Particle-in-Cell Simulations for Ion Propulsion Applications

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This paper presents an overview on some recent advances in particle simulation modeling of ion propulsion. We first discuss two new particle simulation algorithms designed to handle complex boundary conditions accurately while maintaining the computational speed of the standard PIC code.

The first is the parallel, three-dimensional immersed-finite-element particle-in-cell (IFE-PIC) algorithm. Domain decomposition is used in both field solve and particle push to divide the computation among processors. It is shown that the parallel IFE-PIC achieves a high parallel efficiency of >90%. The second is the hybrid IFE-PIC (HG-IFE-PIC) algorithm, extended from IFE-PIC to further reduce the computation time and memory requirement for simulations involving non-uniform plasmas. In HG-IFE-PIC, the meshes used by the IFE field solve and PIC are decoupled and the IFE mesh is stretched according to local potential gradient and plasma density. It is shown that the HG-IFE-PIC can achieve approximately the same accuracy as IFE-PIC. Both the parallel IFE-PIC and HG-IFE-PIC are applied for ion thruster plume modeling and ion optics plasma flow modeling. We next present two simulation studies. The first concerns multiple ion thruster plume interactions for a realistic spacecraft and plume contamination on solar array. The second concerns the simulation of whole sub-scale ion optics gridlet and accelerator grid impingement current. Finally, we present an ongoing research on the development of simulation based design tool. The unsolved issues and future directions in ion propulsion modeling are also discussed.

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Outline

- I. Introduction and Background
- II. Simulation Approach
- III. Ion Thruster Plume Modeling
- IV. Ion Optics Modeling
- V. Simulation Based Design Tool
- VI. Summary and Conclusions

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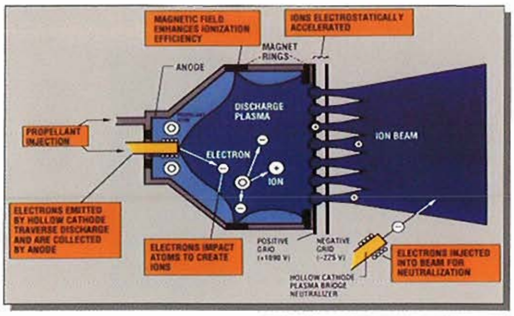
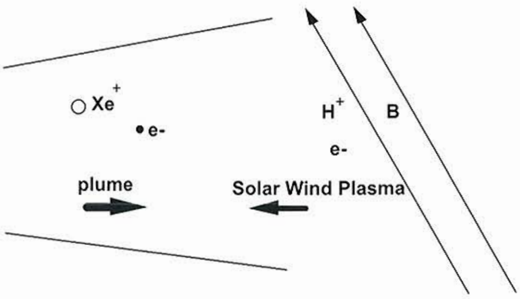
I. Introduction and Background





- Flow Species: (IPS ionizes 80% to 90% of xenon in discharge chamber)
  - beam ions: O(10^3)eV; un-ionized neutrals: O(0.01)eV; electrons: O(1)eV
  - charge-exchange xenon ions: O(0.01)eV

$$Xe^{+}_{beam} + Xe^{0}_{thermal} \longrightarrow Xe^{0}_{beam} + Xe^{+}_{CEX}$$

  - sputtered grid material
- Flow Characteristics:
  - inside optics/near spacecraft: **electrostatic, "space-charge" flow**
  - far from spacecraft: **electromagnetic, quasi-neutral flow**
  - ion flow **"collisionless"**

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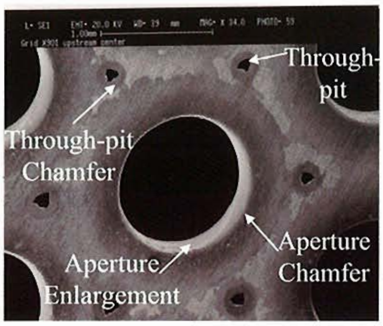
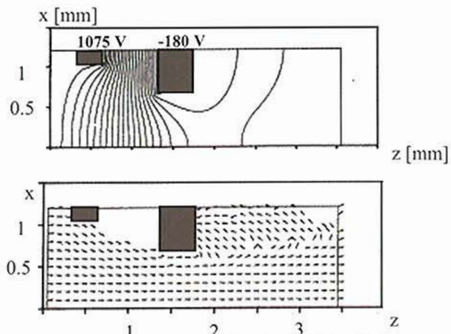
Plasma Interaction Problem I:
Ion Optics Plasma Flow & Grid Erosion





- The behavior of the accel grid current defines the operation envelop of an ion optics system
- Impingement of beam ions and CEX ions cause grid erosion, the primary factor that limits the service life of an thruster
  - Structural failure due to grid erosion from CEX ions
  - Electron backstreaming due to enlargement of grid holes from erosion
- Current modeling status:
  - Many ion optics models (designed for "local" aperture simulations) exist
  - An ion optics model designed for whole grid simulation was also developed recently (Kafafy and Wang, 2006)

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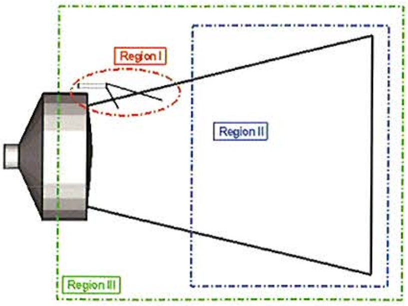
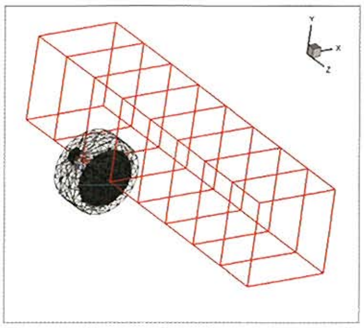
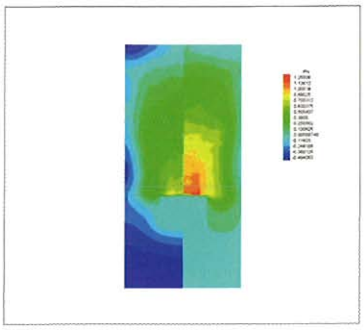
Plasma Interaction Problem II: **Near-Thruster Beam Interactions**







- While ion beam neutralization is readily achieved in experiments, the detailed physics in the near thruster region is still not well understood.
- Current modeling status:
  - Few simulation model exists for near-thruster interaction
    - Full particle PIC simulations using realistic ion/electron mass ratio were carried out for scaled-down thruster models (Wang et al., 2005)
  - Near-thruster simulation remains a significant challenge

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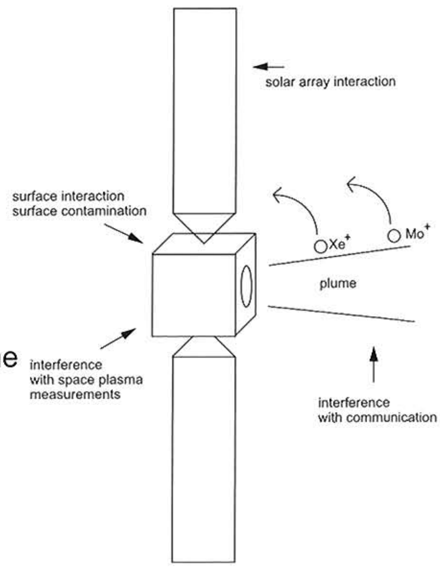
Plasma Interaction Problem III: **Plume-Spacecraft Interactions**



- Low energy ions (Xe^+ and Mo^+) produced in the plume can backflow to interact with spacecraft
  - Xe^+ plasma dominates local plasma environment, affects spacecraft charging and plasma measurements
  - Mo^+ contaminates spacecraft surface
- Current modeling status:
  - Many ion thruster plume models (most designed for simplified spacecraft) exist
  - New simulation algorithms and parallel computing techniques are being applied to perform more realistic simulation (Wang et al., 2006)

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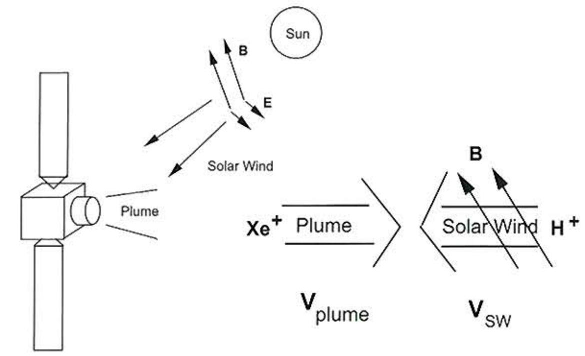
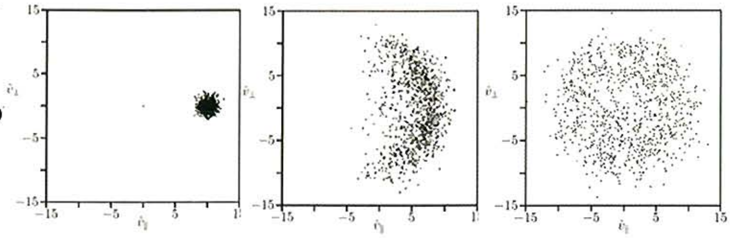
Plasma Interaction Problem IV:
Plume-Solar Wind Coupling

- Thruster produced ions may couple with the solar wind plasma via several mechanisms:
  - Particle/particle coulomb collisions (negligible)
  - Cyclotron pickup
  - Wave particle interactions
- Current modeling status:
  - Hybrid simulations were carried out on coupling by wave-particle interactions (Wang et al.,1999)
  - This problem is primarily o theoretical interest





