MATURATION :
Algorithmes PIC sur grilles parcimonieuses massivement parallèles pour la simulation des plasmas froids hors-équilibres
ANR-22-CE46-0012

CE46 - Modèles numériques, simulation, applications

Laplace

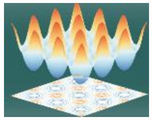
INSTITUT de MATHEMATIQUES de TOULOUSE

Inria

Maison de la Simulation

DUREE : 2023 - 2026 (4 ANS)
BUDGET : 1 341 072 €
AIDE : 355 470 €

label aerospace valley



Ordre du jour

- **10h-10h15 :** point administratif (L. Garrigues)
- **10h15-11h :** derniers résultats 2D (L. Garrigues)
- **11h-11h45 :** mise en place d'un schéma d'ordre 4 (P. Pace)

- **12h-13h15 :** repas – L'Esplanade

- **13h30-16h30 :** discussion générale
  - Recrutement
  - Tâches à venir et liens entre équipes
  - GitLab
  - etc.

Plan de gestion des données

https://aap.agencerecherche.fr

Calendrier du projet

T0 scientifique	Durée scientifique	Tfinal scientifique	T0 administratif	Durée administrative initiale	Durée administrative avec prolongations	Tfinal administratif
01/01/2023	48 mois	31/12/2026	01/10/2022	51 mois 1 jour	51 mois	31/12/2026

Historique des modifications sur le calendrier du projet

Documents de suivi

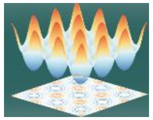
Condition	Nom personnalisé	Date attendue	Date de dépôt	Statut	Bloquante	Abrogation
Plan de gestion des données à 6 mois	Plan de gestion des données à 6 mois	01/07/2023	24/05/2023	Validé par l'ANR	☐	☐
Plan de gestion des données à 24 mois	Plan de gestion des données à 24 mois	01/01/2025		Attendu	☐	☐
Plan de gestion des données final	Plan de gestion des données final	31/12/2026		Attendu	☐	☐
Rapport final	Rapport final	31/12/2026		Attendu	☑	☐

Documents en provenance des partenaires pour l'ANR

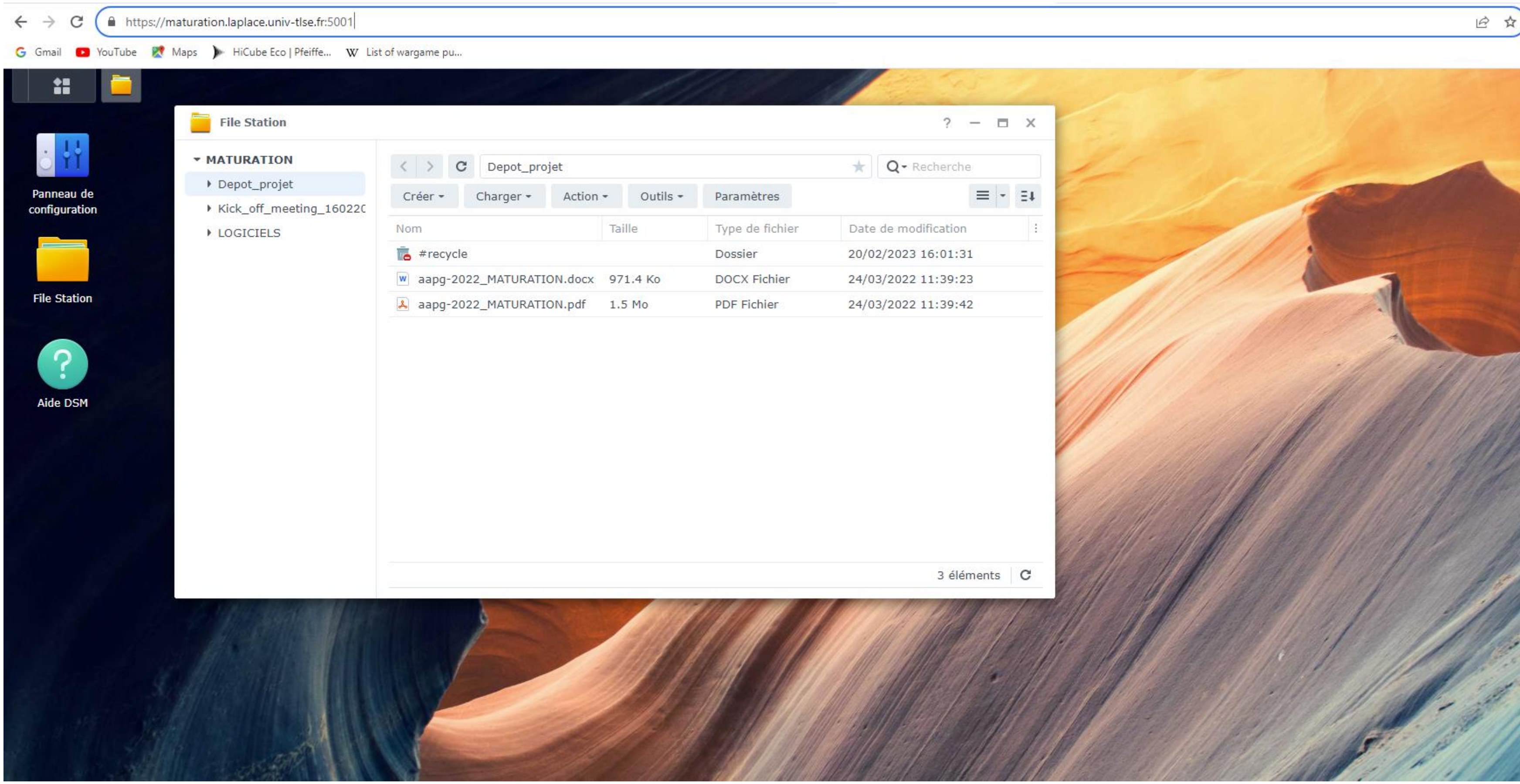
Taille Maximum : Mo.

Choisir un fichier | Aucun fichier choisi | Déposer

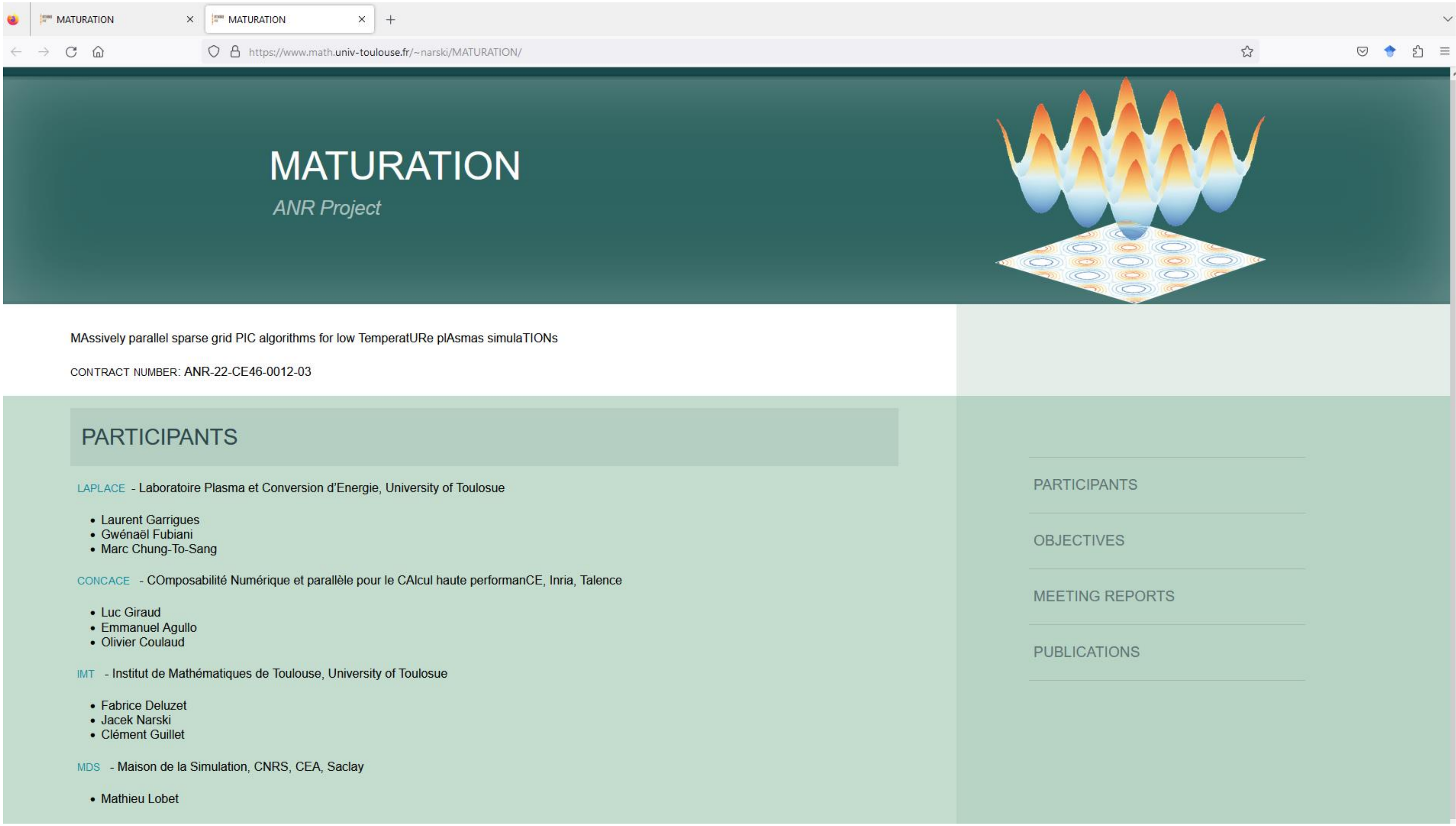
Documents en provenance de l'ANR pour les partenaires



