High-order moment methods for partially-ionized plasmas

Laboratoire de Physique des Plasmas

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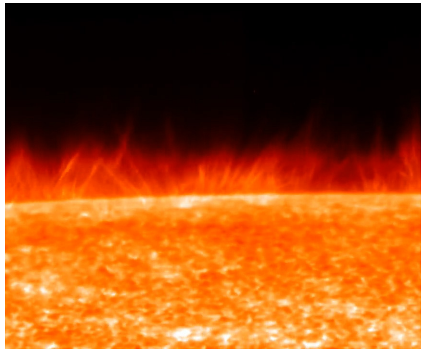
Partially ionized plasmas

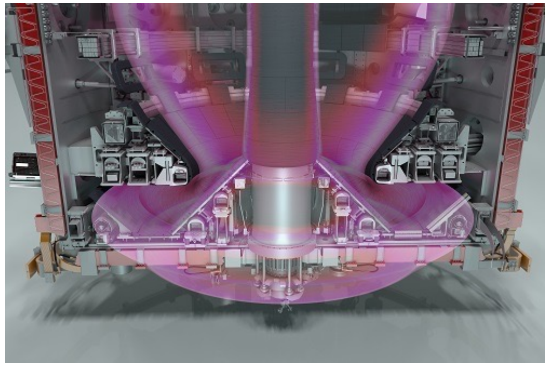
Space plasmas



Sun chromosphere

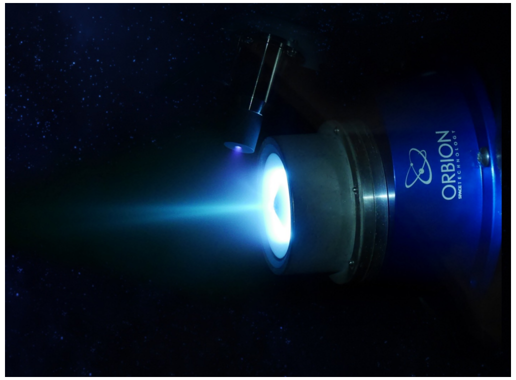
Accretion disks

Fusion plasmas



Divertor region

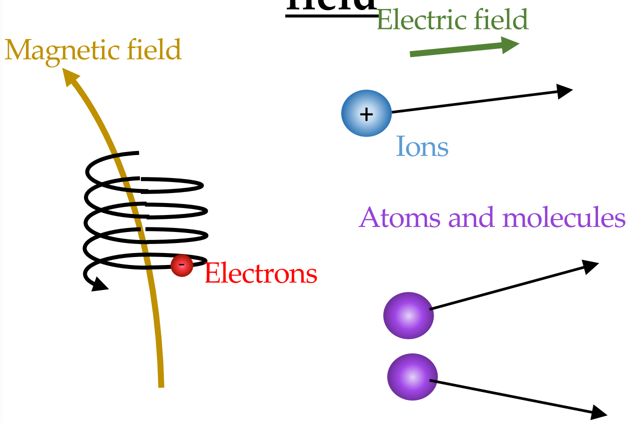
Low temperature plasmas



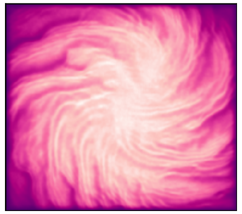
Electric propulsion

Difficulties of modeling partially-ionized plasmas with a magnetic field

Particle motion with magnetic field



Anomalous transport



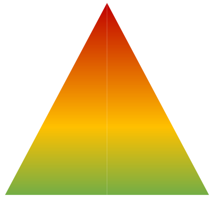
Strong magnetic field

Weak magnetic field

Electrostatic (and electromagnetic) instabilities

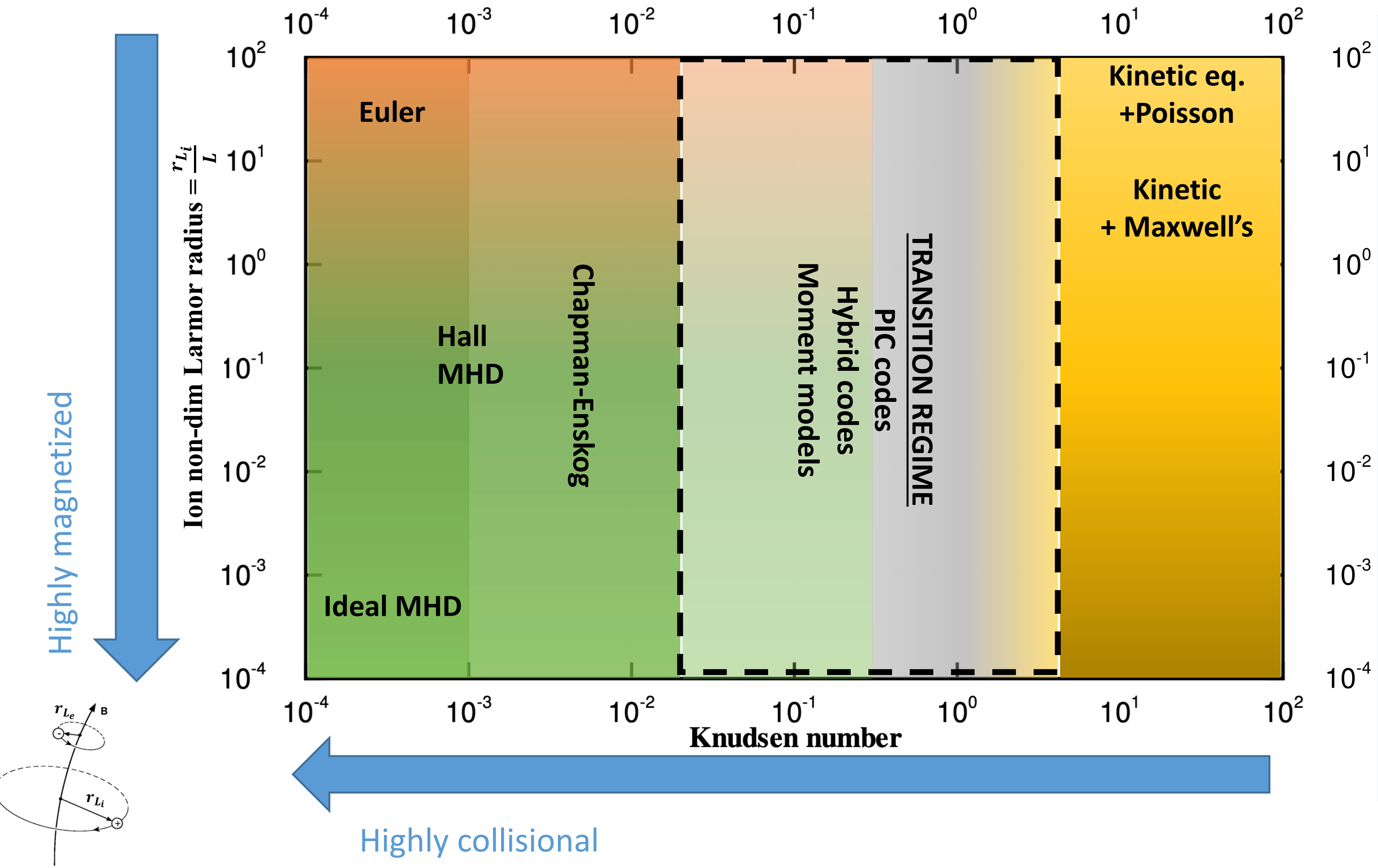
Micro vs macro

Kinetic models: computationally too expensive



Standard MHD models: Neglect important physics

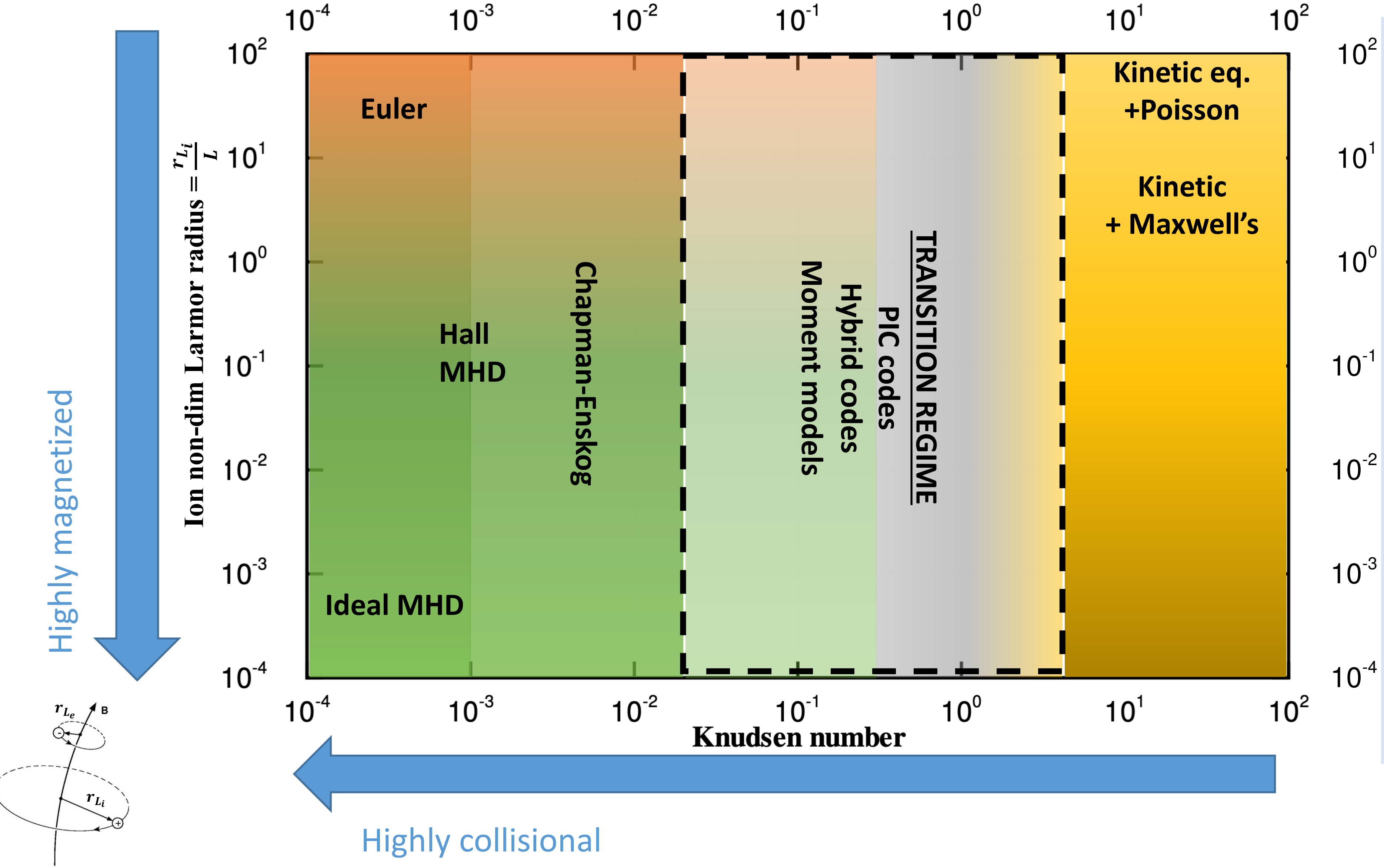
Different mathematical descriptions can model the state of a plasma



Chapman-Enskog models:

- Braginskii (1965)
  - Magnetized and fully-ionized (Landau operator)
- Ern & Giovangigli (1994)
  - Chapman-Enskog in kinetic equation.
- Zhdanov (2002)
  - Magnetized and partially ionized (Boltzmann op.)
- Graille, Magin, Massot (2009)
  - Magnetized & partially-ionized (Boltzmann op.)

Different mathematical descriptions can model the state of a plasma



Moment models:

- Grad's method (1949)
  - Landau and Boltzmann.
- Landau Fluids (1997)
  - Kinetic phenomena
- Levermore's Maximum Entropy (1996)
  - Mostly with BGK
- Pearson IV, angular moments, other closures…

Kinetic equation in plasmas

Microscopic state is defined by position and momentum of particles by the Hamiltonian of the system

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \underbrace{\sum_{i=1}^{N} U(\mathbf{r}_i)}_{\text{External Electro-magnetic field}} + \underbrace{\sum_{\substack{i,j=1\\ i<j}}^{N} u(|\mathbf{r}_i - \mathbf{r}_j|)}_{\text{Interaction potential between pairs.}}$$

From **Liouville's equation**, we can derive the first equation of the **BBGKY hierarchy** (for the one-particle distribution function):

$$\frac{\partial f_1}{\partial t} + \mathbf{v}_1.\boldsymbol{\nabla}_{\mathbf{r}_1} f_1 - \nabla_{\mathbf{r}_1} U_{\text{ext}}(\mathbf{r}_1).\boldsymbol{\nabla}_{\mathbf{v}_1} f_1 = \int \nabla_{\mathbf{r}_1} u(|\mathbf{r}_1 - \mathbf{r}_2|).\boldsymbol{\nabla}_{\mathbf{v}_1} \underbrace{f_2(\mathbf{r}_1, \mathbf{r}_2, \mathbf{v}_1, \mathbf{v}_2, t)}_{\text{Two-particle distribution function}} \, d^3\mathbf{r}_2 \, d^3\mathbf{v}_2.$$

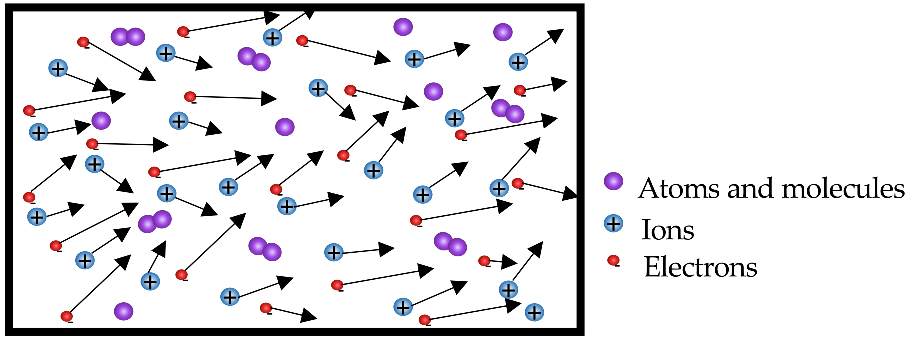
We introduce the two-particle correlation function

$$g_2(\mathbf{r}_1, \mathbf{r}_2, \mathbf{v}_1, \mathbf{v}_2, t) \equiv f_2(\mathbf{r}_1, \mathbf{r}_2, \mathbf{v}_1, \mathbf{v}_2, t) - \underbrace{f_1(\mathbf{r}_1, \mathbf{v}_1, t) f_1(\mathbf{r}_2, \mathbf{v}_2, t)}_{\text{Statistically independent particles}}$$

We integrate the RHS term of the kinetic equation:

$$\int \nabla_{\mathbf{r}_1} u \, .\boldsymbol{\nabla}_{\mathbf{v}_1} f_2 \, d^3\mathbf{r}_2 \, d^3\mathbf{v}_2 = \underbrace{\boldsymbol{\nabla}_{\mathbf{v}_1} f_1 \int n(\mathbf{r}_2, t) \nabla_{\mathbf{r}_1} \mathbf{u} \, d^3\mathbf{r}_2}_{\text{Field of (N-1) particles on particle 1}} + \underbrace{\int \nabla_{\mathbf{r}_1} u \, .\boldsymbol{\nabla}_{\mathbf{v}_1} g_2 \, d^3\mathbf{r}_2 \, d^3\mathbf{v}_2}_{\text{Collisional term}}$$