Solar wind proton pickup through electromagnetic heavy ion-proton instabilities

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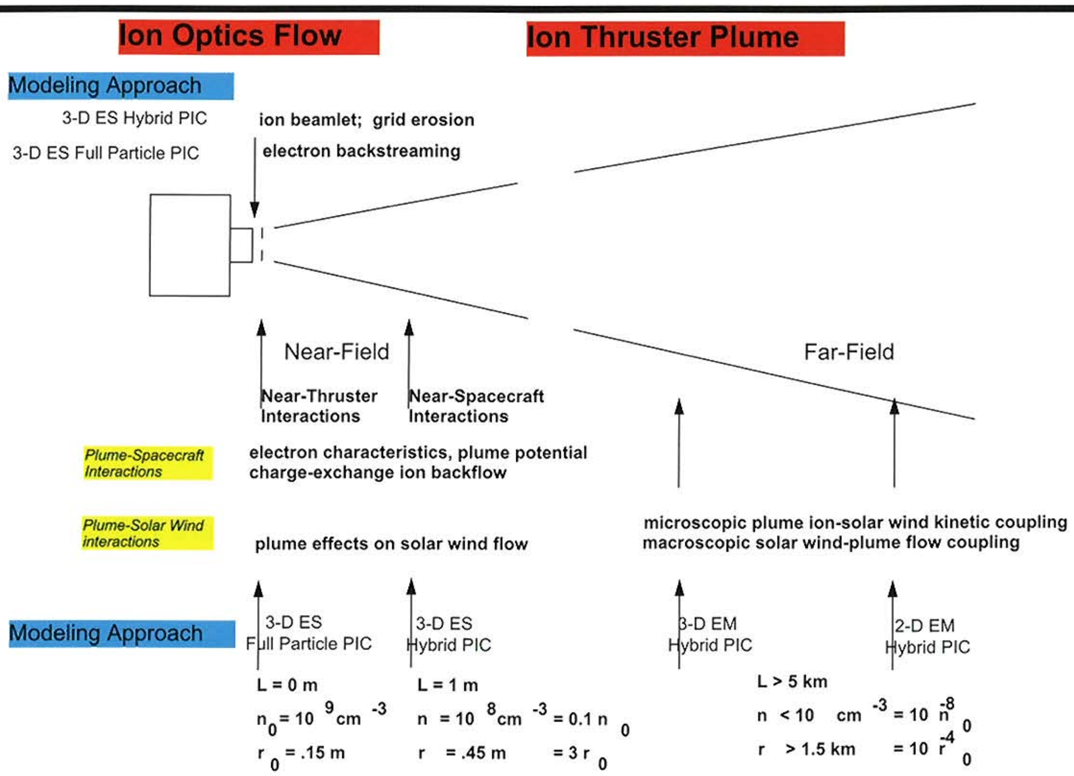
Overview of EP Interaction Modeling at Virginia Tech



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II. Particle Simulation Approach

- There have been significant progress in ion propulsion modeling and simulation in recent years
  - Particle-in-cell has become standard modeling algorithm
  - Numerous PIC based models have been developed for ion thruster plume and ion optics
- Status: Computational time/cost & computer memory restrict the application of particle simulation to small scale problems and simplified spacecraft model
  - Plume simulations typically use simplified spacecraft configuration
  - optics simulations concern single aperture
  - most use simplified model for electrons
  - almost all use small domain…etc
- Challenge: Accuracy and computational speed present conflicting requirements for large-scale PIC simulations involving complex object boundary
  - Accuracy requires the use of tetrahedral cell based or unstructured mesh to body fit the boundary to solve the electric field
    - Very expensive for particle push
  - Computing speed requires the use of structured, preferably Cartesian, mesh to push particles
    - May lose accuracy in field solve in the vicinity of boundary

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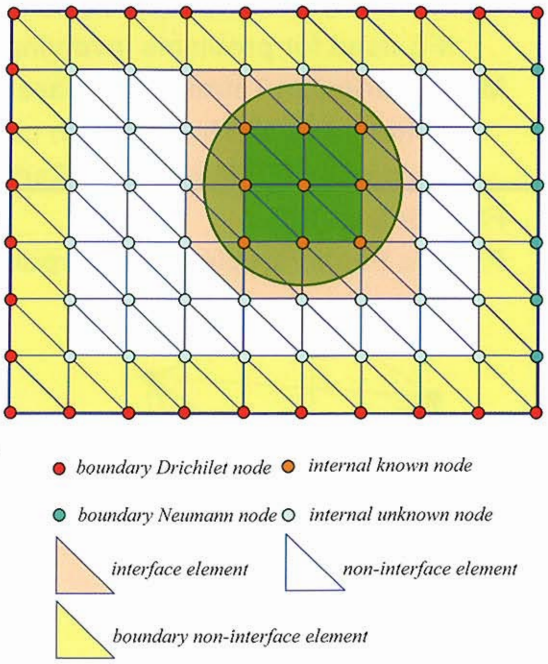
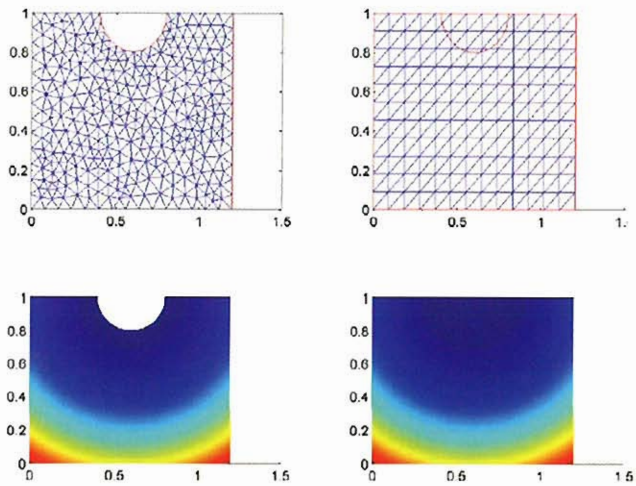
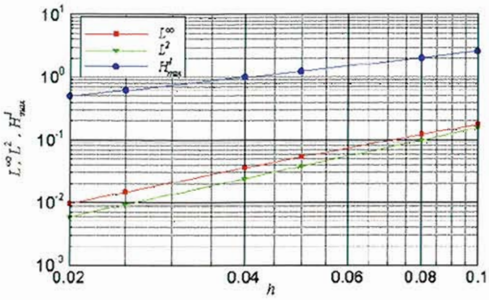
- Existing parallel PIC algorithms:
  - All use domain decomposition
  - Most use either fast Fourier transform (FFT) or a local, non-iterative method (such as finite-difference time-domain or discrete-volume time-domain)
  - Efficient parallel PIC codes have been developed using FFT or local, non-iterative field solve methods for problems involving simple boundary conditions
  - Few parallel PIC codes exists using global, iterative field solve methods for problems involving complex boundary conditions
- Our Recent Research:
  - A new class of ES PIC algorithm is developed using the immersed finite element formulation
  - IFE is designed to accurately resolve boundary effects while maintaining computational speed associated with standard PIC code

Immersed Finite Element Formulation for PIC Code

- Major features of IFE (Kafafy et al, 2005):
  - **Mesh independent of object boundary: Allows the use of Cartesian mesh for complex geometric interface and/or time-varying interface with the approximation capability as the body-fit mesh**
    - **Accuracy: 2nd order convergence**
  - **Electric field solved for both inside and outside the object if needed: material property effects explicitly included**
  - **Trial functions satisfy the jump conditions imposed by material properties at interface : Physics maintained at object interface**
  - **Based on finite element formulation: Nice mathematical properties (e.g. algebraic systems are symmetric & positive definite, etc.)**
  - **Cartesian mesh for PIC: maintains standard particle search and particle push in PIC; avoids numerical diffusion associated with particle shape change**







- IFE allows the use of standard Cartesian mesh based PIC algorithm for problems involving complex boundary conditions
  - **Possibility to maintain standard PIC speed without losing accuracy**
  - **Easy parallel implementation**

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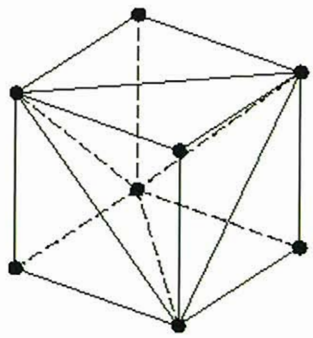
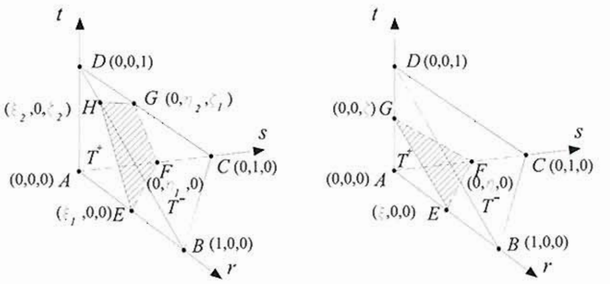
Immersed-Finite-Element PIC (IFE-PIC)

- **IFE-PIC: A hybrid finite-difference finite element PIC**
  - **IFE used for problems involving complex geometric boundary**
- **Mesh: Cartesian Tetrahedron-Based Structured Mesh**
  - **Primary PIC Mesh: Cartesian cells**
  - **Secondary IFE Mesh: each Cartesian cell is divided into 5 tetrahedrons.**
- **Field Solver: IFE**
- **Particle Push/Particle-Grid Interpolation: standard PIC**



