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FULLY THREE-DIMENSIONAL KINETIC SIMULATIONS OF UNSTEADY SHOCK–BOUNDARY LAYER INTERACTIONS

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EXECUTIVE SUMMARY

Hypersonic flow over double-wedge configurations displays what is known as complex Edney type IV interactions. Whether they are modeled using continuum or particle methods, these flows are unsteady in nature. However, modeling of such flows provides an opportunity to study flow stability mechanisms and identify near-transition behavior. Given the importance of continuum breakdown in strong shocks, a kinetic particle treatment of such flows is crucial. However, the continuum-like free stream conditions create a challenging problem because of the multiple shock–shock and shock–boundary layer interaction, separated flows near the hinge, shear layer, and three-dimensional effects. These conditions generate a mesh that is highly nonuniform because of very high levels of refinement near the surface due to extremely high flow gradients in temperature and pressure. The geometry of the double wedge also presents challenges with respect to load imbalance among the processors, which can cause significant increases in communication time.

RESEARCH CHALLENGE

Hypersonic compressible flows are characterized by significant gradients in gas density, high temperatures, and a large degree of nonequilibrium. Simulation of such flows requires due consideration of shocks, the chemistry of diatomic molecules, and the interactions of gases with embedded surfaces. The multiscale nature of these problems makes it a challenge in terms of flow physics and computational intensity.

This work was motivated by the study of laminar shock wave–boundary layer interaction (SWBLI) problems. These have a significant role in determining aerothermodynamic quantities such as heat transfer, skin friction, and pressure loads over different angular sections. The particle-based Direct Simulation Monte Carlo (DSMC) method is a good candidate to simulate such flows because it solves the Boltzmann transport equation and provides the highest fidelity in strong shock regions. However, the extent of its applicability to such problems has been limited by the high computational requirements arising from the need to simulate a large number of particles to satisfy DSMC requirements. Since the DSMC approach is amenable to parallelization, however, these limitations can be overcome with an efficient use of state-of-the-art petascale resources such as Blue Waters and computational tools that have been designed for these resources.

METHODS & CODES

We developed a three-dimensional MPI-parallelized DSMC code known as Scalable Unstructured Gasdynamic Adaptive mesh Refinement (SUGAR). SUGAR uses new techniques to simulate hypersonic compressible flows, such as an octree-based adaptive mesh refinement (AMR) implementation for capturing multiscale physics, linearized representation of an unstructured grid using Morton-Z space-filling curve for efficient access of computational cells, an accurate cut-cell algorithm to compute correct volume of intersected computational cells, algorithmic improvements for efficient gas–surface interactions, and array-based data structures for optimal use of cache memory utilization. We have performed a great deal of work to improve the scalability of the code [1] and have achieved the highest performance in the world for such problems: 87% weak scaling for 8,192 processors for flow over a hemisphere with 24 billion particles.

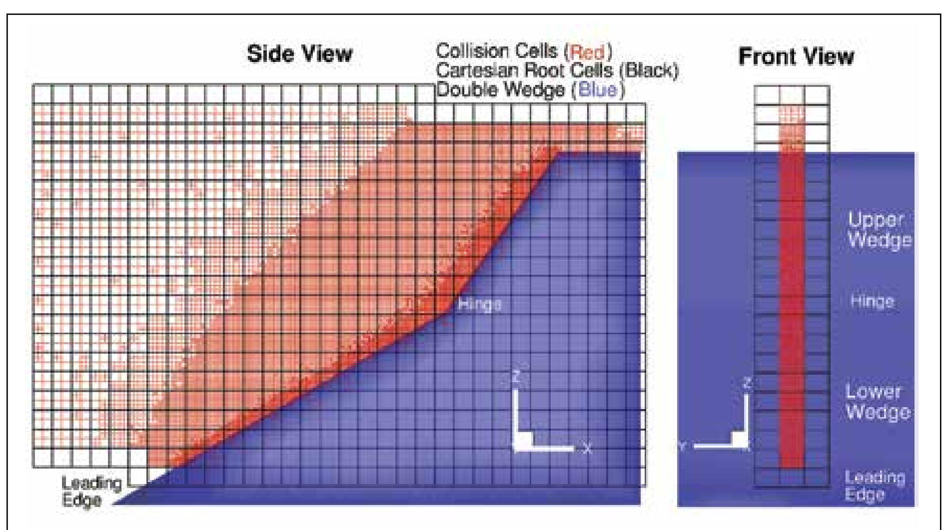

Figure 1: Decomposition of the computational domain held by a single of the 32 processors. Collision and root grids are shown in red and black, respectively. Root grid elements that are blank represent roots held by neighboring processors. The processor needs the location code array data held in both filled and blank roots.