Site web à diffusion interne



Site web à diffusion externe



MATURATION | MATURATION

https://www.math.univ-toulouse.fr/~narski/MATURATION/

MATURATION

ANR Project

MAssively parallel sparse grid PIC algorithms for low TemperatURe plAsmas simulaTIONs

CONTRACT NUMBER: ANR-22-CE46-0012-03

PARTICIPANTS

LAPLACE - Laboratoire Plasma et Conversion d'Energie, University of Toulosue

- Laurent Garrigues
- Gwénaël Fubiani
- Marc Chung-To-Sang

CONCACE - COmposabilité Numérique et parallèle pour le CAlcul haute performanCE, Inria, Talence

- Luc Giraud
- Emmanuel Agullo
- Olivier Coulaud

IMT - Institut de Mathématiques de Toulouse, University of Toulosue

- Fabrice Deluzet
- Jacek Narski
- Clément Guillet

MDS - Maison de la Simulation, CNRS, CEA, Saclay

- Mathieu Lobet

PARTICIPANTS

OBJECTIVES

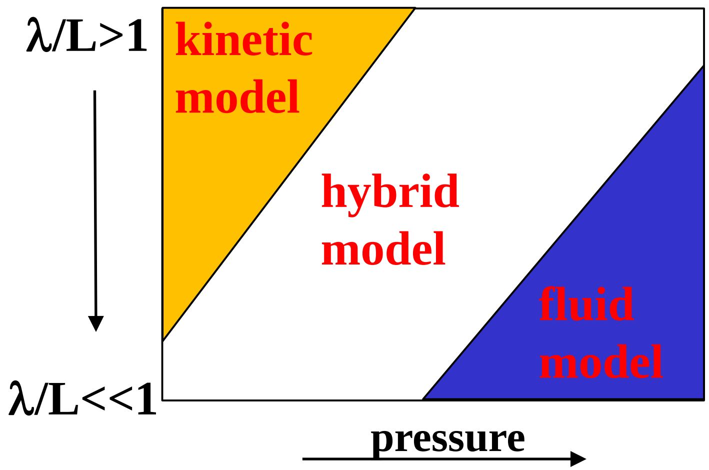
MEETING REPORTS

PUBLICATIONS

Résultats 2D plasma froids basse pression

Présentation ICPIG – juillet 2023

Kinetic vs fluid approaches



Boltzmann equation

$$\frac{\partial}{\partial t} f_s + \vec{v}\frac{\partial}{\partial \vec{r}} f_s + \vec{a}\frac{\partial}{\partial \vec{v}} f_s = \left\{\frac{\partial}{\partial t} f_s\right\}_{coll}$$

$$f_s \equiv f_s(\vec{r}, \vec{v}, t)$$

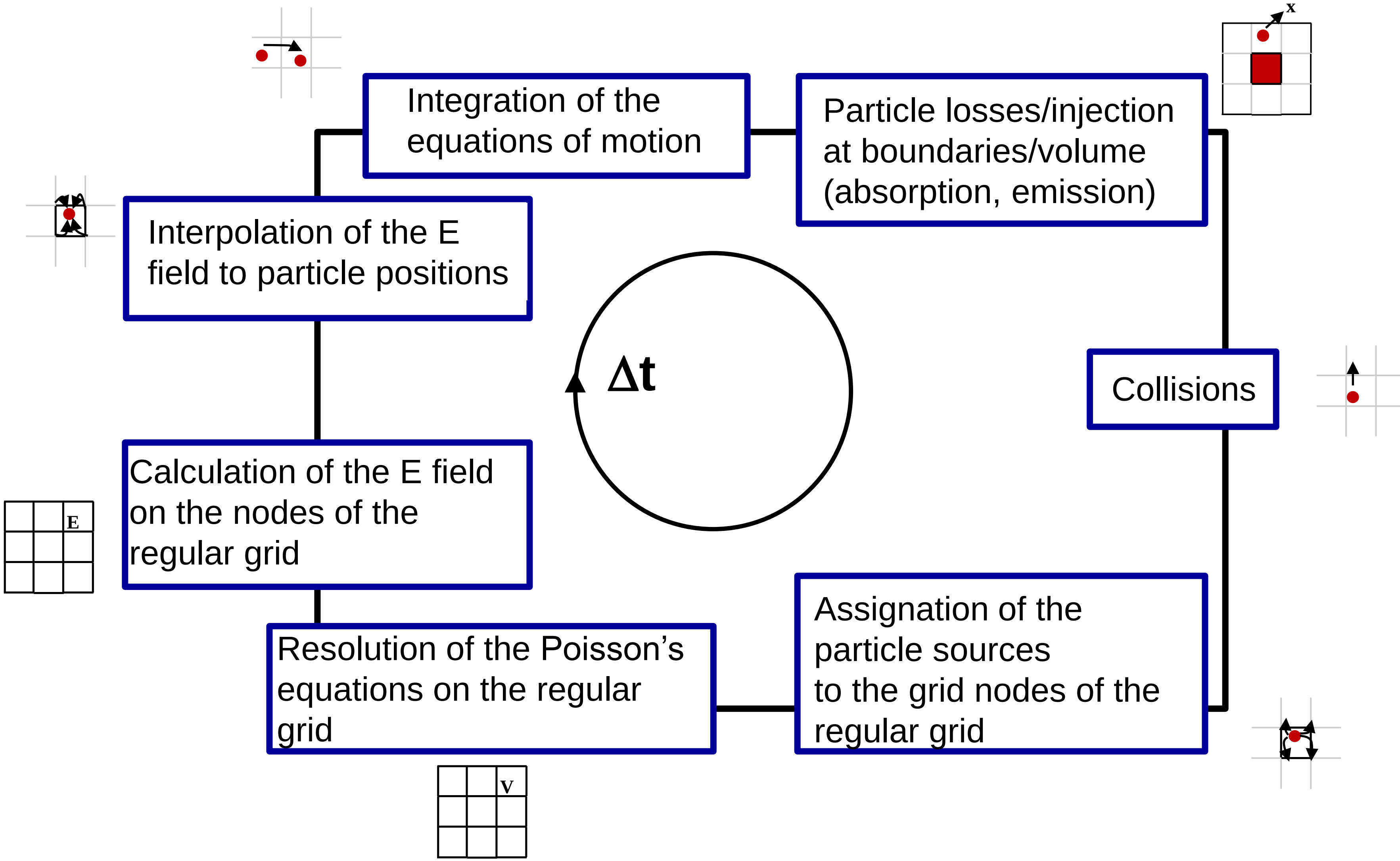
$$\vec{a} = q_s\left(\vec{E} + \vec{v} \times \vec{B}_{ext}\right)/m_s$$

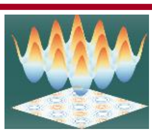
Poisson equation

$$\nabla \cdot \left[\varepsilon \cdot \vec{E}(\vec{r}, t)\right] = \rho(\vec{r}, t)$$