IFE-PIC cell



Intersection of boundary with IFE cell

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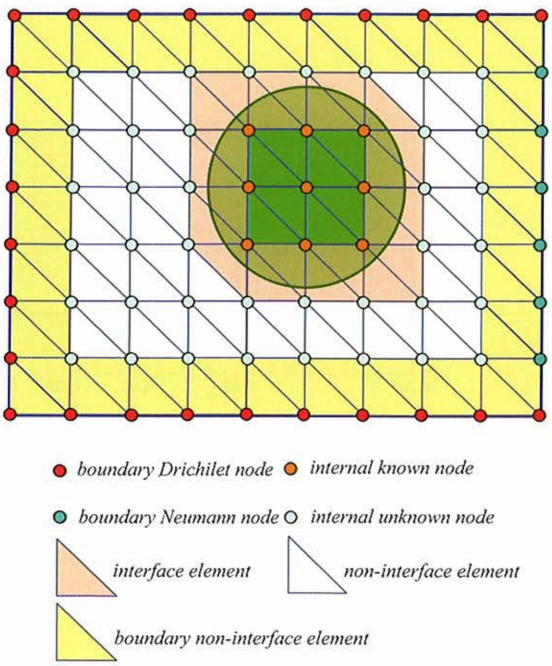
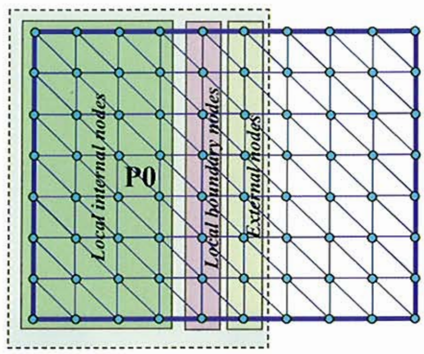
Parallel IFE-PIC





- IFE Sub-domain Mesh
  - Sub-domain IFE mesh includes local and external nodes
  - Pointers are used to local internal, local boundary, and external nodes
  - Boundary conditions are copied from global Mesh definition

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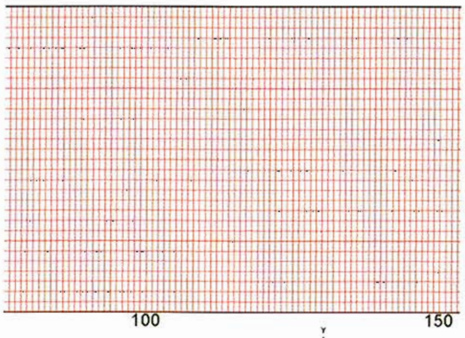
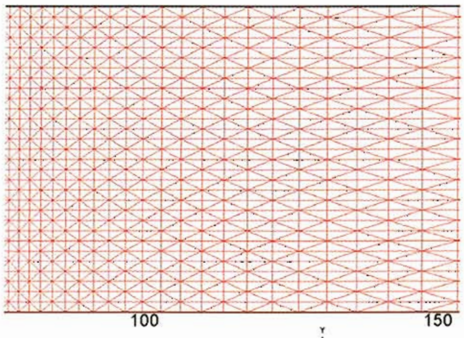
Hybrid-Grid IFE-PIC (HG-IFE-PIC)

- HG-IFE-PIC: Designed for problems involving complex geometric boundary and non-uniform plasma in a large domain
  - In the hybrid-grid version of the IFE-PIC code, the PIC and IFE meshes are further made independent of each other.
    - PIC mesh: Uniform Cartesian mesh
    - IFE mesh: Stretched Cartesian-based tetrahedral mesh
  - Stretched IFE mesh is used for problems involving non-uniform plasmas in large simulation domain.
  - Mesh stretching follows potential gradients and local plasma conditions.



PIC mesh
(uniform Cartesian)



IFE mesh
(Cartesian-based, tetrahedral stretched mesh)

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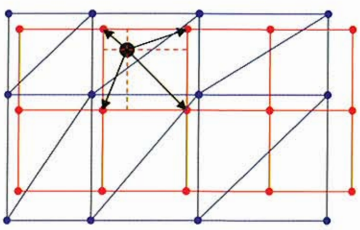
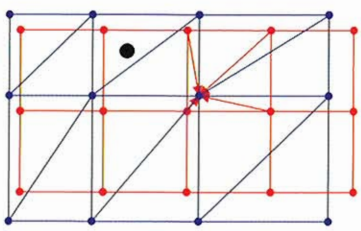
HG-IFE-PIC Details:

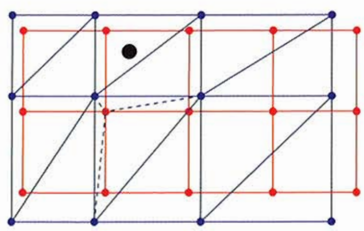
- IFE-PIC-Particle Interpolation Procedure
  - Physical quantities need to be appropriately traded among particle locations, PIC mesh nodes and IFE mesh nodes.
  - Particle charges are deposited onto PIC mesh nodes using linear weighting.
  - Charge densities are linearly interpolated from PIC mesh nodes into IFE mesh nodes.
  - After field solution, field quantities are interpolated from IFE mesh nodes into PIC mesh nodes using the IFE *linear basis functions.*



a) Particle-PIC Deposition



b) PIC-IFE Interpolation



c) IFE-PIC Interpolation

IFE-PIC-Particle Interpolation Process
Particle [black], PIC mesh [red], IFE mesh [blue]

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III. Ion Thruster Plume Modeling

- Previous Study (Wang et al., JSR, 2001):
  - A 3-D simulation model developed for the Deep Space 1
  - Results in excellent agreement with DS1 in-flight measurements
- This study (Wang et al., IEEE Trans. Plasma Science, 2006):
  - Simulation of more complex spacecraft configuration with multiple ion thrusters
  - Parallel IFE-PIC simulation using parallel computer
  - HG-IFE-PIC simulation using PC
  - Predict plume contamination for DAWN spacecraft

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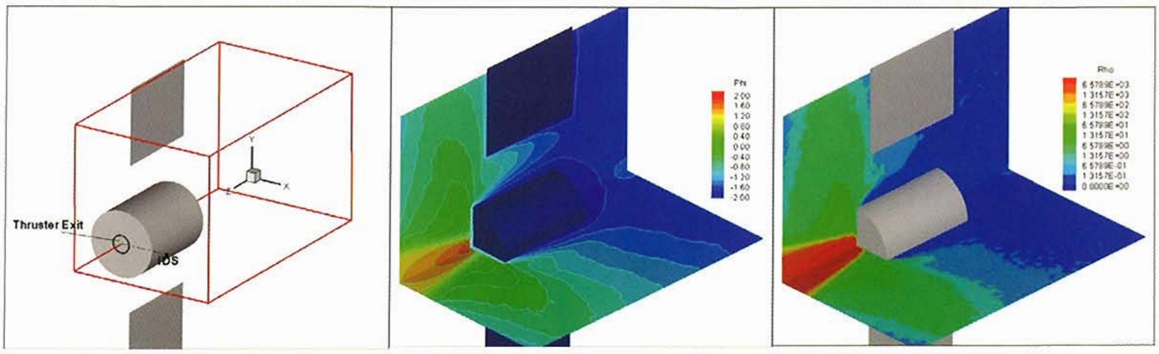
Simulation Model

- Model based on the same physics formulation of our previously developed Deep Space 1 ion thruster plume model (Wang et al., JSR, 38(3), 2001)
- Model validation using Deep Space 1 in-flight data:



NSTAR thruster operating condition ML83:

IDS measurement: IDS potential – center potential: -15V; CEX ion density: 1.2E6cm^{-3}
Simulation: IDS potential – center potential: -13V; CEX ion density: 1.1E6cm^{-3}

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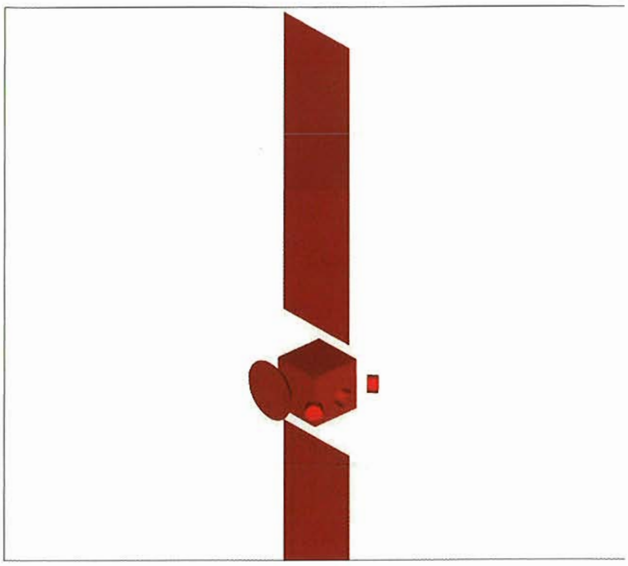
High Resolution IFE-PIC Simulations of Multiple Ion Thruster Plume Interactions

- Objective:
  - multiple ion thruster plume interactions with a realistic spacecraft
  - CEX plasma distribution on solar array surface and payload
- Domain:
  - encloses the entire solar array panel: 9.3mx9.3mx15.4m
- Resolution:
  - resolves the CEX plasma Debye length in the entire domain
  - CEX plasma resolution: 5cm
  - Electric field resolution: 1cm



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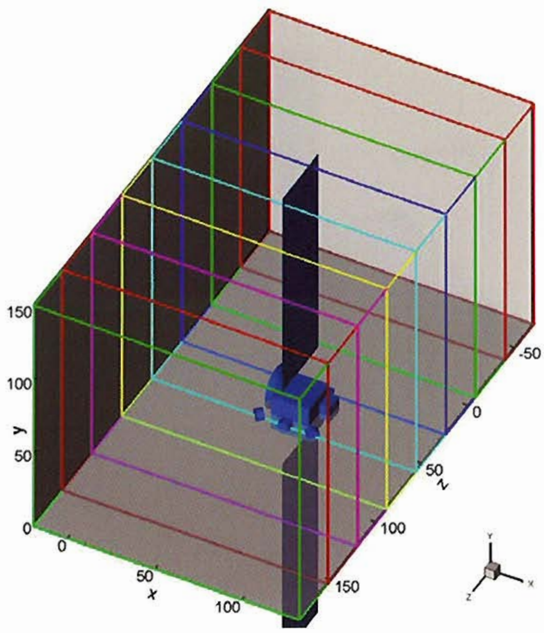
- Simulation Parameters:
  - Particles at steady state: 125 million
  - PIC cells: 155x155x256 (>6.15 million)
  - Tetrahedral elements: 30.8 million
- Typical Computation Time:
  - Full transient to steady state simulation: 10 hrs on 64 processors of Dell cluster for 1000 PIC steps
  - Steady state only simulation: 2 hrs on 64 processors