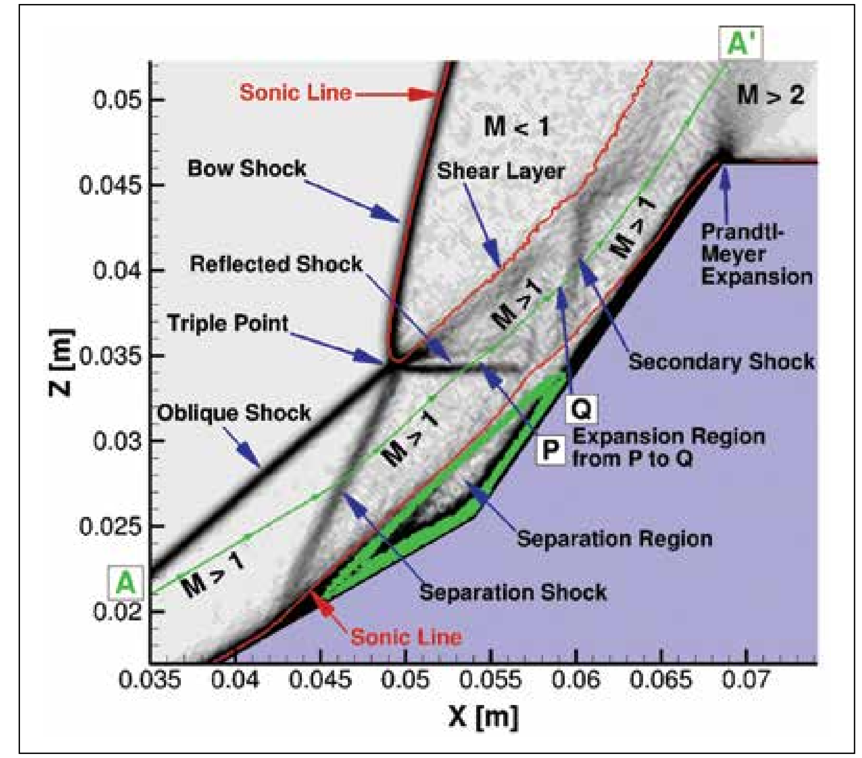

Figure 2: SWBLI features shown based on gradient density magnitude in the symmetry plane based on flow field parameters sampled from ~0.1 to 0.108 ms.

RESULTS & IMPACT

Satisfying the DSMC requirement for a SWBLI case at a Knudsen number of the order of 10^3 requires billions of computational particles and cells, which necessitates very sophisticated memory optimization tactics. The results for the actual case presented here were simulated using 20,000 processors, a number that would only be possible on Blue Waters. Furthermore, the gradients in the flow are so severe that there are many AMR/octree roots and each can have seven levels of refinement. This requires 8 MB of memory per processor to store the location code array that correlates the position of DSMC particles with leaf nodes. The memory requirement is made more tractable by storing this array for only those roots that lie in the portion of the domain assigned to the processor and the neighboring roots, as shown in Fig. 1.

The unsteady simulated Schlieren of the complex shock structure formed in the symmetry plane on the double wedge at ~0.1 ms is shown in Fig. 2. We can see that an oblique and bow shock are formed at the leading edge of the lower wedge and in front of the upper wedge, respectively. As the flow moves up the lower wedge, an adverse pressure gradient is formed and the boundary layer separates, thus generating a separation shock. These three shocks meet at the triple point and with their interaction form a reflected shock, also known as the trailing shock. As the reflected shock reaches closer to the boundary layer, the compression is nearly isentropic with a continuous transition to subsonic velocities. At the reattachment location of the boundary layer, a succession of compression waves are formed that coalesce into a secondary shock. As the flow passes through the oblique, separation, and reflected shocks, the increase in density and temperature results in a reduction in the thickness of the boundary layer downstream of the reattachment location. We observed strong recirculation in the separation zone embedded between the hinge, separation point, and the reattachment point. Note that the flow downstream of the bow shock is subsonic, but the flow going through the oblique, separation, and reattachment shocks remains supersonic. Therefore, a contact surface, also known as the shear layer, is formed, across which the pressure is constant although the velocities and temperatures differ.

WHY BLUE WATERS

The time-accurate, large-scale DSMC simulations performed to obtain the results shown in Fig. 2 require on the order of 100,000 node-hours, 24 billion computational particles, and 2.2 billion collision cells to reach one millisecond. Blue Waters is one of the few computer architectures that can host and execute these simulations.