Implicit Conservative Particle-In-Cell kinetic simulations of magnetic nozzles

Pedro Jimenez, Luis Chacon, Mario Merino



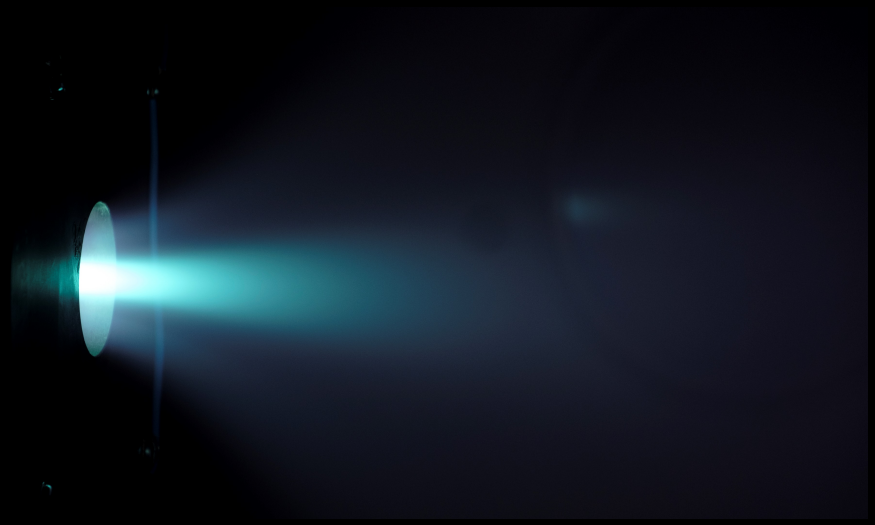


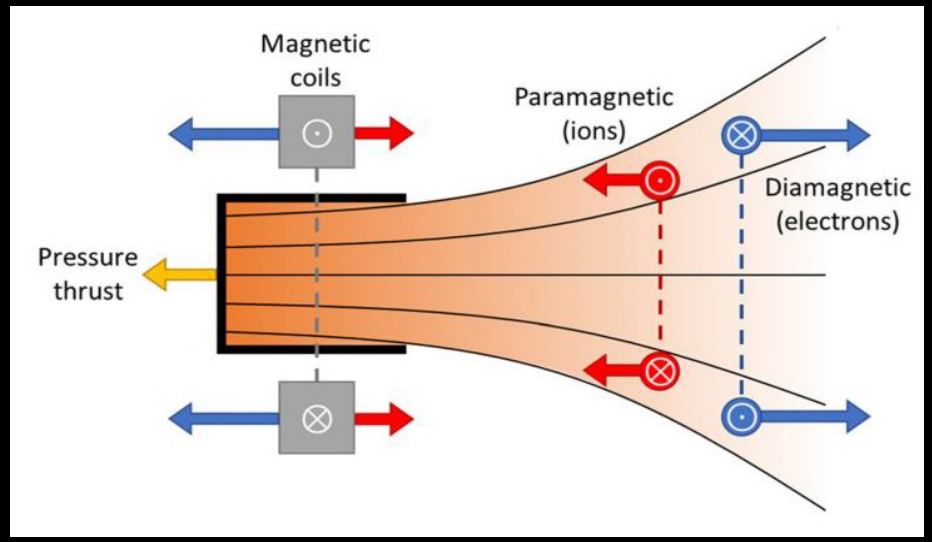
Magnetic Nozzles (MN)

- Magnetic nozzles are used as the acceleration stage in some plasma thrusters. Diverging $\boldsymbol{B}_a$ created by coils or magnets.

- Basic mechanisms well understood from fluid models
  - Quasineutral, near-collisionless operation
  - Radial confinement and axial acceleration by Lorentz force
  - Thrust generation
    - Azimuthal plasma current induces $\boldsymbol{B}_p$; reaction force on coils
  - Thermal electron energy to ion kinetic energy conversion via the electrostatic potential
  - Supersonic acceleration of ions

- However, fluid models fail to provide an accurate description of electrons, which lack local thermodynamic equilibrium in the near-collisionless regime
  - Electron kinetics, subpopulations and cooling need high fidelity and fast kinetic simulations (Implicit PIC)





