spacecraft-plasma interaction modelling

development needs

Richard Marchand
University of Alberta
Canada

Needs

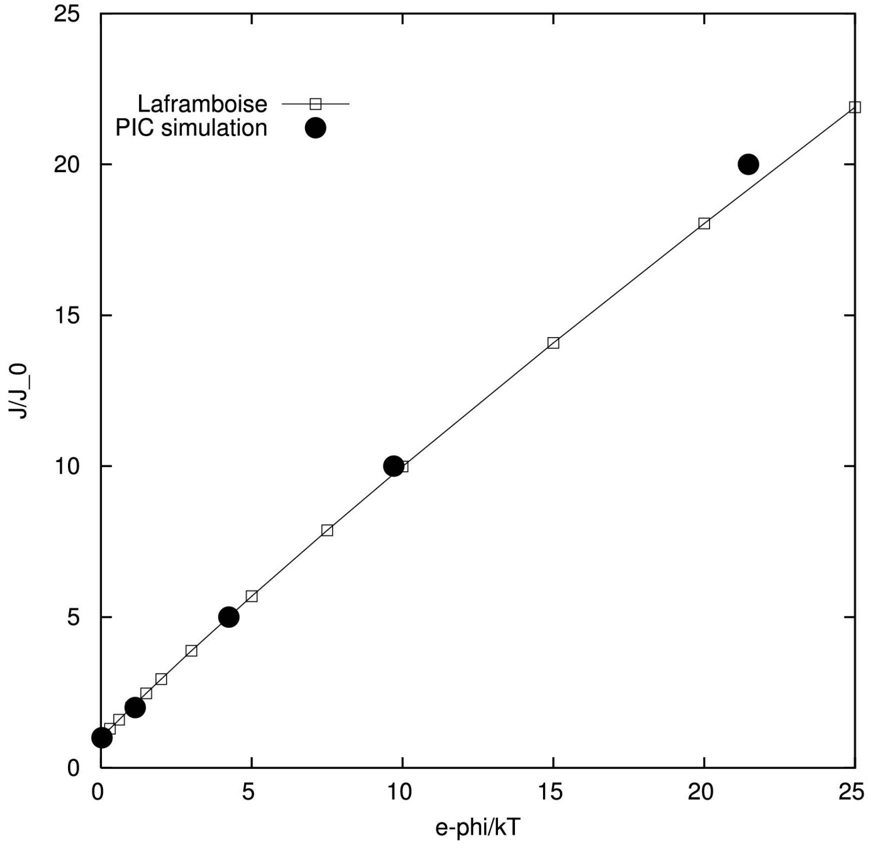
- Validity
- Physical completeness
- Accuracy
- Efficiency
- Interoperability and modularity
- Readability

Validity

- Numerical algorithms and their implementation must be validated.
- Standard validation procedures must be established and documented.
- Validations should be done periodically, and following major updates.
- Validation tests should be done by the developers, and users should be able to repeat them independently.
- Validation must bare on numerics (particle trajectories, solution of Poisson's equation, calculation of mutual capacitances, boundary conditions, etc.) and physics (the ability to reproduce analytic results or compare results with those obtained with other models).

Example 1: Characteristic of a positively biased spherical probe

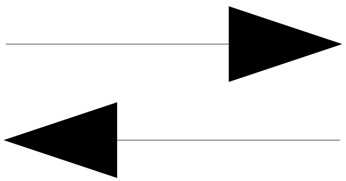
- Spherical probe of diameter 2cm.
- $n_e = 2.8 \times 10^{10}\ m^{-3}$
- $T_e = 0.2$ eV
- Debye length ~ 2cm
- Consider the normalised collected electron current vs. the normailsed applied voltage.
- Compare with results obtained by Laframboise



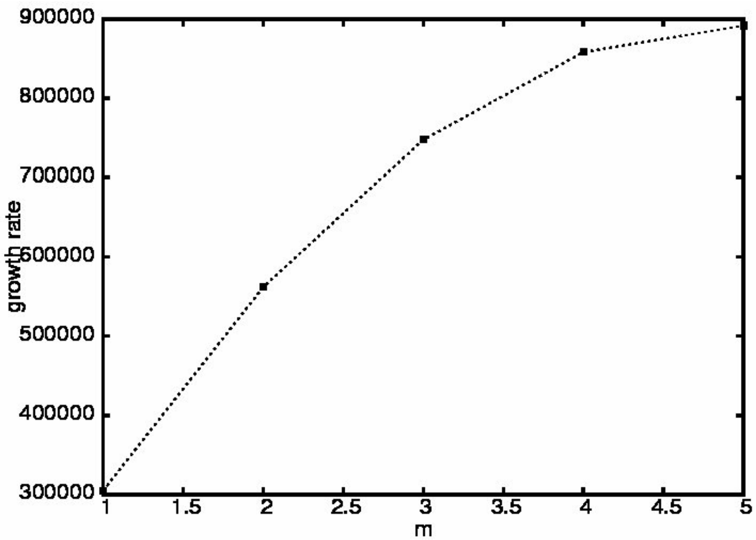
Obtained with Ptetra, a 3D PIC simulation model with tetrahedral mesh.

