Modeling low temperature plasmas

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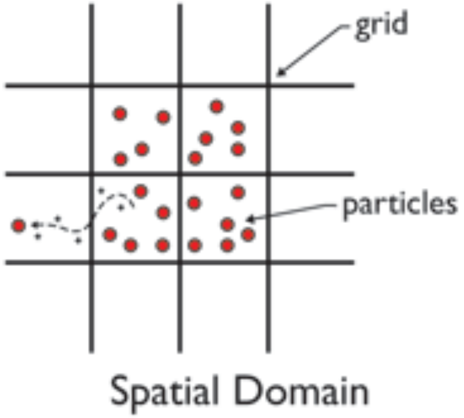
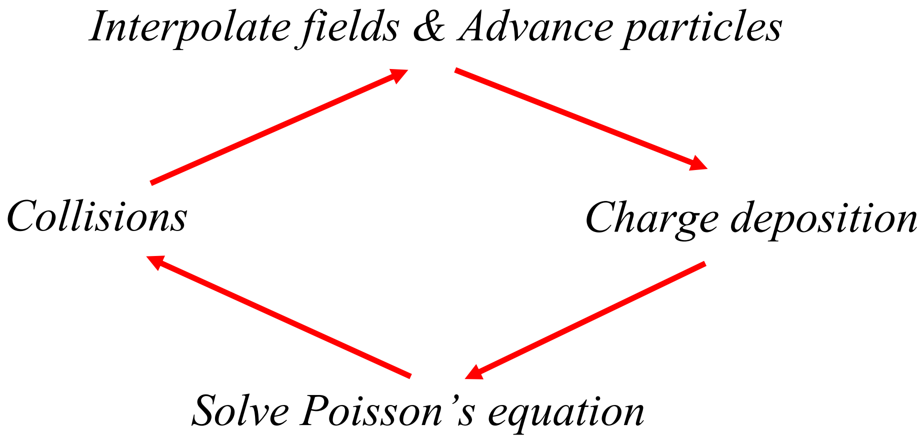
Numerical tools: Particle in Cell (PIC) with Monte-Carlo-Collisions (MCC)



- The model* is fully “homemade”, explicit and electrostatic
- 1D/2D/3D Cloud-In-Cell.
- Parallelized (hybrid MPI and OpenMP)
- Poisson solver is a multi-grid (2D/3D) or direct solver (2D, Pardiso)
- Magnetic field is prescribed

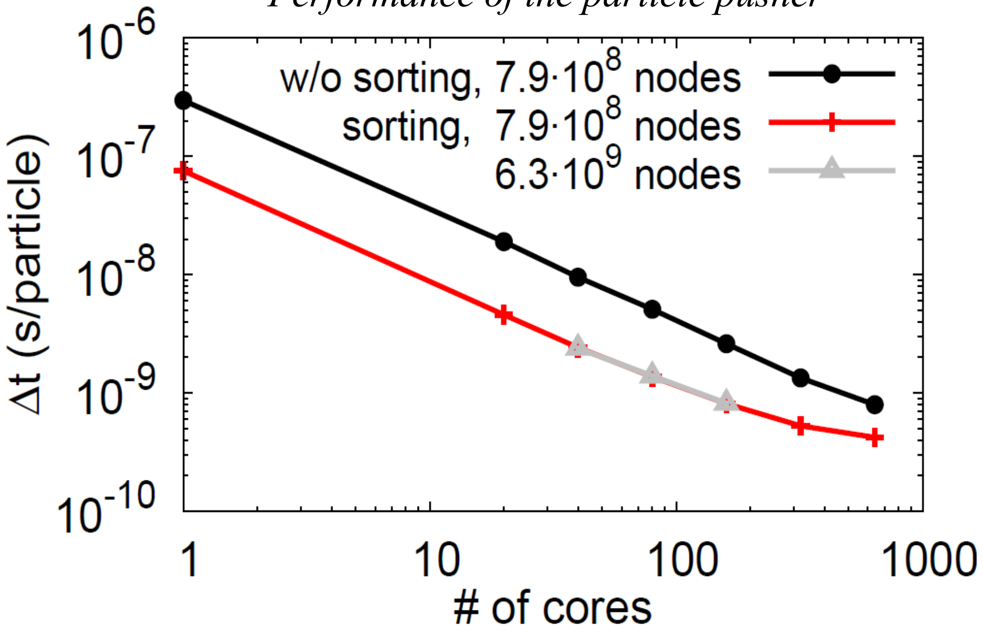

Interpolate fields & Advance particles

Collisions

Charge deposition

Solve Poisson’s equation

Performance of the particle pusher



**Developed by the LAPLACE (G. Fubiani & L. Garrigues). Other similar models designed by other groups (LPP, etc.)*

Inclusion of a comprehensive physical chemistry: for instance, hydrogen gas with negative ions

~60 reactions implemented in the PIC-MCC model

Table 1. Electron collisions.