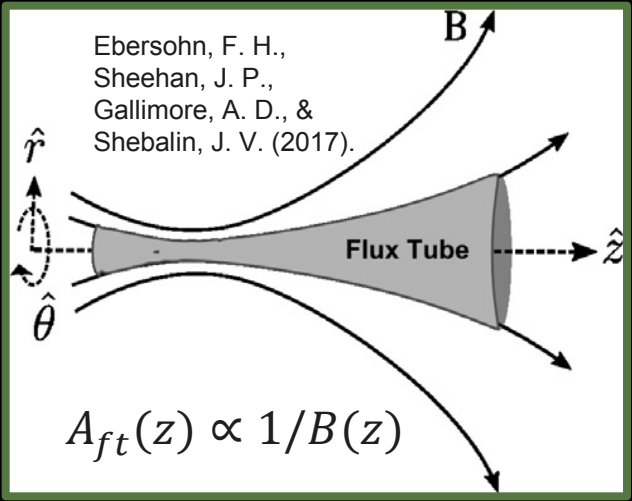
Governing equations

$$\frac{\partial f_s}{\partial t} + \frac{1}{B(\mathbf{x})}\left[\nabla\cdot\left(v_\parallel \mathbf{B} f_s\right) + \frac{\partial}{\partial v_\parallel}\left(\left(\frac{q_s}{m_s}E_\parallel - \tilde{\mu}\mathbf{b}\cdot\nabla B\right) B f_s\right)\right] = 0$$

$$f_s(z, v_z, \tilde{\mu}, t) = \sum_{p\in s} w_p \delta(z - z_p(t))\delta(v_z - v_{z,p}(t))\delta(\tilde{\mu} - \tilde{\mu}_p(t))$$

$$v_\parallel \approx v_z \;;\; E_\parallel \approx E_z \;;\; \mathbf{B} \approx B(z)\mathbf{z}.$$

- Drift-kinetic Vlasov equation (DKE). Perpendicular drifts can be neglected by virtue of the Paraxial approximation.
- Particle discretization of the EDFs.
- Paraxial approximation



Ebersohn, F. H., Sheehan, J. P., Gallimore, A. D., & Shebalin, J. V. (2017).

$$\nabla\cdot\mathbf{B} = \frac{1}{J^B}\partial_z(J^B B) = 0$$

$$A_{\mathrm{ft}}(z) \propto 1/B(z) = J^B$$

$$\frac{\mathrm{d}z_p}{\mathrm{d}t} = v_{z,p},$$

$$\frac{\mathrm{d}v_{z,p}}{\mathrm{d}t} = \frac{q_p}{m_p}E_z(z_p) - \tilde{\mu}_p \left.\frac{\mathrm{d}B}{\mathrm{d}z}\right|_{z_p}$$

- Evolution equations for the particles
  - Reduction to 1D geometry
  - Magnetic mirror force with μ conserved

Modification of the divergence operator to recover solenoidal B. Conservation of the flux in magnetic tube

Implicit PIC Algorithm

- Limitation of explicit PIC codes:
  - $\Delta x < \lambda_{Debye}$ (finite-grid instability $\longrightarrow$ enforces a minimum spatial resolution)
  - $\omega_{pe}\Delta t < 1$ (CFL-type instability $\longrightarrow$ enforces a minimum temporal resolution)
  - Inefficient for long time and large-scale simulations

- Basic implicit scheme based on Chen et al. 2011
  - The evolution of the particles is a function of the potential; non-linear elimination of the particle coordinates (**Particle enslavement**)

$$x_p^{n+1} = x_p[\Phi^{n+1}]; \quad v_p^{n+1} = v_p[\Phi^{n+1}]$$

$$G\left(x_p^{n+1}, v_p^{n+1}, \Phi^{n+1}\right) = G(x[\Phi^{n+1}], v[\Phi^{n+1}], \Phi^{n+1}) = \tilde{G}(\Phi^{n+1})$$

  - The residual is only a function of the potential
    - Major reduction of the non-linear system unknowns
    - Solution achievable with modern non-linear solvers. JFNK, Anderson …

- Fully Implicit Crank Nicolson discretization
  - Time centered, 2nd order, non-dissipative
  - This work adds the magnetic mirror
    - Conserving μ, E_{tot} and local charge

