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CONSISTENT CONTINUUM-PARTICLE MODELING OF HYPERSONIC FLOWS AND DEVELOPMENT OF HYBRID SIMULATION CAPABILITY

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14. ABSTRACT

Space vehicles re-entering the atmosphere generate flow conditions that range from highly rarefied to fully continuum. However, even within a continuum flow, there may exist regions of flow that are locally rarefied leading to strong non-equilibrium. These local areas of non-equilibrium are generated around sharp leading edges, within shock waves, wake regions, and boundary layers or are exhibited in rocket plumes in space. For accurate simulation of such flows, a hybrid CFD-DSMC technique is required. While great strides have been made in developing a robust hybrid method, further work is necessary before a single hybrid hypersonic tool capable of 3D, parallel simulations, employing high fidelity chemistry models can be completed. In particular, two advancements are necessary; the hybrid method must be extended to fully 3D complex geometries with scalable parallel performance, and vibrational, chemical, and ultimately weak ionization models must not only be incorporated but also made physically consistent between the CFD and DSMC components. The current proposal focuses mainly on the second advancement, demonstrating full consistency between CFD and DSMC solutions for chemically reacting flows in the near-continuum regime. The proposed work will demonstrate such consistency for the first time and demonstrate preliminary de-coupled hybrid CFD-DSMC solutions for challenging flows.

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1 Project Summary

This research project was aimed at developing and implementing consistent models in both particle (direct simulation Monte Carlo – DSMC) simulations and continuum CFD simulations of hypersonic flows, and in addition, implementing a number of numerical procedures required to perform hybrid particle-continuum calculations.

The main numerical procedures added to the Molecular Gas Dynamic Simulator (MGDS) particle method (DSMC) code included (i) a parallel Adaptive Mesh Refinement (AMR) algorithm that can process large grids accurately and efficiently, (ii) a parallel post-processing algorithm that enables rapid (low cost and low memory) analysis of large solution files using the **hdf5** file format, (iii) the capability for users to specify arbitrary inflow/outflow planes and therefore simulate only the flow region of interest, and (iv) the capability to generate inflowing particles on such arbitrary surfaces and therefore perform decoupled CFD-DSMC simulations, where inflowing particles to DSMC can be specified from a CFD solution extracted along an arbitrary surface.

Large-scale DSMC simulations were performed of near-continuum canonical flows, such as the Hollow Cylinder Flare (HCF) geometry. Prior to comparing DSMC and CFD solutions for these near continuum flows, research was required in order to develop a consistent dissociation model for both particle and continuum methods. A preliminary model was developed, using quantum chemistry collision data from a related project. The new DSMC model accurately reproduces the quantum chemistry data and also analytically integrates to provide a continuum two-temperature dissociation rate model that could be used in CFD.

The progress made on this research project is a significant advancement in the development of a state-of-the-art hybrid DSMC-CFD of general applicability to complex hypersonic flows.

2 DSMC ADVANCEMENTS

As discussed in the proposal, the current state of hybrid DSMC-CFD research is that this capability has been demonstrated on simple geometries (cylinders, planetary probe geometries, etc.) [1-5], internal energy physics for nitrogen has been included [6], and preliminary results for multispecies mixtures [7-8] have been presented. However, hybrid DSMC-CFD capability for complex 3D vehicle geometries and, most importantly, including chemical reactions, has not yet been demonstrated.

As a result of the current grant research, we are now in a position to pursue hybrid DSMC-CFD capability including chemical reactions and also for computationally demanding 3D flows. The DSMC code under development at the University of Minnesota, called the Molecular Gas Dynamic Simulator (MGDS) code [9-11], is now capable of large-scale DSMC simulations of near-continuum flow conditions. This is essential for a hybrid DSMC-CFD code, since the flow conditions of most interest are continuum flows where only localized regions exhibit strong non-equilibrium. In contrast, if the entire flow is rarefied then pure DSMC simulations would be computationally feasible. The real need for hybrid DSMC-CFD capability is for challenging near-continuum flows where key regions of thermochemical nonequilibrium must be accurately resolved, and therefore, the capability to run near-continuum DSMC calculations is essential.