Ionized gas



Kinetic equation for the charged particles:

$$\frac{\partial f}{\partial t} + \mathbf{v}.\boldsymbol{\nabla}_{\mathbf{r}} f + \underbrace{\frac{q(\mathbf{E} + \mathbf{v} \times \mathbf{B})}{m}}_{\text{External + field created by other particles.}} .\boldsymbol{\nabla}_{\mathbf{v}} f = \left(\frac{\delta f}{\delta t}\right)_c$$

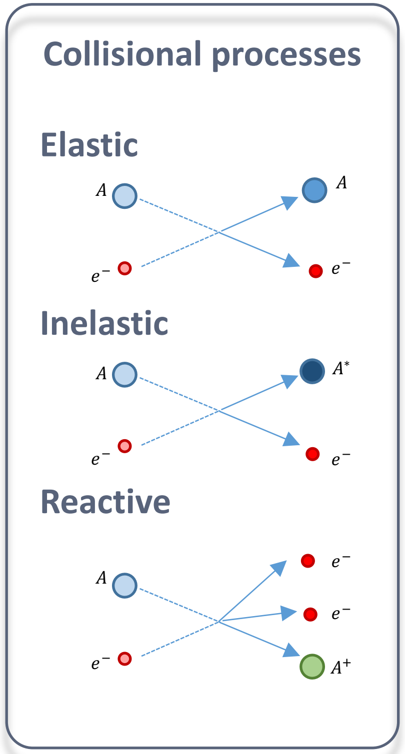
Maxwell's equations

$$\begin{aligned} \frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} &= 0 \\ \frac{\partial \mathbf{E}}{\partial t} - c^2 \nabla \times \mathbf{B} &= -\frac{1}{\mu_0} \sum_\beta q_\beta \int d\mathbf{v} \mathbf{v} f^\beta \\ \nabla \cdot \mathbf{B} &= 0 \\ \nabla \cdot \mathbf{E} &= \frac{1}{\epsilon_0} \sum_\beta q_\beta \int d\mathbf{v} f^\beta \end{aligned}$$

Collisional term models (electrons)

We consider the following collisional processes:

$$\left(\frac{\delta f_{\mathfrak{e}}}{\delta t}\right)_c = \left(\frac{\delta f_{\mathfrak{e}}}{\delta t}\right)_{\mathfrak{eg}}^{(elast.)} + \left(\frac{\delta f_{\mathfrak{e}}}{\delta t}\right)_{\mathfrak{eg}}^{(inelast.)} + \left(\frac{\delta f_{\mathfrak{e}}}{\delta t}\right)_{\mathfrak{ee}} + \left(\frac{\delta f_{\mathfrak{e}}}{\delta t}\right)_{\mathfrak{ei}}$$



Collisional models

electron-gas elastic collisions

- Boltzmann operator
- Lorentz gas
- BGK operator

$$\left(\frac{\delta f_{\mathfrak{e}}}{\delta t}\right)_{\mathfrak{eg}}^{(Boltz)} = \int\int \left(f'_{\mathfrak{e}} f'_{\mathfrak{g}} - f_{\mathfrak{e}} f_{\mathfrak{g}}\right) g\sigma d\Omega d\boldsymbol{v}_{\mathfrak{g}}\,.$$

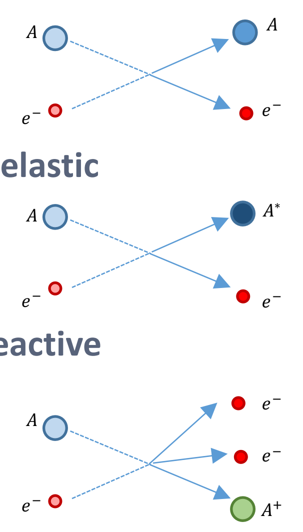
$$\left(\frac{\delta f_{\mathfrak{e}}}{\delta t}\right)_{\mathfrak{eg}}^{(Lorentz)} = n_{\mathfrak{g}} v_{\mathfrak{e}} \int \left(f'_{\mathfrak{e}} - f_{\mathfrak{e}}\right) \sigma(v_{\mathfrak{e}}, \chi) d\Omega$$

$$\left(\frac{\delta f_{\mathfrak{e}}}{\delta t}\right)_{\mathfrak{eg}}^{(BGK)} = \nu_m (f_{\mathfrak{g}} - f_{\mathfrak{e}})$$

Collisional term models (electrons)

We consider the following collisional processes:

$$\left(\frac{\delta f_{\mathfrak{e}}}{\delta t}\right)_c = \left(\frac{\delta f_{\mathfrak{e}}}{\delta t}\right)_{\mathfrak{eg}}^{(elast.)} + \left(\frac{\delta f_{\mathfrak{e}}}{\delta t}\right)_{\mathfrak{eg}}^{(inelast.)} + \left(\frac{\delta f_{\mathfrak{e}}}{\delta t}\right)_{\mathfrak{ee}} + \left(\frac{\delta f_{\mathfrak{e}}}{\delta t}\right)_{\mathfrak{ei}}$$



Collisional models

Coulomb collisions

- Landau operator
- Boltzmann operator (screened at Debye length)
- Lennard-Balescu and Instability-enhanced collisional operators

$$\left(\frac{\delta f_{\mathfrak{e}}}{\delta t}\right)_{\mathfrak{e}\alpha}^{(Fokker-Planck)} = \partial_{v_r}\left(D^{\alpha}_{rs}\partial_{v_s} f_{\mathfrak{e}}\right) - \partial_{v_r}\left(A^{\alpha}_{r} f_{\mathfrak{e}}\right)$$

$$\left(\frac{\delta f_{\mathfrak{e}}}{\delta t}\right)_{\mathfrak{e}\alpha}^{(Boltz)} = \int\int \left(f'_{\mathfrak{e}} f'_{\alpha} - f_{\mathfrak{e}} f_{\alpha}\right) g\sigma d\Omega d\boldsymbol{v}_{\alpha} \quad \alpha \in \{\mathfrak{e}, \mathfrak{i}\}$$

More info: Balruud et al., Physics of Plasmas 17, 055704 (2010);

Moment (multi-fluid) hierarchies: closure problem

Microscopic description

Multi-fluid description

Average in velocity space

$$\mathbf{M}_\alpha(\vec{x},t) = \int_\infty \mathbf{V}_\alpha f_\alpha d^3v = \langle \mathbf{V}_\alpha f_\alpha \rangle$$

$$\mathbf{V}_\alpha(\vec{v}) = \left(m_\alpha,\ m_\alpha v_i,\ \frac{1}{2} m_\alpha v_i v_j,\ m_\alpha v_i v_j v_k,\ \cdots \right)^T$$

Boltzmann equation

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

$$\alpha \in \{\text{electrons, ions, gas}\}$$

Moment hierarchy

$$\frac{\partial \mathbf{M}_\alpha}{\partial t} + \vec{\nabla}\cdot\langle \vec{v}\mathbf{V}_\alpha f_\alpha\rangle = -\left\langle \mathbf{V}_\alpha \frac{\vec{F}_\alpha}{m_\alpha}\cdot\vec{\nabla}_{\vec{v}} f_\alpha \right\rangle + \left\langle \mathbf{V}_\alpha \left(\frac{\delta f_\alpha}{\delta t}\right)_{coll} \right\rangle$$

Macroscopic variables

Fluxes

Electromagnetic forces

Collisional terms

Mass, Momentum, Energy, Heat flux:

$$\begin{pmatrix} \rho \\ \rho u_i \\ \frac{1}{2}\rho u_i u_j + \frac{1}{2}P_{ij} \\ \rho u_i u_j u_k + P_{ij}u_k + P_{jk}u_i + P_{ik}u_j + Q_{ijk} \\ \vdots \end{pmatrix} \quad \begin{pmatrix} \rho u_i \\ \rho u_i u_j + P_{ij} \\ \rho u_i u_j u_k + 3P_{(ij}u_{k)} + Q_{ijk} \\ \rho u_i u_j u_k u_l + 6u_{(i}u_j P_{kl)} + 4u_{(i}Q_{jkl)} + R_{ijkl} \\ \vdots \end{pmatrix} \quad \begin{pmatrix} 0 \\ q_\alpha n E_i \\ 2q_\alpha n u_{(j}E_{i)} \\ 3q_\alpha\left(nE_{(i}u_j u_{k)} + \frac{E_{(i}P_{jk)}}{m}\right) \\ \vdots \end{pmatrix}$$

Closure problem:

- How many moments?
- The fluxes depend on next moment

Collisional integrals:

- Depend on cross-section data and VDF

Coupling Euler + Maxwell's equations

More info in :

A. Alvarez Laguna, et al., J. Comput. Phys., 419, 15 (2020).
A. Alvarez Laguna, et al., Comput. Phys. Commun., 231, (2018).
A. Alvarez Laguna, et al., J. Comput. Phys., 318, 15 (2016).

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“Collisionless” isothermal Euler/Poisson equations

Electron mass: $$\partial_t n_e + \partial_x \cdot (n_e u_e) = 0$$

Electron momentum: $$m_e \partial_t (n_e u_e) + \partial_x \cdot (m_e n_e u_e \otimes u_e + p_e) = -n_e e E$$

Ion mass: $$\partial_t n_i + \partial_x \cdot (n_i u_i) = 0$$

Ion momentum: $$m_i \partial_t (n_i u_i) + \partial_x \cdot (m_i n_i u_i \otimes u_i + p_i) = n_i e E$$

Gauss law: $$\partial_x \cdot E = \frac{n_i - n_e}{\epsilon_0} e$$

We normalize with: n_0, L_0, T_e

$$u_0 = \sqrt{\frac{kT_0}{m_i}}$$

$$t_0 = L_0/u_0$$

$$p_0 = n_0 k T_0$$

Difficulties of the Euler/Poisson system:

- Explicit discretizations are unconditionally unstable.*
- Implicit discretizations are not well conditioned.
- Disparity of time-scales and stiff source terms.

*Sylvie Fabre, Stability analysis of the Euler-Poisson equations, J. Comp. Phys. 101, 445 (1992).

"Collisionless" isothermal Euler/Poisson equations

Electron mass: $$\partial_{\bar{t}}\bar{n}_{\mathfrak{e}} + \partial_{\bar{x}} \cdot (\bar{n}_{\mathfrak{e}}\bar{u}_{\mathfrak{e}}) = 0$$

Electron momentum: $$\partial_{\bar{t}}(\bar{n}_{\mathfrak{e}}\bar{u}_{\mathfrak{e}}) + \partial_{\bar{x}} \cdot \left[\bar{n}_{\mathfrak{e}}\left(\bar{u}_{\mathfrak{e}}^2 + \varepsilon^{-1}\right)\right] = \varepsilon^{-1}\bar{n}_{\mathfrak{e}}\partial_{\bar{x}}\bar{\phi},$$

Ion mass: $$\partial_{\bar{t}}\bar{n}_{\mathfrak{i}} + \partial_{\bar{x}} \cdot (\bar{n}_{\mathfrak{i}}\bar{u}_{\mathfrak{i}}) = 0$$

Ion momentum: $$\partial_{\bar{t}}(\bar{n}_{\mathfrak{i}}\bar{u}_{i}) + \partial_{\bar{x}} \cdot \left[\bar{n}_{\mathfrak{i}}\left(\bar{u}_{\mathfrak{i}}^2 + \kappa\right)\right] = -\bar{n}_{\mathfrak{i}}\partial_{\bar{x}}\bar{\phi},$$

Gauss law: $$\partial_{\bar{x}\bar{x}}^2\bar{\phi} = \mu^{-1}(\bar{n}_{\mathfrak{e}} - \bar{n}_{\mathfrak{i}})$$

We define the non-dimensional numbers

Mass ratio: $\varepsilon = \frac{m_{\mathfrak{e}}}{m_{\mathfrak{i}}} \sim 10^{-5}$

Temperature ratio $\kappa = \frac{T_{\mathfrak{i}}}{T_{\mathfrak{e}}} \sim 10^{-2}$

Debye length $\mu = \left(\frac{\lambda_D}{L_0}\right)^2 \sim 10^{-5}$

Dimensional quantities			
Neutral density	$n_{\mathfrak{n}}$	1.25×10^{20}	m^{-3}
Electron density	$n_{\mathfrak{e},\mathfrak{i}}$	10^{16}	m^{-3}
Ion and neutral temperature	$T_{\mathfrak{n},\mathfrak{i}}$	0.05	eV
Electron temperature	$T_{\mathfrak{e}}$	2	eV
Distance between plates	l	3	cm
Ion-neutral collisional cross section	$\sigma_{\mathfrak{in}}$	10^{-18}	m^2
Electron-neutral collisional cross section	$\sigma_{\mathfrak{en}}$	10^{-19}	m^2
Ionization constant	K_{ion}	8.16×10^{-18}	$\mathrm{m}^3\mathrm{s}^{-1}$
Ionization potential	ε_{ion}	17.44	eV
Electron plasma period	ω_{pe}^{-1}	$1.77 \cdot 10^{-10}$	s

Asymptotic limit with respect to the Debye length and ion-to-electron mass ratio

Complete problem

$$
{}^{\mu}F^{\varepsilon}: \begin{cases} \partial_{\bar{t}}\bar{n}_{\mathfrak{e}} + \partial_{\bar{x}}\cdot(\bar{n}_{\mathfrak{e}}\bar{u}_{\mathfrak{e}}) = 0, \\ \partial_{\bar{t}}\bar{n}_{\mathfrak{i}} + \partial_{\bar{x}}\cdot(\bar{n}_{\mathfrak{i}}\bar{u}_{\mathfrak{i}}) = 0, \\ \partial_{\bar{t}}(\bar{n}_{\mathfrak{e}}\bar{u}_{\mathfrak{e}}) + \partial_{\bar{x}}\cdot\left[\bar{n}_{\mathfrak{e}}\left(\bar{u}_{\mathfrak{e}}^2 + \varepsilon^{-1}\right)\right] = \frac{\bar{n}_{\mathfrak{e}}}{\varepsilon}\partial_{\bar{x}}\bar{\phi}, \\ \partial_{\bar{t}}(\bar{n}_{\mathfrak{i}}\bar{u}_{i}) + \partial_{\bar{x}}\cdot\left[\bar{n}_{\mathfrak{i}}\left(\bar{u}_{\mathfrak{i}}^2 + \kappa\right)\right] = -\bar{n}_{\mathfrak{i}}\partial_{\bar{x}}\bar{\phi}, \\ \partial^2_{\bar{x}\bar{x}}\bar{\phi} = \mu^{-1}\left(\bar{n}_{\mathfrak{e}} - \bar{n}_{\mathfrak{i}}\right). \end{cases}
$$

$\varepsilon \to 0$ and $\mu \to 0$

$$
{}^{0}F^{0}: \begin{cases} \partial_t \bar{n}_{\mathfrak{e}}^{(0,0)} + \partial_{\bar{x}}\cdot\left(\bar{n}_{\mathfrak{e}}^{(0,0)}\bar{n}_{\mathfrak{i}}^{(0,0)}\right) = 0, \\ \partial_t \bar{n}_{\mathfrak{i}}^{(0,0)} + \partial_{\bar{x}}\cdot\left(\bar{n}_{\mathfrak{i}}^{(0,0)}\bar{u}_{\mathfrak{i}}^{(0,0)}\right) = 0, \\ \frac{1}{\bar{n}_{\mathfrak{e}}^{(0,0)}}\partial_{\bar{x}}\bar{n}_{\mathfrak{e}}^{(0,0)} = \partial_{\bar{x}}\phi^{(0,0)}, \\ \partial_t \bar{n}_{\mathfrak{i}}^{(0,0)} + \partial_{\bar{x}}\cdot\left[\bar{n}_{\mathfrak{i}}^{(0,0)}\left({\bar{u}_{\mathfrak{i}}^{(0,0)}}^2 + \kappa\right)\right] = -\bar{n}_{\mathfrak{i}}^{(0,0)}\partial_x\phi^{(0,0)}, \\ \bar{n}_{\mathfrak{e}}^{(0,0)} = \bar{n}_{\mathfrak{i}}^{(0,0)}. \end{cases}
$$

- Charge neutrality and massless electrons (Boltzmann electrons) are two asymptotic limits of the system.
- Formally, we have an elliptic relation to compute the electric potential from the electron density.

