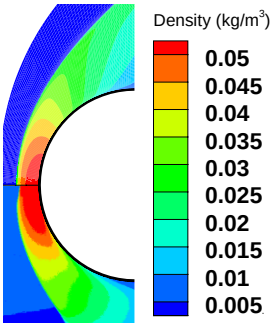

Figure 1. Density field around the cylinder.

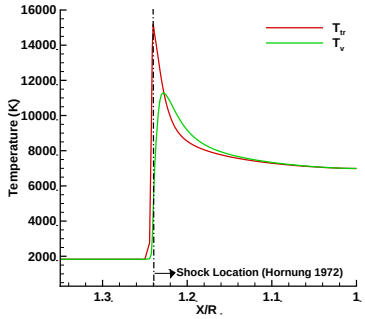

Figure 2. Temperature variation across the shock wave in CFD.

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The authors would like to thank ANSYS for providing the research licenses to facilitate this research.

Extension and Application of the Modular-Particle Continuum Method to Transient Flows

T. R. Deschenes, B. D. Smith, J. Quenneville, R. S. Taylor

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Many engineering flows of interest contain spatial and temporal variation in continuum and rarefied flow domains. Continuum-based methods, based on the Navier-Stokes equations, can introduce physical errors in regions of rarefied flow. The Direct Simulation Monte Carlo (DSMC) method maintains accuracy throughout the continuum and rarefied regions, but its use in continuum regions results in significant computational cost. Hybrid methods that couple continuum and rarefied modules have been successfully demonstrated for a wide variety of steady-state flows [1]. For example, the Modular Particle-Continuum method has been demonstrated to reproduce full DSMC results using a fraction of the computational time and memory [2-3]. In this talk, we extend the MPC method to model transient flows. The implementation of the unsteady MPC method couples the US3D code [4] with the SPARTA DSMC software [5]. The method is applied to a transient, mixed continuum-rarefied flow field where a one-dimensional shock of N_2 gas propagates from an inviscid wall. For example, Figure 1 shows a snapshot of the flow field predicted by CFD, DSMC, and the MPC method. The flow contains a moving rarefied region and rarefied continuum interfaces in both supersonic and subsonic regions of the flow. The MPC results are compared with full CFD and full DSMC results. Similar to previously published steady-state hybrid results [2-3], the unsteady MPC method can reproduce the full DSMC results, while only applying the DSMC method in rarefied regions. For example, the left figures compare the translational and rotational temperatures of the gas at two snapshots, while the right figure compares the velocity distribution function predicted by the DSMC and MPC methods within the interior of the shock snapshot highlighted on the lower left.

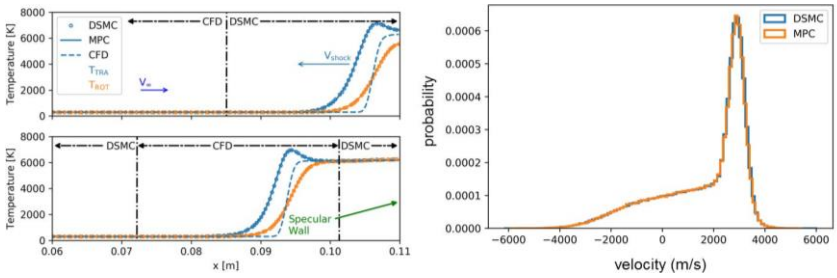

Figure 1. (left) Snapshot of translational and vibrational temperatures for early shock formation (top) and later shock formation (bottom); (right) comparison of velocity distribution function in the x-direction within the interior of the shock (shown in the lower left panel), as predicted by full DSMC and the MPC method.

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On-Average Error in Zero-Dimensional DSMC

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It is known that DSMC [1] converges to solutions of the Boltzmann equation as the number of simulated particles increases [2], but of course in practice simulations will use as few particles as possible in order to run faster. This yields noisy instantaneous results, so macroscopic properties such as temperature are often obtained by averaging over multiple time steps or multiple independent simulations [1,3]. Averaging is used for other noisy quantities too, such as ion populations or reaction rates, and in many cases the future state of the simulation depends on a noisy variable. However, for some quantities of interest, it is not the case that either time or ensemble averages converge to the correct value as the number of time steps or number of independent simulations increases—DSMC is on-average wrong when using finite numbers of simulated particles. This is a well-known issue for complex flows [4], but we demonstrate bias for simple 0D relaxation problems. We show that even elastic collisions are an important source of error: even if a collection of computational particles is initially representative of the underlying physical distribution, collisions sever this relationship. We present two simple cases demonstrating on-average error in DSMC and explore why the method produces them.

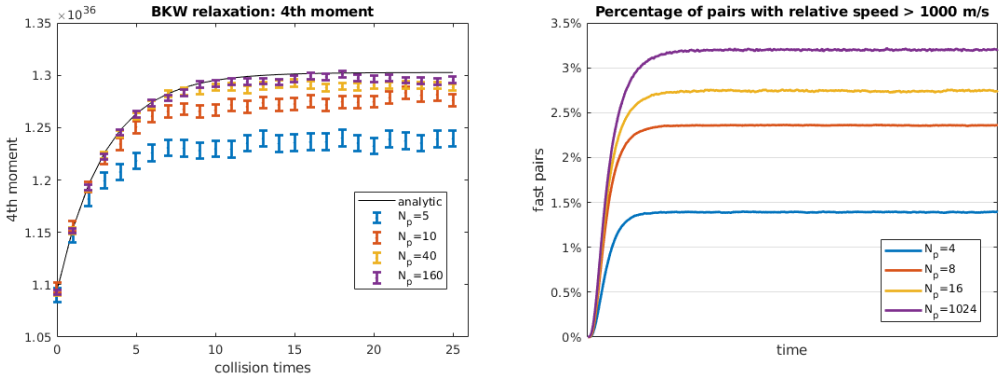

Figure 1. (left) 95% confidence intervals of the 4th moment from tens of thousands of simulations of the relaxation of the Bobylev-Krook-Wu distribution [5] with argon. (right) The average fraction of fast pairs over time for a double-delta-function distribution (where all particles are initialized at ±413 m/s in the x direction).

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Potential Energy and Angular Momentum Conservation in Particle Merging and Collision Models

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Despite consistency with the Boltzmann equation when converged in the limit of infinitesimal cell size [1] and therefore collision partner separation, it has long been known that the DSMC method fails to exactly conserve angular momentum for finite collision partner separation distances. While Meiburg attributed differences observed between DSMC and MD results [2] to this lack of angular momentum conservation, Bird quickly showed that this was more likely a result of the misapplication of DSMC to a flow that violates the dilute gas assumption and that an alternative version of DSMC where post-collision positions are modified to ensure conservation of angular momentum performed no better than the original method on a test case of a forced vortex in a box [3]. Further, Nanbu analyzed the problem directly showing that, not only is vorticity actually related to conservation of linear momentum, but that the angular momentum is conserved in expectation with variance that diminishes rapidly with cell size [4]. Though this analysis served as a strong basis for the continued use of DSMC for high-vorticity fluid flows, this lack of angular momentum conservation is still periodically revisited as the fact that it is a collisional invariant and one of the conserved quantities for global Maxwellian equilibrium distributions [5] suggests that even small random walks in angular momentum may be detrimental to flows more sensitive to the quantity. As conservation of these invariants is of particular interest also in particle-merging methods used to resample velocity distributions, it was similarly shown that modifying the octree particle-merging method [6] for angular momentum conservation by appropriate selection of spatial scatter with respect to the merge pair center of mass could improve dispersion resulting from merging in a collisionless radial potential energy well as presented in Ref. [7]. This suggests that the conservation of angular momentum may be more critical in scenarios where the random walk of small deviations may interact nonlinearly with other system quantities such as fields. For the addition of binary collisions or particle merging in simulations of magnetized plasma like E×B transport simulations described in Ref. [8], the conservation of angular momentum appears to have additional consequences. This effect is not dissimilar to the observed enhanced numerical heating that a failure to account for finite collision pair separation distances in potential energy causes when coupling binary collisions of charged particles to PIC simulations [9]. In this presentation, these conservation effects will be studied in the context of adding Nanbu's binary Coulomb collisions model [10] and particle merging to enhanced E×B transport simulations.

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Hybridizing DSMC and Discrete Velocity Methods in Velocity Space

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The present work is concerned with investigation of a new approach to modeling of rarefied gas flows, based on a hybridization in velocity space. The bulk of the distribution function is represented via DSMC [1] particles, while the tails of the distribution function are modelled via a discrete velocity method [2-4].

While velocity-space hybridization schemes have been proposed previously [5-8], they were usually limited to a BGK model equation solver [5-7] and were not investigated in detail. In the present work, the proposed hybridization scheme, based on a variable-weight DSMC scheme and a discrete velocity solver of the full Boltzmann equation, is applied to spatially homogeneous problems. Various numerical aspects of the scheme are considered, and the influence of different parameters on the on the fidelity of the solutions and the computational speed is evaluated.

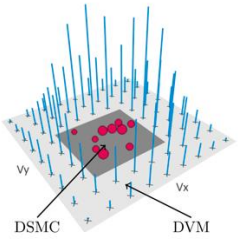

Figure 1. Schematic of hybrid velocity-space representation for a fixed z-component of the velocity.

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This work was supported by Sandia National Laboratories. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525. This paper describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the paper do not necessarily represent the views of the U.S. Department of Energy or the United States Government.

Accurate Particle Time Integration for Solving the Vlasov-Fokker-Planck Equation

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The Vlasov-Fokker-Planck equation (together with Maxwell's equations) provides the basis for plasma flow calculations. While the terms accounting for long-range forces are established, different drift and diffusion terms are used to describe Coulomb collisions. Here, linear drift and a constant diffusion coefficient are considered, and the electromagnetic fields are imposed, i.e., plasma frequency is not addressed. The solution algorithm is based on evolving computational particles of a large ensemble according to a Langevin equation, whereas the time-step size is typically limited by plasma frequency, Coulomb collision frequency, and cyclotron frequency. To overcome the latter two time-step size constraints, a novel time integration scheme for the particle evolution is presented. It requires that only gradients of mean velocity, bath temperature, magnetic field and electric field need to be resolved along the trajectories. In fact, if these gradients are zero, then the new integration scheme is statistically exact, no matter how large the time step is chosen. This is demonstrated by the result in Fig. 1. A large number of deuterium ions, initially at rest at the origin, were accelerated and deviated in a constant electromagnetic field, while interacting with a bath of constant temperature. Shown are the mean trajectory and the ion locations after a finite time interval. It is noteworthy that the final locations and velocities can be computed in one time step and that the resulting statistics is exact; despite the tortuous trajectories, which do not have to be resolved. Obviously, if employed within a particle-based solution algorithm, this provides a huge computational advantage compared to classical integration schemes. Besides single ion trajectories, plasma flow in spatially varying electromagnetic fields was also investigated, that is, the influence of time-step size and grid resolution on the final solution was studied.

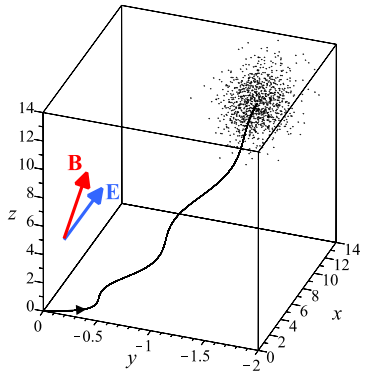

Figure 1: Position cloud and mean trajectory of a large deuterium ion ensemble. The ions were initially at rest at the origin and got accelerated and deviated in a constant electromagnetic field, while interacting with a bath of constant temperature.

