Coupling Non-Maxwellian View Factor Model to Octree Based Particle VDF Compression for Accelerated Spacecraft-Plume Simulation

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Much of the cost of simulating Spacecraft-Plume interactions results from modeling the slow evolution to steady-state of the neutral gas densities. Accurate estimation of these densities is important because charge-exchange collisions outside the thruster represent an important source of ions traveling at high angles relative to the thruster beam that pose a particularly large risk to spacecraft surfaces located behind the thruster exit plane. This free-molecular flow requires the use of fully kinetic numerical methods such as time-averaged particle Monte Carlo or ray tracing. Particle methods in particular have poor computational efficiency in resolving the flow-field distant from the thruster source, especially in three dimensions, because particles are inefficient at representing densities that span many orders of magnitude as encountered in expanding flows. Controlling statistical fluctuations and asymptotically slow convergence to steady state make these models extremely computationally expensive despite representing relatively simple physics. The view factor model, developed as an extension of ray tracing, was designed to overcome this challenge by directly computing the steady state density fields given the velocity distribution on an emitting surface. The method has recently been extended to non-Maxwellian velocity distributions on the source, but prior to this work, had not yet been adapted for arbitrary spatially varying non-Maxwellian distributions. This work extends the non-Maxwellian view factor model to this regime by connecting it to a virtual probe model which captures and compresses velocity distributions by sampling the flow of particles that cross a discretized surface. In this work, the coupling of these two models is described. The resulting density fields are then compared to time-averaged Monte Carlo results for two test cases. The first is a basic streaming Maxwellian distribution emitted by a finite area circular orifice. The second is the neutral density in a spacecraft plume resulting from the highly non-Maxwellian velocity distribution captured in the near-field region of an annular Hall thruster simulation. This demonstrates the ability to mitigate the high cost of resolving complex neutral flow-fields, accelerating the computation by more than two orders of magnitude. However, additional work is still required to determine the effective error contributions due to velocity distribution sampling and velocity mesh resolution to quantify the speedup at equivalent error levels. Approaches to further extend this model to both accelerate and generalize it to more realistic spacecraft plume problems are also discussed as potential future work.

I. Introduction

Much of the computational cost of electric propulsion plume-spacecraft interaction modeling results from resolving highly non-equilibrium extremely low density flows distant from thruster plasma sources. Due

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to the low collisionality of the plasma in these regions, kinetic techniques such as particle methods or ray tracing are required to capture the flow-field. Particle methods are particularly challenging because the low densities result in particularly poor statistics for the interactions of the plume with regions of the spacecraft far from the plasma source. These challenges are further exacerbated by the requirement to wait for the slowest particles to fill a large volume surrounding the thruster. Though relatively collisionless, accurate estimation of neutral density in the far-field is still important because ion-neutral charge-exchange (CEX) collisions outside the thruster represent an important source of ions that pose potential hazards to spacecraft surfaces behind the exit plane of the thruster.

For neutral flow, these challenges have led to the development of an alternative method related to ray tracing called the view factor model.[1–3] This method was developed to provide a reasonable approximation to the neutral density field without statistical noise even far from the particle source. The method has recently been adapted for use with arbitrary velocity distribution function (VDF),[4,5] but it is still fundamentally focused on steady state neutral density. Though much of the volume of a spacecraft plume is of such low density that both collisions and the accelerations due to the plasma potential are negligible, the method has not been extended to these regions due to the complexity of connecting the higher density particle models to these view factor models. This work represents a first effort towards directly coupling particle methods to the non-Maxwellian view factor method for rapidly bridging the large volumes of low density collisionless plasma inherent to plume simulations.

The major outstanding challenge for coupling the particle and view factor models for realistic particle sources addressed here is in the definition of this outgoing continuum velocity distribution at the particle/view factor interface surface. The cost of griding and storing arbitrary unknown velocity distributions for each surface element of an interface surface is in general prohibitive. To handle a related challenge for storing arbitrary velocity distributions, a modified numerical retarding potential analyzer (RPA) probe, described in Section II, has been developed within the thermophysics universal research framework (TURF).[6] This modified virtual probe captures all particles crossing rectangular elements of a spherical surface. As storing these particles would soon become prohibitive, the virtual probe then uses a modified version of the octree particle merging[7,8] to compress the particle distribution into a manageable distribution per surface element. In this process, an octree in velocity space is constructed which is used to locally conserve mass, momentum, and energy within adaptive velocity cell bins that are based on the incoming distribution.

