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DEI PLASMI
Consiglio Nazionale delle Ricerche

The computational virtual lab of electric propulsion at CNR-ISTP, Bari

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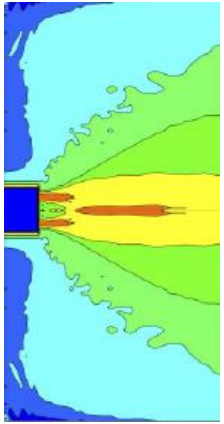
Contents

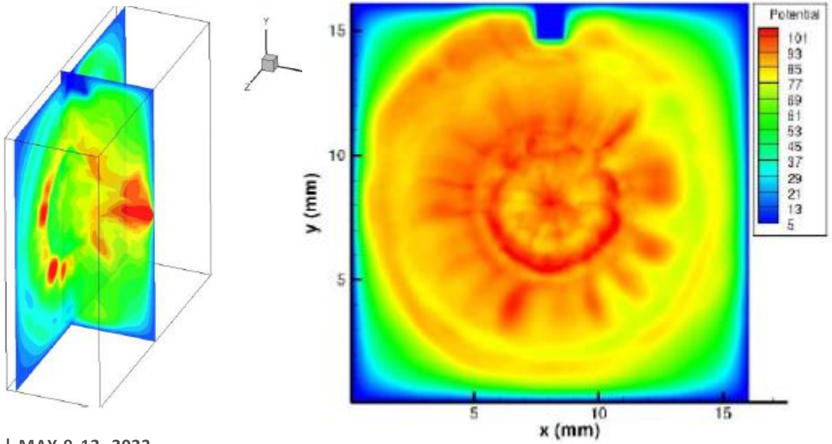
Overview of past and present simulation activities at ISTP (I)

- In the last 2 decades, ISTP has gained significant experience in PIC codes for different applications:
  1. 2D and 3D hybrid PIC/fluid codes for plasma thruster plume expansions
  2. Fully 3D (with geometrical scaling) near Hall thruster (HT) plume simulations
  3. Fully 1D (θ or r) simulations of a HT discharge

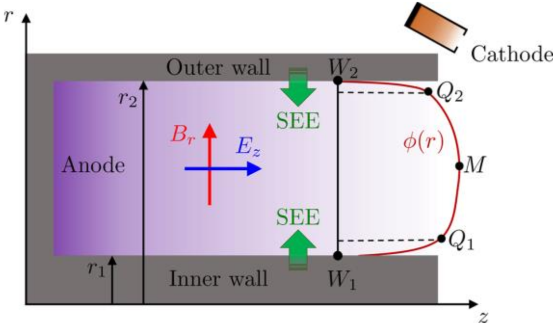
[1] 2D hybrid HT plume simulation



[2] Fully kinetic 3D simulation of a HT near plume

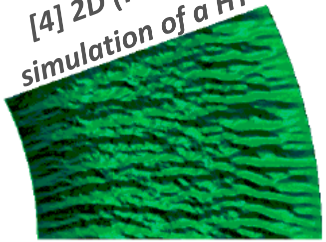


[3] Fully kinetic 1D simulation (radial coordinate) of a HT discharge



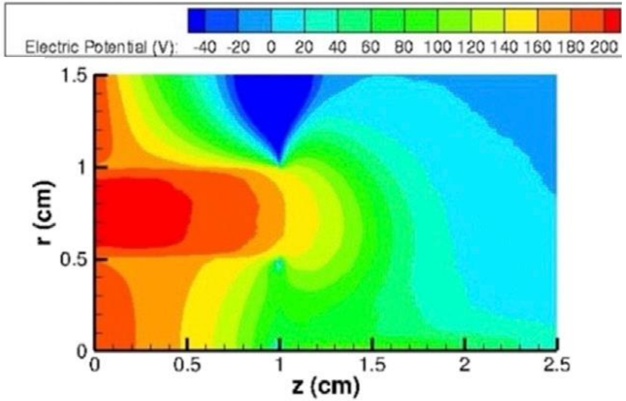
Overview of past and present simulation activities at ISTP (II)

4. Fully kinetic 2D ($r-\theta$ and $\theta-z$) PIC simulations of a HT channel
5. Fully kinetic 2D ($r-z$) PIC simulations of a HT channel and near plume
6. Fully kinetic 3D (z, r, θ) PIC simulations of a HT channel
7. Fully kinetic 3D (ϵ_0 scaling) PIC simulations of negative ion sources
8. Fully kinetic 2D planar simulations of plasma-divertor interaction in a fusion reactor

