HIGH-PERFORMANCE COMPUTING OF HYPERSONIC, SHOCK–SHOCK INTERACTIONS USING KINETIC, PARTICLE APPROACHES

Allocation: Illinois/70 Knh
PI: Deborah A. Levin[1]

[1]University of Illinois at Urbana–Champaign

EXECUTIVE SUMMARY:

When steep gradients occur in the strong shocks of hypersonic flows, the use of continuum formulations such as the Navier Stokes equations is questionable. Instead, the direct simulation Monte Carlo (DSMC) method provides a numerical solution to the Boltzmann equation of transport, particularly for modeling thermochemical non-equilibrium shock-dominated flows. In the DSMC method, the flow is modeled by a series of collisions that occur by using simulated particles, each of which represents a large number of real molecules. The approach is computationally tractable and well suited to parallelization because the particle collisions and movement are decoupled. Recently we have implemented an approach that uses octree grids to reduce the cell size only in regions where the mean free path is small (i.e. distance travelled between particle collisions is small, so lots of particle collisions), thus reducing the required number of computational particles.

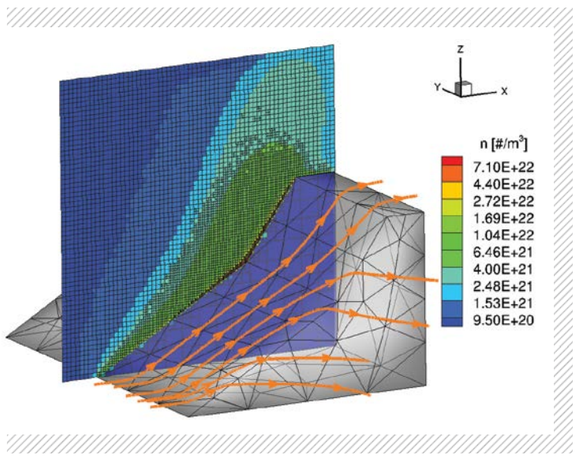

FIGURE 1: Streamlines and number density contours over a double wedge for Mach-7 flow showing increased density near the surface and the presence of 3D effects.

INTRODUCTION

In direct simulation Monte Carlo (DSMC) the flow is modeled by a series of binary collisions that occur by using simulated or numerical particles, each of which represents a large number of real molecules. The time step is selected to be small compared to the mean time between collisions. We are developing a novel, in-house DSMC code, known as scalable unstructured gas dynamics adaptive refinement (SUGAR), using the adaptive mesh refinement (AMR)/octree grids has been applied to the study of 3D ion thruster plumes [1]. The case being considered here, hypersonic flow over a double wedge, presents different challenges because a high level of spatial refinement is needed to capture shock-shock and shock-boundary layer interactions that create regions of separation and shear layers for low Knudsen number flows.

METHODS & RESULTS

The basic steps of our DSMC code involve the movement of particles through the computational domain, collisions of these particles with other particles and with surfaces, mapping of the particles onto the collision and sampling meshes, mesh refinement (when required), and sampling of the macro-parameters in each Cartesian collisional cell. Depending on the gas-wall surface interaction model, the particle is reflected specularly, diffusively, or mixed specularly and diffusively. After the movement of all the computational particles in the domain, each particle is checked to see if it is still on the same processor, has been transferred to another processor, or has exited the computational domain.

For the computational particles that are transferred to another processor, each processor creates linked lists to store the corresponding particle lists that need to be transferred. Once each processor has the information regarding which processor it must send to or receive computational particles from, communication is accomplished in a point-to-point fashion via MPI. After each processor has the list of its particles, these particles are put in the basic Cartesian cells overlying the computational domain. These Cartesian cells are refined based on criteria such as a required number of particles per cell and that the cell size is smaller than the local, spatially varying, mean free path. The SUGAR code performs AMR on two octree meshes: the collision mesh and the sampling mesh. During the collision phase, particles are selected to participate in a collision from collision cells using the appropriate physical cross section (e.g., elastic, inelastic, reaction) and their post-collision velocities are updated based on the statistical outcome. The octree grid is destroyed and recreated until it meets the refinement criteria and the flow reaches steady state.

To date we have modeled shock-dominated flows corresponding to flows over a sphere and a wedge. In figs. 1–2, the nature of the oblique and bow shocks can be observed, with the highest temperatures observed downstream of the bow shock. Three-dimensional effects were important in allowing for pressure relief at the edges of the wedge, as seen by the streamlines falling over the wedge's sides. The level of octree refinement was four in the recirculation region that formed at the intersection of the two wedges.

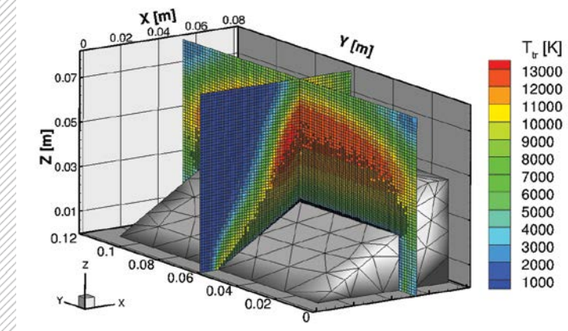

FIGURE 2: Maximum temperature (T_{tr}) decreases along the span-wise direction due to pressure-relief effects.

WHY BLUE WATERS

The starting point for modeling Edney type IV shock interactions with DSMC involves 7 billion particles (approximately 3 per collision cell) and 200 GB of physical memory. With the Blue Waters petascale facility, we have the ability to use thousands of cores to reduce the time taken for modeling a flow from a few weeks to a few days. We expect that we will generate approximately 1 TB of data per case. In order to improve the scaling performance of our new code, we are using the CPMAT profiler specifically built for CRAY systems for quick visualization.

PUBLICATIONS

Sawant, S., B. Borkut, O. Tumulku, and D. Levin, Development of an AMR Octree DSMC Approach for Shock Dominated Flows, *AIAA SciTech 2015,* Orlando, Fla., January 5, 2015. [AIAA Paper No.-2015-0070].