

Particle in cell simulations

PTetra workshop
January 27, 2022

Richard Marchand
University of Alberta

Outline

- Introduction
- PTetra
- A few examples

Problem and objective

- Plasma dynamics is a complicated many-body problem.
- It can be modelled with fluid equations, kinetically, or with a combination of the two.
- Interaction of satellites and mounted instruments with plasma environment is determined by kinetic processes in non equilibrium perturbed plasma.

Fluid description

Based on conservation equations,

- Mass conservation → continuity equation
- Momentum conservation → momentum equation
- Energy equation → energy equation

and moments of kinetic equations

Advantages

- Simplicity
- Applicable to large scales (entire solar system)
- Robust, because of conservation laws

Limitations

- Reliance on an assumed approximate particle distribution function; e.g., Maxwellian.
- Breaks down when deviations from the assumed distribution is important.
- Incompleteness. The set of equations requires ad hoc closure. This is related to the BBGKY hierarchy.

Kinetic approaches

Imitate nature

- Particle-particle interactions
 - Straightforward and easy to implement.
 - With N particles: $N(N-1)/2$ interactions and N trajectory integrations every time step.
- Particle-cluster interaction
 - PP interaction between nearby particles,
 - PC interaction with “distant” clusters
 - Less straightforward to implement.
- Particle-mesh interaction
 - Interpolate particles on a mesh to get charge and current densities
 - Solve Maxwell equations
 - Interpolate fields from the mesh back to the particles
 - Integrate particle trajectories for one time step, and repeat.
- Hybrid simulations
 - Some species are approximated as a fluids, and others kinetically.
- Vlasov approach
 - Solve the Vlasov equation in 6-dimensional space.
 - Similar to the fluid approach, but in phase space.

(“Computer simulation using particles”, Hockney and Eastwood)

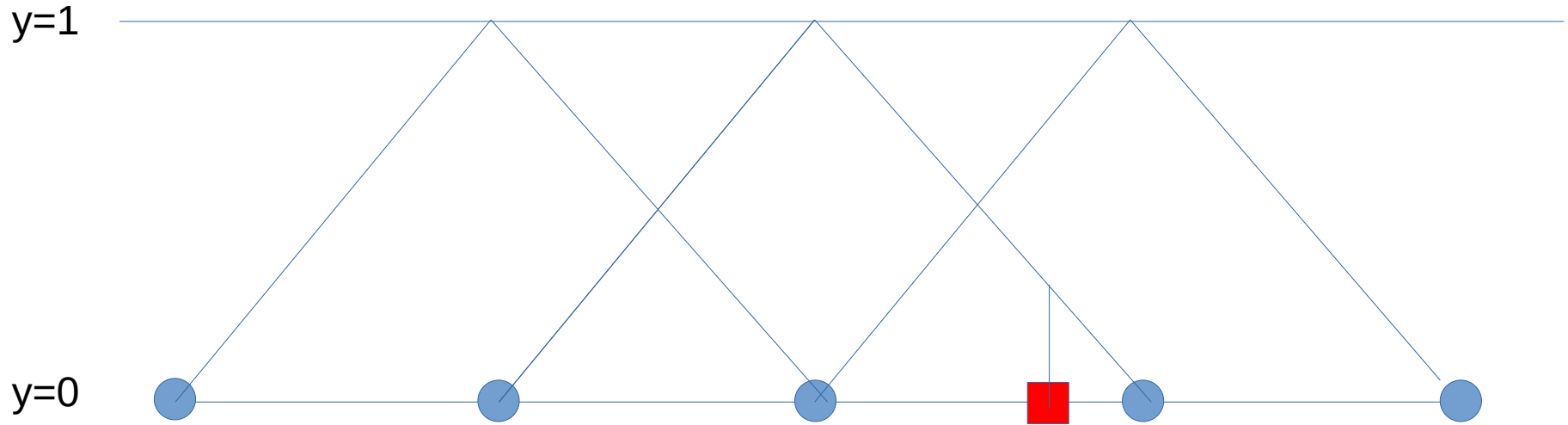
Hybrid approach

- Certain species (often electrons) are described with fluid equations.
- Others (ions) are treated kinetically.

Particle In Cell

The particle in cell approach

illustration in 1D



Distribution of a point charge on a grid

Solution: Fast Fourier Transform, finite difference, ...
Boundary conditions: periodic, reflecting absorbing/emitting, ...