- Jacobian Free Newton Krylov (JFNK)
  - No need to compute the Jacobian Matrix
  - Jacobian vector product for Krylov subspace method (GMRES)
  - Easily preconditioned -> Potential for acceleration

Vlasov-Ampere Formulation

- Advantages of **Vlasov -Ampere** vs Vlasov-Poisson
  - Exact **global energy** conservation
  - Exact **local charge** conservation $\frac{d\rho}{dt} + \nabla \cdot \boldsymbol{j} = 0$
  - Amenable to orbit averaging
  - Can be extended to electromagnetic algorithms

- Ampere's equation

$$\epsilon_0 \partial_t E + j = \nabla \times \boldsymbol{B}$$

  - Taking the divergence to eliminate $\nabla \times \boldsymbol{B}$

$$\epsilon_0 \partial_t \nabla \cdot \boldsymbol{E} + \nabla \cdot \boldsymbol{j} = 0$$

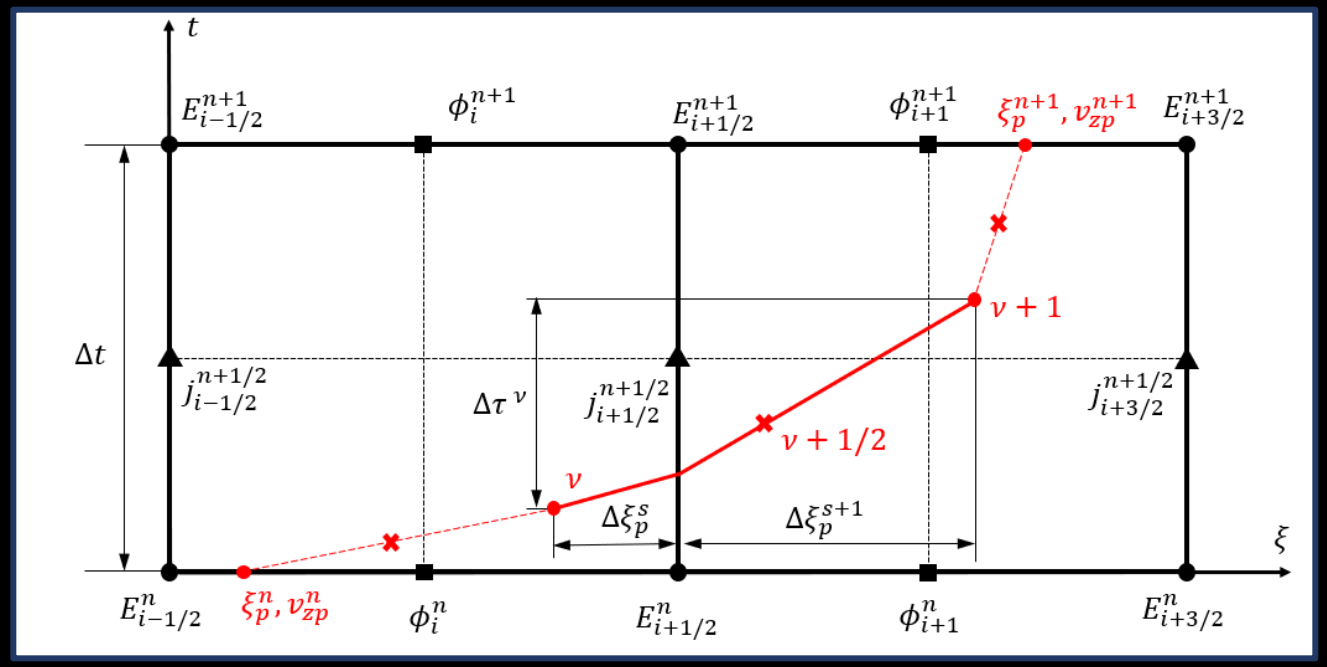
  - Introducing the scalar potential $E = -\nabla \phi$

$$\epsilon_0 \partial_t \nabla^2 \phi - \nabla \cdot \boldsymbol{j} = 0$$

(equivalent to the time derivative of Poisson equation with charge conservation)

Subcycling and mesh map

- In MN problems of interest,
  - Fields vary slowly (Δt)
  - Electron times are much faster ($\Delta\tau \ll \Delta t$)
- Particle orbits need to be resolved to avoid large errors, even when using large Δt
  - Use small substeps such that $\sum\Delta\tau = \Delta t$