The non-Maxwellian view factor model, reviewed in Section III, is adapted in Section IV to sample VDF densities from velocity distribution functions resulting from this virtual VDF probe collection. The resulting density fields are then compared to the direct long time averaging of the computational particles in Section V for a streaming Maxwellian distribution and a Hall thruster based spacecraft plume simulation.

This work is envisioned as a necessary first step towards a fully bi-directional coupling of the particle and view-factor models of steady state spacecraft-plume interaction modeling. In Section VI the outlook for this hybridization along with potential next steps will be reviewed.

II. Numerical VDF Probe

The fundamental assumption of the RPA-probe/RPA-source pair as implemented in numerical plume models[9] is that the particles which are captured and emitted are essentially traveling purely radially on spheres centered at some point, usually the center of the thruster face. Though reasonable when the probe and source surfaces are very far from the thruster, this does not account for the finite offset of the annular thruster face. To demonstrate this distinction for finite size source, a numerical VDF probe was created.

A. Adaptation of Numerical RPA Probe to Capture VDFs

The numerical RPA probe in TURF was adapted to collect copies of all the particles that intersect the probe surface. This normal flux is converted back to a sample of the velocity distribution crossing the surface by dividing the computational weight of the particle by the normal velocity. The number of particles collected in this manner would quickly overwhelm the memory capacity of the system as potentially a copy of every particle modeled in the plume simulation would have to be saved. To overcome this difficulty, an octree based conservative particle merging technique was adapted from prior work.[7]

Instead of merging in spatial volumes, the collected particles were binned in cells defined by the azimuthal and polar angles on the surface of the virtual probe sphere so that particles merged are spatially nearby.

B. Qualitative VDF Probe Results

Figure 1 shows two views of the velocity distribution function (VDF) collected at a 0.6mm radius sphere centered on an HPHall[10] thruster simulation for a spot on the centerline designed to be qualitatively geometrically comparable to the laser induced fluorescense (LIF) tomography results.[11] In one view, the particles are visualized by the accumulation of semi-transparent particles in velocity space to simulate the volume rendering effect of the tomography plots using unstructured particle data. In the other view, the back half (+Vx) of the velocity distribution binned in uniform cells is depicted so that the cross section is visible comparable to the cut-planes visualized in the tomography results.[11]

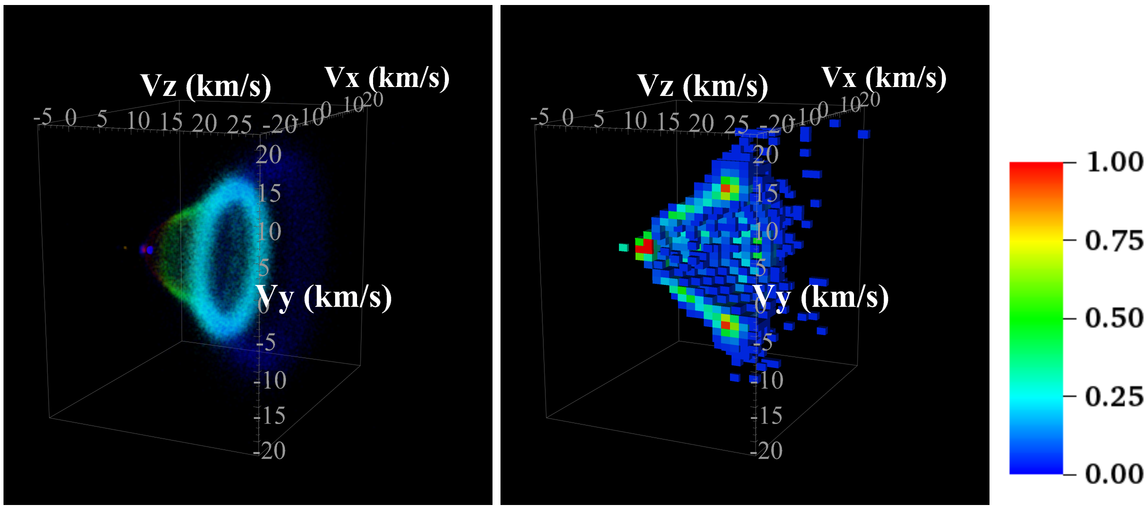

Figure 1. Volume rendering (left) of particle compuatational weights and +Vx sliced, binned velocity distribution (right) of sampled numerical probe particles captured one mean channel radius downstream of thruster face (arbitrary scale).

