MODELING PLASMA FLOWS WITH KINETIC APPROACHES USING HYBRID CPU–GPU COMPUTING

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EXECUTIVE SUMMARY

The main objective of our Blue Waters proposal has been to characterize the backflow contamination environment due to plasma created by electric-propulsion (EP) plumes and their interaction with the spacecraft environment and neutralizer sources, using state-of-the-art high-performance petascale computations. In terms of modeling and simulation, we have built on our earlier work where we developed an object-oriented C++ Direct Simulation Monte Carlo (DSMC) code that uses AMR/Octree grids to capture the vast length scales inherent in supersonic expansions to vacuum for neutral–neutral and neutral–ion collisions. A key aspect of this computational work has been to take advantage of our recent unique advances in GPU multithread parallelization applied to tree-based computational strategies. Blue Waters has been especially crucial to this modeling since we were able to use up to 256 GPUs per run for the plasma plume simulations on the XK nodes. During this work, we implemented the first DSMC calculations coupled to the particle-in-cell method with a particle approach for electrons as well.

RESEARCH CHALLENGE

The main objective of our work is to characterize the backflow contamination environment due to the plasma created by EP plumes, and their interaction with the spacecraft environment and neutralizer sources, using state-of-the-art high-performance GPU-based petascale computations. The improved predictability of key surfaces of solar cell arrays and spacecraft charging in the backflow environment of chemical and EP thrusters is crucial, particularly for small satellites and CubeSats where there is close placement of thrusters and solar cell arrays. To model the spacecraft environment, multiple sources and processes that must be considered include both neutral and charged species in the backflow region of an onboard EP thruster as well as highly reactive ion thrusters and ambient neutral species that occur over multiple time and length scales. The indirect environmental exposure of spacecraft material such as the micron-sized glass and aluminized Mylar coatings of solar arrays can cause appreciable sputtering and erosion. Sputtering and erosion are hard to quantify and predict because the backflow ion fluxes are about five orders of magnitude less than those due to main ion beam impingement. In addition, the external hollow cathodes are a source of electrons that must be modeled kinetically if one is to truly understand how charge-exchange (CEX) ions affect the erosion of solar cell panels.

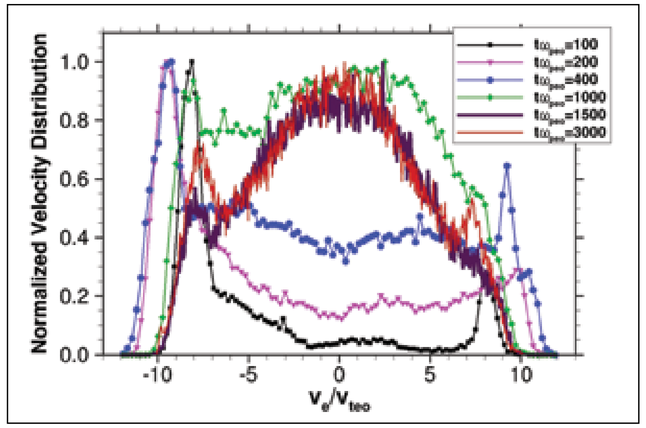

Figure 1: Non-Maxwellian Electron velocity distribution functions of a shifted source plume as a function of the evolution time of an electric propulsion xenon ion plume. The asymmetry of the main xenon beam and the electron neutralizer means that the electrons cannot be described by an electron temperature.

METHODS & CODES

Our plasma modeling is an outgrowth of our DSMC code, CHAOS (Cuda-based Hybrid Approach for Octree Simulations), that was developed under a previous Blue Waters effort to study neutral flows through porous media. The approach is unique in that in order to compute volume of cut-leaf nodes it utilizes the Morton Z-curve octree structure, a volume-of-fluids (VOF) method, and ray-tracing, which is very efficient on GPUs. Since the space conditions are such that the local mean free path for collisions is about three orders of magnitude larger than the local Debye length (~10^{-6} m), we have implemented two linearized Morton-ordered forests of octrees (FOT) so that these grids can be adapted to meet these two diverse numerical criteria. We have shown in [1] that when a leaf node may only be one level larger than its smallest-faced neighbor (the "2:1 criterion") we are able to obtain first-order accuracy in the gradient calculations. In our AMR/octree approach, the DSMC cells of variable size satisfy the mean-free-path and Debye length criteria, but do not automatically satisfy the 2:1 ratio. Implementation of this on an AMR/octree grid is nontrivial and has been accomplished through the use of local (on a single processor) and local–global (across processors) stages.

In addition, we have implemented new boundary conditions that enable us to model a stable, steady plume as the beam-front crosses the computational domain. Further, we have obtained a physically reasonable result where the electron distribution function remains Maxwellian for a co-located ion and electron source with an electron temperature less than about 2 eV. This computational complexity could be avoided by modeling a much larger computational domain, but the computational cost increases to the point where the number of resources would be prohibitive. Finally, as is shown in [1], we obtained ideal scaling up to 128 GPUs. This work received a prestigious best paper award at the 45th International Conference on Plasma Science in 2018 [2].