In particular, during this grant, a number of advancements were made to the MGDS DSMC code. First, the adaptive mesh refinement algorithm (AMR) was separated from the main MGDS source code. Adaptive mesh refinement is now compartmentalized such that every L1 cell can be adapted independent of all other L1 cells. Recall, each L1 cell (the largest cell structure) contains many L2 and L3 cells, where L3 cells are sized to the local mean-free-path. This enables AMR to be performed in parallel where each L1 cell is refined independently by a different processor. The MGDS code is now able to rapidly perform AMR for the very large grids required for near-continuum flows. Second, the post-processing code has been compartmentalized in a similar fashion. Specifically, each L1 cell (including all L2/L3 cells and all particles within them) can be interrogated by direct access to the **hdf5** data file format. This avoids the process of loading the entire grid and solution into memory before post-processing. Rather, a precise region of the flow can be interrogated directly from the **hdf5** solution file with little memory and cost. This is a significant upgrade for the MGDS code in terms of its ability to simulate near-continuum flows.

Such near-continuum flows require an enormous number of computational cells, which must be sized to the local mean-free-path for the DSMC method, and an enormous number of simulated particles. Since the DSMC grid (sized to the local mean-free-path) is dependent on the solution (the local density within the flowfield), adaptive mesh refinement (AMR) is essential. As a result of the current grant, the MGDS code now has an efficient and precise AMR strategy.

An example grid, created using AMR, for hypersonic flow over a Hollow Cylinder Flare (HCF) geometry is shown below in Fig. 1.

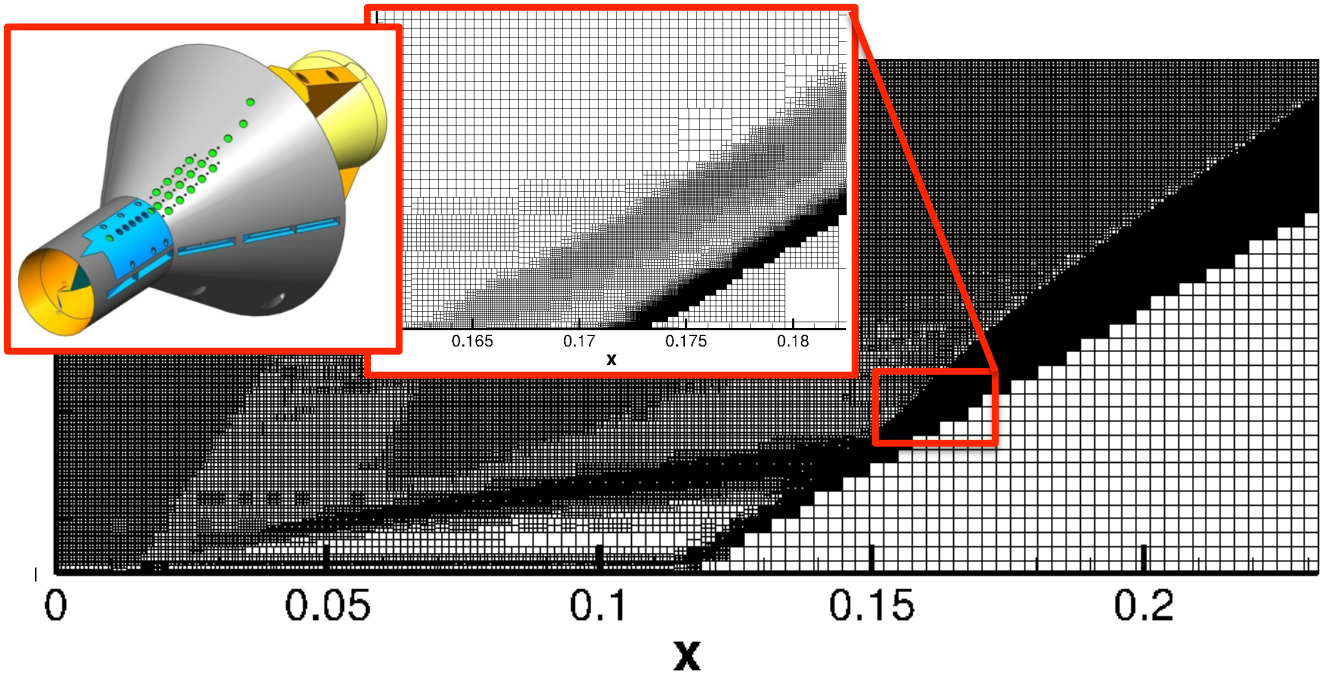

Figure 1: MGDS –DSMC adapted grid for hypersonic flow over a hollow cylinder flare geometry. Insets show the CUBRC test model geometry, and a close-up view of the grid near the shock-boundary layer interaction, the location of peak heating seen experimentally. Simulation contains ~0.5 billion particles.

