Italian National Agency for New Technologies,
Energy and Sustainable Economic Development

Particle simulations of plasma-wall interaction at the divertor, plasma sources and plumes

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Contents

- Plasma simulation models
- The particle-in-cell (PIC) method
  - **DESPICCO**: plasma-wall interaction at the divertor walls
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- The hybrid PIC/fluid method
  - **EP2PLUS**: plasma thruster plumes and S/C interaction
- Ongoing and foreseen activities

Plasma simulation models (I)

- Given a set of **boundary conditions** on **electric/magnetic** fields and particles, a plasma model aims at either:
  - obtaining the particle distribution function $f(\boldsymbol{r},\boldsymbol{v},t)$ satisfying Maxwell-Boltzmann's equation (**kinetic models**):

$$\frac{\partial f_s}{\partial t} + \frac{\boldsymbol{p}_s}{m_s} \cdot \nabla f_s + q_s(\boldsymbol{E} + \boldsymbol{v} \times \boldsymbol{B}) \cdot \frac{\partial f_s}{\partial \boldsymbol{p}_{\boldsymbol{s}}} = \left(\frac{\partial f_s}{\partial t}\right)_c$$

$$\iiint f(\boldsymbol{r},\boldsymbol{v},t)\mathrm{d}^3v = n(\boldsymbol{r},t) = \text{number density}$$

  - solving different moments of the Maxwell-Boltzmann's equations (**fluid models**) in terms of fluid properties $\boldsymbol{u}$**,** n, p, $\boldsymbol{q}$, T:

higher order moments $\downarrow$

$\iiint [\text{Boltz.eq.}]\mathrm{d}^3v \longrightarrow$ Mass conservation equation: $G_0(n,\boldsymbol{u},t) = 0$

$\iiint [\text{Boltz.eq.}]\boldsymbol{v}\mathrm{d}^3v \longrightarrow$ Momentum balance equation: $\boldsymbol{G}_1(n,\boldsymbol{u},p,t) = \boldsymbol{0}$

$\iiint [\text{Boltz.eq.}]\frac{mv^2}{2}\mathrm{d}^3v \longrightarrow$ Energy balance equation: $G_2(n,\boldsymbol{u},T,\boldsymbol{q},t) = 0$

Plasma simulation models (II)

- Plasma equations are always coupled with Maxwell's equations:

MAXWELL'S EQUATIONS (SI)

$$\nabla \cdot \boldsymbol{B} = 0 \qquad \nabla \cdot \boldsymbol{E} = \frac{\rho_c}{\epsilon_0}$$

$$\nabla \times \boldsymbol{E} = -\frac{\partial \boldsymbol{B}}{\partial t} \qquad \nabla \times \boldsymbol{B} = \mu_0 \boldsymbol{j} + \frac{1}{c^2}\frac{\partial \boldsymbol{E}}{\partial t}$$

charge and current density are **moments** of the plasma species **distribution functions**

- Plasma models can thus be classified into:
  - **Kinetic models** directly solving for **Maxwell-Boltzmann's equation**:

$$\frac{\partial f_s}{\partial t} + \frac{\boldsymbol{p}_s}{m_s} \cdot \nabla f_s + q_s(\boldsymbol{E} + \boldsymbol{v} \times \boldsymbol{B}) \cdot \frac{\partial f_s}{\partial \boldsymbol{p_s}} = \boxed{\left(\frac{\partial f_s}{\partial t}\right)_c}$$

COMPLEX MODELING

  - **Kinetic models** based on **particles** (particle-particle, particle-mesh methods)
  - **Fluid models**: assumptions of Maxwellian distribution and equation closures
  - **Hybrid PIC-fluid models**: different treatment (kinetic/fluid) according to species

The particle-in-cell method (I): shape and interpolation functions

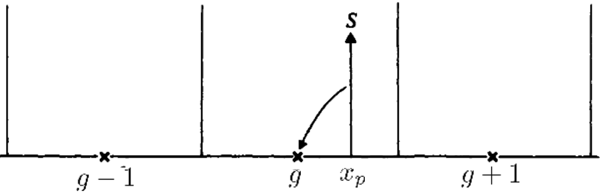
- **Lagrangian-Eulerian particle-mesh method**, consisting in discretizing the distribution function with macro-particles (Lagrangian), while solving for the fields at the mesh nodes (Eulerian):

$$f(\boldsymbol{r},\boldsymbol{v}) = \sum_{p=1}^{N} w_p \delta(\boldsymbol{v}-\boldsymbol{v}_p)\boxed{S(\boldsymbol{r}-\boldsymbol{r}_p)}$$

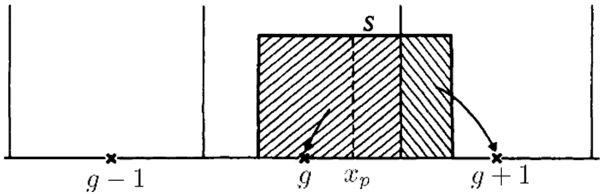
Macro-particle weight

SHAPE FUNCTION

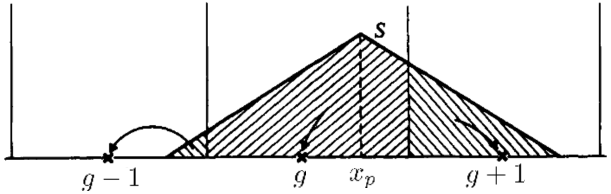
NEAREST GRID POINT (NGP)



CLOUD IN CELL (CIC)



TRIANGULAR SHAPED CLOUD (TSC)



WEIGHTING FUNCTION

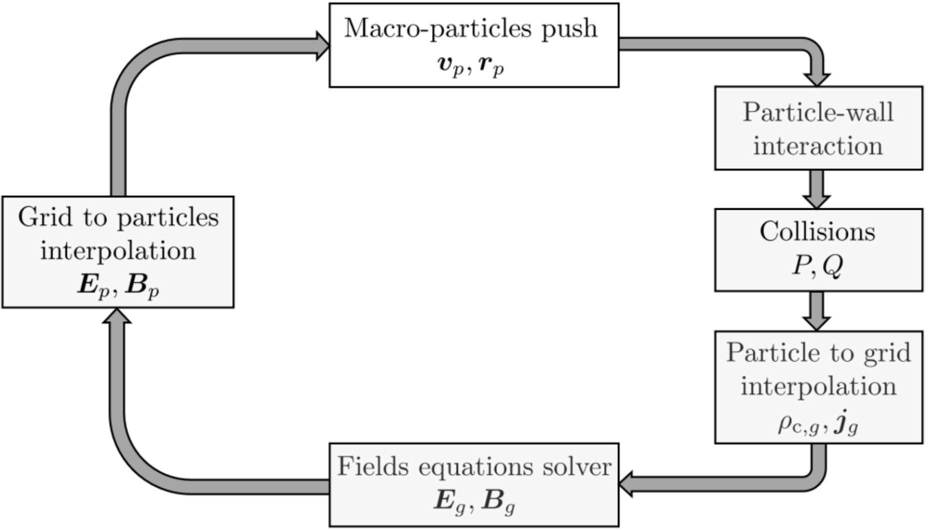
$$W(\boldsymbol{r}) = \iiint S(\boldsymbol{r}')\, b_0\left(\frac{\boldsymbol{r}-\boldsymbol{r}'}{\Delta r}\right) \mathrm{d}^3 r'$$

$$\rho_{c,g} = \frac{1}{V_g}\sum_{p=1} w_p q_p W(\boldsymbol{r}_g - \boldsymbol{r}_p)$$

node volume

$$\boldsymbol{j}_g = \frac{1}{V_g}\sum_{p=1} w_p q_p \boldsymbol{v}_p W(\boldsymbol{r}_g - \boldsymbol{r}_p)$$

The particle-in-cell method (II): the computational cycle



Macro-particles push $\boldsymbol{v}_p, \boldsymbol{r}_p$

Particle-wall interaction

Collisions P, Q

Particle to grid interpolation $\rho_{c,g}, \boldsymbol{j}_g$

Fields equations solver $\boldsymbol{E}_g, \boldsymbol{B}_g$

Grid to particles interpolation $\boldsymbol{E}_p, \boldsymbol{B}_p$

*from «Taccogna 2023, **J. Appl. Phys.*** **134**, 150901»