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Monday, September 23, 2019

Session 5: Non-Continuum Flows

Chair: F. E. Lumpkin III

3:20-3:40	**DSMC Simulations of Diffuse Shocks in Molecular Beam Experiments** E. Geistfeld, T. E. Schwartzentruber
3:40-4:00	**Leading Edge Velocity-Slip and Temperature-Jump in Hypersonic Flows** P. Bhide, T. E. Schwartzentruber
4:00-4:20	**On Temperature Discontinuity at an Evaporating Liquid-Vapor Interface** P. Jafari, H. Ghasemi
4:20-4:40	**Kelvin-Helmholtz Instability with Thermal Nonequilibrium** M. Lee, J. H. Chen, M. A. Gallis
4:40-5:00	**SPARTA Kokkos: The Quest for Performance Portable DSMC** S. G. Moore, A. K. Stagg
5:00-6:00	**SPARTA Users Meeting** S. J. Plimpton

DSMC Simulations of Diffuse Shocks in Molecular Beam Experiments

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A molecular beam, when targeted at a small blunt object, can generate a diffuse hypersonic shock layer that exhibits noticeable dissociation physics (Fig. 1). Unlike large shock-tunnel facilities, the beam can be pulsed to generate shock layers two times per second for hours or even days with repeatable conditions. Such test frequency and repeatability may enable existing optical diagnostic techniques to measure thermochemical quantities with unprecedented accuracy and precision at a fraction of the cost of existing facilities. Essential inputs for CFD and DSMC models include internal energy relaxation rates and chemical reaction rate coefficients accurate for thermal-nonequilibrium conditions. Existing models [1,2] are based on relatively few experiments performed over a limited range of conditions, but new experiments could improve these models and validate new ones.

This work presents DSMC simulations of diffuse shock layers in molecular beams to investigate the feasibility of a new type of experimental facility to study nonequilibrium chemistry. We simulate the current molecular beam facility at Montana State University [3], now with a blunt target placed in the scattering chamber of the hyperthermal molecular beam. This setup is similar to that described in [3]; the target is exposed to pulses of highly energetic gas mixtures for time scales of ~20 microseconds. The shock layer produced does not precisely match hypersonic flight conditions but may still provide a novel way to optically measure chemical processes in fine detail.

Preliminary DSMC simulations show that the beam source as it exists today can produce such diffuse shock layers around small targets with considerable oxygen and partial nitrogen dissociation. The simulated energy distributions are highly nonequilibrium with overpopulated high-energy tails compared to the equivalent Boltzmann distributions. Stagnation line profiles and velocity and energy distribution functions for each component of a five-species air mixture are analyzed. The location and thickness of the shock layer, the degree of nitrogen and oxygen dissociation, and the energy distributions of the gas, predicted by DSMC, may serve as valuable guidelines for spectroscopic measurement techniques, source strength, sample positioning, and overall design of the final apparatus.

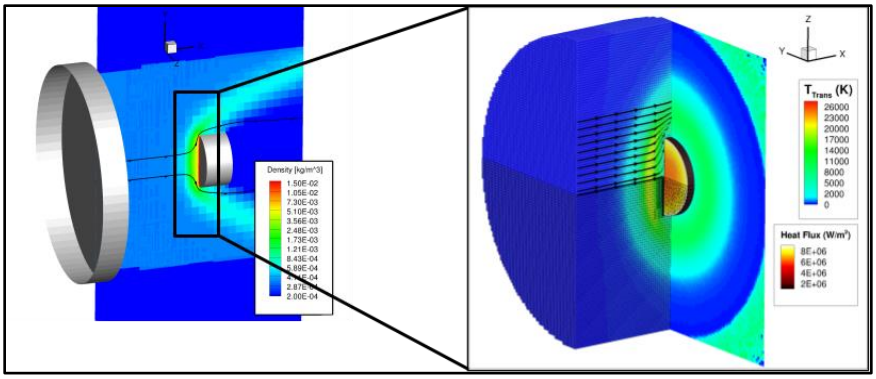

Figure 1. Example DSMC simulation showing a molecular beam impacting a blunt object.

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The speaker would like to thank his advisor, Professor Thomas E. Schwartzentruber, for his invaluable expertise, guidance, and support during the project, without which this work would not have been possible.

Leading Edge Velocity-Slip and Temperature-Jump in Hypersonic Flows

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The modeling of shock-dominated hypersonic flows over geometries with sharp leading edges can pose substantial difficulties for continuum methods. Such flows may contain regions with strong thermal/chemical non-equilibrium, sharp flow gradients and significant velocity-slip/temperature-jump at the wall which may not be captured accurately by traditional CFD solvers. It has been shown previously that the continuum assumption is valid for small deviations from the equilibrium distribution function [1] and may not hold in regions of large flow gradients [2], such as those observed in the attached boundary layer flow past the leading edge. The DSMC method can be used for modeling flow conditions ranging from free-molecular to continuum. DSMC also has an advantage over continuum solvers in capturing 'slip flow' at the wall in that separate phenomenological models are not required and instead the velocity slip and temperature jump are obtained as results of the simulation.

We present flow-field comparisons between CFD and DSMC for the attached boundary layer downstream of the sharp leading edge of three geometries, namely the Hollow Cylinder Flare (HCF), Double-cone, and Double-wedge. The no-slip and slip boundary conditions [3] are both used in the CFD simulations. The magnitudes of velocity slip and temperature jump at the wall as predicted by CFD (with slip) and DSMC are compared to assess the accuracy of the slip models. We also look at the degree of thermal non-equilibrium in the attached boundary layer and investigate the effect of these phenomena on surface properties such as heat flux. Figure 1 shows the CFD temperature contours for flow over the Double-cone geometry, with a zoomed-in view of the flow near the leading edge on the right, displaying locations of 'stations' where we extract boundary layer profiles to make the aforementioned comparisons. The flows are analyzed in terms of the Knudsen number Kn_{gl} based on flow gradients, proposed by Boyd et al. [2].

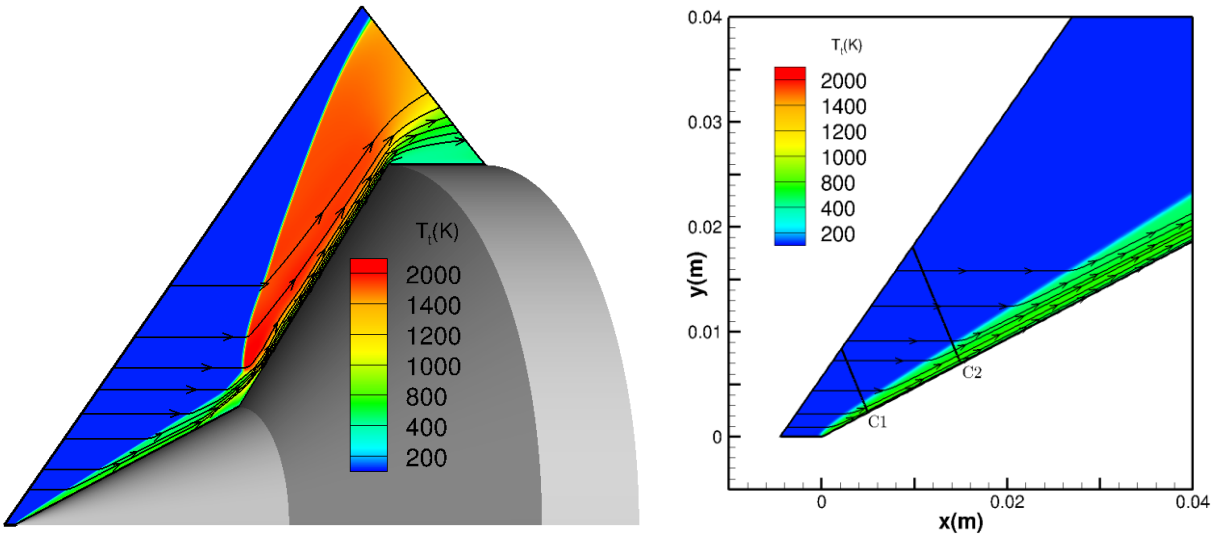

Figure 1. CFD temperature contours for flow over the Double-cone geometry.

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[2] I. D. Boyd, G. Chen, and G. V. Candler, "Predicting Failure of the Continuum Fluid Equations in Transitional Hypersonic Flows," *Physics of Fluids*, **7** (1), 210-219 (1995).

[3] T. Gökçen, R. W. MacCormack, and D. R. Chapman, "Computational Fluid Dynamics Near the Continuum Limit," AIAA-1987-1115, American Institute of Aeronautics and Astronautics, Reston, VA (1987).

On Temperature Discontinuity at an Evaporating Liquid-Vapor Interface

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Numerous experimental studies have indicated that a temperature discontinuity exists across an evaporating liquid-vapor interface. However, the magnitude of the discontinuity has been contentious. Various values of temperature discontinuity at the liquid-vapor interface from 0.1 K to 15 K have been measured, and the reported values are open to question. The possible factors affecting measurement of the interfacial temperature discontinuity, including radiation, thermocouple bead diameter, and evaporative cooling of the thermocouple bead, were investigated and concluded to be negligible. Investigators have found that the magnitude of the interfacial temperature discontinuity can depend mainly on the experimental conditions at the vapor side of the interface. Here, we studied the influence of vapor-side thermal boundary conditions on the temperature profile along the Knudsen layer formed in the steady evaporation of a vapor. The vapor polyatomic molecules behave as rigid rotators, and the vapor motion is obtained by the numerical solution of the Boltzmann equation by the Direct Simulation Monte Carlo (DSMC) method. The adopted numerical method allows us to obtain an accurate interfacial temperature profile, which can be used as a benchmark to determine interfacial temperature discontinuity at different thermal boundary conditions. The obtained temperature profiles at different thermal boundary conditions are also validated by the previous experimental studies.

Kelvin-Helmholtz Instability with Thermal Nonequilibrium

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The Kelvin-Helmholtz (K-H) instability is one of the most important instability mechanisms present in many engineering applications and occurring in nature. The instability occurs when a strong velocity gradient exists at the interface of two fluids flows. The most significant characteristic of the K-H instability is the roll-up of vortical structures, and this mechanism transfers kinetic energy from small-scale to large-scale motions. In this study, we investigate the effect of strong thermal non-equilibrium from the primary unstable K-H mode and energy-transfer mechanisms. Multiple studies showed that DSMC (Direct Simulation Monte Carlo) is an excellent tool to study various hydrodynamic instabilities with multi-physics, including the Richtmyer-Meshkov and Rayleigh-Taylor instabilities [1-3]. First, we demonstrate that DSMC with the Sandia SPARTA code is capable of studying K-H instability in low-Knudsen-regime flows by comparing results from DSMC and DNS (Direct Numerical Simulation). Second, we investigate the effect of strong non-equilibrium between translational, rotational, and vibrational energy modes on energy-transfer rate from small-scale to large-scale motions and mixing of fluids.

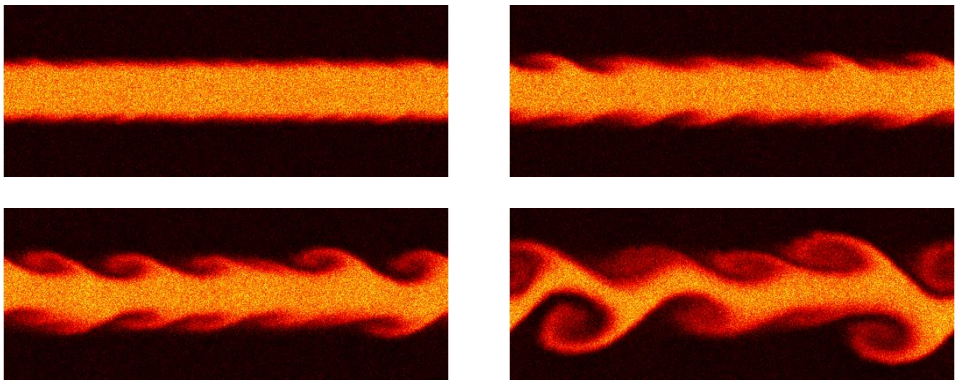

Figure 1. Temporal evolution of Kelvin-Helmholtz instability: argon (orange), neon (black).

