Particle in cell simulations

PTetra workshop
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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

Limiatatations

- 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)

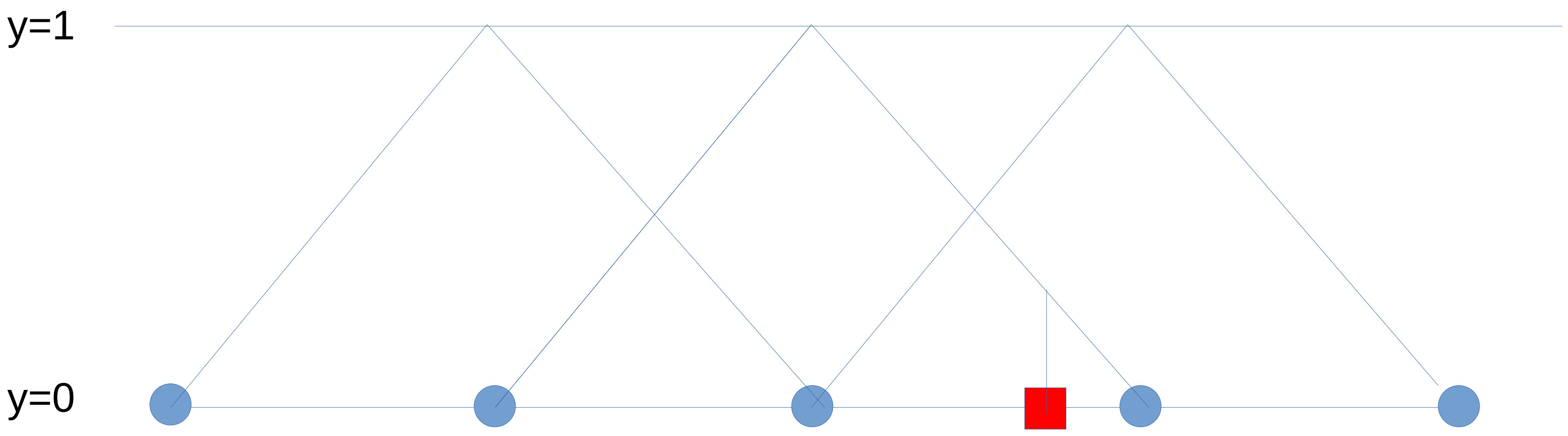
Hybrid approach

- 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 etrahedral adaptive in PTetra
- Boundary conditions,
  - Dirichlet (used in PTetra for all boundaries).
  - Newmann
  - Mixed

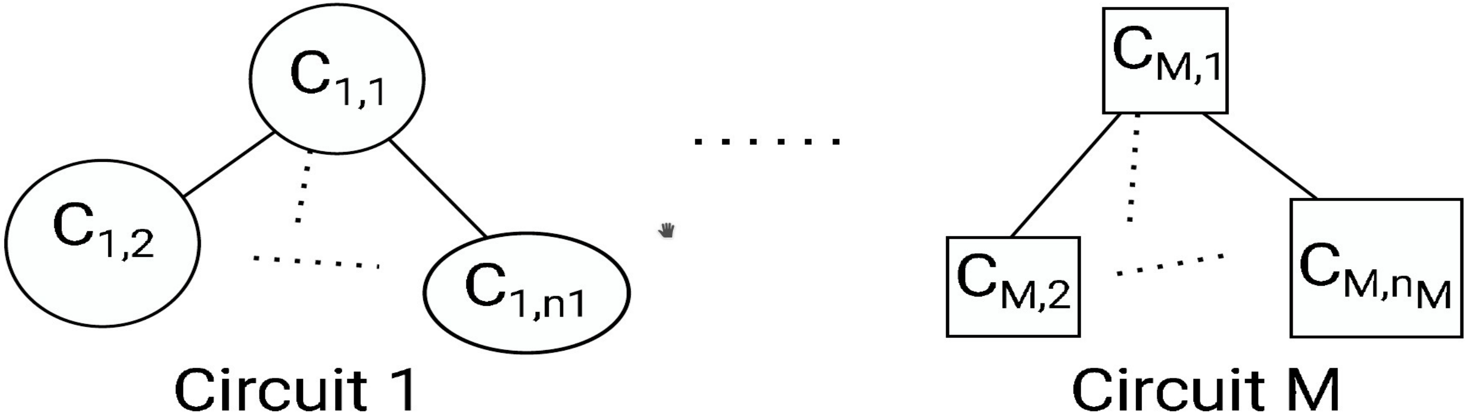
Boundary conditions in PTetra

- Dirichlet boundary conditions are set as seen in the satellite reference frame.
- V = (vxB).r at the boundary, from the motional electric field E = -vxB
- “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

