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3D sparse PIC modeling of a Hall thruster: Comparisons with experimental results

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This work presents a new approach of the explicit electrostatic Particle-In-Cell (PIC) method. It uses the sparse grids as an alternative representation of the full grid domain. These grids are built with coarser anisotropic and isotropic grids through a combination technique. Change of basis allows to move from the sparse grid to the regular grid and vice versa. The method when integrated to the PIC scheme gives significant speed up in computational time by reducing the number of particles needed to reduce the statistical noise, and by making Poisson equation solved on coarser grids, especially for 3D simulations. Drawbacks of the method are that the combination technique introduces an additional grid approximation of the solution it reconstructs, so that the sparse grid and combination technique must be chosen wisely depending on the physics it aims to represent. Also, sparse grid methods are yet to be adapted to complex geometries and are limited to cubes in this work. As this work aims to compare numerical simulation with experimental data of a Hall thruster, adaptation of the method has been made to represent both the plume where experimental measures are taken and the channel of the Hall thruster. First results in transient state are presented for a 3D sparse PIC simulation, and computational time estimated to 20 days for fully converged simulation with electron density reaching $2 \times 10^{18} m^{-3}$.

I. Nomenclature

PIC	=	Particle-In-Cell
N	=	Grid level
G_r	=	Number of cells in the regular grid
M	=	Number of points in each direction for a grid level N
G_{sparse}	=	Number of cells in all sub-grids
$G_{hierarchical}$	=	Sparse grid, namely hierarchical grid
$G_{I,J}$	=	Two-dimensional sub-grid of level I in horizontal direction and J in vertical direction

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II. Introduction

Standard electrostatic Particle-In-Cell (PIC) method uses a kinetic model to compute particle trajectory and a grid approach to solve the Poisson equation to obtain electric potential to the grid. Then electric field is computed to particle position by differentiating the electric potential and interpolation. This explicit approach introduces constraints of grid spacing and time step related to the resolution of electron properties (Debye length and inverse of plasma frequency). These inner limitations induce exponential dependence on dimension for numerical complexity and large number of particles to compute to reduce statistical noise which result in high computational time in three dimensional simulations. Such problems invite us to look into an alternative sparse PIC method exchanging a significant increase in computational time with an additional approximation over the grid potential.

III. Gains in Sparse PIC Method

The sparse PIC method defines a hierarchy of anisotropic and isotropic sub-grids with coarser mesh ([1] and [2]). It applies to initial grids with $2^N + 1$ points in each direction of space, where N is the grid level, and thus are limited to simple geometry such as square in two dimensions and cubes in three dimensions, up to the author's knowledge. Charge deposition is done on these sub-grids as well as solving Poisson equation. The ratio between the total number of cells in a regular grid and the number of cells of these sub-grids reaches a factor 1000 when considering a 512^3 -cells three dimensional regular grid and scales as shown in Fig.1 . It means that there are less operations to make for charge deposition as well as avoiding solving Poisson equation on fine grids, resulting in a direct gain in computational time and making the use of efficient direct solver possible. Less cells means also less particles if we keep the same number of particles per cell. Sparse grids have proven to be reducing statistical noise ([3]) and thus have a good synergy with PIC algorithm.

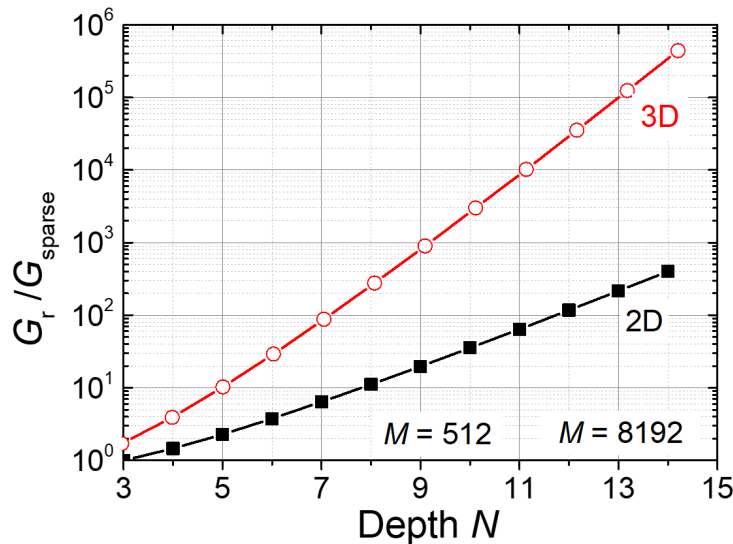


Fig. 1 Scaling of the ratio of regular grid number of cells over sparse method number of cells with the grid level N . M is the number of points in each direction for grid level $N=9$ and $N=13$.