Example 2: Two-stream instability

- Consider a cube of extent 2x2x2 m^3
- Spatial resolution ~ 4.4 cm
- $n_e = 10^9\ m^{-3}$, $T_e = 10^{-4}$ eV, $V_{ez} = \pm\ 10^5$ m/s

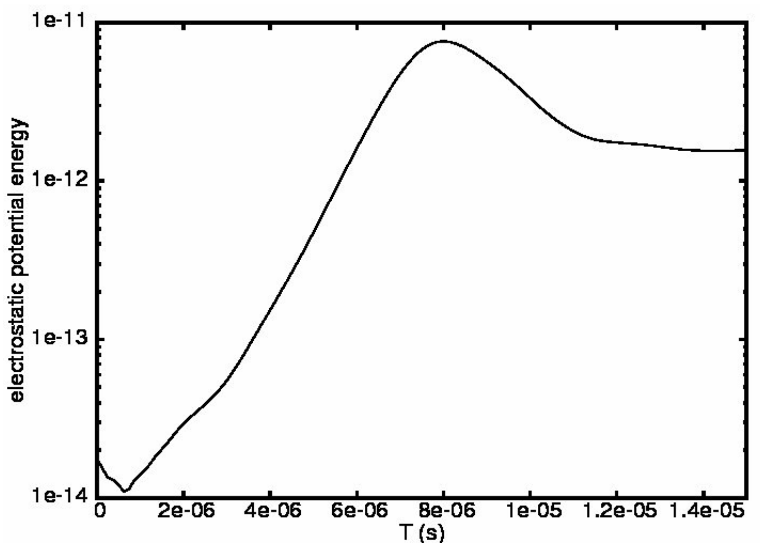


$V_e = 10^5$ m/s
$n_e = 10^9\ m^{-3}$



Analytic growth rates for different m modes

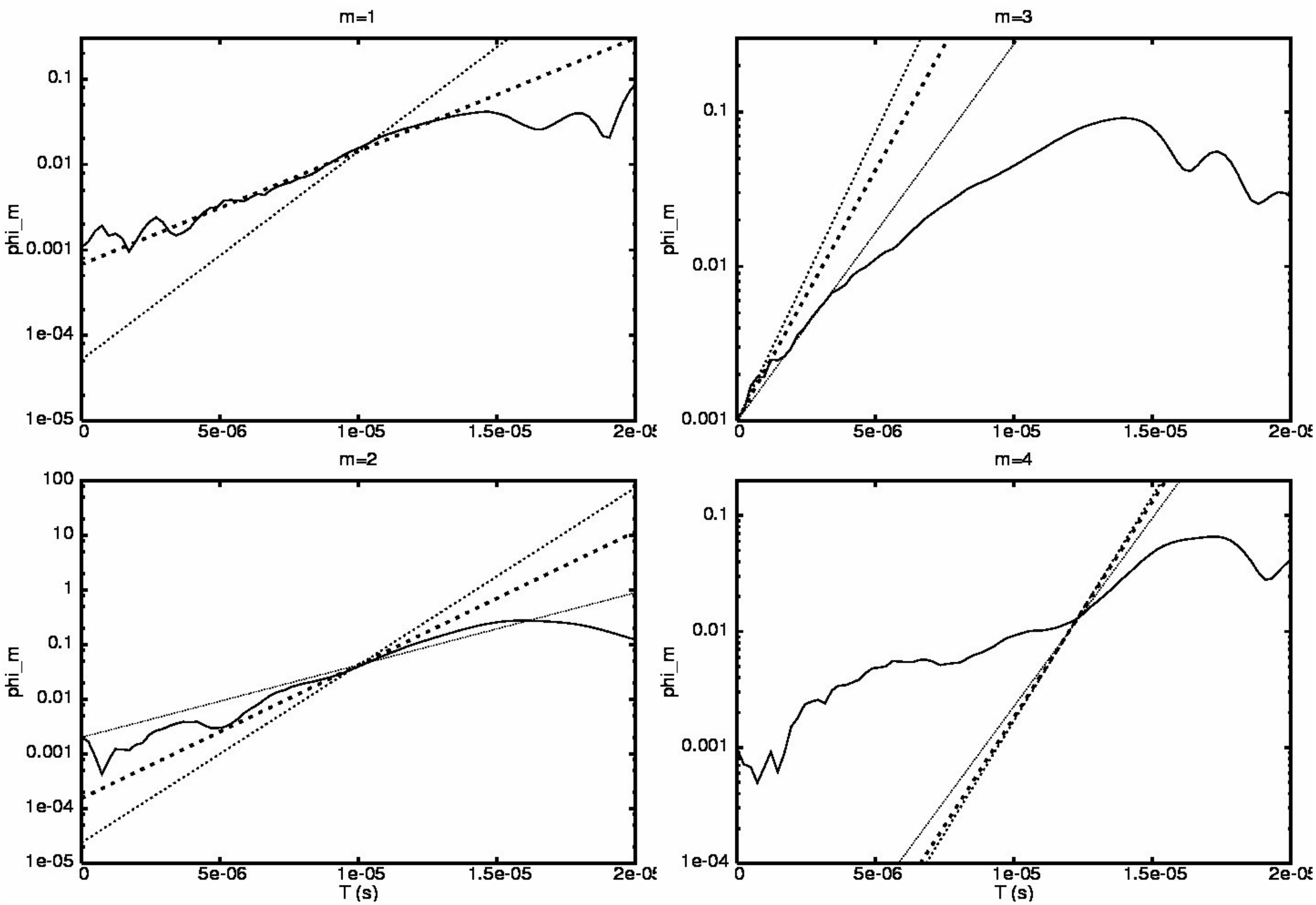
Example 2: Exponential growth of the total electrostatic energy