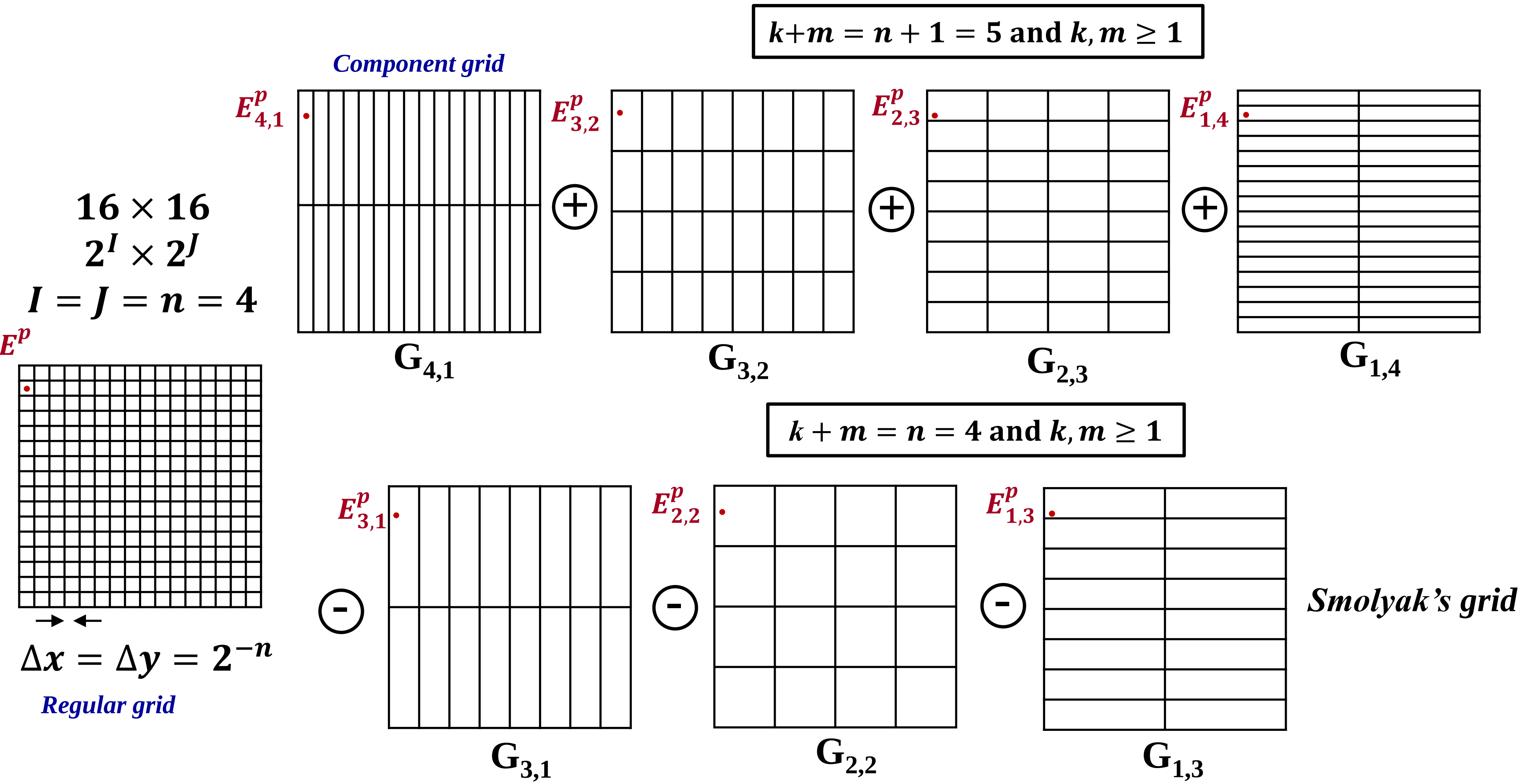
$$\rho(\vec{r}, t) = \sum_s q_s \int f_s(\vec{r}, \vec{v}, t)\, d\vec{v}$$

PIC cycle with standard approach





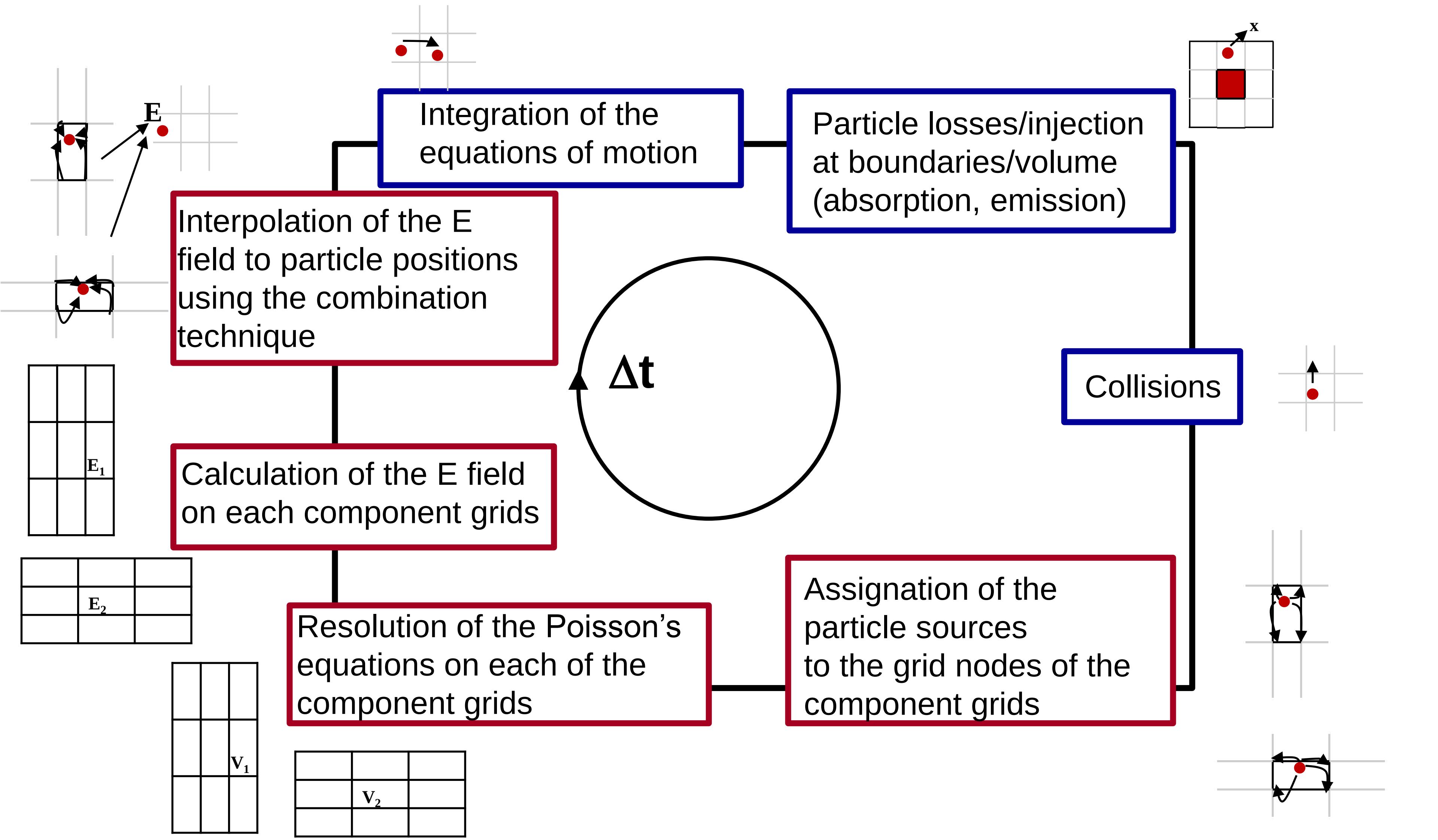
Construction of sparse grid domains



Combination technique

$$E^p \cong \sum_{k+m=n+1} E^p_{k,m} - \sum_{k+m=n} E^p_{k,m}$$

PIC cycle with revisited with sparse approach



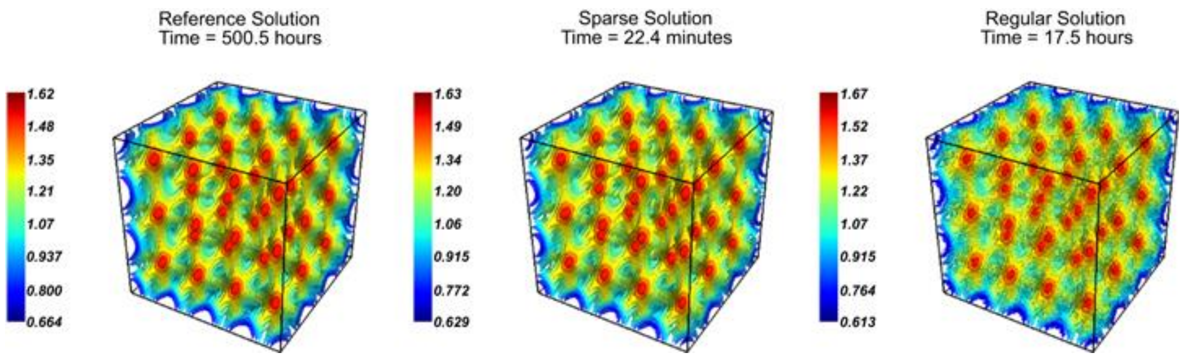
First plasma simulations

- **Applicability to PIC techniques**

L. F. Ricketson and A. J. Cerfon, PPCF 59, 024002 (2017)

  - Ions at rest
  - Periodic boundary conditions
  - No collisions

- **Numerical tests**
  - Linear/non linear Landau damping
  - Diocotron instability