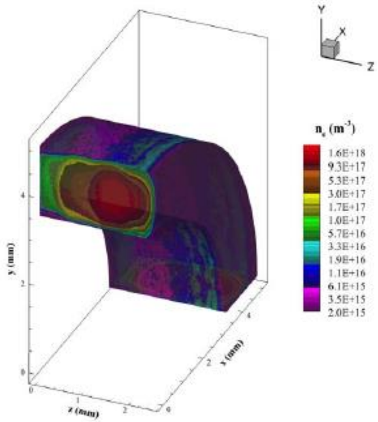


[4] 2D $(r-\theta)$ simulation of a HT

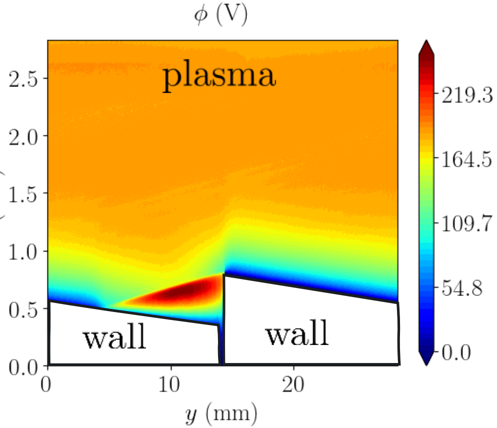
[5] 2D $r-z$ simulation of an SPT-20 operating with molecular nitrogen



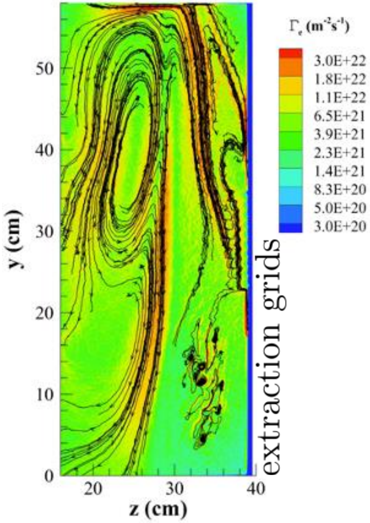
[6] 3D (z, r, θ) simulation of a micro- HT channel



[8] 2D (y, z) simulation of plasma-wall interaction in ITER divertor



[7] 3D (x, y, z) simulation of NIS negative ion source

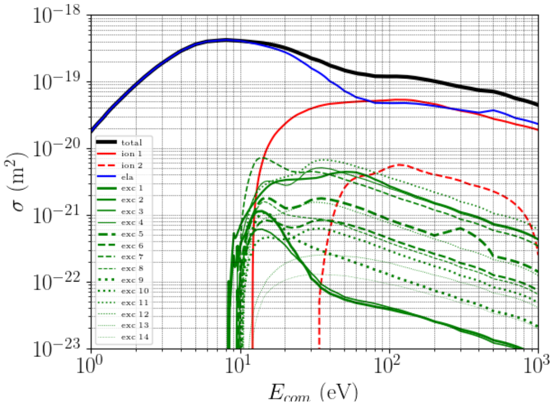


A new collisional database for PIC codes (I)

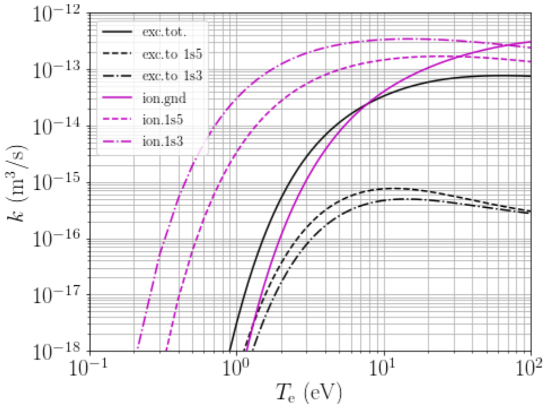
- The large variety of developed codes urges to use a unique collisional processes database for PIC codes, including:
  - Cross sections for ionization, excitation of **ground** and **metastable states**, elastic collisions, charge exchange collisions, recombination collisions
  - For molecules: cross sections for dissociation, dissociative attachment and ionization, vibration and rotation
- The complex chemistry required for molecules will be dealt with two main approaches:
  1. Inclusion of certain metastable excitation and vibrational levels as **new PIC species** with their corresponding cross sections → no added complexity at PIC code level
  2. Inclusion of excitation and vibrational levels as **additional state vector components** of a single heavy neutral PIC species
- Inclusion of gas species relevant for electric propulsion and fusion: hydrogen, deuterium, helium, molecular oxygen and nitrogen, atomic oxygen, xenon, etc…