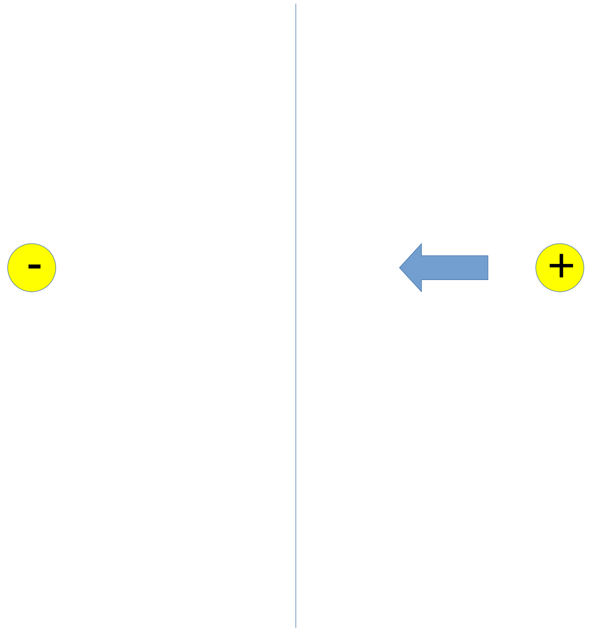


Alternatively, potentials can be fixed a priori, relative to the background plasma.

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.



V=0