Mesh

- Meshes can be
 - 1, 2, and 3D
 - Structured / unstructured
 - Unstructured tetrahedral adaptive in PTetra
- Boundary conditions,
 - Dirichlet (used in PTetra for all boundaries).
 - Neumann
 - Mixed

Boundary conditions in PTetra

- Dirichlet boundary conditions are set as seen in the satellite reference frame.
- $V = (\mathbf{v} \times \mathbf{B}) \cdot \mathbf{r}$ at the boundary, from the motional electric field $\mathbf{E} = -\mathbf{v} \times \mathbf{B}$
- “absolute” or self-consistent

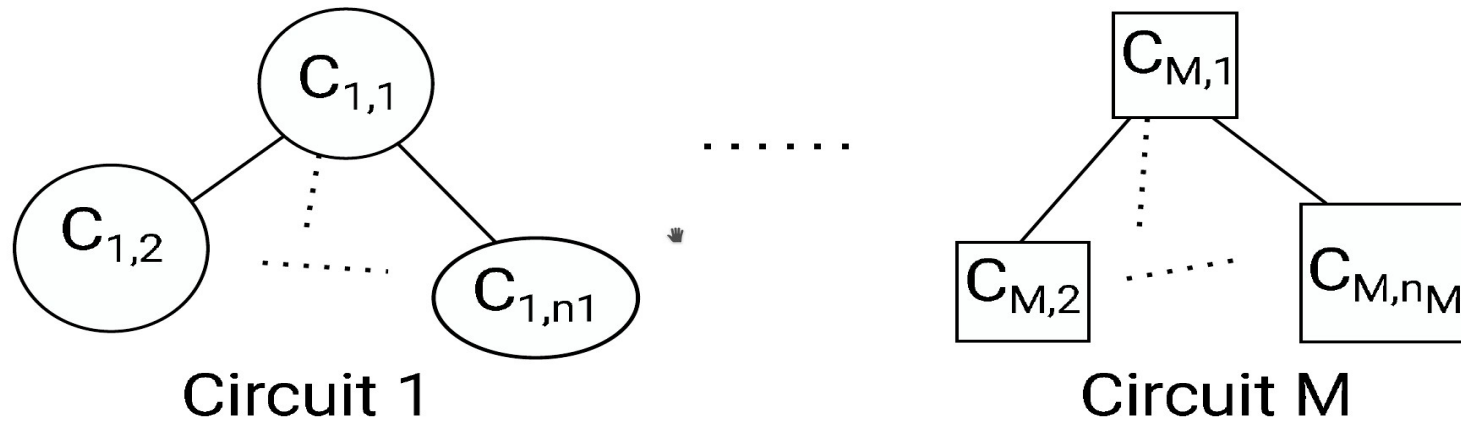
- Absolute: independent of plasma conditions.

Every physical structure is assigned a potential.

- Self-consistent: relative potentials are specified between different elements.

different disjoint sets of elements can be considered

Networks with relative biases

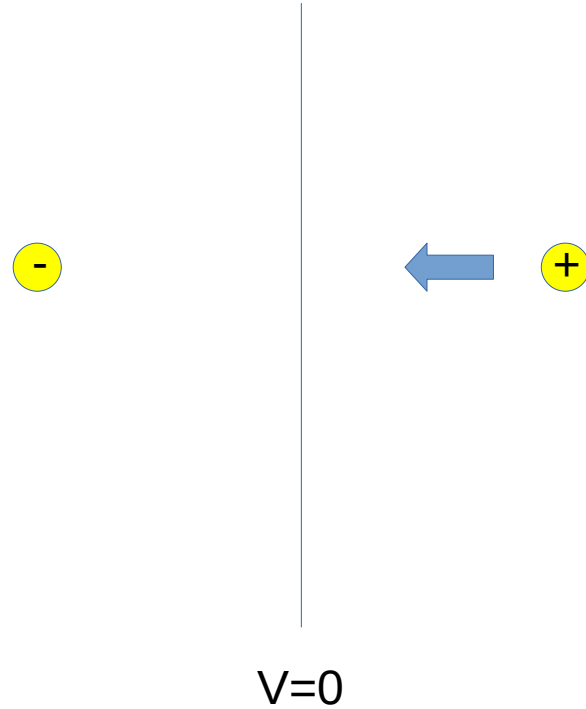


Alternatively, potentials can be fixed a priori, relative to the background plasma.

Special features

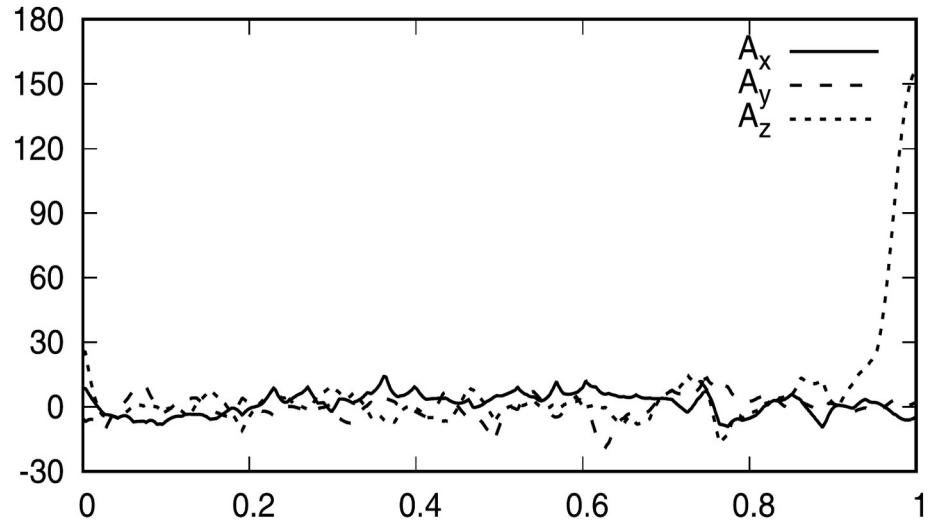
Unphysical features

- Self force
 - General boundary conditions produce **nonphysical** self-forces.
- Mirror force
 - Appears at boundaries.
- These are negligible with large numbers of particles per cell.