Lagrange-projection operator splitting

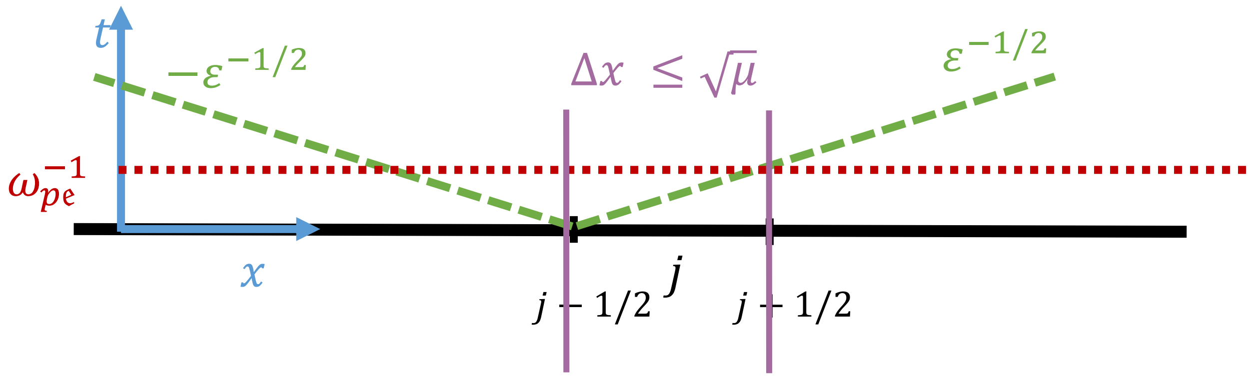
We propose to solve the system of equations as the succesive solution of the two following systems:

Electron acoustic and electrostatic system

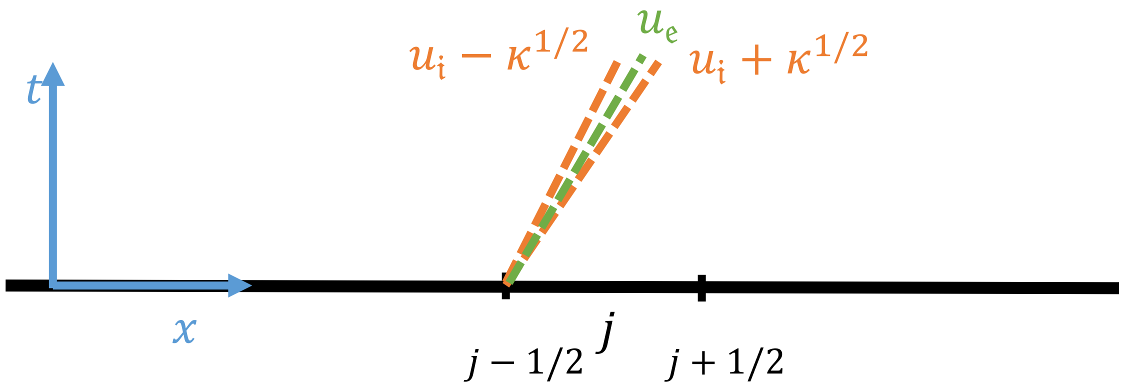
$$
\begin{aligned}
\partial_{\bar t}\bar n_{\mathfrak e} + \bar n_{\mathfrak e}\partial_{\bar x}\cdot \bar u_{\mathfrak e} &= 0,\\
\partial_{\bar t}(\bar n_{\mathfrak e}\bar u_{\mathfrak e}) + \bar n_{\mathfrak e}\bar u_{\mathfrak e}\partial_{\bar x}\cdot \bar u_{\mathfrak e} + \partial_{\bar x}\bar p_{\mathfrak e} &= \frac{\bar n_{\mathfrak e}}{\varepsilon}\partial_{\bar x}\bar\phi,\\
\partial^2_{\bar x\bar x}\bar\phi &= \frac{\bar n_{\mathfrak e} - \bar n_{\mathfrak i}}{\mu},
\end{aligned}
$$

Electron transport and ion dynamics.

$$
\begin{aligned}
\partial_{\bar t}\bar n_{\mathfrak e} + \bar u_{\mathfrak e}\cdot\partial_{\bar x}\bar n_{\mathfrak e} &= 0\\
\partial_{\bar t}(\bar n_{\mathfrak e}\bar u_{\mathfrak e}) + \bar u_{\mathfrak e}\cdot\partial_{\bar x}(\bar n_{\mathfrak e}\bar u_{\mathfrak e}) &= 0,\\
\partial_{\bar t}\bar n_{\mathfrak i} + \partial_{\bar x}\cdot(\bar n_{\mathfrak i}\bar u_{\mathfrak i}) &= 0\\
\partial_{\bar t}(\bar n_{\mathfrak i}\bar u_{i}) + \partial_{\bar x}\cdot\left[\bar n_{\mathfrak i}\left(\bar u_{\mathfrak i}^2 + \kappa\right)\right] &= -\bar n_{\mathfrak i}\partial_{\bar x}\bar\phi,
\end{aligned}
$$

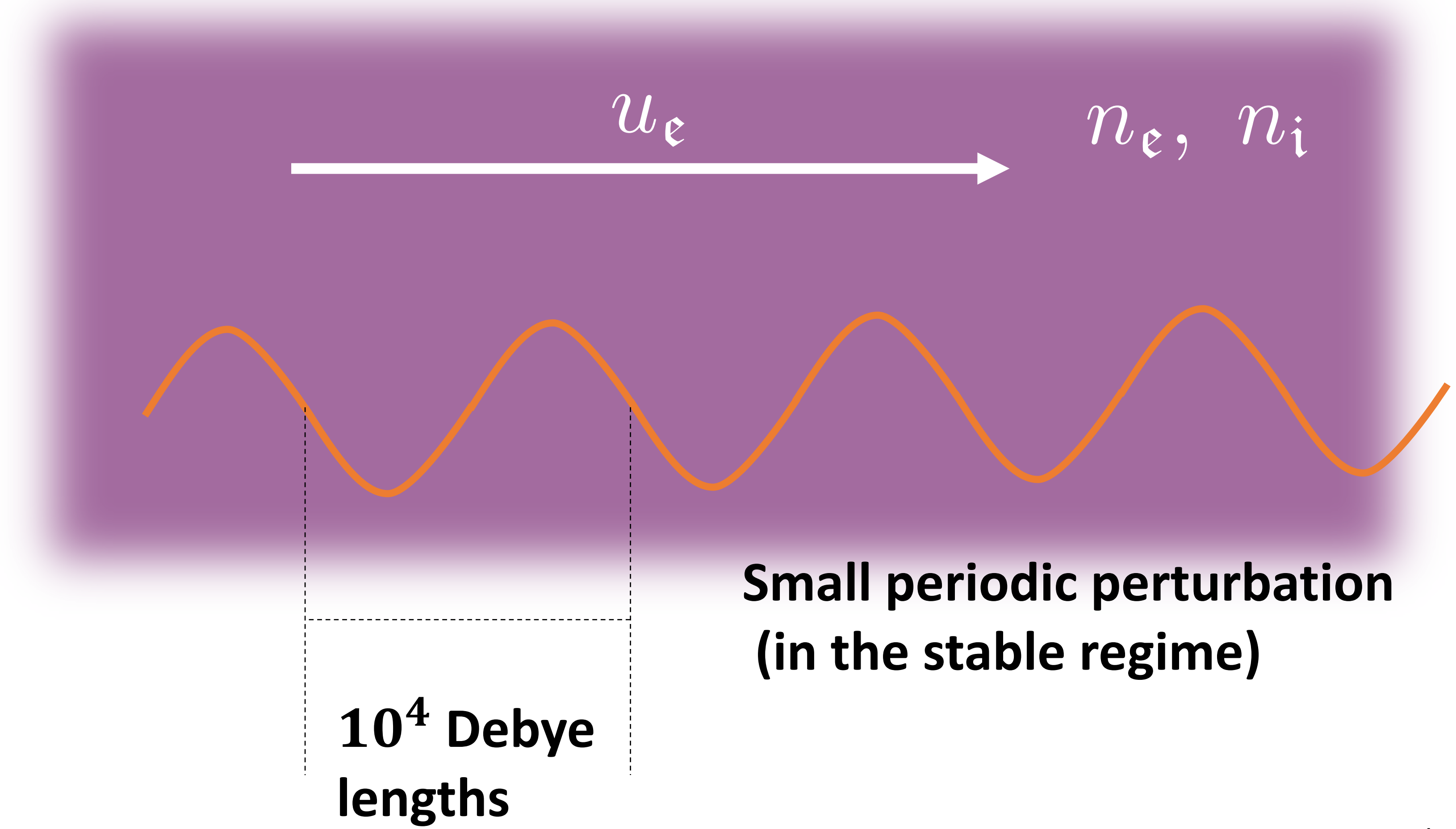


Slow dynamics: Ion dynamics + electron advection



Two-stream perturbation in an isothermal plasma

- We choose a case with $\varepsilon = 10^{-4}, \mu = 10^{-8}$, resolved with 100 cells and $\mathrm{CFL} = 0.7$



Alvarez Laguna et al., JCP (2020)

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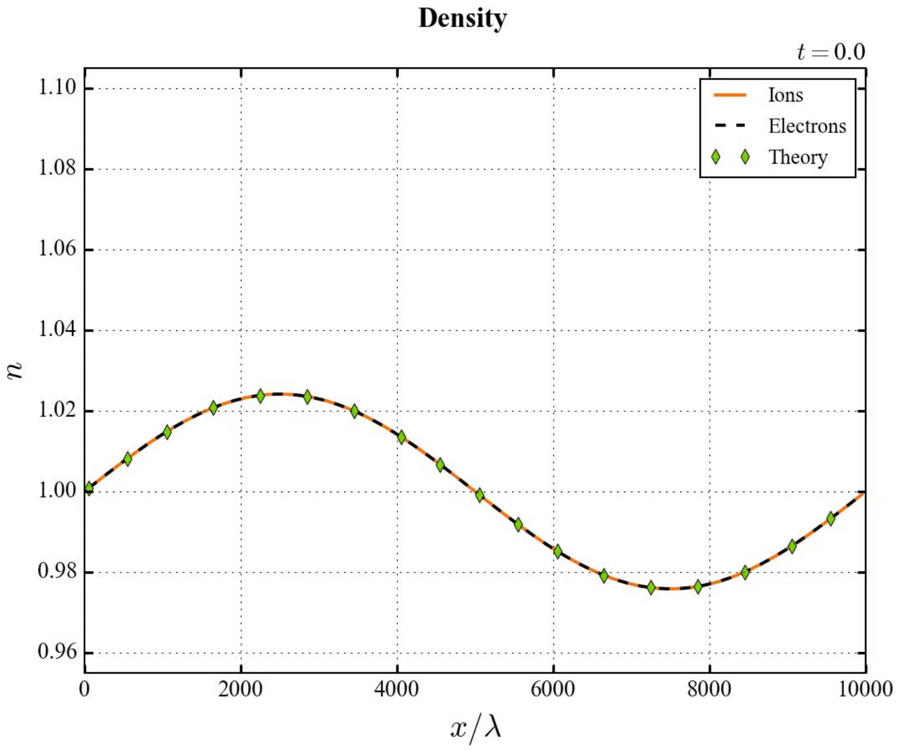
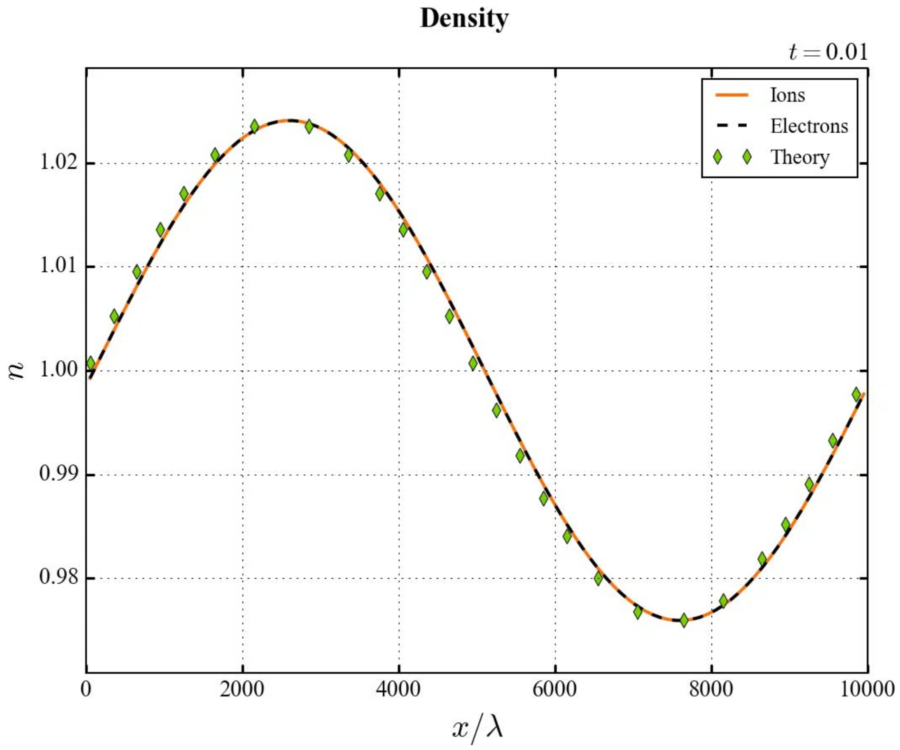
Standard discretization