After getting potential on these sub-grids, the coefficients expressed in the nodal basis are moved to the hierarchical basis thanks to a hierarchization algorithm. In this basis, an appropriate sum of the sub-grids, namely the combination technique, see example in Fig.2, results in the construction of the sparse grid also called hierarchical grid. This first part of the algorithm is easily parallelised on OpenMP/MPI architecture. Though its principle is based on the cancellation of errors in the coarse grids solving, the combination technique used can be critical to the reconstruction of the solution as it adds an additional grid error. The choice of the appropriate sub-grids used for combination technique remains a topic of interest to capture the whole plasma physics in the Hall thruster and is also being investigated but let for future prospects in this work.

Then a dehierarchization algorithm transforms the hierarchical solution into the nodal solution on the regular grid, allowing to perform standard differentiation on the regular grid to compute electric field and interpolate it to the particle

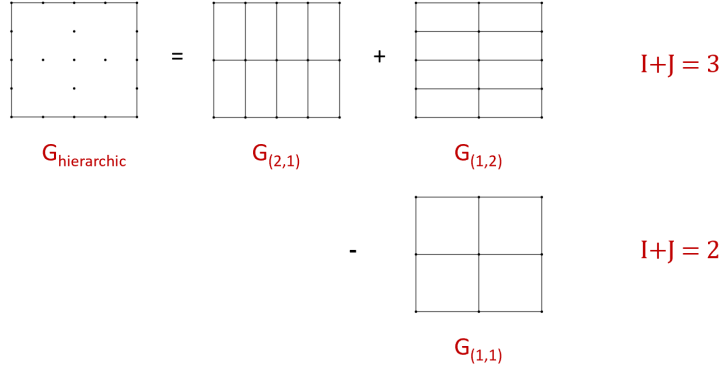


Fig. 2 Example of combination technique in two dimensions for grid level $N=2$

position. Using this implementation allows to avoid interpolating electric field for all sub-grids which are dozens in number in three dimension; for instance, they are 64 for a $N = 7$ grid. However it is more difficult to parallelize on OpenMP/MPI architecture, and other solution using GPU might be considered.

The rest of the algorithm is the same than standard PIC scheme. Particles are pushed with the Boris algorithm and no collisions are taken into account in this work. It is important to notice that the sparse PIC algorithm requires far less memory usage than the standard PIC algorithm, making memory requirements not critical.

IV. Towards comparison with experimental data

The experimental setup of the PIVOINE 2021 measurement campaign at ICARE, Orléans, calls for numerical simulation adaptation. Incoherent Thomson scattering measurements along radial and azimuthal directions of a PPS 1350 Hall thruster were made for Xenon and Krypton and could give the electron density, temperature and drift velocity profiles. Considering one measure needs 10 minutes of data acquisition (6000 laser pulses with an acquisition window of 10 nanoseconds every 0.1 second), simulation must have converged to give time averaged profiles.

Also, laser measurements catch photons coming from a small volume equivalent to a cylinder of 0.9 mm of diameter and 1.5 mm of length due to glass fibers and optics so that profiles must be space averaged.

Measurements being made out of the canal at 1 mm of distance from the exit, the plume must be part of the simulation domain. Specific functioning regime has been used for the campaign with 130V at the anode and a radial magnetic field gradient has been measured. This implies that the source term in the Hall thruster simulation is not uniform in the radial direction, which makes it difficult to model as it is often a fixed parameter of the simulation. Results of the experimental campaign are presented in [4] and tend to show a divergence of the plume with outer electron density and temperature being superior to inner one.

V. 3D sparse PIC computation of a Hall like thruster

All figures in this section are presented in Appendix: Figures for clarity, with international unit system. The simulation domain used for this preliminary work is being represented in Fig. 3 and 4. Key simulation parameters are presented in Table. 1. Initial density profiles are uniform for both ions and electrons. For each ion leaving the domain, we inject an electron-ion pair with cosine distribution in the ionization zone. A neutralization current equal to the difference between the electron and ion current at the anode is injected close to the cathode like in [5]. We impose periodic conditions in the azimuthal direction and Dirichlet conditions in the others.

