

# Moment (multi-fluid) models for low-pressure discharges



Laboratoire de Physique des Plasmas



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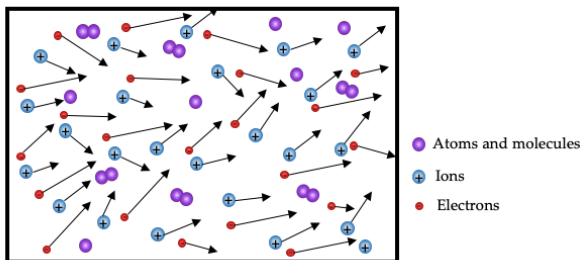
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Laboratoire de physique des plasmas

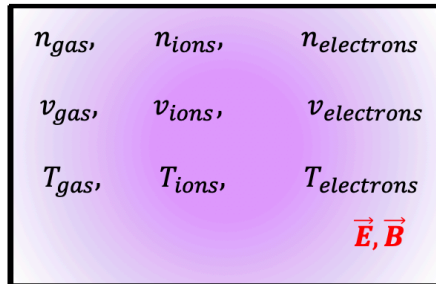
# Outline of the talk

## Part I: From microscopic to macroscopic

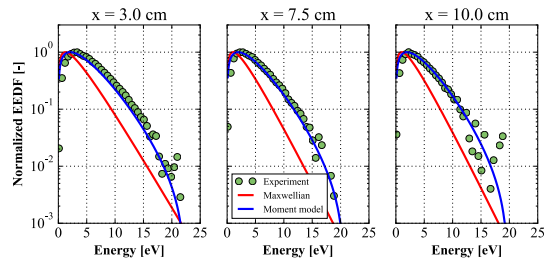
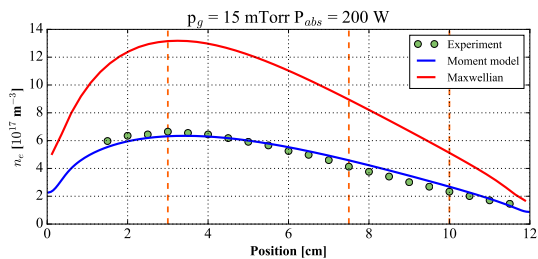
### Microscopic description



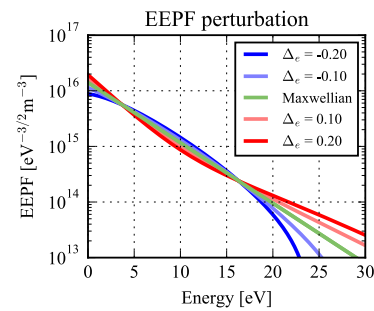
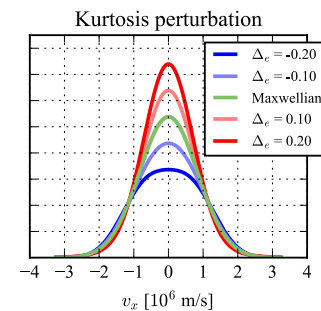
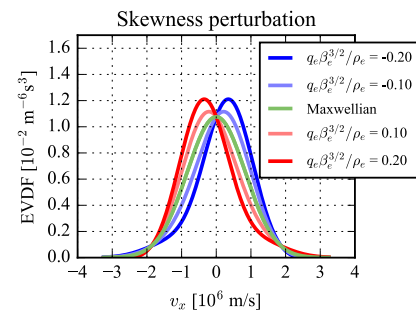
### Macroscopic description



