

# MODELING PLASMA FLOWS WITH KINETIC APPROACHES USING HYBRID CPU-GPU COMPUTING

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## EXECUTIVE SUMMARY

Our main objective is to characterize the backflow contamination environment due to plasma created by electric-propulsion plumes, 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 build on our earlier work where we have developed an object-oriented C++ Direct Simulation Monte Carlo (DSMC) code that uses adaptive mesh refinement (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 our computational work is to take advantage of our unique, recent advances in GPU (graphics processing unit) multi-thread parallelization applied to tree-based computational strategies. Blue Waters is especially suited to this modeling since we expect to use 128 to 256 GPUs per run for the plasma plume simulations on the XK nodes. Initial results demonstrate that our approach has been successfully extended to couple DSMC and particle-in-cell (PIC) simulations on an AMR/octree grid using GPUs.

## RESEARCH CHALLENGE

With the space environment becoming a home to constellations of small satellites and cube satellites, improved predictability of key surfaces of solar cell arrays and spacecraft charging in the backflow environment of chemical and electric-propulsion (EP) thrusters is crucial. Fig. 1 shows a schematic of the multiple sources and processes that must be considered. Because there are both neutral and charged species in the backflow region of an onboard EP thruster, the modeling of these highly reactive ions with thruster and ambient neutral species involves multiple time and length scales. Indirect environmental exposure of spacecraft material such as the micron-sized coatings of solar array cover glass and aluminized Mylar can cause appreciable sputtering and erosion. This is often hard to quantify and predict over the lifetime of the mission because backflow ion fluxes are about five orders of magnitude less than those due to main ion beam impingement. The well-known charge-exchange (CEX) process between xenon thruster neutrals and beam ions also occurs among plume/beam ions and ambient species such as Xe<sup>+</sup> and O, although these processes are not presently modeled in spacecraft environment effect models. In addition, external hollow cathodes are a source of electrons and also emit xenon ions and neutrals. Inclusion of their plumes is essential as the electrons play an important role in the charge density distribution, which influences the generation of the slow CEX ions, and, in turn, affects the erosion of solar cell panels.

## METHODS & CODES

Our new plasma modeling is an outgrowth of our DSMC code, CHAOS (Cuda-based Hybrid Approach for Octree Simulations) that was developed to study neutral flows through porous media [1]. We have adapted this approach now to include both neutral and ion species in an external electric field. Because the local mean free path for collisions is about three orders of magnitude larger than the local Debye length ( $\sim 10^{-6}$  m), two linearized Morton-ordered forests of octrees (FOTs) have been implemented so that these grids can be adapted to meet these two diverse numerical criteria. To accurately model the electric field, using a Boltzmann distribution at a fixed electron temperature, or to solve Poisson's equation, a leaf node should be only one level larger than its smallest face neighbor, i.e., a "2:1 criteria." When this criterion is adhered to, any numerical discontinuities in the

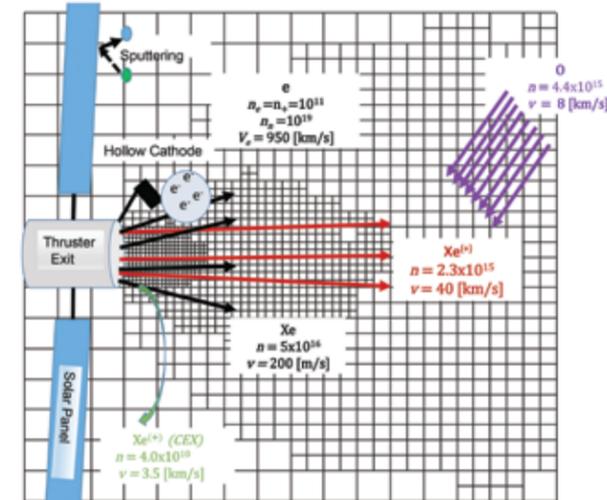


Figure 1: Key species, velocities, and concentrations (m<sup>3</sup>) in the backflow and beam region for a spacecraft in a low- to mid-earth orbit space environment. Approximate scale is 1 m.