A new collisional database for PIC codes (II)

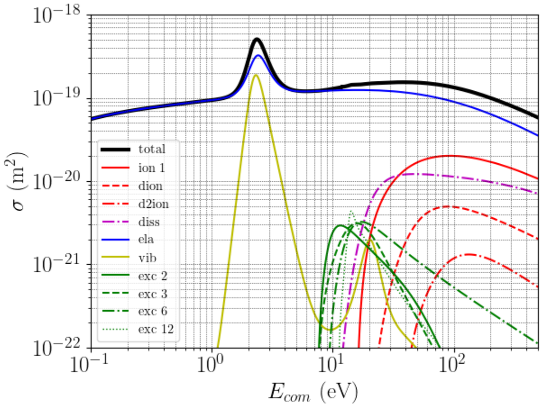
Electron-Xe atom cross sections



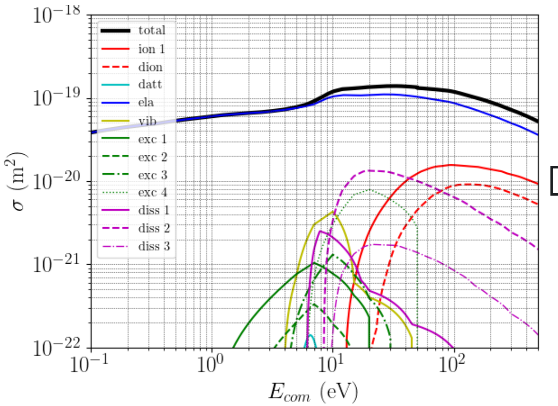
Reaction rates of metastable Xe states



Electron-N_2 molecule cross sections



Electron-O_2 molecule cross sections



- Ongoing collaboration with **EP2 research group (UC3M)** to assess the effects of metastable Xe states on plasma thruster discharge properties

- Studies on **air-breathing Hall thruster** concepts using alternative propellants: [5] F. Taccogna et al (2022), Front. Phys. 10:1006994.

Development of a multi-purpose simulator: PICCOLO

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- Flexible massively parallelized particle-in-cell code
  - **MPI / Open MP** parallelization with domain decomposition
  - High performance parallelization techniques (particle resorting, vectorization, optimized field gathering, etc…)
  - **Cartesian** or **Cylindrical** geometry
  - Possibility to tackle **quasi-1D** or **quasi-2D** simulation scenarios, through appropriate periodic boundary conditions for fields and particles along the zero-gradient directions
  - Use of the **HDF5 collisional database**
  - **Complex chemistry collisions** (MCC and DSMC sampling algorithms)
  - **Complex secondary electron emission** models, differentiating true secondaries and backscattered electrons

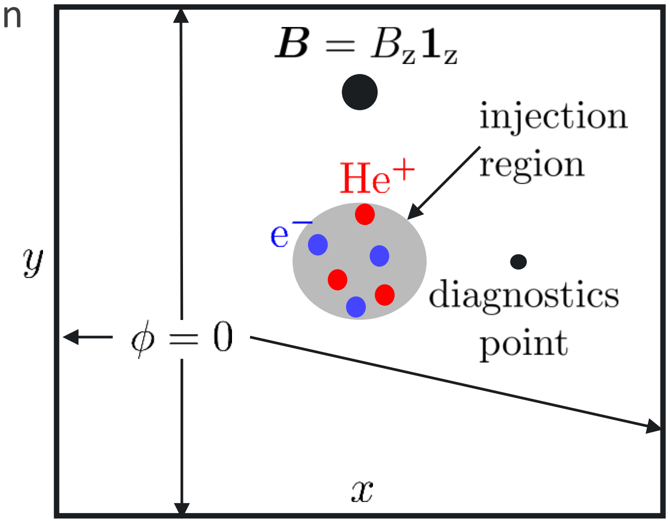
  - Tested over **more than 1000 cores** with good scalability

Benchmarking the code: Penning spoke discharge (I)

- International benchmark within program LANDMARK (**L**ow temper**A**ture mag**N**etize**D** plas**MA** benchma**RK**s): https://jpb911.wixsite.com/landmark/test-cases
- 2D simulation box ($x - y$) with z-directed magnetic induction field
- Injection of different ion/electron currents from a "cylindrical region" at the box center