#	Reaction	Cross section reference
1	$e + H \rightarrow e + H$ (elastic)	[71–75]
2	$e + H \rightarrow e + H$ (inelastic, 4 proc.)	[32]
3	$e + H \rightarrow 2e + H^+$	[32]
4	$e + H_2 \rightarrow e + H_2$ (elastic)	[76]
5	$e + H_2 \rightarrow 2e + H_2^+$	[32]
6	$e + H_2 \rightarrow 2e + H^+ + H$ (2 proc.)	[32]
7	$e + H_2 \rightarrow e + H_2$ (inelastic, 16 proc.)	[32–38]
8	$e + H_2 \rightarrow e + 2H$ (3 proc.)	[32, 77]
9	$e + H_3^+ \rightarrow 3H$	[32]
10	$e + H_3^+ \rightarrow H + H_2$	[32]
11	$e + H_3^+ \rightarrow e + H^+ + 2H$	[32]
12	$e + H_3^+ \rightarrow e + H^+ + H_2$	[32]
13	$e + H_2^+ \rightarrow 2H$	[32]
14	$e + H_2^+ \rightarrow e + H^+ + H$ (2 proc.)	[32, 77]
15	$e + H_2^+ \rightarrow 2e + 2H^+$	[77]
16	$e + H^- \rightarrow 2e + H$	[32]
17	$e + H_2^* \rightarrow H^- + H$ (1% of H_2)	[77]
18	$e + H_2^+ \rightarrow e + H_2^+$	(Coulomb) [22]
19	$e + H^+ \rightarrow e + H^+$	(Coulomb) [22]
20	$e + H_3^+ \rightarrow e + H_3^+$	(Coulomb) [22]

Table 2. Heavy particle processes.

#	Reaction	Cross section reference
1	$H_3^+ + H_2 \rightarrow H_3^+ + H_2$ (elastic)	[78]
2	$H_3^+ + H \rightarrow H_3^+ + H$ (elastic)	
3	$H_2^+ + H_2 \rightarrow H_3^+ + H$	[43, 78]
4	$H_2^+ + H_2 \rightarrow H_2 + H_2^+$	[78]
5	$H_2^+ + H \rightarrow H_2^+ + H$ (elastic)	[79]
6	$H^+ + H \rightarrow H + H^+$	[80]
7	$H^+ + H \rightarrow H^+ + H$ (elastic)	[80]
8	$H^+ + H_2 \rightarrow H^+ + H_2$ (elastic)	[78]
9	$H^+ + H_2 \rightarrow H^+ + H_2$ (inelastic, 4 proc.)	[41–43, 78]
10	$H^- + H \rightarrow e + 2H$	[32]
11	$H^- + H \rightarrow e + H_2$	[32]
12	$H^- + H_2 \rightarrow H^- + H_2$ (elastic)	[43]
13	$H^- + H \rightarrow H^- + H$ (elastic)	[43]
14	$H^+ + H^- \rightarrow 2H$ (2 proc.)	[32]
15	$H^+ + H^- \rightarrow H_2^+ + e$	[32]
16	$H^- + H_2 \rightarrow H_2 + H + e$	[32]
17	$H^- + H \rightarrow H + H^-$	[81]
18	$H + H \rightarrow H + H$	[80]
19	$H + H_2 \rightarrow H + H_2$	[80]
20	$H_2 + H_2 \rightarrow H_2 + H_2$	[82]

MAGNIS fluid model* @ LAPLACE Toulouse

- Multi-fluid: electrons, ions, neutrals
- Continuity equations with chemistry source terms
- Full momentum equations including inertia terms
- Electron energy equation with magnetized heat flux
- Quasi-neutrality: plasma potential deduced from current continuity
- Boundary conditions from sheath theory, allowing for different wall materials: grounded, biased, dielectric
- Evolution in time and 2D plane perpendicular to magnetic field lines
- Parallel losses (along field lines) included via effective source terms (2D+½D) allowing for dielectric, grounded, or biased walls
- Magnetized fluxes handled through original numerical scheme using prediction/correction on shifted numerical grids

R. Futtersack, PhD thesis (University of Toulouse, 2014)

S. Sadouni, PhD thesis (University of Toulouse, 2020)

**Developed by G. Hagelaar*

Main fluid model equations

- Continuity & momentum equations for each species α:

$$\frac{\partial n_\alpha}{\partial t} + \nabla_\perp \cdot (n_\alpha \mathbf{w}_\alpha) = S_\alpha - L_{//\alpha} \qquad\qquad L_{//\alpha} = \overline{\nabla_{//} \cdot (n_\alpha \mathbf{w}_\alpha)} \propto n_\alpha$$

$$m_\alpha \frac{\partial \mathbf{w}_\alpha}{\partial t} + m_\alpha \mathbf{w}_\alpha \cdot \nabla \mathbf{w}_\alpha + m_\alpha \left(\nu_\alpha + \frac{S_\alpha}{n_\alpha} \right) \mathbf{w}_\alpha + q_\alpha \mathbf{B} \times \mathbf{w}_\alpha = -q_\alpha \nabla \Phi - \frac{\nabla (n_\alpha T_\alpha)}{n_\alpha}$$

- Quasi-neutrality & current conservation:

$$n_e = \frac{1}{e} \sum_i q_i n_i \qquad\qquad \nabla_\perp \cdot \left(e n_e \mathbf{w}_e(\Phi) \right) = \nabla_\perp \cdot \left(\sum_i q_i n_i \mathbf{w}_i \right) + \sum_\alpha q_\alpha L_{//\alpha}$$

- Electron energy:

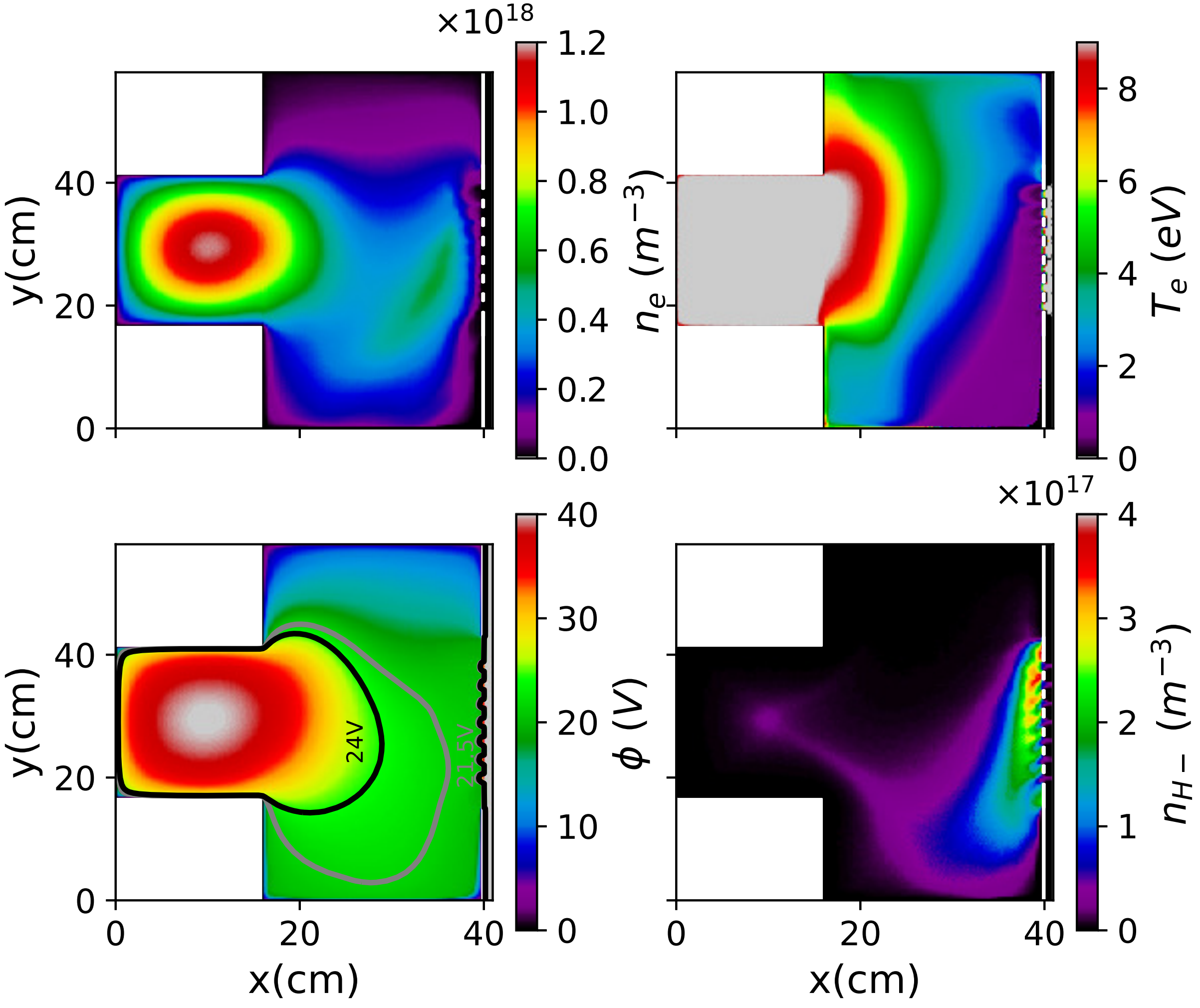
$$\frac{3}{2} \frac{\partial n_e T_e}{\partial t} + \frac{5}{2} \nabla_\perp \cdot (n_e \mathbf{w}_e T_e) + \nabla_\perp \cdot \mathbf{Q}_e = P_{\text{ext}} + e n \mathbf{w}_e \cdot \nabla_\perp \Phi - L_{\text{col}} - L_{//T}$$

$$\frac{\partial \mathbf{Q}_e}{\partial t} + \nu \mathbf{Q}_e - \frac{e}{m_e} \mathbf{B} \times \mathbf{Q}_e = -\frac{5 n_e T_e}{2 m_e} \nabla T_e$$

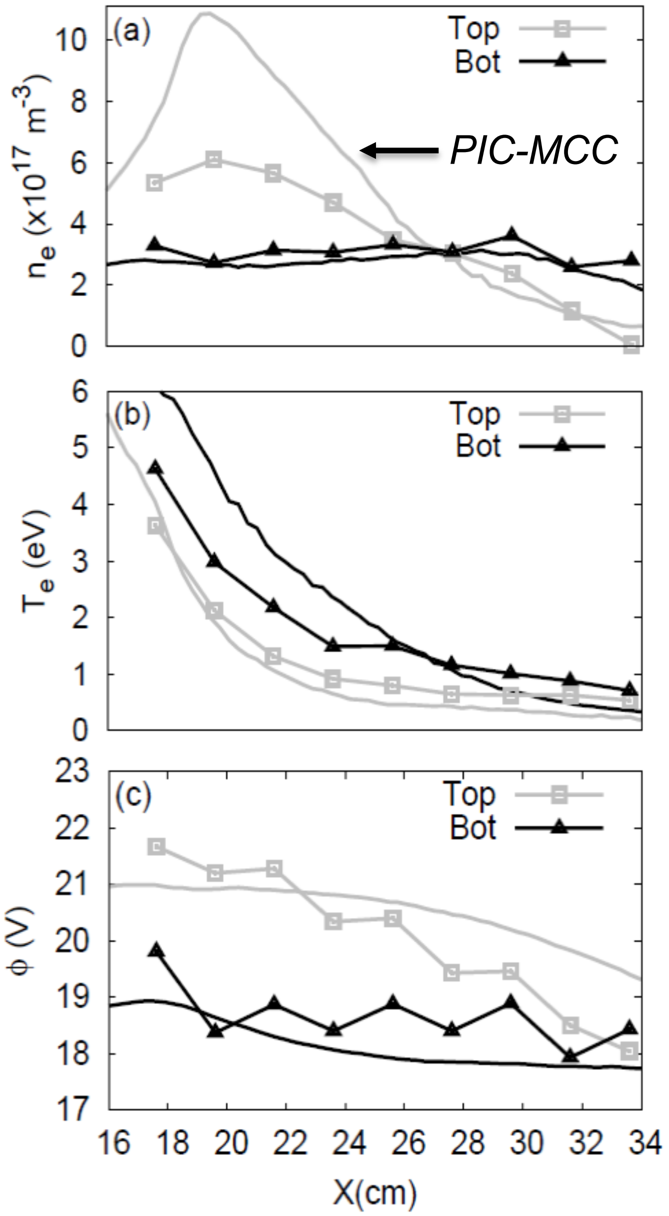
- Boundary conditions from sheath theory: $\mathbf{w}_i \cdot \mathbf{n} \geq \left(T_e / m_i \right)^{1/2}$

