Multi-fluid simulations of instabilities and sheaths in low-temperature partially-magnetized plasmas: advanced numerical methods and comparison with PIC

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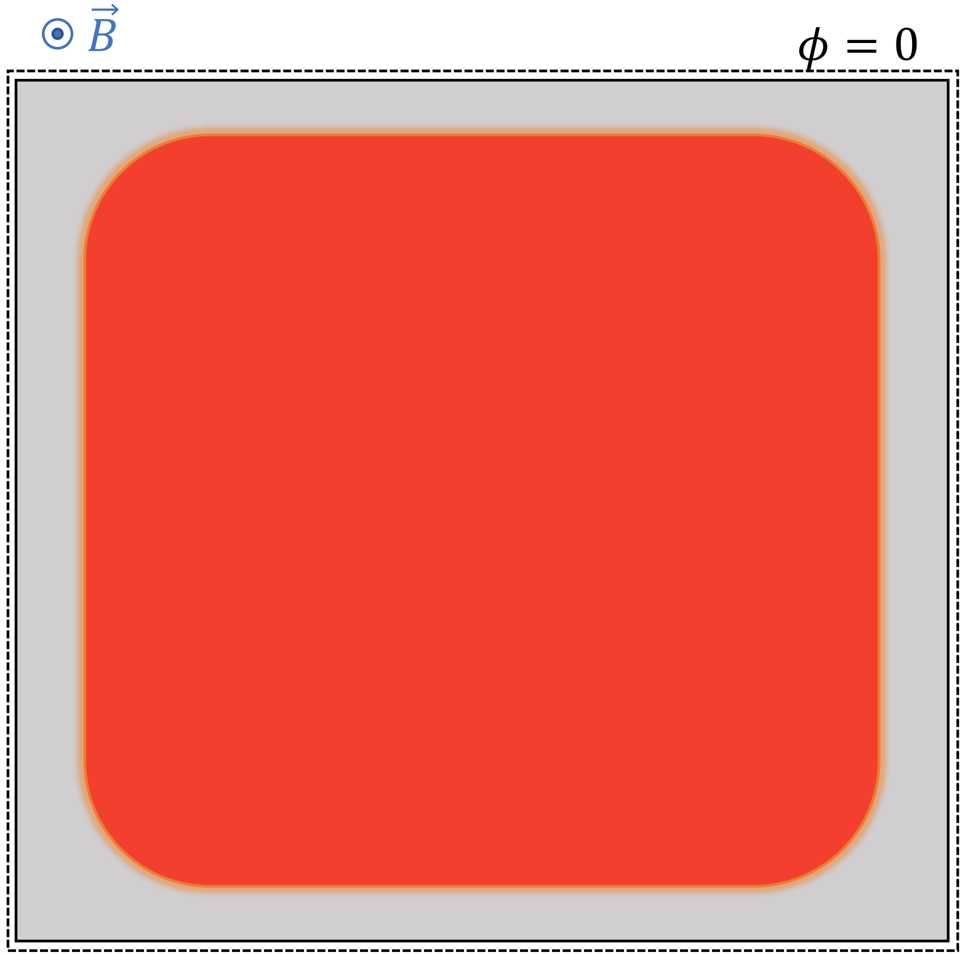
Electron transport in magnetized rectangular plasma discharge



Relevance of this configuration:

- Features kinetic effects (sheath), instabilities
- Strongly Multiscale (hydrogen, helium)
- 2D geometry

Representative of the main difficulties in modeling and simulating applications such as electric propulsion or ICP magnetized columns

Electron transport in magnetized rectangular plasma discharge

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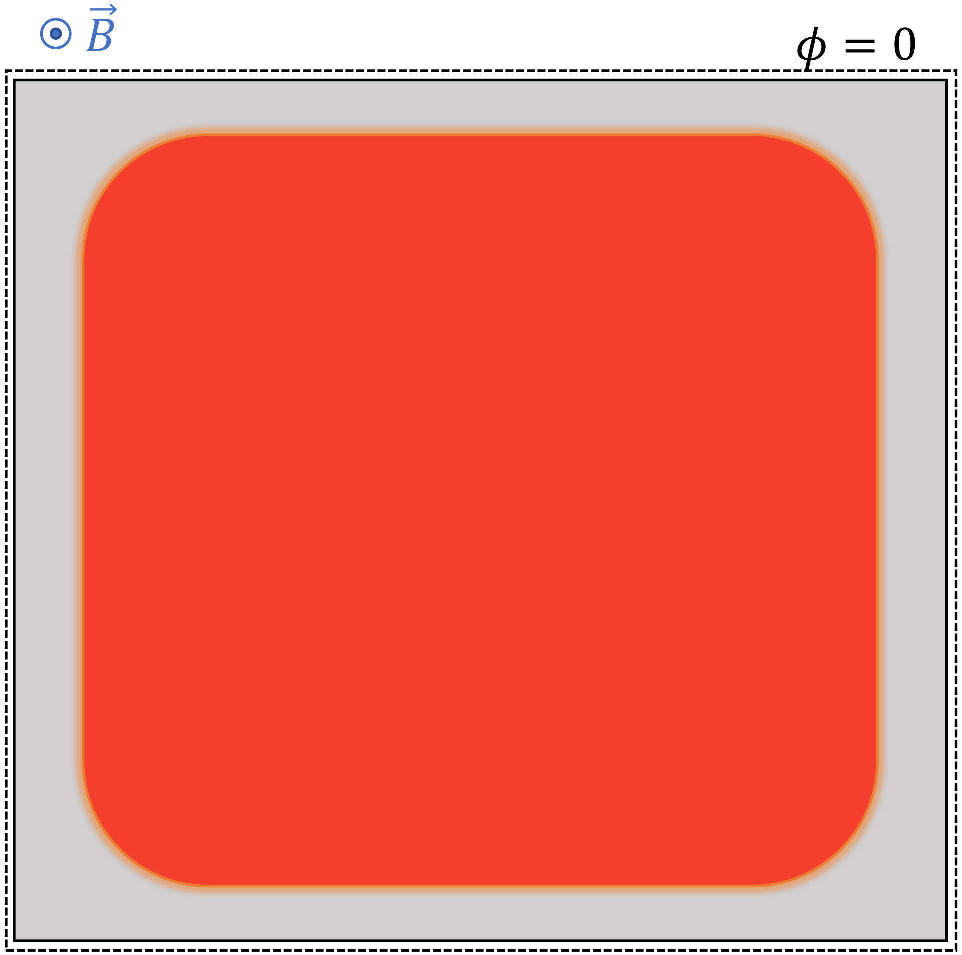
- Features kinetic effects (sheath), instabilities
- Strongly Multiscale (hydrogen, helium)
- 2D geometry

Good candidate to discriminate between models and numerical methods



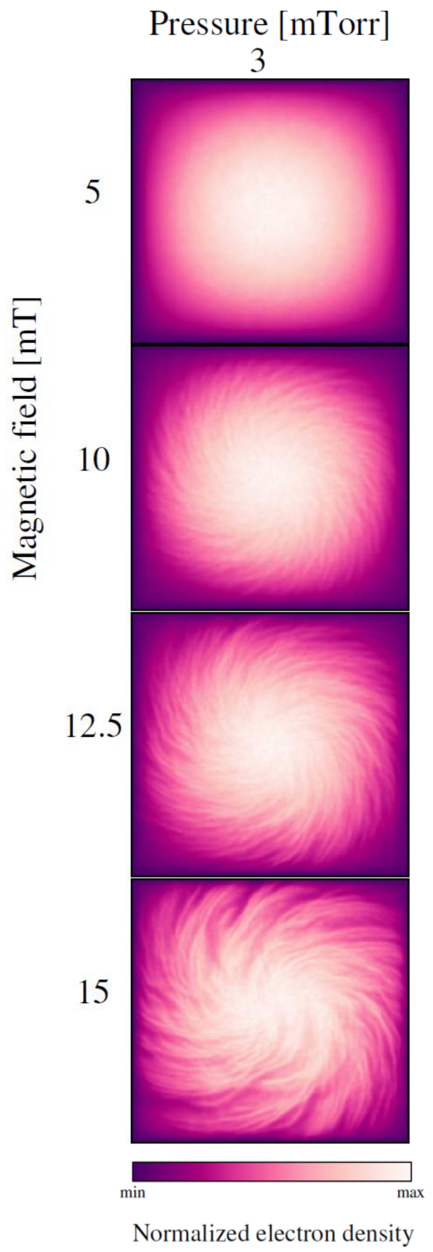
Kinetic approach of the problem:

- The multi-fluid model is derived by taking moment of the Boltzmann equation for each considered species α:

$$\partial_t f_\alpha + \vec{v}.\vec{\nabla} f_\alpha + \frac{\vec{F}_\alpha}{m_\alpha}.\vec{\nabla}_{\vec{v}} f_\alpha = \left(\frac{\delta f}{\delta t}\right)_{coll}$$