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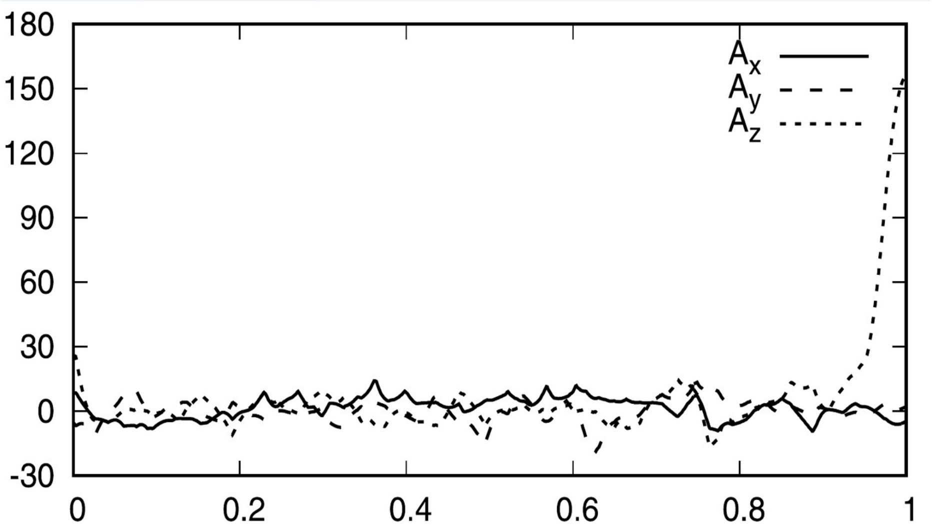
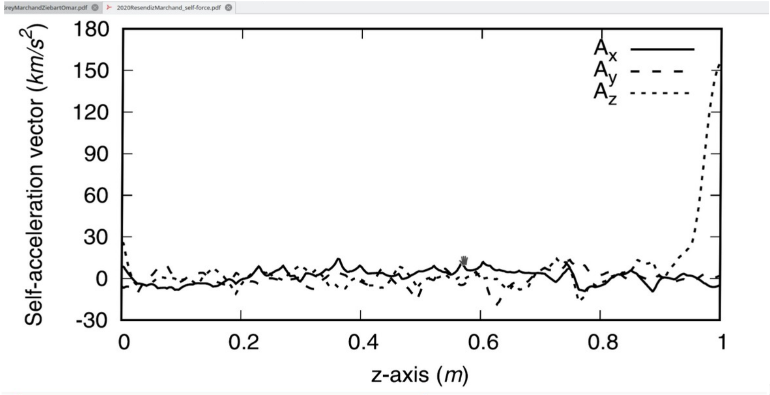
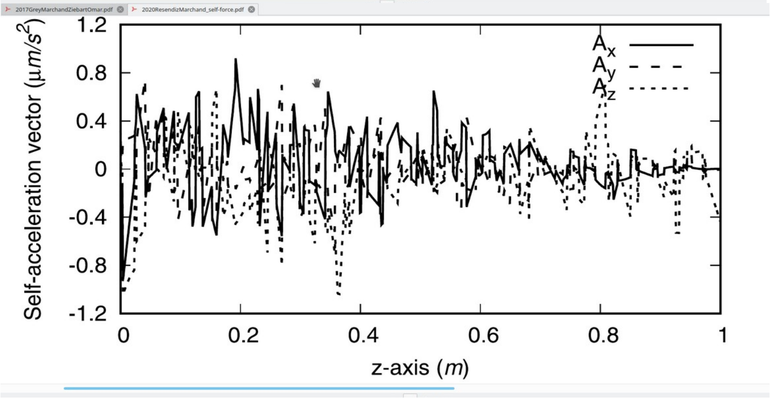
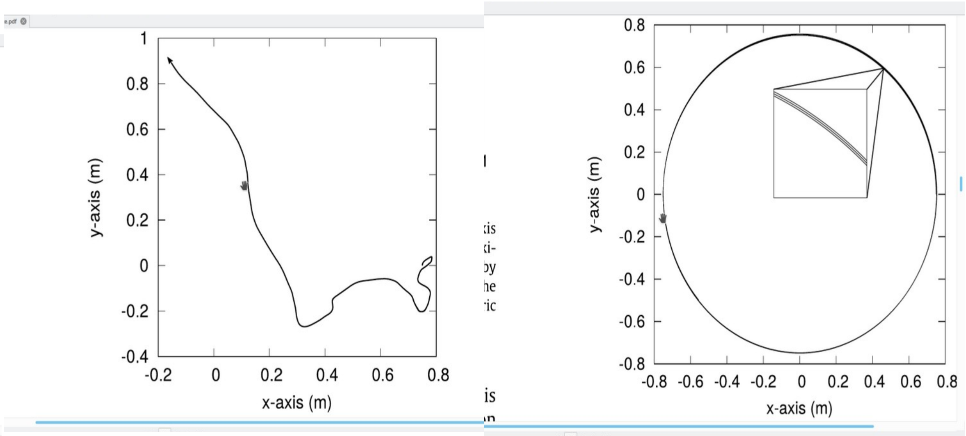