Domain Decomposition

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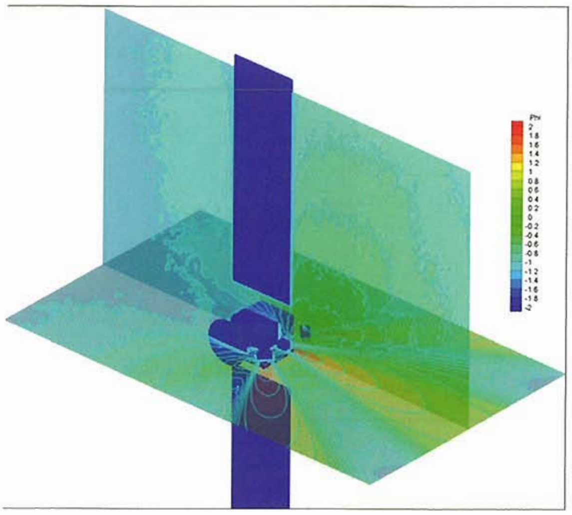

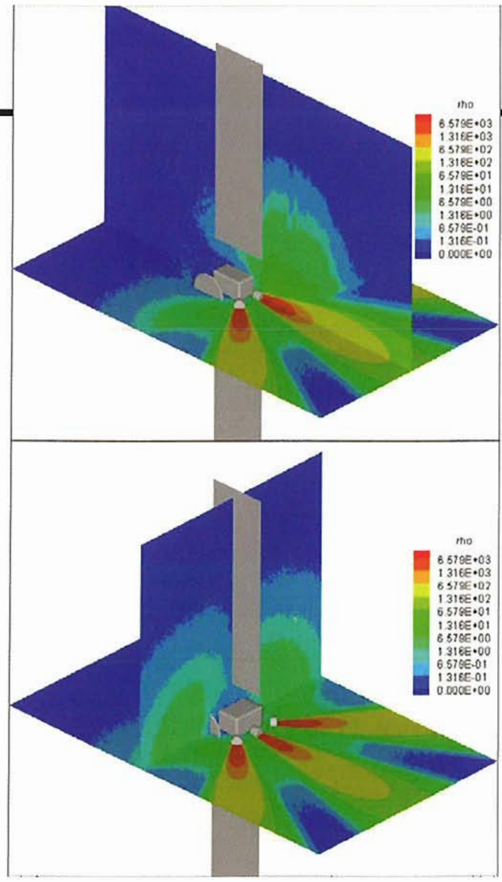

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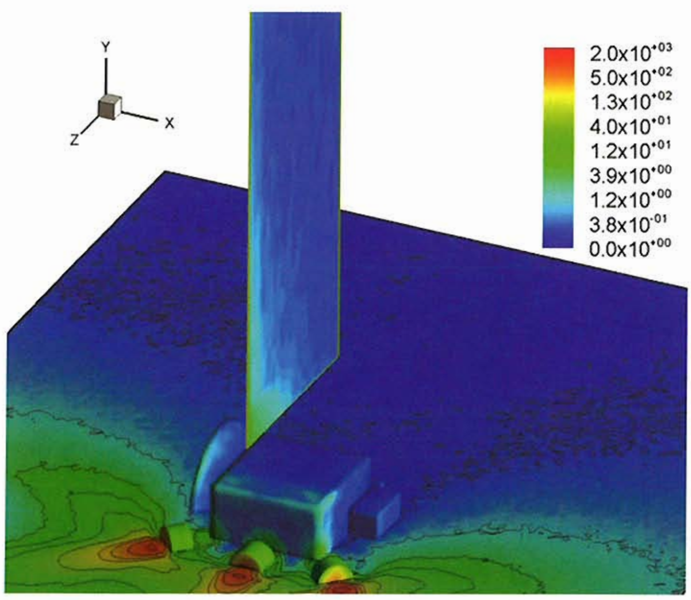

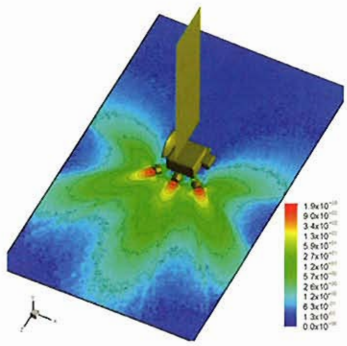

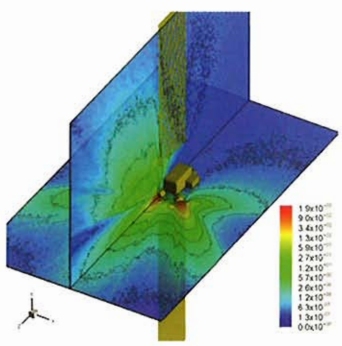

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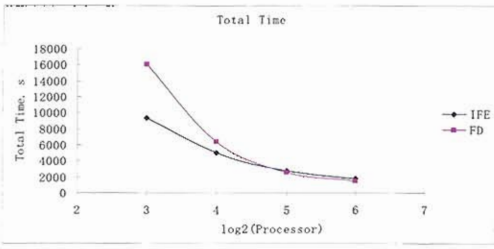
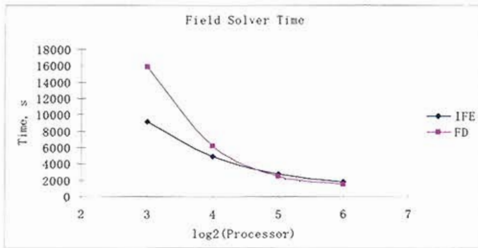
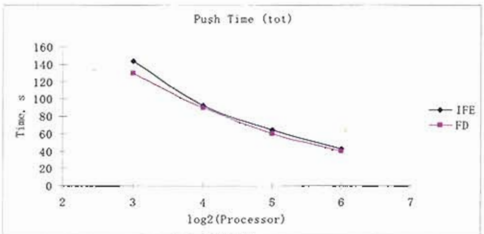
Computational Time: IFE-PIC vs. FD-PIC





Code speed on 64 processors of the Dell Xenon cluster:

steady state: 125 million particles and 30million tetrahedral elements



IFE-PIC loop time = 38s/step
Particle push time = 21.2 ns/particle/step

IFE field solve time = 4986 ns/cell/step (997 ns/element/step)

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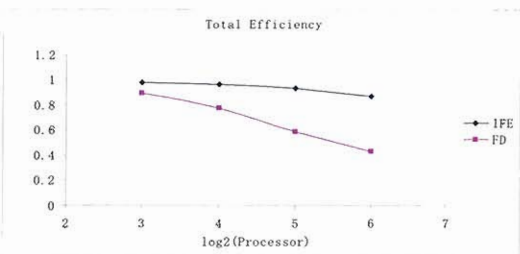
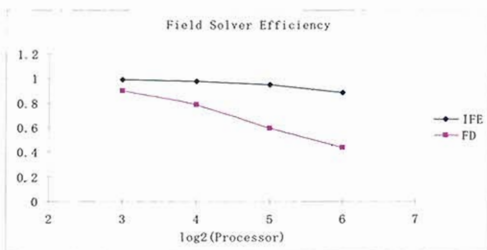
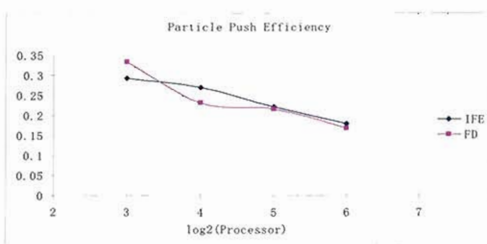
Parallel Efficiency: IFE-PIC vs. FD-PIC





Parallel efficiency for IFE-PIC at steady state on 64 processors: ~ 90%



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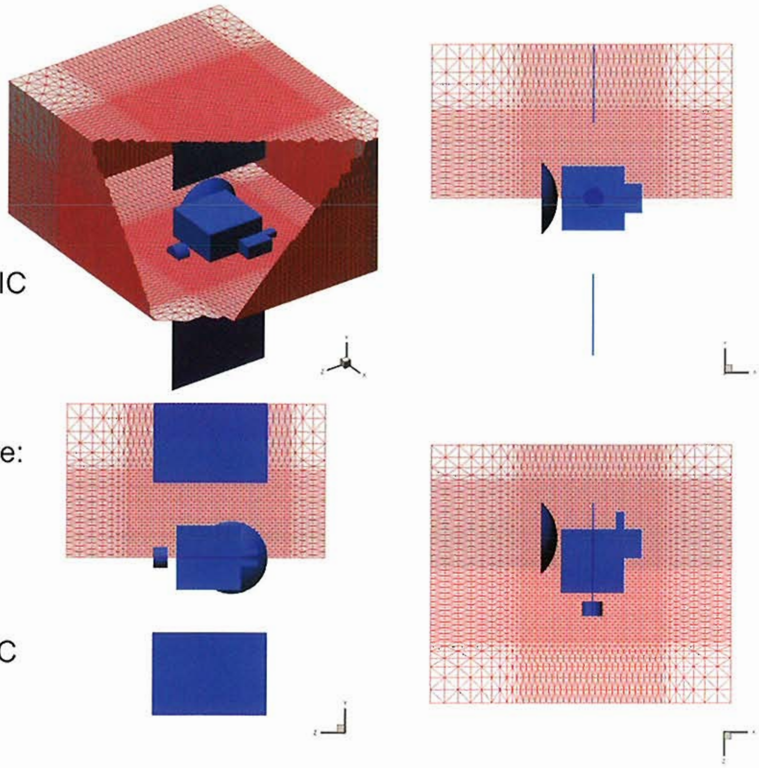
Hybrid Grid IFE-PIC Simulations of Multiple Ion Thruster Plume Interactions

- Objective:
  - To further reduce computation time and memory requirement
- Domain:
  - 2-zone mesh
  - Inner zone uses IFE-PIC
  - Outer zone uses HG-IFE-PIC
- Resolution:
  - PIC cell same as before: 5cm
  - IFE cell:
    - Inner zone: 5cm
    - Outer zone: Vcell_IFE/Vcell_PIC =1 to ~ 7



