Development, validation and benchmarking of LPPic for **ExB** discharges.

A. Tavant, V. Croes, R. Lucken, T. Charoy, A. Bourdon, P. Chabert

ExB workshop, PPPL, November 1-2, 2018

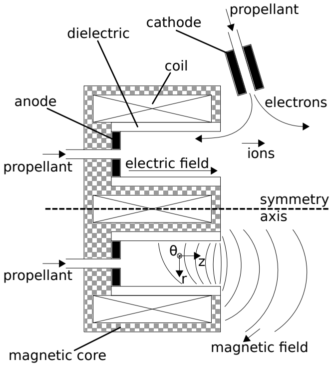
Introduction

What is **LPPic** ?

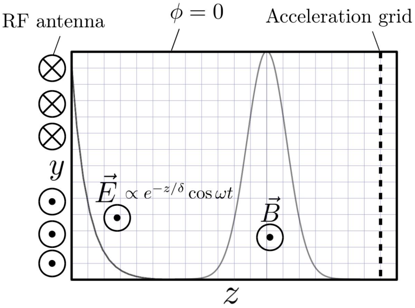
- Particle in Cell simulation code of magnetized plasma
- Started in 2014
- Particular care taken on computing performance and model validity

Plasma for space propulsion

Hall effect Thruster and Pegases



Hall Effect Thruster



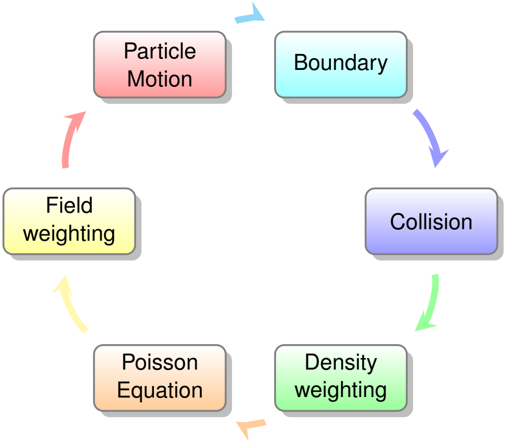
Gridded Thruster: Pegases

LPPic: presentation

PIC loop

Standard Particle in Cell simulation:

- Explicit
- Electrostatic
- Numerous gases
  - Helium
  - Argon
  - Krypton
  - Xenon



- **Electrostatic** $\Rightarrow$ Solving Poisson Equation (*Hypre* or *PetsC*)
- **Particle Motion** : Boris scheme [1] or Leapfrog [2]
- **Cloud-in-Cell** : bi-linear interpolation
- **Collision** Monte-Carlo algorithm[3] using LXcat[4] data base

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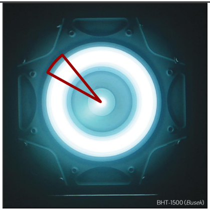
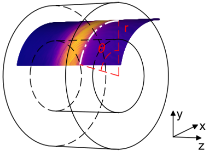
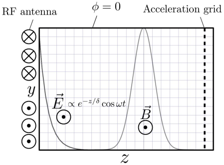
[1] Boris 1970.
[2] Birdsall and Langdon 1985.
[3] Vahedi and Surendra 1995.
[4] Phelps 2005.

LPPic: presentation

Simulation cases

Simulation case	HET: $R - \theta$ (case 2b)	HET: $Z - \theta$ (case 2a)	Pegases
			
Computational time with 360 CPUs	$10 \mu s \rightarrow 50h$	$20 \mu s \rightarrow$ 2 weeks	$40 \mu s \rightarrow 20h$

Verification

assessing the **numerical accuracy** of the solution to a computational model.[5]

- Convergence of a solver
- Unit Test or Test cases

Validation

addresses the physics modeling accuracy of a simulation by comparing it with reality (experiments, theory).[5]

- Mezzanine tests
- Benchmarks

[4] Oberkampf and Trucano 2008.

Unit tests

- Poisson solver
- Particle Pusher
- Boundary conditions
- Monte-Carlo Collision
- Diagnostics
- ...

Verify :

- physical results vs. analytical solutions
- validity domain of the module
- error (e.g $\mathcal{O}(\Delta_x)$, *etc.*)

Unit tests

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- ...

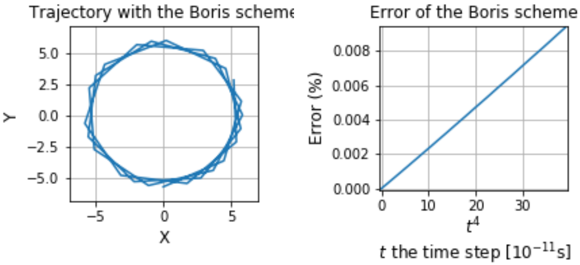

Figure: Verification of the Boris scheme

Unit tests

- Poisson solver
- Particle Pusher
- Boundary conditions
- Monte-Carlo Collision
- Diagnostics
- ...

- Fast (even on PCs)
- Systematic (with Continuous Integration tools)

Back reproducibility: Can we reproduce previous results ?

- "Verify" all of the code
- We have three cases (HET R-θ, Z-θ, Pegases)
- Longer to run (few days), need cluster

Validation : comparing the code results with...

Theory : Easier

- Simplified cases can be simulated
- Can validate parts of the code
- [M. Turner (2016) *PSST*]

Experiments: more Difficult

- Some physics is missing
- Large uncertainties
- "What to compare ?"