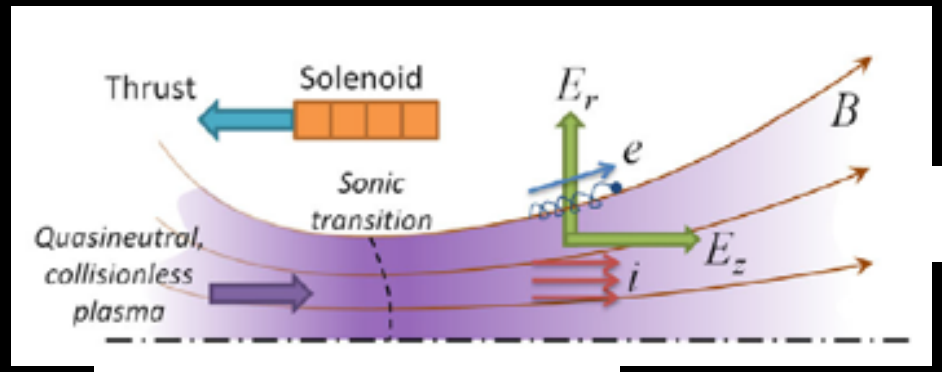


- Hybrid push in mapped meshes
  - Particle positions are advanced in a Cartesian logical (computational) space and velocity advanced in physical space
- New mover:
  - Particles are allowed to cross several cells in a suborbit
  - Averaged splines are used to recover energy and charge conservation

- Estimator for the selection of $\Delta\tau$ based on CN truncation error
  - $\Delta\,\tau_e^{\nu} = \left(\frac{12\,\mathcal{E}_{\Delta\tau}}{||(d\,a\,/\,d\,\tau)^{\nu}||}\right)^{\frac{1}{3}}$
    - Reduces error in momentum conservation

Magnetic nozzle study

- From previous studies and experimental evidence
  - The plasma is quasi-neutral and ambipolar
  - There will be a potential drop in the entrance followed by a slow monotonic decay
    - Accelerates ions and reflects some electrons
  - The plasma is almost collisionless
- We consider a small convergent part + long divergent region

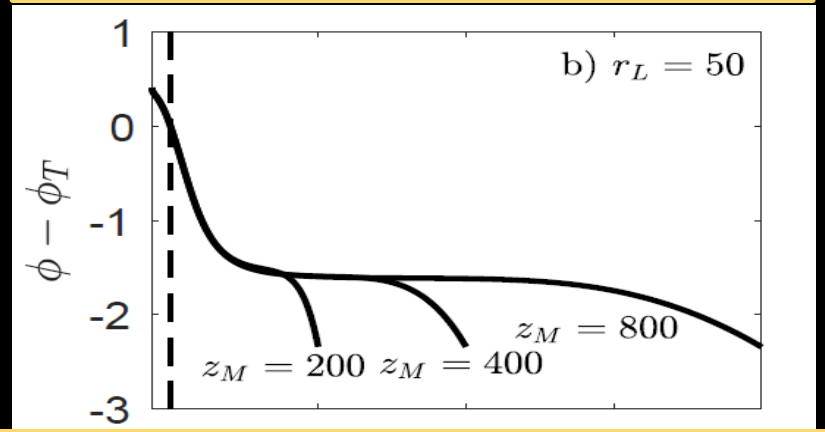


Injection boundary, $\phi = \phi_{ref}$

Freeloss / reflection BC for ϕ ?

Downstream particle and field BCs ?
Expansion to infinity in a finite domain

- Fixing ϕ. [Sanchez et al. 2018]
  - Does not guarantee $j_z = 0$
  - Also, sheath development



- Li, Merino et al. 2019
  - Some electrons must be reflected downstream the boundary
    - Reflection controlled to get $j_z = 0$
  - Fixing E=0 still limiting