$$\mathbf{w}_e \cdot \mathbf{n} = \left(T_e / 2\pi m_e \right)^{1/2} \exp\left(-e(\Phi - \Phi_{\mathrm{w}}) / T_e \right) \qquad\qquad \mathbf{Q}_e \cdot \mathbf{n} = n_e \mathbf{w}_e \cdot \mathbf{n} \left(e(\Phi - \Phi_{\mathrm{w}}) - \tfrac{1}{2} T_e \right)$$

Examples: plasma properties of a fusion-type negative ion source (2.5D-3V PIC-MCC)

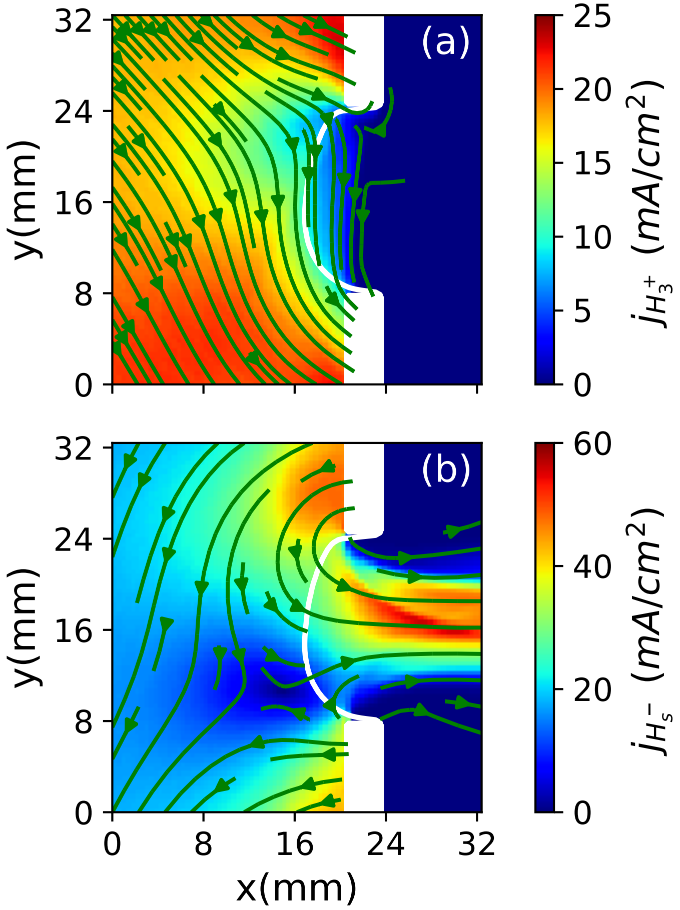


Comparison with experiments

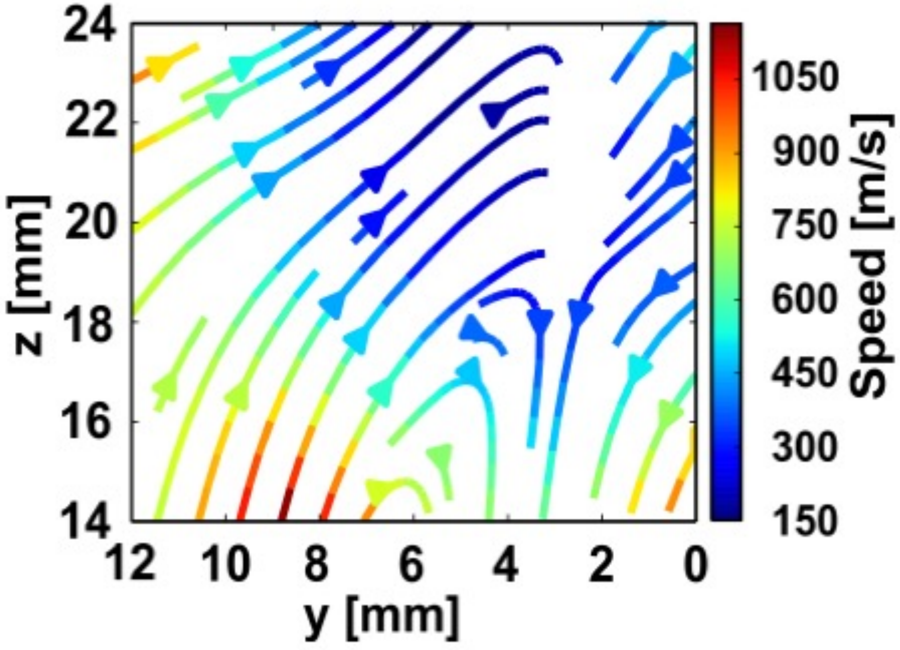


Extraction of negative ions (PIC-MCC)