Self- and mirror force removal







Electron gravitation around a fixed proton at the centre of a 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

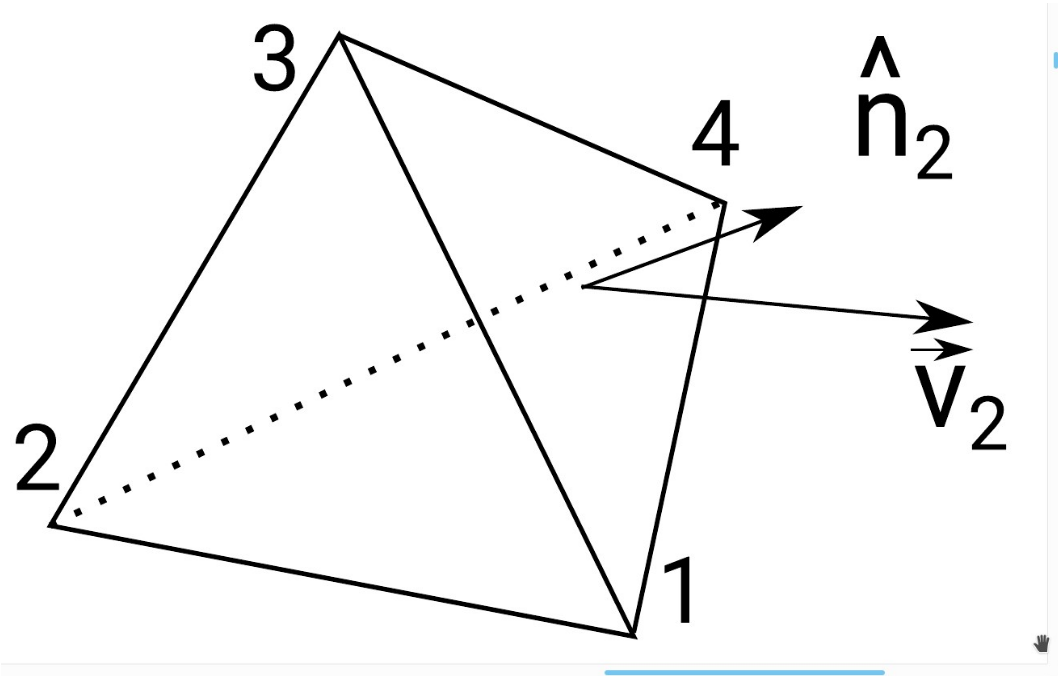
```
$coord
ncoord=      293984
    1   0.0000000000000000E+00   5.7499999999999996E-01   2.5000000000000001E-02
    2   0.0000000000000000E+00  -5.7499999999999996E-01   2.5000000000000001E-02