The hollow cylinder flare is a canonical geometry that has been the focus of many experimental test campaigns at the Calspan University of Buffalo Research Center (CUBRC) over many years. This geometry involves a very sharp leading edge, which induces a degree of "slip flow" in the boundary

layer. The shock wave from the flare ultimately causes the boundary layer to separate leading to a complex shock-boundary layer interaction that is challenging to accurately predict and is relevant for hypersonic control surfaces. The conditions for this flow are near-continuum and the DSMC simulation requires a large number of cells and particles, and precise AMR. In fact, for visualization purposes, the grid in Fig. 1 is actually 4x coarser than was used for the simulation. The simulation involves a 5 species reacting air chemistry model and requires approximately 0.5 billion particles.

Another advancement in the MGDS code, developed during the current grant, is the capability to impose arbitrary boundary surfaces. Such surfaces can be seen in the Hollow Cylinder Flare solution depicted in Fig. 2, which allows the user to simulate only the flow region (cells) of interest, instead of always being restricted to rectangular flow domains. As seen in Fig. 2, inflow conditions are imposed on the surfaces shown (planes shaded in grey). An outflow surface is also placed inside the cylinder portion of the HCF geometry to remove particles that enter the hollow portion of the geometry. Since we are not interested in the flow inside of the HCF, only the small region around the leading edge need be simulated in order to accurately capture the weak leading edge shock wave. All particles outside of these surfaces are removed. The ability to restrict the flow domain to only the regions of interest is a necessary step when simulating near-continuum, large-scale DSMC problems.

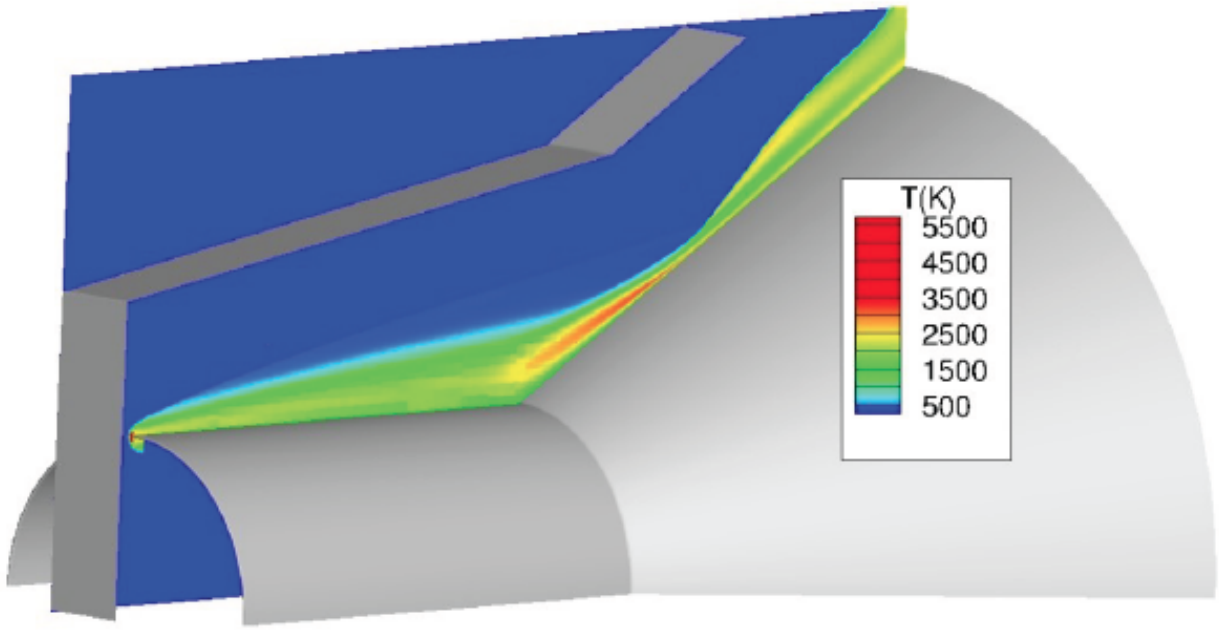

Figure 2: MGDS –DSMC solution for the Hollow Cylinder Flare problem employing arbitrary inflow/outflow planes. These planes ensure that particles are only simulated in regions of interest, resulting in significant cost and memory savings.