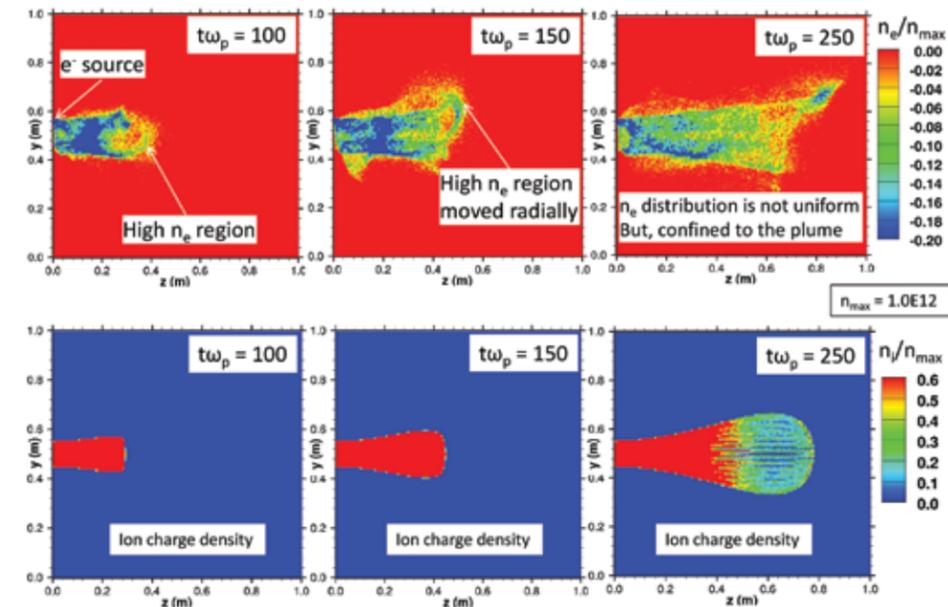


Figure 2: Unsteady behavior of ions and electrons emitted by two spatially separate sources with an electron thermal velocity, plasma frequency,  $\omega_p$ , and electron to ion thermal-to-bulk velocity ratio of  $5.9 \times 10^5$  m/s,  $1.78 \times 10^8$  rad/s, and 1.25, respectively.

E-octree are smoothed out and we are able to maintain 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.

## RESULTS & IMPACT

We have recently run simulations of mesothermal, collisionless plasmas for shifted electron and ion sources [2]. We discovered very interesting unsteady plume dynamics by modeling a *shifted* electron source (in contrast to co-located electron and ion sources) as summarized in Fig. 2. The electron source, with a radius of  $R_e = 0.01$  m, was placed above the ion source, with an electron thermal to ion drift velocity of 1.25. The Xe<sup>+</sup> and electron number densities were  $5 \times 10^{12}$  and  $1.0 \times 10^{13}$ , (#/m<sup>3</sup>), respectively. Temperatures and bulk velocities were assumed to be 0.04 and 2 eV and 472,000 and 0 m/s, for ions and electrons, respectively. For this simulation, both ions and neutrals had the same time step of  $2.8 \times 10^{-10}$ s. Fig. 2 shows a summary of the interesting time-varying behavior, which is very different for the ions versus the electrons. The electron dynamics were found to be complex, and as soon as electrons are released, they accelerate toward the beam and travel *beyond* the beam front. The positively charged beam front then decelerates the electrons that have escaped and reflects them back in the reverse direction, resulting in negative electron velocities. The continual exchange between electron kinetic and potential energy results in a meandering/bouncing movement, as can be seen in the top row of the figure, as time (normalized by plasma frequency) increases. The ion beam, however, more or less propagates away

from its emitting source as time increases. Nevertheless, some diffusion of ions can be seen, particularly in the beam front at later times. In comparison to the electrons, the large ion mass keeps them moving primarily away from the source. In addition, as time progresses, the electron bouncing region is elongated with the multiple bouncing motions increasing the electron temperature. The increase in temperature is contrary to what is expected in an expanding plume and, not surprisingly, the actual electron velocity distribution obtained in the beam front region is very non-Maxwellian.

## WHY BLUE WATERS

Blue Waters has allowed us to test on a large number of GPUs the potential computational savings to enable three-dimensional, fully kinetic plasma simulations. Compared to the present state-of-the-art plasma simulations, a uniform grid in 3D would require about a factor of seven more cells than our use of AMR/octree. The use of a single K20x GPU decreases the runtime by a factor of five compared to a single Interlagos processor. Very conservatively, we estimate that the octrees in combination with GPUs, decrease the total runtime by at least a factor of 10, compared to uniform grid solvers on multi-core CPUs.