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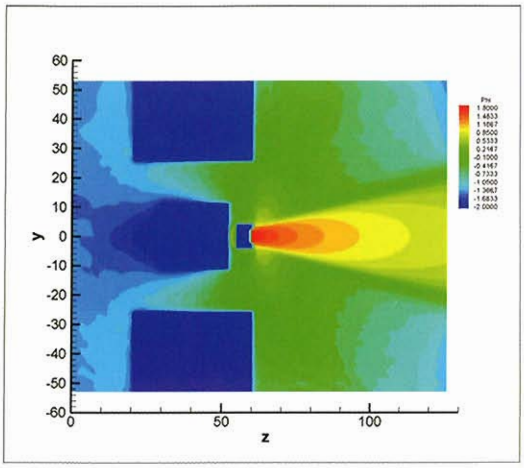
- Simulation Parameters:
  - Particles at steady state: 6 million
  - PIC cells: 105x54x90
  - Tetrahedral elements: 0.83 million
- Typical Computation Time:
  - Steady state only simulation: ~ 3 to 5 hours on P4 @ 2.2 GHz



Comparison of

IFE-PIC and HG-IFE-PIC

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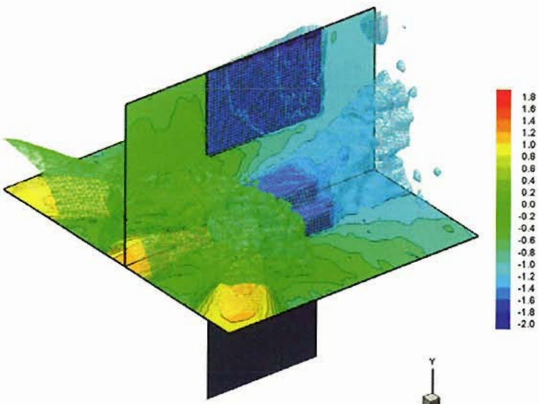
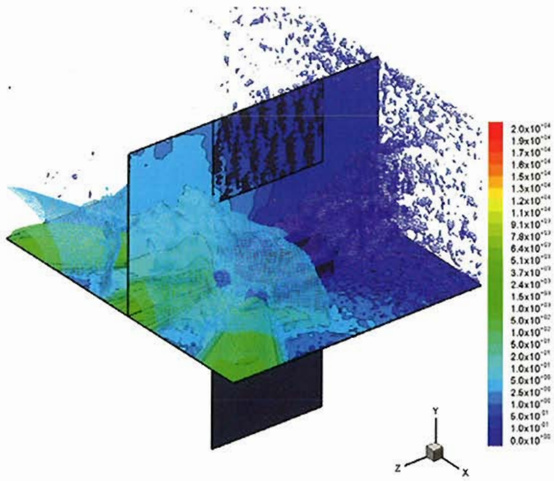


Electric Potential



Ion density

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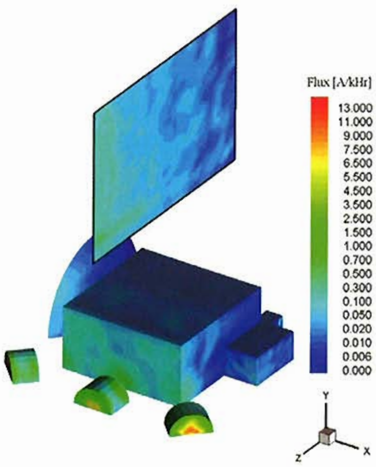

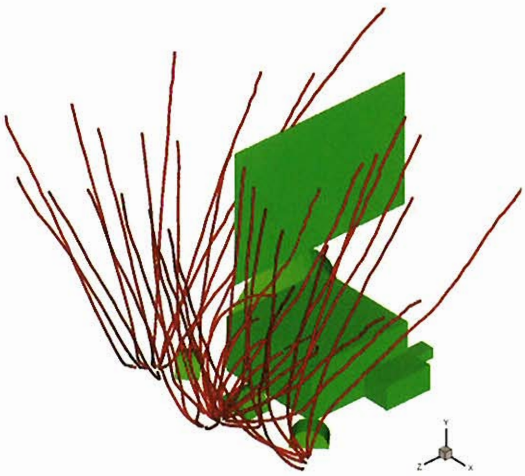

Prediction of Plume Contamination on Solar Array

- A primary concern for space missions using solar electric propulsion is plume induced contamination on solar cell
  - power loss; temperature change; catastrophic shorting
- Deposition of contaminants is calculated by tracing Mo+ particles from plume to solar array surface
- For an ion thruster similar to the NSTAR thruster, the contamination effect on the solar array is very moderate for DAWN configuration
- For multiple ion thruster plumes, deposition on solar array in general is NOT the sum of the contamination produced by individual thrusters

	Cases	1	2-A	2-B	2-C	3
Solar Array	Ave (A/kHr)	0.014	0.014	0.018	0.0501	0.0704
	Max. (A/kHr)	0.2513	0.216	0.0357	0.4085	0.4717

IV. Ion Optics Modeling

- Previous Study (Wang et al., JPP, 2003):
  - A 3-D "local" simulation model developed for NSTAR ion optics
  - Results in excellent agreement with measured erosion pattern and erosion depth
- This study (Wang et al., 2006):
  - Simulation of a whole ion optics gridlet
    - **new model explicitly includes apertures located at the edge and fully accounts for the effects of geometric asymmetry**
  - HG-IFE-PIC simulation using PC
  - Predict erosion from direct impingement at cross-over for CSU subscale ion optics

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- **The behavior of the accel grid current defines the operation envelop of an ion optics system.**
- **Accurate prediction of the cross-over and preveance limit is essential to ensure long-term ion thruster operation.**
- **Model predictions of ion impingement limits are currently based on extrapolations of single beamlet simulations**
  - Existing ion optics models are either axi-symmetric or 3-D with symmetric boundaries.
  - The geometric asymmetry associated with the edge apertures are not resolved.
- **Previous simulations of CBIO gridlet were not able to accurately predict the cross-over limit**
- **Both the disagreement between simulation and experiment and ongoing experimental studies suggest that the effects of geometry asymmetry and sheath interaction between adjacent holes may have a significant influence on the cross-over limit**

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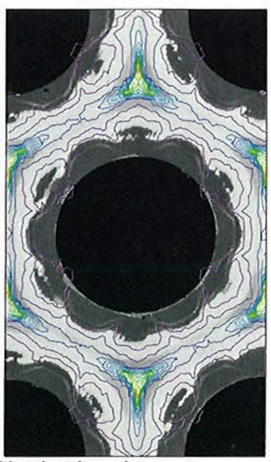
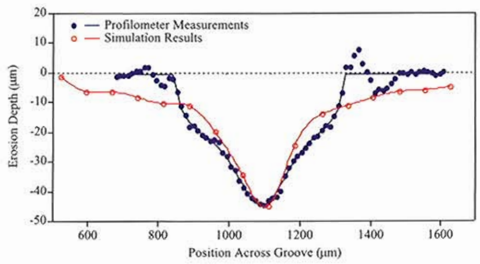
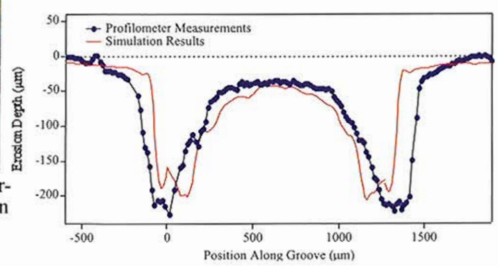
- **"Local" optics simulation of grid erosion for normal operation condition (Wang et al., J. Propulsion & Power, 2003)**

Downstream face of accelerator grid after 8200 hours at 2.3 kWe


Simulated erosion contours overlaid on measured erosion pattern





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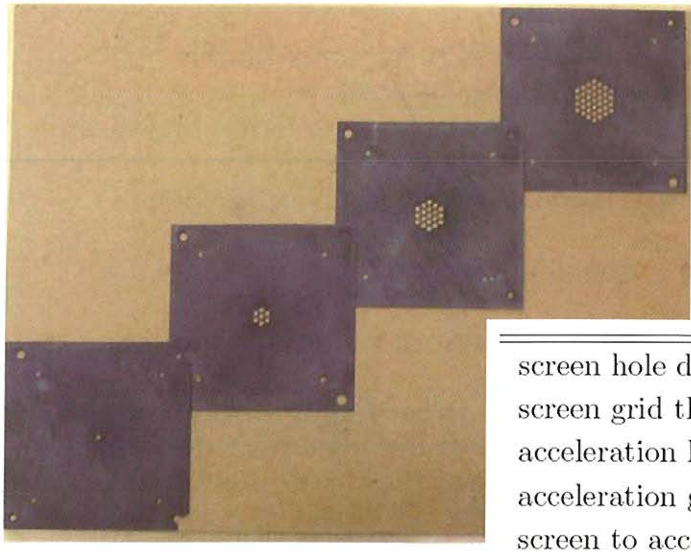
CSU Subscale Gridlet



screen hole diameter, d_s	2.305 mm
screen grid thickness, t_s	0.461 mm
acceleration hole diameter, d_a	1.396 mm
acceleration grid thickness, t_a	1.016 mm
screen to acceleration grid gap, l_g	0.810 mm
center-to-center hole spacing, l_{cc}	2.674 mm)

Sub-scale CBIO-style Poco graphite grids.