Figures 5,6,7 and 8 show transient state of the Hall thruster discharge at one microsecond obtained with 3D sparse PIC simulation for ion density profile and the azimuthal electric field associated in the axial azimuthal plane, and axial electric field and potential in the axial radial plane. Comparison with other codes ([5] and [6]) fully converged ExB Hall thruster discharges will be performed in future work.

Table 1 Key simulation parameters.

Grid level	8
Simulation domain	$4.5 \times 1.5 \times 3 \text{ cm}^3$ – four cubes of $1.5 \times 1.5 \times 1.5 \text{ cm}^3$
Channel	$1.5 \times 1.5 \times 1.5 \text{ cm}^3$
Plume	$4.5 \times 1.5 \times 1.5 \text{ cm}^3$
Source term	$z=0.93 \text{ cm} - 1.5 \text{ cm}$. Cosine both directions radial x and axis z
Axis-position of cathode electron injection	2.9cm
Anode potential	200V
Cathode potential potential	0V
Magnetic field maximum at the center of the channel	100G
Initial density	$5 \times 10^{16} \text{ m}^{-3}$
Time step	$5 \times 10^{-12} \text{ s}$
Final time	$1 \times 10^{-6} \text{ s}$
Computational time	1 day and 1 hour

VI. Conclusion

This work has presented the Sparse PIC method adapted to a three dimensional Hall thruster model and shown qualitative figures in transient state. As a recent numerical technique, many questions still remain. We address several points of discussion and considerations:

- 1) Gains in computational time depend on level of sparse grids with the current optimization and domain (3.8s/dt for N=9, 0.46s/dt for N=8 , 0.08s/dt for N=7 with 1440 cpus shared between 80 sockets). Charge deposition costs more than 75% of the computational time for $N \leq 7$ and remains important for $N \geq 8$ as the number of sub-grids grows too.
- 2) Sparse cubes used as elementary brick to represent some types of geometries have slight effects at cube frontiers and this alternative method needs investigation. It also needs to be adapted to more complex geometries, such as the curved walls of the Hall thruster.
- 3) MPI/OpenMP architecture might not be relevant for dehierarchization algorithm which reconstructs potential on the regular grid for all sockets to avoid expensive MPI communications.
- 4) The model of the Hall like thruster will be completed for taking into account non-uniform radial ionization, and investigation over electron secondary emission effects will be pursued.
- 5) Use of different combination techniques can be investigated to get more precision in the results, especially with truncated/offset approaches ([7]).

We would like to emphasize that this work aims to compare numerical Sparse PIC simulation with experimental data and that any comparison with other PIC simulation is welcomed.