[1] G. A. Bird, *Molecular Gas Dynamics and the Direct Simulation of Gas Flows*, Oxford University Press, Oxford, UK (1994).
[2] M. A. Gallis, T. P. Koehler, J. R. Torczynski, and S. J. Plimpton. "Direct Simulation Monte Carlo Investigation of the Richtmyer-Meshkov Instability," *Physics of Fluids*, **27** (8), 084105 (2015).
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The work at Sandia National Laboratories was supported by the US Department of Energy, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences, and Biosciences. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525. This paper describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the paper do not necessarily represent the views of the U.S. Department of Energy or the United States Government. This research used resources of the National Energy Research Scientific Computing Center (NERSC), a U.S. Department of Energy Office of Science User Facility operated under Contract No. DE-AC02-05CH11231.

SPARTA Kokkos: The Quest for Performance Portable DSMC

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SPARTA, an open-source, massively parallel direct simulation Monte Carlo (DSMC) code [1-3], has been extended to use the Kokkos performance portability library [4] to enable multithreaded CPU and GPU parallelism. The Kokkos library is developed by Sandia National Laboratories as a single-source system, meaning C++ code is written once in a form that looks independent of the target hardware and then target-specific code (i.e., OpenMP or CUDA) is generated based on compile-time options. This is helpful for dealing with a wide variety of ever-changing hardware and protects developers from having to maintain multiple versions of the code. SPARTA Kokkos has been used to perform large-scale DSMC simulations on 3 of the world's top 10 supercomputers (Trinity, Sequoia, and Sierra), and it also runs on small clusters and desktop machines. Benchmarking results on several different hardware such as NVIDIA V100 GPUs and Intel Xeon Phis will be presented, and a few challenges to obtaining performance portability and running at large scale (looking toward exascale computing) will be discussed.

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Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525. This paper describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the paper do not necessarily represent the views of the U.S. Department of Energy or the United States Government.

Tuesday, September 24, 2019

Session 6: Keynote Lecture

Chair: A. L. Garcia

8:00-9:00	**Graeme A. Bird Keynote Lecture:** **Taming Fire: Molecular Simulations of Combustion** A. A. Alexeenko

Taming Fire: Molecular Simulations of Combustion

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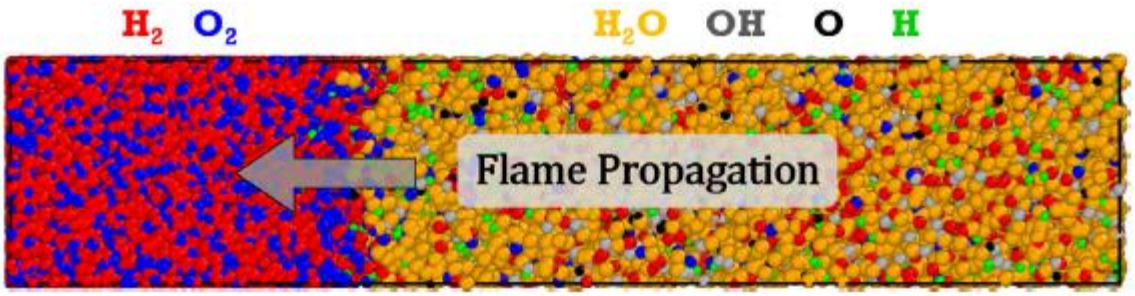
The Direct Simulation Monte Carlo (DSMC) method [1] allows combustion phenomena to be studied at the molecular level, including state-to-state processes at conditions far from thermal equilibrium. The evolution of computational platforms and the availability of highly scalable DSMC software provide an opportunity for molecular simulations to enable improved combustion diagnostics and control. Such modeling is especially useful for combustion at high speeds and at the microscale due to nonequilibrium transport and chemistry. In this talk, we review the necessary elements for a framework for applying DSMC to model combustion at the molecular level. Notably the standard DSMC approach employing Total Collision Energy (TCE) chemistry and Larsen-Borgnakke (LB) energy exchange models is not applicable for combustion simulations, which are dominated by exchange and recombination reactions. A modified TCE-LB method is developed to ensure detailed balance and relaxation toward thermal equilibrium regardless of the internal energy relaxation rates. First, we consider a benchmark of H_2-O_2 premixed flame and compare with continuum modeling and experimental data. The DSMC simulations based on the extended TCE-LB framework are then applied for other combustion examples. In particular, we consider a novel microcombustor concept based on field-emission dielectric barrier discharge (FE-DBD). Field-emission-based microplasma actuators generate highly positive space charges that can be used to preheat, pump, and mix reactants in microscale geometries and that offer promising solutions to the problems associated with initiating and sustaining microcombustion.

[1] G. A. Bird, *Molecular Gas Dynamics and the Direct Simulation of Gas Flows*, Oxford University Press, Oxford, UK (1994).



Tuesday, September 24, 2019

Session 7: Chemistry I

Chair: B. M. Stewart

9:00-9:20	**Bird's Chemistry Model for Given Reaction Rates** I. J. Wysong, S. F. Gimelshein
9:20-9:40	**Direct Molecular Simulation of Dissociating Oxygen in 0D Adiabatic Reactor** E. Torres, T. E. Schwartzentruber
9:40-10:00	**State-Resolved Treatment of Transport Properties for the $O(^3P)+O_2(^3\Sigma_g^-)$ System in DSMC** S. Subramaniam, T. Pan, K. Swaminathan-Gopalan, K. A. Stephani
10:00-10:20	**Break**

Bird's Chemistry Model for Given Reaction Rates

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The work focuses on the Total Collision Energy (TCE) model of chemical reactions, derived through the application of the collision theory in the pioneering work of Graeme Bird in 1977-1978 [1-2]. Here, we analyzed several subtle, and often omitted in the literature, aspects of the model, such as the inclusion of the quantum structure of the internal energy modes, the number of internal degrees of freedom, the detailed balance, as well as some numerical limitations such as the reaction probability exceeding unity, as well as ways to overcome them. The applicability of the TCE model to the dissociation, exchange, and ionization reactions is examined.

An example of TCE model performance is shown in Fig. 1, where the cross section of the exchange reaction $N_2+O \rightarrow NO+N$ is obtained using the collision theory of the TCE approach and the quasi-classical trajectory (QCT) calculations [3]. The translational energy dependence of the cross section is illustrated for the rotational and vibrational states J = 0 and v = 5, respectively. The vibrational energy dependence is given for E_t = 2.5 eV and J = 0. The results indicate that the TCE model captures the energy dependence of the nitrogen exchange reaction cross sections quite reasonably. For a fixed vibrational level, the difference between the TCE and QCT results is within a factor of two. For a fixed relative translational energy, TCE somewhat underpredicts QCT for low vibrational energies and overpredicts for high energies, but the difference is mostly within a factor of three.

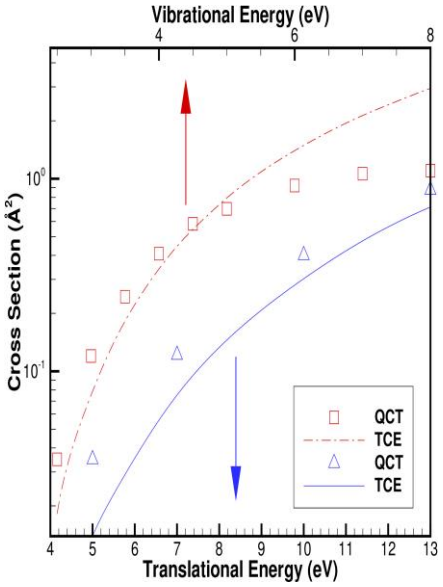

Figure 1. Dependence of the exchange reaction cross section on translational and vibrational energies.

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[2] G. A. Bird, "Monte Carlo Simulations in an Engineering Context," *Progress in Astronautics and Aeronautics*, **74**, 239-255 (1981).

[3] D. Bose and G. V. Candler, "Thermal Rate Constants of the $N_2 + O \rightarrow NO + N$ Reaction Using Ab Initio ^{3}A" and ^{3}A' Potential Energy Surfaces," *Journal of Chemical Physics*, **104**, 2825-2833 (1996).

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

Direct Molecular Simulation of Dissociating Oxygen in 0D Adiabatic Reactor

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In this paper, we present direct molecular simulations (DMS) of rovibrational excitation and dissociation of an oxygen mixture in a constant-volume reactor under adiabatic conditions. The DMS method is a variant of Direct Simulation Monte Carlo (DSMC) wherein collision outcomes are determined directly based on quasi-classical trajectory calculations (QCT) on multi-body potential energy surfaces (PESs), instead of the semi-empirical chemistry models that are commonplace in DSMC. Since it relies entirely on the PES to determine collision outcomes, DMS is capable of naturally predicting the rates of internal energy excitation and dissociation under nonequilibrium conditions without any tuning parameters. Thus, its primary use is as a benchmark tool for the development of reduced-order nonequilibrium chemical-kinetics models for DSMC or computational fluid dynamics (CFD) codes. In this study, we use the set of ab initio potentials for ground-electronic-state oxygen recently generated at the computational chemistry group at the University of Minnesota by Paukku et al. [1, 2] and Varga et al. [3]. Due to the spin and spatial degeneracies of oxygen, three distinct PESs are used for the QCT calculations involving O_2-O_2 and an additional 9 PESs for O_2-O interactions.

Unlike the recent DMS simulations of Grover and Schwartzentruber [4] where a similar oxygen mixture was studied under isothermal conditions, in the current case no energy is added to or removed from the system between collision steps. This adiabatic reactor is more representative of the conditions behind a strong shock wave, such as the ones generated in shock-tube facilities or formed at the bow of hypersonic flight vehicles. In this work, we restrict ourselves to the simulation of a static gas in a 0D reservoir without flow coupling, but we carefully select the initial conditions to mimic the state observed behind the shock fronts during the recent oxygen shock-tube experiments of Ibraguimova et al. [5]. We examine rotational and vibrational energy distributions of the O_2 molecules, as well as the temperatures associated with these modes to compare to the ones found in the experiments.

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State-Resolved Treatment of Transport Properties for the $O(^3P)+O_2(^3\Sigma_g^-)$ System in DSMC

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Internal energy non-equilibrium in hypersonic flows described by state-to-state (StS) models have been successfully developed for use in both computational fluid dynamics (CFD) and Direct Simulation Monte Carlo (DSMC) codes, where each internal energy (ro-vibrational) level is treated as a 'pseudo' species [1]. Since CFD methods are typically limited to *near-equilibrium* velocity distribution functions (VDF), hybrid CFD/DSMC methods may be employed to provide accurate flow predictions in combined continuum/rarefied flows. Ongoing efforts toward development of a StS hybrid CFD/DSMC framework for chemically reacting flows have introduced a StS dissociation/recombination model for DSMC based on the $O+O_2$ [2] system and continuum breakdown parameters for chemically reacting flows [3,4]. Our focus here is on developing consistent StS transport properties for both CFD and DSMC solution methods.