3D non linear Landau damping
Comparison of density reference solution computed (128 × 128 × 128)
using regular PIC (left), ~ 30 simulations,
sparse solution on grid with N_{pc} = 800 (center),
and regular-PIC solution on grid with N_{pc} = 800 (right)

- **Extension to low temperature plasmas?**

RF capacitive discharges

- **Self-consistent description of the discharge**
- **Motion of ions**
- **Time and space evolution of sheaths**
- **Collisions between electrons/ions and neutrals**
- **Dual-frequency RF capacitive discharges**
  - HF: control of the plasma discharge
  - LF: control of the ion properties

P. C. Boyle *et al.*, Plasma Sources Sci. Technol. 13, 493 (2004)

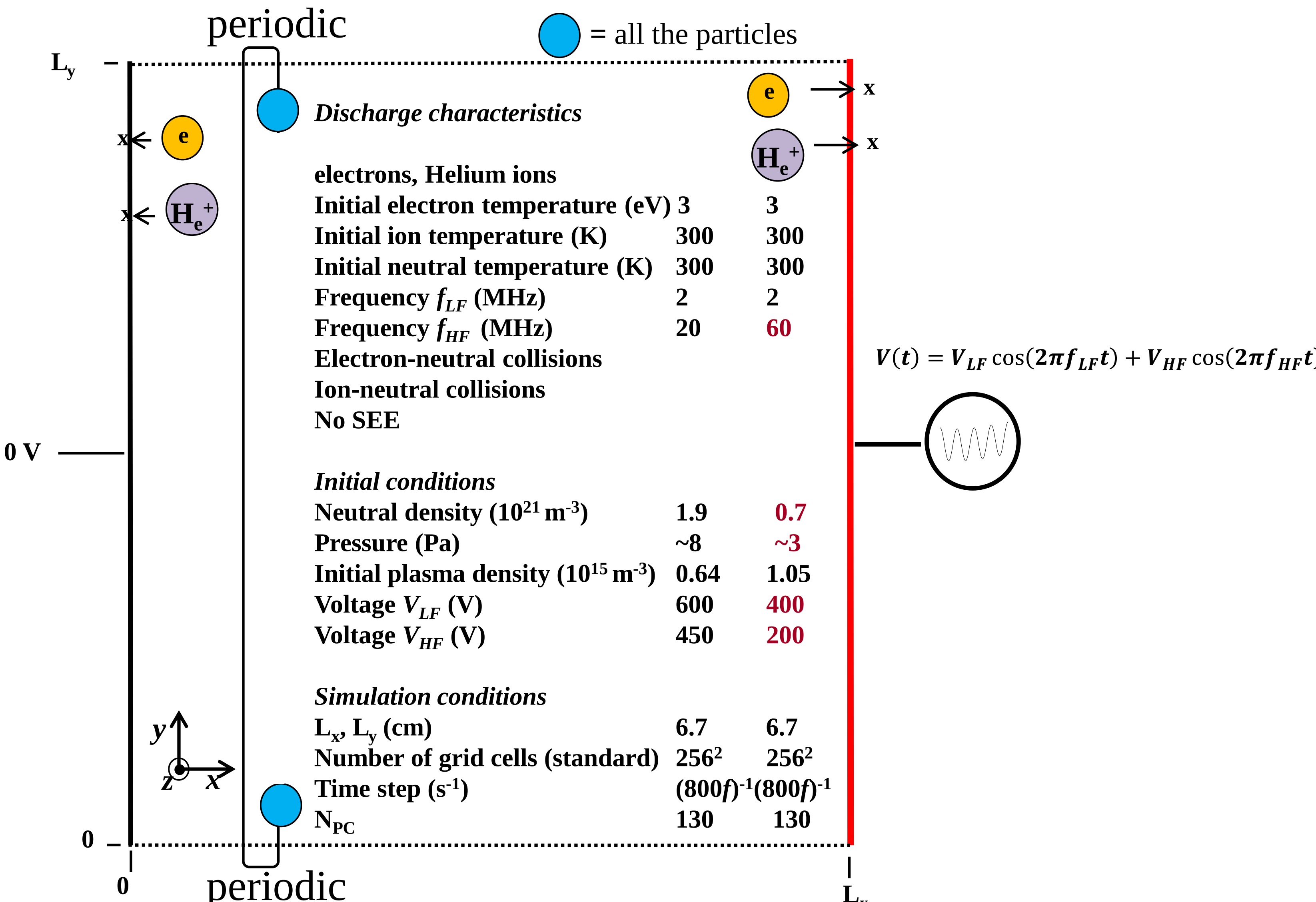
J. K. Lee *et al.*, Plasma Sources Sci. Technol. 14, 89 (2005)

J. Schulze *et al.*, Plasma Sources Sci. Technol. 20, 045007(2011)

Z. Donko, Plasma Sources Sci. Technol. 30, 095017 (2021)

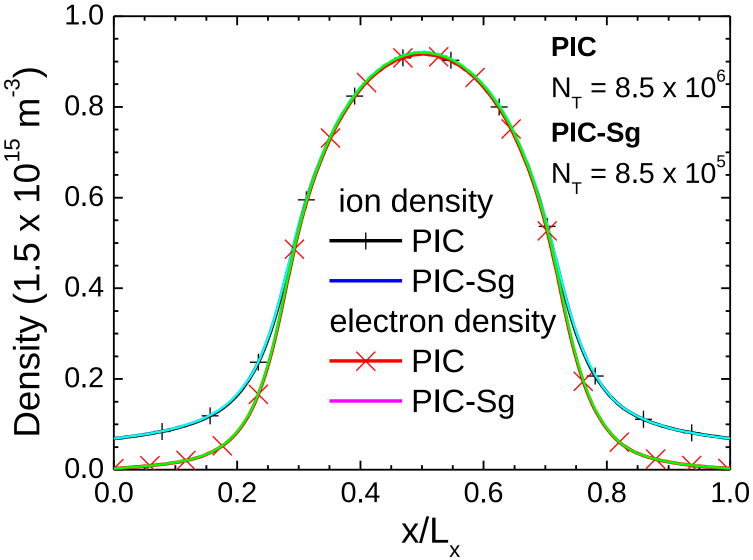
CCP discharges
P1.6, P1.41, P2.49, P3.11, P3.37, P4.21

