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Progress and future prospects for particle-based simulation of hypersonic flow

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ABSTRACT

The direct simulation Monte Carlo method (DSMC) has evolved over 50 years into a powerful numerical technique for the computation of thermochemical nonequilibrium gas flows. In this context, nonequilibrium means that velocity and internal energy distribution functions are not in equilibrium forms due to a low number of intermolecular collisions within a fluid element. In hypersonic flow, nonequilibrium conditions occur at high altitude and in regions of flow fields with small length scales. This article highlights significant developments in particle simulation methods (since 2001) applied specifically to hypersonic flows, which now includes Molecular Dynamics in addition to DSMC. Experimental measurements that have led directly to improved DSMC models will be highlighted. Algorithm development for DSMC aimed at increasing computational efficiency is discussed with a focus on hybrid particle-continuum methods. New research that applies all-atom Molecular Dynamics simulation and trajectory-based DSMC simulation to normal shock waves is summarized. Finally, a discussion of state-resolved DSMC modeling is included with reference to future prospects for particle simulation methods and in particular for the DSMC method.

1. Introduction

When modeling gases in nonequilibrium, the atomistic/molecular nature of the gas must be explicitly accounted for. This is especially true for gases in thermochemical nonequilibrium which involve finite-rate translational–rotational–vibrational–electronic relaxation as well as chemical reactions. Such finite rate processes, when coupled with low densities, small length-scales, high gradient regions, or high flow speeds, can result in strong thermochemical nonequilibrium in the bulk flow and next to vehicle surfaces. Understanding and prediction of the precise thermochemical gas state within the flow field surrounding a vehicle and within the boundary layer next to a vehicle's surface is crucial in order to design hypersonic flight vehicles and thermal protection systems. Particle simulation methods have proven to be a valuable tool for fundamental understanding and design of hypersonic systems and have enormous potential as computational power continues to rapidly increase.

Since changes in the state of a dilute gas occur via molecular collisions, the relevant spatial scale is the mean free path (λ) and the relevant temporal scale is the mean collision time (τ_c). Below this temporal scale, $O(\tau_c)$, no variations in the gas state are possible and likewise, no changes are possible below a spatial scale of $O(\lambda)$. Furthermore, in a dilute gas there are an enormous number of molecules within a volume of λ^3, ranging from tens-of-thousands at sea level to billions (per λ^3 volume) at altitudes typical of hypersonic flight. It is unnecessary to account for the properties of all real molecules, rather, their local distribution functions (for velocity, internal energy, chemical species, etc.) are sufficient to completely describe the nonequilibrium state of the gas. Such distribution functions can be accurately constructed by considering only a small fraction of the real molecules. In addition, the pre-collision orientations (the impact parameters) of colliding molecules are completely random in a dilute gas. The direct simulation Monte Carlo (DSMC) method takes advantage of these three inherent properties of dilute gases by using simulator particles that each represent a large number of identical real molecules, moving simulator particles with timesteps on the order of τ_c, and stochastically selecting collision pairs and initial/final orientations within volumes (computational cells) on the order of λ. These are rigorous simplifications based on sound physical principles. Present DSMC methods then go one step further and use probabilistic rules to determine the local collision rate and collision outcomes, thus introducing collision *models*.

The DSMC method was first introduced by Bird [1]. Since that time, Bird has written three books on the method [2–4] and thousands of research papers have been published that report on

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development and application of the technique. The significance of the DSMC technique has been its ability over 50 years of development to provide a method of analysis for high Knudsen number flows (conditions ranging from continuum to free-molecular). Strong nonequilibrium in a flow is characterized by large Knudsen numbers ($Kn=\lambda/L>0.01$), where L is a characteristic length of interest in the flow. A DSMC simulation emulates the same physics as the Boltzmann equation. In fact, it has been demonstrated that DSMC converges to the solution of the Boltzmann equation in the limit of a very large number of particles [3]. For low Knudsen numbers ($Kn=\lambda/L<0.01$), through Chapman-Enskog theory [5], the Boltzmann equation reduces exactly to the Navier–Stokes equations, which are the governing equations for computational fluid dynamics (CFD) simulations. Therefore, DSMC and CFD methods provide a highly consistent modeling capability for gas flows spanning the entire Kn range.

DSMC collision models are extremely flexible in that they can be phenomenological and formulated to be consistent with continuum thermochemical rate data or they can directly incorporate ab initio quantum chemistry results. This flexibility in physical modeling enables DSMC to provide high fidelity calculations of multispecies gases in strong thermochemical nonequilibrium over full vehicle geometries. For example, DSMC has been used recently to support the Columbia Space Shuttle orbiter accident investigation [6], to support the 2001 Mars Odyssey aerobraking mission [7], and to analyze the post-flight data from the Stardust mission [8–11]. The utility of DSMC and its range of applications continues to expand in-step with advances in computational resources.