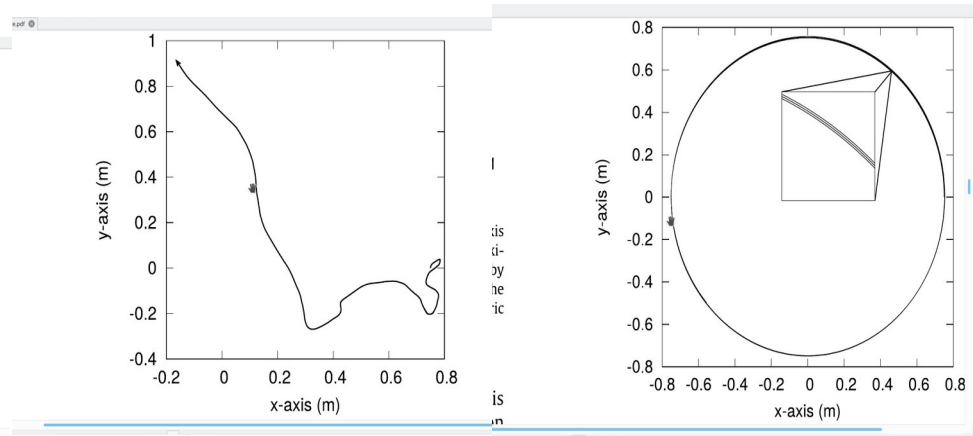
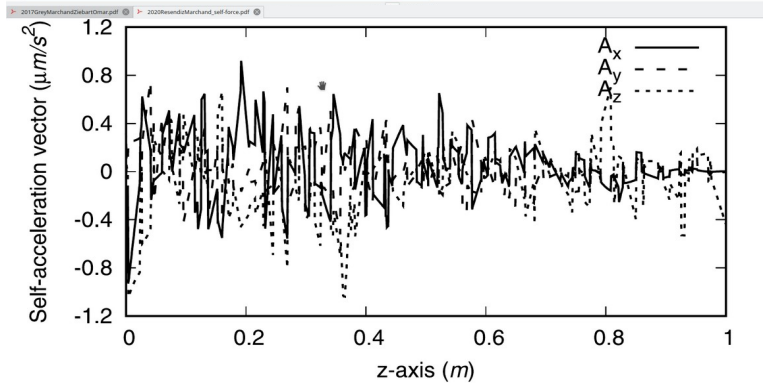
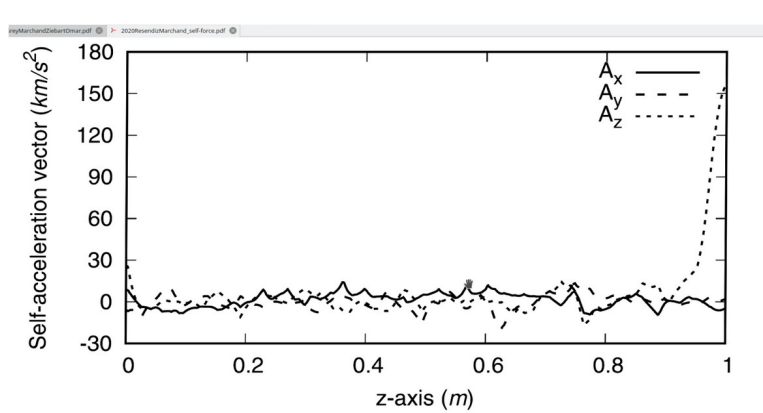


Unphysical features

- Self force
 - General boundary conditions produce **nonphysical** self-forces.
- Mirror force
 - Appears at boundaries.
- These are negligible with large numbers of particles per cell.



Self- and mirror force removal



Electron gravitation around a fixed proton at the centre of a spherical simulation domain without (left) and with (right) SF subtraction.

(Resendiz and Marchand, Computer Physics Communications 254 (2020) 107212)

Mesh and the topo file

Structure of the topo file

- Generate a mesh with gmsh → filename.msh.
- Convert the msh file to “topo” format with msh2topo → msh2topo.out
- Rename msh2topo.out to something more convenient, such as mygeometry01.topo
- The topo file contains
 - Vertices used to define the mesh
 - 4 Indices of vertices forming each tetron + the indice of the 4 neighbouring tetrahedra opposite each of the 4 vertices

Inside topo

\$coord

ncoord= 293984

1	0.0000000000000000E+00	5.7499999999999996E-01	2.5000000000000001E-02
2	0.0000000000000000E+00	-5.7499999999999996E-01	2.5000000000000001E-02
3	0.0000000000000000E+00	6.9169999999999995E-02	7.8920999999999997E-01
4	0.0000000000000000E+00	-6.9169999999999995E-02	7.8920999999999997E-01

...