- **Push**: given **long-range** Lagrangian $\boldsymbol{E}_p$, $\boldsymbol{B}_p$ → update of macro-particles positions/velocities

$$\begin{cases} m_p \dfrac{\mathrm{d}\boldsymbol{v}_p}{\mathrm{d}t} &= q_p(\boldsymbol{E}_p + \boldsymbol{v}_p \times \boldsymbol{B}_p), \\ \dfrac{\mathrm{d}\boldsymbol{r}_p}{\mathrm{d}t} &= \boldsymbol{v}_p, \end{cases}$$

- Short-range particles interaction (**collisions**) modeled as instantaneous collisional events, with sampling based on MCC/DSMC algorithms
- Instantaneous **particle-wall** interaction
  - ion/electron induced SEE, thermionic, sputtering, recombination, reflection, etc…

- Macro-particles **weighting** to mesh nodes → Eulerian charge and current densities $\rho_{c,g}$, $\boldsymbol{j}_g$
- **Maxwell's equation solver** → Eulerian electric and magnetic fields $\boldsymbol{E}_g$, $\boldsymbol{B}_g$
- Interpolation to particle positions → Lagrangian electric and magnetic fields $\boldsymbol{E}_p$, $\boldsymbol{B}_p$ → **New step**

The particle-in-cell method (III): the constraints

1. Courant–Friedrichs–Lewy (CFL) condition:
   - Electrostatic PIC: $v_e \Delta t_{\mathrm{PIC}} < \Delta r$
   - Electromagnetic PIC: $c \Delta t_{\mathrm{PIC}} < \Delta r$

Further limitation on time step

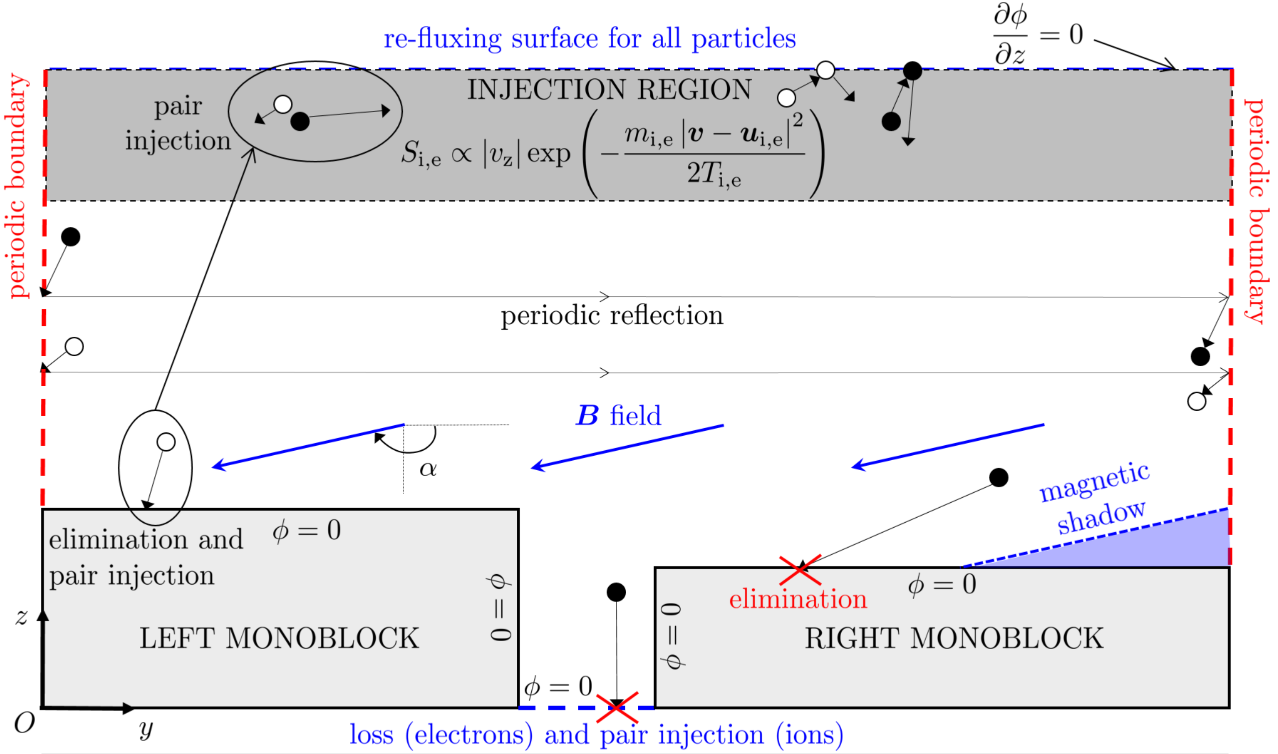
2. Grid resolution to avoid numerical heating: $\Delta r \leq \zeta \lambda_{\mathrm{De}}$ with $\zeta = O(1)$
   - Implicit (more complex) PIC schemes do not have to comply with this → Large savings in computational time

3. Plasma frequency resolution: $\omega_{\mathrm{pe}} \Delta t_{\mathrm{PIC}} < 0.2$

4. Cyclotron frequency resolution: $\omega_{\mathrm{ce}} \Delta t_{\mathrm{PIC}} < 0.35$
5. Cyclotron radius resolution: $\Delta r \leq r_{\mathrm{Le}}$

6. Collisional time constraint: $\Delta t_{\mathrm{PIC}} < 0.05\ \Delta t_{\mathrm{coll,min}}$

DESPICCO: Divertor Edge Simulator of Plasma-wall Interaction with Consistent COllisions



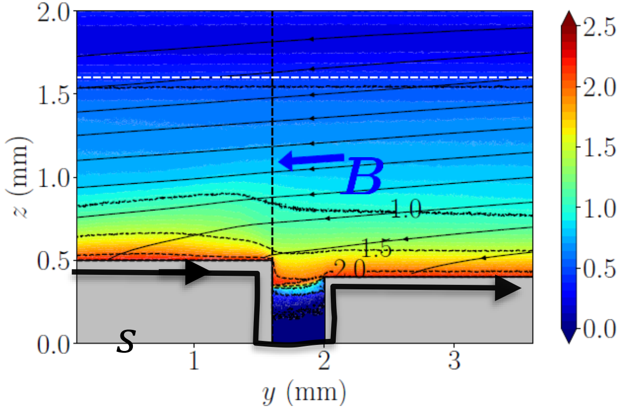
from «Cichocki 2023, ***Nucl Fusion 63****,* 086022»

- 2D-3V code developed within DTT (2021-2023) to study the plasma-wall interaction in the vicinity of the divertor in collaboration with **ISTP-CNR** (**Bari**)
- Complex divertor monoblocks geometries
- Parallelized with either **Open-MP** or **CUDA** on a single node

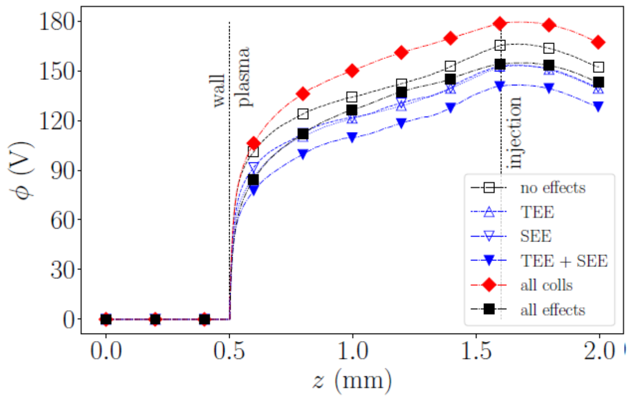
DESPICCO results: exposed edges in ITER

- Code validated against theoretical predictions
- For a poloidal gap scenario featuring exposed edges in ITER:
  - Code results were benchmarked against SPICE2 code
  - A parametric analysis on the effects of electron wall emission and collisions was carried out

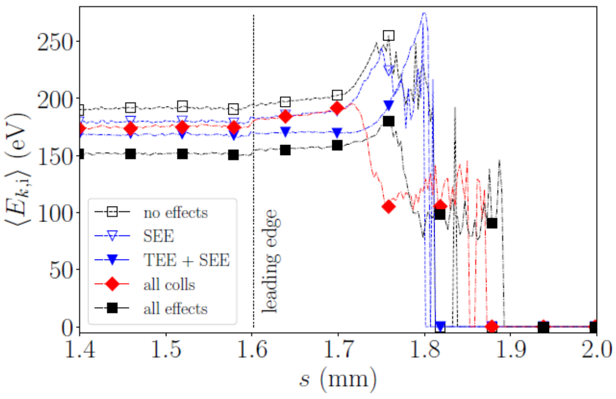
Ion Mach number [-]