    3   0.0000000000000000E+00   6.9169999999999995E-02   7.8920999999999997E-01
    4   0.0000000000000000E+00  -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.

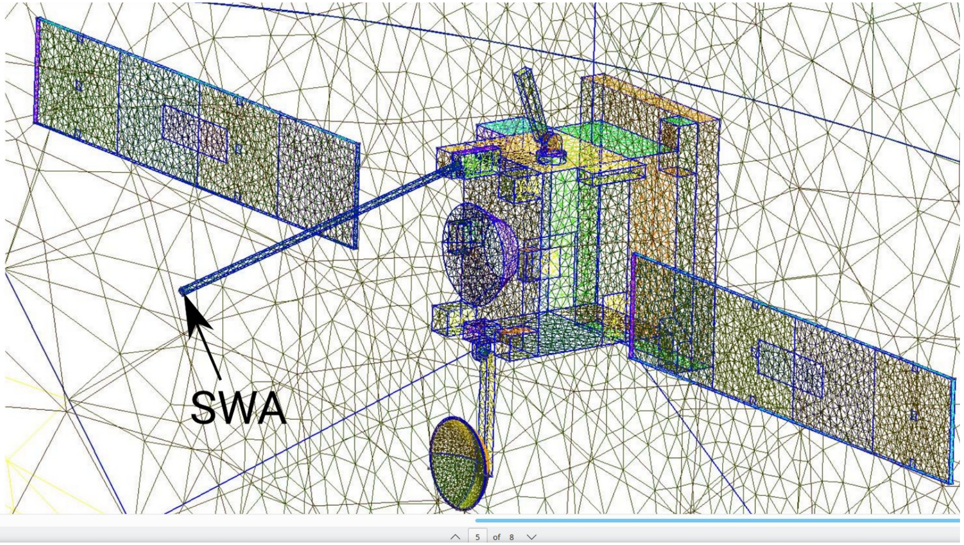
Finding a point in the mesh



Selected examples

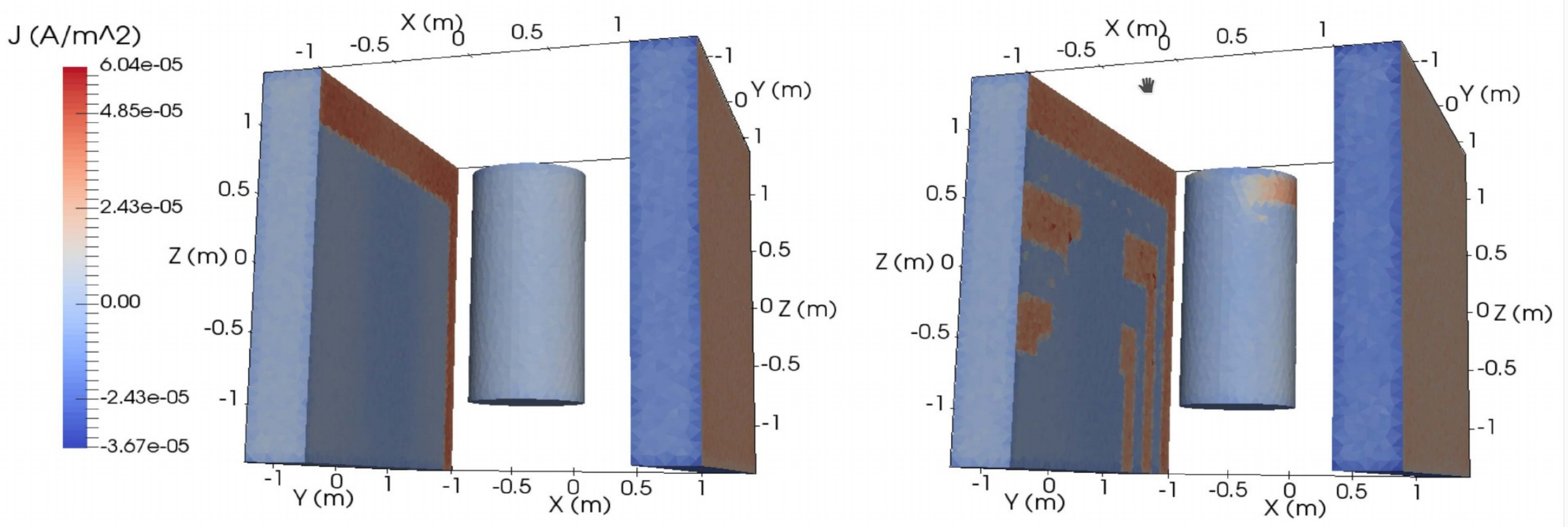
3D – mesh

- 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)