\$elements nodes (1-4) and adjacency (1-4)

nelem= 1664501

1	42859	192516	139632	222048	45316	2290	769089	87995
2	69416	109371	109955	182807	77273	258049	8832	1559
3	62254	99707	124127	144835	13117	148202	238368	125905
4	69747	89573	118673	147577	46264	465323	75943	2599

...

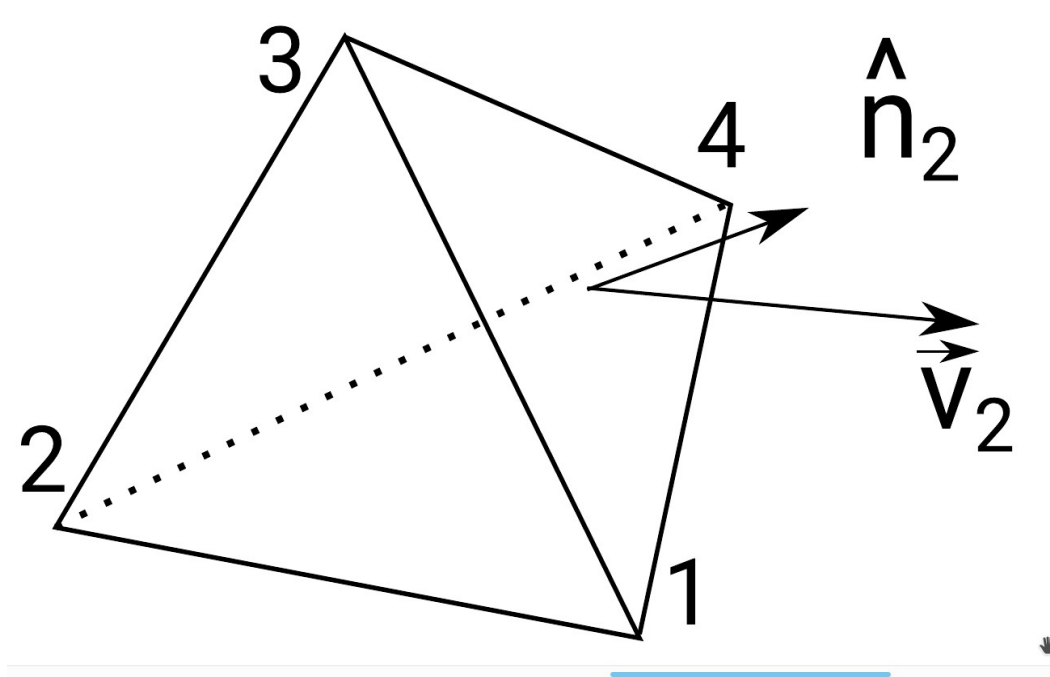
1062	7595	9970	117807	267393	23061	32582	789	420655
1063	52897	97	1157	130068	480618	174510	3062	-9
1064	39318	142508	122745	175421	340709	642754	86591	4154
1065	27243	30485	27245	94959	129731	1600927	5170	-1

...

topo file convention

- When a tetrahedron face is on a physical structure (numbered with an integer index in gmsh), the “neighbour” opposite the vertex opposite that face is the negative of that index.
- From the first vertex listed in a tetrahedron, vertices 2, 3, 4 rotate clockwise.