Open Downstream Boundary BC: new approach

- Integral condition coming from Ampere's equation in the Electrostatic limit

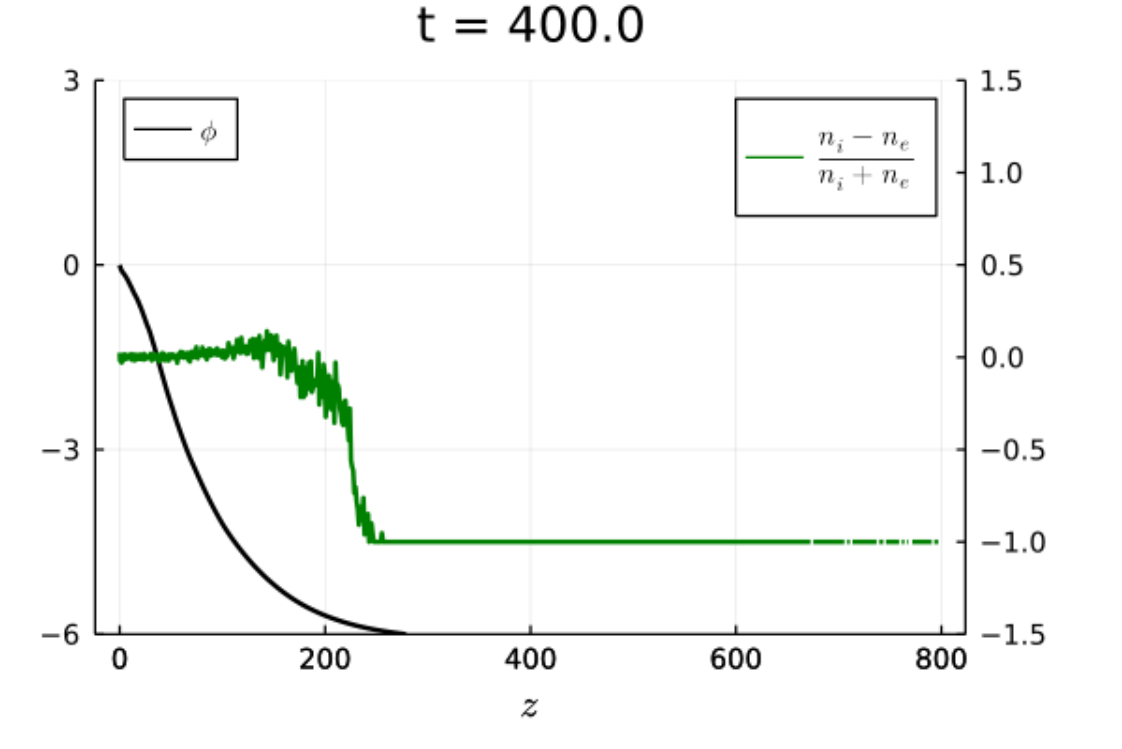
$$\partial_t E + j = C(t)/J^A$$

  - $C(t)$ constant in 1D domain
    - If we evaluate at z $= \infty \Rightarrow \partial_t E + j = 0$
  - Results in **Dynamic Inhomogeneous Neumann** condition for exit field $E^{n+1}_{n_z+1/2} = E^{n}_{n_z+1/2} - \Delta t \cdot j^{n+1/2}_{n_z+1/2}$
    - Current vanishes at steady state j $= 0,\ I = 0$
    - **No need for a current control!**
    - Correct physics during the transient

  - Downstream electron reflection control
    - Critical energy E_{crit} related to the potential at infinity ϕ_∞
      - Electrons are reflected upon arrival to the boundary if $K_p < E_{crit}$
    - We adjust E_{crit} to get a quasi-neutral plasma at the exit. Heuristic proportional control
      - $\Delta E_{crit} = \rho_{n_z} \cdot G$
      - Stationary solution $\Delta E_{crit} = 0$ & $\rho_{n_z} = 0$