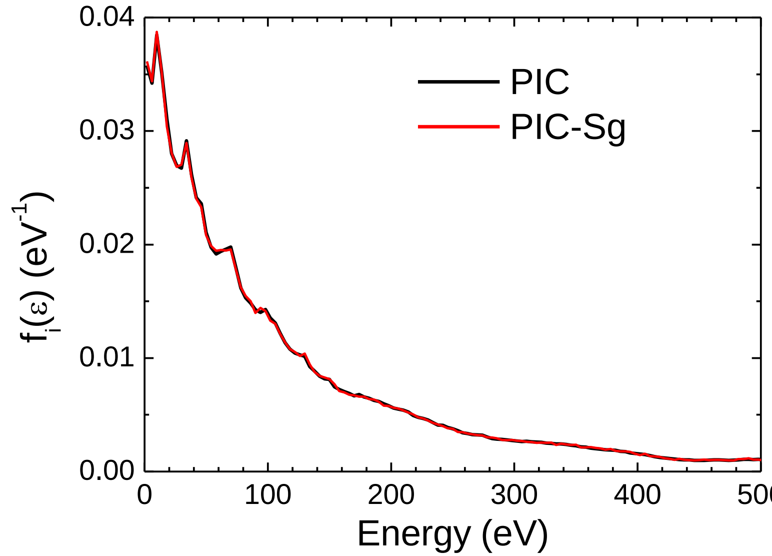
Quasi 1D benchmark conditions

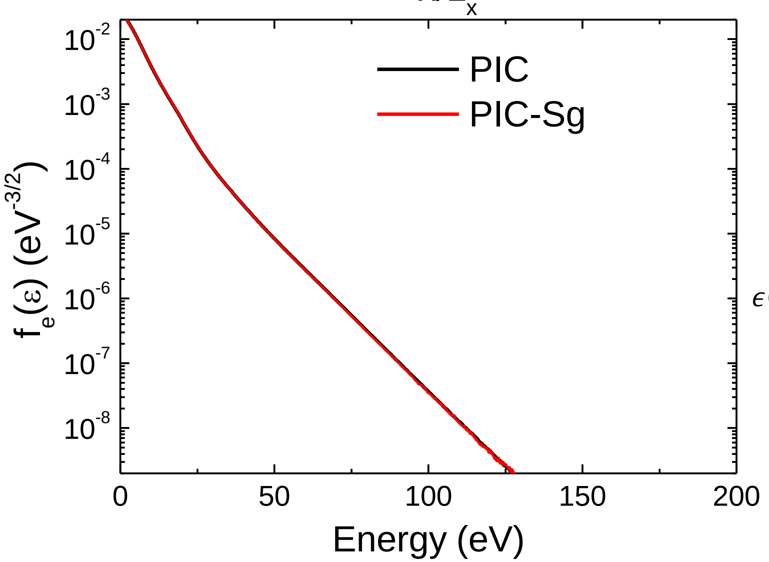


Discharge characteristics		
electrons, Helium ions		
Initial electron temperature (eV)	**3**	**3**
Initial ion temperature (K)	**300**	**300**
Initial neutral temperature (K)	**300**	**300**
Frequency f_{LF} (MHz)	**2**	**2**
Frequency f_{HF} (MHz)	**20**	**60**
Electron-neutral collisions		
Ion-neutral collisions		
No SEE		
Initial conditions		
Neutral density (10^{21} m^{-3})	**1.9**	**0.7**
Pressure (Pa)	**~8**	**~3**
Initial plasma density (10^{15} m^{-3})	**0.64**	**1.05**
Voltage V_{LF} (V)	**600**	**400**
Voltage V_{HF} (V)	**450**	**200**
Simulation conditions		
L_x, L_y (cm)	**6.7**	**6.7**
Number of grid cells (standard)	**256^2**	**256^2**
Time step (s^{-1})	**$(800f)^{-1}$**	**$(800f)^{-1}$**
N_{PC}	**130**	**130**

Results @ 20 MHz



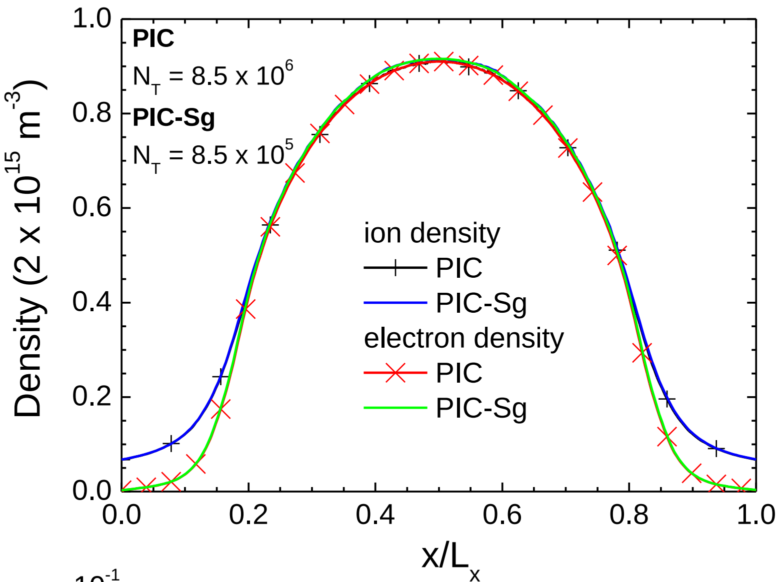


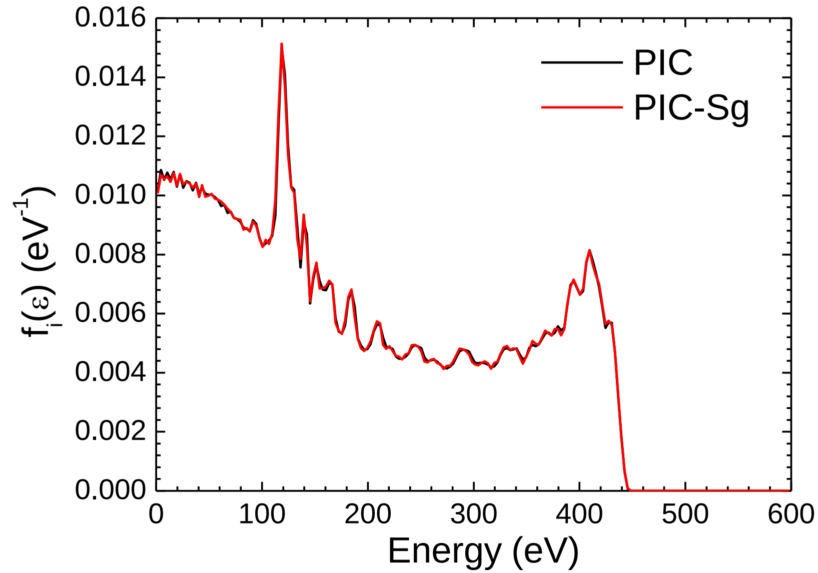


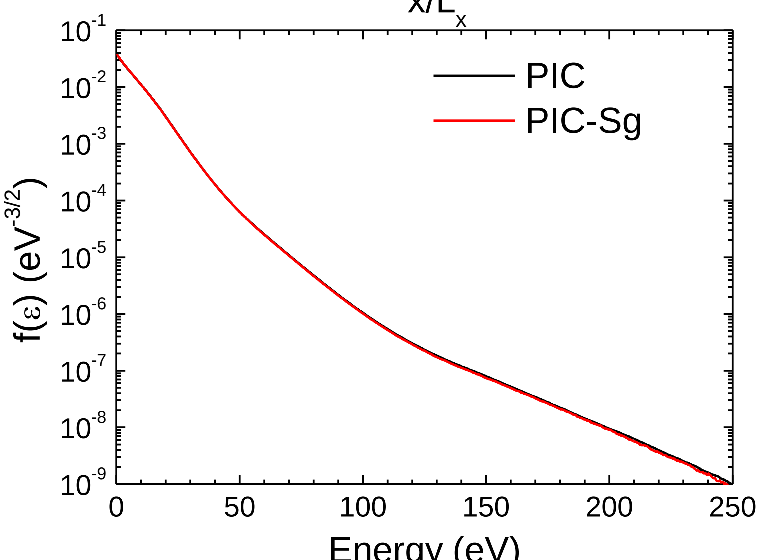
$$\epsilon(\varphi) = \frac{\|\varphi - \varphi_{\mathrm{ref}}\|_{L^2}}{\|\varphi_{\mathrm{ref}}\|_{L^2}} = \sqrt{\frac{\int |\varphi - \varphi_{\mathrm{ref}}|^2 \mathrm{du}}{\int |\varphi_{\mathrm{ref}}|^2 \mathrm{du}}}$$

	Error (%)
n_i	0.5
n_e	0.45
$EEDF$	0.02
$IEDF$	0.14

Results @ 60 MHz



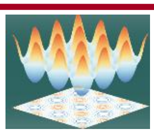




$$\epsilon(\varphi) = \frac{\|\varphi - \varphi_{\mathrm{ref}}\|_{L^2}}{\|\varphi_{\mathrm{ref}}\|_{L^2}} = \sqrt{\frac{\int |\varphi - \varphi_{\mathrm{ref}}|^2 \mathrm{du}}{\int |\varphi_{\mathrm{ref}}|^2 \mathrm{du}}}$$

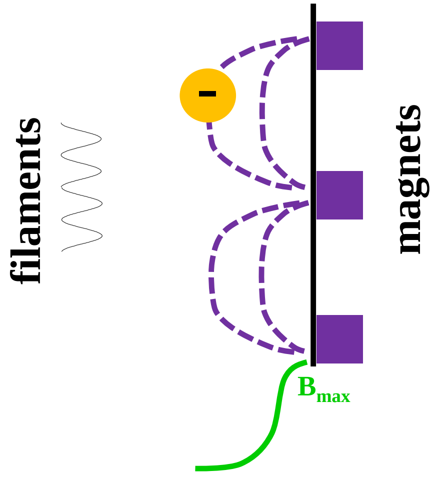
	Error (%)
n_i	1
n_e	1
$EEDF$	0.08
$IEDF$	0.15