- With
  - The Lorentz force: $\vec{F}_\alpha = q_\alpha\left(\vec{E} + \vec{v} \times \vec{B}\right)$
  - The collisions : $\left(\frac{\delta f}{\delta t}\right)_{coll} = J_\alpha + J_\alpha^r$
    - Elastic term : $J_{\alpha\beta}(f_\alpha, f_\beta) = \iint \left(f'_\alpha f'_\beta - f_\alpha f_\beta\right)\sigma_{\alpha\beta}|\vec{v}_\alpha - \vec{v}_\beta| d\widehat{\Omega} d\vec{v}_\beta$
    - Reactive term : $J_\alpha^r = \frac{1}{2}\Sigma_{\beta\gamma\delta}\iint\left(f'_\gamma f'_\delta\left(\frac{m_\alpha m_\beta}{m_\gamma m_\delta}\right)^3 - f_\alpha f_\beta\right)\sigma^r_{\alpha\beta\gamma\delta}|\vec{v}_\alpha - \vec{v}_\beta| d\widehat{\Omega} d\vec{v}_\beta$

Particle-In-Cell (PIC) is a popular way to solve these equations in the low-temperature plasma community



[1] Romain Lucken PhD thesis, 2019, LPPic

Fluid approach of the problem

We consider moments of the Boltzmann equation to obtain the evolution of macroscopic quantities:

Number density : $n_\alpha = \int f_\alpha d\vec{v}$ Particle flux : $n_\alpha \vec{u}_\alpha = \int \vec{v} f_\alpha d\vec{v}$ Particle flux : $\frac{3}{2} n_\alpha k_B T\_\alpha = \frac{m_\alpha}{2} \int (\vec{v} - \vec{u}_\alpha) f_\alpha d\vec{v}$

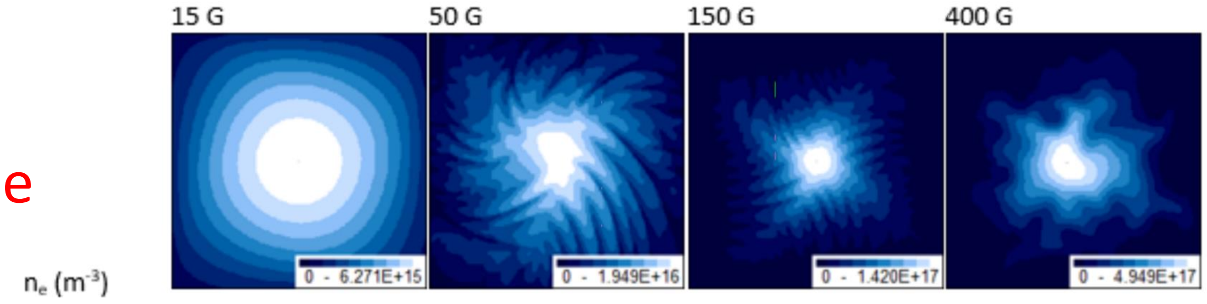
This leads to conservation equation for mass, momentum and energy:

Mass $\frac{\partial n_\alpha}{\partial t} + \vec{\nabla} \cdot (n_\alpha \vec{u}_\alpha) = \dot{n}_\alpha$

Momentum $m_\alpha \frac{\partial n_\alpha \vec{u}_\alpha}{\partial t} + \vec{\nabla} \cdot (m_\alpha n_\alpha \vec{u}_\alpha \vec{u}_\alpha + p_\alpha \bar{\bar{I}}) = \vec{\nabla} \cdot \bar{\bar{\Pi}}_\alpha + \vec{F}_\alpha + \sum_{\beta \neq \alpha} \vec{R}_{\alpha\beta}^{elastic} + \vec{R}_\alpha^{react}$

Energy $\frac{\partial}{\partial t} \left[\mathcal{U}_\alpha + m_\alpha n_\alpha \frac{u_\alpha^2}{2} \right] + \vec{\nabla} \cdot \left[\left(\mathcal{U}_\alpha + m_\alpha n_\alpha \frac{u_\alpha^2}{2} \right) \vec{u}_\alpha \right] = \vec{\nabla} \cdot (\vec{u}_\alpha \cdot \bar{\bar{\Pi}}_\alpha - \vec{q}_\alpha - p_\alpha \vec{u}_\alpha) + \rho_\alpha \vec{F}_\alpha \cdot \vec{u}_\alpha + \sum_{\beta \neq \alpha} \dot{Q}_{\alpha\beta}^{elastic} + \dot{Q}_\alpha^{react}$

This method can be much faster than PIC methods provided that it does not solve the Poisson equation



[2] Sarah Sadouni PhD thesis, 2020, MAGNIS

Advantages of using both particle-based and fluid approaches:

	Particle-based models	Fluid models
MODEL	• Stochastic resolution of the **kinetic equations** • Capture kinetic phenomena	• Hierarchy of **moments equations**, using specific hypothesis of closure • Proper framework to study macroscopic instabilities
NUMERICAL METHOD	**Particle-In-Cell (PIC)** • Statistical noise • Complex quantification of numerical error • **1D-2D settings**	**Finite Volume Methods** • Deterministic • Benefit from the experience of the CFD community • **Potentially 3D settings**

$$\Delta t \leq \omega_{pe}^{-1} = \sqrt{\frac{m_e \epsilon_0}{n_e q_e^2}}$$

$$\Delta x^2 \leq \lambda_D^2 = \frac{\epsilon_0 K_B T}{n_e q_e^2}$$

Problematic : can we predict the 2D sheath structure and magnetic-related instabilities with a fluid model and corresponding numerical methods?

Collisional isothermal Euler-Poisson equations

$$\partial_t n_e + \boldsymbol{\nabla}.\left(n_e \mathbf{u}_e\right) = n_e \nu^{iz}, \qquad \text{Mass equation}$$

$$m_e \partial_t \left(n_e \mathbf{u}_e\right) + \boldsymbol{\nabla}.\left(m_e n_e \mathbf{u}_e \otimes \mathbf{u}_e + p_e \mathbf{I}_d\right) = -n_e e \left(\mathbf{E} + \mathbf{u}_e \times \mathbf{B}\right) - m_e n_e \nu_e \mathbf{u}_e, \qquad \text{Momentum equation}$$

$$\partial_t n_i + \boldsymbol{\nabla}.\left(n_i \mathbf{u}_i\right) = n_e \nu^{iz}, \qquad \text{Mass equation}$$

$$m_i \partial_t \left(n_i \mathbf{u}_i\right) + \boldsymbol{\nabla}.\left(m_i n_i \mathbf{u}_i \otimes \mathbf{u}_i + p_i \mathbf{I}_d\right) = n_i e \left(\mathbf{E} + \mathbf{u}_i \times \mathbf{B}\right) - m_i n_i \nu_i \mathbf{u}_i, \qquad \text{Momentum equation}$$

$$\boldsymbol{\nabla}.\mathbf{E} = \frac{n_e - n_i}{\epsilon_0} e, \qquad \text{Gauss Law}$$

$$\boldsymbol{\nabla} = \begin{pmatrix} \partial_x \\ \partial_y \end{pmatrix}$$

$$\mathbf{I}_d = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$p_e = n_e \mathrm{k_B} T_e$$

$$p_i = n_i \mathrm{k_B} T_i$$

Boundary Conditions:

$$n_e u_e|_{wall} = n_e|_{wall} \sqrt{\frac{\mathrm{k_B} T_e}{2\pi m_e}}$$

Choice of model: low order moment-method compatible with some level of kinetic effect (sheath) [3]

[3] A. Alvarez-Laguna, T. Magin, M. Massot, A. Bourdon, P. Chabert. Plasma-sheath transition in multi-fluid models with inertial terms under low pressure conditions: Comparison with the classical and kinetic theory. Plasma Sources Science and Technology, 2020, ⟨10.1088/1361-6595/ab6242⟩.

Normalized equations

We normalize with: n_0, L_0, T_e

$$u_0 = \sqrt{\frac{kT_e}{m_i}}$$

$$t_0 = L_0/u_0$$

$$p_0 = n_0 k_B T_e$$

$$\phi_0 = \frac{k_B T_e}{e}$$

$$B_0 = \frac{e}{m_i t_0}$$

We define the non-dimensional numbers

Mass ratio: $\varepsilon = \frac{m_e}{m_i}$

Temperature ratio $\kappa = \frac{T_i}{T_e}$

Debye length $\chi = \left(\frac{\lambda_D}{L_0}\right)^2$

$$\partial_{\bar{t}} \bar{n}_e + \bar{\boldsymbol{\nabla}} . \left(\bar{n}_e \bar{\mathbf{u}}_e\right) = \bar{n}_e \bar{\nu}^{iz},$$

$$\partial_{\bar{t}} \bar{n}_i + \bar{\boldsymbol{\nabla}} . \left(\bar{n}_i \bar{\mathbf{u}}_i\right) = \bar{n}_e \bar{\nu}^{iz},$$

$$\partial_{\bar{t}} \left(\bar{n}_e \bar{\mathbf{u}}_e\right) + \bar{\boldsymbol{\nabla}} . \left(\bar{n}_e (\bar{\mathbf{u}}_e \otimes \bar{\mathbf{u}}_e + \varepsilon^{-1} \mathbf{I}_d)\right) = \varepsilon^{-1} \bar{n}_e \left(\bar{\boldsymbol{\nabla}} \bar{\phi} - \bar{\mathbf{u}}_e \times \bar{B}\right) - \bar{n}_e \bar{\nu}_e \bar{\mathbf{u}}_e$$

$$\partial_{\bar{t}} \left(\bar{n}_i \bar{\mathbf{u}}_i\right) + \bar{\boldsymbol{\nabla}} . \left(\bar{n}_i (\bar{\mathbf{u}}_i \otimes \bar{\mathbf{u}}_i + \kappa \mathbf{I}_d)\right) = \bar{n}_i \left(-\bar{\boldsymbol{\nabla}} \bar{\phi} + \bar{\mathbf{u}}_i \times \bar{B}\right) - \bar{n}_i \bar{\nu}_i \bar{\mathbf{u}}_i,$$

$$\bar{\Delta} \bar{\phi} = \chi^{-1} \left(\bar{n}_e - \bar{n}_i\right),$$

Boundary Conditions:

$$\bar{n}_e \bar{u}_e \big|_{wall} = \bar{n}_e \big|_{wall} \sqrt{\frac{1}{2\pi\varepsilon}}$$