Potential [V] versus wall distance



Mean ion impact energy [eV] along the wall

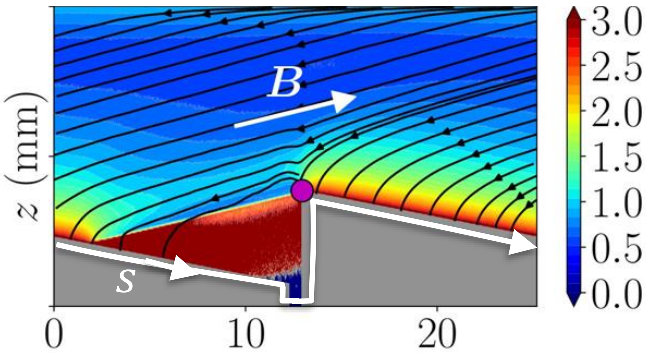


*from «Cichocki 2023, **Nucl Fusion 63**, 086022»*

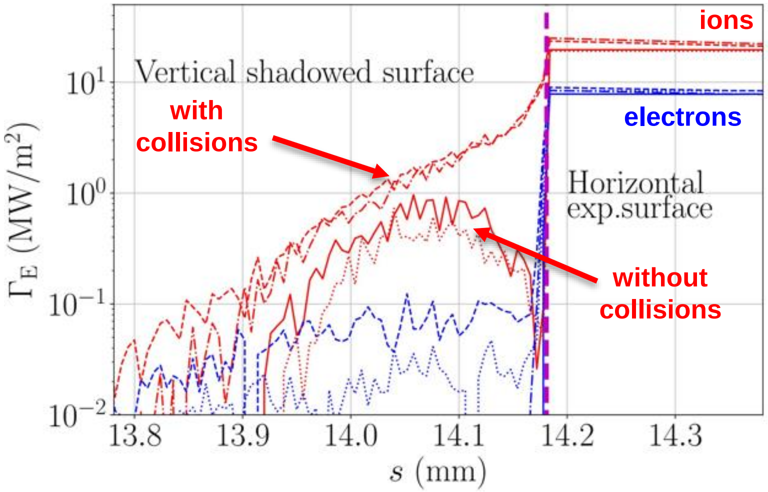
DESPICCO results: DTT shadowed edges

- An **attached divertor condition** with SN magnetic configuration was considered (invited talk EPS 2023, *Cichocki 2024, Plasma Phys. Control. Fusion 66, 025015*)
- Worst energy flux points on both IVT and OVT
- Effect of bevelling and collisions/wall emission on energy fluxes and ion impact distribution function was assessed

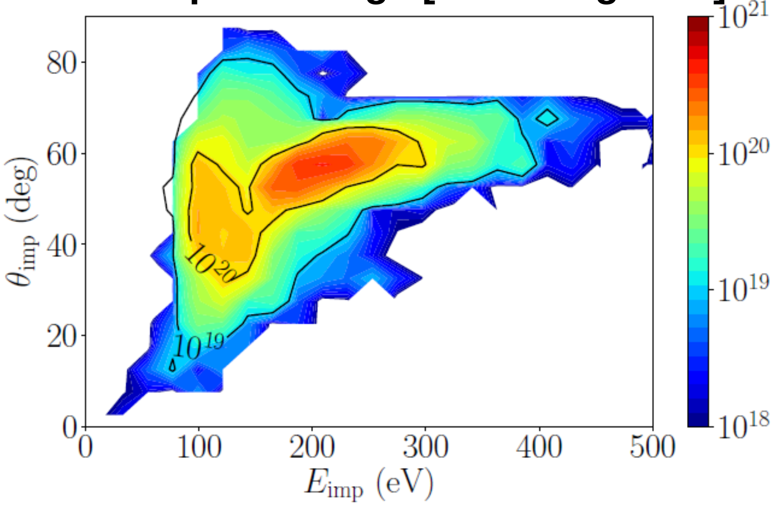
Ion Mach number at OVT [-]



Ion/electron energy fluxes around corner at OVT



Ion impact distribution function at OVT close to exposed edge [$m^{-2}\,s^{-1}deg^{-1}eV^{-1}$]

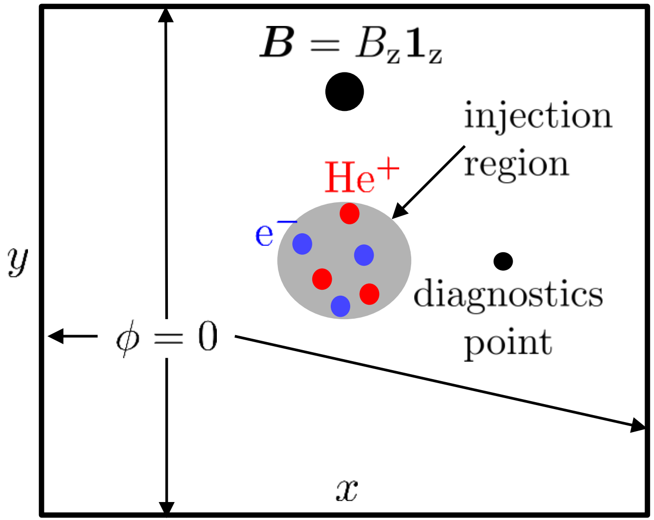


PICCOLO: PIC COde for LOw temperature plasmas

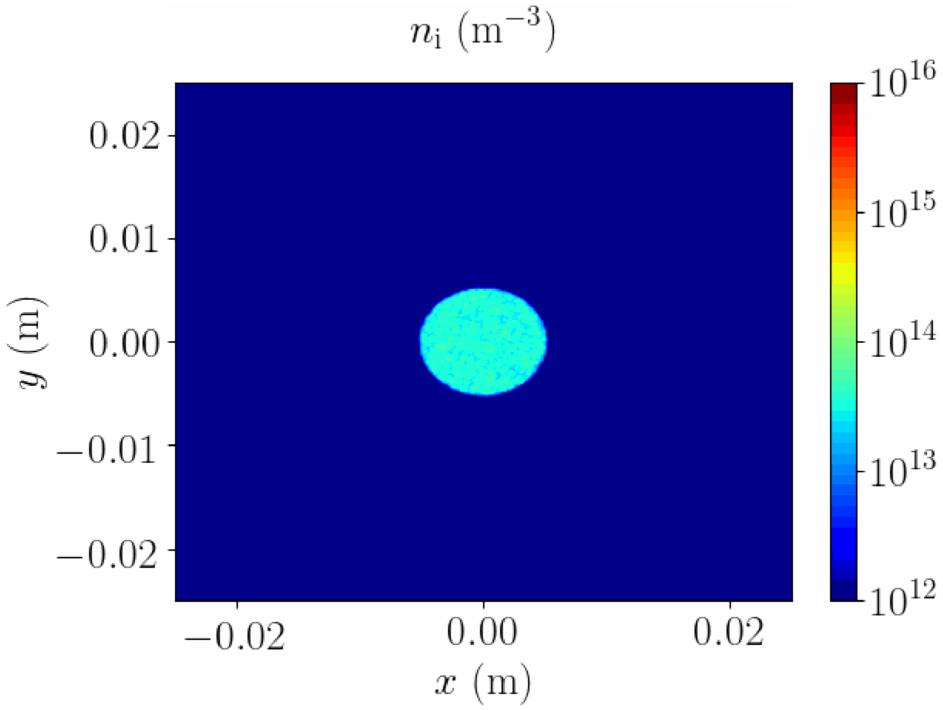
- General purpose PIC code for **multi-dimensional simulations** (1D, 2D, 3D) in **cylindrical** and **cartesian** coordinates
- Developed in collaboration with ISTP-CNR (Bari)
- Parallelized with **MPI** and **tested** over more than **3000 CPU cores**, with good scalability
- Currently **electrostatic PIC code** $\nabla^2\phi = -\frac{\rho_c}{\epsilon_0}$
- It already **incorporates DESPICCO functionalities**
- Benchmarked against other codes within **LANDMARK, L**ow temper**A**ture mag**N**etize**D** plas**MA** benchma**RK**s, https://jpb911.wixsite.com/landmark/test-cases
- Apart from divertor scenarios, already applied for:
    - Hall thruster chamber simulations (SPT100)
    - Negative ion sources chamber simulations (SPIDER, ITER)
    - Streamer simulations (high pressure discharge ignition)