L. Garrigues *et al.*, in preparation



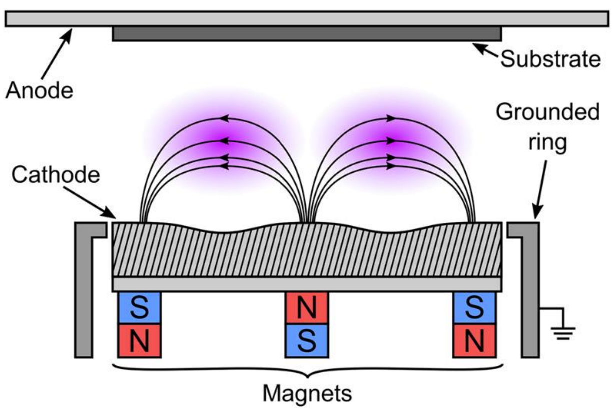
Multipolar cusp confinement

- **Multipolar cusp confinement**
  - Reduce electron losses on chamber walls
  - Larger plasma densities
  - Permanent magnets placed behind the electrode/dielectric wall

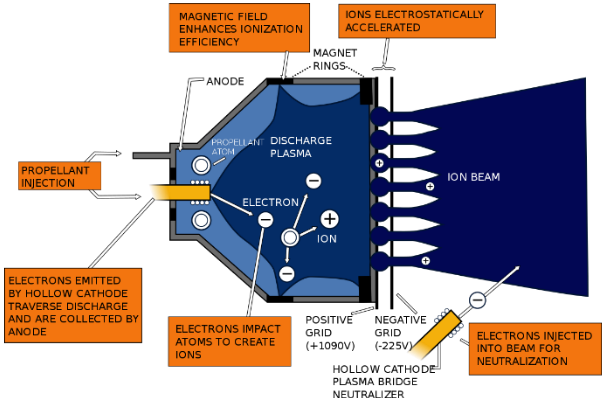


- **Partially magnetized low temperature plasmas ion sources**

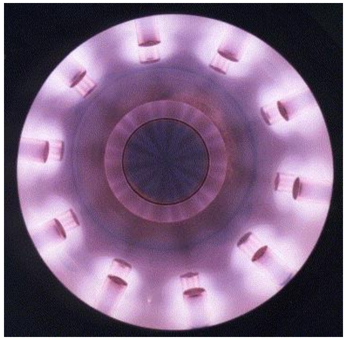
DC magnetron for sputtering



Kaufman ion source



DECR source



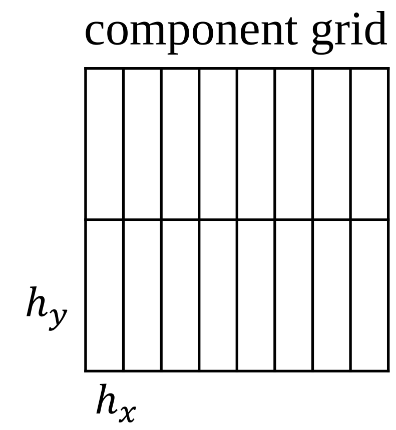
D. Lunedin *et al.*,
"High Power Impulse Magnetron Sputtering"

D. M. Goebel and I. Katz,
"Fundamentals of Electric Propulsion"

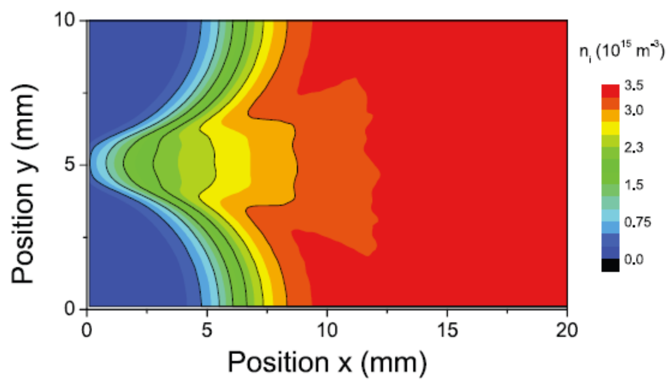
S. Bechu *et al*, Surf. Coat. Technol. 186, 170 (2004)

More about the grid-based error

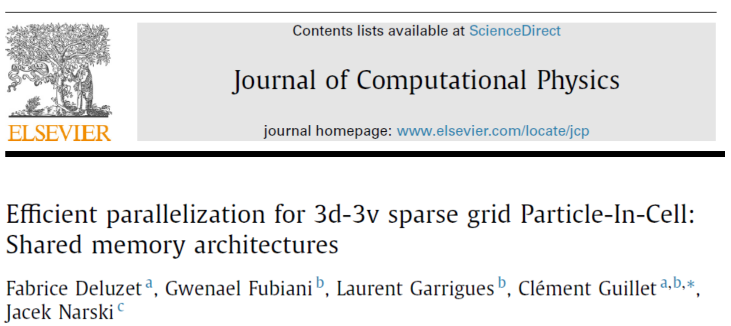
- **Grid-based error in 2D**
  - Terms along x and y directions cancel out with combination technique … but not along mixed directions
  - Error associated with ρ



$$\varepsilon_s = \underbrace{b_1 \frac{\partial^2 \rho}{\partial x^2} h_x^2}_{\text{error along } x} + \underbrace{b_2 \frac{\partial^2 \rho}{\partial y^2} h_y^2}_{\text{error along } y} + \underbrace{b_{1,2} \frac{\partial^4 \rho}{\partial x^2 \partial y^2} h_x^2 h_y^2}_{\text{error along mixed directions}} + O(h_x^4, h_y^4)$$



Y. Jiang *et al.*, Phys. Plasmas 27, 113506 (2020)


Contents lists available at ScienceDirect

Journal of Computational Physics

journal homepage: www.elsevier.com/locate/jcp

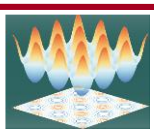
ELSEVIER

Efficient parallelization for 3d-3v sparse grid Particle-In-Cell: Shared memory architectures

Fabrice Deluzet [a], Gwenael Fubiani [b], Laurent Garrigues [b], Clément Guillet [a,b,*], Jacek Narski [c]

- **Oversampled method to reduce the grid-based error in the mixed directions**

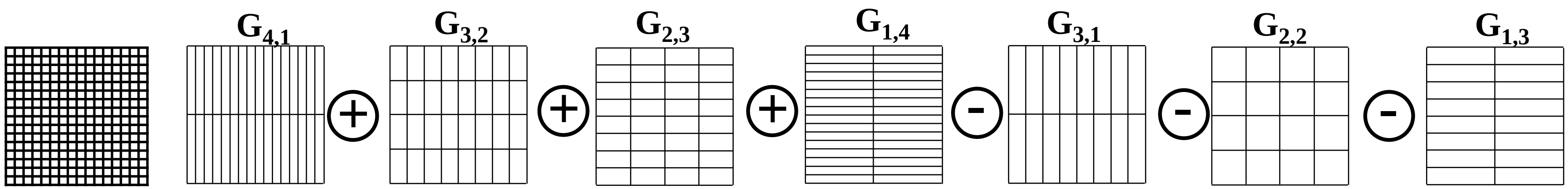
S. Muralikrishnan *et al.*, J. Comput. Phys. X 11, 100094 (2021)



The offset sparse method – component grids

$$l^0 = 0, l^1 = 0 \text{ and } k, m \geq 1$$

$k + m = n + l^0 - l^1 + 1 = 5$ $\qquad$ $k + m = n + l^0 - l^1 = 4$



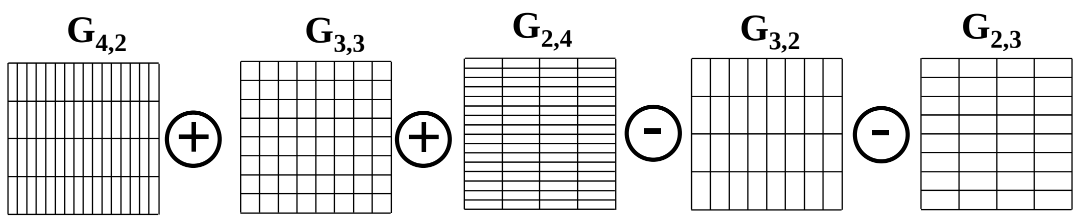
16×16

$2^I \times 2^J$

$I = J = n = 4$

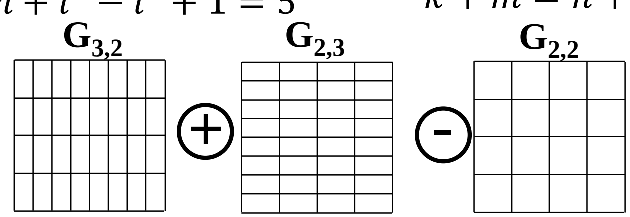
$$l^0 = 1, l^1 = 0 \text{ and } k, m > l^0$$

