Three Dimensional Coupled Particle-in-Cell and DSMC Simulations of Backflow Contamination from Electric Propulsion Device Plumes

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Background and Previous Work

- EP devices, being reliable, low-cost and efficient, are the best candidate for present and future space propulsion applications.
- Considerable research on increasing the performance as well as its integration and interaction with the spacecraft itself.
  - The modeling of *Hyakutake et al.*(*) did not include full coupling of neutral and ion species
  - The work of *VanGilder**(**) lacked three dimensionality and expressed concerns about the accuracy of various cross-section data.

Motivation of This Work

• Since EP thrusters are usually used in array forms, the interaction between each single thruster can effect the performance and the entire spacecraft health.

• The interaction with the spacecraft is crucial since mission specific sensitive systems and instruments can be effected causing unexpected mission failures and resulting in a decrease in the lifetime of the spacecraft.

• A state of the art approach is essential which will address these issues. Three dimensionality is important for complex geometries where arrays of thrusters are used and full coupling between neutral and ion species will help quantify the degree of spacecraft contamination.
PIC Results Revisited

- The figure shows a PIC simulation of a colloid ion thruster plume downstream of the extractor ring.
- No significant backflow can be observed because collisions between the particles were not modeled.
- A more realistic simulation must include interactions between particles through collisions.
DSMC approach

• In order to improve the previous results, the interaction between the particles will be modeled more accurately. This is where DSMC plays an important role where it will account for the interaction of particles that cannot be captured by the Coulombic interaction.

• PIC and DSMC approaches must work harmoniously in order to capture the complexity of the problem. Coupling of DSMC and PIC in the literature is mainly used in simulations of plasma flows and electric propulsion devices.

• The interaction of PIC and DSMC routines is at the particle movement routine. PIC effectively calculates the acceleration of particles due to electrostatic forces and DSMC calculates the velocity change due to collisions.
Neutral Flow Simulation

• A preliminary study of a flow consisting of only neutral species from a nozzle plume is simulated.

• This is important and necessary because majority of the EP device plumes are neutral (1%-10% ionization) and this study can give an estimate on the flow characteristics.

• The future work will include the major interaction between charged and neutral species which are due to the charge exchange (CEX) reactions (1). CEX is the major mechanism for depositing energy to the neutrals.

\[ Xe_{fast}^+ + Xe_{slow} = Xe_{slow}^+ + Xe_{fast} \]  

(1)
Neutral Flow Results (1/3)

- A 2-D asymmetric Xe flow with uniform velocity of 270 m/s at the thruster exit is simulated. Thruster is represented as the black box.

- The figure shows the expansion of the flow from the thruster. Streamlines show the divergence of the plume. One can also see the acceleration of the flow along the centerline.
It can be seen from the above figure that the lateral velocity is very high along the lateral direction near the nozzle exit. This will trigger mechanisms (i.e. CEX reactions) that can cause collisions of ions and neutrals with the spacecraft surface.
• The plot on the right shows the number density variation along the centerline of the domain. It can be observed that almost 2 orders of magnitude decrease in number density is present.

• This plot illustrates the presence of multi scale physics in the problem and motivates the choice of the grid system.
Multistep Algorithm

- Ions have $O(2-3)$ higher velocity than the neutrals, so the timestep and grid cell size criteria for DSMC calculation differs greatly from the neutral species. Particle interaction and movement routines becomes inefficient if a single time step is employed.

- It is possible to maintain the close coupling between the cross-species using the multi-step algorithm discussed in Serikov et al(*). The fundamental idea is to extrapolate the impact of collisions between fast and slow species at the short time interval of the fast species.

Results for Multistep Algorithm

• A 3-D box containing 2 species initialized with different temperatures. Different timesteps were used for each species.

• These species represent the ions (Xe+) and neutrals (Xe) which will be used in the larger parallel simulation. Xe and Ar are typical species used as fuels in EP applications.

• In order to validate and verify the DSMC module, preliminary studies have been conducted. Once the DSMC module is fully validated, full simulations coupled with PIC will be run.
Multistep Algorithm

• The algorithm involved (*) can be summarized as follows for cross-species, where \( g, \sigma \) and \( W \) represent relative velocity, collision cross-section and weighting factor respectively;

  \[ \text{Step 1: Sample a pair of particles } A_i^s \text{ and } A_g^r \ (s = 1, \ldots, N_i; r = 1, \ldots, N_g) \text{ at random.} \]

  \[ \text{Step 2: Calculate } g_{ig}^{sr} = |c_i^s - c_g^r|. \text{ Call a standard random number } U, \text{ i.e., } 0 < U < 1. \text{ If } U > \left( g_{ig}^{sr} \sigma_T (g_{ig}^{sr}) / g_{\text{max}} \sigma_T^{\text{max}} \right), \text{ then no collision occurs, hence go to Step 1. If not, go to Step 3.} \]

  \[ \text{Step 3: Replace } c_i^s \text{ by } c_i'^s \text{ with probability } W_g / \max\{W_i, W_g\} \times \max\{\tau_i, \tau_g\} / \tau_g \ (= 1), \text{ and } c_g^r \text{ by } c_g'^r \text{ with probability } W_i / \max\{W_i, W_g\} \times \max\{\tau_i, \tau_g\} / \tau_i \ (W_i / W_g \times \tau_g / \tau_i). \]

Temperature Relaxation

- Species #1(Xe) and #2(Xe+) are initialized at 300 K and 3000 K, respectively.

**Case 1 (single timestep)**

Timestep($\Delta t=1.0E-9$ s) for both species are set to the faster species(Xe+).

* Time axis is normalized by 12 mean collision times which is based on the calculation of the collision frequency.
Case 2 (multi timestep, Xe ($\Delta t=1.0E-6$ s), Xe+ ($\Delta t=1.0E-9$ s))

Different timesteps for 2 species which have a $O(3)$ difference which are typical for ion and neutral pairs.
Temperature Relaxation Conclusions

• Cases 1 and 2 produce identical results as expected.

• The advantage of using multi timestep algorithm is to improve the computational efficiency. For the preliminary case, the speed up was found to be 42.8%.

• The efficiency is likely to be higher as the complexity of the simulations increases (i.e. inclusion of more species with greater variability in their velocities).

• These studies were run in serial and will be supplied to the parallel PIC code under development.
Numerical Grid Considerations

• Different length and time scales involved in the problem necessitates a novel grid system for the numerical simulation.

• Adaptive Mesh Refinement (AMR,*) provides this flexibility and numerical efficiency. AMR is becoming widely used in high fidelity simulation. An efficient data storing method called “octree” representation will also be used.

Algorithm of Octree Meshing

- **Active**
- **Deactive**

Parent-Children Connectivity

Active Cells List
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