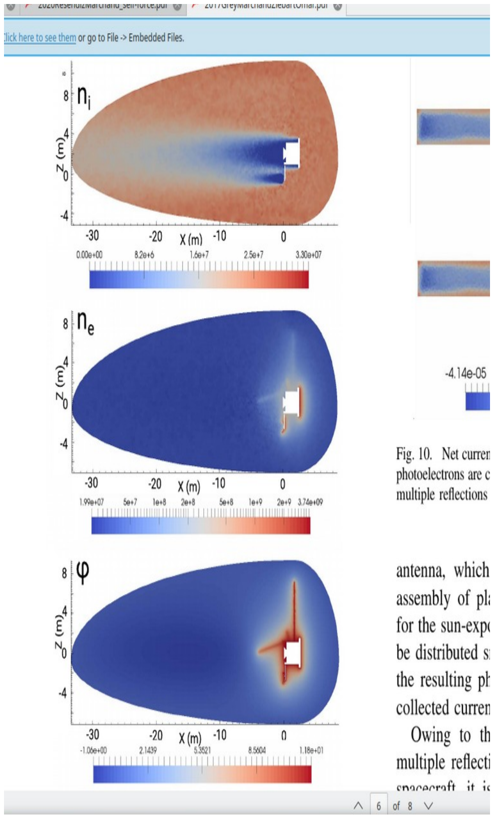
Photo-electron emission from multiple reflections

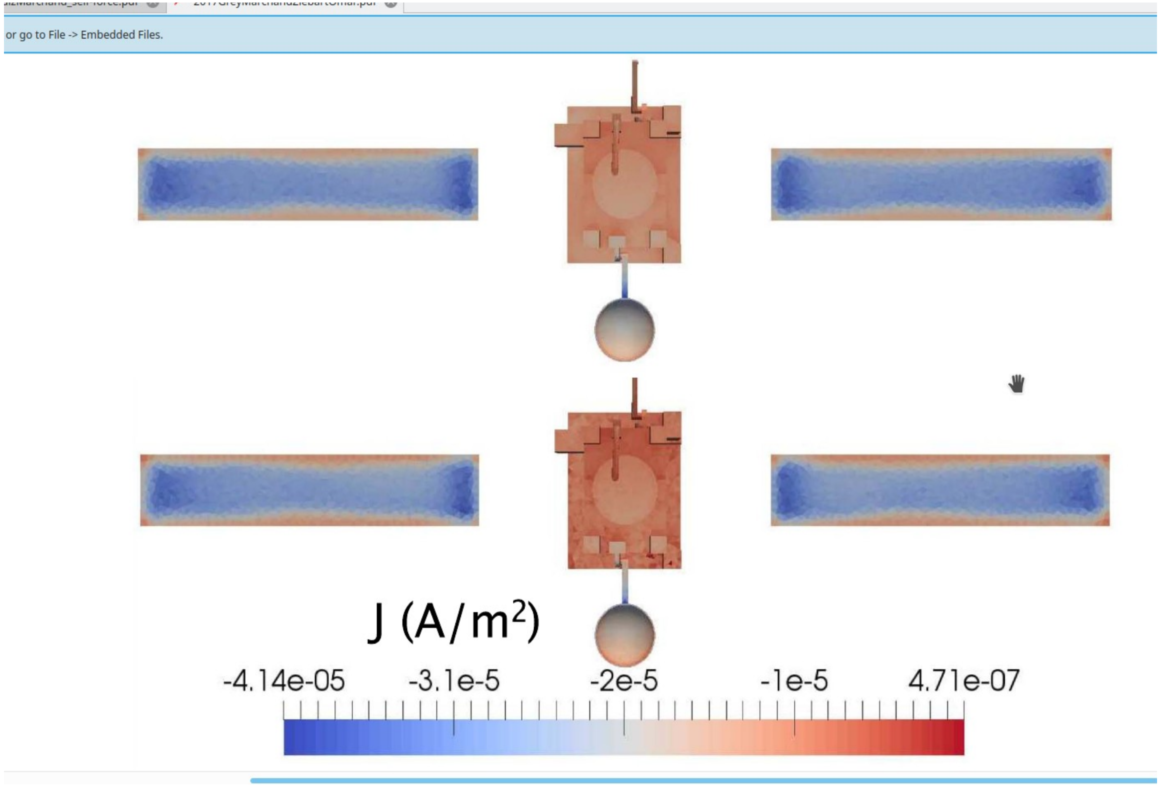


“Multiple reflections of solar radiation and photoelectron emission in satellite interaction with space environment”, R. Omar, MSc thesis 2016, https://doi.org/10.7939/R3PZ51S0B

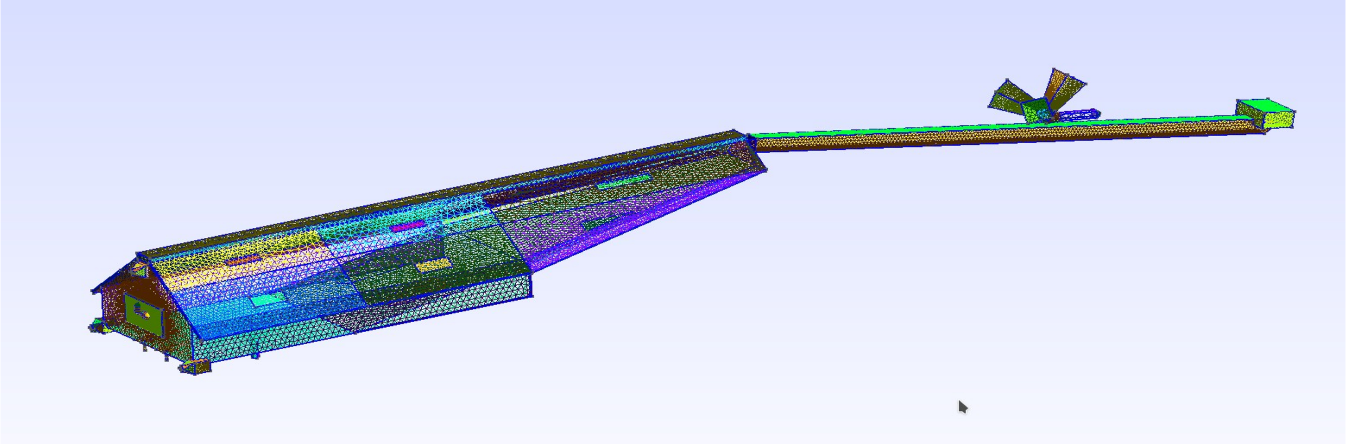
Application to Solar Orbiter