Within hybrid solvers, to ensure that differences in the methodologies arise only due to the inherent continuum assumption in CFD, models describing chemical kinetics, relaxation and transport processes need to be treated consistently in CFD and DSMC. Here, we focus on faithfully representing transport quantities in CFD and DSMC, computed from ab initio potential energy surfaces (PES). Within CFD, StS collision integrals calculated from the PES using collision dynamics are employed for computing transport properties [5] (Fig. 1(b)), whereas, a collision cross-section model like the variable soft sphere (VSS) is used in DSMC for elastic collisions. In the present work, we calibrate the parameters for a StS, $O+O_2$ VSS model, based on the same StS *collision integral* values that are employed in CFD [6]. However, such a calibration procedure introduces an equilibrium VDF assumption in DSMC through the definition of collision integrals. Therefore, we propose to calibrate the VSS model parameters directly from StS *collision cross sections* obtained from collision dynamics calculations (Fig. 1(a)). This approach will ensure that the fit remains valid under strong non-equilibrium conditions. Finally, the StS scattering angles calculated from both fitting procedures will be compared to the 'true' scattering profiles calculated directly from the PES.

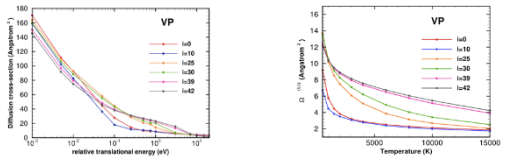

Figure 1. (a) StS diffusion cross-section; (b) StS collision integrals for the $O+O_2$ system.

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This work was supported by an Early Career Faculty grant from NASA's Space Technology Research Grants Program and the Air Force Office of Scientific Research under award number FA9550-17-1-0127.

Tuesday, September 24, 2019

Session 8: Chemistry II

Chair: S. F. Gimelshein

10:20-10:40	**Ab Initio Collisional Models for Direct Simulation Monte Carlo for Hypersonic Flows** N. Singh, T. E. Schwartzentruber
10:40-11:00	**A Monte Carlo Method with Negative Particles for Coulomb Collisions** D. S. Silantyev, B. Yan, R. E. Caflisch
11:00-11:20	**Cubic Kinetic Vlasov Fokker Planck Model for Plasma Applications** K. Chung, M. H. Gorji, P. Jenny
11:20-11:40	**Suppression and Distortion of Non-Equilibrium Fluctuations by Transpiration** A. L. Garcia, D. R. Ladiges, A. J. Nonaka, J. B. Bell
11:40-1:00	**Lunch**

Ab Initio Collisional Models for Direct Simulation Monte Carlo for Hypersonic Flows

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Recently, using quantum chemistry methods, accurate potential energy surfaces (PESs) for air species have been constructed [1]. Using these PESs as input, Master-Equation (ME) and Direct Molecular Simulation (DMS) have been used to study the evolution of a gas in strong thermo-chemical non-equilibrium conditions representative of shock waves. However, these methods are computationally infeasible to simulate flow over full vehicles. The DSMC method [2,3], on the other hand, can be used to simulate flow over 3D complex geometries; however, the current phenomenological models in DSMC do not agree with ab initio methods. For instance, in Fig. 1, DMS simulation of the evolution of pure nitrogen gas initialized at low ro-vibrational energy and excited isothermally to T = 20,000 K is shown. The nitrogen molecules excite ro-vibrationally before dissociating and reaching a quasi-steady state (QSS). In the same figure, DSMC predictions using the standard Parker model for the rotational collision number, the Millikan-White correlations for vibration, and the Total Collision Energy (TCE) model with the parameters recommended by Park, are also shown. For internal energy redistribution, the Borgnakke-Larsen (BL) model, which samples post-collision energies from an equilibrium distribution based on the collision energy, is used in DSMC. As shown in Fig. 1, there are significant differences between DMS and DSMC results in dissociation rates, internal energy relaxation, and the quasi-steady state. Using ab initio results, we construct new DSMC models and compare them with ab initio methods.

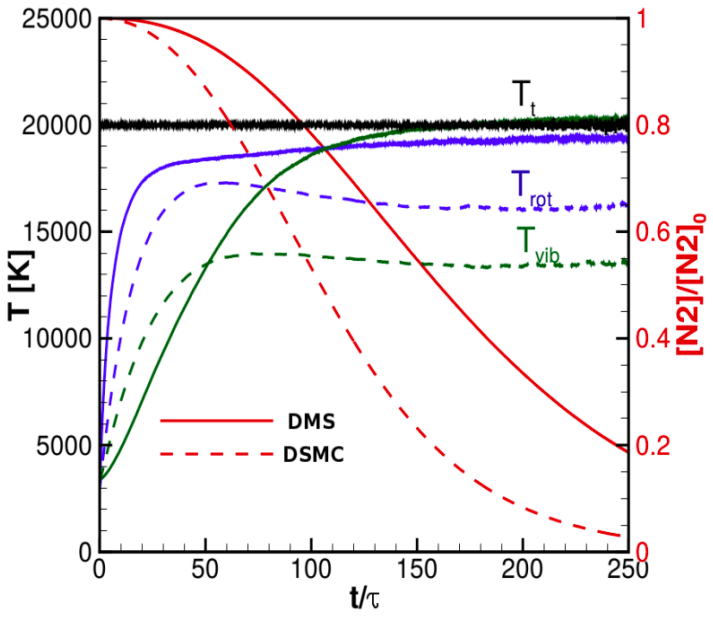

Figure 1. Comparison of DMS and DSMC predictions for high-temperature dissociation in nitrogen. Solid lines denote DMS, and dashed lines denote DSMC.

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[3] I. D. Boyd and T. E. Schwartzentruber, *Nonequilibrium Gas Dynamics and Molecular Simulation*, Cambridge University Press, Cambridge, UK (2017).

A Monte Carlo Method with Negative Particles for Coulomb Collisions

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Firstly, for a homogeneous case, we describe a novel method with negative particles [1] for the general bilinear collision operators and apply it to Coulomb collisions. We split the distribution into a Maxwellian part and a deviational part simulated by numerical particles. These particles, named deviational particles, could be both positive and negative. The method is fully nonlinear with the greatest advantage in the near-fluid regime. We focus on certain important aspects of the method—taming the growth of number of particles, particle resampling, source-term sampling, variance reduction, and acceleration techniques.

Secondly, for a non-homogeneous case, we describe a Hybrid method with Deviational Particles (HDP) [2] for non-homogeneous plasma modeled by the Vlasov-Poisson-Landau system. As before, we split the distribution into a Maxwellian part evolved by a grid-based fluid solver and a deviation part simulated by numerical particles. This method is a combination of the Monte Carlo method proposed in [1], a Particle-in-Cell method and a Macro-Micro decomposition method [3] and is applicable all regimes and significantly more efficient than a PIC-DSMC method near the fluid regime.

Lastly, we propose a uniformly efficient method in all regimes of plasma simulation, based on the HDP method and optimal combination of deviational particle and coarse particle (regular DSMC) solutions to obtain a method that is maximally and universally efficient, in a suitable sense.

Various numerical simulations are performed to demonstrate the accuracy and efficiency of the method in both homogeneous and non-homogeneous cases compared to a standard DSMC and PIC- DSMC methods.

[1] B. Yan and R. E. Caflisch, "A Monte Carlo Method with Negative Particles for Coulomb Collisions," *Journal of Computational Physics*, **298**, 711-740 (2015).
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Cubic Kinetic Vlasov Fokker Planck Model for Plasma Applications

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In this study, we present a novel time integration scheme to solve the Vlasov Fokker Planck equation with a cubic drift (CD) kinetic model for plasma applications. We extended a previous work [1] by introducing a nonlinear polynomial function for the fluctuating velocities in the drift term [2]. Together with a constant diffusion coefficient, Coulomb interactions of charged particles in the presence of electro-magnetic fields are handled. The devised model fulfills the required conservation laws, and in the equilibrium limit the solutions converge to Maxwellian distributions.

For validation, spatially homogeneous relaxation with different initial conditions is considered. The results show that the proposed integration scheme has no dependency on the time step size. This leads to computational advantages, especially in comparison to other commonly used particle methods, e.g., DSMC [3-4]. Furthermore, unlike the linear drift (LD) model introduced in [1], the CD model ensures the correct relaxation behavior of not only the second but also the third velocity moment, which is crucial for studies of heat-transfer phenomena. This kinetic model also shows good agreement with DSMC results.

Beside homogeneous studies, the influence of time step size and grid resolution on plasma flow in spatially varying electromagnetic fields was also investigated. Computational efficiency and accuracy of the new scheme are demonstrated with numerical studies.

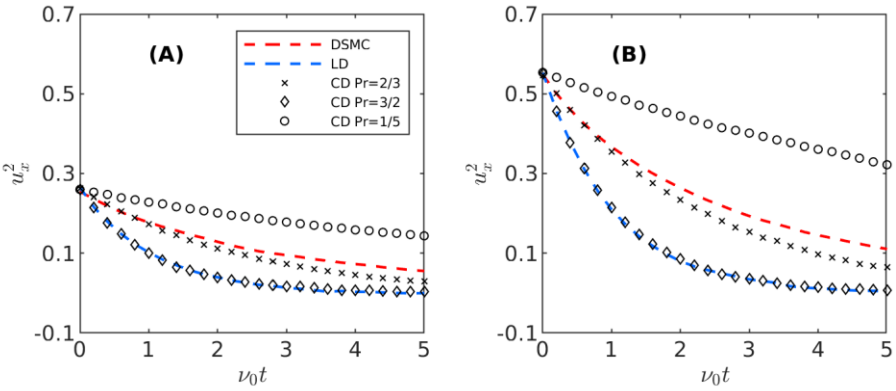

Figure 1. Heat-flux relaxation with two different initial conditions using the Cubic-Drift model compared to results from DSMC and the Linear-Drift model. Symbols refer to results with different model constants.

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Suppression and Distortion of Non-Equilibrium Fluctuations by Transpiration

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A fluid in a non-equilibrium state exhibits long-ranged correlations of its hydrodynamic fluctuations [1,2]. In this talk, we examine the effect of a transpiration interface on these correlations—specifically, we consider a dilute gas in a domain bisected by the interface. The system is held in a non-equilibrium steady state by using isothermal walls to impose a temperature gradient. The gas is simulated using both direct simulation Monte Carlo (DSMC) [3] and fluctuating hydrodynamics (FHD) [4]. For the FHD simulations, two models are developed for the interface based on master-equation and Langevin approaches.

For each approach, we quantify the effects of transpiration on long-ranged correlations in the hydrodynamic variables [5]. Good agreement is observed between DSMC and FHD results, with the latter showing a significant advantage in computational speed. Several qualitative differences in the correlations were observed; however, the principal effect of the interface was to reduce their magnitude proportionally to the effusion probability. This outcome can largely be explained by changes in the temperature gradient induced by the interface. We also observe a distortion of the temperature correlations, specifically the appearance of a new peak located near the interface; this effect is qualitatively described by a simple heat-equation model.

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[5] D. Ladiges, A. Nonaka, J. B. Bell, and A. Garcia, "On the Suppression and Distortion of Non-Equilibrium Fluctuations by Transpiration," *Physics of Fluids,* **31**, 052002 (2019).