Consistent with the LIF results,[11] the VDF probe results depict a primarily toroidal particle distribution. Along with the torus, both LIF and VDF probe results include another low speed population near the origin which results from ion-neutral charge exchange collisions. This distribution shape is obviously distinctly non-Maxwellian even at this close proximity to the thruster face where densities and hence collisionalities are considerably higher than further out in the plume. This flow demonstrates the principle difficulty with the approach of linearly extrapolating the cumulative flux distributions from RPA probes. Though the mean velocity is axial on the centerline as is required for axisymmetric flows, the fact that this axial flow is actually composed of the average of interpenetrating flows from around the annulus indicates why extrapolating a linear flow-field does not work well along the centerline axis. This further highlights a fundamental incompatibility of applying a fluid model in this highly kinetic near-plume flow region.

The captured VDF can be sampled to produce a source model consistent with the actual HPHall model as a replacement for the purely radial injection of the RPA source model. However, this does not achieve the goal of supplanting the RPA source models derived from experimental data. Doing this would require inferring VDF data from the experiment as is done with the LIF tomography.

III. Review of non-Maxwellian View Factor Model

An initial effort to apply the radiosity view factor model to the three dimensional neutral gas plume of a Hall effect thruster has been attempted previously.[3] However, it was found that the computed density field did not agree with the results from the particle methods because the ionization collisions in the thruster resulted in a highly non-Maxwellian VDF at the thruster exit face. To address this issue, the radiosity view factor model was extended to support arbitrary velocity distributions[4] and further extended[5] to incorporate diffuse surface reflections.

In the traditional view factor model, the flux parallel to the ray from source to destination point may be evaluated analytically assuming a Maxwellian distribution. For the non-Maxwellian view factor model, this flux was instead numerically integrated along that ray.[4] This was accomplished by binning the full velocity distribution on a Cartesian mesh and then using the trapezoidal rule for uniform steps on the ray along with trilinearlly interpolated probability density values.

The basic formulation for the flux of particles at a differential destination element, d, from a differential source element, s, is given in Equation 1.

$$d\dot{N}_{sd} = n_s dA_s \iiint_d \hat{n} \cdot \vec{v} f(\vec{v}) \hat{n} d\vec{v} \tag{1}$$

This equation is then converted to polar coordinates so that the integration can be split into a geometric factor and an integration through a one-sided speed distribution, $g(C)$. This integration is performed parallel to the ray connecting the source to the destination point as shown in Equation 2.

$$d\dot{N}_{sd} = n_s dA_s \int_0^\infty C^3 g(C) dC \iint_d cos\theta sin\theta d\theta d\phi \tag{2}$$

The second integral is purely a function of the geometry of the source and destination point locations and can be precomputed as F_{sd}. For source and destination elements well separated, this total flux to the destination is approximated by the centroid flux using the area and normal of a triangular source element as shown in Equation 3.

$$\dot{N}_{sp} = n_s A_s \int_0^\infty C^3 g(C) dC \cdot F_{sd} \tag{3}$$

Using continuity, the number density at a points downstream caused by the arbitrary VDF flux through a surface can then be evaluated from the flux using Equation 4.

$$n_{sp} = n_s \int_0^\infty C^2 g(C) dC \cdot F_{ds} \tag{4}$$

This model was evaluated with respect to several general velocity distributions and compared to Monte Carlo particle results in prior work.[4] Though this allowed for the neutral density downstream of an orifice with a uniform velocity distribution to be estimated rapidly, it did not directly address the original challenge of estimating the neutral field downstream of a Hall effect thruster simulation because the velocity distribution on the outflow surface is both unknown and spatially varying. To address that issue the model must be provided with this spatially varying velocity distribution.

IV. Coupling VDF Probe and non-Maxwellian View Factor Models

The numerical VDF probe naturally collects the required velocity distributions across a discretization of the source model's outflow surface. To connect the VDF probe to the generalized view factor model, the challenge is principally that of data management.