Appendix: Simulation Figures

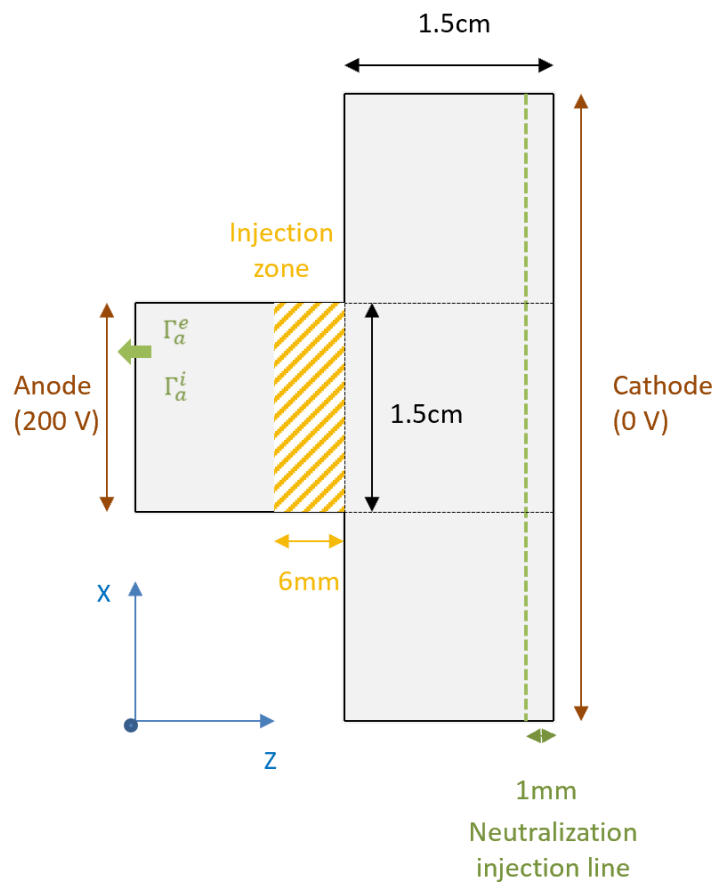


Fig. 3 Simulation domain - 2D axial/radial cut

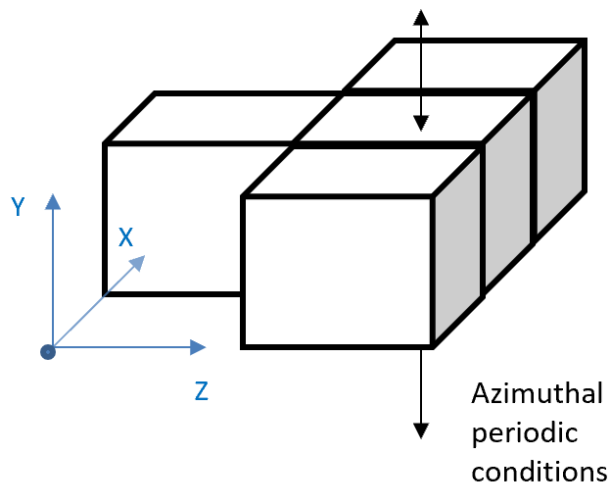


Fig. 4 Simulation domain - 3D view

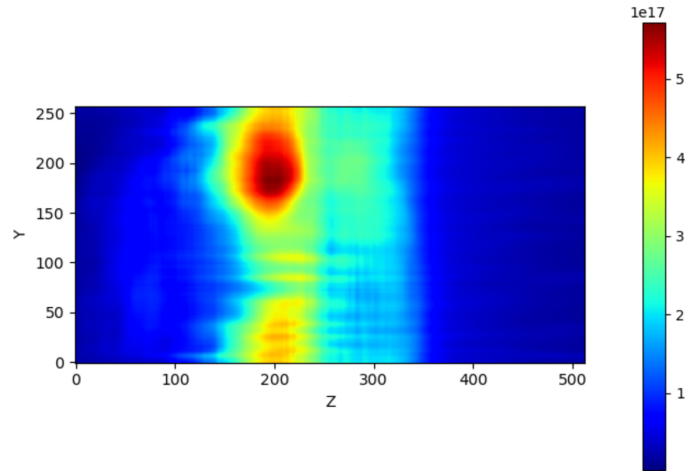


Fig. 5 Ion density 2D axial-azimuthal profile.

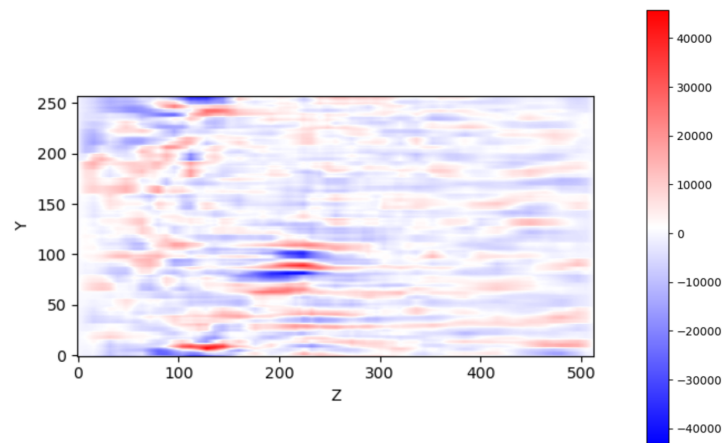


Fig. 6 Azimuthal electric field 2D axial-azimuthal profile.