  - Magnetic induction field confines particles within one Larmor radius (much smaller than the simulation box) away from injection region, until a rotating spoke instability is triggered
  - In this quasi-2D simulation, 2 cells along z are considered → plasma uniformity along z must be enforced to minimize non-2D effects related to polarization drifts $mq/B^2 \frac{\mathrm{d}\boldsymbol{E}}{\mathrm{d}t}$

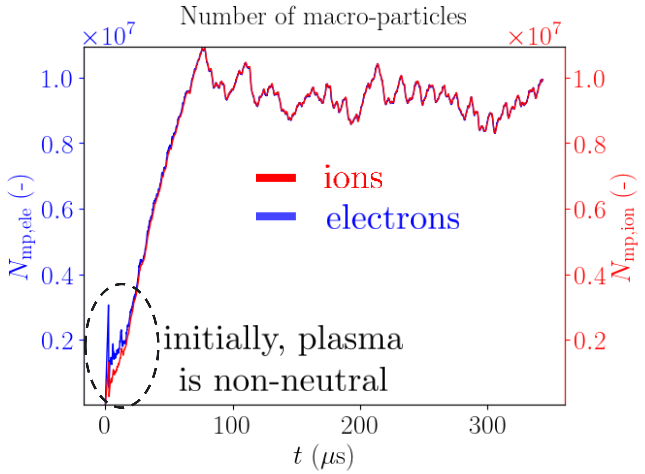
SIMULATION DOMAIN



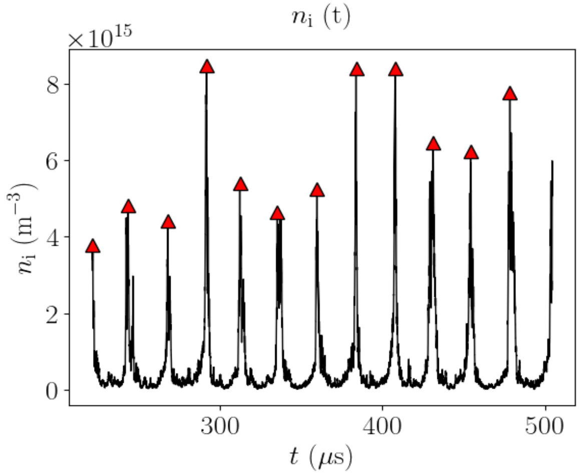
Benchmarking the code: Penning discharge (II)

- Collisionless plasma: particles can move radially outward only through drifts
    1. After an initial phase of accumulation of macro-particles, azimuthal non-uniformities and strong electric fields appear
    2. Radial drifts due to $E_\theta B_z$ transport particles away from injection region
    3. After approx. 100 μs, a steady state is reached, featuring a rotating spoke