$k + m = n + l^0 - l^1 + 1 = 6$ $\qquad$ $k + m = n + l^0 - l^1 = 5$

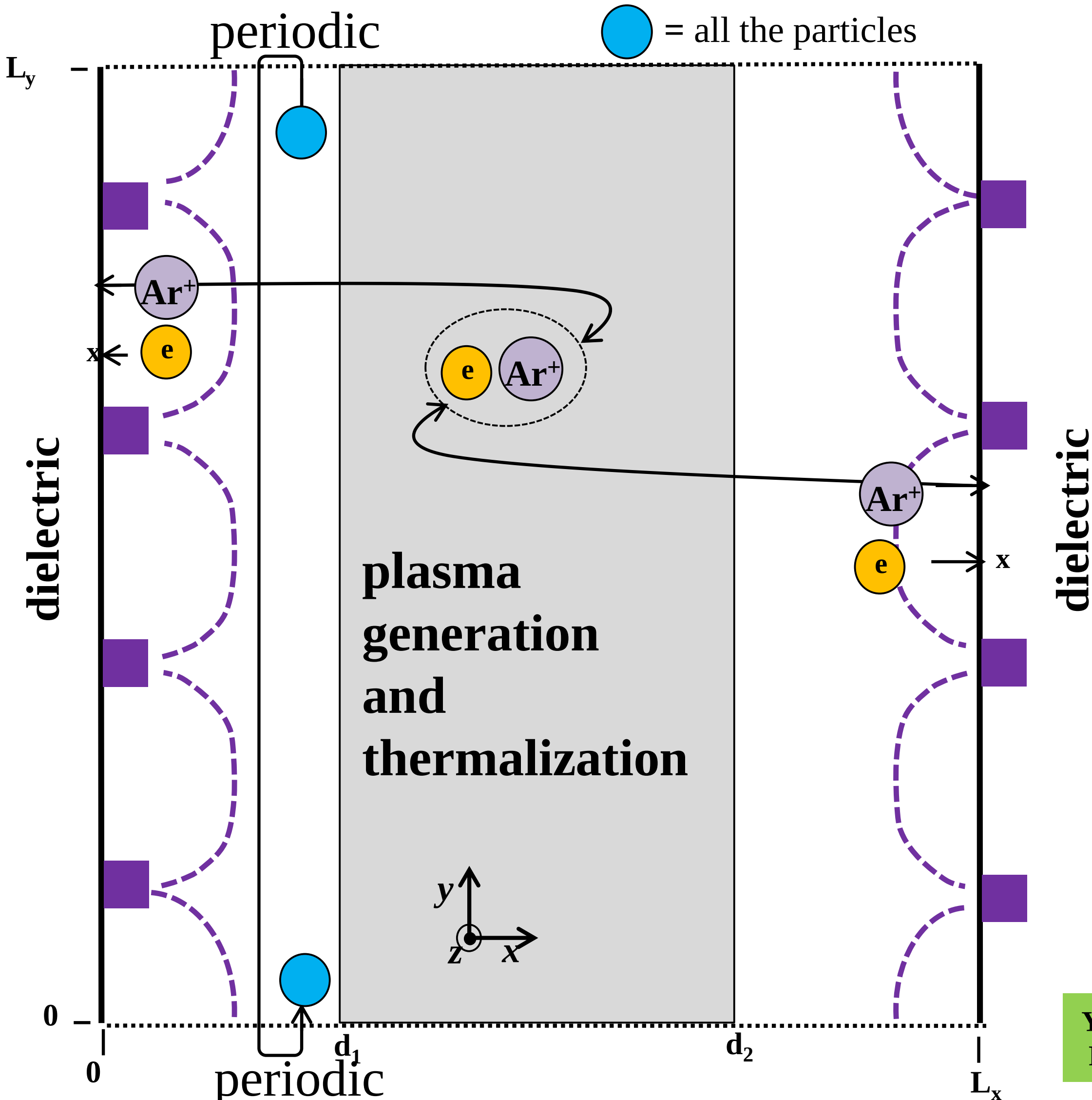


$$l^0 = 1, l^1 = 1 \text{ and } k, m > l^0$$

$k + m = n + l^0 - l^1 + 1 = 5$ $\qquad$ $k + m = n + l^0 - l^1 = 4$



Simplified 2D modeling of a cusp discharge



Discharge characteristics

Magnetized electrons, argon ions
Initial electron temperature (eV) 3
Thermalization temperature (eV) 3
Initial ion temperature (eV) 0.1
Electron-neutral collisions

Initial conditions

Pressure (mTorr)	**0.1**
Neutral density (10^{18} m^{-3})	**3.2**
Initial plasma density (10^{15} m^{-3})	**1**
Magnetic field max (G)	**400**

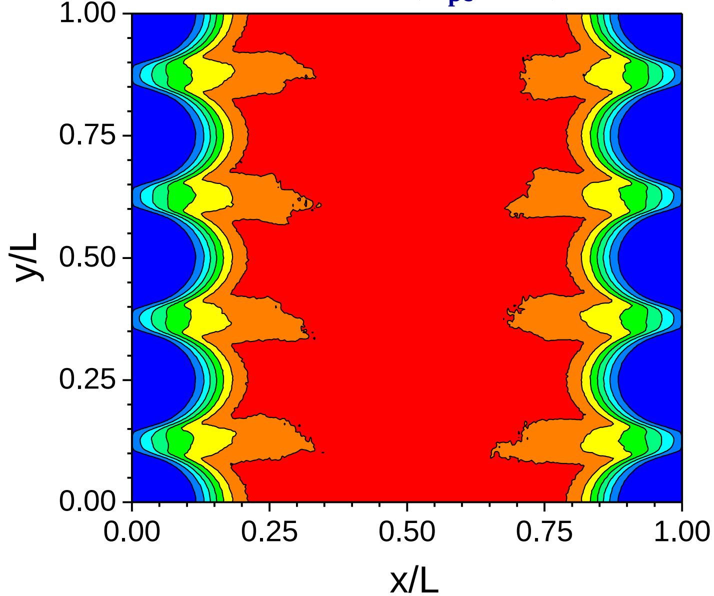
Simulation conditions

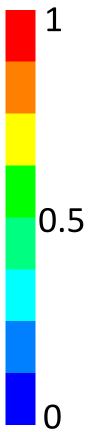
$L_x = L_y$ (cm)	**4**
d_1, d_2 (cm)	**1.6, 2.4**
Number of grid cells (std)	**256^2**
Time step (s^{-1})	**$0.2/\omega_p$**
N_{PC}	**50**

Y. Jiang, G. Fubiani, L. Garrigues, and J. P. Boeuf, Phys. Plasmas 27, 113506 (2020)

Results @ 0.1 mTorr - 400 G (1/2)

Standard (N_{pc} = 50)

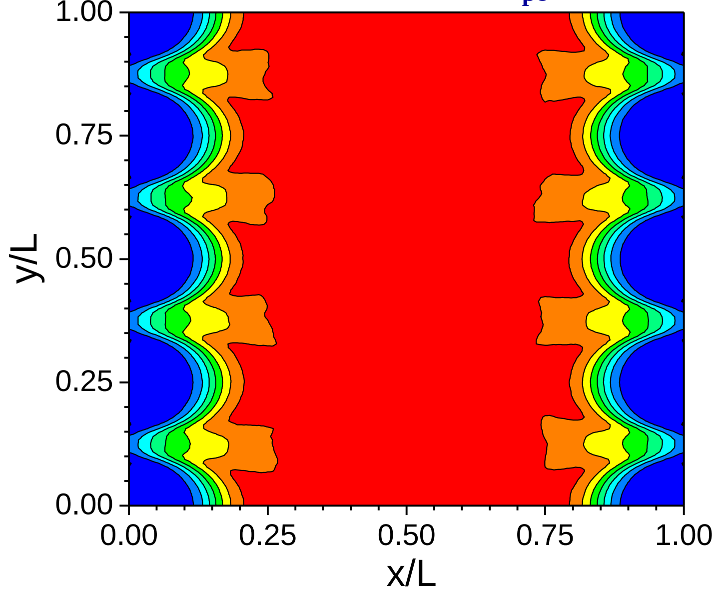


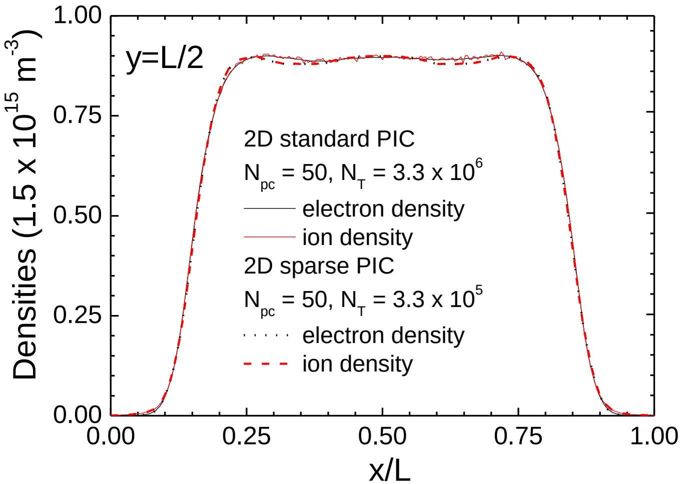


Ion density

1.4×10^{15} m^{-3}

Sparse $l^0 = 4, l^1 = 1$ (N_{pc} = 50)