Zoom near one aperture



Experimental validation

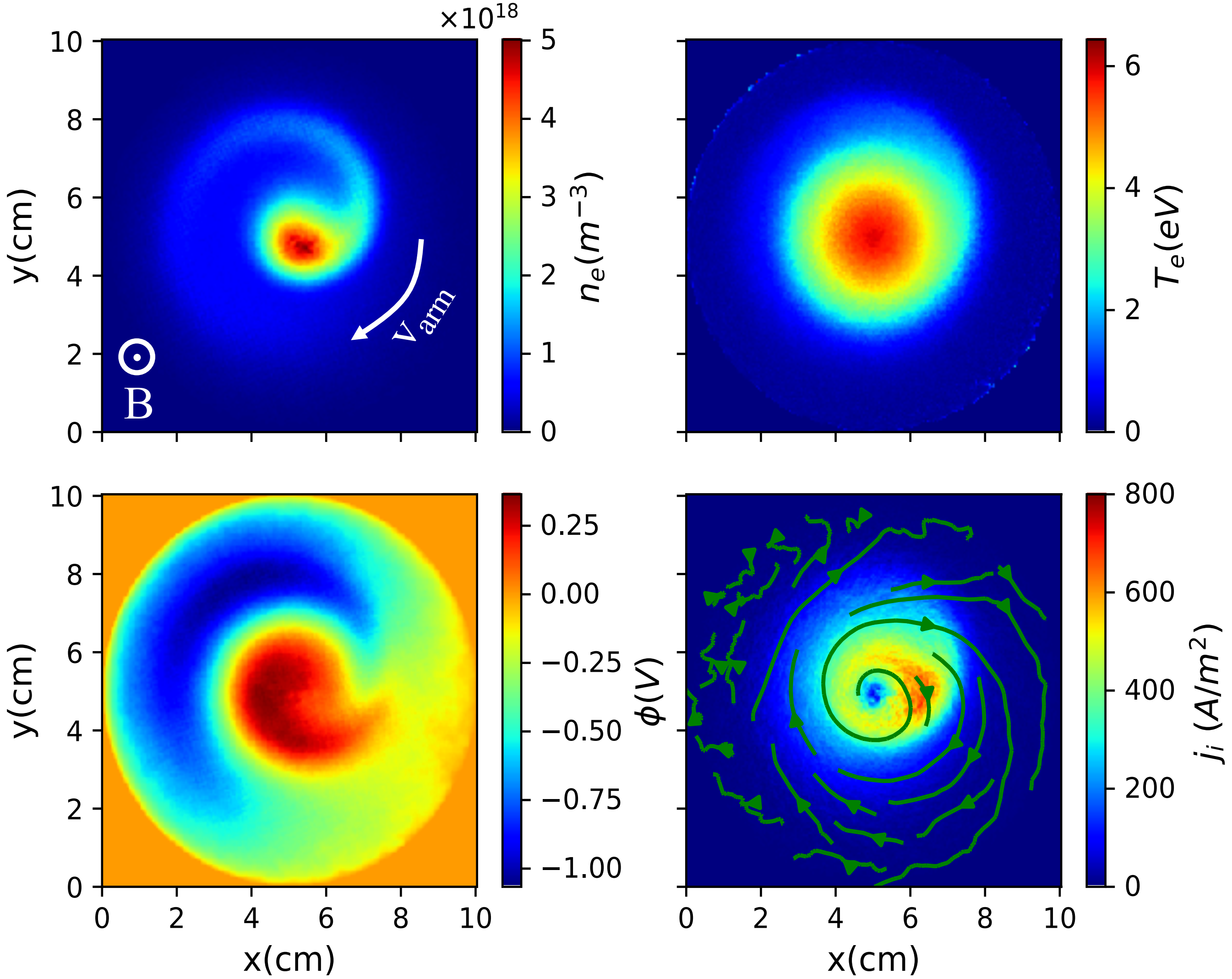


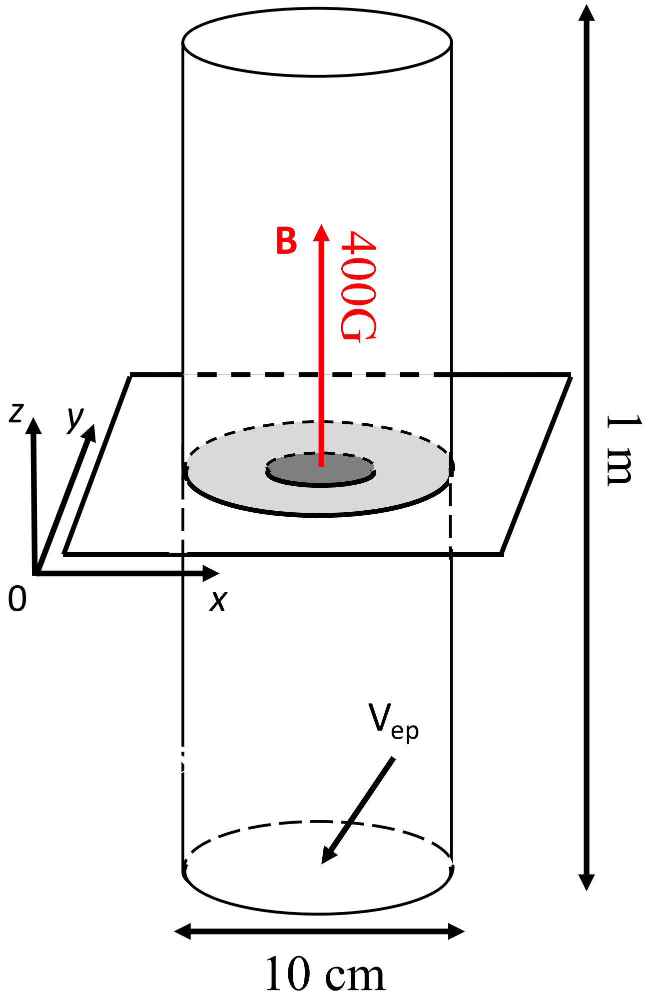
Courtesy of Tsumori et al., NIFS, Japan

Slight magnetization of the negative ions affects the beamlet current density profile

Rotating structures in RF Penning discharges (2.5D-3V PIC-MCC)