Small scales that are challenging on a numerical level are present in our normalized model

A well-known problem of the CFD literature: excessive numerical diffusion in low-Mach regime

- The **convective part** of electron can be written:

$$\partial_t n_e + \partial_x(n_e u_e) = 0$$
$$\partial_t(n_e u_e) + \partial_x\left(n_e\left(u_e^2 + c^2\right)\right) = 0$$

With $c^2 = \varepsilon^{-1}$ and $\mathrm{M} = \sqrt{\varepsilon}$

$$\xrightarrow{\varepsilon \to 0}$$

$$\partial_x n_e = O(\varepsilon)$$
$$\partial_x u_e \approx -\frac{\partial_t n_e}{n_e} \approx 0 \text{ for periodic BC}$$

- This is solved in the **conservation law** formalism and **Lax-Friedrichs**:

$$\partial_t w + \partial_x f(w) = 0 \Rightarrow w_j^{n+1} = w_j^n - \frac{\Delta t}{\Delta x}\left(F_{j+1/2}^{LF} - F_{j-1/2}^{LF}\right)$$

With $F_{j+1/2}^{LF} = \frac{f\left(w_{j+1}^n\right)+f\left(w_j^n\right)}{2} - \lambda_{max}\left(w_{j+1}^n - w_j^n\right)$ and $\lambda_{max} = \max\left(\left|u_{j+1}^n\right|, \left|u_j^n\right|\right) + c$

There scheme is expected to be too diffusive, especially in 2D (Dellacherie 2009 [4])

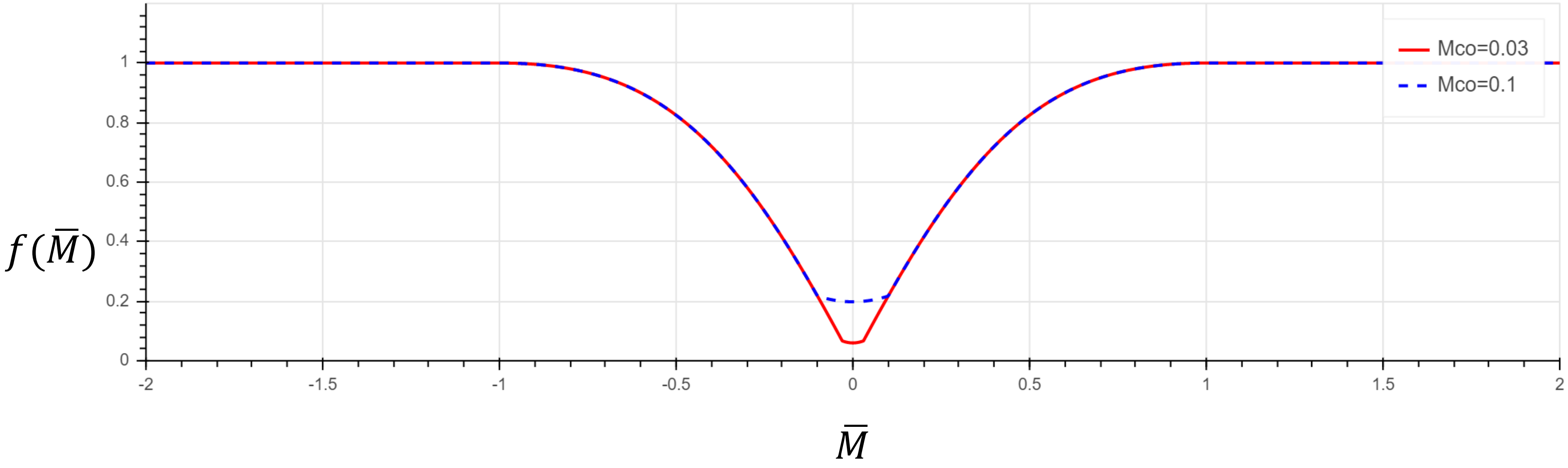
Low Mach Correction (LMC) adapted from Liou (2006) and Rieper (2011)

$$\lambda_{max} = \max\left(\left|u_{j+1}^n\right|, \left|u_j^n\right|\right) + f(\bar{M})c \qquad \bar{M} = \frac{|\hat{u}| + |\hat{v}|}{c}$$

$$f(\bar{M}) = \frac{\sqrt{(1-M_0)^2\bar{M}^2 + 4M_0}}{1+M_0^2} \qquad \hat{u} = \frac{\sqrt{\bar{n}_{eL}}\bar{u}_{eL} + \sqrt{\bar{n}_{eR}}\bar{u}_{eR}}{\sqrt{\bar{n}_{eL}} + \sqrt{\bar{n}_{eR}}}$$

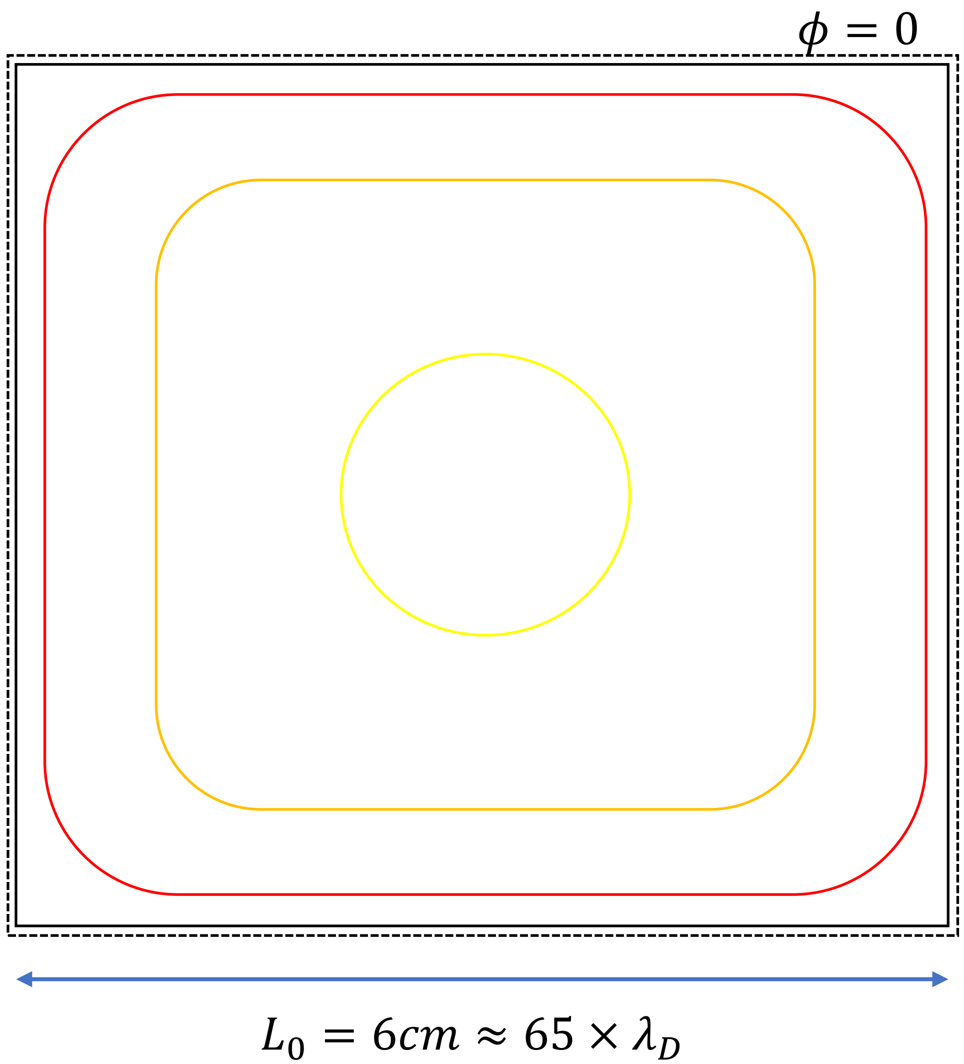
$$M_0 = \sqrt{\min\left(1, \max\left(\bar{M}^2, M_{co}^2\right)\right)}$$

The cut off value M_{co} is a critical parameter to control the effect of the correction, usually $M_{co} \sim \sqrt{\varepsilon}$



FVM/PIC comparison on Helium case

- Plasma parameters
  - $\varepsilon = \frac{m_e}{m_i} = 1.37\text{e}{-04}$
  - $\bar{\lambda}_D = 1.50\text{e}{-02}$
  - $\kappa = \frac{T_i}{T_e} = 2.86\text{e}{-03}$
  - $\bar{t}_f = 2$
- Simulation parameters:
  - 256×256 cells, $\Delta x \approx \bar{\lambda}_D/3$
  - $\Delta t \leq CFL \times \frac{\Delta x}{\lambda_{max}} \approx 10^{-6}$
  - $t_{simu} \approx 2\ days$ on 64 CPUs