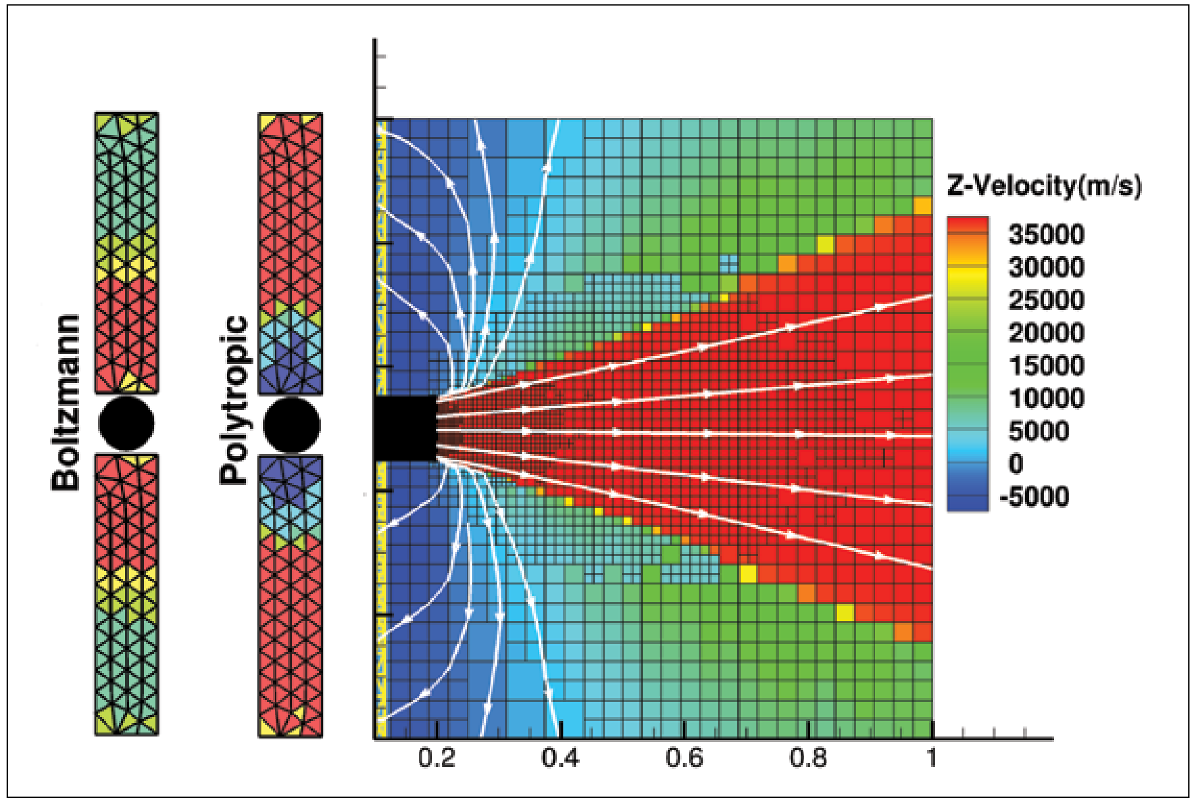

Figure 2: CEX ion streamlines (white) superimposed on an ion thruster, ion velocity field. Vertical strips are notional solar cell arrays. Ion impact fluxes differ for two electron models (Boltzmann vs. polytropic).

RESULTS & IMPACT

Modeling of electron species directly requires very small timesteps to accommodate typical velocities of 200 km/s. Therefore, previous modeling of electrons as a separate species in electric-propulsion plumes assumed a much smaller ion-to-electron mass ratio than the true system and was limited to two-dimensional cases. With this research on Blue Waters we are able to model the actual xenon-to-electron mass ratio for three-dimensional geometries. Fig. 1 shows the evolution of the electron cross-stream velocity component at a location close to the thruster exit (z = 0.005m, normalized by the electron plasma frequency, $\omega_e = 1.78\text{x}10^8$ rad/s. The electrons were initialized with a temperature of 2 eV and an initial number density of $1.0\text{x}10^{13}/\text{m}^3$. The figure shows that at $t\omega_e = 400$, the spacing between the two peak locations decreases, and the normalized probability of electrons with zero cross-stream velocity increases to 0.4. This supports the hypothesis that the ion beam is trapping the electrons, which, in turn, damps the electron oscillations. As the plume evolves to $t\omega_e$ =1000, 1500, and 3000, the peak of the y-EVDF (electron velocity distribution function) lies at $v_e/v_{teo} = 0$, with a smaller peak at $v_e/v_{teo} = -8$ showing that most electrons do not oscillate, and the electrons emitted from the shifted source are immediately attracted toward the plume.

Fig. 2 shows an extension of these simulations, taking the fundamental output to a very practical level. Streamlines moving from right to left along the core of the plume (red region) produce thrust, whereas ions that stream back to the solar cell arrays (yellow vertical strip on the main plot) cause damage. Because the distribution of ions flowing in the backward direction toward the spacecraft depends on the electron model, only a fully kinetic approach can give a truly predictive answer.

WHY BLUE WATERS

Blue Waters has allowed us to test and develop our algorithms on a large number of GPUs for three-dimensional, fully kinetic plasma simulations. Compared to the present state-of-the art plasma simulations, a uniform grid in 3D would require a factor of at least ten more cells than our use of AMR/octree. The use of GPUs vs. CPUs decreased the runtime by at least another factor of five.