This work was supported by the U.S. Department of Energy, Office of Science, Office of Advanced Scientific Computing Research, Applied Mathematics Program under contract DE-AC02-05CH11231. This research used resources of the National Energy Research Scientific Computing Center, a DOE Office of Science User Facility supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

Tuesday, September 24, 2019

Session 9: Non-Equilibrium

Chair: P. Jenny

1:00-1:20	**Combined Experimental and Computational Efforts for Hypersonics Validation at Sandia** S. P. Kearney, J. L. Wagner, D. R. Richardson, R. M. Wagnild, M. A. Gallis
1:20-1:40	**Modeling Chemical Equilibrium with a Variance Reduction Collision Method** Y. K. Poondla, P. L. Varghese, D. B. Goldstein
1:40-2:00	**Application of Machine Learning to Molecular Gas Dynamic Simulations** P. Valentini, M. Grover, E. Josyula
2:00-2:20	**Modeling of Internal Energy Relaxation in a Kinetic Fokker-Planck Solver** C. Hepp, M. Grabe, K. Hannemann
2:20-2:40	**Investigation of Coarse-Grain Models for Energy Transfer and Dissociation/Recombination in DSMC** T. J. Pan, K. A. Stephani
2:40-3:00	**A Unified Stochastic Particle Bhatnagar-Gross-Krook Scheme and Its Combination with DSMC for Multiscale Gas Flows** F. Fei
3:00-3:20	**Break**

Combined Experimental and Computational Efforts for Hypersonics Validation at Sandia

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New experimental and computational efforts for improved validation of air chemistry and nonequilibrium models for hypersonic flows will be discussed. A three-pronged approach that includes facility development, diagnostics, and computational modeling is undertaken. We present Sandia's newly constructed free-piston shock tube facility, which allows us to reach enthalpies in excess of 10 MJ/kg. Upcoming efforts to convert this facility to a fully operational shock tunnel are discussed, and the expected range of operating conditions is summarized. This facility will be co-located with reacting-flow diagnostics based on pulse-burst laser technology. Imaging and spectroscopic tools based on laser-induced fluorescence (LIF) and coherent anti-Stokes Raman scattering (CARS) are pursued for measurements of temperature, vibrational distribution function, and concentrations of key reacting species, including NO and O-atom. This experimental infrastructure will be capable of producing high-quality validation data sets, where multiple measured flow-field quantities can be combined with surface measurements, including well-characterized freestream and stagnation conditions and quantifiable measurement uncertainty. Our experimental program will be guided by needs of DSMC and continuum simulation codes, which will be used to design canonical validation experiments that include normal shock waves and bluff-body flows under conditions of significant thermodynamic nonequilibrium.

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525. This paper describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the paper do not necessarily represent the views of the U.S. Department of Energy or the United States Government. The current work is additionally supported by Sandia's Laboratory Directed Research and Development (LDRD) program.

Modeling Chemical Equilibrium with a Variance Reduction Collision Method

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This work focuses on efforts to model chemistry in Quasi-Particle Simulation (QuiPS), a novel rarefied gas solver that models a population of molecules via a discretized, truncated velocity distribution function (VDF) made up of fixed-velocity quasi-particles [1-3]. Particle weights are continuously variable, which enables accurate resolution of the tails of the VDF. Each particle also has quantized internal energy distribution functions (rotational and vibrational levels are decoupled). A typical chemistry model in DSMC (the total collisional energy, or TCE [4, 5]) is implemented in QuiPS using the variance reduction collision method [6-8]. In this method, the VDF is split into equilibrium and deviational components, and computational effort is focused on collision integral terms involving the deviational components. The method is applied to a zero-dimensional adiabatic relaxation, specifically an N_2+N system, to demonstrate its capability to arrive at chemical equilibrium. The evolution of internal energy distribution functions due to chemistry can be trivially visualized in QuiPS and provides an additional level of insight.

Figure 1. Schematic of 1D deviation distribution function. Collisions between equilibrium distributions are assumed to have no effect and are not performed. Equilibrium-deviation and deviation-deviation collisions are performed. Near equilibrium, the deviation density is small, and the number of collisions computed is correspondingly small.

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This work was supported by a NASA Space Technology Research Fellowship, grant NNX16AM87H. Additional support was provided by the National Science Foundation grant CBET-1438530. Y. Poondla would also like to thank Chris Moore and George Oblapenko for their input and insight.

Application of Machine Learning to Molecular Gas Dynamic Simulation

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We describe the application of artificial neural networks (ANNs) to construct potential energy surfaces (PESs) from ab initio energy data sets for application to trajectory calculations [1] or direct molecular simulation [2]. Permutation invariance is guaranteed by mapping the interatomic distances onto a set of permutation invariant inputs, known as fundamental invariants [3], that generate the permutation invariant polynomial ring. With an appropriate energy decomposition, we impose the correct 2-body energy contribution. Spurious long-distance interactions between diatoms are removed with a tapering function that smoothly cuts off the interaction below an energy threshold at which many-body interactions are negligible. This guarantees the correct long-range behavior to properly describe threshold near-dissociation events in trajectory integration. In this work, the application of neural networks to PES training is specialized for the N4 system using the ab initio data set of Bender and co-workers [1]. The ANN-PES is shown to be as accurate or to have reduced root-mean-square error compared to the standard permutation invariant polynomial (PIP) description. Results from quasi-classical trajectory calculations show excellent agreement between dissociation probabilities obtained from trajectories performed on the ANN-PES and on the PIP-PES. Similar agreement is seen at the level of internal energies distributions. For the test case considered, the ANN-PES is also generally more computationally efficient than the PIP-PES at comparable root-mean-squared error levels, achieving a speed-up of up to 4 in the current implementation.

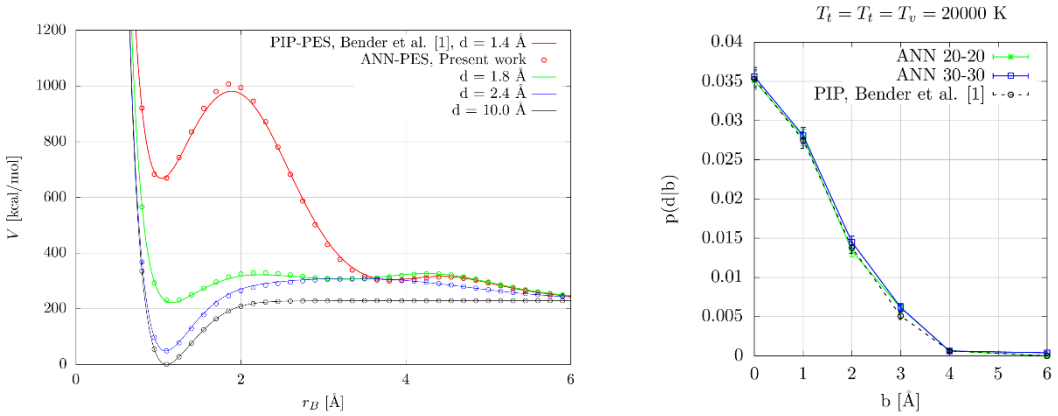

Figure 1. Left: comparison between ANN-PES (symbols) and PIP-PES (solid line, Ref. [1]) for the A-shape N_2+N_2 arrangement. Right: dissociation probabilities at fixed impact parameters obtained from trajectories on the ANN-PES and the PIP-PES (Ref. [1]).

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Approved for Public Release/Unlimited Distribution; Case File Number 88ABW-2019-3017; PA clearance date: 17 June 2019.

Modeling of Internal Energy Relaxation in a Kinetic Fokker-Planck Solver

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The Direct Simulation Monte Carlo (DSMC) [1] method is widely used to model non-equilibrium rarefied gas flows, such as shock waves or strong expansion flows. However, its application to practical problems at rather high density is costly, as the computational effort for DSMC increases strongly with decreasing Knudsen number. It is therefore common practice to couple DSMC with less accurate but faster methods, applying those to flow domains in which the resolution and modeling depth of DSMC is not required. One recently proposed method employs a kinetic Fokker-Planck (FP) model [2]. The FP method employs a large number of simulator particles that are moved through the computational domain and updates particle velocities in a separate step, as is the case in the DSMC method. This algorithmic similarity fosters a simple coupling of both methods.

Correct modeling of internal energy modes is relevant for simulating non-equilibrium molecular flow. While well-established models for internal energy relaxation exist for DSMC, only few approaches are documented in the open literature [3, 4] for the FP method. In particular, according to the authors' knowledge, no models for describing discrete internal energy levels within FP have yet been developed. In this talk, a scheme is presented to extend arbitrary monatomic Fokker-Planck models to describe polyatomic species. A master-equation approach is used to model internal energy relaxation, but instead of solving the master equation directly, the underlying random process is simulated. Three different models are suggested, describing internal particle energies as continuous scalars or as a set of discrete levels. The proposed models are implemented in the well-known cubic Fokker-Planck model [5] using the SPARTA particle simulation framework [6], and relaxation, expansion-flow, and shock-flow test cases (Fig. 1) are investigated to demonstrate their performance.

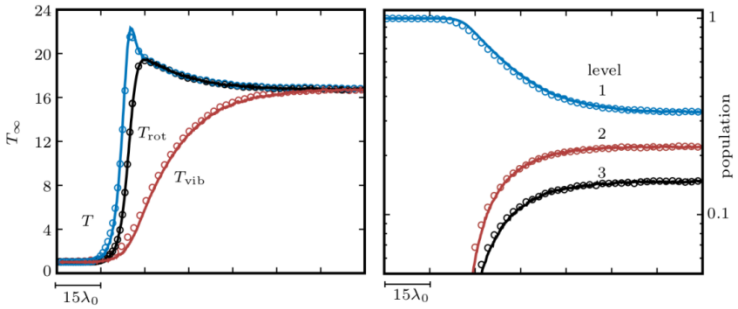

Figure 1. DSMC (lines) and FP (circles) results for a 1D shock flow. Left: Distribution of translational, rotational, and vibrational temperatures. Right: Populations of the first three vibrational levels.

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[2] M. H. Gorji and P. Jenny, "Fokker–Planck–DSMC Algorithm for Simulations of Rarefied Gas Flows," *Journal of Computational Physics*, **287**, 110-129 (2015).
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Investigation of Coarse-Grain Models for Energy Transfer and Dissociation/Recombination in DSMC

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Modeling the flow field surrounding hypersonic vehicles poses a significant challenge owing to the complex thermochemical processes in the shock-heated region, the boundary layer, and the wake. These regions are characterized by both thermal and chemical non-equilibrium owing to the disparity in characteristic relaxation times. Models based on state-to-state kinetics have received considerable attention and have been developed for use in the Direct Simulation Monte Carlo (DSMC) method [1, 2] in place of widely used phenomenological models. In the state-to-state approach, the collisional cross-sections of all possible channels from each internal energy state are required, which are obtained by quasi-classical trajectory (QCT) calculations based on the given ab initio potential energy surfaces (PES). Although the fully state-to-state model provides the most accurate description of non-equilibrium processes, its use for practical 3-D engineering applications is not feasible owing to its high computational cost.

Several coarse-grain models have been proposed for computational-fluid-dynamics (CFD) solvers [3, 4] to reduce the number of equations and for DSMC [5, 6] to reduce the number of cross sections which needs to be evaluated in each collision. However, the previous DSMC work only focused on employing coarse-grain models for energy transfer and dissociation due to the lack of a compatible recombination model. In this work, the state-specific recombination model [2] is extended to include two different types of coarse-grain models for DSMC: (i) *energy-based grouping* and (ii) *vibrational-based grouping*. In the *energy-based grouping*, the internal states with a similar amount of energy are grouped together, while in the *vibrational-based grouping*, the internal states with the same vibrational quantum number are grouped together. The performance of the coarse-grain models for energy transfer and dissociation/recombination in both dissociative and recombinative regimes will be explored.

Figure 1. Schematic of energy-based (left) and vibrational-based (right) grouping strategies for O_2+O system.