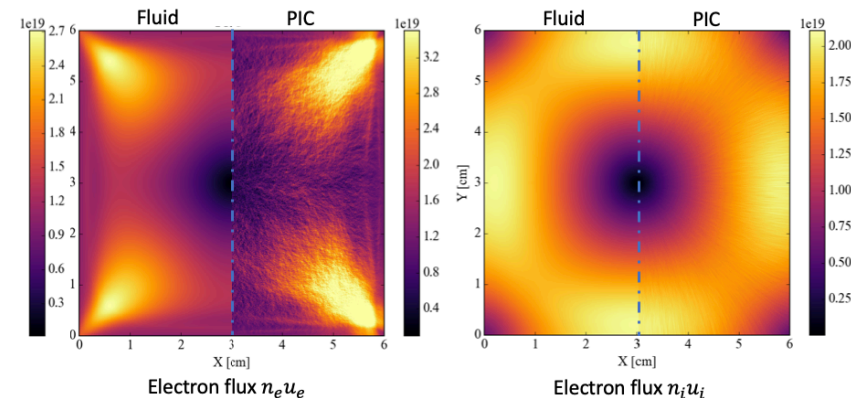
## Part III: Resolution of the moment equations and comparison to experiments



## Part II: How to close a high-order moment set of equations



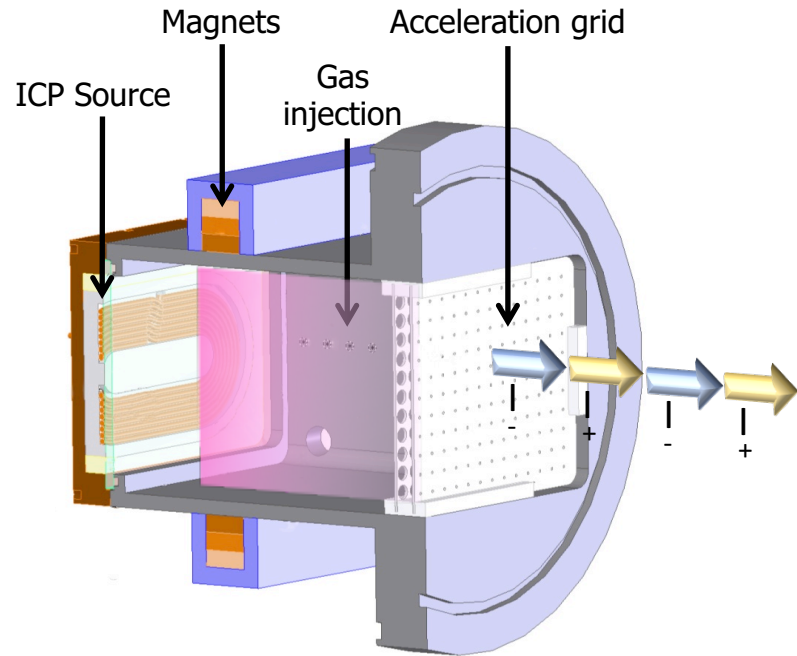
## Part IV: Non-ambipolar models, future developments and conclusions





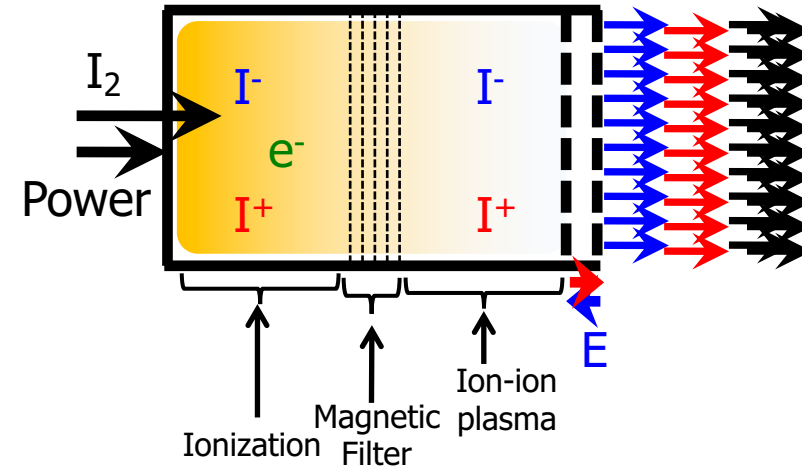
# Motivation: Plasma Propulsion with Electronegative gases