PICCOLO: 2D Penning discharge benchmark

Simulation domain



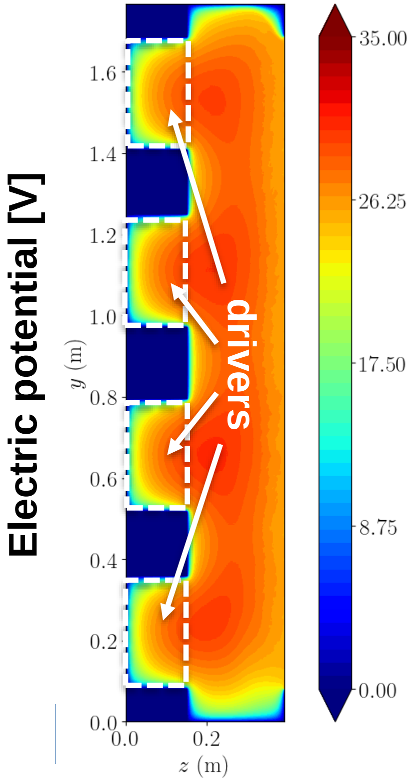
Ion density video

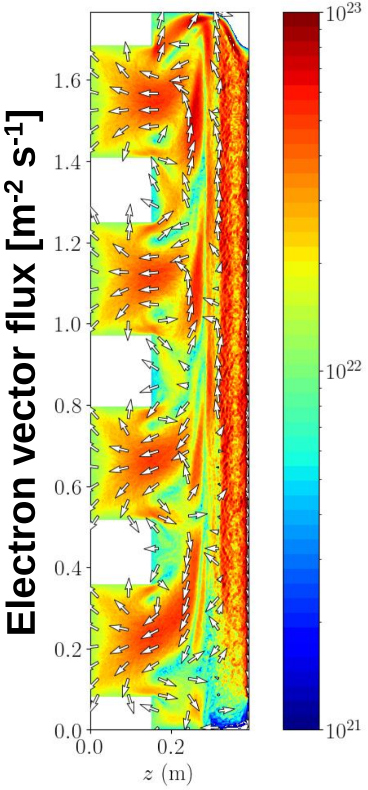


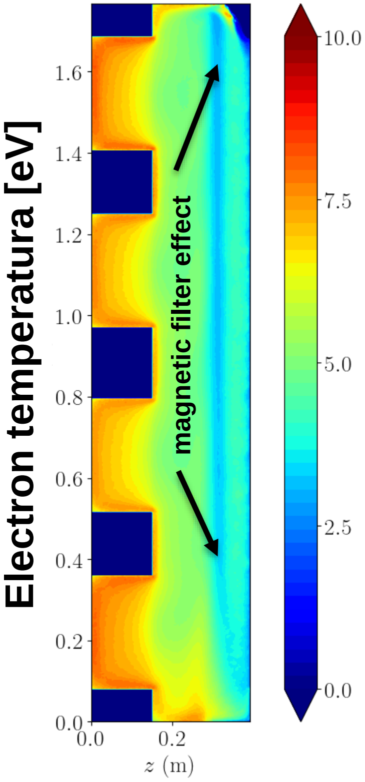
A collisionless plasma diffuses out of the box through the onset of instabilities (rotating spoke

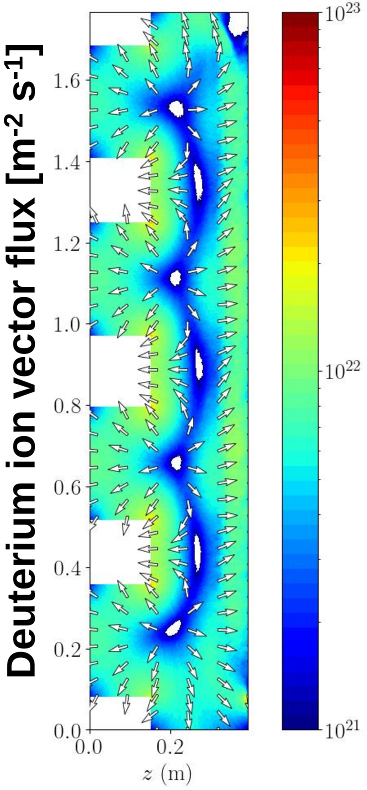
PICCOLO: SPIDER chamber 2D y-z simulation

- ➢ Increased artificially the dielectric constant to reduce the computational cost (x 22500)
- ➢ Applied magnetic field perpendicular to the page, to filter electrons

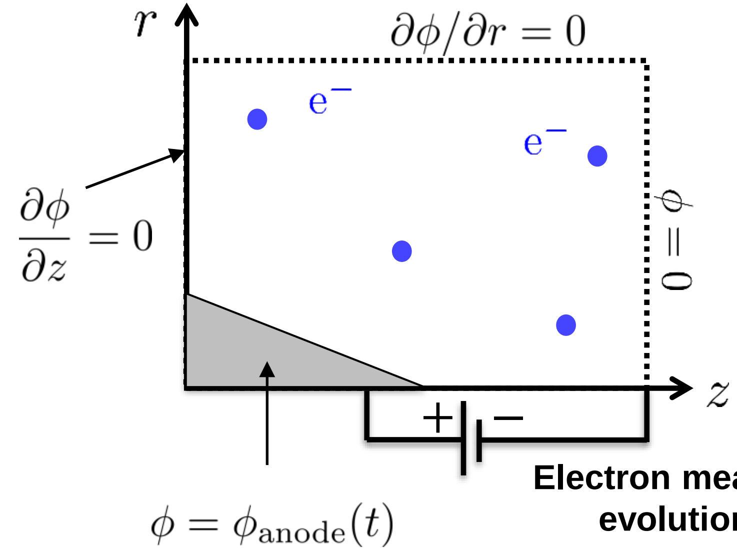




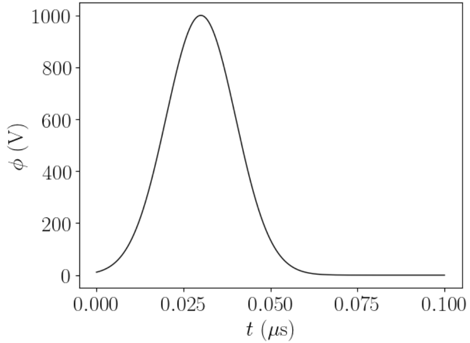




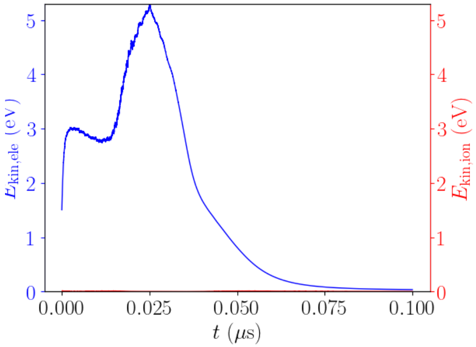
PICCOLO: streamer 2D r-z simulation



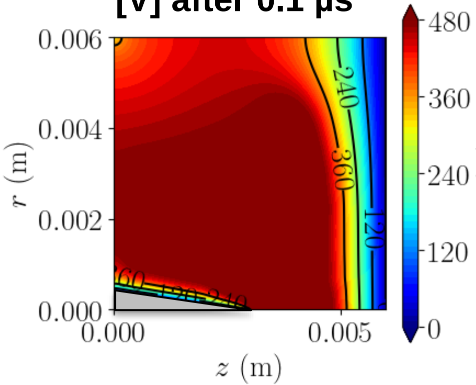
- Experimental setup for **plasma processing experiments** featuring a high-voltage conical needle
- 2D simulation in cylindrical coordinates
- Self-consistent **high pressure discharge ignition**
  - Electrons ionize a background gas (at 1 atm), starting from a few free electrons distributed in space
- Time-varying boundary conditions → Study of transient phenomena



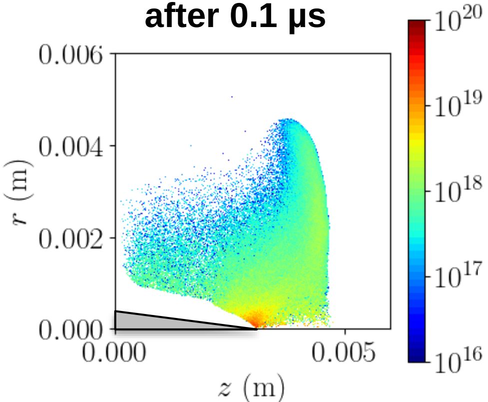
Electron mean energy evolution [eV]