Asymptotic-preserving discretization



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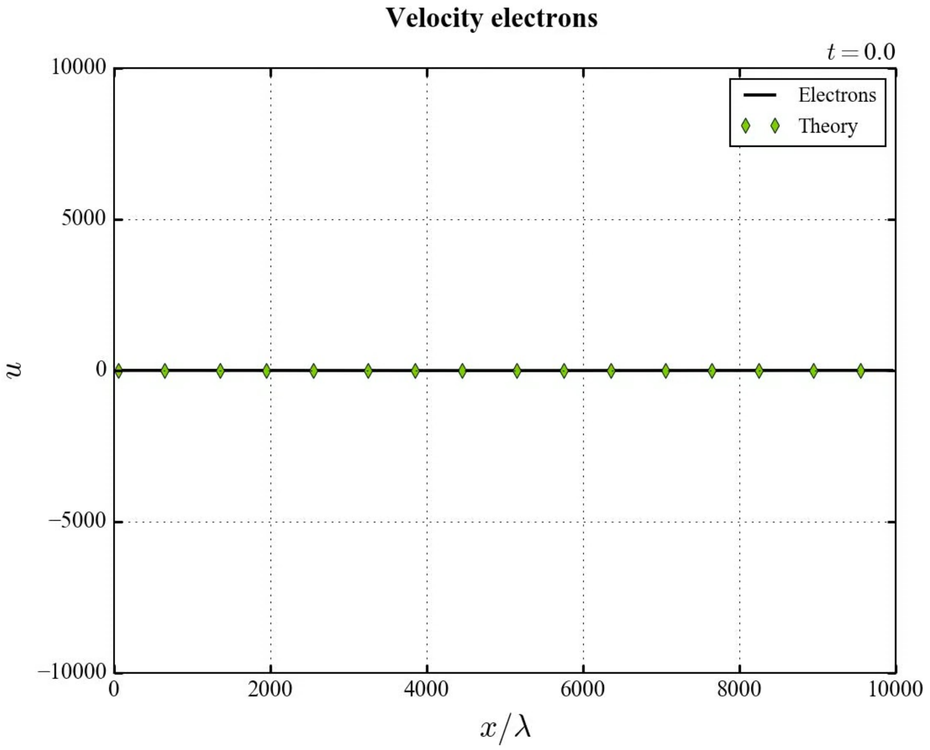

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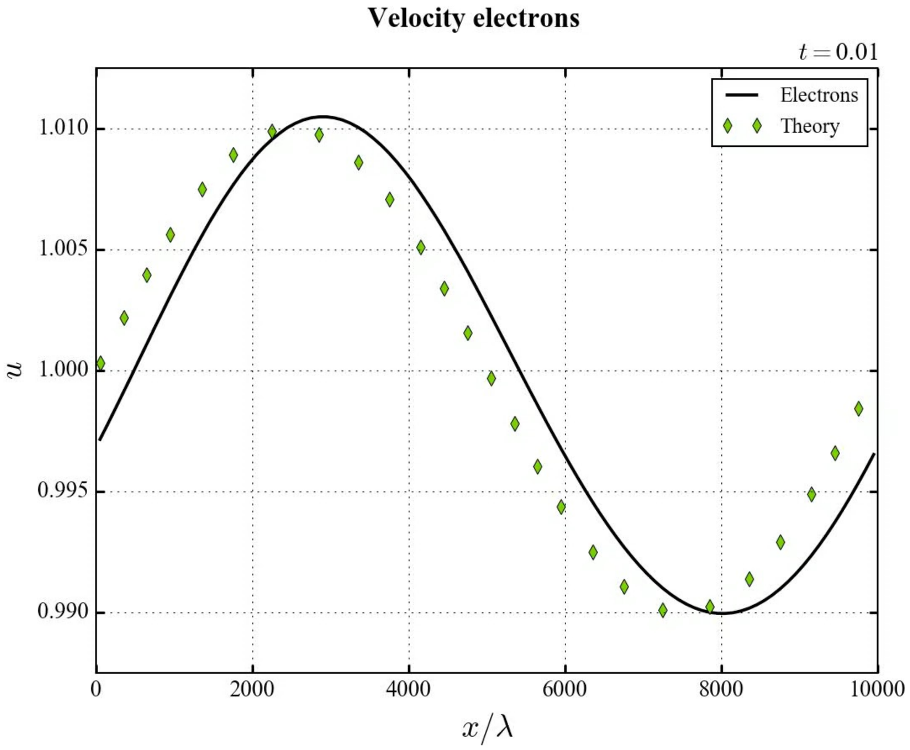


Alvarez Laguna et al., JCP (2020)

"Collisionless" isothermal Euler/full Maxwell's equations

Electron density: $\partial_t n_e + \partial_x \cdot (n_e u_e) = 0$

Electron momentum: $\partial_t (n_e u_e) + \partial_x \cdot (n_e u_e^2 + n_e \varepsilon^1) = \varepsilon^1 (n_e \partial_x \phi - \beta^2 u_e \times B)$

Ion density: $\partial_t n_i + \partial_x \cdot (n_i u_i) = 0$

Ion momentum: $\partial_t (n_i u_i) + \partial_x \cdot \left(n_i u_i^2 + n_i \kappa\right) = (-n_i \partial_x \phi + \beta^2 u_i \times B)$

Maxwell's equations:

$$\beta^2 \partial_t B + \partial_x \times E = 0$$

$$\mu\, (\alpha^2 \partial_t E - \beta^2 \partial_x \times B) = \alpha^2\, (n_e u_e - n_i u_i)$$

$$\partial_x \cdot\ B = 0$$

$$\mu\, \partial_{xx} \phi = (n_e - n_i)$$

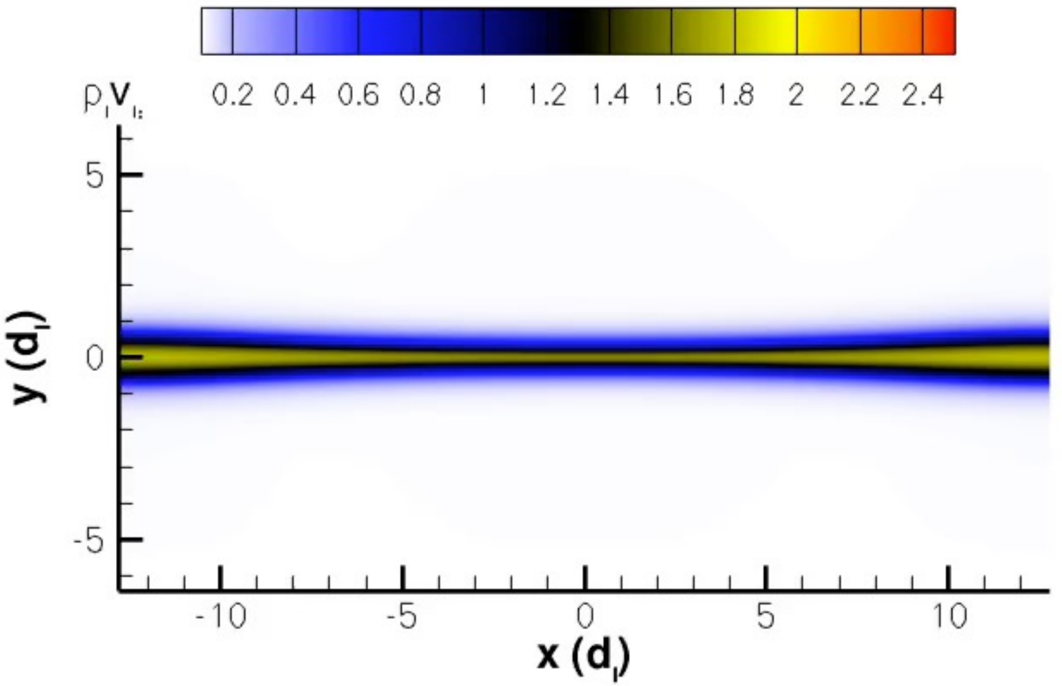
non-dimensional numbers

Mass ratio:	$\varepsilon = \frac{m_e}{m_i}$
Temperature ratio	$\kappa = \frac{T_i}{T_e}$
Debye length	$\mu = \left(\frac{\lambda_D}{L_0}\right)^2$
Magnetization	$\beta^2 = \frac{u_0 B_0}{E_0}$
Relativistic regime	$\alpha^2 = \frac{u_0}{c}$

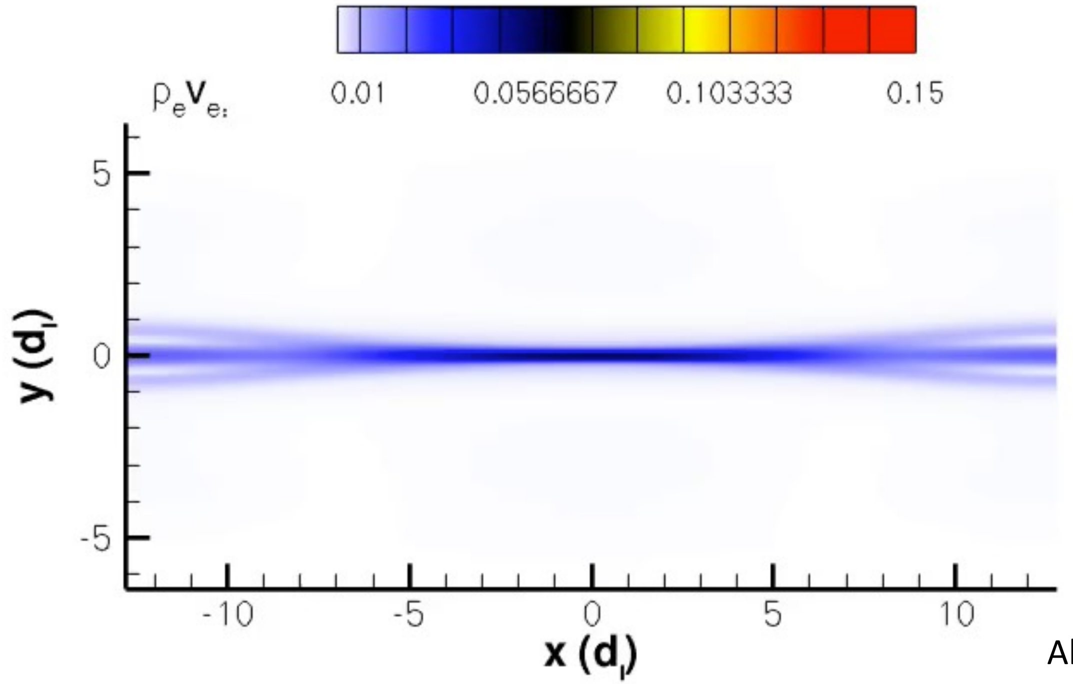
More info: Alvarez Laguna et al., CPC (2018)

Example: Magnetized plasma

Ion Momentum



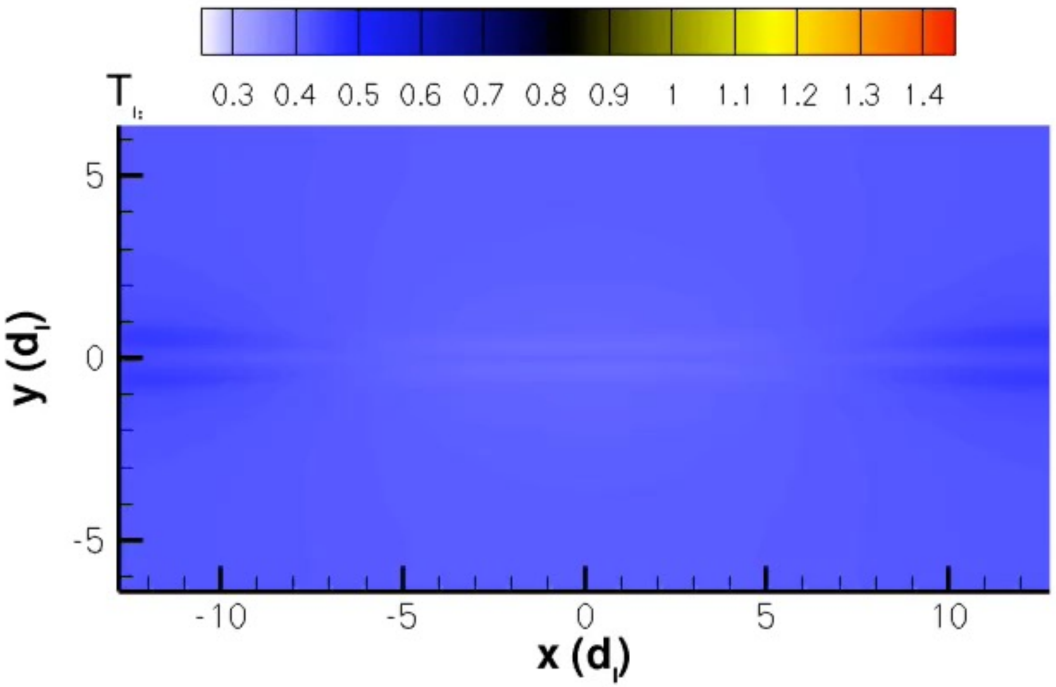
Electron Momentum



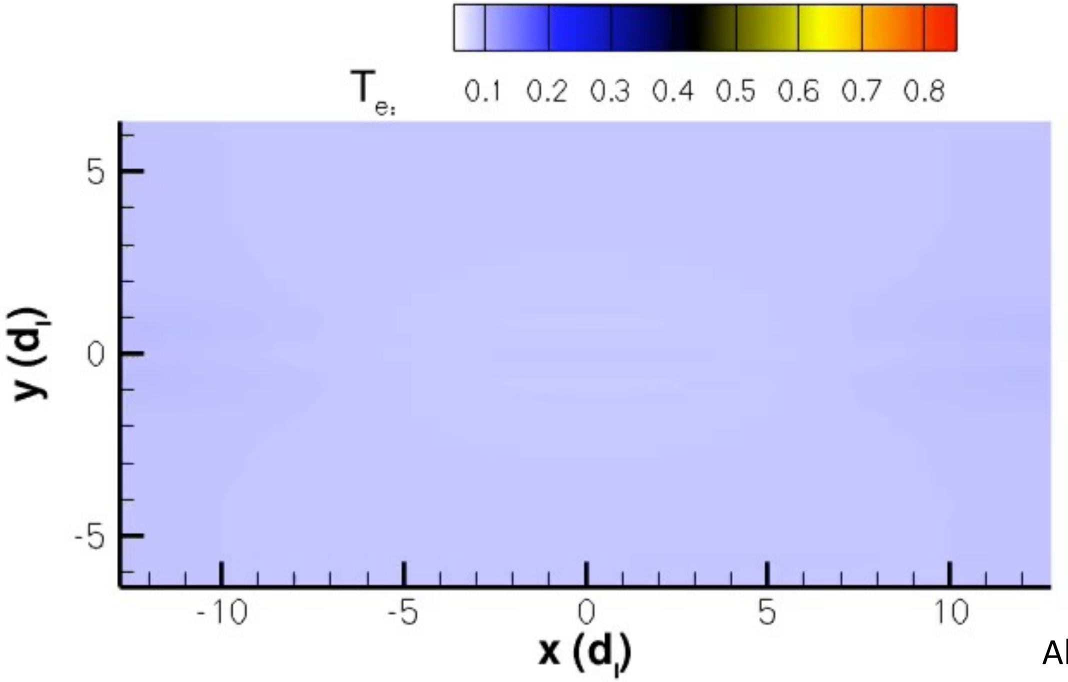
Alvarez Laguna et al., CPC (2018)

Example: Magnetized plasma

Ion Temperature



Electron Temperature



Alvarez Laguna et al., CPC (2018)

Summary and conclusions to this section:

- The moment plasma equations have the disadvantage to **have very restricting constraints** and numerical stability issues

- **Stiffness** related to the fast dynamics of the electron equations and the electrostatic and electromagnetic modes:

    - Plasma wave (related to quasi-neutrality)
    - Speed of light (in electro-magnetic solvers)

- We propose an **asymptotic-preserving scheme based on the Lagrange-projection** operator splitting and a **fully-implicit well-balanced discretization.**

Grad’s closure for electrons in partially-ionized plasmas

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Grad's method: Derivation of the equations

We propose a Grad's closure with the following number of moments

Moment weights:

$$\psi = \left(m_e,\ m_e \boldsymbol{v},\ \frac{m_e}{2}c_e^2,\ \frac{m_e}{2}c_e^2\boldsymbol{c}_e,\ \frac{m_e}{2}c_e^4\right)^T$$ Total = (9 eqs.)