Obtained with Ptetra, a 3D PIC simulation model with tetrahedral mesh.
Number of particles: 2 million per electron beam.

- The total electrostatic energy grows nearly exponentially until saturation at ~ 8μs
- This growth is the result of the superposition of several unstable m-modes
- The growth of individual modes is obtained from a 3D Fourier transform of φ.

Example 2: Comparison between computed and analytic growth of different modes



Growth rate Corresponding to m

Growth rate Corresponding to m+1

Growth rate Corresponding to m-1

Example 2: Observations

- Exponential growth of the instability is visible, over more than one order of magnitude for the lower modes (m=1, 2).
- For these modes, there is agreement between the linear growth rates and the observed exponential growth phase.
- Higher mode numbers don't show a clear exponential growth rate. This is likely due to the increase relative noise for these modes, and to their lower saturation levels.

Physical completeness

Most (ideally all) important physical effects must be accounted for.

- Material properties (conductivity, self/mutual-capacitances, photo/ secondary electron emission, work functions, …)
- Volume charge density and surface charge densities are straightforward for conducting surfaces.
- Surface charge densities on dielectrics are more problematic. Models probably need to be developed.
- Static magnetic fields. They complicate the sheath and wake structures. They may probably require larger simulation domains, ad hoc transport perpendicularly to **B**, and better empirical boundary conditions.
- Time varying magnetic fields: Solve the full set of Maxwell equations instead of only Poisson.

Accuracy

Accuracy needs to be quantified for the various numerical algorithms used. To the extent that it is practical, choices should be available to the user.

- Poisson solver: Gauss-Seidel, GMRES, ..., convergence criteria
- Electric field: piecewise constant per element or continuous. The former allows analytic particle trajectories, but the latter may give more physical solutions.
- Particle trajectories: analytic if possible, or leapfrog
- Models should come with standard diagnostics to monitor robustness and overall accuracy (conservation laws)

Efficiency

- Large PIC simulation **MUST** make use of parallel computing possibilities available on modern computers and desktops.
- For C, C++ and FORTRAN programs, this is possible with OpenMP (shared memory) and MPI (clusters).