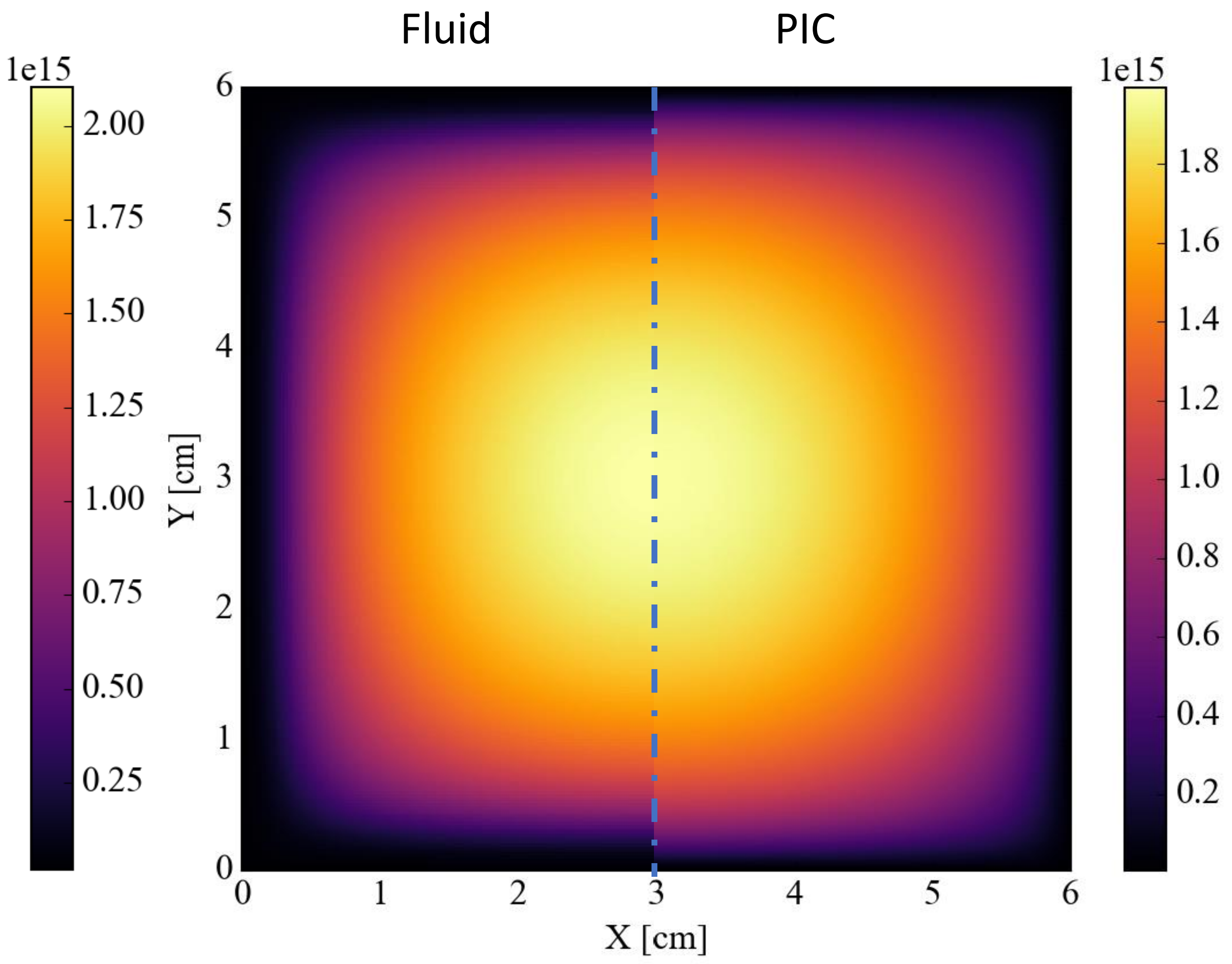


$n_0 = 1.2 \times 10^{-15} m^{-3}$

$T_e = 17.5eV$

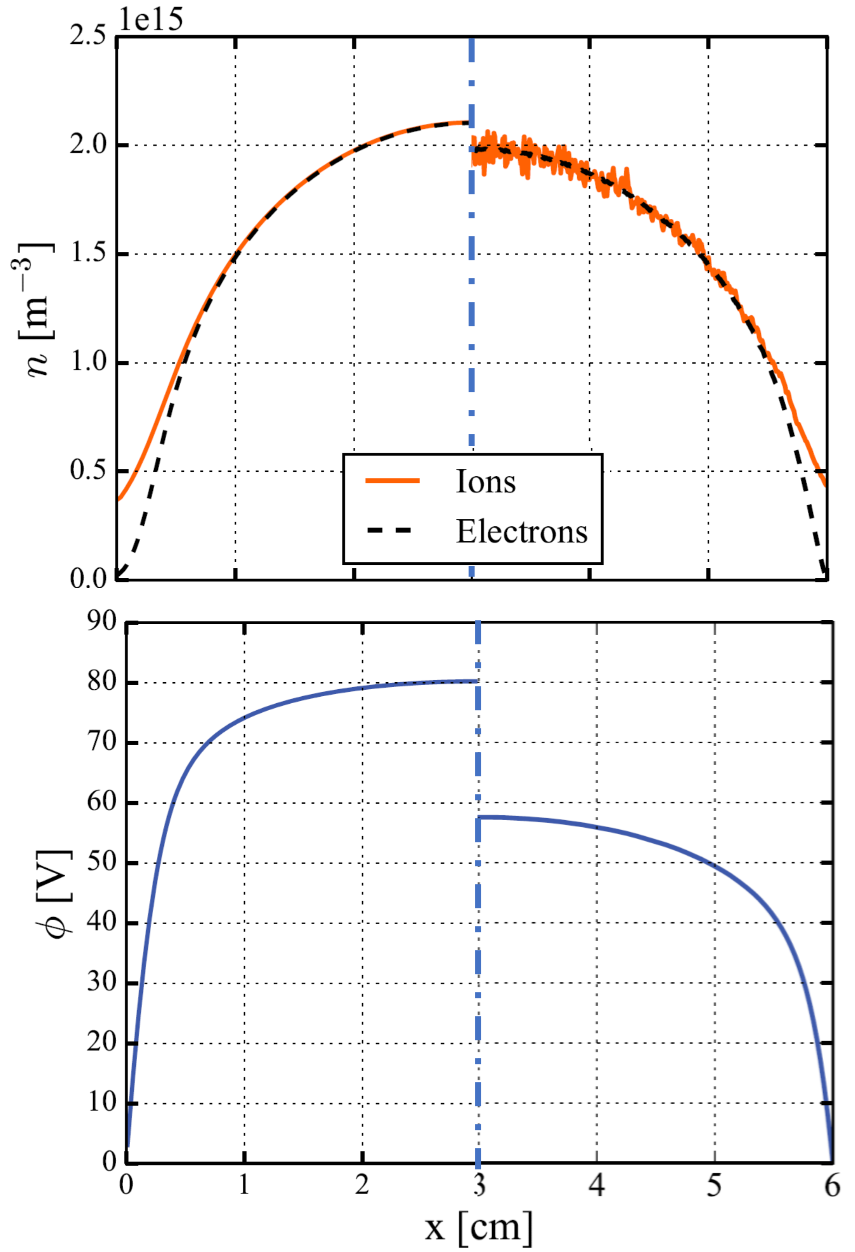
$t_{real} \approx 6\sim7\ \mu s$

Electron density comparison



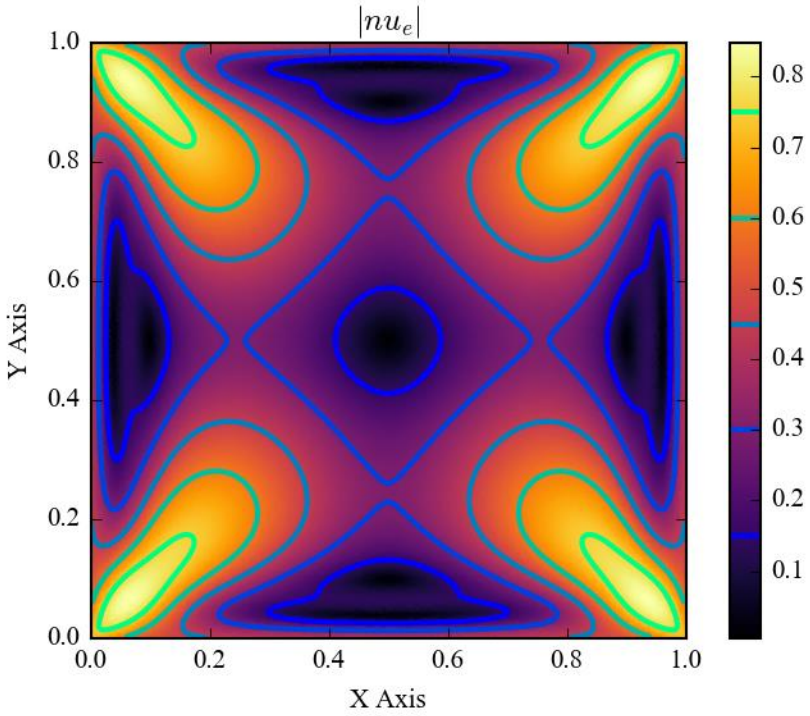