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This work was supported by an Early Career Faculty grant from NASA's Space Technology Research Grants Program and by the Air Force Office of Scientific Research under award number FA9550-17-1-0127.

A Unified Stochastic Particle Bhatnagar-Gross-Krook Scheme and Its Combination with DSMC for Multiscale Gas Flows

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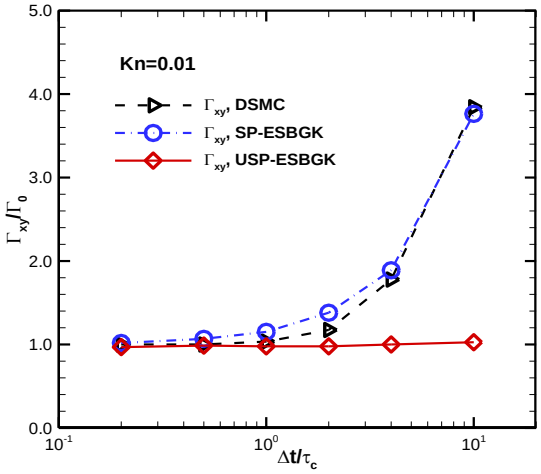
The stochastic particle method based on the Bhatnagar-Gross-Krook (BGK) or ellipsoidal statistical BGK (ESBGK) model approximates the pairwise collisions in the Boltzmann equation using a relaxation process [1]. Therefore, it is more efficient to simulate gas flows at small Knudsen numbers than the counterparts based on the original Boltzmann equation, such as the Direct Simulation Monte Carlo (DSMC) method [2]. However, the traditional stochastic particle BGK (SP-ESBGK) method is implemented using the time-splitting algorithm in analogy to the DSMC method, i.e., molecular motions and collisions are decoupled. Therefore, its numerical transport coefficients scale linearly with the time step size, which lets solutions significantly deviate from physical values as the time step size increases, which is shown in Fig. 1. In order to reduce the numerical dissipation in the stochastic particle BGK method, a unified stochastic particle ESBGK (USP-ESBGK) method is proposed by solving the molecular motions and collisions coupled during the particle transport. Benefiting from the linear interpolation and a Crank-Nicolson scheme [3], the USP-ESBGK method is of second order accuracy in both space and time. Therefore, the proposed method can be applied using larger temporal-spatial discretization, which is useful and efficient for the simulation of multiscale gas flows ranging from rarefied to continuum regimes. Further, since the BGK model fails in the non-equilibrium regime with high Mach and/or Knudsen numbers (Fig. 2), a particle-particle hybrid method based on the USP-ESBGK and DSMC methods, which further extends the application domain of the proposed USP-ESBGK method, was developed.



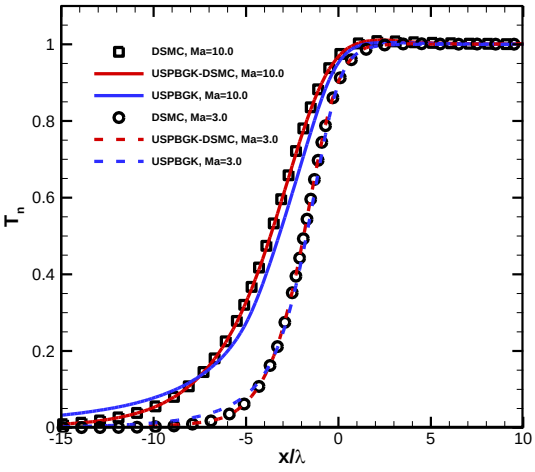


Figure 1. Left: Comparison of shear stresses in Couette flow obtained by the SP-ESBGK, USP-ESBGK and DSMC methods with different time steps.

Figure 2. Right: Temperature destitutions in shock waves obtained with DSMC, USP-ESBGK and the hybrid method based on DSMC and USP-ESBGK.

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Tuesday, September 24, 2019

Session 10: Chemistry Verification and Validation

Chair: I. J. Wysong and S. F. Gimelshein

3:20-3:40	**Roundtable Discussion on Nonequilibrium Air Models** I. J. Wysong, S. F. Gimelshein
3:40-5:00	**Open Discussion** Session Participants
6:30-9:00	**Conference Banquet**

Roundtable Discussion on Nonequilibrium Air Models

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This session will be a roundtable discussion on the topic of nonequilibrium air models, with many individuals participating.

We plan to start with a brief review of the HyNECC (Hypersonic Nonequilibrium Comparison Cases) effort to compare some reaction rates for air (both in equilibrium and two-temperature limits). We'll present the results we have gathered so far. If others have any results such as new rates derived from QCT or new simplified approaches that lead to effective 2-T rates, these can be presented during this section.

We will then move on to discuss existing and possible validation cases, including 1D and 2D flows where the gas could be nitrogen, oxygen, or air mixtures. We will give very brief synopsis and lessons learned for the following three cases: O_2 shock data from Moscow State (Ibraguimova JCP 2013), LENS-XX double-cone (Maclean AIAA Aviation 2014), and HEG cylinder (Karl AIAA 2003-4252). We will solicit inputs for key comments on those 3 cases and for other possible validation cases that are currently available.

Any slides or results presented will be limited to 5 minutes and will be coordinated in advance. We will also welcome comments and discussion that arise during the meeting, as much as time will allow, but we will give priority to the material that is coordinated in advance.

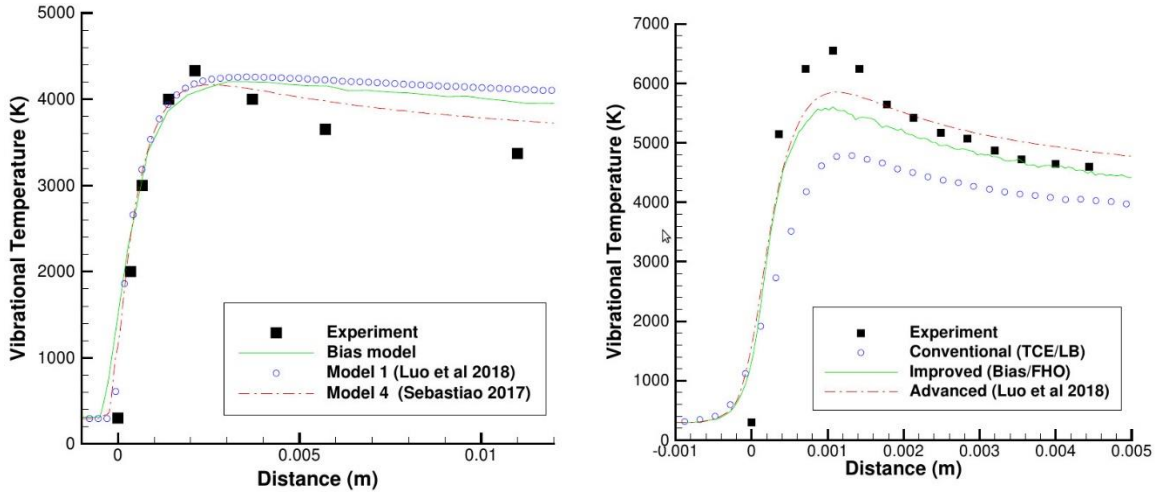

Figure 1. Vibrational temperature profiles in a 1D oxygen shock wave with a freestream velocity of 3.07 km/s (left) and 4.44 km/s (right).

Wednesday, September 25, 2019

Session 11: Planetary Flows

Chair: E. Jun

8:00-8:40	**Invited: A Quick Overview of Planetary Exploration Missions** J. Rabinovitch, C. Sotin
8:40-9:00	**Influence of the Mars Atmosphere Model on 3-D Aerodynamics of an Entry Capsule** G. Zuppardi
9:00-9:20	**Direct Simulation Monte Carlo Applied to Reentry of Debris** P. Van Hauwaert, M. Spel, J. Annaloro, P. Omaly
9:20-9:40	**Differential Drag and Plume Interactions for a CubeSat Swarm** A. Chinnappan, P. Kazarin, R. Kumar, A. A. Alexeenko
9:40-10:00	**DSMC Simulations of Hypervelocity Sampling in Venus' Upper Atmosphere** A. Borner, M. A. Gallis, J. Rabinovitch, C. Sotin
10:00-10:20	**Break**

A Quick Overview of Planetary Exploration Missions

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Starting with the Explorer 1 satellite launch in 1958, which enabled the discovery of the Van Allen Radiation Belts, NASA has been exploring space and making new discoveries for over 60 years. NASA planetary missions range in scope and size from low-cost small-satellite science missions to multi-billion-dollar flagship-class missions. Each mission has specific scientific objectives, a different risk posture, and different stages of formulation, design, and execution. Currently, in order to focus future scientific investigations, if a planetary mission is going to receive NASA funding, it should address key scientific/technical objectives specifically outlined in the Decadal Survey reports [1]. The last decadal survey, entitled "Vision and Voyages for Planetary Science in the Decade 2013-2022," defines three cross-cutting themes (Building New Worlds, Planetary Habitats, and Workings of the Solar System) that lead to ten priority questions that can be responded to by exploring different targets in our Solar System. It explicitly supports Mars Sample Return (MSR) and prioritizes five flagship missions. Mars 2020, which is potentially the first element of MSR, and Europa Clipper are under development and will be launched in 2020 and 2023, respectively.

DSMC simulations and analysis play a large role in space missions—ranging from entry analysis and thruster plume analysis to contamination control calculations and many things in between. However, space missions take extremely large teams, are extremely multi-disciplinary, and require many complex analyses outside of DSMC. Understanding the complex interactions between the different systems of a spacecraft can help one understand where DSMC analysis fits into the overall spacecraft design process.

For any space mission, in order to relate scientific objectives to specific mission and instrument requirements, a Science Traceability Matrix (STM) is created. The STM creates a direct link between specific science objectives and the required measurements to meet the scientific objectives and also justifies what accuracy and precision specific instruments must be able to accommodate for their measurements [2]. Spacecraft requirements flow down from science requirements, not vice versa.

This work will give examples of planetary missions of different scales and different scopes and emphasize how the science return of a mission will always drive its design. Furthermore, an overview of how JPL addresses different aspects of mission formulation will be provided, with a brief description of JPL's Innovation Foundry, which includes JPL's A-Team and Team-X internal design teams [3]. Interesting design anecdotes from the MSL and InSight missions will be used in order to illustrate the complexities associated with planetary exploration missions.

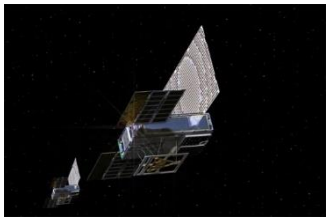

Figure 1. An artist's rendering of the twin Mars Cube One (MarCO) spacecraft. Image credit: NASA/JPL-Caltech.