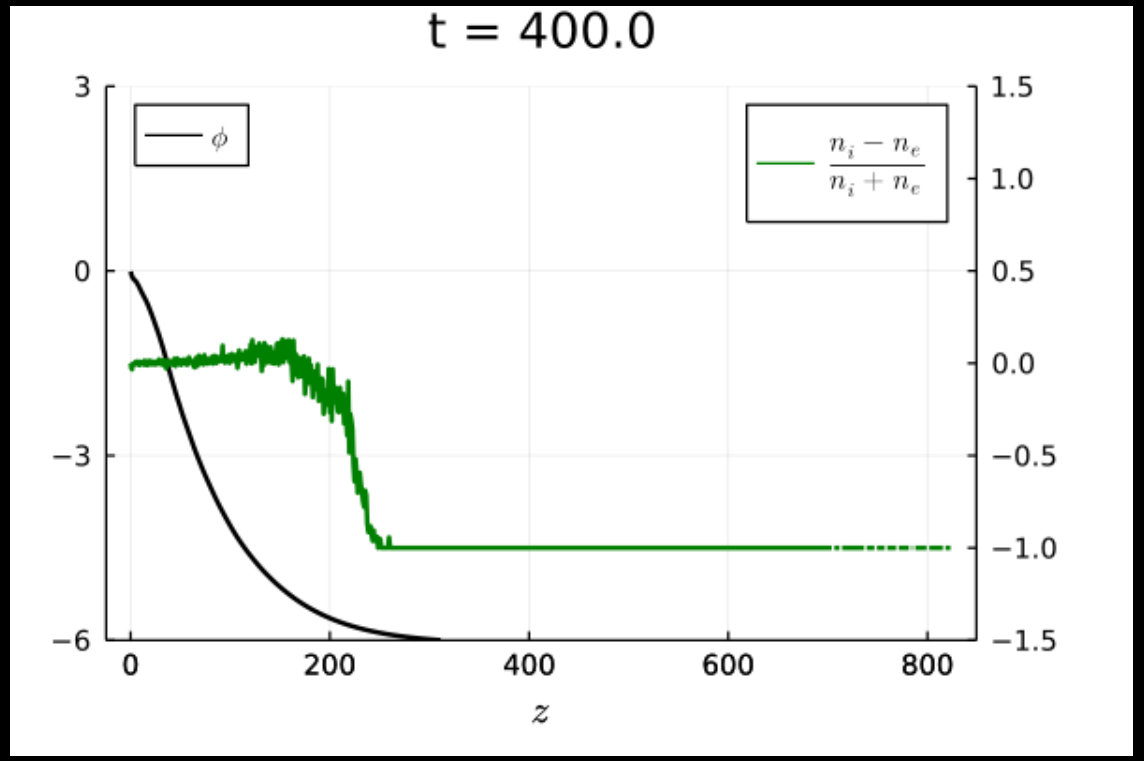
System evolution

Downstream dielectric wall



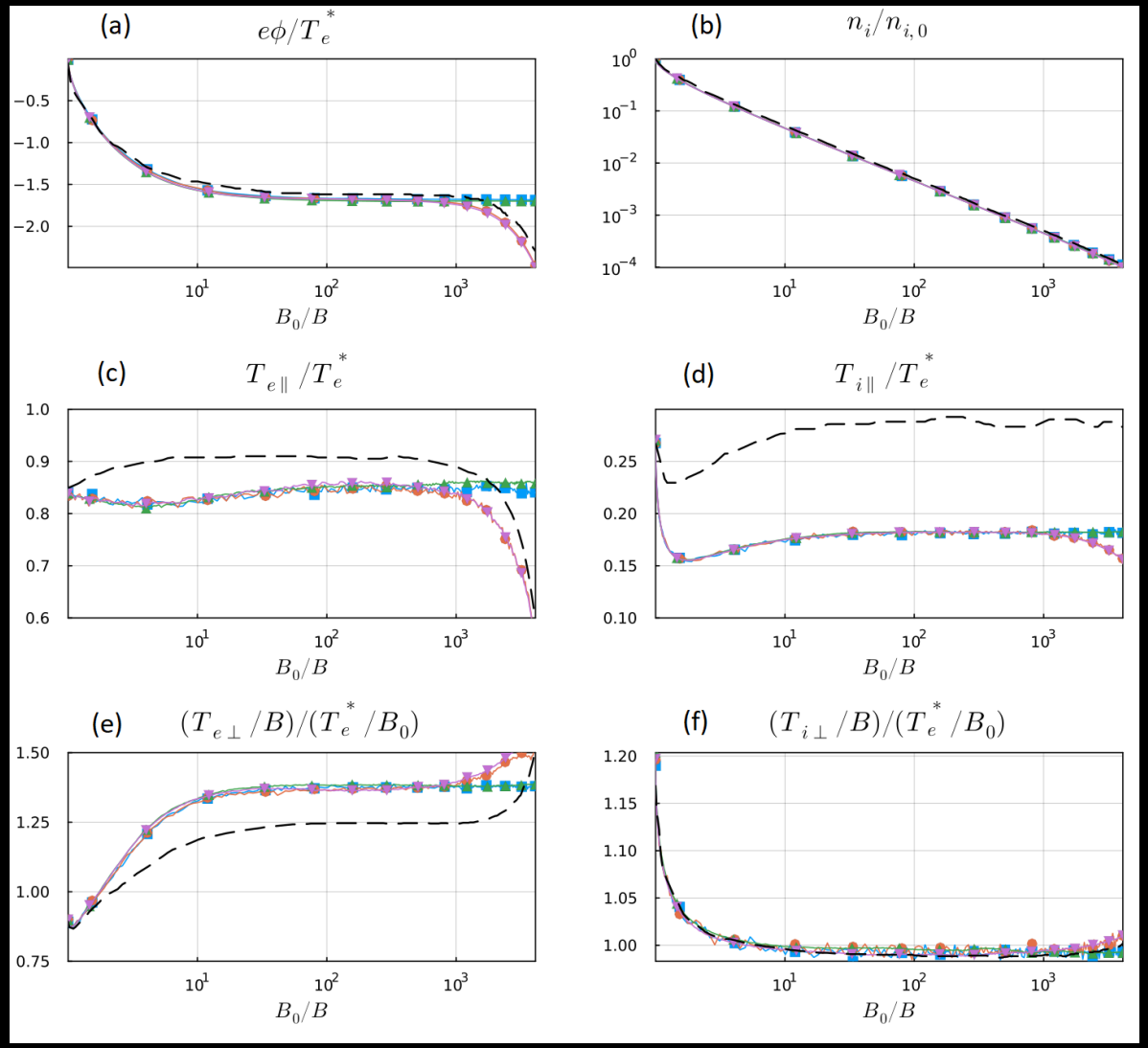
- We get a similar $\phi_\infty = -2.82\ to\ -2.75$ and sheath
  - New potential is self-consistent, not imposed