Electric potential [V] after 0.1 μs



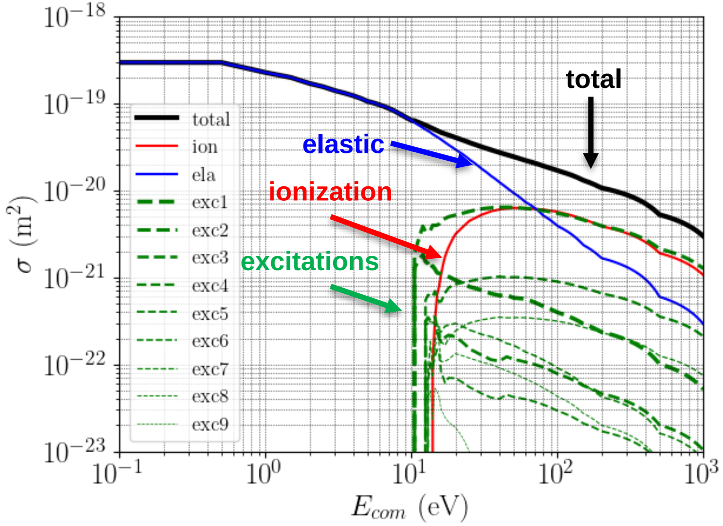
Ion density [m^{-3}] after 0.1 μs



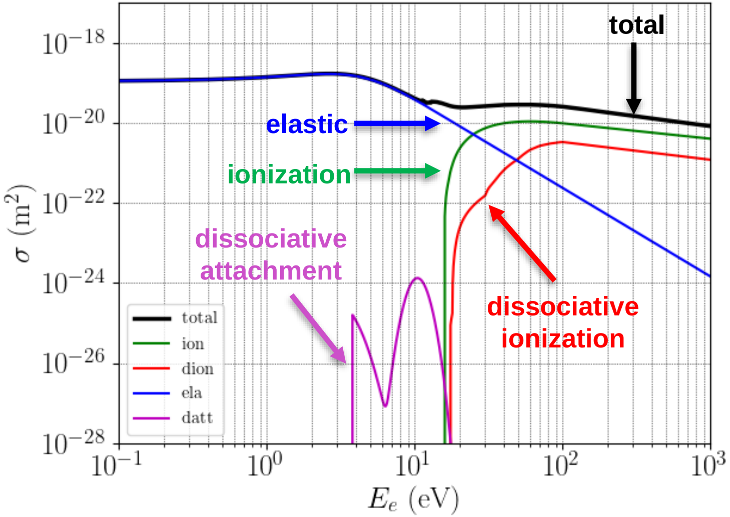
PIC codes collisional database

- The collisional cross sections are stored in a **common PIC codes HDF5 database**
- Vast variety of collisional processes: elastic, ionization, excitation, charge exchange, dissociative ionization, vibration, recombination, etc…
  - Currently only state-independent cross sections
  - We are working also on **state-dependent** (vibration/excitation) **cross sections**

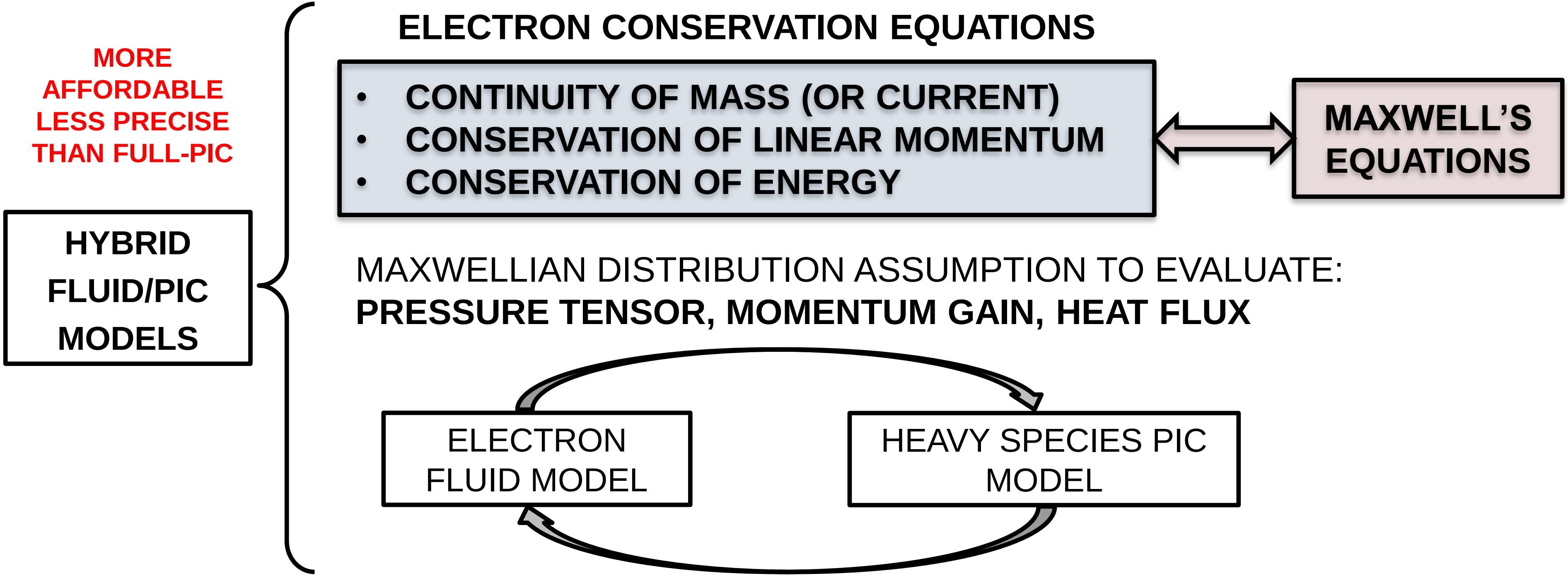
electron-deuterium atom cross sections



electron-H molecule cross sections



The hybrid PIC/fluid method



MORE AFFORDABLE
LESS PRECISE THAN FULL-PIC

HYBRID FLUID/PIC MODELS

ELECTRON CONSERVATION EQUATIONS

- **CONTINUITY OF MASS (OR CURRENT)**
- **CONSERVATION OF LINEAR MOMENTUM**
- **CONSERVATION OF ENERGY**

MAXWELL'S EQUATIONS

MAXWELLIAN DISTRIBUTION ASSUMPTION TO EVALUATE:
PRESSURE TENSOR, MOMENTUM GAIN, HEAT FLUX

ELECTRON FLUID MODEL

HEAVY SPECIES PIC MODEL

EP2PLUS: Extensible Parallel Plasma PLUme Simulator

- **Hybrid 3D** code developed at UC3M (University of Madrid “Carlos III”) during my PhD studies
- Ions and neutrals followed as PIC macro-particles
- Electrons modeled as a magnetized fluid subject to conservation equations:

$$\nabla \cdot (\boldsymbol{j}_{\mathrm{e}} + \boldsymbol{j}_{\mathrm{i,PIC}}) = -\partial \rho_{\mathrm{c}} / \partial t$$

CURRENT CONTINUITY

$$0 = -\nabla p_{\mathrm{e}} - e n_{\mathrm{e}} \left(\boldsymbol{E} + \boldsymbol{u}_{\mathrm{e}} \times \boldsymbol{B} \right) - \sum_s \nu_{\mathrm{e}s} m_{\mathrm{e}} n_{\mathrm{e}} \left(\boldsymbol{u}_{\mathrm{e}} - \boldsymbol{u}_s \right)$$

MOMENTUM BALANCE

$$\frac{T_{\mathrm{e}}}{T_{\mathrm{e0}}} = \left(\frac{n_{\mathrm{e}}}{n_{\mathrm{e0}}} \right)^{\gamma - 1}$$