[1] National Research Council 2011, *Vision and Voyages for Planetary Science in the Decade 2013-2022*, The National Academies Press, Washington, DC (2011), https://doi.org/10.17226/13117.
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Influence of the Mars Atmosphere Model on 3-D Aerodynamics of an Entry Capsule

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The present paper is a step forward in the study of the subject "Aerodynamics in Mars atmosphere" carried on by Zuppardi [1-4]. Due to the forthcoming manned missions to Mars, this subject is topical and deserves to be studied even more deeply. On the other hand, the success of the study of such a problem is linked also to the availability of a reliable mathematical model of the atmosphere. Unfortunately, a single and completely reliable model is not yet available for Mars. In literature, in fact, there are two different models (NASA Glenn and GRAM-2001) providing very different parameters (density, temperature) at altitudes higher than 40 km, therefore different entry trajectories (velocity) and different fluid-dynamic conditions or different Mach, Reynolds and Knudsen numbers. Zuppardi carried on the aerodynamic analysis considering the Mars Pathfinder capsule in the altitude interval 50-100 km and using a homemade code for the computation of the entry trajectories and a DSMC code (DS2V 4.5 64 bits) for the solution of 2-D/axial-symmetric flow fields. Zuppardi already quantified the effects of the: i) different fluid-dynamic conditions linked to the atmosphere models, ii) chemical reactions, iii) surface temperature on local (pressure, skin friction, etc.) and on global (drag) aerodynamic quantities, iv) surface catalytic reactions. The results showed that, because of the much higher values of both free stream dynamic pressure ($\rho_\infty V_\infty^2$) and energy flux ($\rho_\infty V_\infty^3$) by the NASA Glenn model, the effects on the aerodynamic quantities of an entry capsule are stronger than those by the GRAM-2001 model. The present paper is aimed at the evaluation of the atmosphere models on 3-D aerodynamics of a Mars entry capsule. Computations are carried on by the 3-D DSMC code DS3V at the altitudes (h) of 60, 80 and 100 km, in the interval of angles of attack (α) 0-180° and considering, once again, the Mars Pathfinder capsule. Figs. 1(a) and 1(b) show the profiles of the drag coefficient (CD) and the longitudinal moment coefficient (C_{Mz}, the reduction pole is the gravity center) at h = 60 and 100 km. The GRAM-2001 model, because of the very different Mach, Reynolds and Knudsen numbers, produces, at h = 100 km, C_D and C_{Mz} profiles very different both from those at h = 60 km and from those by the NASA Glenn model. Despite this difference, the C_{Mz} profile agrees with others in fixing equilibrium (C_{Mz} = 0): 1) unstable ($dC_{Mz}/d\alpha > 0$) at α = 0° and stable ($dC_{Mz}/d\alpha < 0$) at α = 180°, 2) also at α = 80°. The influence of the two Mars atmosphere models on the aerodynamic force and moment, as well as on the related coefficients, will be considered. The stability derivatives will be also computed to quantify the stability/instability levels.

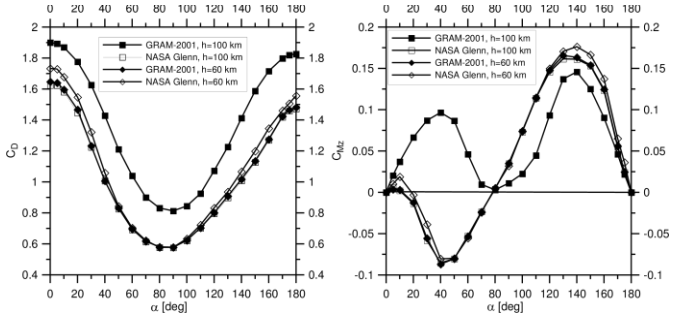

Figure 1. Pathfinder's drag (a) and longitudinal moment (b) coefficients.

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Direct Simulation Monte Carlo Applied to the Reentry of Debris

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With the French Space Operation Act (SOA) [1] signed in 2008 that applies for every mission launched and operated from the French territory, predicting the debris survivability during an atmospheric re-entry and assessing the prospective risk on ground has become a concern. CNES is in charge of ensuring the right application of that law. With computational fluid dynamics, Direct Simulation Monte Carlo [2] is one of the tools used to predict the aero-thermo coefficients and the demise of debris for which a database of thousands of simulations is needed. The diversity of the geometries requires automating the simulations. The structure of a C++ DSMC code to carry out this task is presented. A cut-cell approach similar to [3] is combined with a Cartesian grid adaptation. With the exception of the wall surfaces, the simulation is distributed using the MPI protocol with the help of the METIS library. Cross code comparison and validation on a hypersonic flat plate is presented. The code is applied to various debris primitives in order to compute the random tumbling coefficients, and the corresponding simulation setup to carry out the computations is outlined.

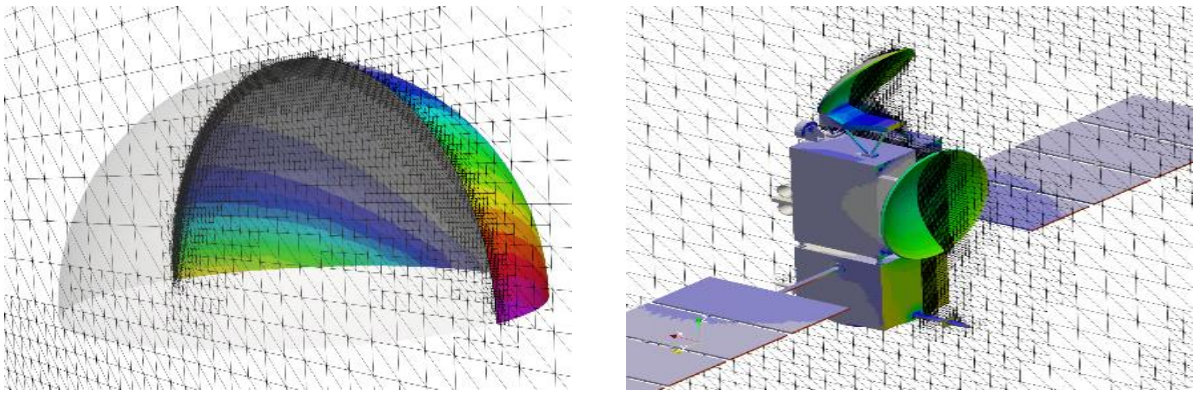

Figure 1. Example of grid adaptation both on a hollow sphere and on a more complex dummy satellite. Colormap at the wall represents the non-dimensional heat rate.

[1] Loi n° 2008-518 du 3 juin 2008 relative aux Opérations Spatiales (LOS).
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[3] D. Gao, C. Zhang, and T. E. Schwartzentruber, "A Three-Level Cartesian Geometry Based Implementation of the DSMC Method," AIAA-2010-450, American Institute of Aeronautics and Astronautics, Reston, VA (2010).

Differential Drag and Plume Interactions for a CubeSat Swarm

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Recent advances in technology and miniaturization of spacecraft bus components have led to the proliferation of small satellites including kilogram-class CubeSats [1]. CubeSat constellations involving multiple spacecraft in a precise formation are considered an enabling approach for high-priority geospace science missions. Aerodynamic forces on multiple satellites operating in close proximity contribute to the overall orbital perturbations and are important for formation control. Free-molecular theory and collisionless Monte Carlo test-particle methods can be used to estimate aerodynamic forces for individual spacecraft. However, collisional interactions become significant for maneuvering spacecraft in the presence of thruster plumes. The Direct Simulation Monte Carlo (DSMC) method [2] is highly suitable to study this problem. The goal of the current study is to estimate the aerodynamic drag of a CubeSat at different configurations using the SPARTA DSMC solver [3].

The problem under consideration involves three 3-U satellites, which are separated by 10 m. A freestream velocity of 8 km/s and flow parameters corresponding to the altitude of 400 km are considered. The velocity flow field for three 3-U CubeSat configurations is shown in Fig. 1. Due to the shadow effect of the first CubeSat, the drag forces on the second and third CubeSats are decreased significantly. The drag forces for three different CubeSats without a plume are computed by the DSMC method and compared with the free-molecular theory, as shown in Table 1. The aerodynamic shadow effect of the leading CubeSat is not taken into account for the free-molecular-theory calculations. A parametric study is performed to investigate the effect of the plume-spacecraft interaction on CubeSat drag and spacecraft trajectories for a few candidate thrusters [4,5].

Spacecraft	Drag, μN DSMC	Cd DSMC	Cd FM
CubeSat1	9.21	2.02	2.18
CubeSat2	5.26	1.15	2.18
CubeSat3	0.13	0.37	4.19

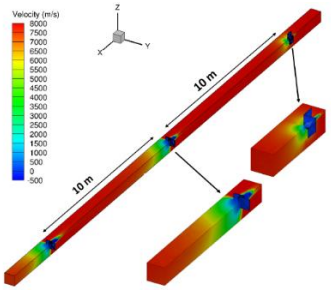

Table 1. Comparison of DSMC results with free-molecular-theory calculations.
Figure 1. Velocity field for three 3-U CubeSats.

[1] H. Heidt, J. Puig-Suari, A. S. Moore, S. Nakasuka, and R. J. Twiggs, "CubeSat: A New Generation of Picosatellite for Education and Industry Low-Cost Space Experimentation," *Proceedings of the 14th Annual AIAA/USU Conference on Small Satellites*, Paper SSC00-V-5, 1-19 (2000).
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Acknowledgment. The first author is funded by Science and Engineering Research Board (SERB) from the Department of Science and Technology, India for his visit to Purdue University, USA. The work is partially supported by NASA SSTP grant NNX18035512.

DSMC Simulations of Hypervelocity Sampling in Venus' Upper Atmosphere

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Measuring the abundances of noble gases and their isotope ratios in Venus atmosphere is an essential investigation required to understand Venus' global evolution, on a planetary scale. Cupid's Arrow is a small satellite mission concept that would skim through Venus' atmosphere below the homopause to collect samples that would be analyzed in deep space by a JPL-developed miniaturized quadrupole ion trap mass spectrometer [1]. The numerical simulations are intended to assess the amount of noble gas fractionation that would occur during hypervelocity sampling.

The DSMC code SPARTA [2], used in this work, is able to model hypervelocity reacting flows in strong chemical and thermal non-equilibrium. Therefore, it is well suited to determine relevant flow properties for the Cupid's Arrow mission concept and to numerically investigate the possibility of elemental and/or isotopic fractionation in the sampled gases. The composition of Venus' atmosphere is modeled as a mixture of N_2 and CO_2 with trace amounts of noble gases (Ar, Xe, Kr, He, Ne). The chemical model includes a number of species such as O, O_2, CO, N, NO, C_2, CN, and C with reaction rates derived from laboratory experiments. The effects of ionization and catalytic versus non-catalytic surfaces are being investigated. 2D axisymmetric simulations with one sample tank and 3D simulations using a more representative geometry (Fig. 1), which includes valves that are present at the back and at the front of the sampling tanks, are utilized to investigate different phenomena.

The preliminary numerical simulations show that fractionation does occur in the sampling system. The ratio Ar/Xe decreased by several times in the tanks, demonstrating that the system favors the transport of heavier species. The standard deviation on this value increases with decreasing amount of noble gases in the freestream, demonstrating that this is an effect of the number of particles used in the simulation. Similarly, the isotope ratios show an enhancement in the heavier component for both Ar and Xe. The difference between these two numbers is attributed to the fact that the relative mass difference between Ar isotopes is much larger than that of Xe isotopes, yielding a larger discrepancy in mass diffusion for Ar isotopes vs. Xe isotopes. The numerical simulations also provide the chemical composition of the non-noble gas species being present in the sampling tanks. Simulation results also predict the time required to fill the tanks as the mass flux of gas into the sampling tanks is limited by the characteristics of the valves.

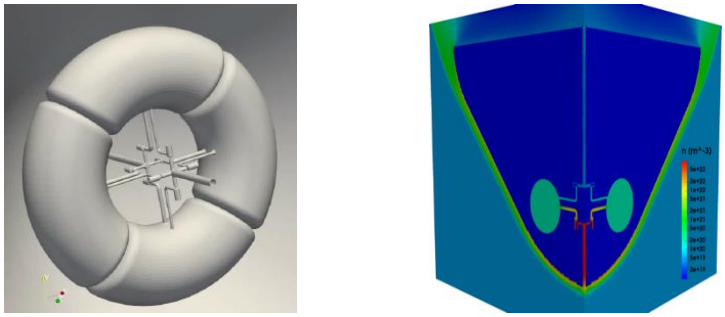

Figure 1. (Left) View of the four tanks that will be filled while skimming through Venus' atmosphere. (Right) Total number density for a 3D geometry.