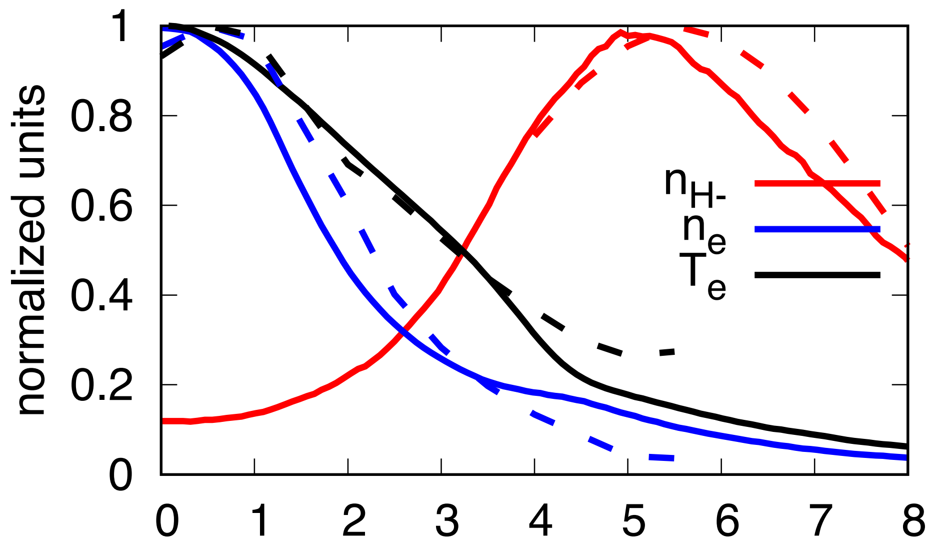
Hydrogen gas, 400G, 0.3 Pa, 2.4 kW, floating end-plates