Other desirable features

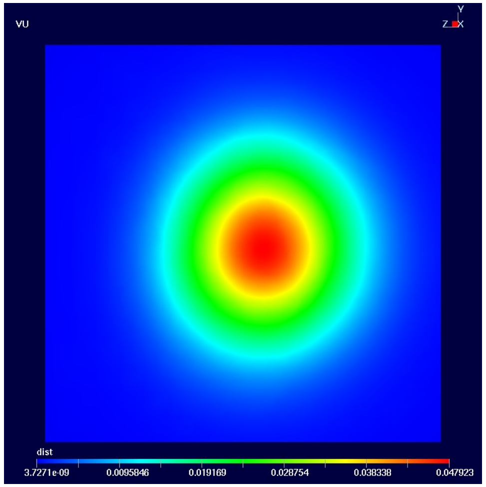
- The possibility of generating restart files at the end, or at any time, during a simulation
- The possibility to end a simulation gracefully at any time (thus producing normal diagnostics, output files and optionally, a restart file).
- The possibility of continuing a simulation from a restart file, with the option of changing some input parameters (the parameters that may be changed must be selected with caution).

Interoperability and modularity

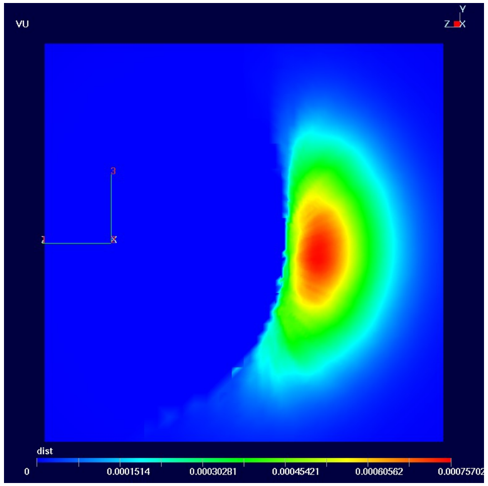
- Enable and facilitate the use of other software for providing input and for analysing (post processing) results.
  - Mesh generation (standalone gmsh, gambit, ...).
  - Visualisation (TECPLOT, Vu, ...).
  - Postprocessing with particle backtracking, or other methods.
- Concentrate on the specificity and strength of PIC satellite-plasma modelling and, as much as possible, use available software (open or proprietary) to do ancillary tasks.
- Enable and facilitate the use modules from other models, possibly written in a different programming language.

Example: Distribution function near IAP on DEMETER, from particle backtracking

Φ~-0.5^0
θ~-0.4^0

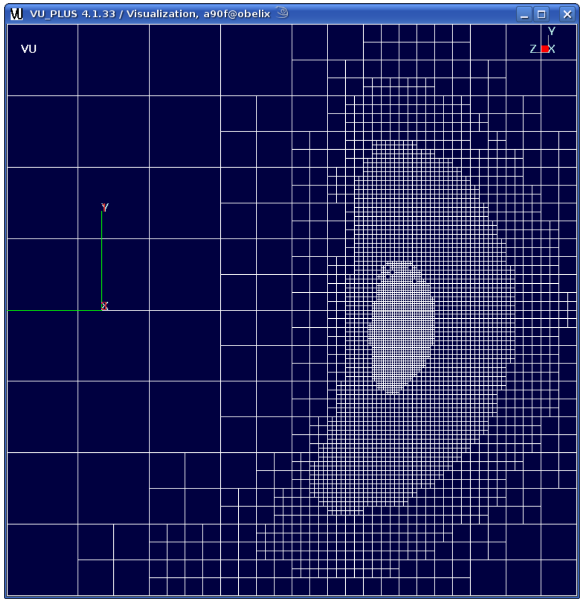


O$^+$

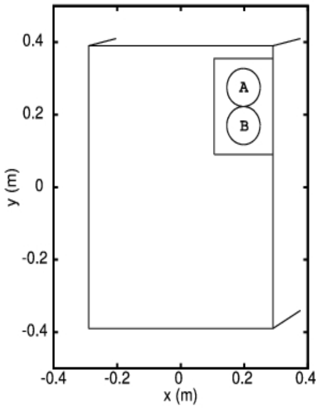


H$^+$

Φ~-4.3^0
θ~-3.8^0



- The computed electrostatic potential is used *a posteriori* by a particle backtracking code, to compute the distribution function at given locations (A in the figure).
  - Use is made of an adaptive grid in momentum space, based on octree decomposition.
  - From there, moments can be computed and compared with observations (e.g., the angle of incidence of the plasma flow).
  - Advantage: Other than the errors in the computed electrostatic potential, this method is free of statistical noise.



Readability

- Provide high level documentation describing
  - the physics
  - the numerical algorithms
  - examples that can be reproduced by the reader
- Documentation should be comparable to (and probably should be the basis for) articles in Comp. Phys. Comm. or J. Comp. Phys.