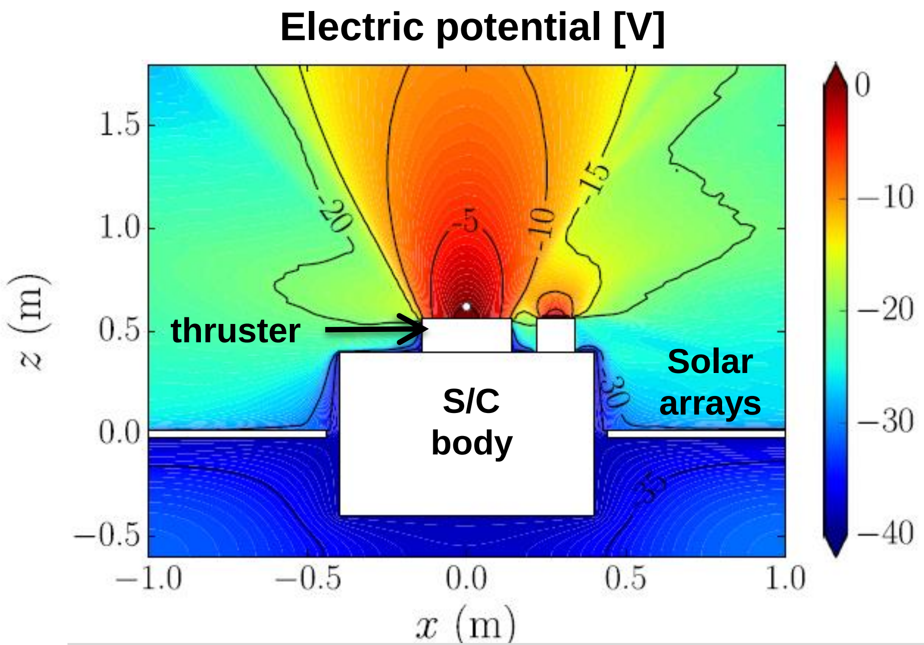
POLYTROPIC APPROXIMATION

- Quasineutral approximation ($n_e = \sum_s Z_s n_s$), except in rarefied regions where a non-linear Poisson’s equation solver is considered:

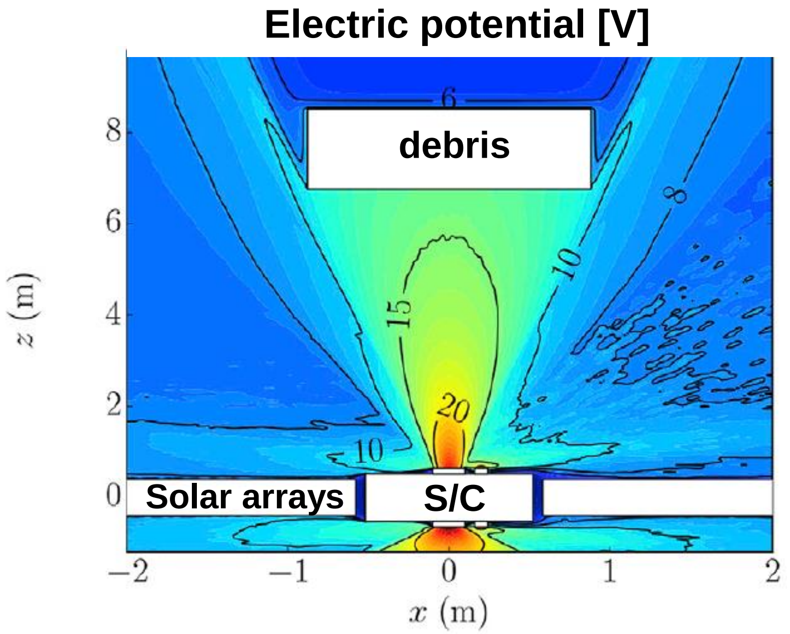
$$\nabla^2 \phi = \frac{\left[e n_{\mathrm{e}}(\phi) - \rho_{\mathrm{c,PIC}} \right]}{\epsilon_0}$$

- Deformed structured PIC meshes can be used
- Studies on different plasma thruster plumes scenarios

EP2PLUS applications (I): plasma plumes - S/C interaction



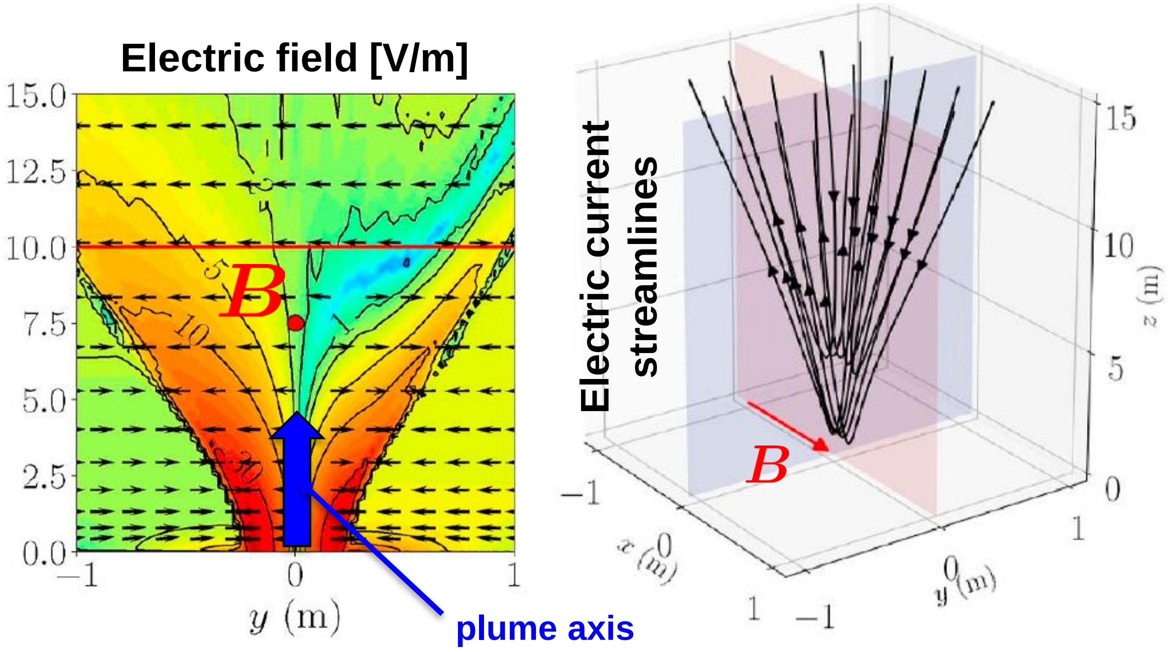
from «Cichocki 2017, ***Plasma Sources Sci. Technol. 26***,125008»



from «Cichocki 2018, ***Acta Astronautica* 146**, 216–227»

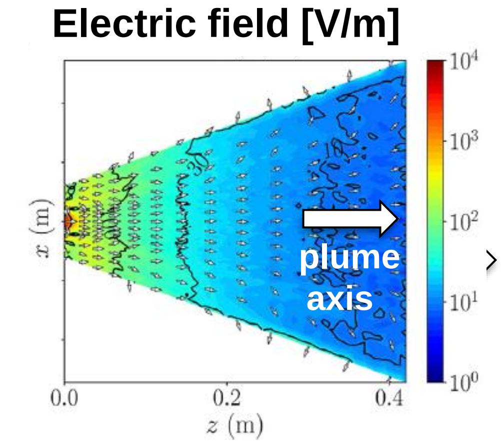
EP2PLUS applications (II): plumes

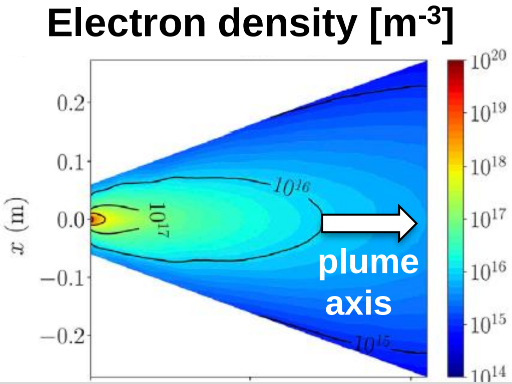
Plasma plume expanding in geomagnetic field



from «Cichocki 2020, **Acta Astronautica 175**, 190–203»

Helicon plasma plume expansion in a magnetic nozzle





from «Cichocki 2022, **Front. Phys. 10**, 876684»