Electron density n_e

1D horizontal cut

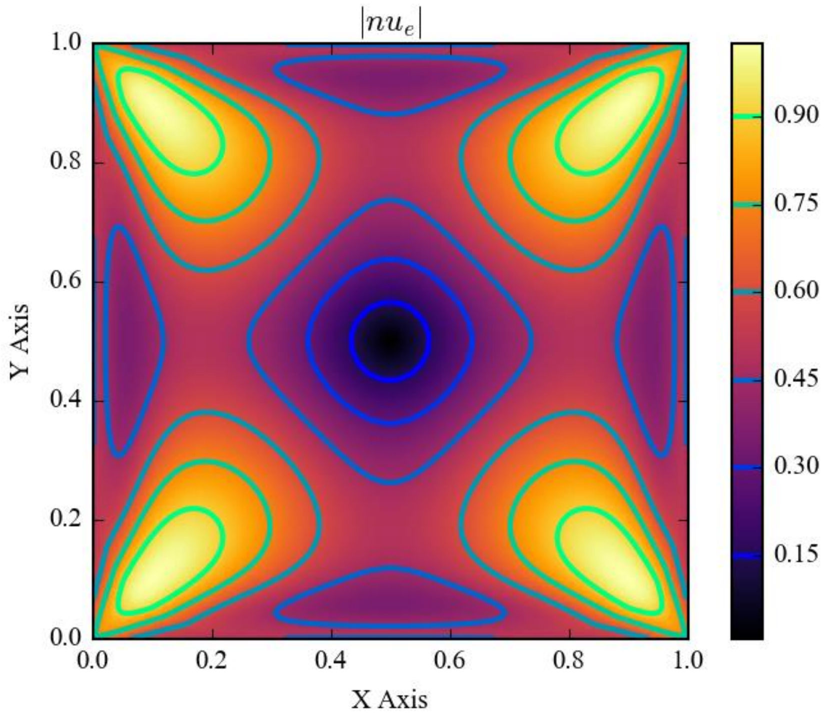


Comparative results for electron fluxes

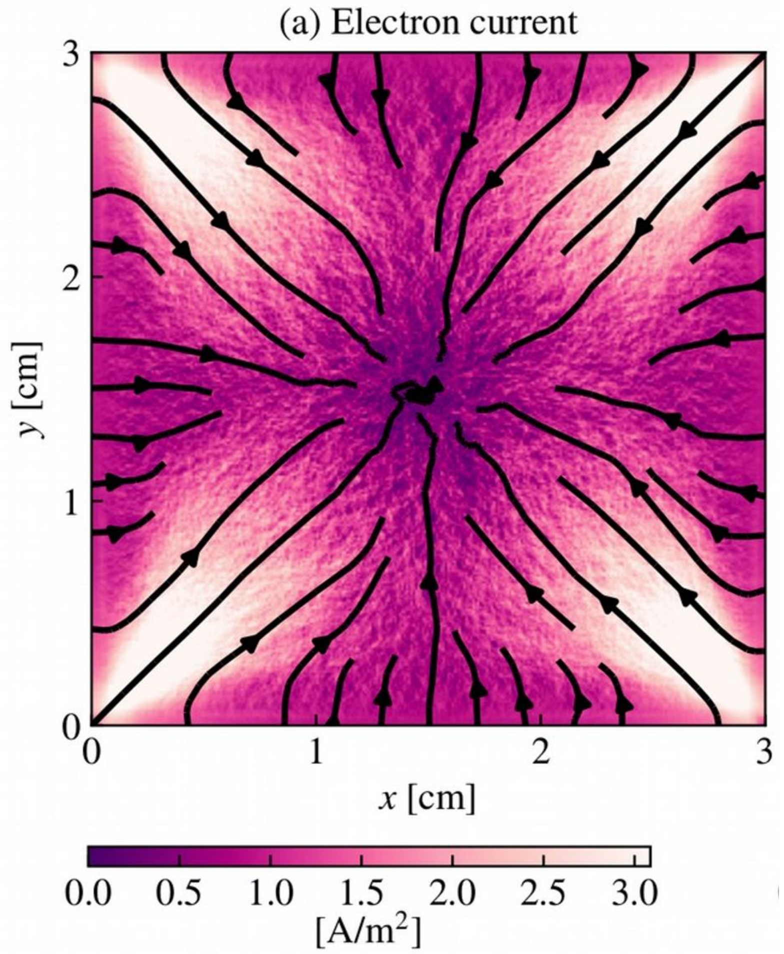
The same scale is used for both figures:



No Low Mach correction



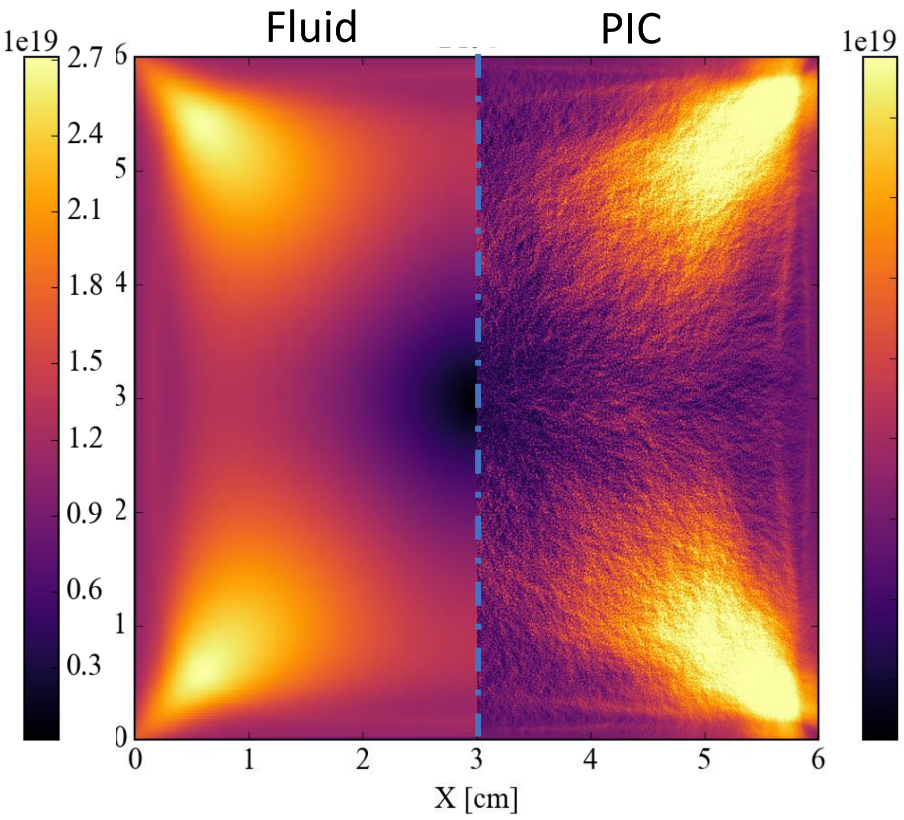
$M_{co} = 0.3$



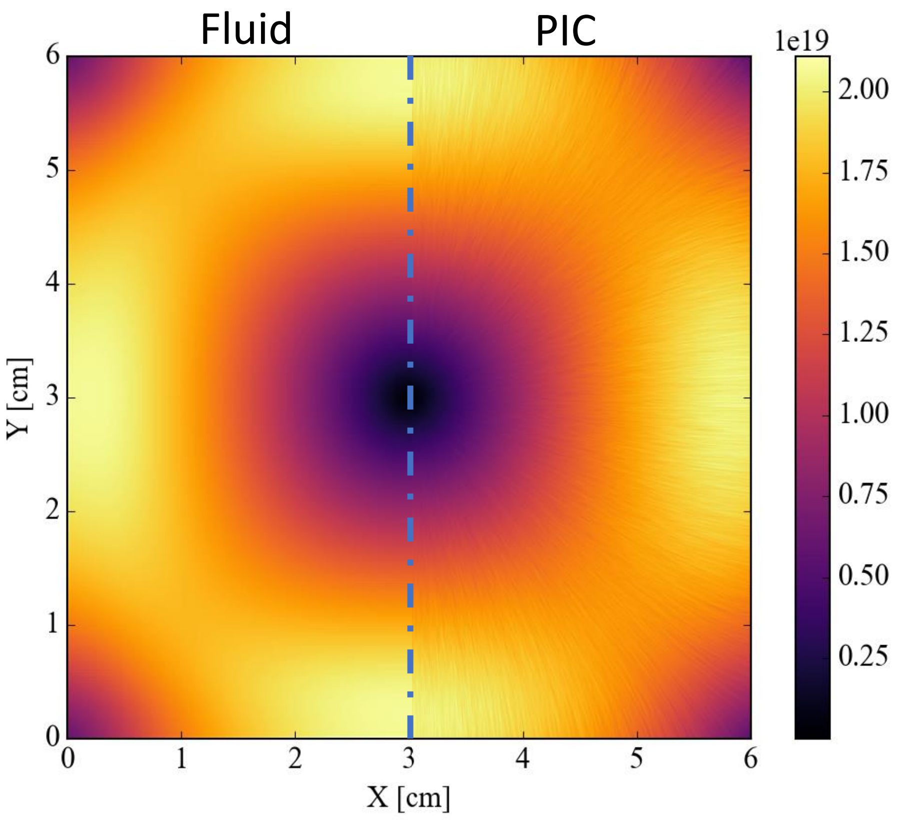
Source: Romain Lucken's PhD, 2019

The Low Mach Correction significantly reduces the diffusivity of the scheme

Flux Comparison

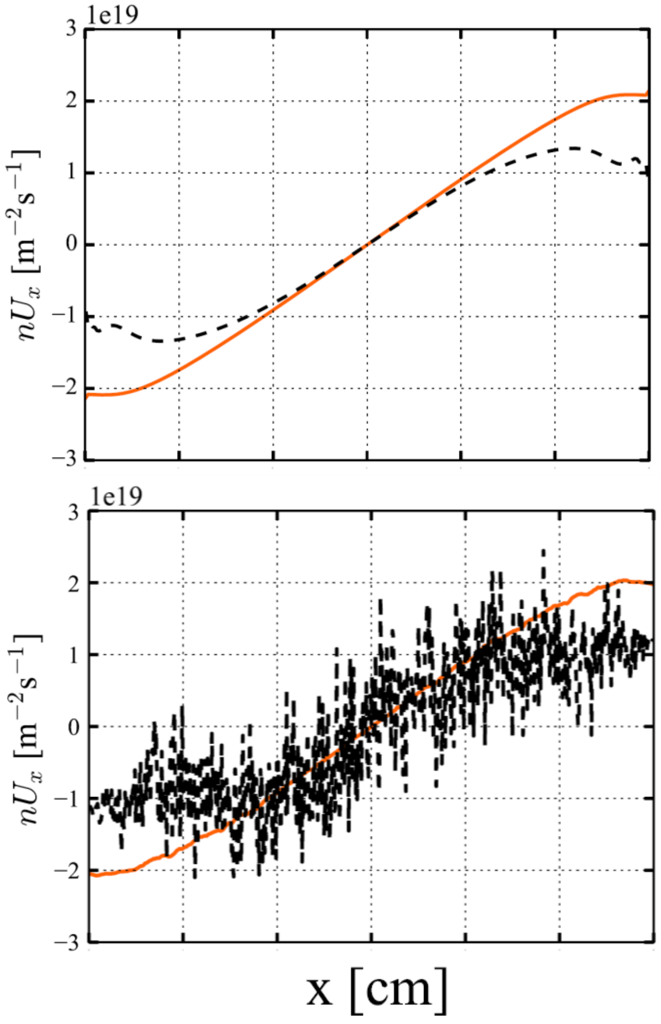


Electron flux $n_e u_e$



Electron flux $n_i u_i$

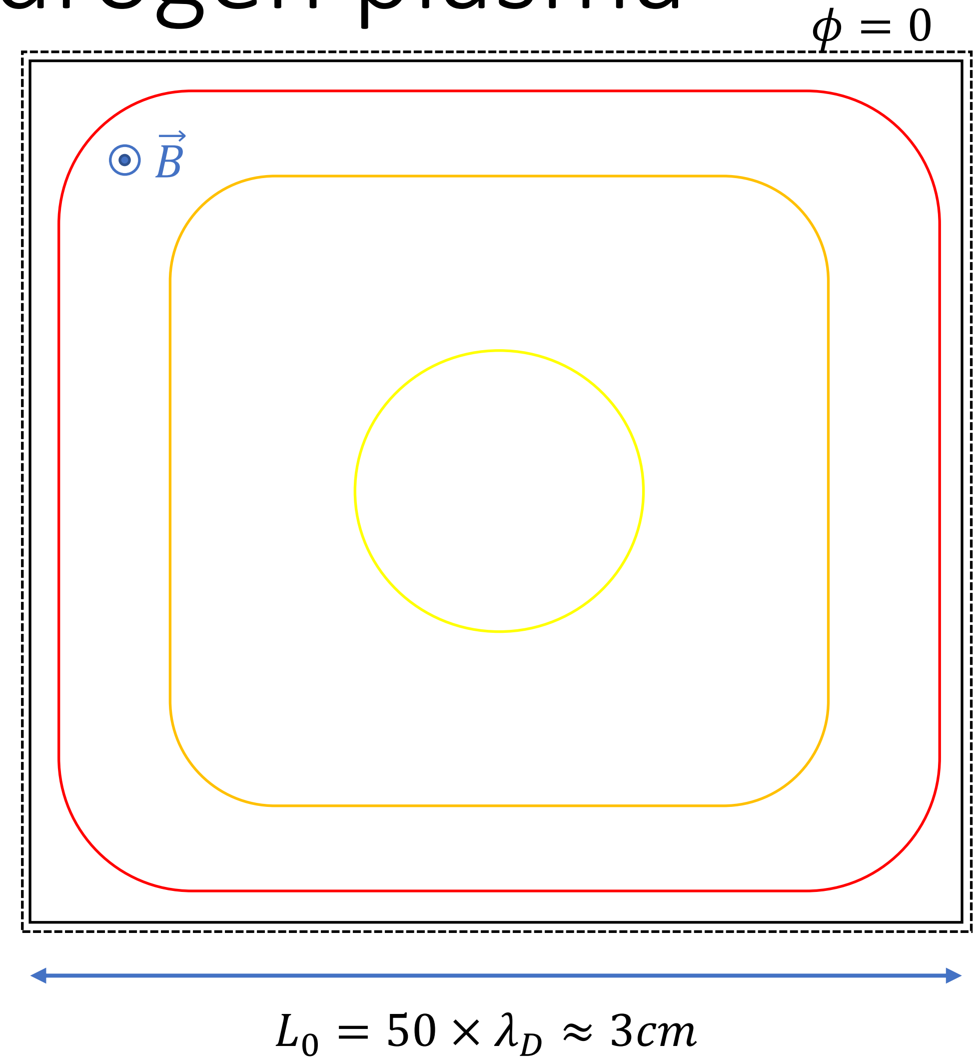
1D horizontal cut



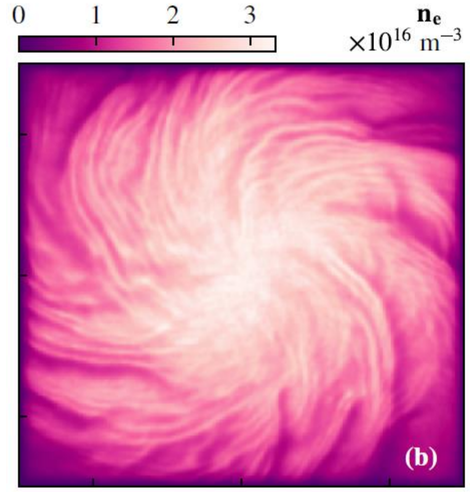
The structure of the fluxes for both ions and electrons is well-described by the fluid approach while the magnitude of the fluxes is more accurate for ions.

Magnetized configuration: Proof of concept with simplified Hydrogen plasma

- Plasma parameters
  - $\varepsilon = \frac{m_e}{m_i} = \frac{1}{1836}$ (proton plasma)
  - $\bar{\lambda}_D = 0.02$
  - $\kappa = \frac{T_i}{T_e} = 0.025$
  - $\bar{t}_f = 4$
- Simulation parameters:
  - 256×256 cells, $\Delta x \approx \bar{\lambda}_D/5$
  - $\Delta t \leq CFL \times \frac{\Delta x}{\lambda_{max}} \approx 10^{-5}$
  - $t_{simu} \approx 10h \sim 20h$ on 64 CPUs