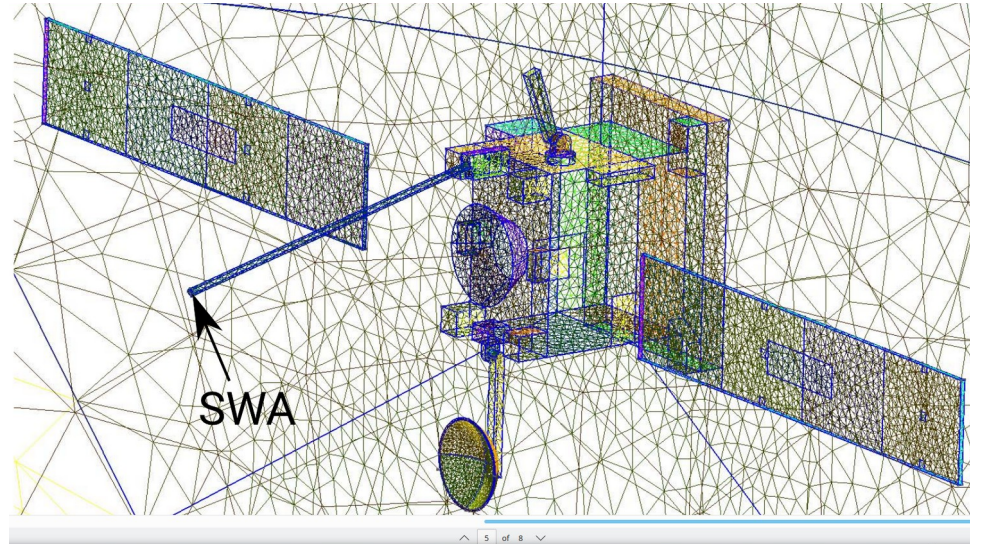
Finding a point in the mesh



Selected examples

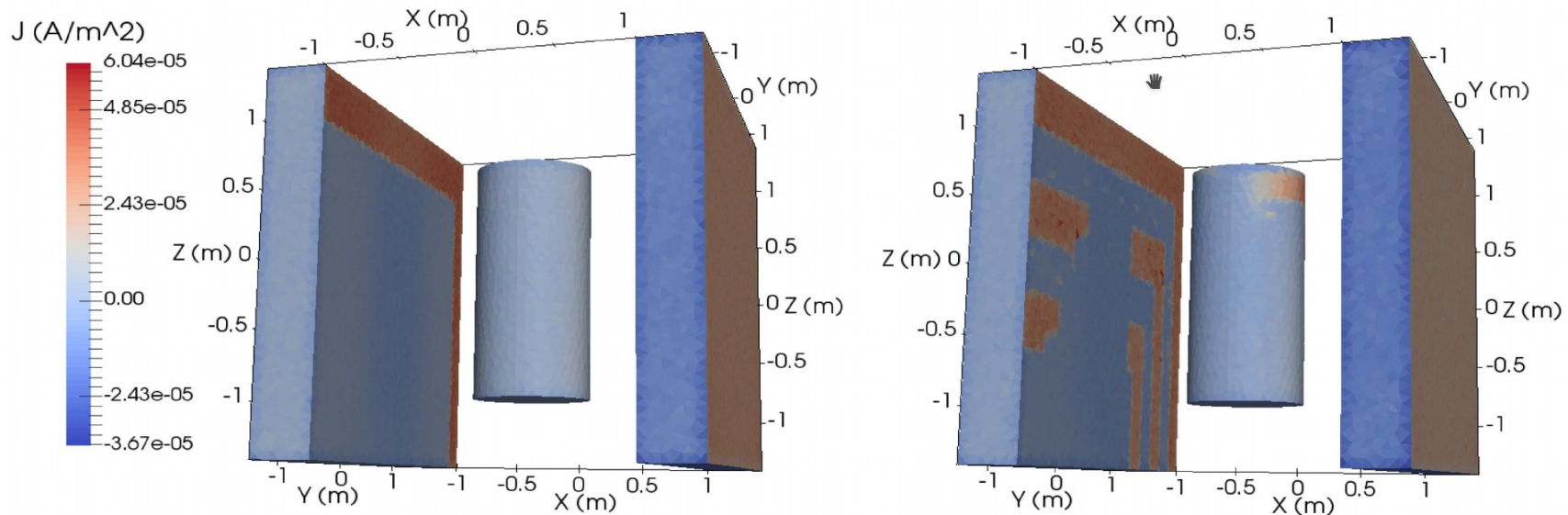
3D – mesh

- Unstructured tetrahedral mesh.
- Used to represent objects in realistic geometry.
- Spatial resolution can be used to represent curved or small components



Simulation of an early Solar Orbiter geometry
Grey, et al. IEEE Trans. Plasma Sci. **45** (2017)

Photo-electron emission from multiple reflections



“Multiple reflections of solar radiation and photoelectron emission in satellite interaction with space environment”, R. Omar, MSc thesis 2016, <https://doi.org/10.7939/R3PZ51S0B>

Application to Solar Orbiter

Grey, et al. IEEE Trans. Plasma Sci. 45 (2017)