In addition to the large-scale parallel capability of the MGDS code, the current research grant has led to the development of key hybrid DSMC-CFD related algorithms. A hybrid code requires capabilities to interpolate solutions between CFD and DSMC computational grids and also requires the capability to perform DSMC simulations of sub-regions of an overall flowfield (i.e. only use DSMC for regions in strong nonequilibrium). Figure 3 depicts a DSMC solution for flow over a cylinder, where only the wake is simulated. Specifically, flow information from the forebody flow is prescribed as in inflow boundary condition (along the inflow plane shown in Fig. 3) to a DSMC

simulation of *only* the wake region. The MGDS DSMC code now has the capability to surround DSMC simulation regions by arbitrary inflow surfaces, where the flow properties for the inflow surfaces can be provided by any general means (such as data from an accompanying CFD [12] simulation). In this manner (Fig. 3), we now have the capability to transfer information between CFD and DSMC grids for general 3D flows.

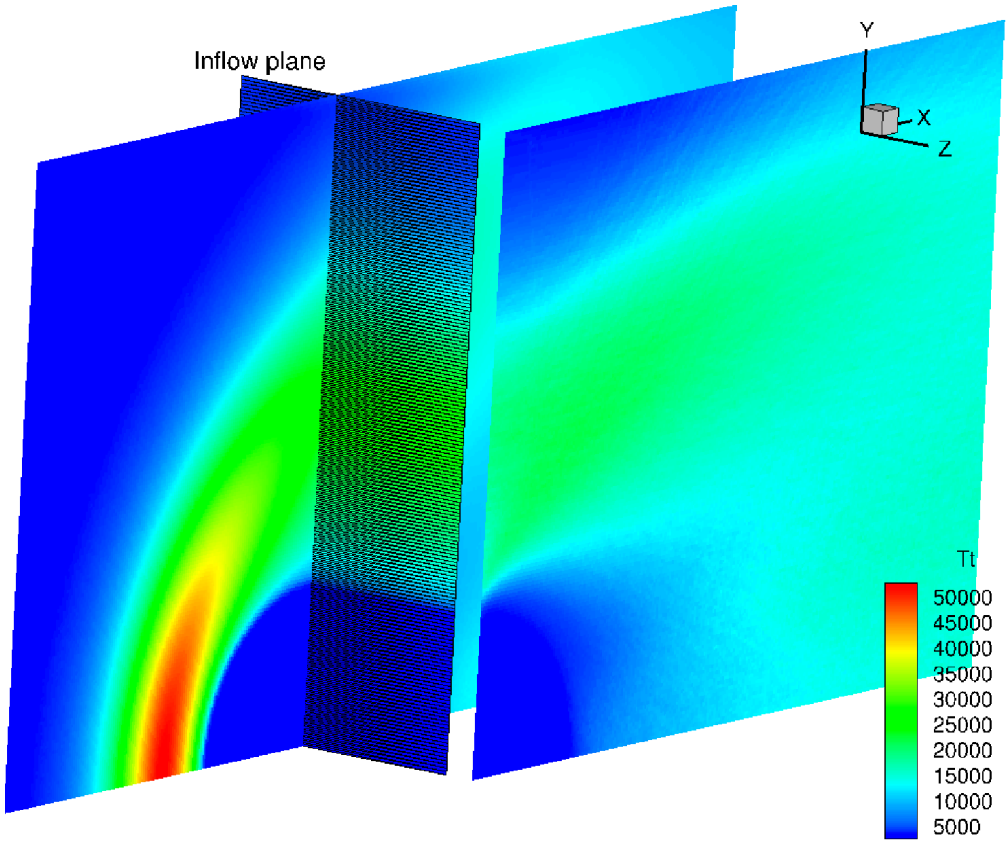

Figure 3: Hypersonic flow over a cylinder. Decoupled simulation where flow information from the forebody region is extracted along an "Inflow Plane", which is used as an inflow boundary condition for a DSMC simulation of only the wake region.