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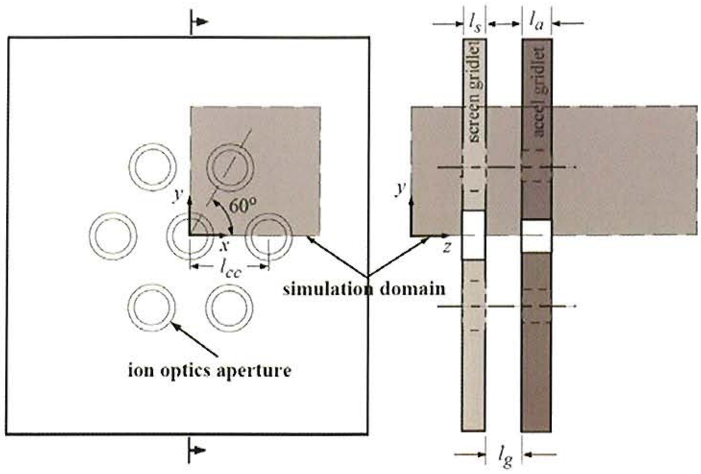
Simulation Model

- Simulation model are based on the HG-IFE-PIC algorithm (Kafafy and Wang, JPP, 2006)
  - **Explicitly includes apertures located at the edge**
  - **Fully accounts for the effects of multiple ion beamlets and geometric asymmetry**

7-hole gridlet model:

Assume uniform upstream plasma density



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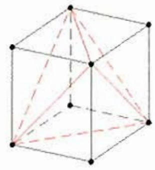
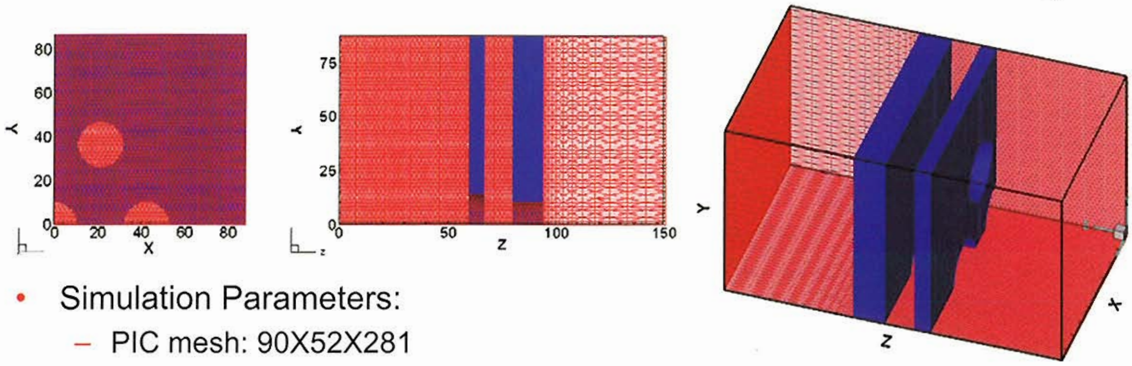
Simulation Mesh and Simulation Parameter

- PIC Mesh:
  - Uniform Cartesian
- IFE Mesh:
  - Multi-zone stretched Cartesian-based tetrahedral mesh





- Simulation Parameters:
  - PIC mesh: 90X52X281
  - IFE mesh: 90X52X280 (4,704,400 elements)
  - Upstream resolution: h=5.2E-5m
  - ~ 117,000 streamlines per simulation loop.

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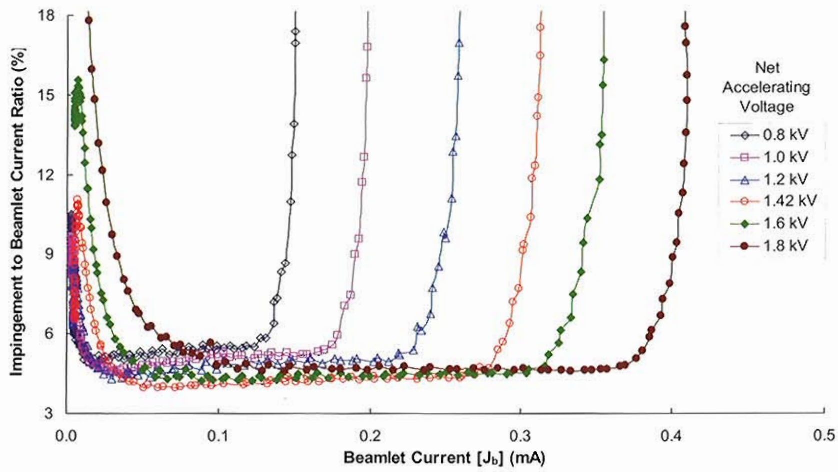
Experimental Results: Accel Grid Impingement Current for 7-hole Gridlet



net acceleration V_N	screen grid voltage V_s	accel grid voltage V_a
800V	770V	-140V
1000 V	970V	-150 V
1200 V	1170V	-166 V
1420 V	1390V	-170 V
1600 V	1570V	-176 V

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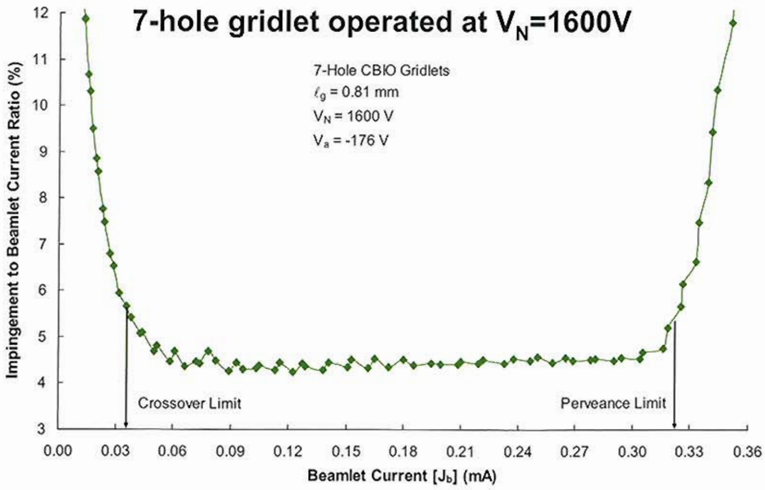
Experimental Results: Cross-over and Preveance Limit Definition



$$J_a = J_{imp} + J_{cex} + J_{leakage}$$ **Jcex ~ 4.5%Jb**

Cross-Over and Preveance Limit is defined at Ja/Jb=5.5%

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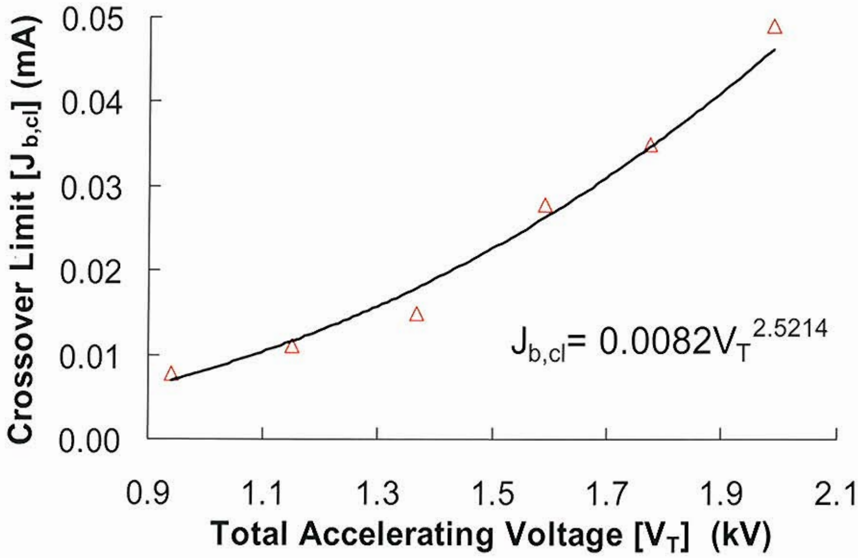
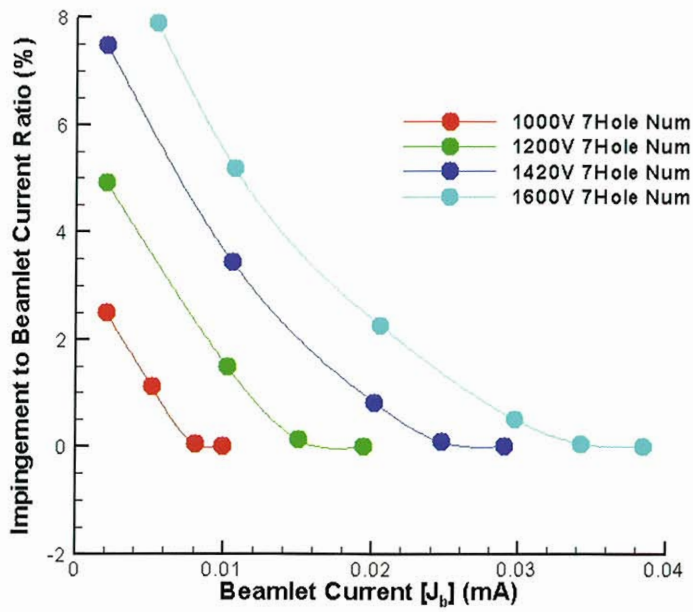
Experimental Results: Cross-Over Limit Behavior for 7-hole Gridlet

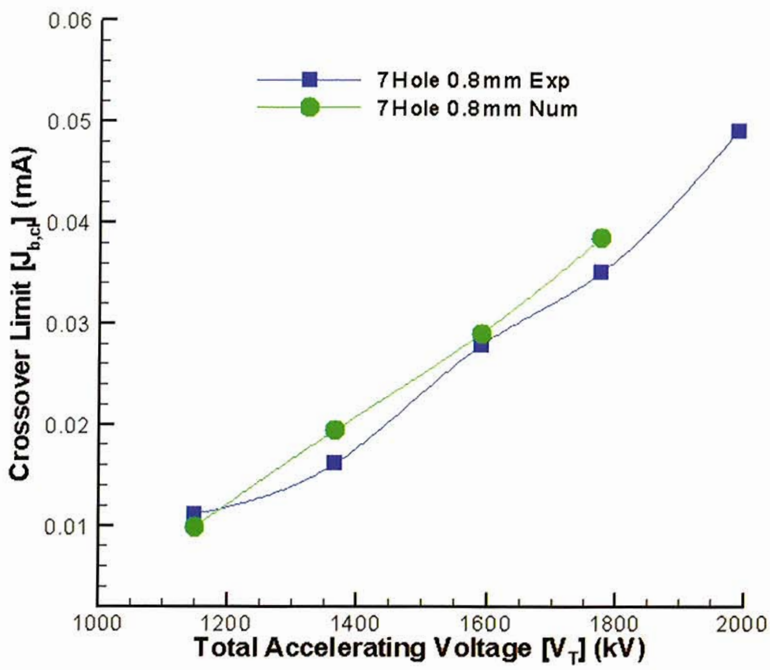


Simulation Results: Accel Grid Impingement Current for 7-hole Gridlet



Simulations do no include CEX ions and leakage current

Simulation vs. Experiment: Cross-Over Limit Behavior for 7-hole Gridlet



Cross-over limit in experiment:

Ja – Jcex=1%Jb

Cross-over limit in simulation:

Ja>=0

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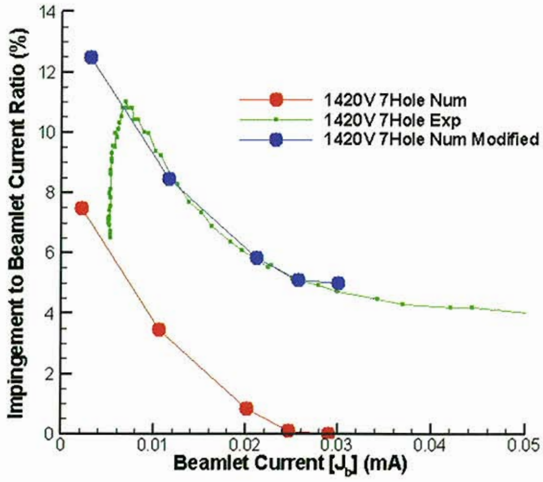
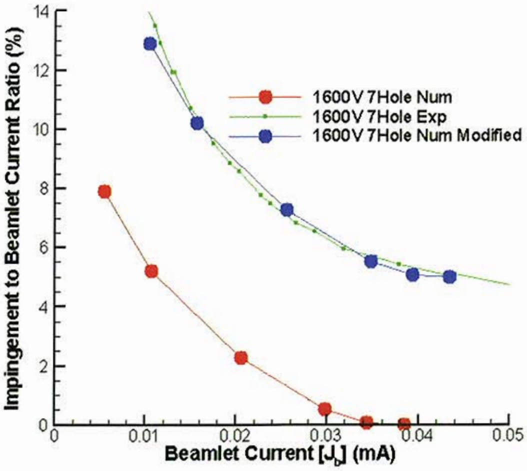
Simulation vs. Experiment: Accel Grid Impingement Current for 7-hole Gridlet



Blue line: origin of the simulation curve shifted from (0,0) to (0.001,4.5)



Blue line: origin of the simulation curve shifted from (0,0) to (0.005,4.5)

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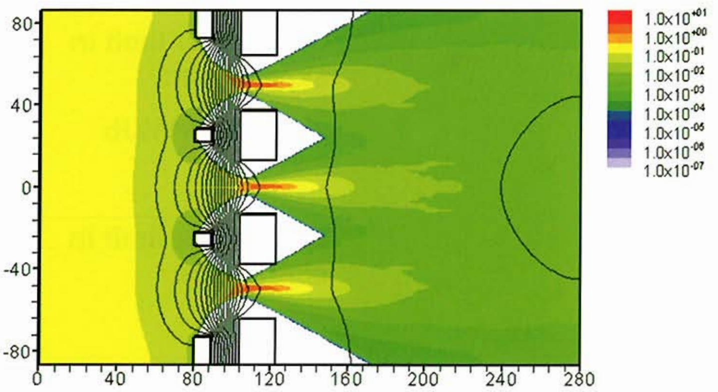
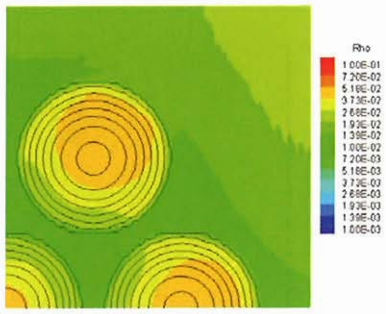
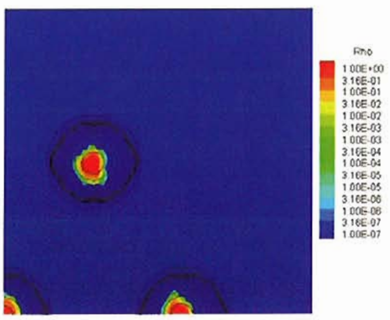
Simulation Results: Beamlet Profile at Cross-Over



$n_0 = 0.15 \times 10^{17} m^{-3}$





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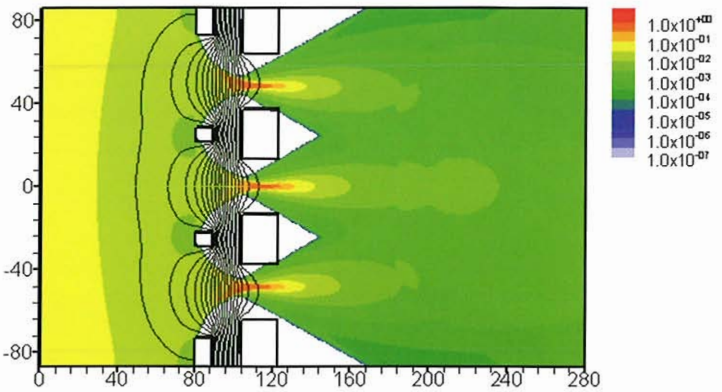
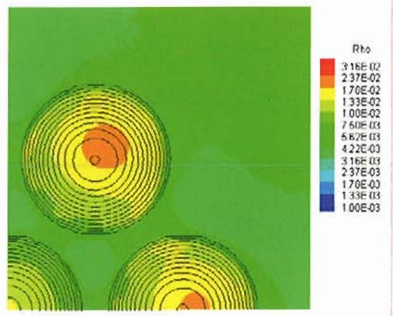
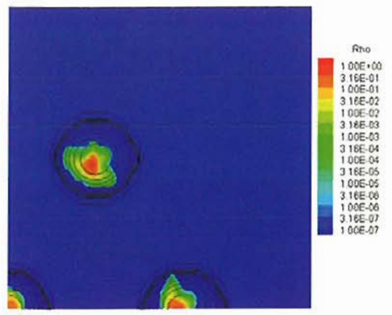
Simulation Results: Beamlet Profile beyond Cross-Over







$n_0 = 0.05 \times 10^{17} \mathrm{m}^{-3}$

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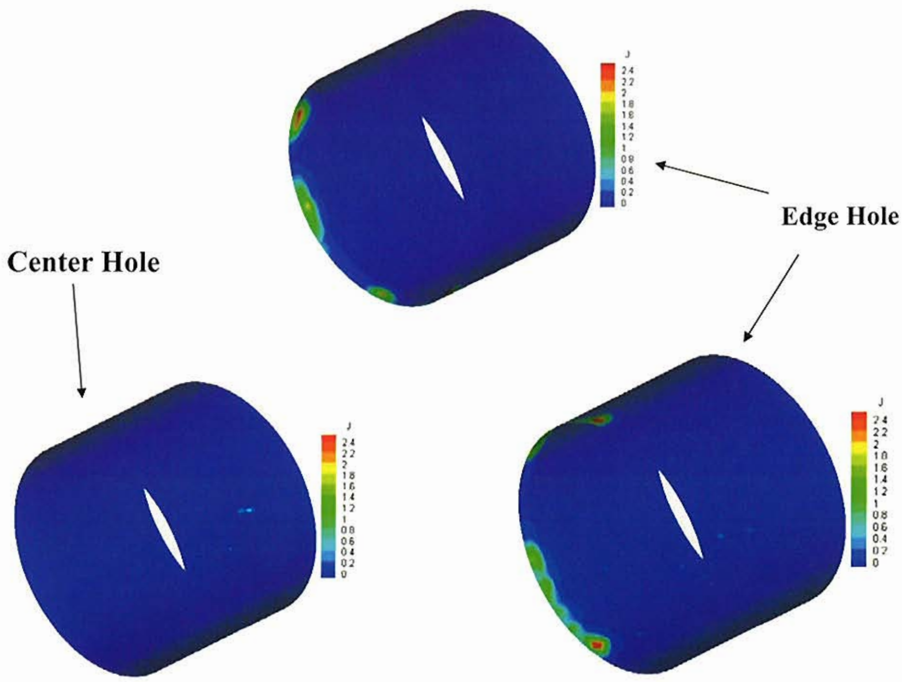
Simulation Results: Ion Impingement Distribution at Cross-Over



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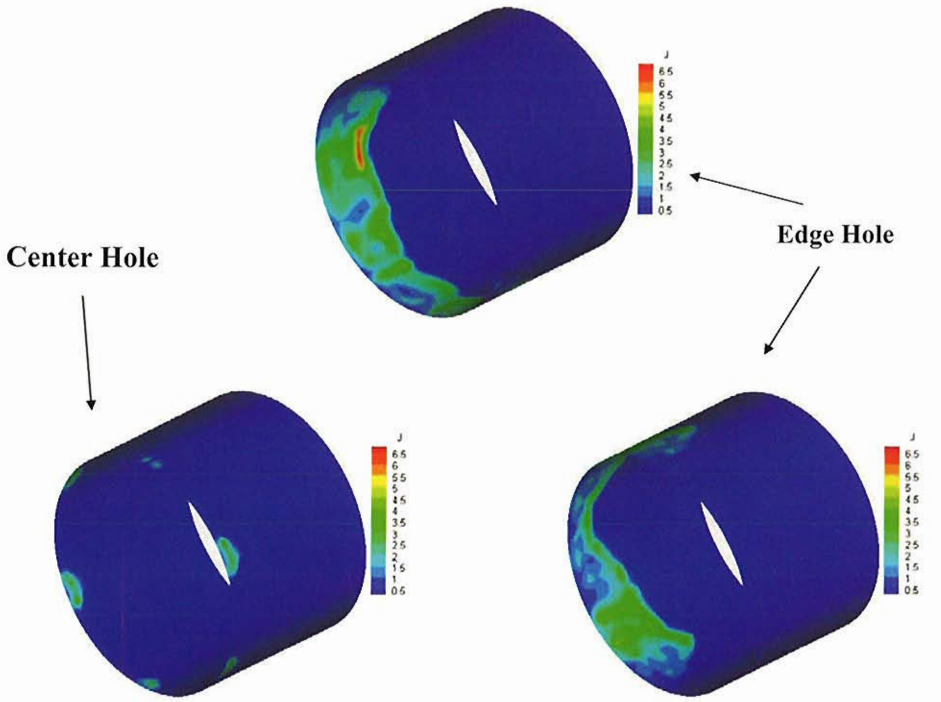
Simulation Results: Ion Impingement Distribution beyond Cross-Over