As described in Section II, the collected flux of particles through the surface becomes unmanageable as the simulation time becomes large. Instead, an approximation of the VDF is collected in a finite number of merged sample particles. To make this distribution compatible with the necessary integration, the particles are first converted back into densities on a gridded velocity space. Note that a similar approach could be developed by simply collecting samples of the VDF directly onto the meshed velocity space, but this makes storage of the intermediate source distribution between sampling of the source and application of the view factor model considerably more challenging.

Following research previously presented,[12] the conversion of the particle distribution back to a useful velocity space density involves some challenges related to the fact that the pointwise delta-function particles carry with them no intrinsic phase space volume. Following the manner in which the velocity space cells are generated for the merging of near neighbors in velocity space, the phase space density is approximated by constructing an octree from the Morton coded velocity coordinates of the sampled velocity distribution as shown in Figure 2. The deepest level of the tree at which the particle is alone within a velocity cell can then be rapidly identified by identifying the first unique digits relative to the neighbors in the sorted list of velocity Morton codes. The particle's numerical 'weight' (i.e. number of physical particles represented by each computational particle) is then distributed uniformly across the velocity space cell represented by the particle.

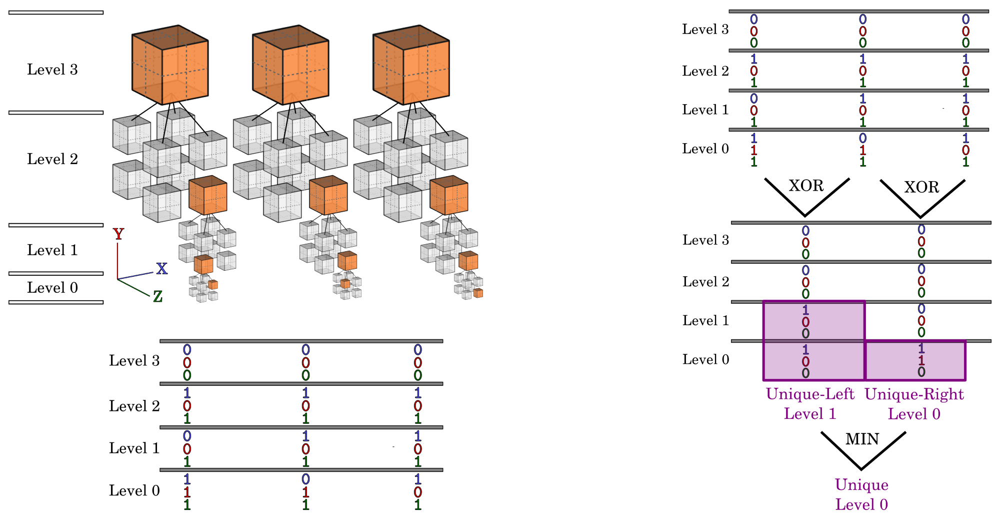

Figure 2. Morton coded ordering for identifying octree depth at which particles are alone in velocity cells. The left half depicts how the integer bits are encoded to idenfity a particle's position in the octree tree. The right half depicts how the encoded integers can be used to identify the level at which bits first differ from most to least significant octant for identifing unique level depth.

As discovered in the prior work, this approach results in a somewhat problematic estimated velocity distribution in that the constant number of particles per cell results in a high variance that does not improve with additional particles. For the sake of demonstrating the combination of view factor and VDF probe models, however, the estimated approximate velocity distribution is sufficient. This is particularly true as the line integrals in velocity space help smooth high variance regions. As the velocity distribution is collected on a uniform mesh in velocity space to be compatible with the existing velocity space interpolation and integration techniques required for the view factor model, this issue is further mitigated as the high variance is restricted to regions of velocity space where the velocity density is small compared to the mean density. Improved velocity space density estimates by direct integration on highly adaptive velocity space density representations are expected to produce dramatically enhanced results with lower memory and computational budgets, but this is left to future work.

V. Numerical Results

A. Streaming Maxwellian Distribution

As in the prior work,[4] a Maxwellian Distribution with a fixed streaming velocity is used as a first test case. Xenon gas emitted from a 1m diameter circular orifice with a temperature of 300K, peak normal velocity of 100m/s, and density of 1e20/m^3 into the center of one side of a 10m cube. The baseline case uses Monte Carlo particle simulation, but the equivalent results using the modified view factor model was demonstrated in the prior work.