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Other codes: **Intermediate**

- Easy to compare the results
- What if the results differ ?

Comparing with other codes: Benchmark
1D CCP Benchmarks [M. Turner (2013) *PoP*]

- **5+** independent PIC codes
- **4** cases with different parameters
- Quite complet:
  - Poisson (1D)
  - Pusher (Leapfrog)
  - Wall boundary conditions
  - MCC ionization (He)
- Validated: error $< 5\%$

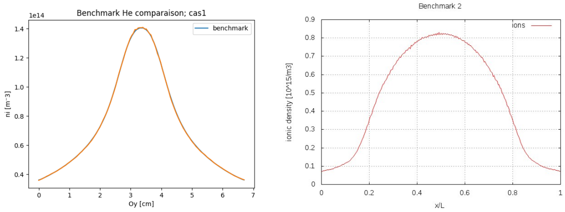

Figure: Results of the benchmarks n° 1 & 2

Comparing with other codes: Benchmark

2D CCP Benchmarks (*currently developed*) [5]

- Similare to 1D Benchmark :
  - Poisson (2D)
  - Pusher (Leapfrog)
  - Wall boundary conditions
  - MCC ionization

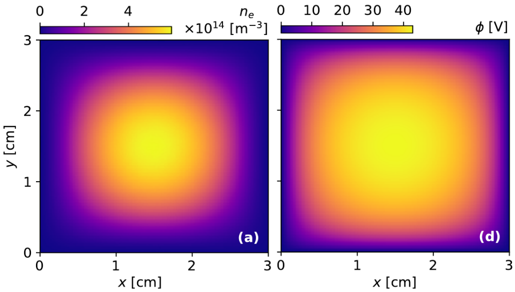

Figure: Proposition for the 2D CCP He benchmark

Turner et al., GEC 2018

How to Validate new results?

When :

- No theory describe the whole simulation
- The models implemented are not validated

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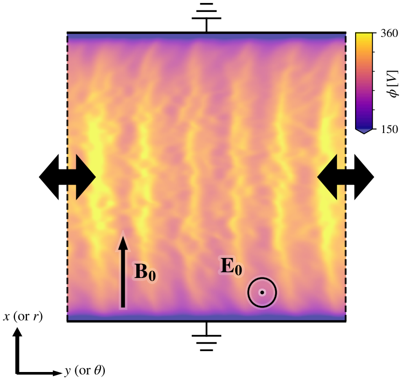
Idea: validate parts of the results with quantitative comparison with theory

LANDMARK case 2B:

R-θ plan of an HET

- 2D simulation of a steady state discharge (Axial boundaries + MCC)



Results of the 2D PIC HET simulation [7,8]

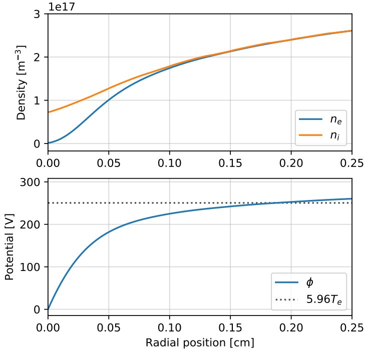
[7] V. Croes (2017), *PSST*

[8] A. Tavant (2018), *PSST*

LANDMARK case 2B:

R-θ plan of an HET

- 2D simulation of a steady state discharge (Axial boundaries + MCC)
- Observed sheath: coherent with Child-Lamguir law



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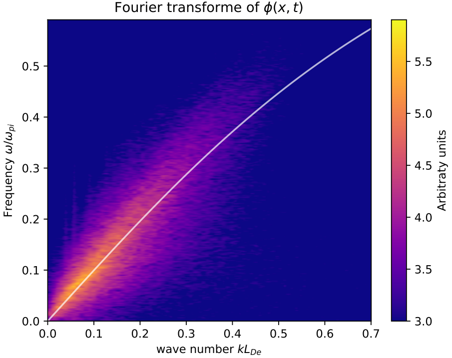
LANDMARK case 2B:

R-θ plan of an HET

- 2D simulation of a steady state discharge (Axial boundaries + MCC)
- Oscillations: Coherent with Ion Acoustic Wave



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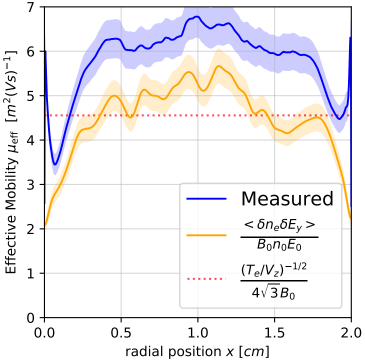
LANDMARK case 2B:

R-θ plan of an HET

- 2D simulation of a steady state discharge (Axial boundaries + MCC)

- Anomalous mobility: agreement with fluid and kinetic theory



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Conclusion

LPPic:

- Versatile and efficient 2D PIC/MCC code
- Can be used for **parametric studies**
- Validated on 1D Benchmark: **Need 2D and/or magnetized Benchmark**

LANDMARK:

- Results obtained for **case 2B** with MCC and axial boundaries
- Presentation **case 2A** $\rightarrow$ talk of T. Charoy
- Validate the results: quantitative comparison with same conditions

The end

Thank you for your attention !

Life is like a PIC simulation

Trevor Lafleur

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