## PEGASE PROTOTYPE\*



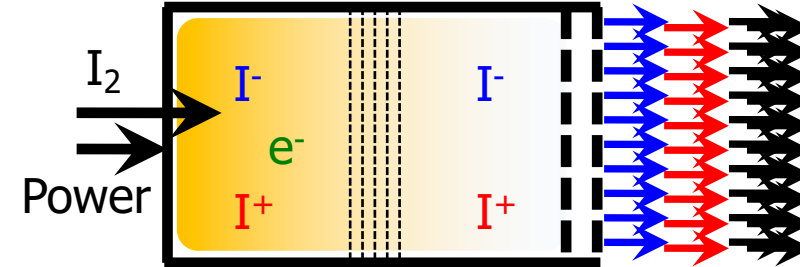
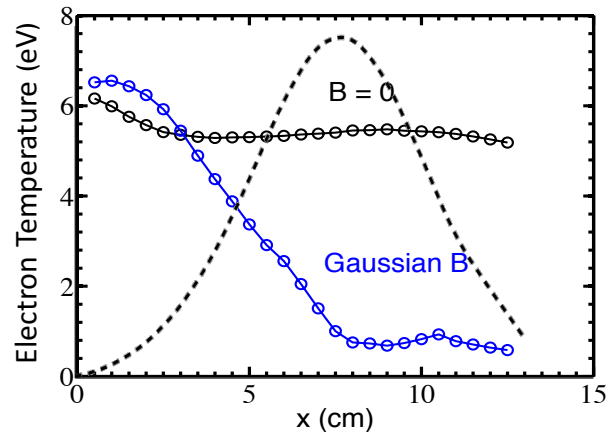
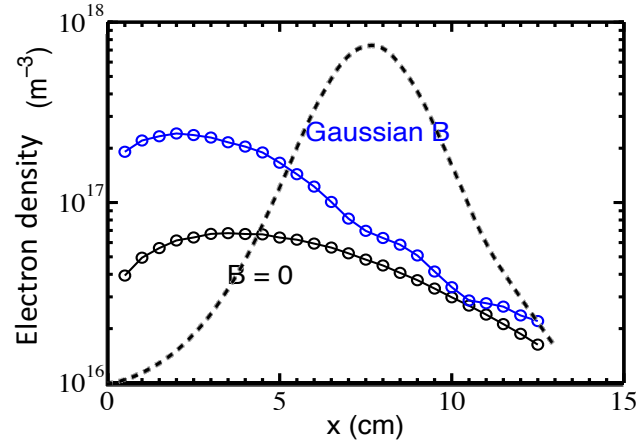
- Size = 8 cm x 12 cm x 12cm
- pressure = 1 – 100 mTorr
- Power = 200 W
- B-Field = 140-245 G

## OPERATING PRINCIPLE



# Motivation: Plasma Propulsion with Electronegative gases

## Density and temperature measurement\*



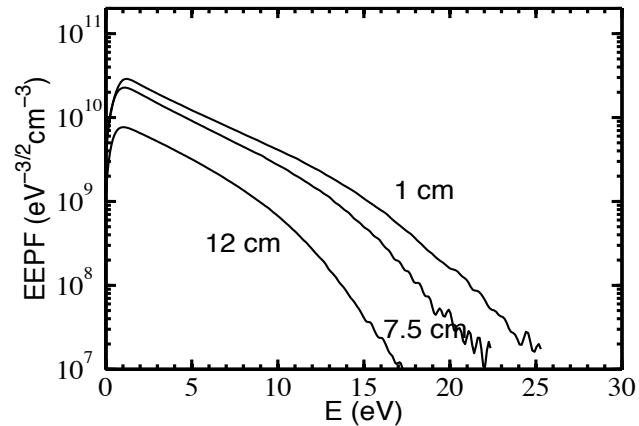
## MODELING CHALLENGES

- **Non-local transport** (Due to geometry and magnetic field)  
✗ Global models cannot describe the discharge