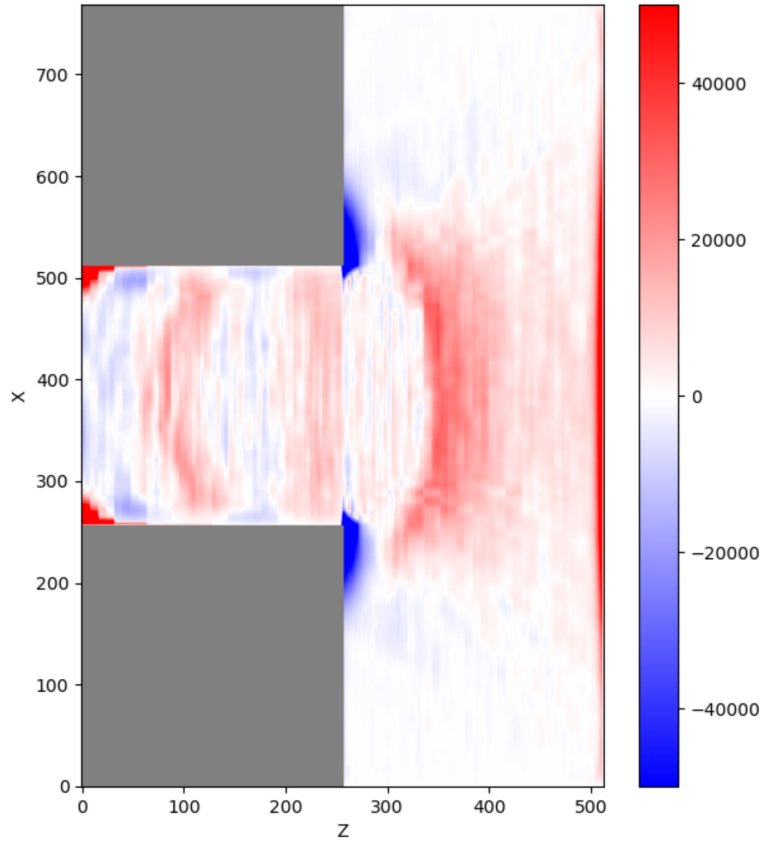


Fig. 7 Axial electric field 2D axial-radial profile.

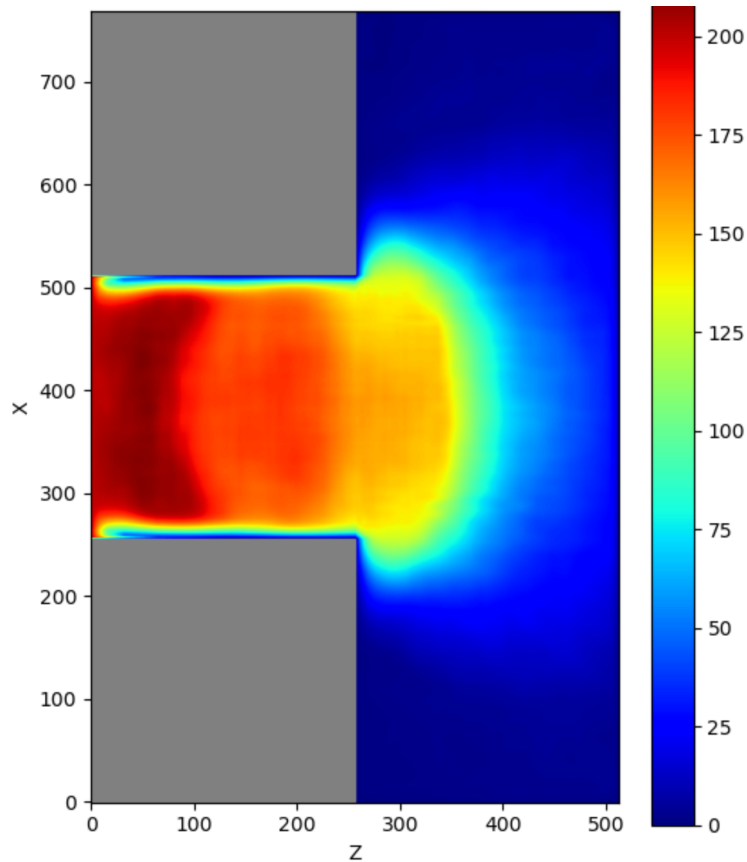


Fig. 8 Potential 2D axial-radial profile.

Acknowledgments

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