- m_e → Mass (1 eq.)
- $m_e \boldsymbol{v}$ → Momentum (3 eq.)
- $\frac{m_e}{2}c_e^2$ → Energy (1 eq.)
- $\frac{m_e}{2}c_e^2\boldsymbol{c}_e$ → Heat Flux (3 eq.)
- $\frac{m_e}{2}c_e^4$ → Contracted fourth-moment (1 eq.)

Fluid variables

$$n_e = \int_\infty f_e d\boldsymbol{v}, \quad \rho_e u_{e_i} = \int_\infty m_e v_i f_e d\boldsymbol{v}, \quad p_e = \frac{1}{3}\int_\infty m_e c_e^2 f_e d\boldsymbol{v},$$

$$q_{e_i} = \frac{1}{2}\int_\infty m_e c_e^2 c_{e_i} f_e d\boldsymbol{v}, \quad \text{and} \quad p_{e_{iijj}} = \frac{1}{2}\int_\infty m_e c_e^4 f_e d\boldsymbol{v}.$$

Deviation of fourth mom from Maxwellian (excess kurtosis)

$$\Delta_e = \frac{p_{e_{iijj}} - p_{e_{iijj}}^{(M)}}{p_{e_{iijj}}^{(M)}} = \frac{2}{15}\frac{\rho_e}{p_e^2}\int_\infty m_e c_e^4 \left(f_e - f_e^{(M)}\right) d\boldsymbol{v}$$

Distribution function: **(Grad's (1949))**

$$f^{(9M)}(c_i) = \underbrace{n_\alpha \left(\frac{m_\alpha}{2\pi e T_\alpha}\right)^{3/2} \exp\left(-\frac{m_\alpha C^2}{2eT_\alpha}\right)}_{\text{Maxwellian}} \underbrace{\left(1 + a + A_i c_{e_i} + B c_e^2 + D_i c_e^2 c_{e_i} + E c_e^4\right)}_{\text{Polynomial Expansion}}$$

→ Coefficients? a, A_i, B, D_i, E

Analysis of non-equilibrium distribution function

Grad's expansion: Maxwellian distribution $f_e^{(0)}$ + perturbation

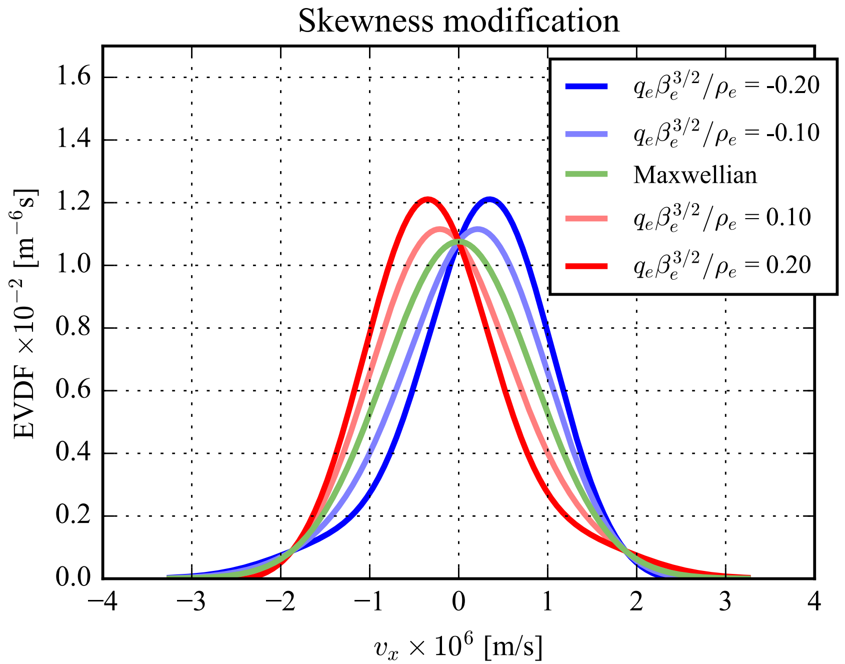
$$f_e(\vec{x},\vec{v},t) = f_e^{(0)}\left\{\left(1+\frac{15}{8}\Delta\right) - \frac{4\beta^2}{\rho}q_iC_i - \frac{5\beta}{2}\Delta C^2 + \frac{8\beta^2}{5\rho}q_i\beta C^2 C_i + \frac{\beta^2}{2}\Delta C^4\right\}$$

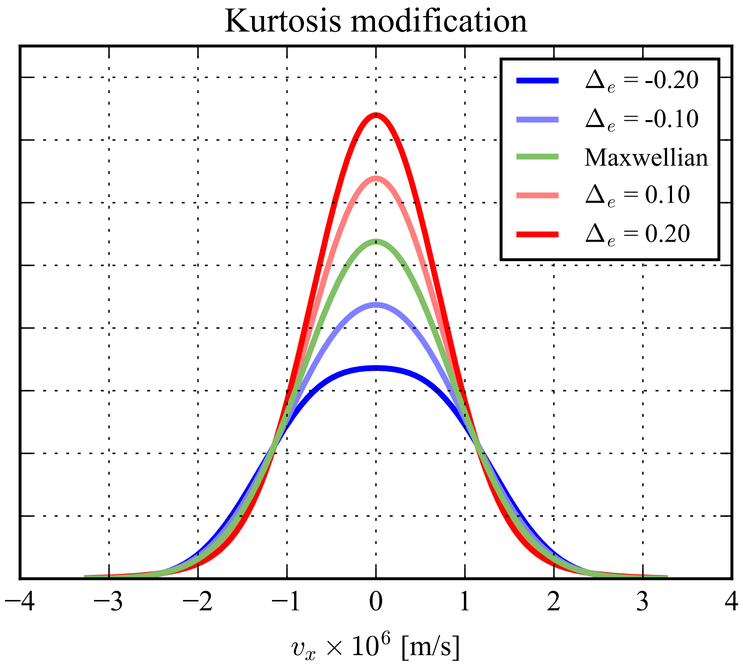
The VDF depends on 5 fluid quantities

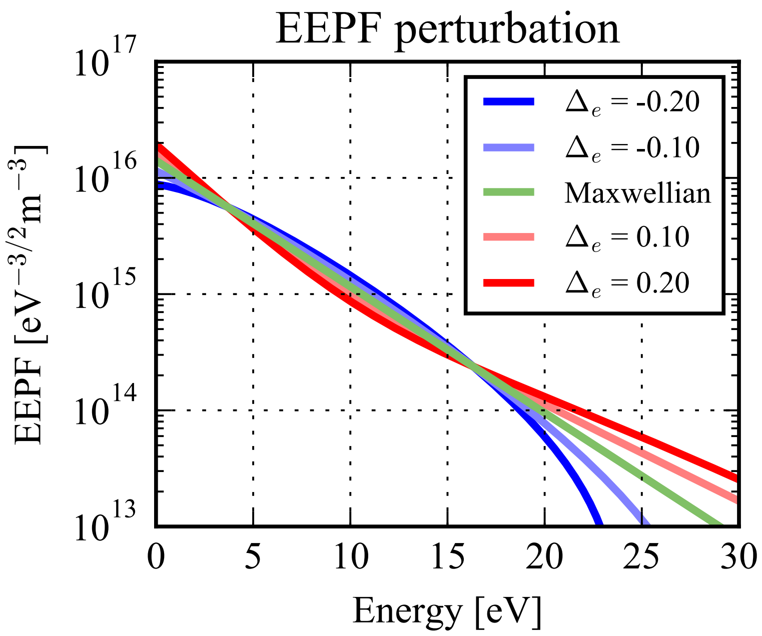
Density	n_e	**Temperature**	T_e
Velocity	$\vec{u}_e$	**Heat Flux**	$\vec{q}_e$

4th-moment

$$\Delta = \frac{1}{15\rho_e}\left(\frac{m_e}{eT_e}\right)^2 \int_\infty m_e C^4 \left(f_e - f_e^{(0)}\right) d^3C$$

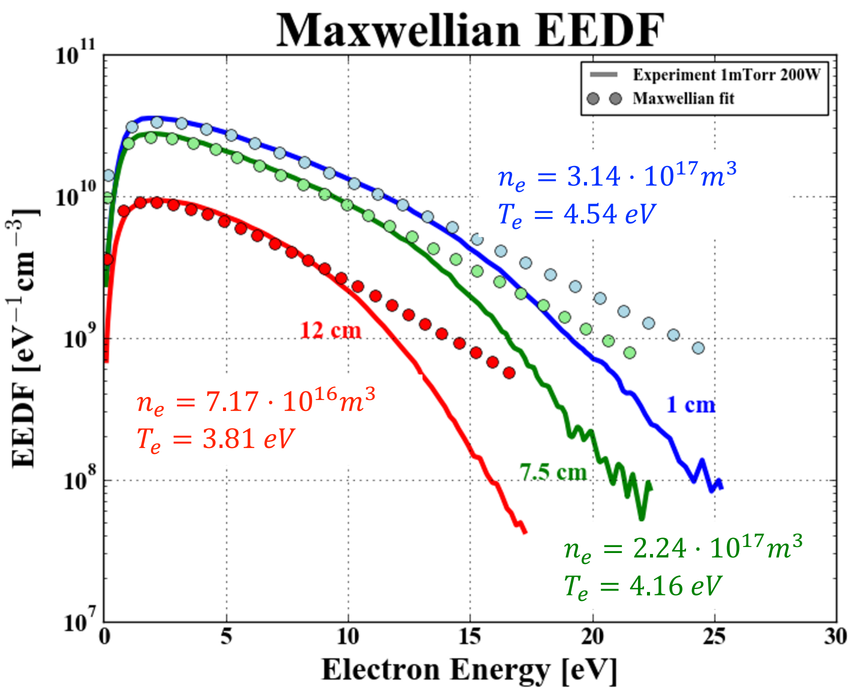


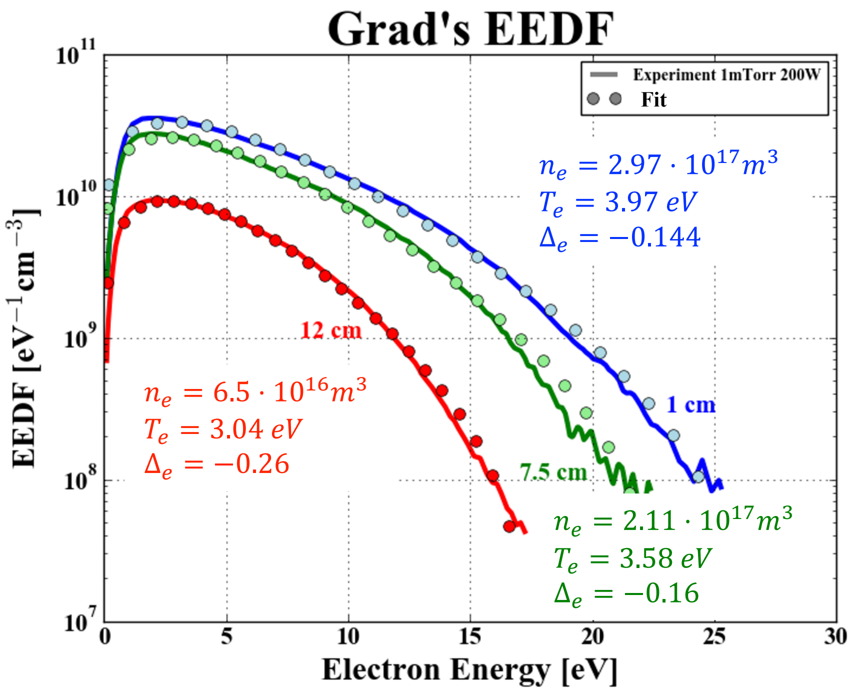




Comparison with experiments: Different positions

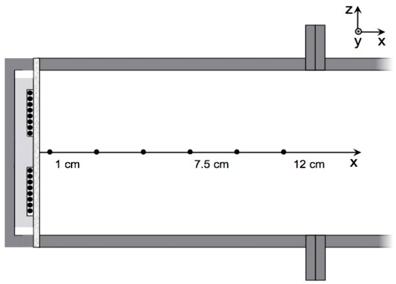
We compare the Grad's EEDF to the experiments:





- Maxwellian EEDF overestimates the temperature and the density
- The EEDF with the 4th moment is able to fit the experimental measurements
- The deviation from Maxwellian of the fourth moment is small, i.e., $|\Delta_e| < 1$

Inductive Argon discharge
- p = 1mTorr
- P = 200 W



*Aanesland, Ane & Bredin, Jérôme & Chabert, Pascal. (2014). Plasma Sources Science and Technology. 23. 044003.

Derivation of collisional source terms: Elastic Collisions

Boltzmann operator $\left.\frac{\delta f_{\mathfrak{e}}}{\delta t}\right|_{\mathfrak{eg}} = \int\int \left(f'_{\mathfrak{e}} f'_{\mathfrak{g}} - f_{\mathfrak{e}} f_{\mathfrak{g}}\right) g\sigma d\Omega d\boldsymbol{v}_{\mathfrak{g}}$

Momentum exchange:

$$\boldsymbol{R}_{\mathfrak{eg}}^{(el)} = \underbrace{-m_{\mathfrak{e}} n_{\mathfrak{e}} \nu_{\mathfrak{eg}}^{(fr,1)} \boldsymbol{u}_{\mathfrak{e}}}_{\text{Frictional force}} \underbrace{- n_e \nu_{\mathfrak{eg}}^{(skew,1)} \frac{\boldsymbol{q}_{\mathfrak{e}}}{p_{\mathfrak{e}}}}_{\text{Soret effect}}$$

Energy exchange:

$$Q_{\mathfrak{eg}}^{(el)} = \underbrace{\frac{m_{\mathfrak{e}}}{m_{\mathfrak{g}}} n_{\mathfrak{e}} \nu_{\mathfrak{eg}}^{(fr,2)} e\left(T_{\mathfrak{g}} - T_{\mathfrak{e}}\right)}_{\text{Temp. relaxation}} + \underbrace{\frac{m_{\mathfrak{e}}}{m_{\mathfrak{g}}} n_{\mathfrak{e}} \nu_{\mathfrak{eg}}^{(kurt,2)} \Delta_{\mathfrak{e}} e T_{\mathfrak{g}}}_{\text{Kurtosis correction}} \underbrace{- n_{\mathfrak{e}} \nu_{\mathfrak{eg}}^{(skew,2)} \frac{\boldsymbol{q}_{\mathfrak{e}}}{p_{\mathfrak{e}}} \cdot \boldsymbol{u}_{\mathfrak{e}}}_{\text{Effect of skewness}}$$

Heat-Flux exchange:

$$\boldsymbol{R}_{\mathfrak{eg}}^{hF,(el)} = \underbrace{-n_{\mathfrak{e}} \nu_{\mathfrak{eg}}^{(fr,3)} e T_{\mathfrak{e}} \boldsymbol{u}_{\mathfrak{e}}}_{\text{Dufour effect}} \underbrace{- \nu_{\mathfrak{eg}}^{(skew,3)} \boldsymbol{q}_{\mathfrak{e}}}_{\text{Skewness relaxation}}$$