  - Same sheath appears downstream at steady state

Expansion to infinity (new BC)

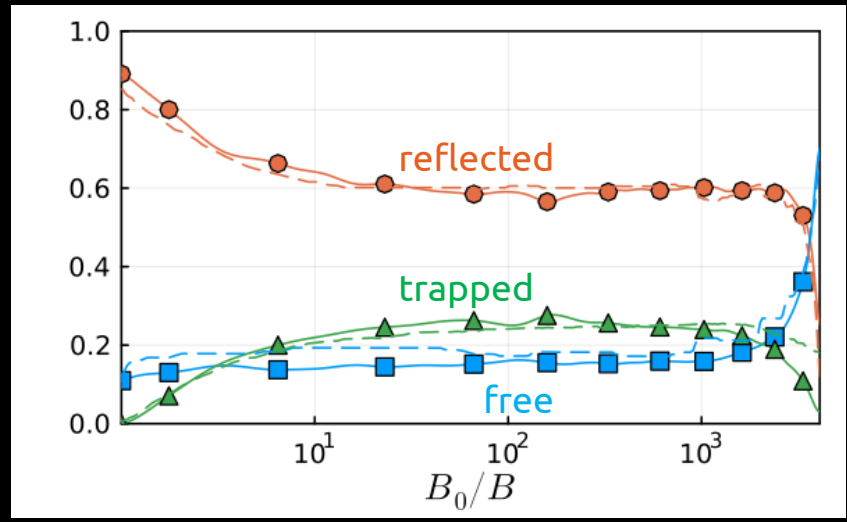


- Electron reflection → Exit is quasi-neutral
  - The sheath disappears
  - The initial drop is equivalent