3 DSMC and CFD MODELING

As described in the previous section, a number of the required capabilities for a hybrid DSMC-CFD code have been developed during this research grant. We have also made progress on one of the most significant remaining obstacles; namely the lack of consistency between DSMC and CFD models for chemistry in flows exhibiting thermochemical nonequilibrium.

Essentially, current chemistry models for both CFD and DSMC are empirical models developed independently for each method. These existing empirical models are not consistent in the continuum limit. As mentioned in the introduction, hybrid simulation capability for reacting flows has not yet been demonstrated in the literature.

Significant progress has been made during the current grant in this area. We have developed a new dissociation model using results from quantum chemistry [13] performed under a grant from AFOSR. The new model was constructed from first-principles, and made inherently consistent at the molecular level (DSMC) and continuum level (CFD).

To summarize, a new simulation approach (called direct molecular simulation – DMS, developed in Schwartzentruber's group [14,15]) is able to directly simulate the rovibrational excitation and coupled dissociation physics of a shock-heated gas, where the only model input is an ab-intio potential energy surface (PES) [16-18]. The DMS method reveals the evolution of non-Boltzmann internal energy distributions and has revealed key details regarding the coupling between vibrational energy and dissociation. These DMS results have been used to construct a coupled vibration-dissociation model for DSMC. In the limit of near-equilibrium flow, this molecular model can then be integrated to obtain a new two-temperature model for use in CFD.

For DSMC, the new dissociation rate model has the following form:

$$P(d|v) = C_1 \exp\left[-\alpha \frac{\epsilon_d}{\langle \epsilon_t \rangle}\right] \exp\left[\frac{\epsilon_v}{\langle \epsilon_t \rangle}\right] \frac{\Gamma[\zeta_{tr}/2, (\epsilon_D - \epsilon_{v_0})/\langle \epsilon_t \rangle]}{\Gamma[\zeta_{tr}/2]}$$

This gives the probability of a molecule dissociating, given its vibrational energy state (ε_v), the average translational energy of the gas ($<\varepsilon_t>$) and the dissociation energy (ε_d). This is the expression that should be used within a DSMC simulation when simulation particles collide and are tested for a dissociation reaction.

A new model for the distribution of vibrational energy in a nonequilibrium gas has also been developed. Specifically, the new model captures deviations from a Boltzmann distribution due to overpopulation of the high-v states due to rapid excitation, and the depletion of high-v states due to dissociation. This non-Boltzmann distribution function is given by:

$$f(\epsilon_v) = \frac{C_2}{\Gamma(\zeta_v/2)} \frac{1}{\langle \epsilon_v \rangle} \left(\frac{\epsilon_v}{\langle \epsilon_v \rangle}\right)^{\zeta_v/2-1} \exp\left[-\frac{\epsilon_v}{\langle \epsilon_v \rangle} + \lambda_1 \left(\frac{\langle \epsilon_t \rangle}{\langle \epsilon_v \rangle} - \frac{\langle \epsilon_v \rangle}{\langle \epsilon_t \rangle}\right)^{\varphi} \left(\frac{\epsilon_v}{k_B \theta_v}\right) - \lambda_2 \frac{\langle \epsilon_t \rangle}{\epsilon_d} \left(\frac{\epsilon_v}{\theta_v}\right)\right]$$

This equation is a Boltzmann distribution based on the average vibrational energy (ε_v), however, it contains two additional exponential terms containing parameters λ_1 and λ_2. The λ_1 term accounts for overpopulation during excitation and the λ_2 terms accounts for depletion during dissociation. Comparisons of this simple model with non-equilibrium distributions during an excitation simulation (using DMS) is shown below in Fig. 4. This model is quite accurate despite it simplicity.

With a simple model for the non-Boltzmann velocity distribution function, one can now integrate the probability of dissociation given a v-level over the population of v-levels. This gives the overall probability of dissociation in the gas, which is directly linked to the reaction rate used in CFD:

$$\langle P_d \rangle = \int_0^\infty P(d|\epsilon_v) f(\epsilon_v) d\epsilon_v$$