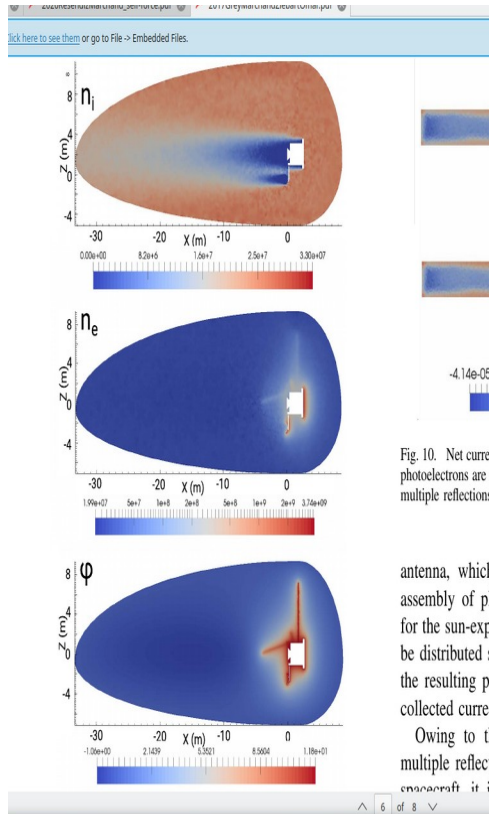
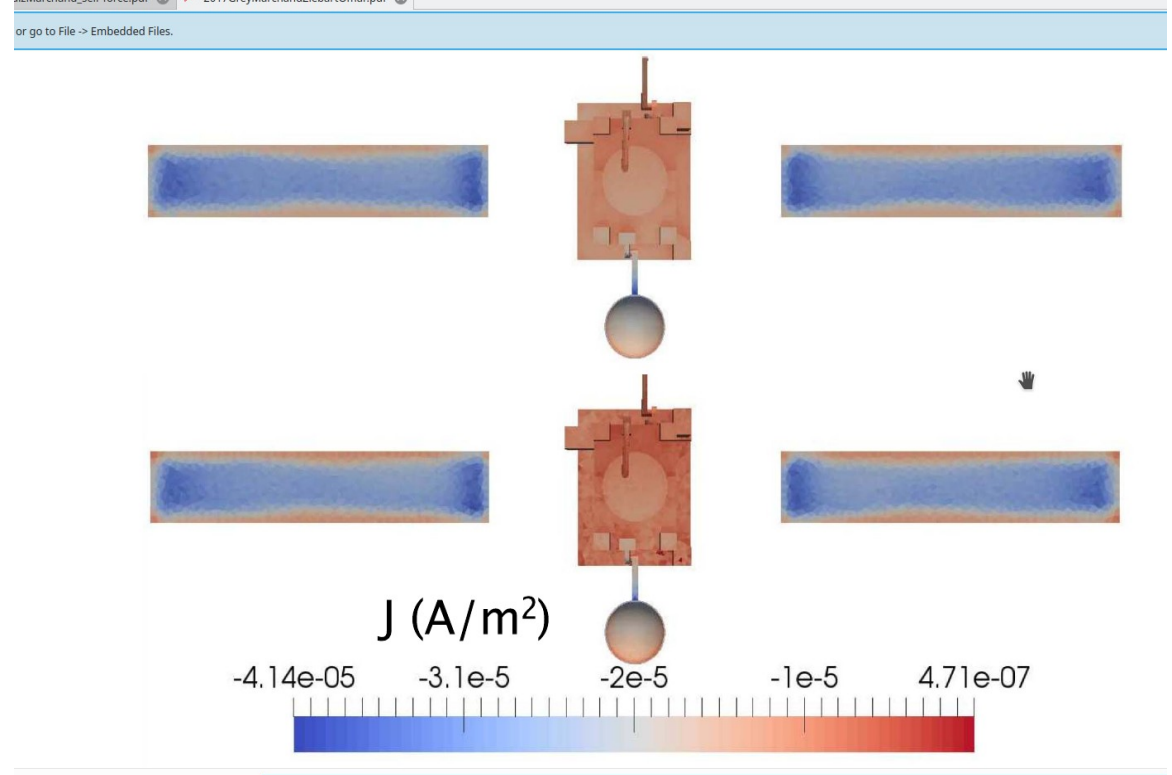
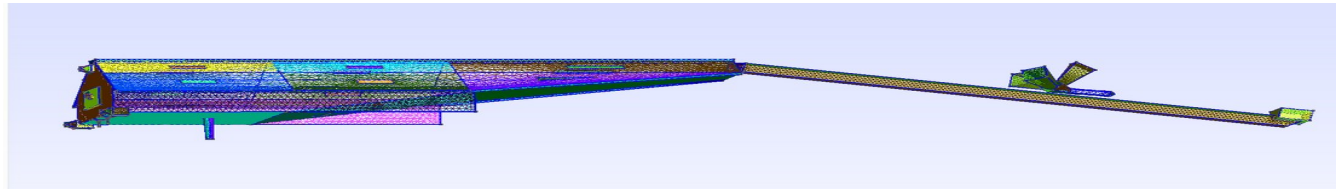
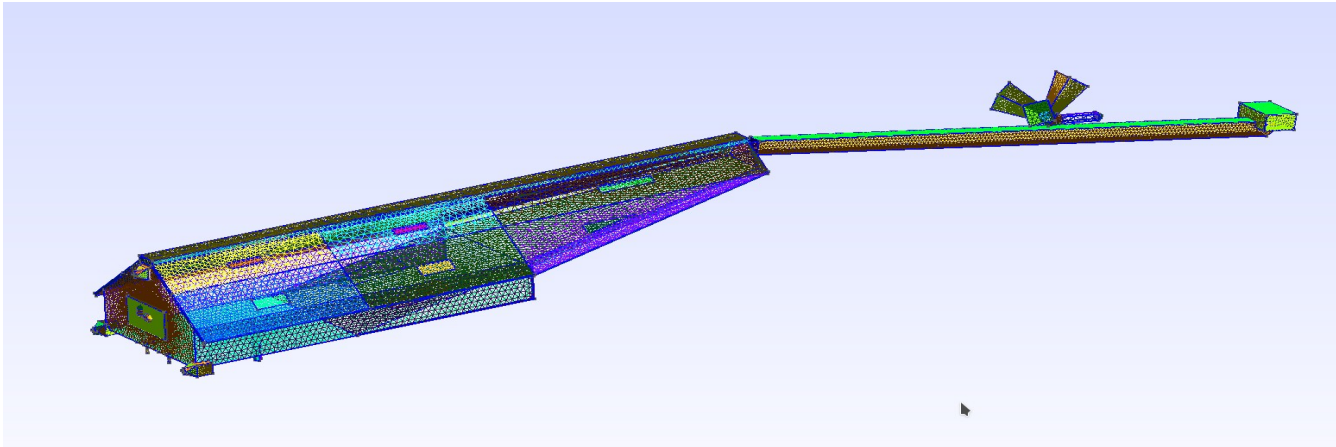