Fourth-moment exchange:

$$Q_{\mathfrak{eg}}^{(el,4)} = \underbrace{n_{\mathfrak{g}} \frac{m_{\mathfrak{e}}}{m_{\mathfrak{g}}} \nu_{\mathfrak{eg}}^{(fr,4)} \frac{p_{\mathfrak{e}}^2}{\rho_{\mathfrak{e}}} \left(\frac{T_{\mathfrak{g}}}{T_{\mathfrak{e}}} - 1\right)}_{\text{Kurtosis relaxation}} + \underbrace{n_{\mathfrak{g}} \frac{m_{\mathfrak{e}}}{m_{\mathfrak{g}}} \nu_{\mathfrak{eg}}^{(kurt,4)} \frac{p_{\mathfrak{e}}^2}{\rho_{\mathfrak{e}}} \frac{T_{\mathfrak{g}}}{T_{\mathfrak{e}}}}_{\text{Additional correction}} + \underbrace{4\nu_{\mathfrak{eg}}^{(skew,3)} \boldsymbol{q}_{\mathfrak{e}} \cdot \boldsymbol{u}_{\mathfrak{e}}}_{\text{Effect of skewness}}$$

BGK operator $\left.\frac{\delta f_{\mathfrak{e}}}{\delta t}\right|_{\mathfrak{eg}} = -\nu_m f_{\mathfrak{e}}$

Momentum exchange:

$$\boldsymbol{R}_{\mathfrak{eg}}^{(el)} = -m_{\mathfrak{e}} n_{\mathfrak{e}} \nu_m \boldsymbol{u}_{\mathfrak{e}}$$

Energy exchange:

$$Q_{\mathfrak{eg}}^{(el)} = -3\frac{m_{\mathfrak{e}}}{m_{\mathfrak{g}}} n_{\mathfrak{e}} \nu_m e T_{\mathfrak{e}}$$

Heat-Flux exchange:

$$\boldsymbol{R}_{\mathfrak{eg}}^{hF,(el)} = -\nu_m \boldsymbol{q}_{\mathfrak{e}}$$

Fourth-moment exchange:

$$Q_{\mathfrak{eg}}^{(el,4)} = -\frac{m_{\mathfrak{e}}}{m_{\mathfrak{g}}} \nu_m \frac{p_{\mathfrak{e}}^2}{\rho_{\mathfrak{e}}} \Delta_{\mathfrak{e}}$$

Derivation of collisional source terms: Electron-electron & Ionization

Mass exchange:

$$\dot{n}_{\mathfrak{e}}^{(iz)} = n_{\mathfrak{e}} n_{\mathfrak{g}} K_{iz}^{(0)}$$

Momentum exchange:

Conserved in electron-electron and neglected in inelastic

Energy exchange:

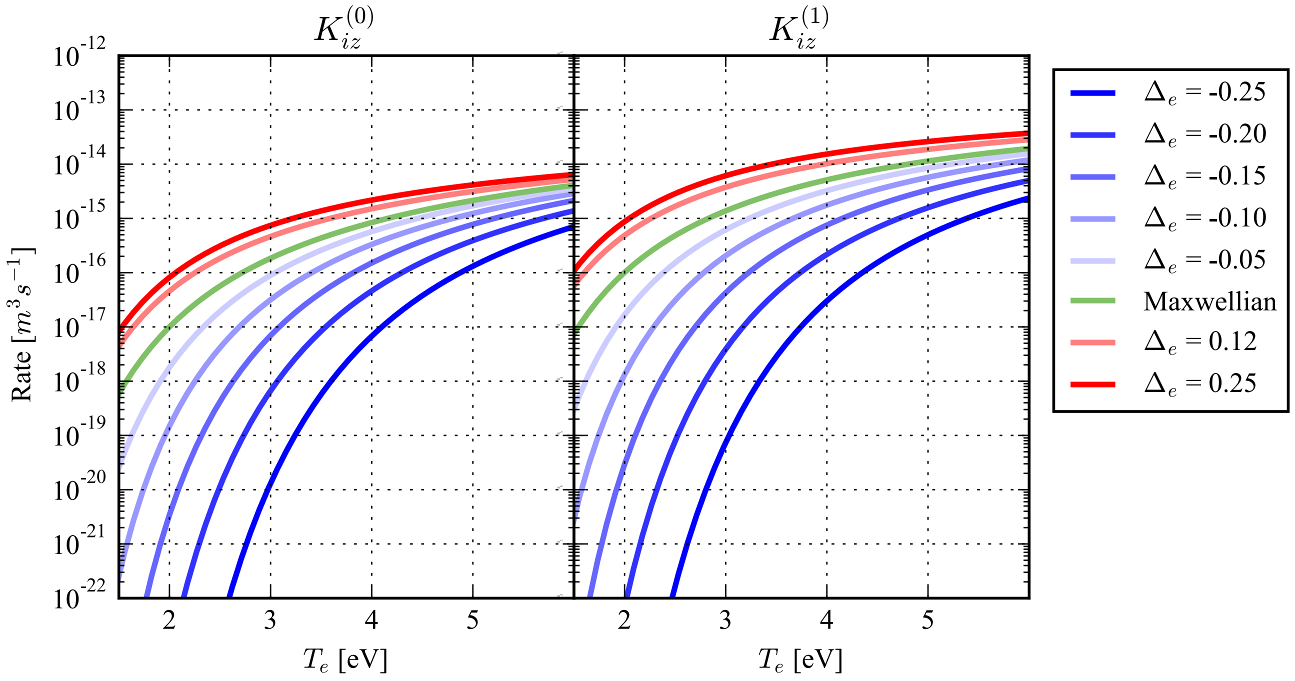
$$Q_{\mathfrak{eg}}^{(inel)} = -\sum_{k=0}^{excit,iz} n_{\mathfrak{e}} n_{\mathfrak{g}} K_{inel,k}^{(0)} n_{\mathfrak{g}} \phi_k^*$$

Heat-Flux exchange:

$$\boldsymbol{R}_{\mathfrak{ee}}^{hF} = -n_{\mathfrak{e}} \nu_{\mathfrak{ee}}^{(skew)} \boldsymbol{q}_{\mathfrak{e}}.$$

Fourth-moment exchange:

$$Q_{\mathfrak{ee}}^{(4)} = -n_{\mathfrak{e}} \nu_{\mathfrak{ee}}^{(kurt)} \frac{p_{\mathfrak{e}}^2}{\rho_{\mathfrak{e}}} \Delta_{\mathfrak{e}} \qquad Q_{\mathfrak{eg}}^{(inel,4)} = -2 \sum_{k=0}^{excit,iz} \left(\frac{p_{\mathfrak{e}}^2}{\rho_{\mathfrak{e}}}\right) K_{inel,k}^{(1)} \left(\frac{\phi_k^*}{T_e}\right)$$



Ionization and inelastic rate largely depend on the kurtosis!

Set of equations with the fourth moment (1D)

Electrons (9 eqs in 3D):

Density
$$\frac{\partial n_e}{\partial t} + \frac{\partial}{\partial x_i} n_e u_{e_i} = \dot{n}_e,$$

Momentum
$$m_e \frac{\partial}{\partial t} n_e u_{e_i} + \frac{\partial}{\partial x_j}\left(m_e n_e u_{e_i} u_{e_j} + p_e \delta_{ij}\right) = -e n_e E_i + R_i,$$

Energy
$$\frac{3}{2}\frac{\partial p_e}{\partial t} + \frac{\partial}{\partial x_k}\left(q_{e_k} + \frac{3}{2} p_e u_{e_k}\right) + p_e \frac{\partial u_{e_k}}{\partial x_k} = Q,$$

Heat flux
$$\frac{\partial q_{e_i}}{\partial t} + \frac{\partial}{\partial x_j}\left(r_{e_{ij}} + q_{e_i} u_{e_j}\right) + r_{e_{ijk}} \frac{\partial u_{e_k}}{\partial x_j} + q_{e_j} \frac{\partial u_{e_i}}{\partial x_j} - \frac{5}{2}\frac{p_e}{\rho_e}\frac{\partial p_e}{\partial x_j}\delta_{ij} = R_i^{hf} - \frac{5}{2}\frac{p_e}{\rho_e}\left(R_i - m_e \dot{n}_e u_{e_i}\right),$$

4th-moment
$$\frac{\partial}{\partial t} p_{e_{iijj}} + \frac{\partial}{\partial x_k}\left(r_{e_{iijjk}} + p_{e_{iijj}} u_{e_k}\right) + 4 r_{e_{ij}} \frac{\partial u_{e_i}}{\partial x_j} - 4\frac{q_{e_i}}{\rho_e}\frac{\partial p_e}{\partial x_j}\delta_{ij} = Q^{(4)} - 4\frac{q_{e_i}}{\rho_e}\left(R_i - m_e \dot{n}_e u_{e_i}\right).$$

Unsteady terms
Flux terms
Electric forces
Collisional terms

Main influence of the fourth moment in the equations:

1. All the collisional rates are modified, e.g., the ionization rate.
2. The heat conduction and diffusion will be modified
3. Non-linear effects due to equations coupling and collisional source terms

Numerical simulations of the moment equations

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Case 1: 0D relaxation in Argon plasma (comparison to kinetic solver)

We study a 0D plasma where the electrons are initially at 5 eV and Maxwellian distribution

- The elastic and inelastic collisions will cool down the electrons as well as change their EEDF.
- We consider the elastic and inelastic processes.
- We compare two models to PIC:
  - **Maxwellian distribution**

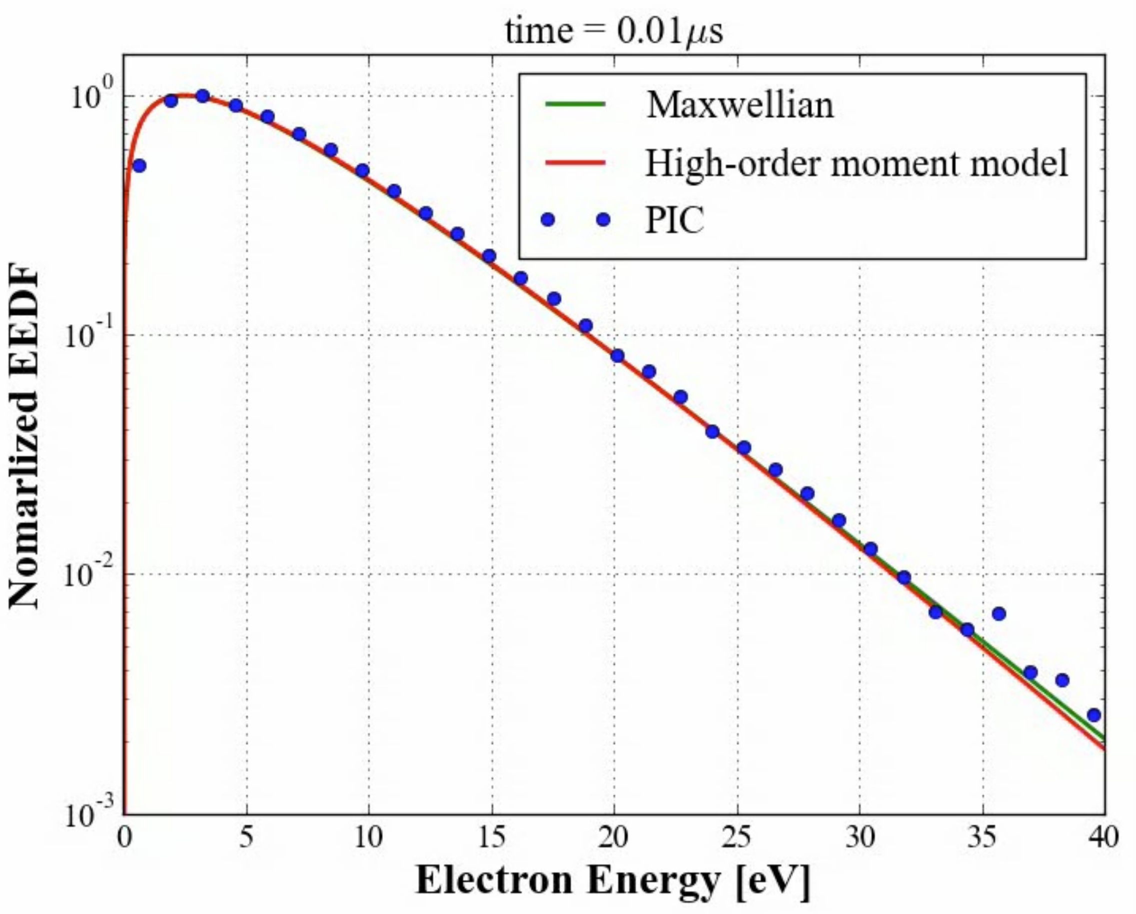
    $$\frac{dn_e}{dt} = \text{Ioniz.}$$

    $$\frac{dT_e}{dt} = \text{Inel. losses} + \text{El. losses}$$
  - **High-order moment**

    $$\frac{dn_e}{dt} = \text{Ioniz.}$$

    $$\frac{dT_e}{dt} = -(\text{Inel. losses} + \text{El. Losses})$$

    $$\frac{d\Delta_e}{dt} = -(\text{Inel. losses} + \text{El. Losses}) + (e - e\ colls.)$$



Case 2: Comparison with a Boltzmann solver with an electric field

We study a 0D plasma with an electric field:

- We compare models to Boltzmann solver:
  - **High-order moment**

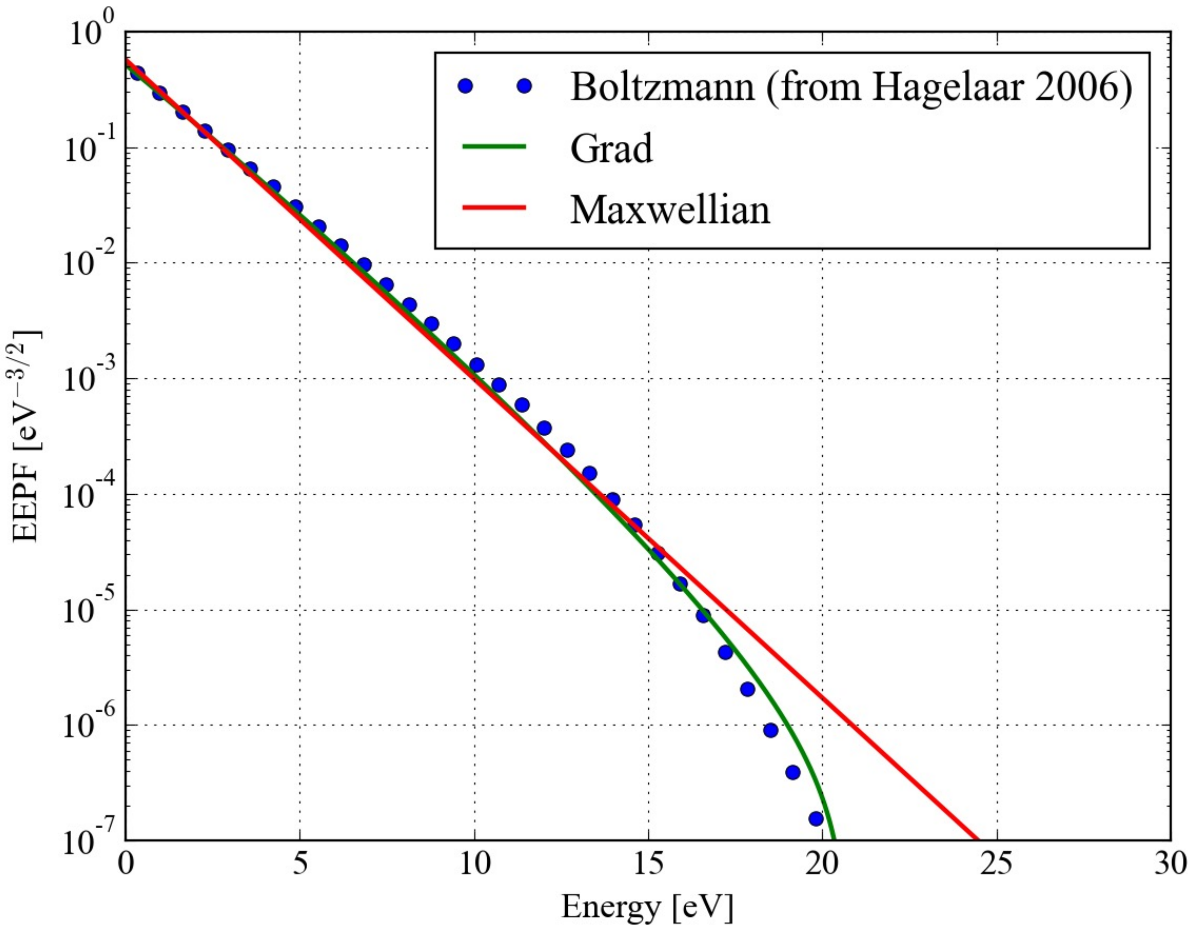
$$\frac{dn_e}{dt} = \text{Ioniz.}$$

$$\frac{du_e}{dt} = \textbf{Electric field} + \text{El. losses}$$

$$\frac{dT_e}{dt} = -(\text{Inel. losses} + \text{El. Losses}) + \textbf{Joule Heating}$$

$$\frac{dq_e}{dt} = \textbf{Electric field} + \text{El. losses} + (e - e\ colls.)$$

$$\frac{d\Delta_e}{dt} = -(\text{Inel. losses} + \text{El. Losses}) + (e - e\ colls.) + \text{"Heating"}$$