NUMBER OF MACRO-PARTICLES



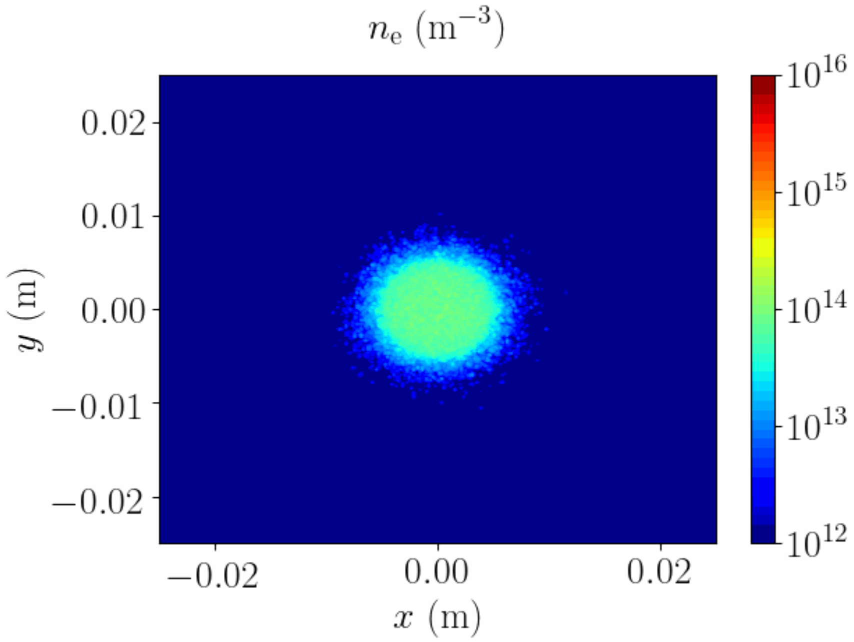
TIME EVOLUTION OF ION DENSITY AT THE DIAGNOSTIC POINT, DURING STEADY STATE



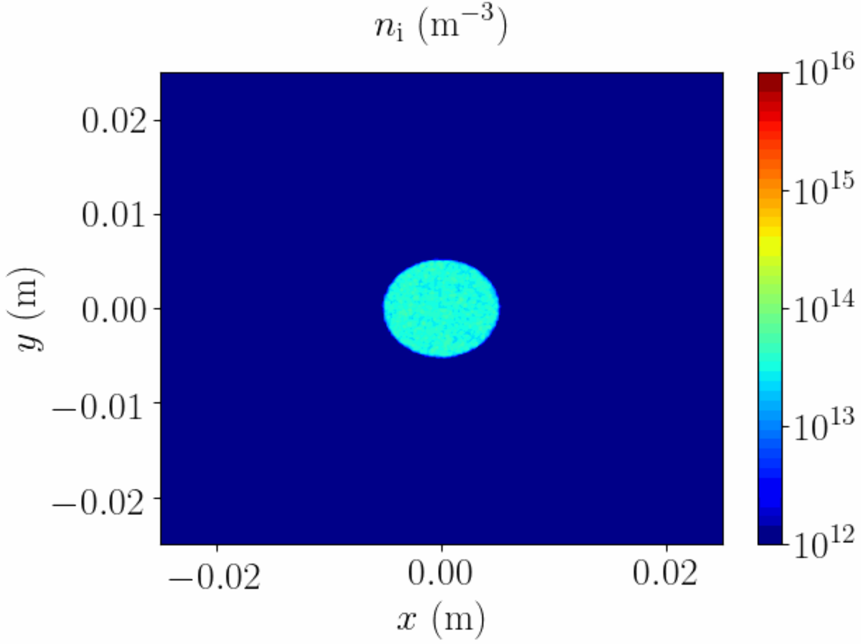
Benchmarking the code: Penning discharge (III)

Onset of the rotating spoke instability. Interval: 0-30 μs

ELECTRON DENSITY



ION DENSITY



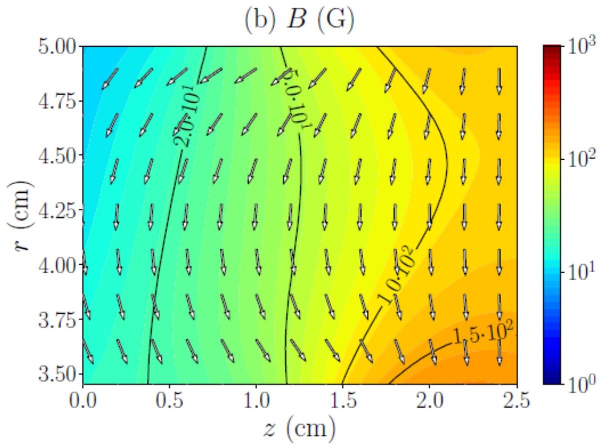
Application to a 2D Hall thruster discharge (I)

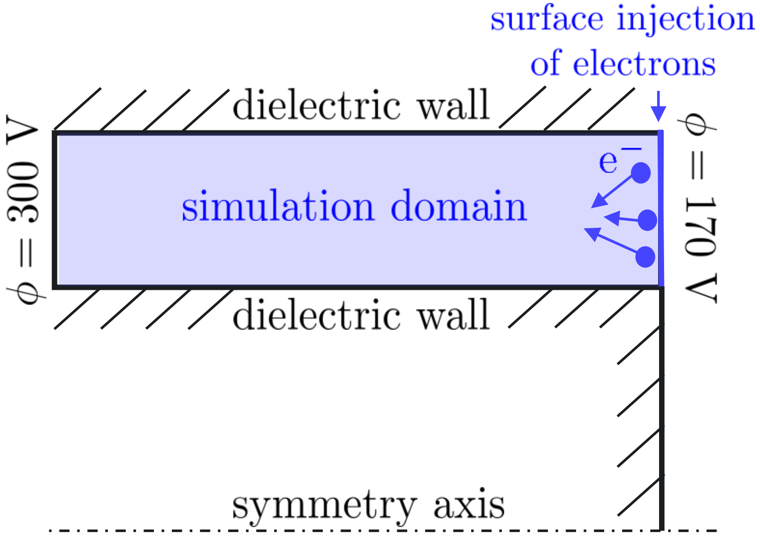
- Goal: quick investigation of **neutral density control** in a simplified 2D scenario
- SPT100-like internal channel simulation
  - Dirichlet conditions at anode/exit plane (300/170 V)
  - Dielectric conditions on lateral walls (Neumann)
  - MCC collisions of ions/electrons with neutral atoms
  - Additional anomalous collisions for electrons, based on Bohm's model
  - Injection of electrons from exit plane:
    - Semi-Maxwellian flux distribution at 10 eV

$$f_{\mathrm{inj}}(\boldsymbol{v}_e, r) \propto \left[|v_{\mathrm{e,z}}| \exp\left(-\frac{m_{\mathrm{e}} v_{\mathrm{e}}^2}{2T_{\mathrm{e0}}} \right) \right] r^2$$