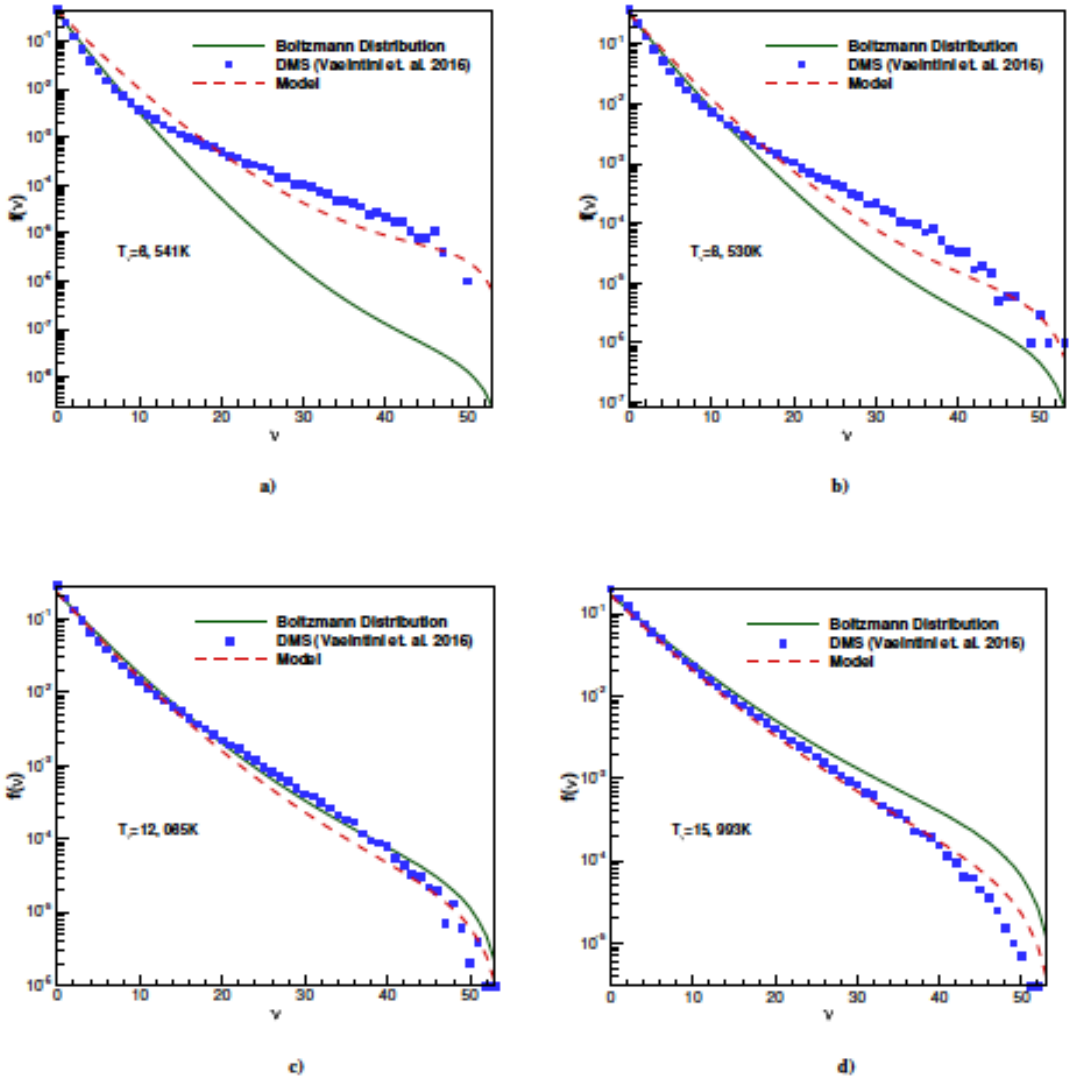

Figure 4: Vibrational energy distribution functions, plotted during an isothermal excitation to 20,000K in nitrogen gas. Direct Molecular Simulation (DMS) results are plotted as symbols. The new model results are plotted as dotted lines and the corresponding Boltzmann distribution is plotted as a solid line. During the excitation, the distribution function transitions from overpopulation compared to Boltzmann to depletion compared to Boltzmann.

We propose to use these new, consistent DSMC and CFD dissociation models and demonstrate hybrid DSMC-CFD solutions for reacting flows in the near future.

References

[1] Schwartzentruber, T. E. and Boyd, I. D., "A hybrid particle-continuum method applied to shock waves," Journal of Computational Physics, Vol. 215, No. 2, 2006, pp. 402–416.

[2] Schwartzentruber, T. E., Scalabrin, L. C., and Boyd, I. D., "A modular particle–continuum numerical method for hypersonic non-equilibrium gas flows," Journal of Computational Physics, Vol. 225, No. 1, 2007, pp. 1159–1174.