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Prediction of Cross-Over for CSU Ion Optics Gridlet

- Cross-Over onset starts at edge apertures!
  - Cross-over occurs at higher J_b than the center aperture
- Beamlet profile is asymmetric for edge apertures
  - Ion beamlets focused more towards the gridlet center due to the asymmetry in E field near grid surface
- Ion impingement distribution is asymmetric for edge apertures
  - Direct impingement concentrated on the aperture side oriented towards the gridlet center
- Ion impingement distribution has a hexagonal pattern for the center aperture
- Edge apertures will experience significant more sputtering erosion than the center aperture.

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V. Simulation Based Design Tool

- **Modeling and simulation are playing an ever more important role in electric propulsion and spacecraft interactions research**
- **The sophistication of the models and the capability of supercomputers have reached such a level that it is becoming feasible to use computer simulations as "virtual" experiments in place of real experiments for many applications**

- **Objective:**
  - **To develop a simulation based design tool for spacecraft using electric propulsion**

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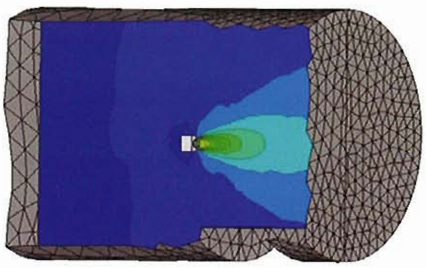
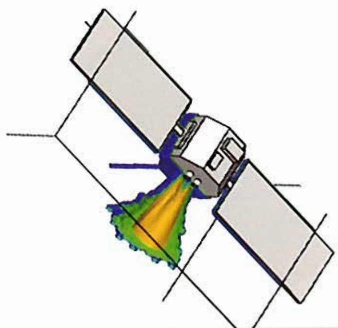
COLISEUM framework

VirginiaTech *Invent the Future*





Surface
- Simulation mesh
- Material specs

Particle Sources
- Exp profile: LIF, j
- HPHall, CHETC

Sputter Model
- Lab measurements
- Model, ***f(E,θ)***

Plasma Simulation:
- RAY (sputtering / deposition)
- PRESCRIBED_PLUME
- AQUILA (Hybrid PIC-DSMC)
- DRACO (Full PIC-MCC)

Collisions
- Cross-sections, literature
- **Limited data**

Results
- Plume properties
- Surface erosion/deposit

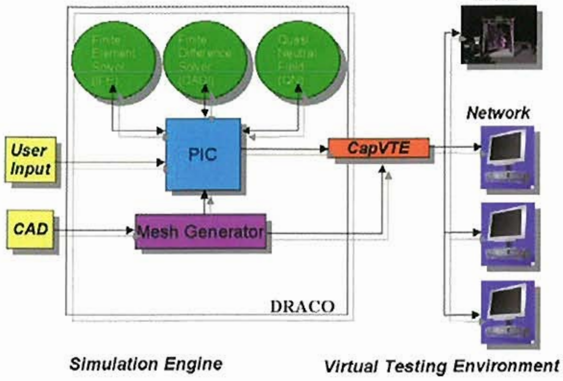
Colorado State University

Advatech Pacific, Inc. Solutions Beyond Services

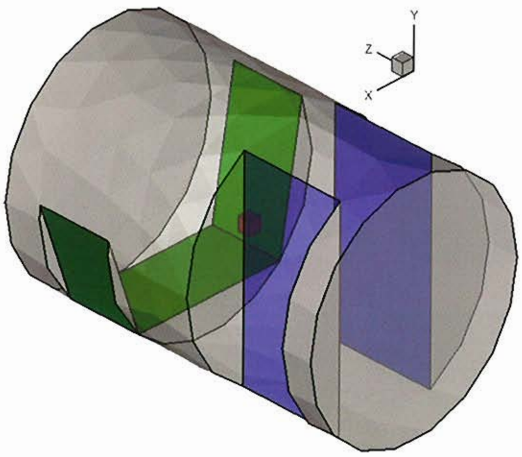
(Spicer, Wang, Brieda, 2006)

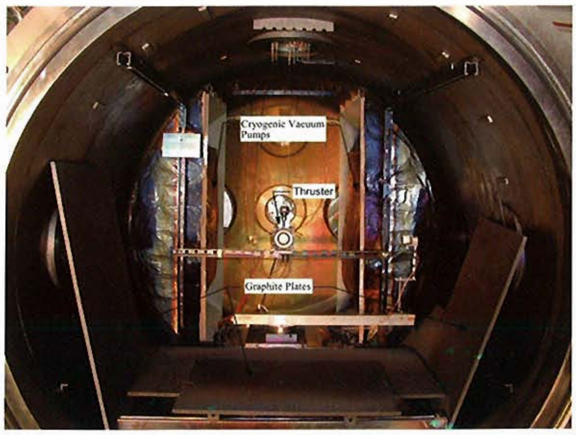
DRACO

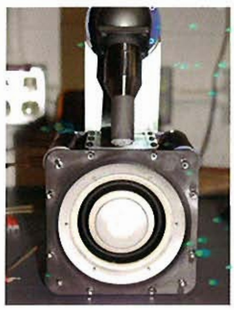
- **A set of multi-purpose 3-D electrostatic PIC codes developed at VT and AFRL**
  - **QN-PIC:**
    - **Quasi-neutral plasma with Boltzmann electrons**
  - **FD-PIC:**
    - **Full particle/hybrid PIC**
    - **Standard finite-difference field solver**
  - **IFE-PIC**
    - **Full particle/hybrid PIC**
    - **Hybrid finite element/finite difference formulation**
    - **Immersed finite element field solver**
  - **Mesh-Object Intersection (VOLCAR)**
    - **Interface between PIC and CAD defined spacecraft model**



Ongoing Work: Simulation of EP Ground Experiment







DRACO Simulation set-up:

Model generated by Solidworks /Hypermesh

Red = Thruster
Blue = Pump
Grey = Tank Walls
Green = Graphite

Comparison with experimental current density sweep at 0.6m

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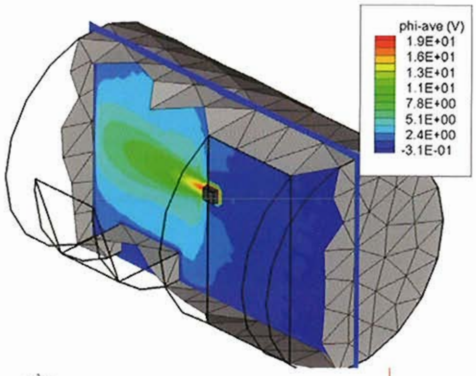
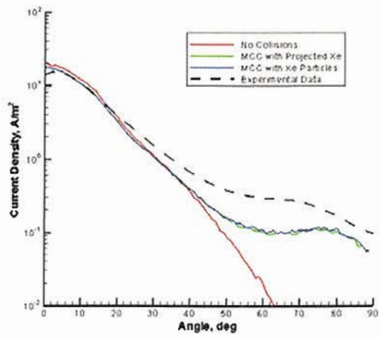
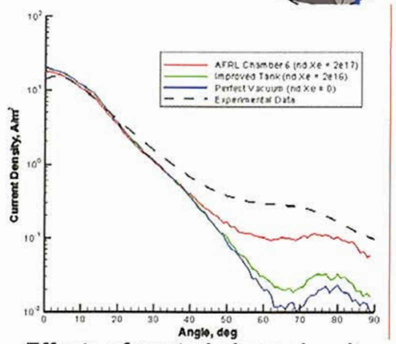
Preliminary Results

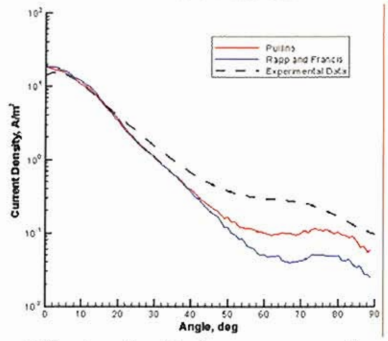




Effects of collision model



Effects of neutral plume density



Effects of collision cross section data

(Spicer, Wang, Brieda, 2006)

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VI. Summary and Conclusions

- **Significant progresses have been made on developing particle simulation models for ion propulsion**
  - Such models are *beginning* to meet user's requirements in *sophistication* (all physics included), *computational speed* (3-D simulations performed routinely), and *accuracy* (agreement with experimental data)
  - Particle simulation models are increasingly being used as engineering design tool in development of new thrusters and in preflight predictions of plume effects
- **However, many challenging issues still remain to be solved**
  - How to accurately incorporate the many "engineering details" of real spacecraft (or thruster) into the model?
    - surface material properties, surface interactions, detailed device configuration, detailed plume characteristics, detailed experimental setup… etc, etc
  - How to account for uncertainties in experimental data?
  - How to avoid mis-interpreting the physics?
  - How to continuously overcome the computation limitation?