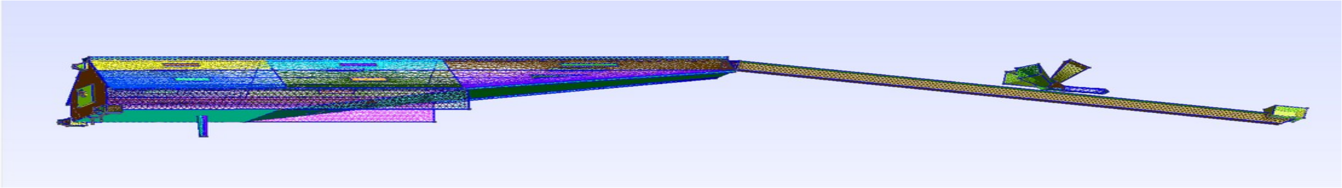
Grey, et al. IEEE Trans. Plasma Sci. **45** (2017)



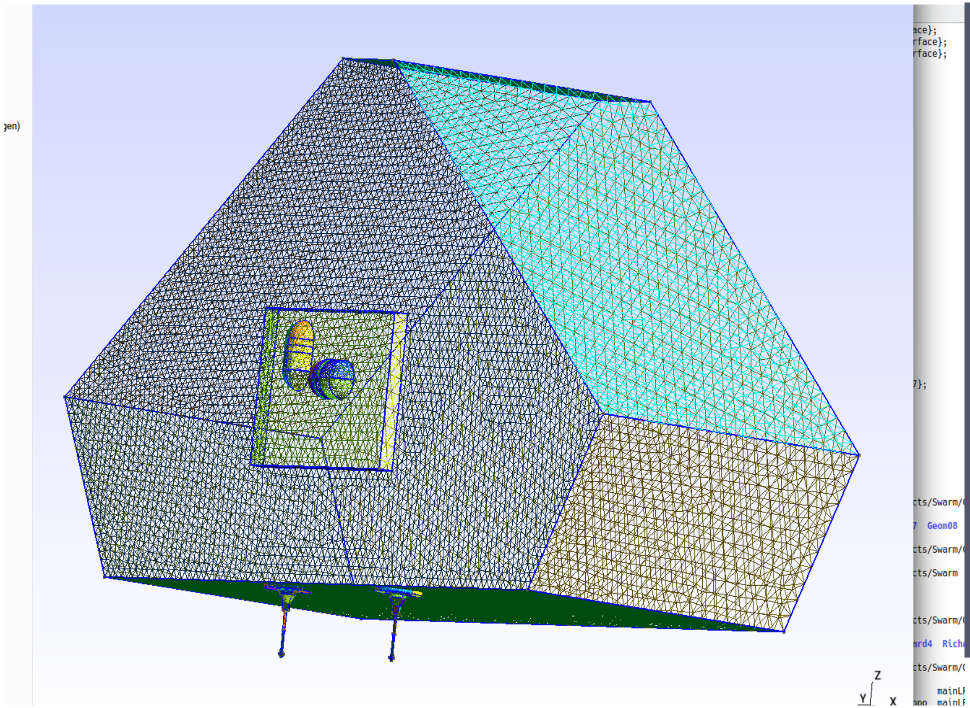


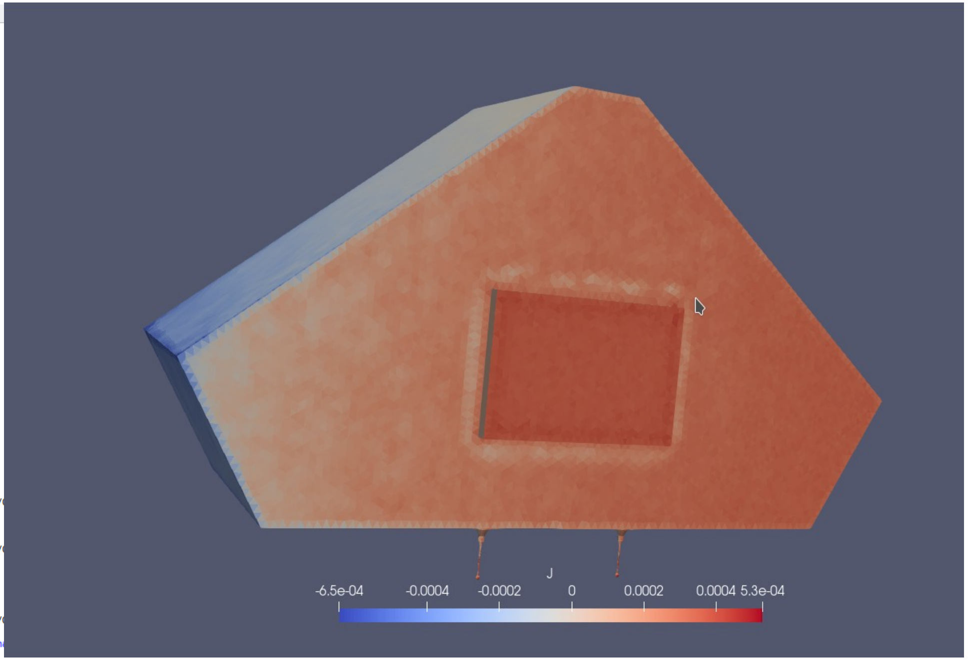
The swarm satellite





Simplified Swarm geometry



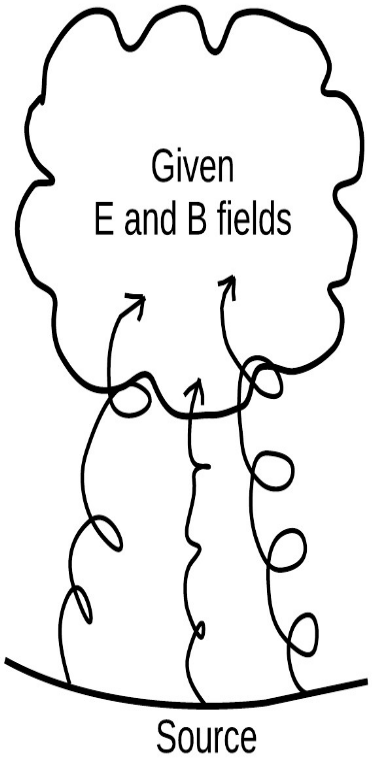


Post processing

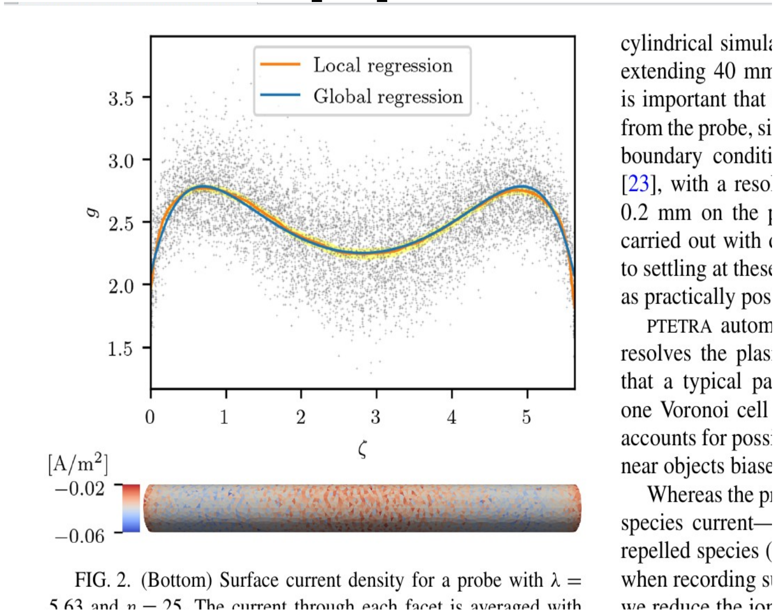
- Relaxation
- Visualisation
- Test-particle simulations