[3] Schwartzentruber, T. E., Scalabrin, L. C., and Boyd, I. D., "Multiscale particle-continuum simulations of hypersonic flow over a planetary probe," Journal of Spacecraft and Rockets, Vol. 45, No. 6, 2008, pp. 1196–1206.

[4] Schwartzentruber, T. E., Scalabrin, L. C., and Boyd, I. D., "Hybrid particle-continuum simulations of nonequilibrium hypersonic blunt-body flowfields," Journal of Thermophysics and Heat Transfer, Vol. 22, No. 1, 2008, pp. 29–37.

[5] Schwartzentruber, T. E., Scalabrin, L. C., and Boyd, I. D., "Hybrid particle-continuum simulations of hypersonic flow over a hollow-cylinder-flare geometry," AIAA journal, Vol. 46, No. 8, 2008, pp. 2086–2095.

[6] Deschenes, T. R. and Boyd, I. D., "Extension of a modular particle-continuum method to vibrationally excited, hypersonic flows," AIAA Journal, Vol. 49, No. 9, 2011, pp. 1951–1959.

[7] Verhoff, A. M. and Boyd, I. D., "Extension of a hybrid particle-continuum method for a mixture of chemical species," 28TH International Symposium on Rarefied Gas Dynamics 2012, Vol. 1501, Zaragoza, Spain, 2012, pp. 342–349.

[8] Stephani, K., Goldstein, D., and Varghese, P., "A non-equilibrium surface reservoir approach for hybrid DSMC/Navier–Stokes particle generation," Journal of Computational Physics, Vol. 232, No. 1, 2013, pp. 468–481.

[9] Gao, D., Zhang, C., and Schwartzentruber, T. E., "Particle simulations of planetary probe flows employing automated mesh refinement," Journal of Spacecraft and Rockets, Vol. 48, No. 3, 2011, pp. 397–405.

[10] Nompelis, I. and Schwartzentruber, T., "Strategies for Parallelization of the DSMC Method," 51st AIAA Aerospace Sciences Meeting, Vol. AIAA Paper 2013-1204, Grapevine, TX, 2013.

[11] Zhang, C. and Schwartzentruber, T. E., "Robust cut-cell algorithms for DSMC implementations employing multi-level Cartesian grids," Computers & Fluids, Vol. 69, 2012, pp. 122–135.

[12] Candler, G. V., Johnson, H. B., Nompelis, I., Gidzak, V. M., Subbareddy, P. K., and Barnhardt, M., "Development of the US3D Code for Advanced Compressible and Reacting Flow Simulations," AIAA 2015-1893, 53rd AIAA Aerospace Sciences Meeting, Kissimmee, FL, 2015.

[13] Singh, N., Valentini, P., and Schwartzentruber, T. E., A Coupled Vibration-Dissociation Model for Nitrogen from Direct Molecular Simulation, to be presented at the 2016 AIAA Aviation Meeting, Washington, D.C., 2016.

[14] Norman, P., Valentini, P., and Schwartzentruber, T., "GPU-accelerated classical trajectory calculation direct simulation Monte Carlo applied to shock waves," Journal of Computational Physics, Vol. 247, 2013, pp. 153–167.

[15] Valentini, P., Schwartzentruber, T. E., Bender, J. D., Nompelis, I., and Candler, G. V., "Direct molecular simulation of nitrogen dissociation based on an ab initio potential energy surface," Physics of Fluids (1994-present), Vol. 27, No. 8, 2015, p. 086102.

[16] Paukku, Y., Yang, K. R., Varga, Z., and Truhlar, D. G., "Global ab initio ground-state potential energy surface of N4," The Journal of Chemical Physics, Vol. 139, No. 4, 2013, p. 044309.

[17] Lin, W., Varga, Z., Song, G., Paukku, Y., and Truhlar, D. G., "Global triplet potential energy surfaces for the N2 (X1S)+ O(3P) NO (X2P)+ N (4S) reaction," The Journal of Chemical Physics, Vol. 144, No. 2, 2016, p. 024309.

[18] Varga, Z., Meana-Pa˜neda, R., Song, G., Paukku, Y., and Truhlar, D. G., "Potential energy surface of triplet N2O2," The Journal of Chemical Physics, Vol. 144, No. 2, 2016, p. 024310.

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