Fig. 10. Net current photoelectrons are multiple reflections

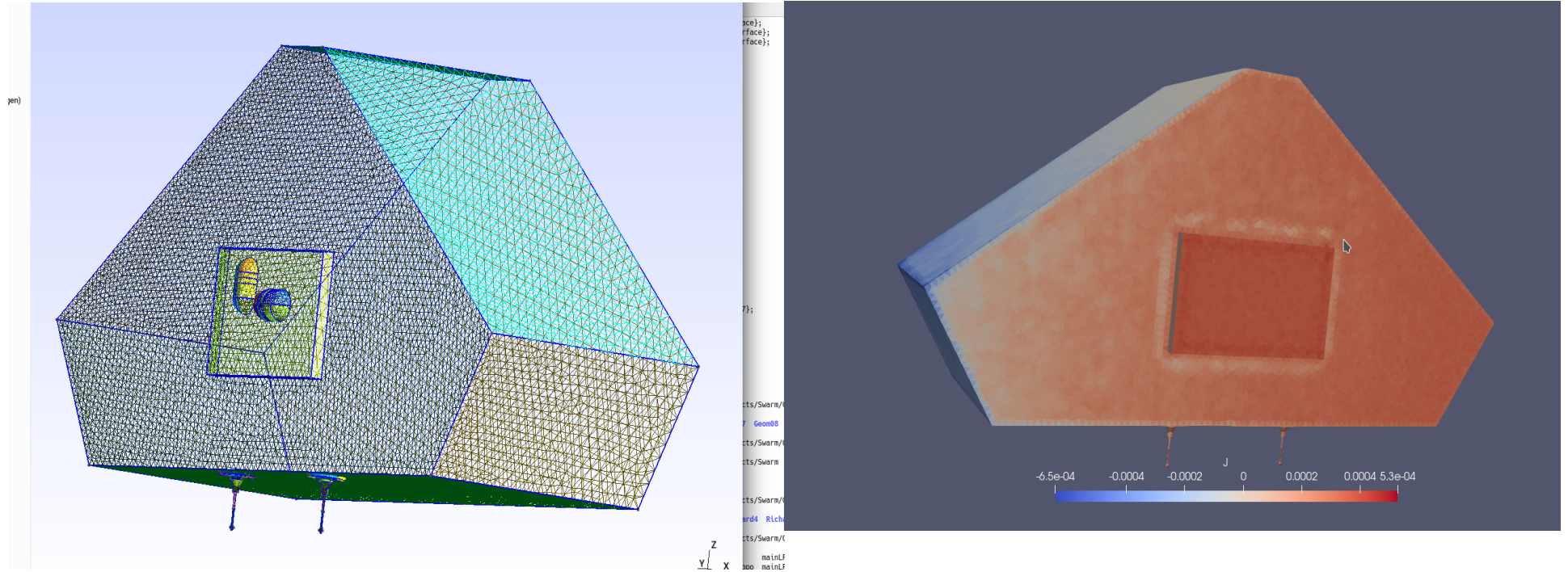
antenna, which assembly of pl for the sun-exposed be distributed so the resulting photo collected current Owing to the multiple reflections spacecraft it is



The swarm satellite



Simplified Swarm geometry

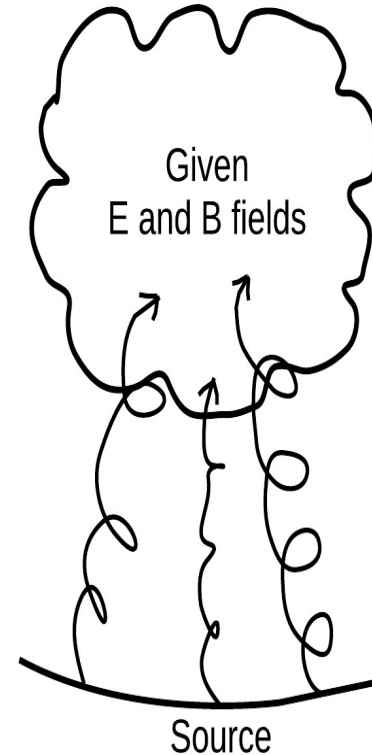


Post processing

- Relaxation
- Visualisation
- Test-particle simulations
 - Used to compute particle distribution functions f
 - Moments of f are calculated numerically
 - Density, fluxes, energy density, pressure, heat flux, ...