  - Background neutrals with z-varying density (**controlled actively**)

MAGNETIC INDUCTION FIELD





Application to a 2D Hall thruster discharge (II)

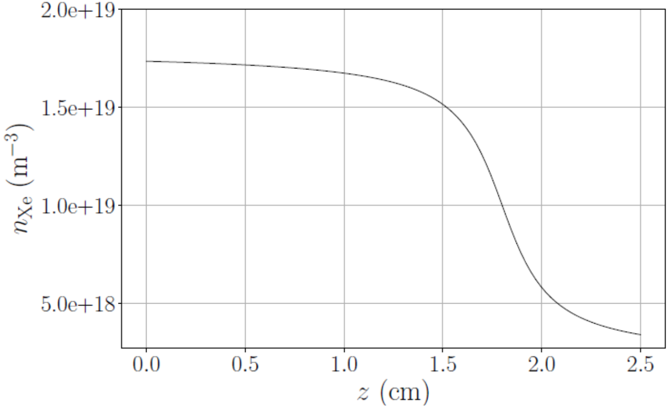
- How to account for neutrals in full-PIC simulations?
  1. Simulation of neutral macro-particles within the same PIC loop → Enormous number of steps: at least 100-200 μs (**50-100 million steps**, feasible only in 2D)

  2. Simulation of neutrals as a fluid, subject to conservation equations → same as above regarding PIC (although with no neutral macro-particles to move)

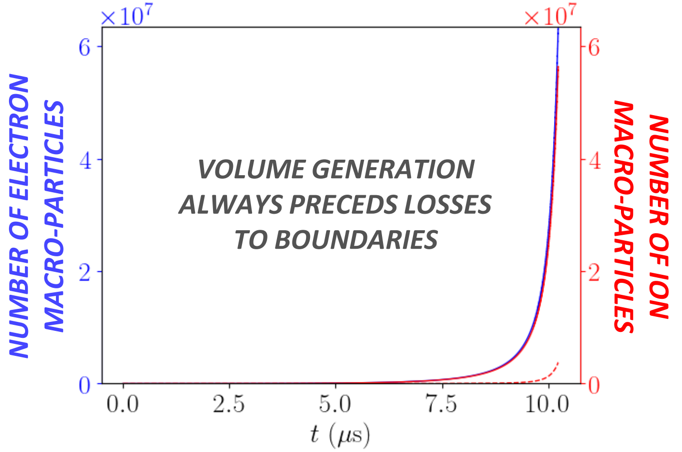
  3. Simulation of neutrals as a **fixed background in time**
     - Volume generation is a run-away process as neutrals are not consumed by ionization
     - Feedback from total ionized mass flow is needed

  4. Simulation of neutrals with a **separate TPMC loop** coupled with PIC loop for charged particles

1D NEUTRAL DENSITY PROFILE



DISCHARGE RUNAWAY WITH NO DENSITY CONTROL

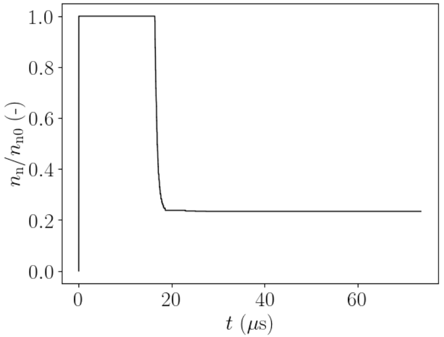


Application to a 2D Hall thruster discharge (III)