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Parts of this work have been performed at the Jet Propulsion Laboratory, California Institute of Technology, under contract to NASA. Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525. A. B. would like to acknowledge funding from the NASA Entry Systems Modeling project and JPL.

Wednesday, September 25, 2019

Session 12: Planetary Flows and Turbulence

Chair: R. S. Martin

10:20-10:40	**Aerothermal Analysis of an Atmospheric Dipper CubeSat** P. Kazarin, A. Chinnappan, A. A. Alexeenko
10:40-11:00	**DSMC Simulation of Nonequilibrium Flow with Classical Impulsive Reaction Model** H. Luo, A. A. Alexeenko, S. O. Macheret
11:00-11:20	**DSMC Simulations of Shock-Vortex Interaction** T. P. Koehler, M. A. Gallis, J. R. Torczynski
11:20-11:40	**DSMC Simulations of Compressible Turbulence** M. A. Gallis, N. P. Bitter, J. R. Torczynski
11:40-1:00	**Lunch**

Aerothermal Analysis of an Atmospheric Dipper CubeSat

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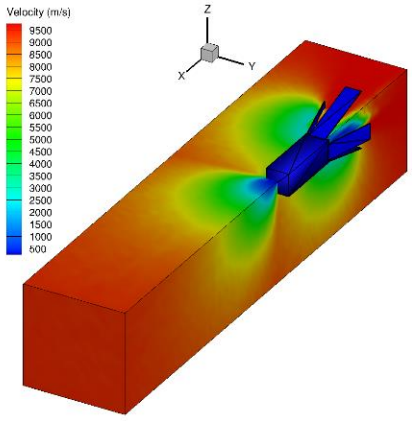
The highly dynamic and complex nature of the atmosphere below 200 km requires the development of special instruments for measurement of the important parameters (e.g., magnetic field, density) in this region. CubeSats have become such an instrument platform and are now being widely used in low Earth orbit for applications such as remote sensing or communications [1, 2]. Thermal analysis is one of the critical aspects which should be addressed at the design stage of a CubeSat in order to ensure that spacecraft bus components work properly during its mission [3]. In this work, aerothermal analysis of an atmospheric dipper CubeSat is performed for further design of probes and sensors incorporated and used to explore the Earth's atmosphere at low altitudes.

High-fidelity and low-fidelity simulations are carried out to predict the thermal load and safe temperature range during the CubeSat's mission. The convective heat flux for different flight conditions was estimated using the Direct Simulation Monte-Carlo (DSMC) method [5]. The SPARTA DSMC solver, developed at Sandia National Laboratories, is used in this work [6]. The DSMC simulations were performed at different altitudes and verified against free-molecular-theory results. The flow field for the flow over a CubeSat with four solar panels deployed at 185 km is shown in Figure 1. Values obtained from DSMC simulations were used as an input to the low-fidelity code developed to model the CubeSat on-orbit temperature variation, shown in Figure 2.



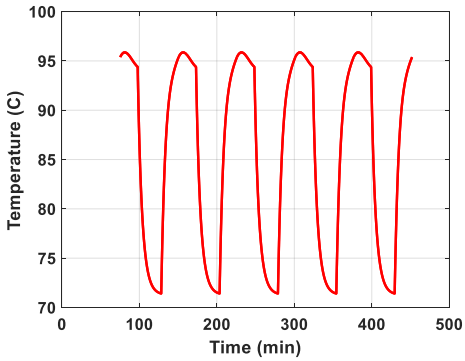


Figure 1. Velocity contour around CubeSat.
Figure 2. Typical temperature evolution of a CubeSat for 5 consecutive orbits.

[1] H. Heidt, J. Puig-Suari, A. S. Moore, S. Nakasuka, and R. J. Twiggs, "CubeSat: A New Generation of Picosatellite for Education and Industry Low-Cost Space Experimentation," *Proceedings of the 14th Annual AIAA/USU Conference on Small Satellites*, Paper SSC00-V-5, 1-19 (2000).

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DSMC Simulation of Nonequilibrium Flow with Classical Impulsive Reaction Model

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Thermochemical nonequilibrium is a phenomenon generated for re-entering vehicles flying at hypersonic speed. The coupling between internal energy of the molecules and chemical reactions complicates the problem, in particular vibration-dissociation coupling. On the one hand, the favoring of a specific internal mode by chemical reactions results in rates different from the equilibrium values. On the other hand, chemical reactions will further drive the development of thermal nonequilibrium if chemical reaction proceeds faster than thermal relaxation. In the DSMC method [1], the total collision energy (TCE) model is widely used to model chemical reaction. The model is based on inverse Laplace transform of Arrhenius equation and has calibration constants that are adjusted to reproduce equilibrium rates. However, it models reaction probability as a function of total energy, and vibrational favoring effect is not accounted, which leads to the development of other phenomenological dissociation models like vibrational favored dissociation model [2] and biased model [3].

In the early 1990s, Macheret et al. developed a theoretical model for nonequilibrium dissociation reaction at high-temperature conditions based on the assumption of classical impulsive collisions [4]. The model was recently re-evaluated, and a new implementation of the model in DSMC was proposed and compared against a QCT-based model [5]. The new model, called the MF-DSMC model, shows good prediction of nonequilibrium rates and average vibrational energy removed by dissociation (Figs. 1-2). A 1D simulation of shock wave experiment also shows the potential of the model being used for high fidelity simulations.

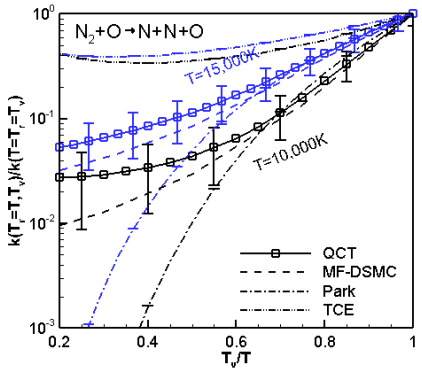

Figure 1. Nonequilibrium factors.

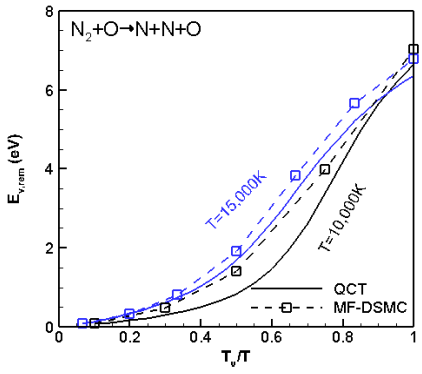

Figure 2. Average vibrational energy removed by dissociation.

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DSMC Simulations of Shock-Vortex Interactions

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Although turbulence is typically studied at the hydrodynamic or continuum level, there are cases in which the Kolmogorov length and time scales are comparable to the mean free path and collision times [1] and a molecular-level approach is required to fully examine the non-equilibrium physics. A practical example is the two-dimensional, unsteady, compressible interaction of a shock wave with a vortex. Traditionally, this interaction has been studied numerically at the continuum level [2] although more recent efforts have used non-continuum techniques [3] to show that non-continuum effects are present. Herein, the shock-vortex interaction is simulated using the Direct Simulation Monte Carlo (DSMC) method of Bird [4] as implemented in Sandia's SPARTA code [5] to study the non-continuum effects on the flow field for various vortex sizes and shock strengths.

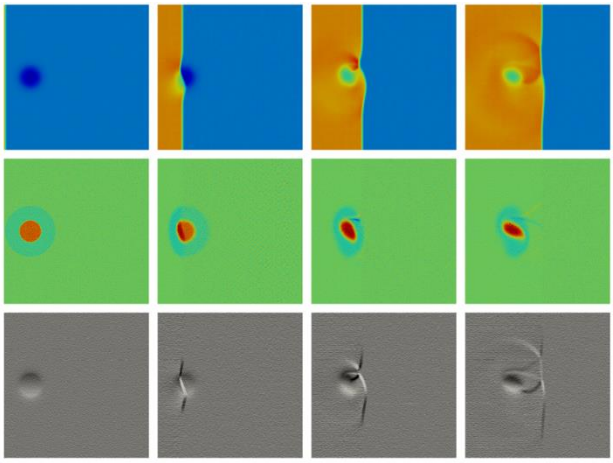

Figure 1. Temporal evolution of the interaction of a Mach 1.5 shock with a Mach 0.7 vortex. Number density (top), vorticity (middle), and numerical Schlieren (bottom) are shown.

[1] M. A. Gallis, N. P. Bitter, T. P. Koehler, J. R. Torczynski, S. J. Plimpton, and G. Papadakis, "Molecular-Level Simulations of Turbulence and Its Decay," *Physical Review Letters*, **118**, 064501 (2017).
[2] O. Inoue and Y. Hattori, "Sound Generation by Shock-Vortex Interactions," *Journal of Fluid Mechanics*, **380**, 81-116 (1999).
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Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525. This paper describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the paper do not necessarily represent the views of the U.S. Department of Energy or the United States Government.

DSMC Simulations of Compressible Turbulence

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The turbulent energy cascade indicates that, in a statistical sense, kinetic energy is generated at large scales, transferred to progressively smaller scales, and ultimately dissipated by viscosity at the Kolmogorov length scale. This inter-scale transfer of kinetic energy is even more complicated and less well understood for compressible turbulence than for incompressible turbulence. In compressible turbulence, nonlinear interactions of vortices, acoustic waves, shock waves, and expansion waves lead to strong coupling between the velocity field and the thermodynamic fields. In this paper, continuum (DNS) and molecular (DSMC) [1] simulations are used to study compressible turbulence in the Taylor-Green (TG) vortex flow [2] for a range of Mach and Reynolds numbers.

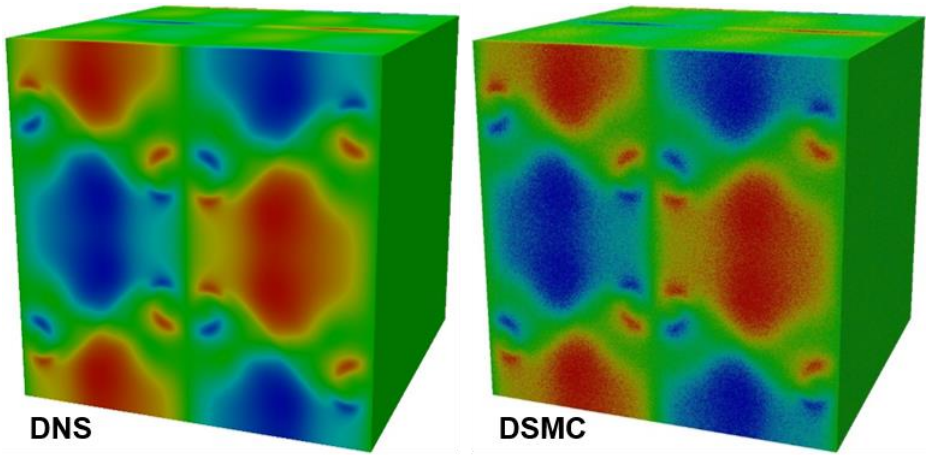

Figure 1. DNS and DSMC velocity fields for incompressible flow at maximum dissipation have almost identical flow structures [3].

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[2] G. I. Taylor and A. E. Green, "Mechanism of the Production of Small Eddies from Large Ones," *Proceedings of the Royal Society of London. Series A, Mathematical and Physical Sciences*, **158** (895), 499-521 (1937).
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