Test-particle simulation

- For a collisionless plasma, $Df/Dt = 0$ along particle trajectories in 6D phase space
- This is the 1-particle equivalent to Louisville's theorem



Application to probes

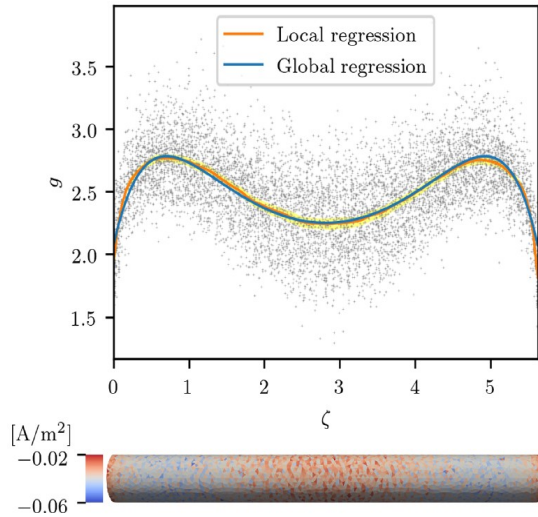


FIG. 2. (Bottom) Surface current density for a probe with $\lambda = 5.63$ and $n = 25$. The current through each facet is averaged with

Collected electron current density along a positive cylindrical probe (left), and electron velocity distribution near the ends and in the middle of the probe (right)

cylindrical simul: extending 40 mm is important that from the probe, si boundary conditi [23], with a reso: 0.2 mm on the p carried out with t to settling at these as practically pos PTETRA autom resolves the plas that a typical pa one Voronoi cell accounts for possi near objects bias Whereas the pi species current—repelled species (when recording si we reduce the ior

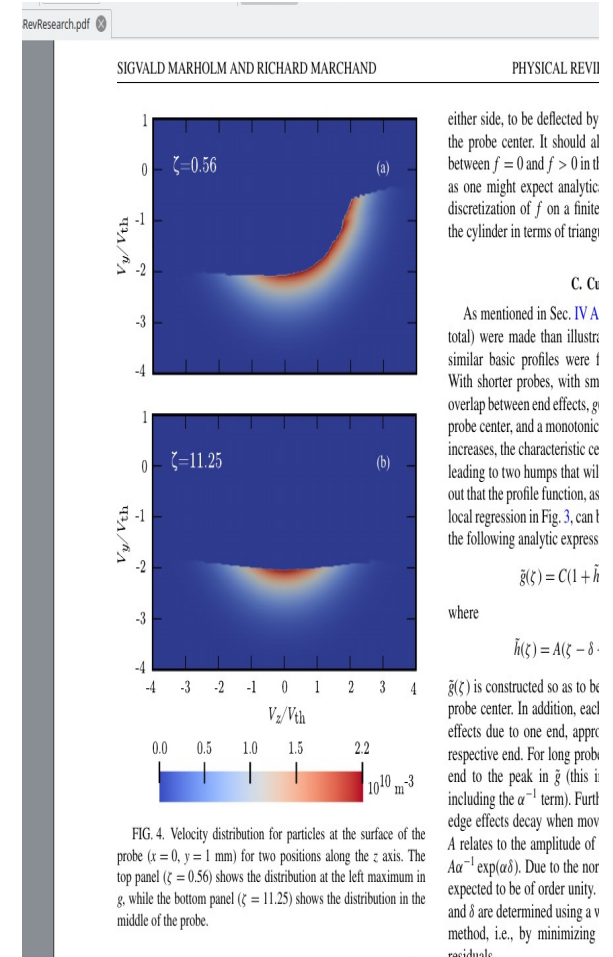


FIG. 4. Velocity distribution for particles at the surface of the probe ($x = 0, y = 1$ mm) for two positions along the z axis. The top panel ($\zeta = 0.56$) shows the distribution at the left maximum in g , while the bottom panel ($\zeta = 11.25$) shows the distribution in the middle of the probe.

either side, to be deflected by the probe center. It should al between $f = 0$ and $f > 0$ in tl as one might expect analytic discretization of f on a finite the cylinder in terms of trian

C. Cu

As mentioned in Sec. IV A total) were made than illustr similar basic profiles were t With shorter probes, with sim overlap between end effects, g probe center, and a monotonic increases, the characteristic ce leading to two humps that wil out that the profile function, as local regression in Fig. 3, can t the following analytic express

$$\tilde{g}(\zeta) = C(1 + \tilde{h}$$

where

$$\tilde{h}(\zeta) = A(\zeta - \delta \cdot$$

$\tilde{g}(\zeta)$ is constructed so as to be probe center. In addition, each effects due to one end, appr respective end. For long prob end to the peak in \tilde{g} (this i including the α^{-1} term). Furt edge effects decay when mov A relates to the amplitude of $A\alpha^{-1} \exp(\alpha\delta)$. Due to the nor expected to be of order unity. and δ are determined using a v method, i.e., by minimizing residuals

Some other codes

- NASCAP-2K: US, proprietary, not widely available, different meshes and comprehensive physics.
- MUSCAT: Japan, proprietary, available at a cost.
- EMSES, Japan, proprietary, structured Cartesian mesh
- SPIS: Europe (ESA sponsored), tetrahedral unstructured meshes, freely available, comprehensive physics packages, written in Java.