$n_0 = 2 \times 10^{-15} m^{-3}$
$T_e = 14eV$
$t_{real} \approx 4\ \mu s$

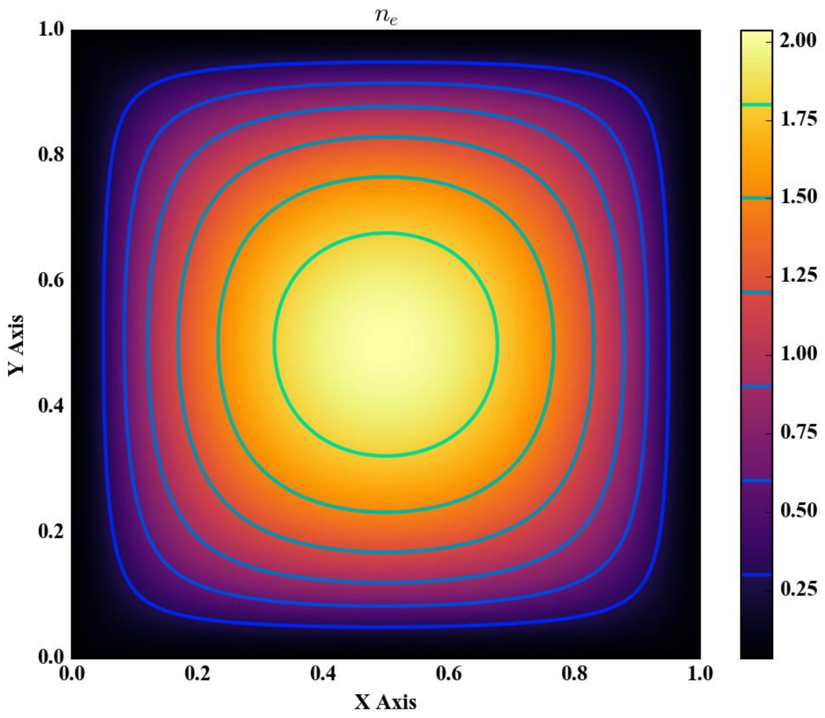


Source: Romain Lucken's PhD, 2019

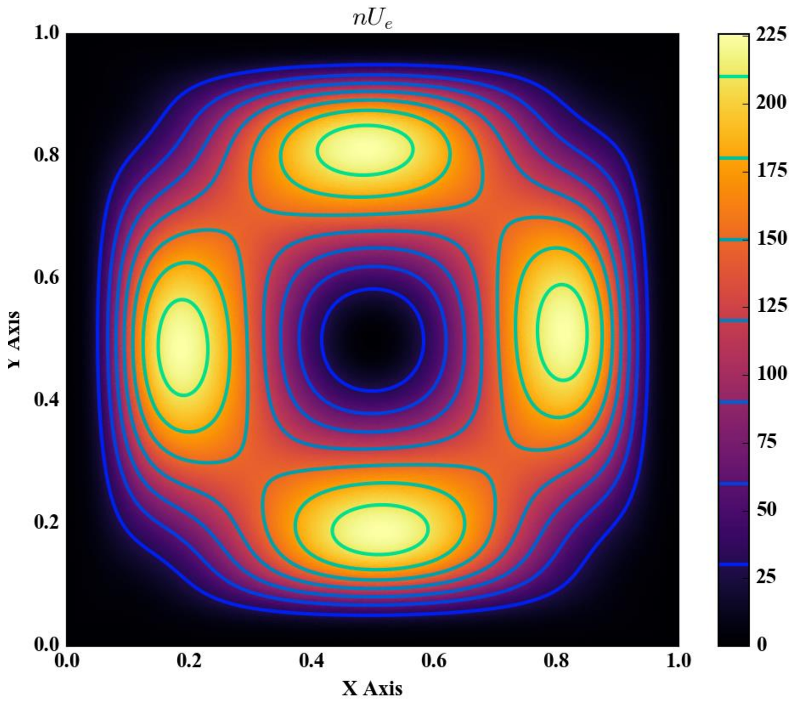
We hope to observe magnetic-related instabilities for a critical value of $\bar{B}$

Magnetized case, moderate magnetic field

$\bar{B} = 0.3,\ \mathrm{B} \approx 1mT, L_0 \approx 5\rho_e, \rho_i \approx 10L_0$



Electron density

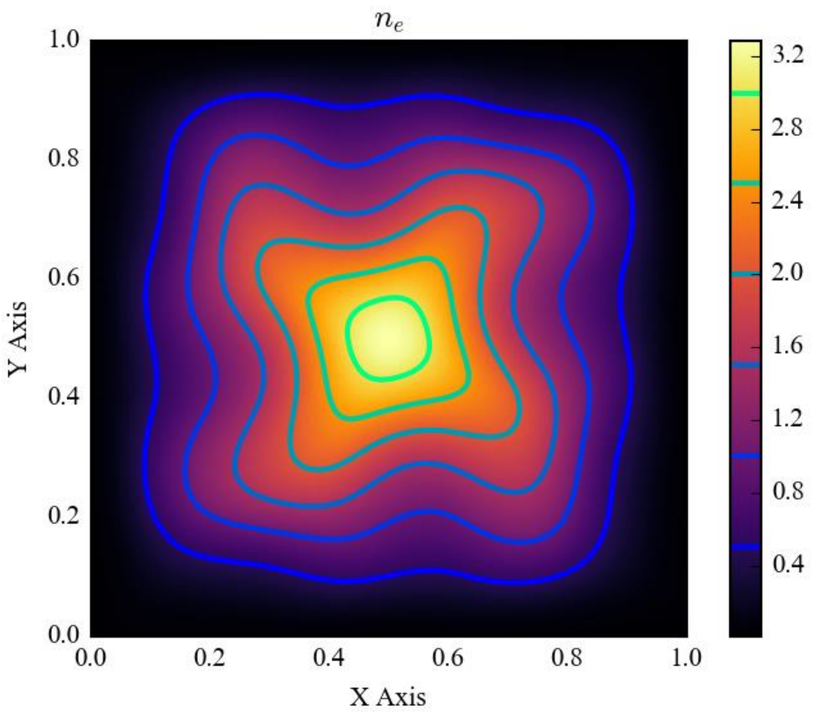


Electron fluxes

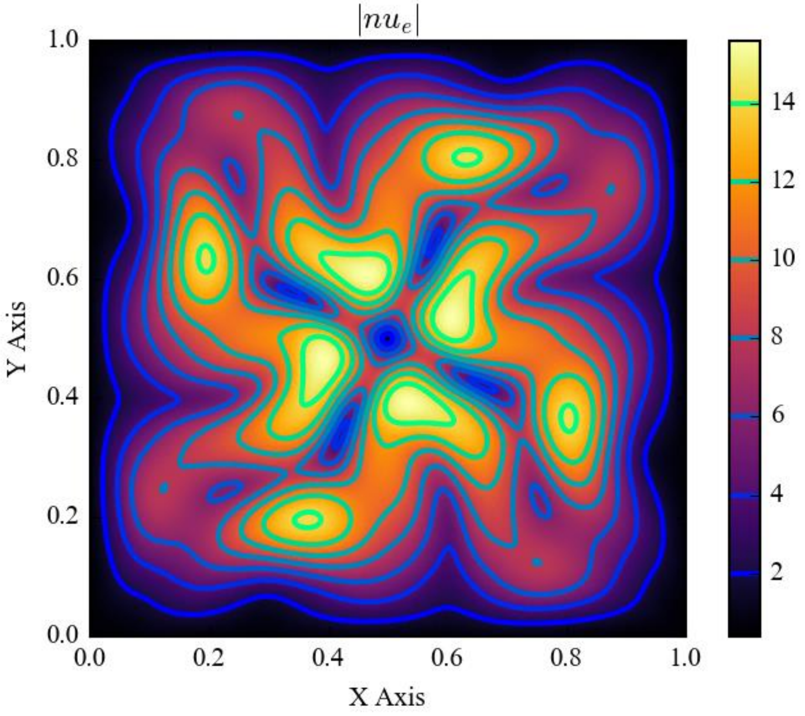
For moderate magnetic fields, a stable structure appears with rotating electrons, similar to that that is obtained via PIC simulations

Magnetized case, high magnetic field

$\bar{B} = 0.5,\ \mathrm{B} \approx 6mT, L_0 \approx 20\rho_e, \rho_i \approx 2L_0$



Electron density

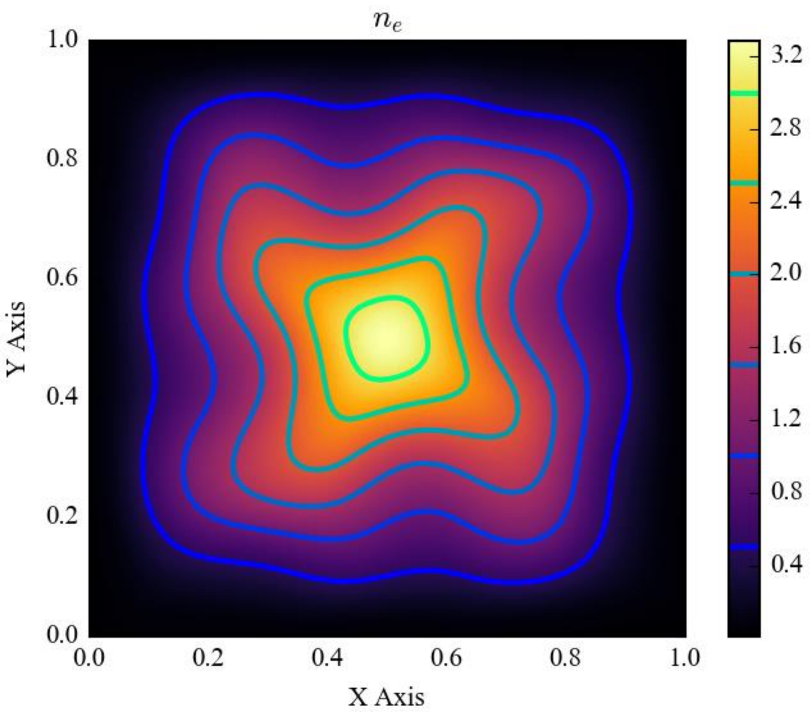


Electron fluxes

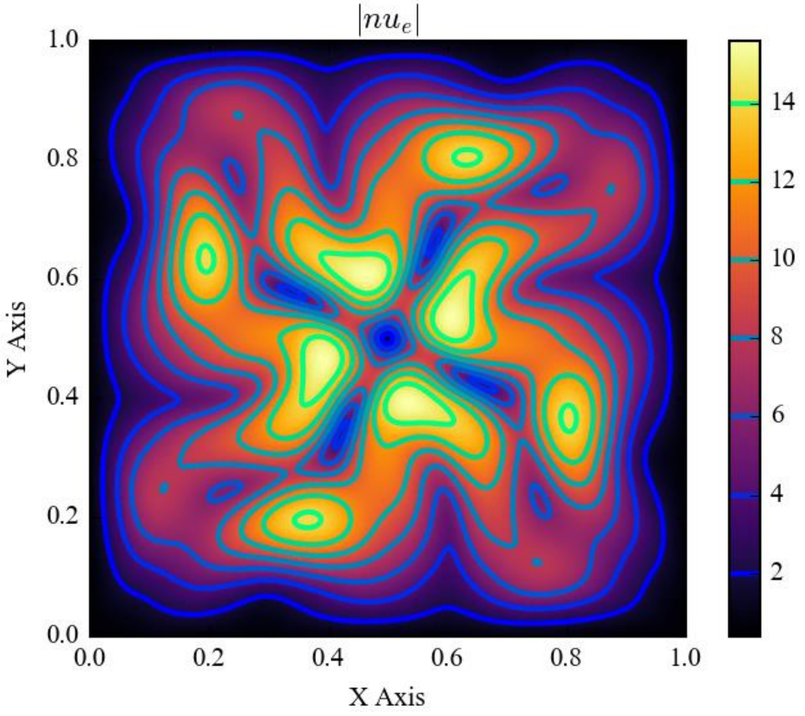
For high magnetic fields, instabilities are triggered

Magnetized case, high magnetic field

$\bar{B} = 0.5,\ \mathrm{B} \approx 6mT, L_0 \approx 20\rho_e, \rho_i \approx 2L_0$



Electron density



Electron fluxes

Simple model encompassing the range of scales describing the relevant physics of our problem and related numerical stiffness that can be used to produce accurate simulations of the instabilities of interest, provided that we use an appropriate numerical strategy.