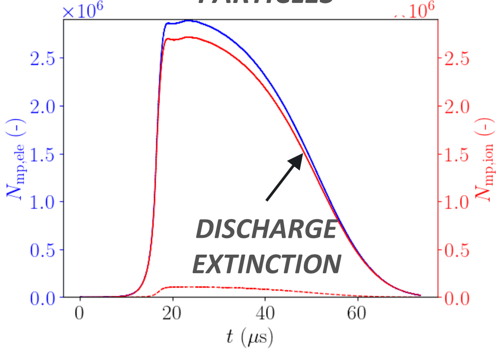
- Targeted ionized mass rate: $\dot{m}_{\text{ion}}^{(TG)}$
- Two control strategies:
  - **One-way control**: neutral density corrected with a factor $\dot{m}_{\text{ion}}^{(TG)}/\dot{m}_{\text{ion}}(t^*)$ only at time instants t^* in which the target value is overcome
  - **Continuous control**: once reached for the first time, targeted ionization rate is maintained by continuously correcting neutral density at all times by a factor $\dot{m}_{\text{ion}}^{(TG)}/\dot{m}_{\text{ion}}(t)$

ONE-WAY CONTROL

CORRECTION FACTORS

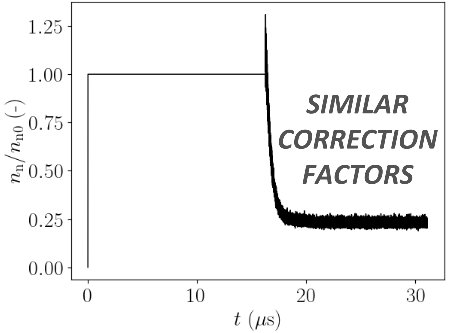


N. MACRO-PARTICLES

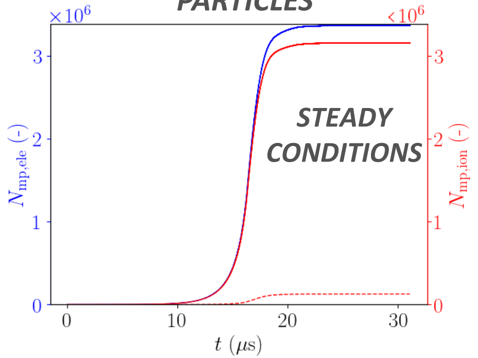


CONTINUOUS CONTROL

CORRECTION FACTORS



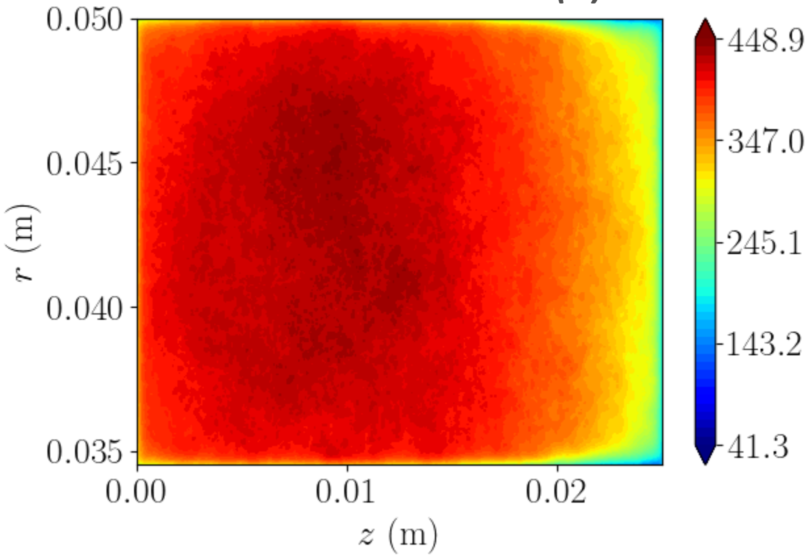
N. MACRO-PARTICLES



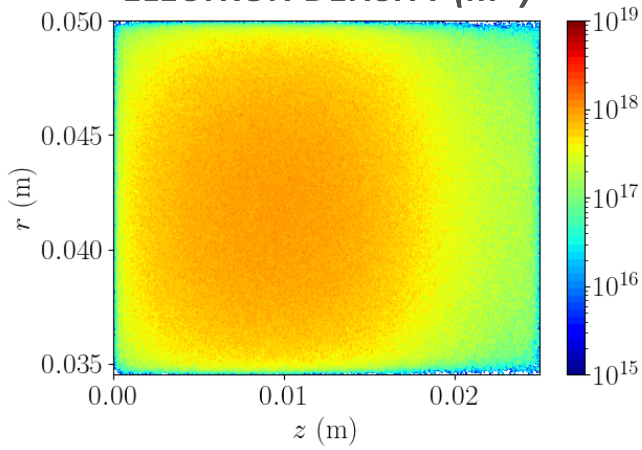
Application to a 2D Hall thruster discharge (IV)

- Preliminary results (instantaneous, no time averaging)
- Simulation inputs (e.g. injected electron current) to be adjusted yet