Steady state results

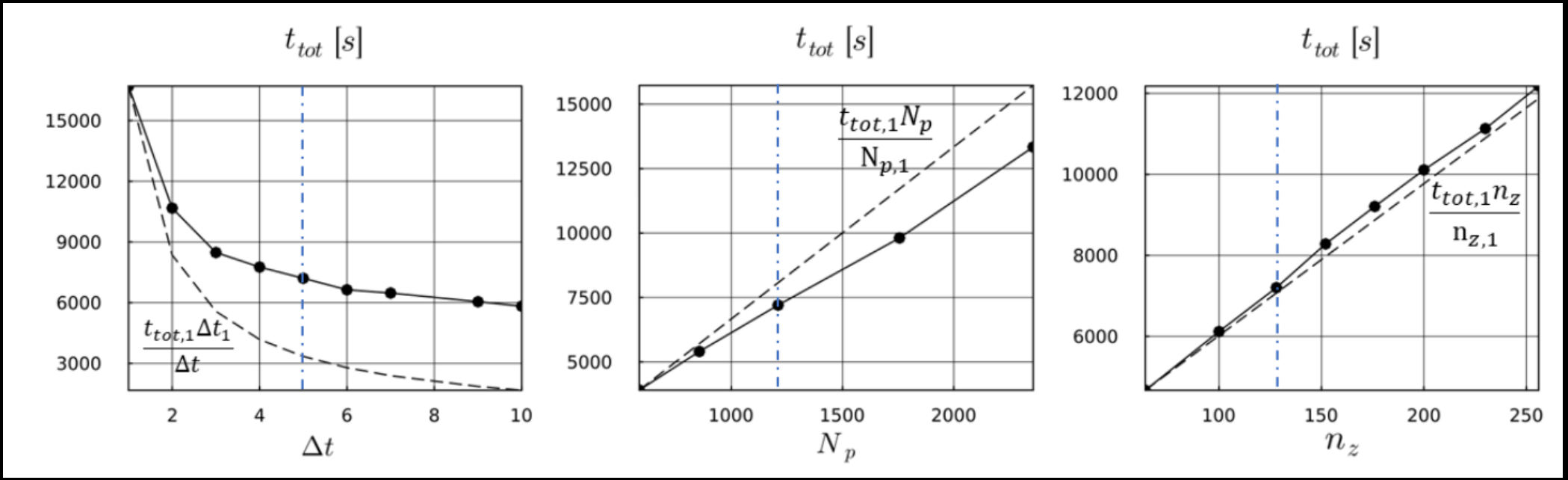


- Excellent convergence of our results
  - We also proved solution is insensitive to our numerical control parameters (e.g. control gains)
- Some differences observed compared with published results [Sanchez et al. 2018]
  - Possible sources of discrepancy
    - Strict conservation properties
    - Steady state dependent on the transient (trapped electrons)



Efficiency and computational scaling

- Linear time scaling with particles/cell and number of cells
- For the first time, $t_{tot} \propto n_z$. New mover allows particles to travel across several cells while exactly conserving energy and local charge
- Speed up of $O(10)$ with respect to explicit PIC
  - Estimation based of typical mesh and timesteps
- Speedup of O(30) with respect to Semi-Langrangian Vlasov code in the MN study [sanc]
  - Plus, strict conservation properties



Conclusions and future work

- Time-implicit → breaks λ_{De} and ω_{pe} constraints
- Cell size and time step can be larger than in explicit PIC
- Exactly global-energy and local-charge conserving
- Adaptive mesh
- Advanced boundary conditions for injection and free space
- Important performance gain compared to state-of-the-art

- Future work:
  - 2D dimensional code -> will require preconditioning
  - GPU parallelization (Julia lang abstractions and packages)
  - Electromagnetic extension -> Darwin approximation

- iPIC Applications in Electric Propulsion
  - Nozzles and expansions
  - Plasma sources
    - Need for collision, plasma chemistry and wall interaction algorithms
  - Anomalous transport studies (oscillations in θ direction)
  - Electrodeless Thrusters (EM version)
    - Helicon, Electron Cyclotron Resonance …
    - Mechanism of plasma heating
      - Electromagnetic power coupling
      - Antennas, inductors …

Acknowledgments

The work of Pedro Jimenez and Mario Merino has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation program (grant agreement No 950466)

Luis Chacon was funded by the Applied Mathematics Research program of the Department of Energy Office of Advanced Scientific Computing Research, and the research was performed under the auspices of the National Nuclear Security Administration of the U.S. Department of Energy at Los Alamos National Laboratory, managed by Triad National Security, LLC under contract 89233218CNA000001





THANK YOU!

CHECKOUT OUR NEW PREPRINT AT

ARXIV.ORG/ABS/2305.07146

pejimene@ing.uc3m.es

ZARATHUSTRA

EP² uc3m erc