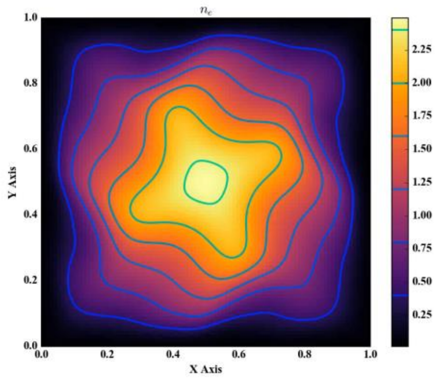
Conclusion

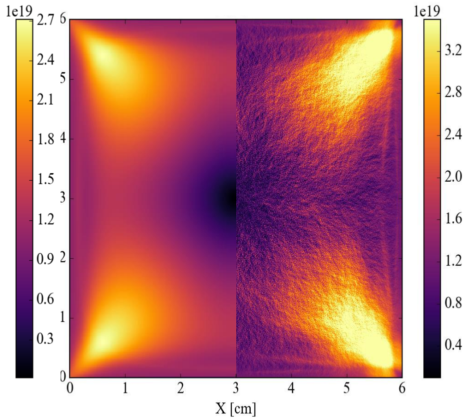
- Simple model encompassing the range of scales describing the relevant physics of our problem and related numerical stiffness. Coupled with an appropriate numerical strategy, it allows to simulate sheath and instabilities in low-temperature partially magnetized plasma.

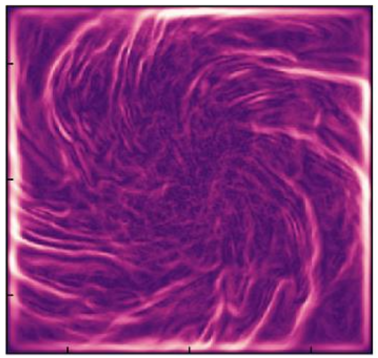
- Paper in preparation on these results (preprint available at VKI PhD symposium)

- This work is part of a larger project at CMAP on new numerical strategies including AP (**asymptotic-preserving**) methods, **AMR** (CanoP), **Multiresolution** (SAMURAI) and **error control** to develop viable alternatives to PIC codes to simulate low-temperature magnetized plasmas

- This work is funded by a joint grant from the French Ministry of Defense (DGA) and the region Île-de-France (DIM Math Innov).







We formulate the problem as a system of conservation law with source term

Both fluids obey an equation of the form:

$$\partial_t w + \partial_x f(w) + \partial_y g(w) = S(w)$$

with

$$w = \begin{pmatrix} n \\ nu \\ nv \end{pmatrix}, \quad f(w) = \begin{pmatrix} nu \\ nu^2 + nc^2 \\ nvu \end{pmatrix}, \quad g(w) = \begin{pmatrix} nv \\ nuv \\ nv^2 + nc^2 \end{pmatrix}, \quad S(w) = \begin{pmatrix} n\bar{\nu}^{iz} \\ qn\left(-\partial_{\bar{x}}\bar{\phi} + v\bar{B}\right) - n\bar{\nu}u \\ qn\left(-\partial_{\bar{y}}\bar{\phi} - u\bar{B}\right) - n\bar{\nu}v \end{pmatrix}$$

with

$$c = \varepsilon^{-1/2} \text{ (electrons) or } c = \kappa^{1/2} \text{ (ions) and } \mathbf{u} = \begin{pmatrix} u \\ v \end{pmatrix}$$

Nonlinear hyperbolic system can form singularities

They can be tackled using Finite Volume Methods [4,5]

[4] Eleuterio F. Toro, Riemann Solvers and Numerical Methods for Fluid Dynamics, Springer, 1997

[5] Randal J. Leveque, Numerical Methods for Conservation Laws, Birkhäuser, 1992

Magnetized case, high magnetic field

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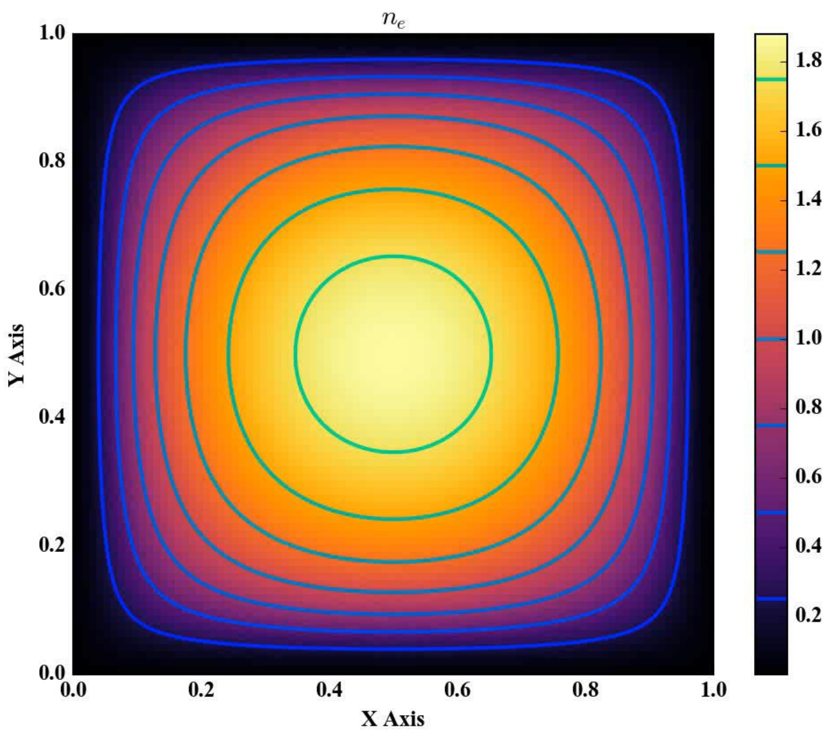
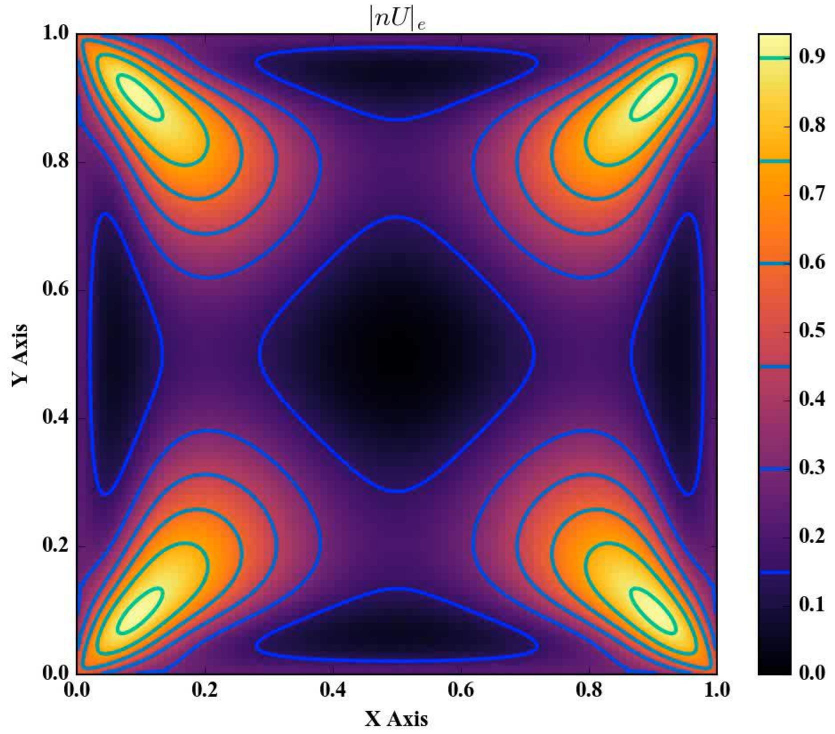


Electron density



Electron fluxes

For high magnetic fields, instabilities are triggered

Simple model encompassing the range of scales describing the relevant physics of our problem and related numerical stiffness that can be used to produce accurate simulations of the instabilities of interest, provided that we use an appropriate numerical strategy.