To demonstrate the coupling of the numerical VDF probe and view factor model, the emitted particles in the Monte Carlo simulation are captured on a 1m radius hemisphere. The captured particles are localized on 20 polar by 32 azimuthal quadrilateral bins with the polar axis aligned with the normal of the emitting surface. Particles are collected from 0.1-4 seconds of physical time and merged to maintain an approximately 2.3 million particle velocity distribution.

The particles are then converted to a velocity distribution by summing the contributions on a Cartesian velocity mesh consisting of 10 m/s cells in a bounding box of $\pm$700 m/s for each of the 640 probe VDF cell bins. The non-Maxwellian view factor model is then applied using the corresponding VDF for a triangulation of the hemisphere mesh where each of the quadrilateral bins is bisected except for the quadrilaterals adjacent to the pole where the resulting degenerate triangles are omitted.

Figure 3 compares the Monte Carlo particle density to the density computed from coupling the non-Maxwellian view factor model to the octree merge particle VDF probe. Here, the Monte Carlo density is the result of time-averaging over 3900 timesteps for the corresponding 0.1-4 seconds of physical time.

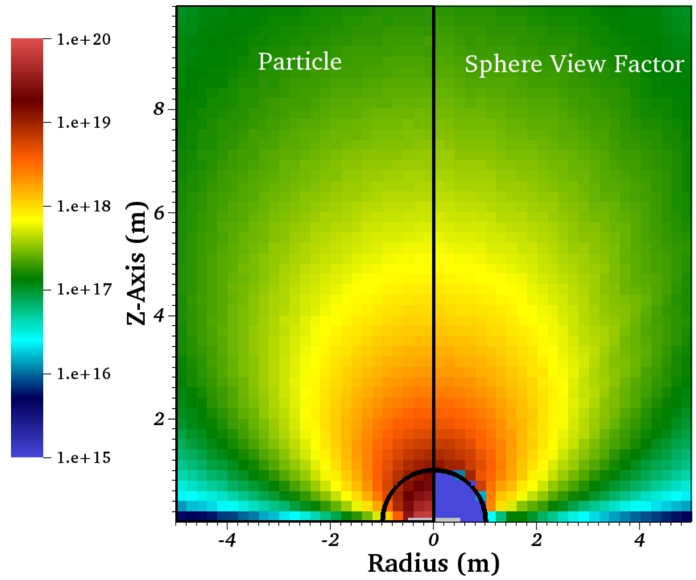

Figure 3. Cross section comparison of Monte Carlo particle and coupled VDF probe + non-Maxwellian view factor model number density (#/m^3) for streaming Maxwellian test case.

The results demonstrate the effectiveness of the combined model to produce results nearly equivalent to the long time average of the particle simulation. Some ray artifacts are noticeable as diagonal streaking. Additional investigation is needed to determine the source of these artifacts. Potential candidates include noise in the VDF resulting from the finite number of merged particles, finite triangulation of the surface as noted in the prior investigations,[3] or the result of the finite velocity cell resolution. These contributions will be explored further in future work.

B. Spacecraft Plume Neutral Gas Distribution

Returning to the original motivating problem, in this section the non-equilibrium neutral plume near the exit of a Hall thruster simulation is revisited. This test case uses the Express-AM6 satellite geometry with SPT-100 like Hall thruster models as in the prior work.[3] The satellite model is placed inside a computational domain of size $12 \times 6 \times 7$ meters meshed with 0.2 meter cubic Cartesian cells. Particles are injected into the simulation from an HPHall simulation where the ions continue to be accelerated by an electric potential computed by inverting the Boltzmann relation assuming quasi-neutrality. Momentum and charge-exchange collisions between ions and neutral atoms are also computed within the computational domain.

Adapting this baseline simulation, the neutral particles are captured on a 0.5 meter radius hemisphere centered on the thruster face and aligned to the thrust axis. The particles are again captured on a mesh of 20 polar and 32 azimuthal bins. The particles are then collected and merged over a range of 0.15-20 ms of physical time using the octree merge algorithm to a distribution composed of approximately 2.2 million particles.

Unlike the streaming Maxwellian case, however, the captured velocity distributions contains two distinctly disparate velocity sub-populations due to the CEX collisions in the thruster and plume simulations. The fast neutral population is the result of ions that have already been accelerated due to the electrostatic potential undergoing CEX collisions to produce a fast neutral and slow ion. To handle this challenge, the collected particle distribution is split between fast and slow populations at a speed of 1 km/s in the view factor simulations.