This article focuses on particle simulation methods applied to hypersonic flows. The long term goals in this field involve (i) large-scale particle simulations that completely overlap with CFD simulations for complex 3D flows (this involves research into computational efficiency and ultimately hybrid DSMC-CFD capability), (ii) advancing phenomenological (reduced-order) models for engineering design and analysis, and (iii) incorporating ab initio based (quantum chemistry) collision models directly into particle simulations to improve our understanding of hypersonic flows at the most fundamental level. As with any numerical modeling approach, these advancements must be validated by experimental data and should also aid in the design of new experiments required to move the science forward.

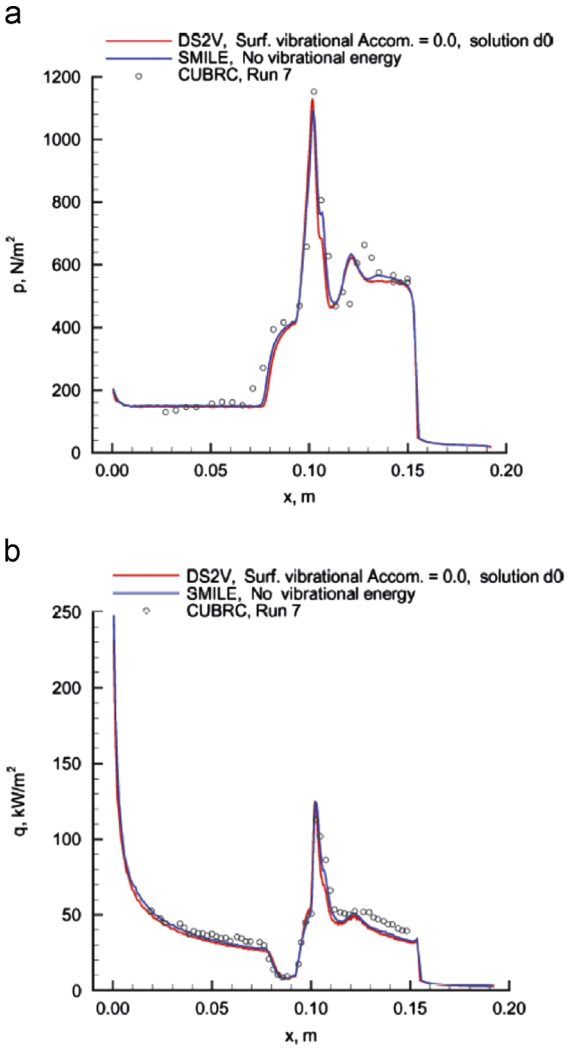

Fig. 1. Measured versus computed surface properties for a double cone geometry tested with nitrogen at Mach 15.6, $Kn=0.002$ [14]. (a) Surface pressure. (b) Surface heat flux.

2. Experimental validation

In this section, a review is provided of the status of the application of the DSMC technique to hypersonic flows. We first consider the application of DSMC to analyze hypersonic experiments conducted in ground-based facilities. Generation of rarefied, hypersonic flows in ground-based facilities presents a technical challenge, and very few data sets exist that enable a detailed assessment of DSMC codes.

In 2001, a code validation exercise (for both DSMC and CFD) was focused on hypersonic viscous interactions that can be generated on slender body configurations. A series of experiments were performed in the LENS facility for a number of configurations including double cones and cylinder-flares [12]. While several groups performed DSMC analyses of some of these cases, Moss and Bird [13] provide the most comprehensive comparisons with the measured data. Fig. 1 shows comparisons for surface pressure and heat flux for a Mach 15.6, $Kn=0.001$ flow of nitrogen over a double cone configuration. DSMC results from two different codes (DS2V and SMILE) are provided and clearly give excellent agreement with the measurements. Similar levels of agreement between DS2V DSMC computations and measurements of pressure and heat flux are also shown in Ref. [14] for a Mach 12.4, $Kn=0.0004$ flow of nitrogen over a cylinder flare configuration. For these flows, the vibrational energy of nitrogen was barely activated, and thus there was no chemistry present under these conditions.

The Bow-Shock Ultra-Violet-2 (BSUV-2) hypersonic flight experiment (a slender vehicle geometry) was flown in 1991 [13]. The vehicle geometry consisted of a spherically-capped 15° cone with a nose radius of about 10 cm. BSUV-2 reentered the atmosphere at 5.1 km/s and provided data in the altitude range from 110 to 60 km. Measurements of the ultra-violet emission due to nitric oxide and vacuum-ultra-violet emission due to atomic oxygen resonance transitions were obtained by on-board instrumentation. Calculation of the radiative emission was performed in a decoupled approach. The chemically reacting flow field was computed using both continuum (CFD) [15–17] and particle (DSMC) methods [18]. Then, the emission was predicted from the flow field solutions using the NASA nonequilibrium radiation code NEQAIR [19]. Initial comparisons between DSMC-based results and measurement produced poor agreement at high altitude. This led to significant activity in the study of the oxygen dissociation and nitric oxide formation chemistry models used in the DSMC computations [20,18]. The final results obtained for nitric oxide radiance as a function of altitude are shown in Fig. 2a [21]. Note that the BSUV-2 Knudsen number ranged from 0.008 at 71 km to