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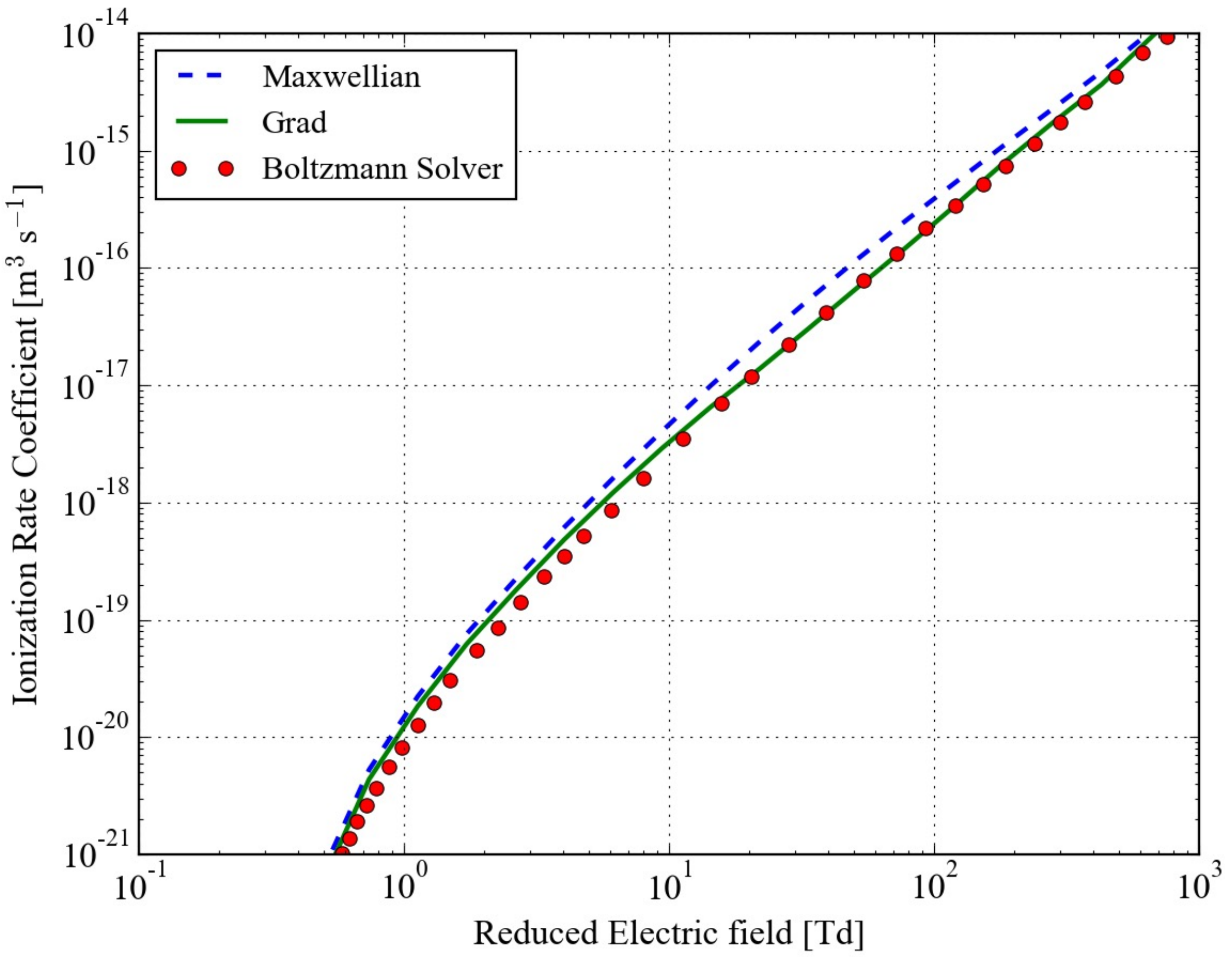

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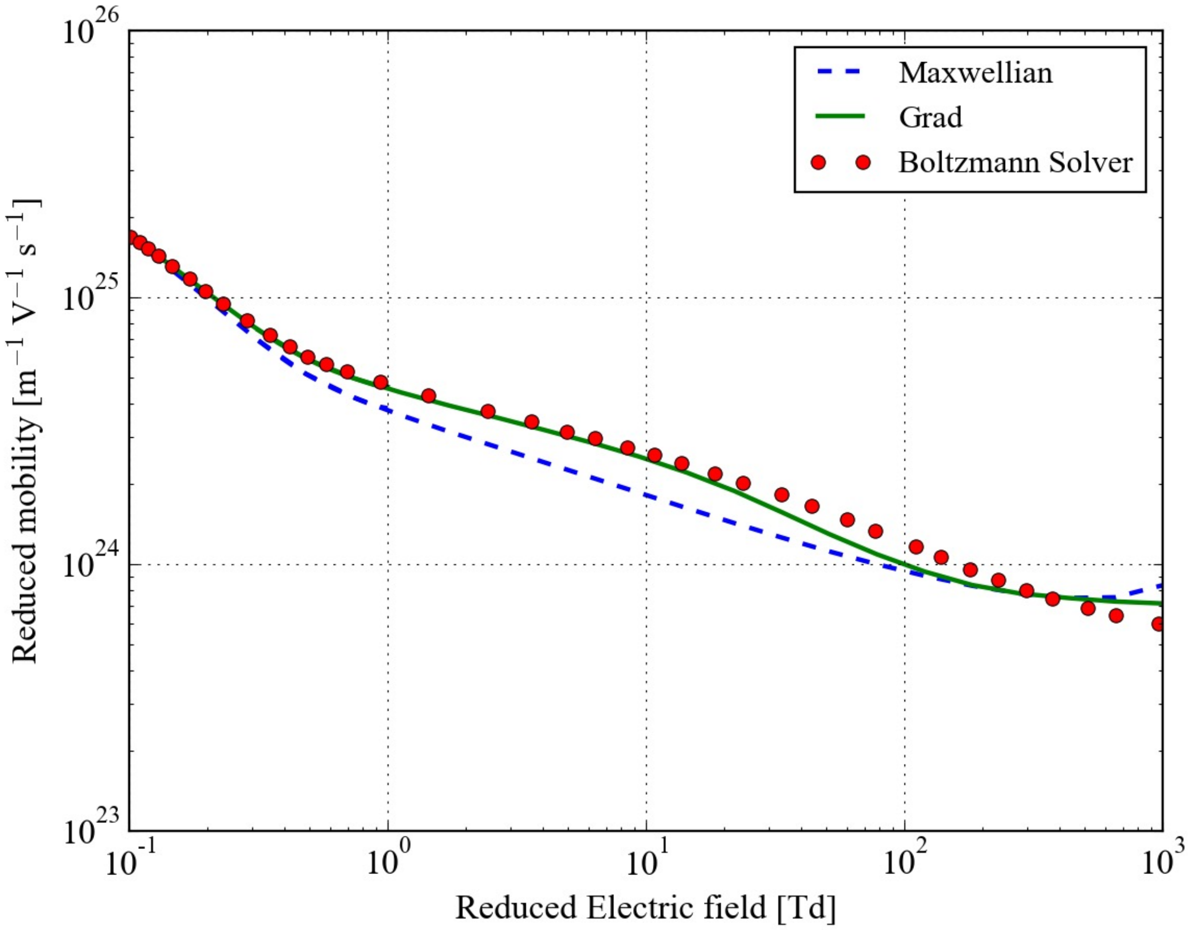
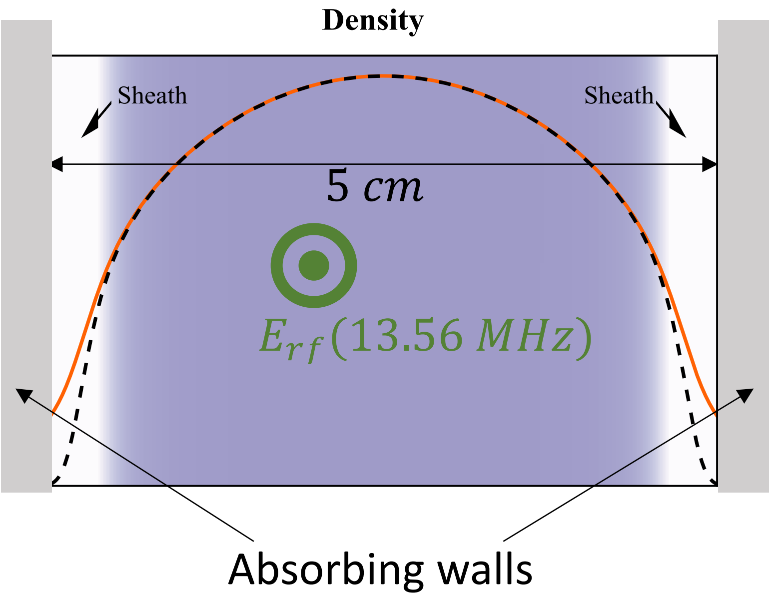
$$\frac{d\Delta_e}{dt} = -(\text{Inel. losses} + \text{El. Losses}) + (e - e\ colls.)$$



Case 3: 1D model of bounded-plasma at low-pressure



We study a 1D ICP Xenon discharge:

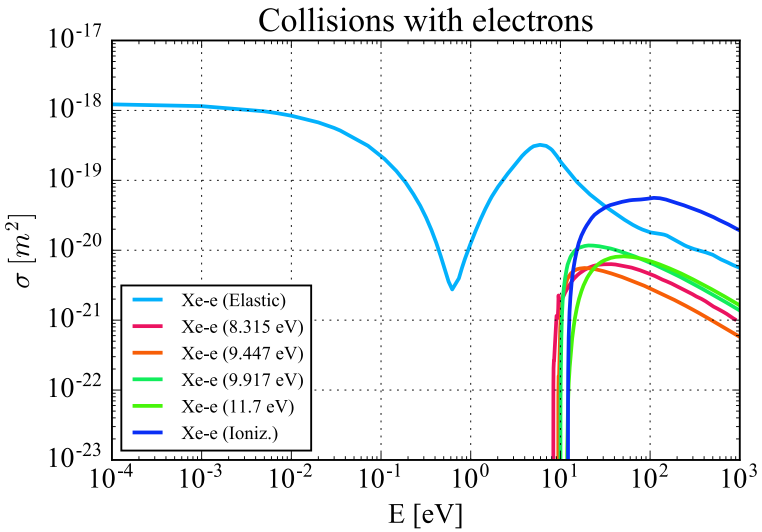
- $\mathbf{p_{gas}} \sim 3\ \boldsymbol{mTorr}$
- $\mathbf{n_e} \sim \mathbf{10^{15}}\boldsymbol{m^3}$
- **4 excitation collisions + single ionization + elastic + backscattering**

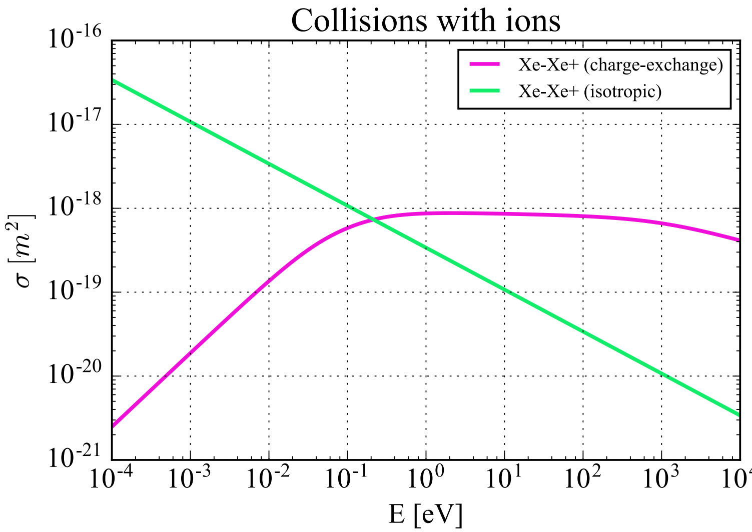
We consider a model solving for:

- **5 moments for electrons**
- **3 moments for ions**
- **Poisson equation**

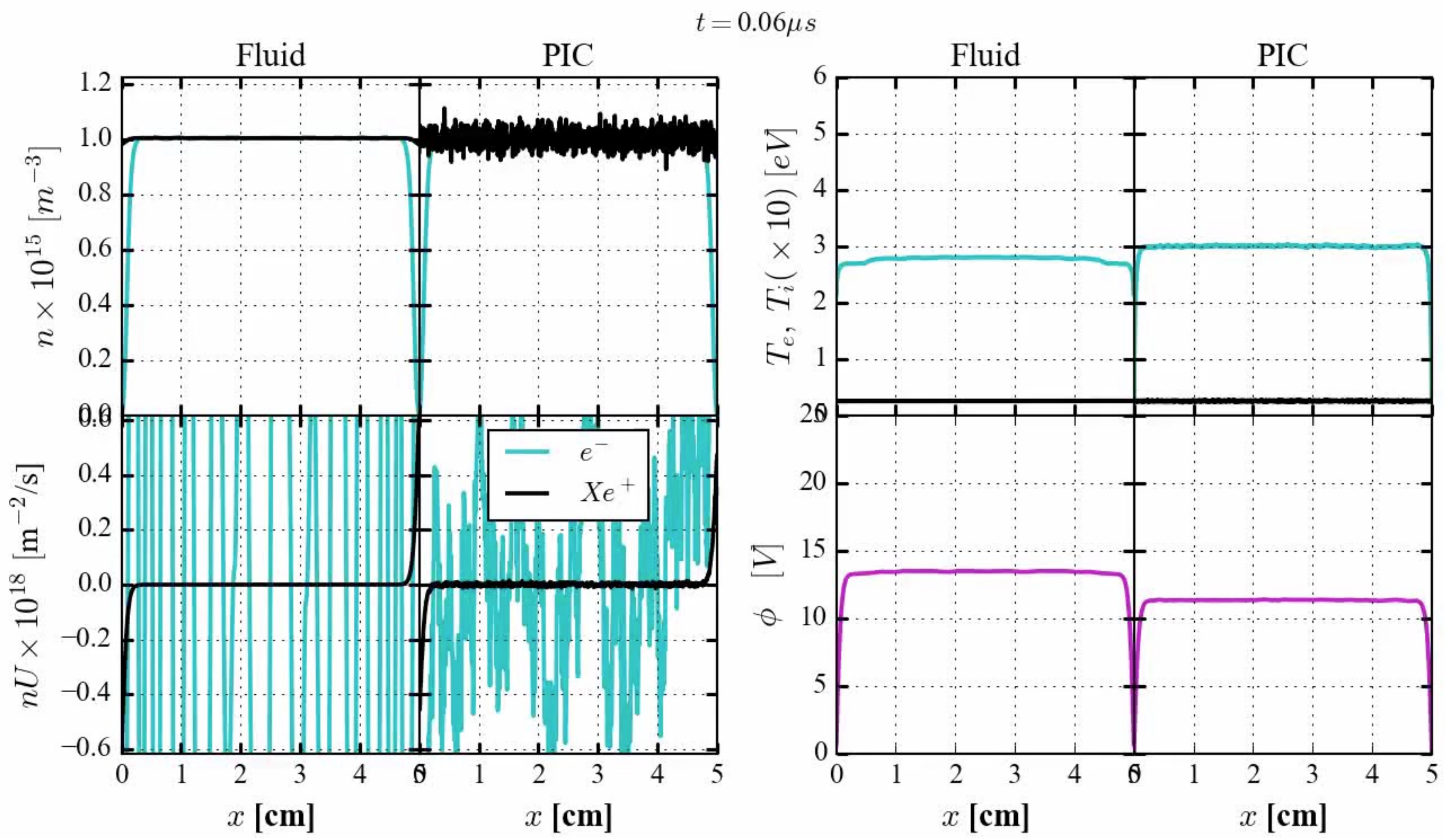
Reaction	Process	Thresh. [eV]
Electron impact Xe		
e + Xe → e + Xe	Elastic	0
e + Xe → e + Xe* (8.315 eV)	Excitation	8.315 eV
e + Xe → e + Xe* (9.447 eV)	Excitation	9.477 eV
e + Xe → e + Xe* (9.917 eV)	Excitation	9.917 eV
e + Xe → e + Xe* (11.7 eV)	Excitation	11.7 eV
e + Xe → Xe⁺ + 2e	Elec. impact ioniz.	12.13 eV
Scattering of ions		
Xe⁺ + Xe → Xe⁺ + Xe	Elastic	0
Xe⁺ + Xe → Xe + Xe⁺	Charge exch.	0

Table : Collisional processes





Comparison electrons (5eqs) + ions (3 eqs) and PIC



Model

Electrons:

- Mass
- Momentum (with inertia)
- Energy
- Heat Flux
- **4th-moment**

Ions:

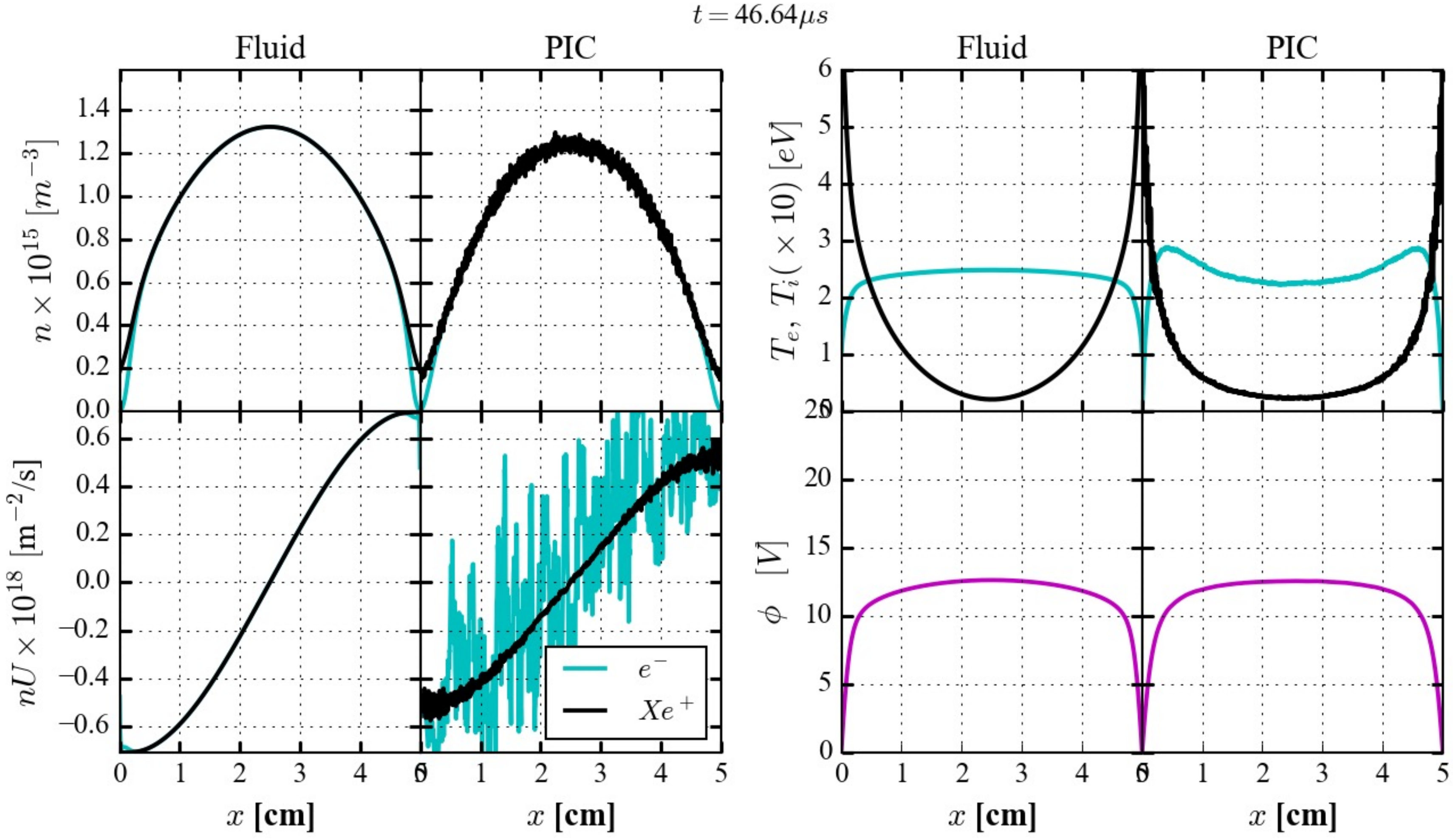
- Mass
- Momentum
- Energy

Collisions follow Benilov (1998)

Poisson Eq.

Comparison electrons (5eqs) + ions (3 eqs) and PIC

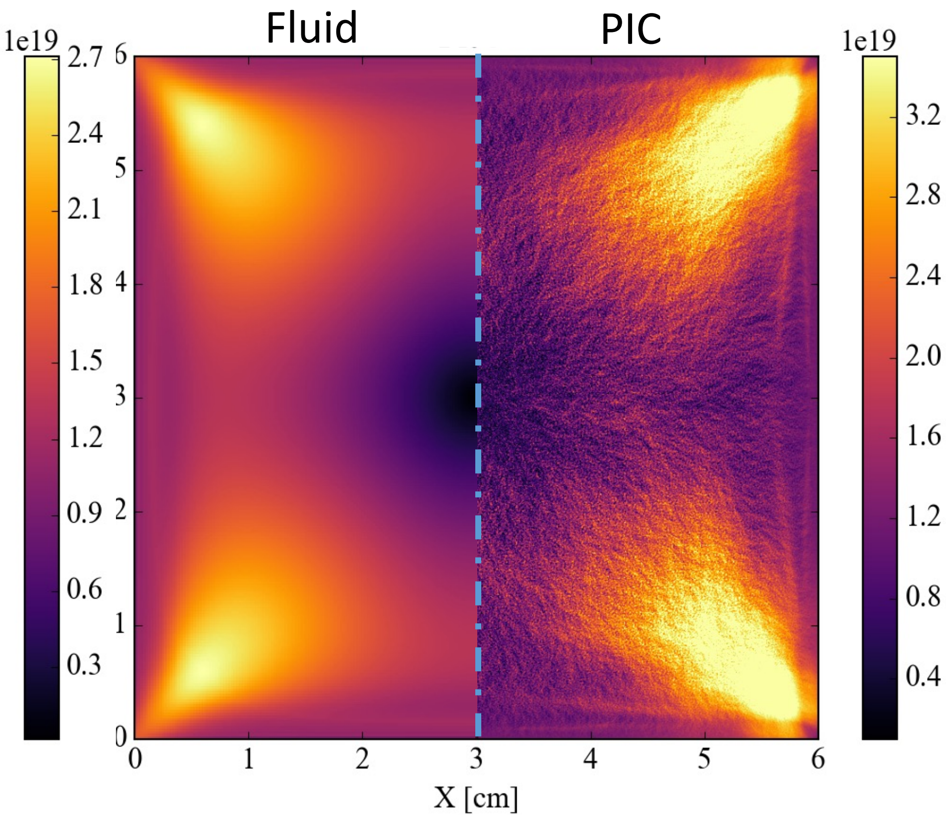
Converged solution



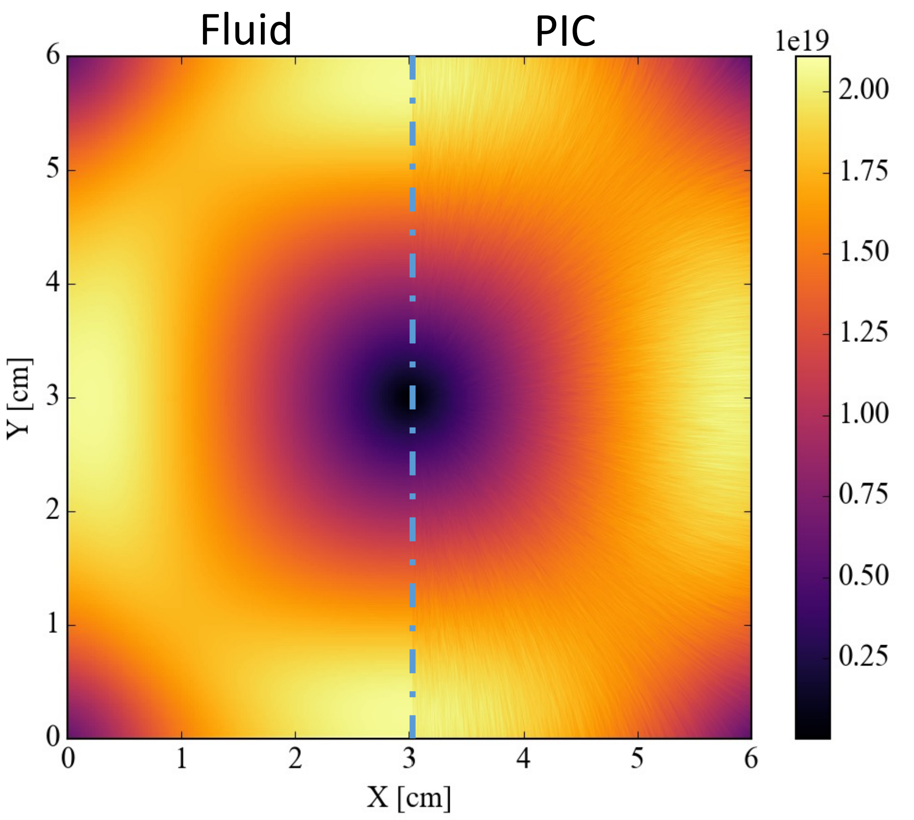
Comparison

- Density is closer
- Temperature drops at the seath
- Ion temperature is well captured
- Flux at the wall is overestimated
- The potential drop is identical

Case4: 2D bounded Helium plasma

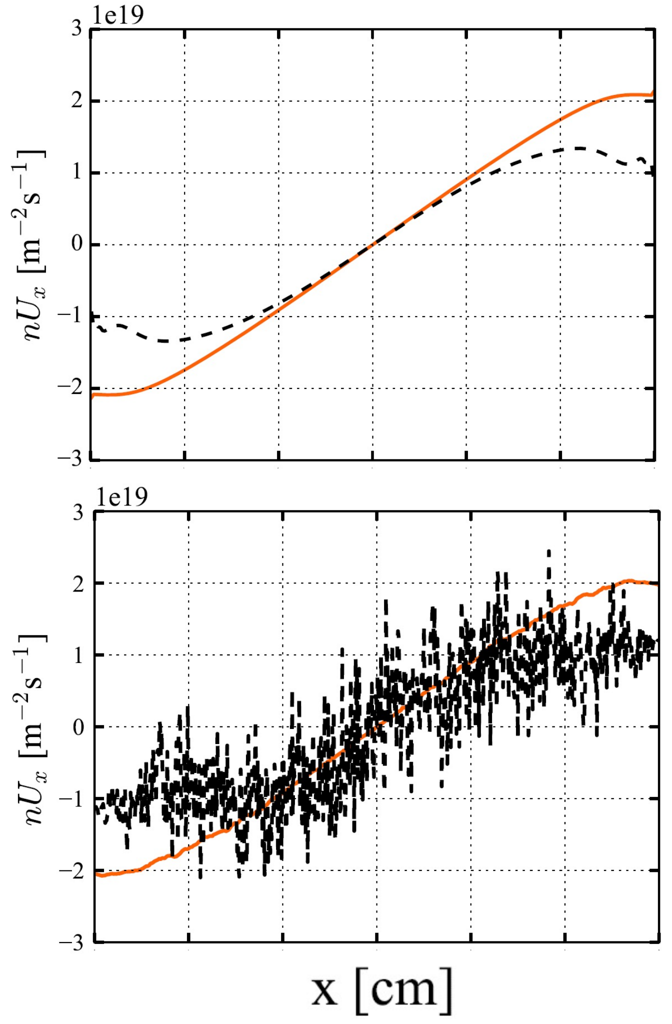


Electron flux $n_e u_e$



Electron flux $n_i u_i$

1D horizontal cut



Work of Louis Reboul's PhD thesis.

Conclusions and future perspectives

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Summary and conclusions

1. Plasmas are complex systems with a large range of scales due mainly to two reasons:

    1. Each species have different dynamics
    2. Coupling with the electromagnetic fields

2. The moment equations need new numerical schemes in order to couple to Maxwell's equations.

3. We propose a Grad's moment expansion for the electron moment equations low-temperature plasma applications. We consider:

    1. Elastic collisions with the gas (Boltzmann operator)
    2. Inelastic collisions with the gas (Lorentz model)
    3. Coulomb collisions (Boltzmann collision)

4. Comparison with kinetic solvers in 0D, 1D and 2D.

5. Paper with derivation of the model and comparison to experiments under review.

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- **VKI:** T. Magin, S. Bocelli, H. Deconinck
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