Ongoing activities

- ❑ Finalization of DESPICCO simulations of **plasma-wall interaction** in the **DTT divertor region**, within work package DTT-PEX 2023
  - ▪ Simulations of the DOME region for an XD magnetic configuration
  - ▪ Inclusion of Neon gas and e-Ne, Ne-D collisions
  - ▪ Larger domain size in the direction normal to the wall → a few cms in 1D simulations
- ❑ Finalization of Eurofusion PARADIGM HPC Project (**PAR**ametric **A**nalysis of **DI**vertor **G**eometry considering **M**ultiple kinetic effects)
  - ▪ Set of > 50 simulations with varying monoblock bevel angles and plasma/magnetic field conditions
- ❑ Update of PICCOLO to simulate **magnetic nozzle expansions** (collaboration with Doct. **F. Napoli** and PhD student **D. Iannarelli**) → propulsive application of **ProtoSphera** and development of Helicon plasma thrusters
  - ▪ At free-loss boundaries, some electrons must be reflected (energy criterion)
- ❑ Collaboration with ISTP-CNR in PIC simulations of various plasma sources:
  - ▪ Negative ion source SPIDER (ITER reactor)
  - ▪ Cylindrical streamer discharge ignition (plasma processing)

Foreseen activities

- ☐ **Short/Medium term activities:**
  1. Application of DESPICCO/PICCOLO to relevant scenarios in **DTT** and **ProtoSphera** (any proposals?)
  2. Study of a **magnetic nozzle plume expansion** with PICCOLO to assess the propulsive performance of both direct fusion drive thrusters (e.g. **ProtoSphera** propulsive application) and other plasma thrusters (Helicon, ECR thrusters, etc…)
     - A study for a **Helicon plasma thruster prototype** will be presented at **38th IEPC** (International Electric Propulsion Conference)
  3. Study of the plasma-divertor wall interaction in **WEST** with DESPICCO (**WPTE 2024**)
  4. Participation as invited speaker to **ESCAMPIG 2024** conference (PIC codes applications)
  5. Inclusion of molecular collisions physics in PIC codes (with vibrational level dependent cross sections)
  6. Modeling of neutrals as particle species (in a separate TPMC module) in DESPICCO/PICCOLO
- ☐ Medium/long term activities:
  1. Experimental activities in ProtoSphera and related projects (to be defined)
  2. Update of PICCOLO to **electromagnetic PIC** → fully consistent simulations of laser-plasma interaction, RF plasma sources, plasma-wall interaction in proximity to ICRH antenas, etc…

References

1. F. Cichocki *et al* 2024, Kinetic modeling of the plasma–wall interaction in the DTT divertor region, ***Plasma Phys. Control. Fusion* 66**, 025015
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5. F. Cichocki *et al* 2020, Three-dimensional geomagnetic field effects on a plasma thruster plume expansion, **Acta Astronautica 175**, 190–203
6. F. Cichocki *et al* 2018, Spacecraft-plasma-debris interaction in an ion beam shepherd mission, ***Acta Astronautica* 146**, 216–227
7. F. Cichocki *et al* 2017, Hybrid 3D model for the interaction of plasma thruster plumes with nearby objects, ***Plasma Sources Sci. Technol. 26,***125008

Thank you very much for the attention

Questions?

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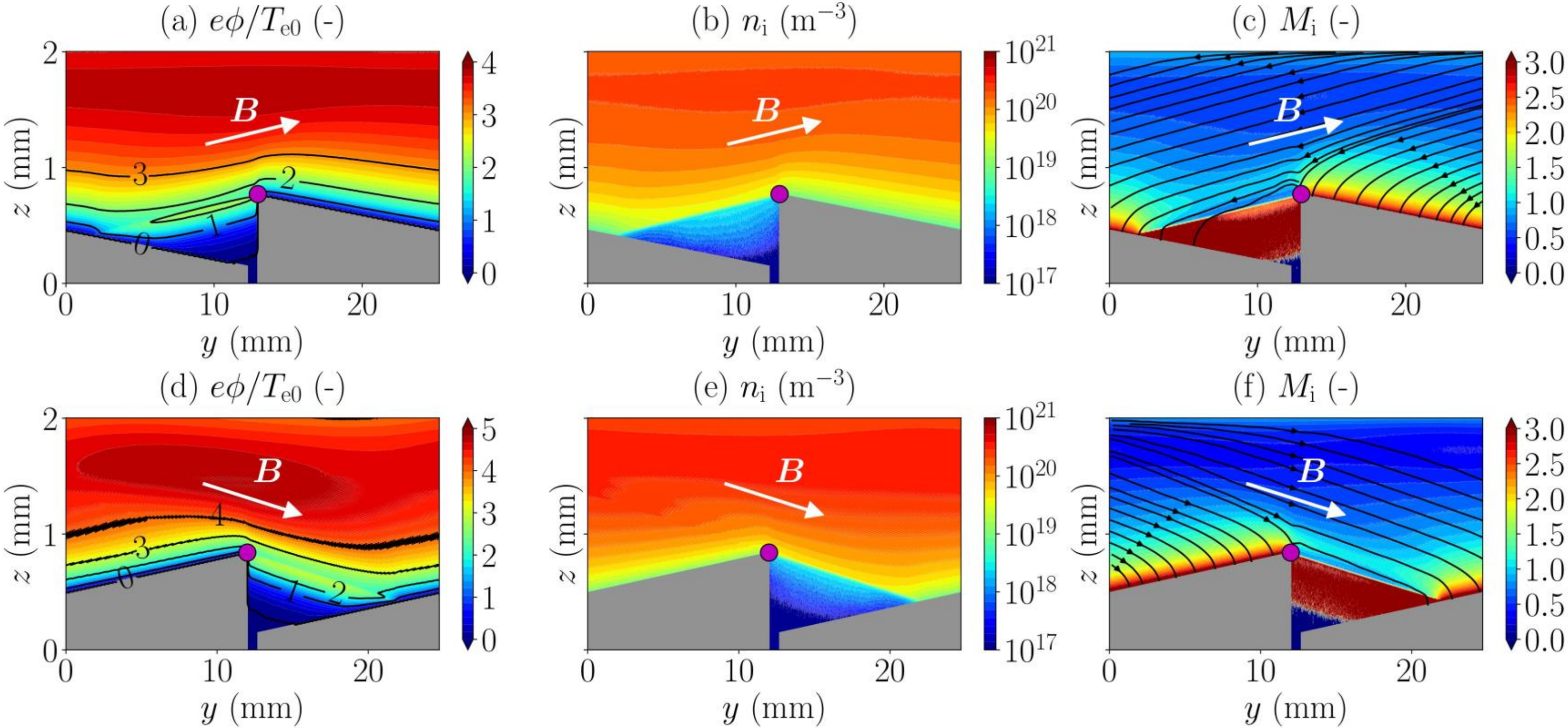
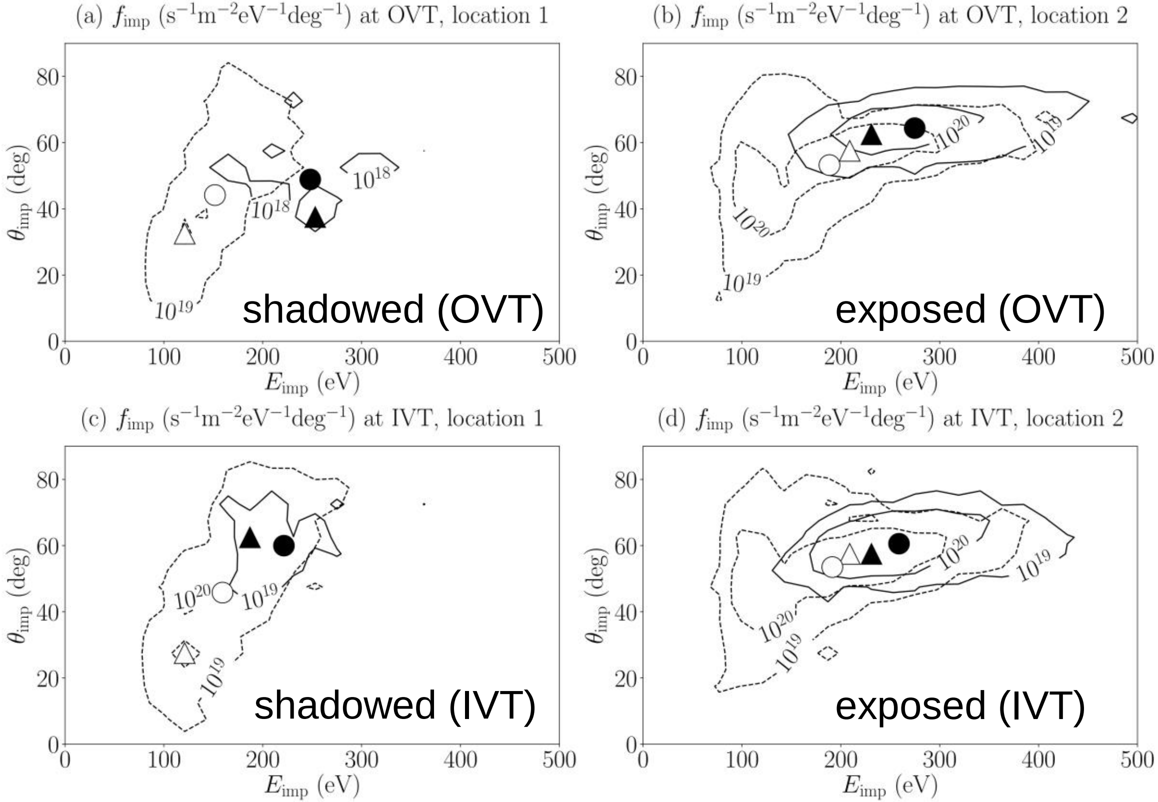
Extra slides (I): PIC simulations for DTT (OVT and IVT)