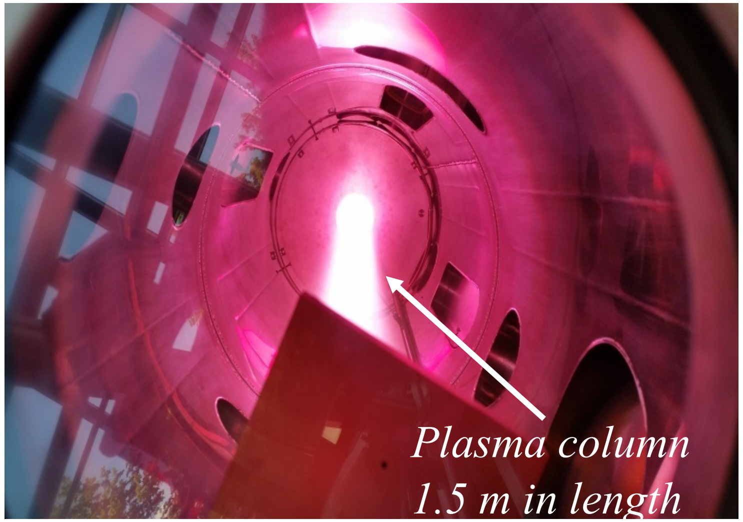


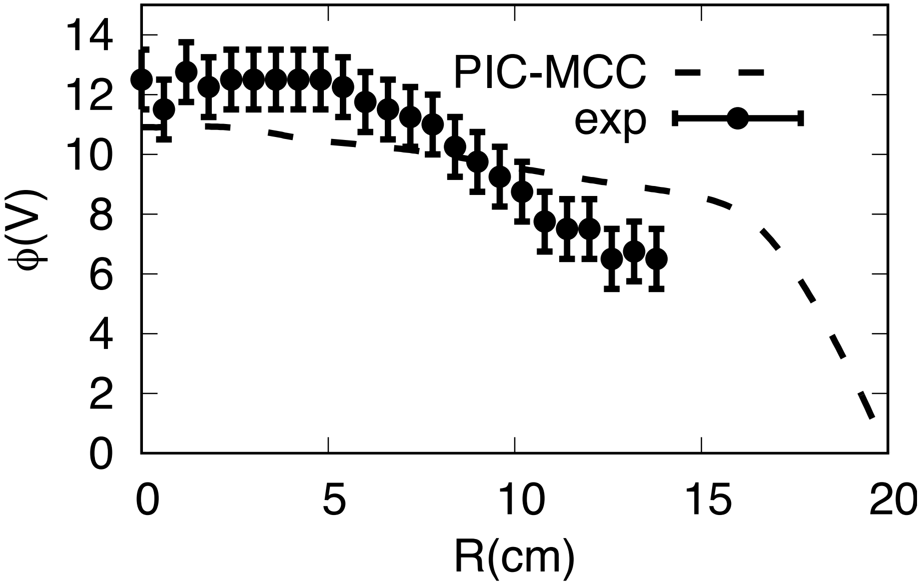


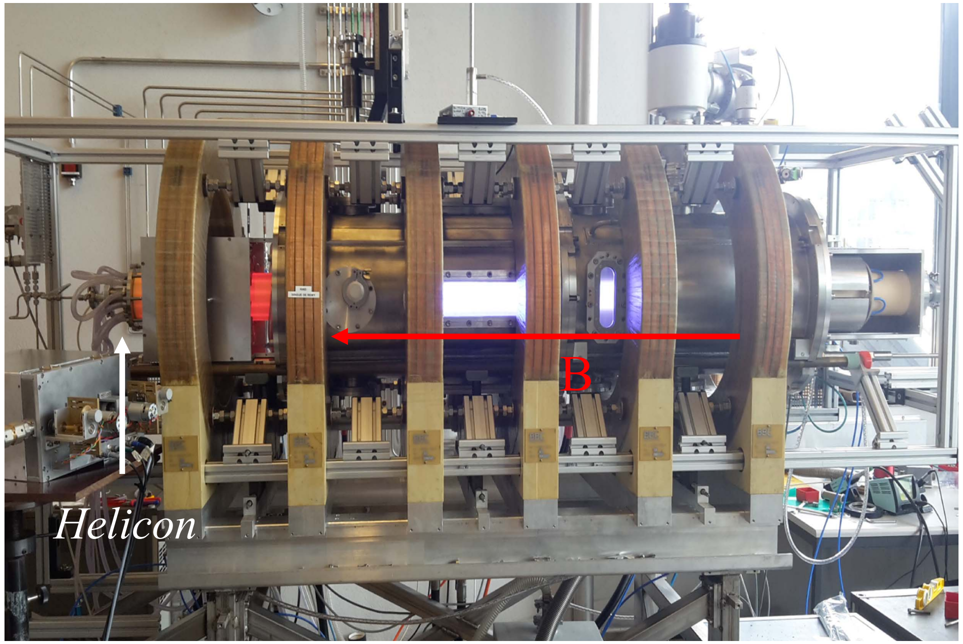
Particle diamagnetic and $E\times B$ drifts are closed