This splitting is necessary because the slow population requires a Cartesian velocity mesh of 20 m/s cubes to provide accurate results, but the fast neutrals require a bounding box on the order of ± 30 km/s. Without adaptive meshing in velocity space, this would correspond to a necessary mesh resolution of $1500 \times 1500 \times 1500$ in each of the 640 cells. Using double precision floating point numbers, this velocity mesh would correspond to a 17.3 terabyte memory footprint.

With the particles split between fast and slow, two separate velocity meshes can be used for the different populations. For the slow population, a ± 1 km/s bounding box is used with 20 m/s velocity cells. The fast population is meshed on a ± 30 km/s bounding box with 1 km/s velocity cells. This results in two separate view factor runs resulting in slow and fast density fields. These can be combined to produce a sum total neutral density. In the prior work,[3] the baseline particle simulation was also split between slow and fast particles at a 1 km/s speed to demonstrate the beam of fast neutrals which allows for direct comparison to the long time averages of both the total and fast neutral densities from that work. Figure 4 shows the neutral density computed using the coupled VDF probe + non-Maxwellian view factor for the slow, the fast, and the combined distribution relative to the time-averaged particle Monte Carlo results.

In the results of Figure 4, it is clear to see that the view factor method can produce reasonably commensurate results as the long time average particle simulation. The low density regions show noticeably lower noise and streaking in the view factor model than in the particle model in this case. This is likely due to the extremely poor sampling of rare high angle particles as compared to the large spatial volume. However, the smoothness seen in the view factor model may also be the result of diffusion in velocity space resulting from the deposition of merged particle density onto the velocity space mesh. As in the streaming Maxwellian case, additional convergence and refinement studies need to be performed to quantitatively compare the errors between the two methods.

Due to the separation of timescales of this problem resulting from the charge exchange collisions, the computational acceleration resulting from using the view factor model is particularly pronounced. The particle case required approximately 112 hours to achieve the depicted level of smoothness over the volume spanning the 5 orders of magnitude density. By comparison, the slow and fast view factor models ran in 20 and 19 minutes respectively with additional speedups already identified for future work. While this still required a relatively long scale particle run to define the source on the source surfaces, it is important to note that the model can then be used to evaluate alternative spacecraft geometries directly at least to the extent that the flux through the source surface is not dramatically modified.

VI. Conclusion and Future Work

This work describes an extension of the non-Maxwellian view factor model to include an array of velocity distributions collected from a particle simulation on the surface of a virtual probe surface. This showed that the problem of complex neutral velocity distribution at the exit plane of a Hall thruster can be successfully resolved such that the far-field neutral distribution can be reproduced without the challenges of poor sampling and expensive long time averaging inherent to the particle simulations. This is particularly relevant for plume simulations involving very large computational domains where the equilibration to steady-state of the slowest neutrals dramatically impedes time to convergence.

It is noteworthy that splitting the velocity between slow and fast distributions was needed to deal with the multiscale velocity space structure of the neutral density population as encoded in the compressed particle VDF for the thruster simulation. At that point of the simulation, the octrees used in the particle merging had already gracefully handled these disparate velocity populations without this ad hoc separation. This highlights an important future direction for adapting the velocity space line integrals. If the non-Maxwellian view factor model was adapted to use integrals on octree mesh constructed on the fly rather than a Cartesian mesh, not only would the memory footprint be dramatically decreased, but the performance would likely be enhanced due to the corresponding dramatic reduction of the required memory bandwidth. This effort is left to future work.

It is also important to note that the current version of the view factor model does not include interactions of the particles within the volume. Though this has been considered previously[2] for the standard view factor model, this means that any CEX collisions happening in the volume outside the source surface are currently omitted. This challenge may be mitigated by extending the ray traced region to begin well into the plume where the densities are low enough that very few collisions occur or by adapting the non-Maxwellian view factor model to allow for collisions.