Extra slides (II): PIC simulations for DTT (dist. functions)

— contours plot for no-effects cases

- - - contours plot for all-effects cases

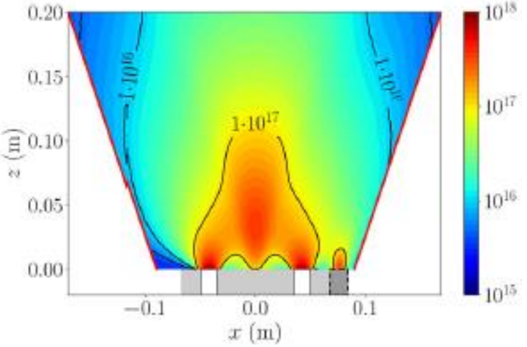


Extra slides (III): EP2PLUS applications to GITs and HETs

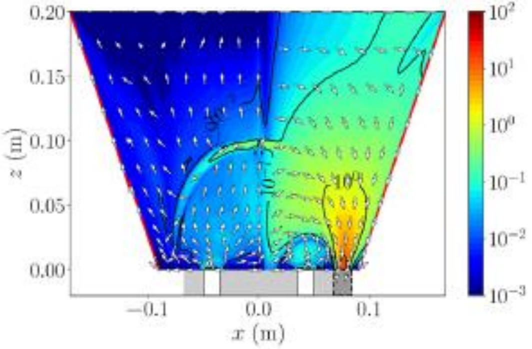
HALL THRUSTER PLUME

«Cichocki 2021, ***Acta Astronautica* 187**, *498–510*»

Electron density [m^{-3}]



Current density [Am^{-2}]



GRIDDED ION THRUSTER PLUMES

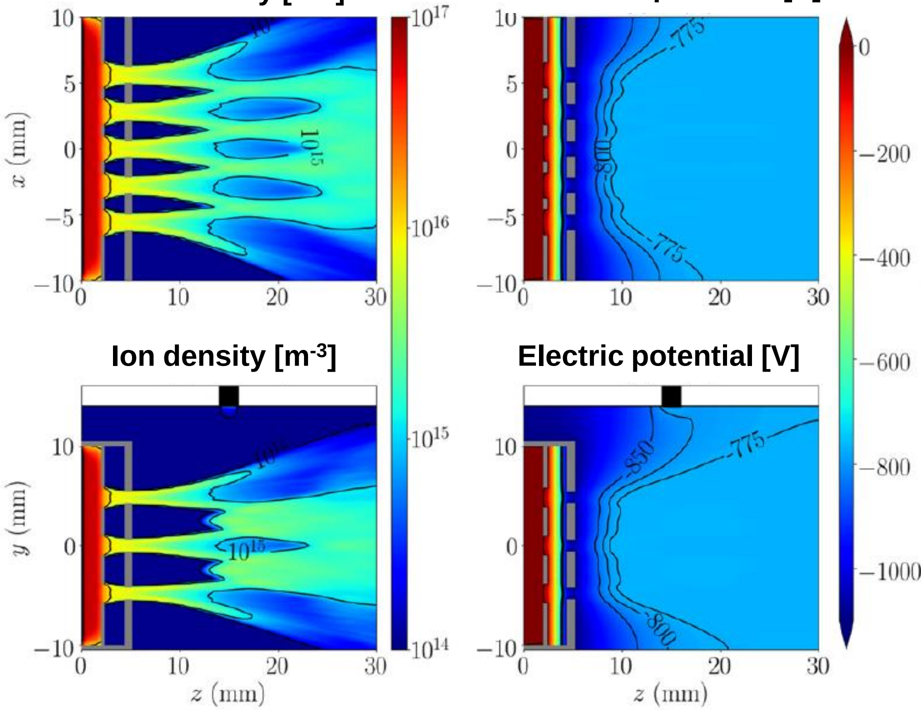
«Perales 2021, ***Plasma Sources Sci. Technol.* 30**, *105023*»

Ion density [m^{-3}]

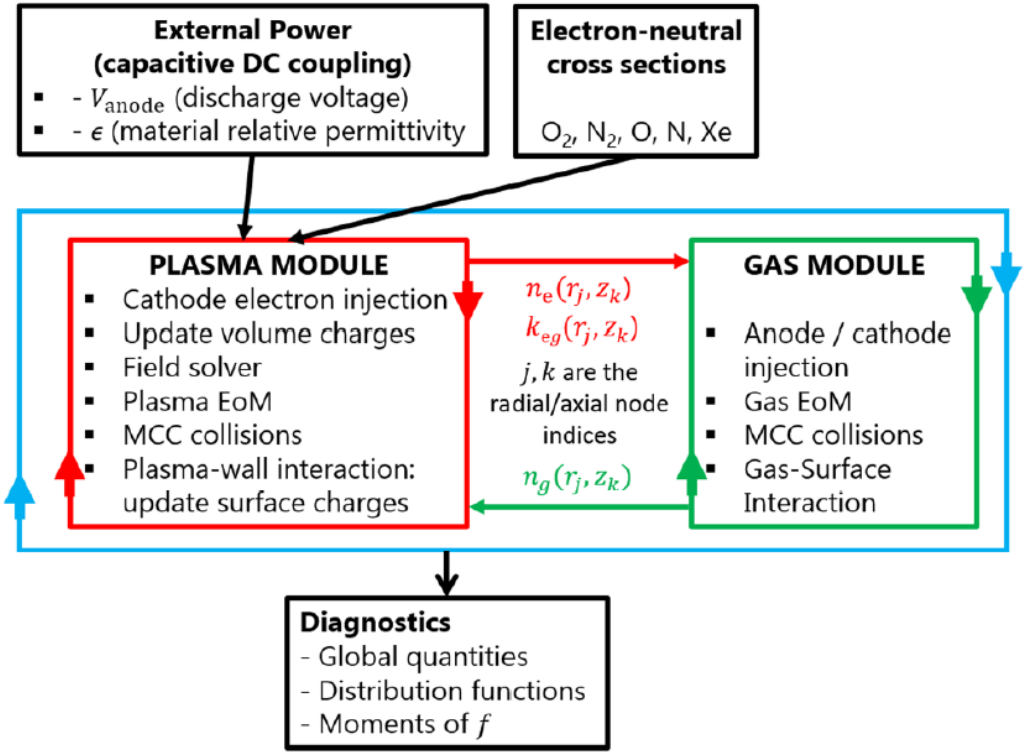
Electric potential [V]

Ion density [m^{-3}]

Electric potential [V]



Extra slides (IV): TPMC-PIC model



External Power (capacitive DC coupling)

- \- V_{anode} (discharge voltage)
- \- ϵ (material relative permittivity

Electron-neutral cross sections

O_2, N_2, O, N, Xe

PLASMA MODULE

- Cathode electron injection
- Update volume charges
- Field solver
- Plasma EoM
- MCC collisions
- Plasma-wall interaction: update surface charges

$n_e(r_j, z_k)$

$k_{eg}(r_j, z_k)$

j, k are the radial/axial node indices

$n_g(r_j, z_k)$

GAS MODULE

- Anode / cathode injection
- Gas EoM
- MCC collisions
- Gas-Surface Interaction

Diagnostics

\- Global quantities

\- Distribution functions

\- Moments of f