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MODELING RAREFIED GAS DYNAMICS USING DIRECT SIMULATION MONTE CARLO METHOD

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Non-equilibrium rarefied gas dynamics effect has been playing an important role in several scientific and engineering disciplines. These include high-altitude hypersonic flow, reentry flight from orbit with considerable chemical reactions, vacuum technology, micro- and nano-scale gas flows, plume impingement on spacecraft, low-pressure materials processing flow, and comet dust and gas plume, to name a few. These gas flows are either highly rarefied or strongly non-equilibrium, which makes the continuum-based Navier-Stokes equations either breakdown or unsuitable for describing these flow phenomena correctly. Instead, the integro-differential Boltzmann equation can faithfully describing these flows. Unfortunately, not only does it have six phase spaces (three positions and three velocities) but also there is a nearly intractable collision integral term. This makes the direct numerical solution of the Boltzmann equation very difficult even with the advanced modern supercomputer system. Thus, an alternative and efficient numerical method for describing these highly non-equilibrium rarefied gas dynamics is necessary.

In early 1960s Bird proposed the direct simulation Monte Carlo method (DSMC) for modeling the non-equilibrium rarefied gas flows. Not until early 1990s, it was mathematically proved that DSMC is equivalent to solving Boltzmann equation statistically [1]. The central idea of DSMC is to reproduce real flow properties with no more than collision kinetics of gas molecules through a large number of pseudo particles that are used to represent real gas molecules. Each pseudo particle represents a fairly large number of real gas molecules. In DSMC, there is an important feature that the motion and the collision of pseudo particles are uncoupled over a time interval. The time interval (time step) should be kept much smaller than the mean collision time. Both the collision between pseudo particles and the interaction between pseudo particles and solid boundaries are computed on a probabilistic basis; therefore, a generator of random number in this method is necessary for producing extensive random numbers. The general procedures of the standard DSMC method [2] are divided into several major steps, including initialization, particle movement, indexing, collision, and sampling. When the flow reaches a steady state, microscopic states (mass, momentum and energy) of particles are continuously sampled until an acceptable statistical uncertainty is

reached.

We have developed a general-purpose parallel 2D/2D-axisymmstric/3D DSMC code using unstructured grid, named **ultra SPARTS** (**S**tatistical **PART**icle **S**imulation: **ultra** computing architecture; SPARTS). Fig. 1a shows the schematic diagram of 25-55° double cone, through which hypersonic nitrogen flow with $M_\infty = 15.6$ [3] passes. Fig. 1b and Fig. 1c, respectively, shows the temperature distribution and comparison of simulated surface heat flux with previous simulation and experimental data. The results show excellent agreement with both of the previous simulation and measurement. Fig. 2a shows the sketch of half Apollo reentry capsule with hypersonic flow ($M_\infty = 34.6$; $Kn_\infty = 0.034$) at an angle of attack of 25° [4]. In the 3D simulation, 5 species (N_2, O_2, NO, N, O) with 34 reactions are considered. Fig. 2b and Fig. 3c, respectively, present the simulated density and temperature (with surface heat flux) distribution. More details will be presented in the meeting.

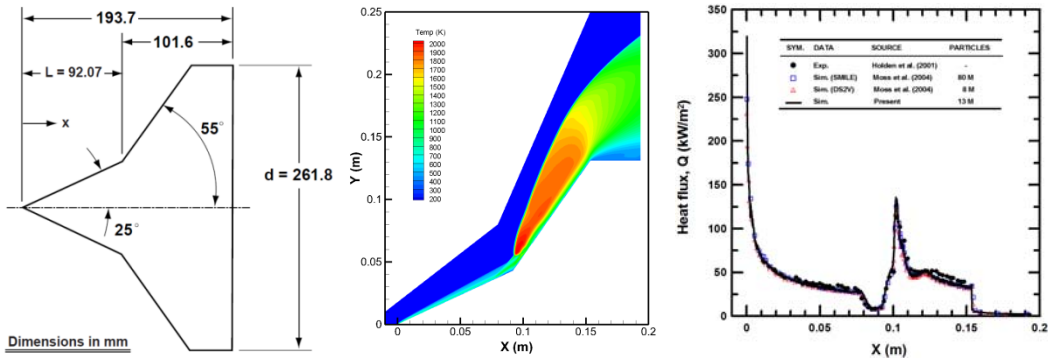

Fig. 2. (a) (left) Sketch of 25-55° double cone; (b) (middle) Simulated temperature contour; (c) (right) Comparison of present simulation with previous published data.

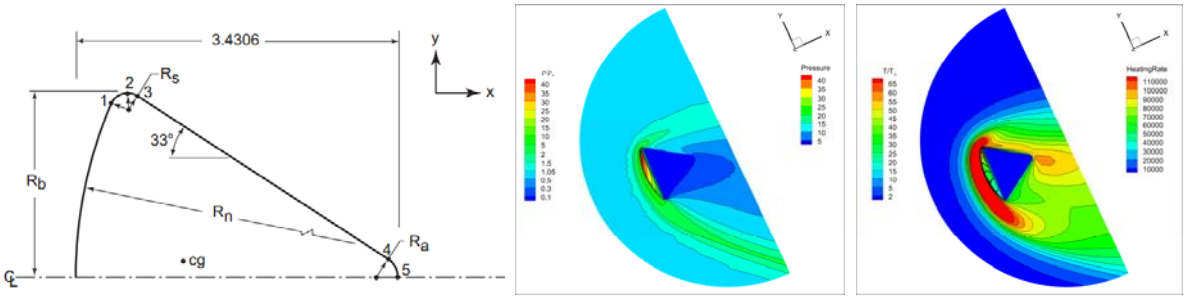

Fig. 3 (a) (left) Sketch of Apollo reentry capsule; (b) (middle) Simulated density contour with surface pressure; (c) (right) Simulated temperature contour with surface heat flux.

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