The splitting of the velocity distributions by speed also hints at an approach to handling energy dependent collision models within the view factor model. The velocity distribution could be further binned into kinetic energy levels such that the densities at points in the field could be partitioned by energy. This would also be useful in evaluating energy dependent sputtering yields and fluxes from the surfaces within the view factor

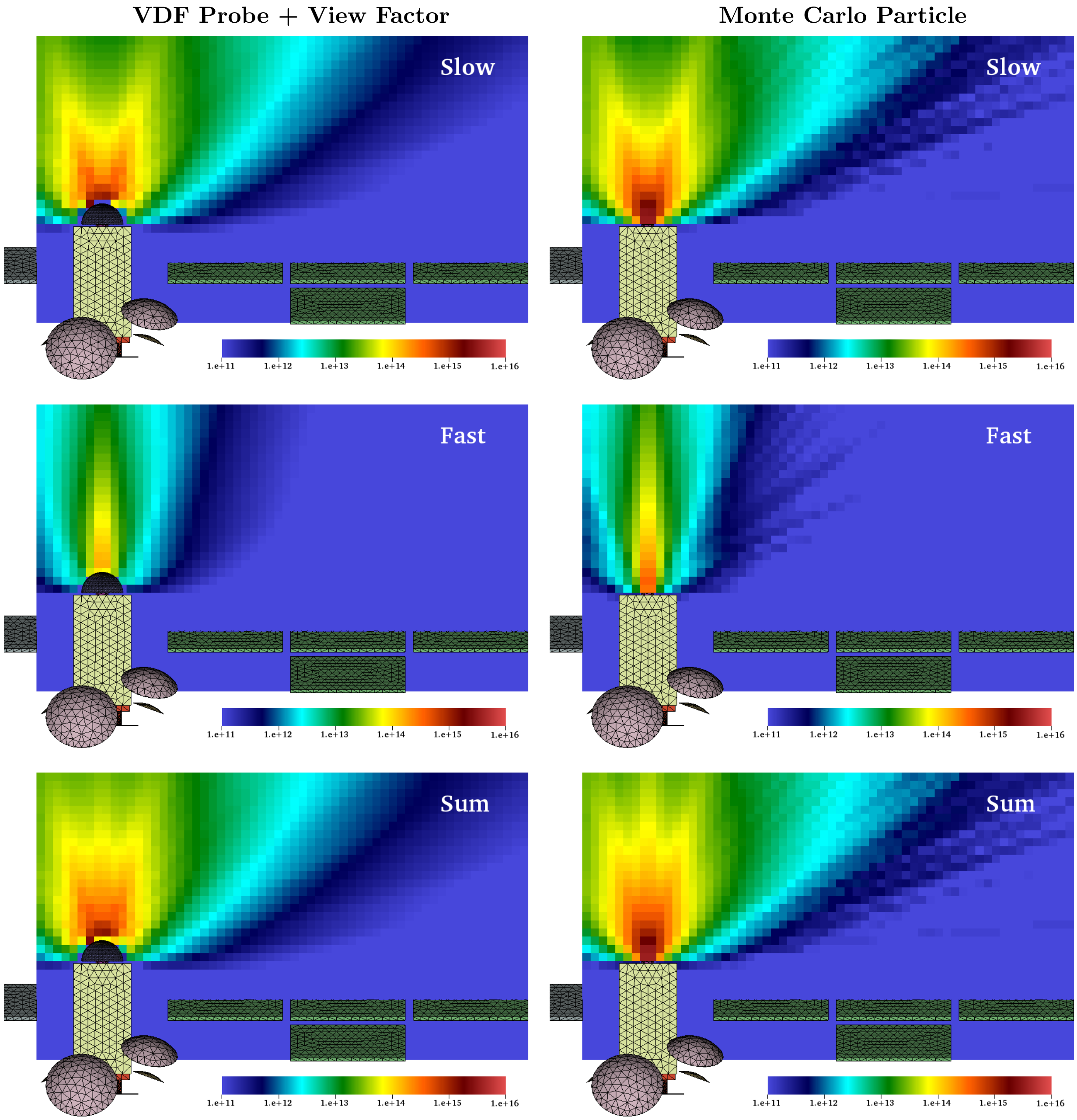

Figure 4. Neutral densities (#/m^3) for the Express-AM6 Satellite resulting from the combined VDF probe + non-Maxwellian view factor model (left) compared to baseline particle Monte Carlo results (right). The subfigures depict the slow-neutral (top), fast-neutral (middle), and total-neutral (bottom) densities.

model.

A further extension would be to couple the view factor model back to a receiving surface to perform Monte Carlo particle simulations in the near surface region of other surfaces of the spacecraft. If a bidirectional coupling could be attained, this would allow for an iteration to steady state for plume simulations that would effectively step over the high computational cost resulting from resolving the large free molecular flow regions of the plume.

Acknowledgments

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