  - Used to compute particle distribution functions f
  - Moments of f are calculated numerically
    - Density, fluxes, energy density, pressure, heat flux, ...

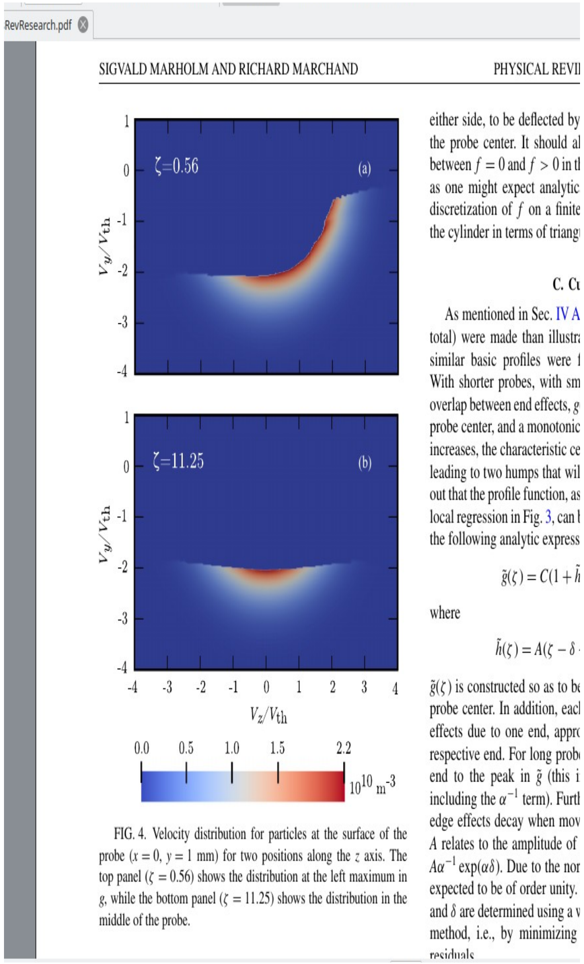
Test-particle simulation

- 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





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

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.