Comparison with experiments performed on RAID at SPC EPFL

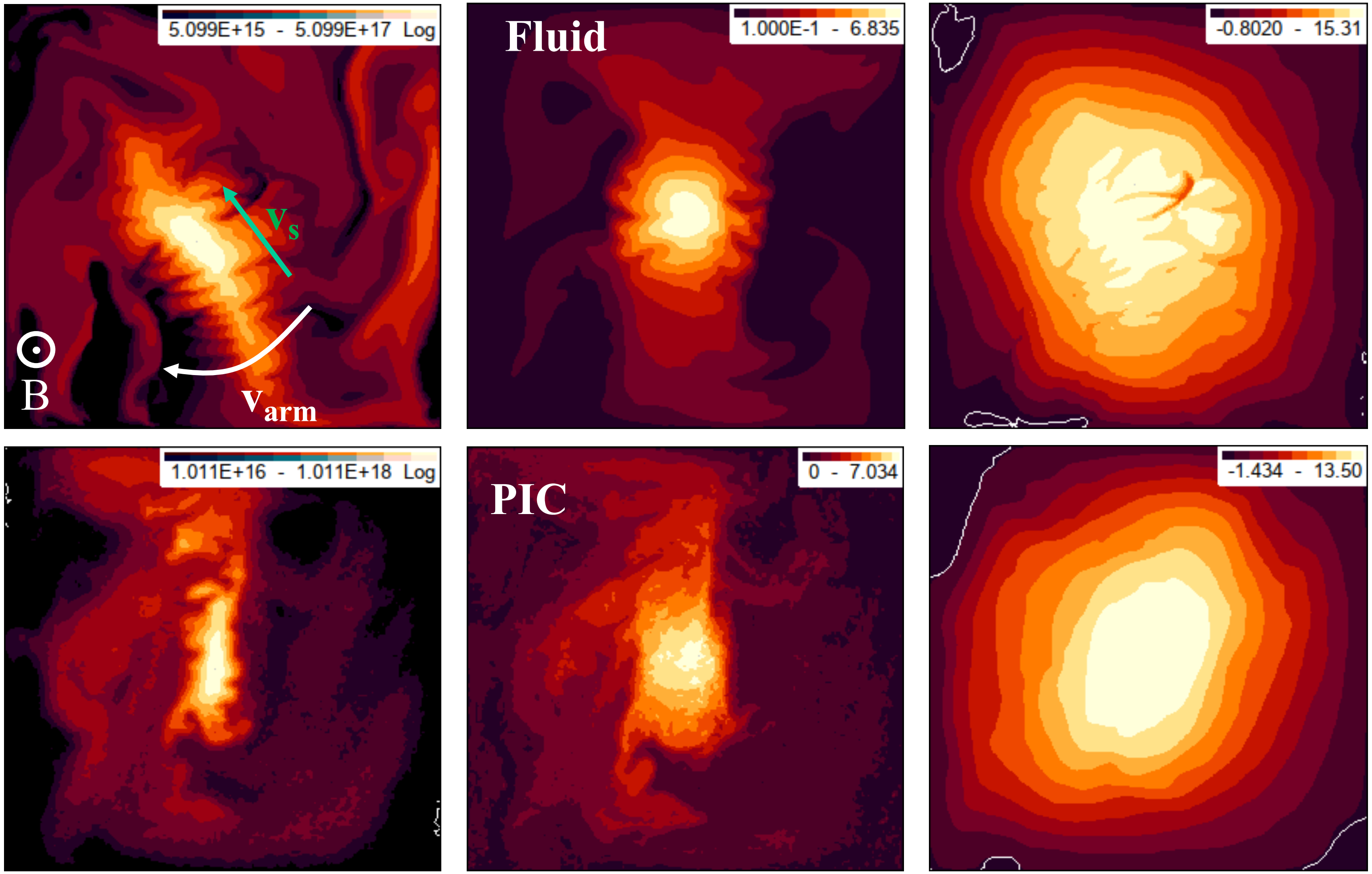








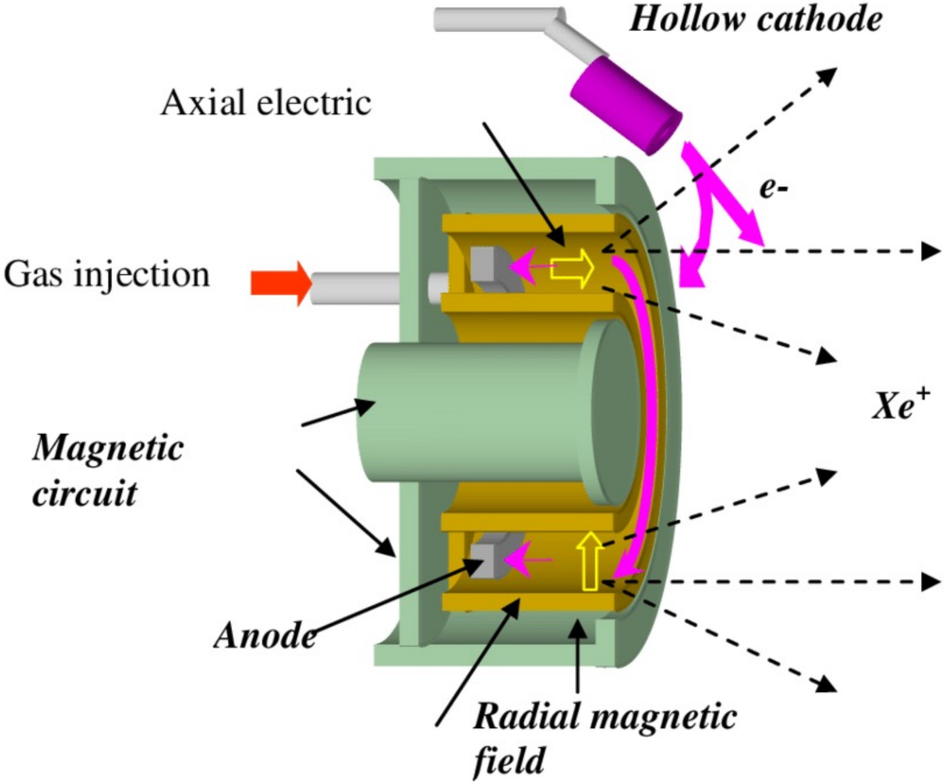
Comparison PIC vs. fluid* models (2.5D). Large scale structure formation in RF Penning discharges

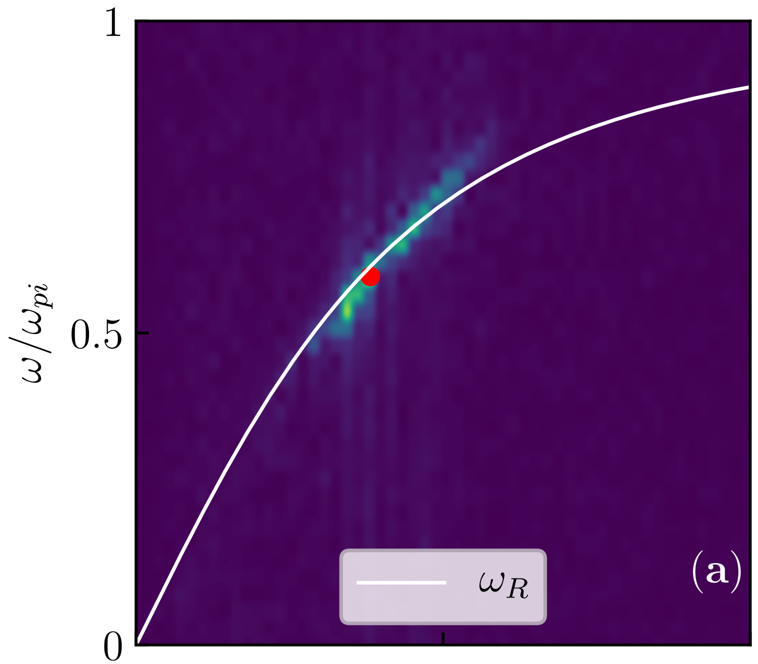


- Arm velocity v_{arm} same direction and magnitude as $E \times B$ drift (also for the ions)
- Fine structures v_s rotate in the direction of the electron diamagnetic drift

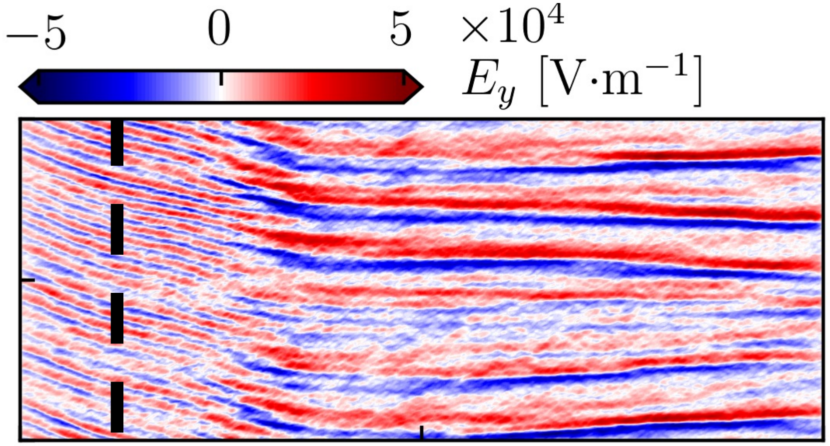
**Model developed by G. Hagelaar*

2D axial azimuthal model of a Hall Thruster* (2D PIC-MCC calculation)





$x = 0.6\ L_x$



$x = 0.12L_x$

*Courtesy of W. Villafana

Conclusion

- Numerical tools are readily available or in development to model Low Temperature (magnetized) Plasma – LTP – devices.
- 1D/2D/3D parallelized OpenMP/MPI explicit PIC-MCC algorithms.
- Electrostatic with prescribed magnetic field maps.
- Can cope with arbitrary physical-chemistry.
- 2.5D fluid models including the magnetic field.
- <u>2D/3D PIC-MCC developments</u> : (i) use of sparse grids, (ii) fully implicit energy and charge conserving algorithms, (iii) electromagnetic.