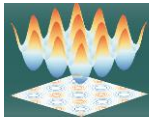




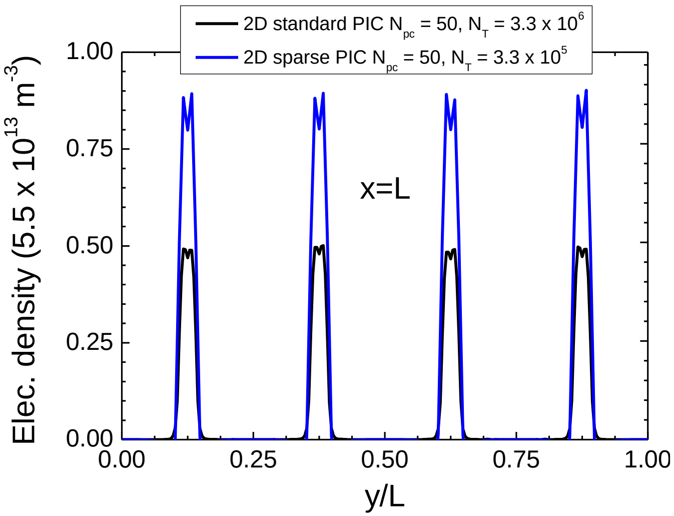
$$\epsilon(\varphi) = \frac{\|\varphi - \varphi_{\mathrm{ref}}\|_{L^2}}{\|\varphi_{\mathrm{ref}}\|_{L^2}} = \sqrt{\frac{\int|\varphi - \varphi_{\mathrm{ref}}|^2 \mathrm{du}}{\int|\varphi_{\mathrm{ref}}|^2 \mathrm{du}}}$$

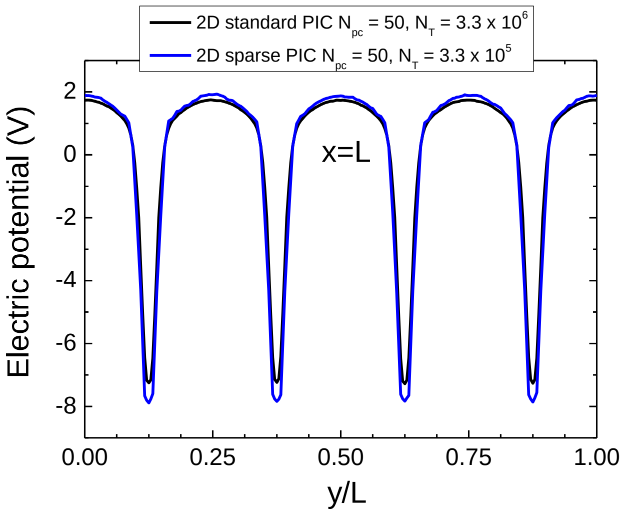
Error (%)	
n_i (2D)	4.5
n_e (2D)	4.5

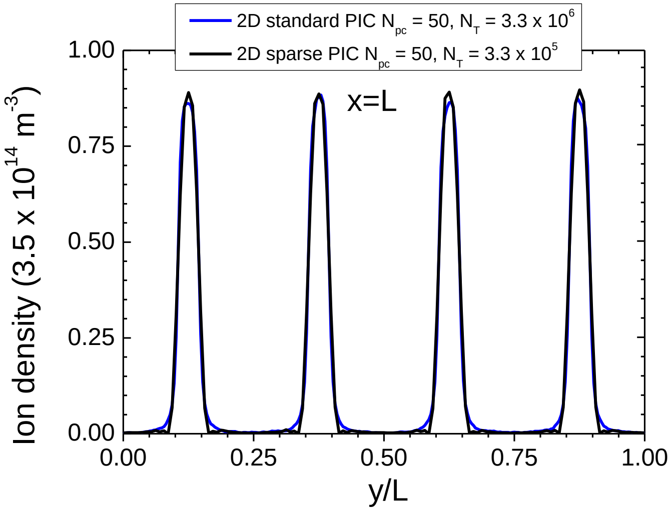
L. Garrigues et al., in preparation



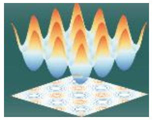
Results @ 0.1 mTorr - 400 G (2/2)







L. Garrigues et al., in preparation



Discussion

Tâches – diagramme de Gantt

Work Packages & Tasks	LAPLACE	CONCACE	IMT	MdS	Year 1				Year 2				Year 3				Year 4			
					T1	T2	T3	T4	T1	T2	T3	T4	T1	T2	T3	T4	T1	T2	T3	T4
WP0 Project management	⊠	×	×	×																
T0.1 – data management	×	×	×	×		M0.1														
T0.2 – meetings	×	×	×	×	D0.1	D0.2		D0.6		D0.3		D0.7		D0.4		D0.8		D0.5		D0.9
T0.3 – hiring of persons	×	×	×	×				M0.2				M0.3	M0.4							
T0.4 – annual reports	×	×	×	×				D0.10				D0.11				D0.12				D0.13
T0.5 – collaborative tool	×	×	×	×		M0.5														
WP1 Opt. 3D sparse PIC model	⊠	×	×	×																
T1.1 – construction	×	×	×	×															D1.1	
T1.2 – scalability	×	×	×	×																D1.2
WP2 Benchmarks	⊠	×	×																	
T2.1 – definition of test cases	×						M2.1													
T2.2 – implementation	×	×	×								M2.2			D2.1						
T2.3 – verification	×	×	×												M2.3			D2.2		
WP3 Numerical analysis	×	×	⊠																	
T3.1 – Sparse grid reconstruction	×	×	×								M3.1							D3.1		
T3.2 – hierarchization strategy	×	×	×									M3.2						D3.1		
T3.2 – Vlasov-Maxwell system	×	×	×													M3.3				D3.2
WP4 3D solvers & parallelization	×	⊠	×	×																
T4.1 – 3D parallelization	×	×	×	×								M4.1						D4.1		
T4.2 – parallel Poisson solver	×	×	×									M4.2						D4.1		
T4.3 – parallel perform. benc.	×	×	×															D4.1		
WP5 Sparse PIC optimization	×	×		⊠																
T5.1 – cache-based optimization	×	×		×										M5.1						
T5.2 – vectorization	×	×		×													M5.2	D5.1		
WP6 Commun. & dissemination	×	×	⊠	×																
T6.1 – communication	×	×	×	×	M6.1															
T6.2 – archive	×	×	×	×	M6.2															
T6.3 – dissemination	×	×	×	×		D6.1		D6.2		D6.3		D6.4		D6.5		D6.6		D6.7		D6.8

Budget

	Partner 1 LAPLACE	Partner 2 Concace	Partner 3 IMT	Partner 4 MdS
Staff expenses	103 196 € (2-year post-doc)	48 000 € (1-year post-doc)	57 180 € (1-year post-doc)	3 900 € (1 Master Internship)
Instruments and material costs (including the scientific consumables)	13 000 €	3 000 €	14 000 €	4 000 €
Building and ground costs	0 €	0 €	0 €	0 €
Outsourcing / subcontracting	2 000 €	2 000 €	2 000 €	2 000 €
General and administrative costs & other operating expenses	17 200 €	22 000 €	15 200 €	5 900 €
Administrative management & structure costs (13 %)	17 601 €	9 750 €	11 489 €	2 054 €
Sub-total	152 997 €	84 750 €	99 869 €	17 854 €
Requested funding	355 470 €