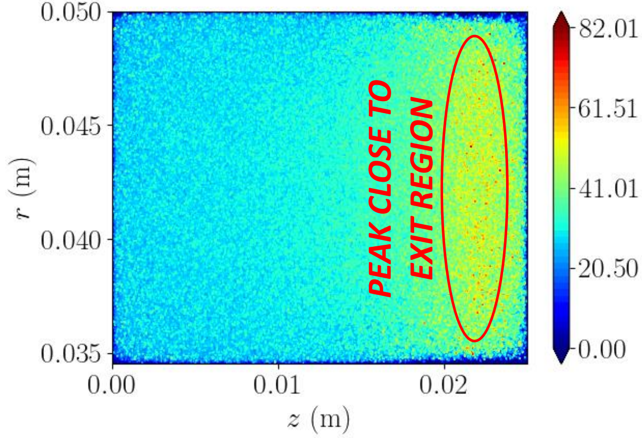
ELECTRIC POTENTIAL (V)



ELECTRON DENSITY (m^{-3})



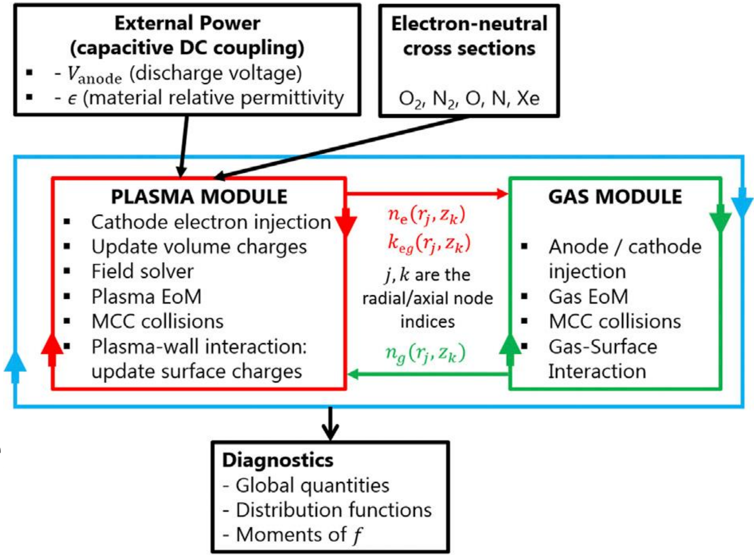
ELECTRON TEMPERATURE (eV)



Conclusions and future work

- The new PICCOLO code has completed the initial development and benchmarking phase
  - Multi-purpose, multi-dimensional, massively parallelized MPI code
- ISTP collisional database for PIC simulation keeps growing, including more and more complex chemistry and propellants
- PICCOLO benchmarks (ongoing):
  - Rotating spoke benchmark
  - HET 2D channel scenario
- Coming next:
  - Implementation of complex chemistry in collisional module (handling of vibration, rotation, and metastable excitation states within a given PIC species)
  - Implementation in PICCOLO of coupled TPMC/PIC architecture to simulate self-consistently the neutrals
  - Reproduction of a 3D HT discharge with a quasi-2D code tailoring anomalous transport model

COUPLED PIC/TPMC LOOPS (FROM REF. [5])



REFERENCES

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- [2] N. Oudini, F. Taccogna, P. Minelli, *3D fully kinetic simulation of near-field plume region*, 33rd International Electric Propulsion Conference, IEPC2013-419
- [3] A. Domínguez-Vázquez, F. Taccogna, E. Ahedo, *Particle modeling of radial electron dynamics in a controlled discharge of a Hall thruster*, Plasma Sources Science and Technology 27 (6), 064006
- [4] F. Taccogna, R. Schneider, S. Longo, M. Capitelli, *Fully kinetic 2D (r, theta) model of a Hall discharge*, 43rd AIAA/ASME/SAE/ASEE Joint Propulsion Conference & Exhibit, 5211
- [5] F. Taccogna, F. Cichocki and P. Minelli (2022), *Coupling plasma physics and chemistry in the PIC model of electric propulsion: Application to an air breathing, low-power Hall thruster*. Front. Phys. 10:1006994
- [6] F. Taccogna, P. Minelli, *Three-dimensional particle-in-cell model of Hall thruster: the discharge channel*, Physics of Plasmas 25 (6), 061208
- [7] F. Taccogna, P. Minelli, *PIC modeling of negative ion sources for fusion*, New Journal of Physics 19 (1), 015012

Thank you very much for your attention

Any questions?