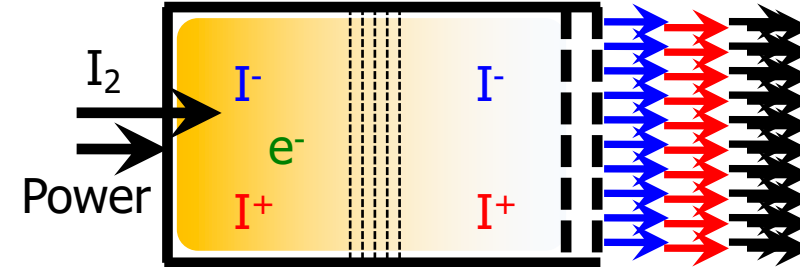
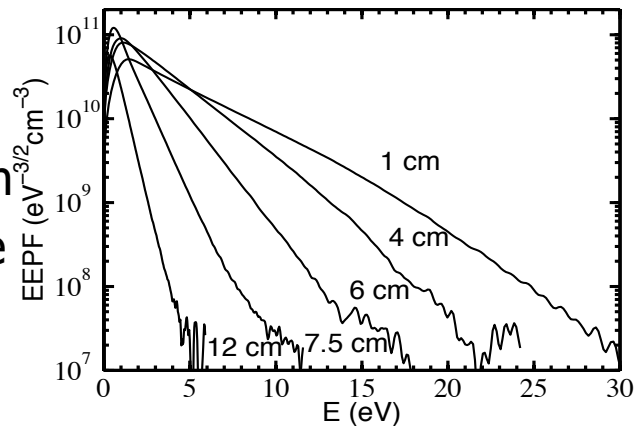
# Motivation: Plasma Propulsion with Electronegative gases

## EEDF Measurements\*

$B = 0$



Gaussian  
B profile

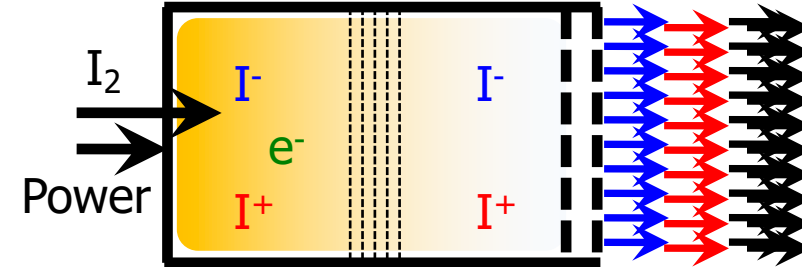
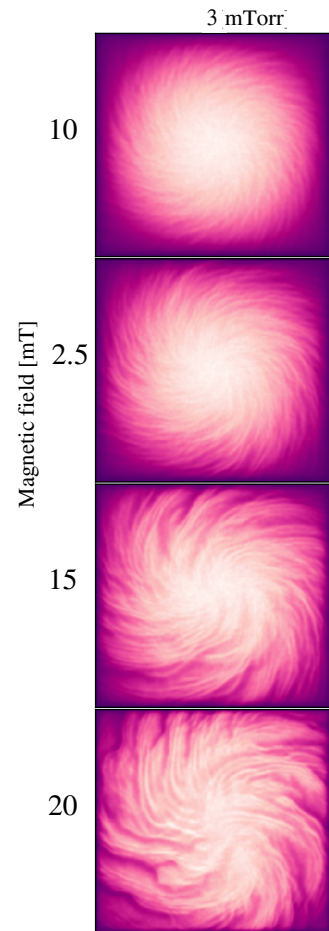


## MODELING CHALLENGES

- Non-local transport (Due to geometry and magnetic field)  
✗ Global models cannot describe the discharge
- **Non-Maxwellian EEDF**  
✗ Domain is too big for PIC simulation

# Motivation: Plasma Propulsion with Electronegative gases

## PIC simulation\*

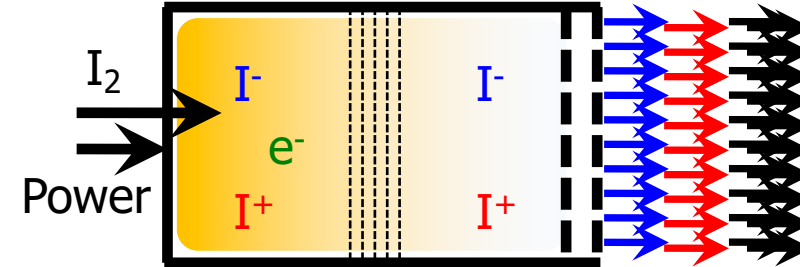
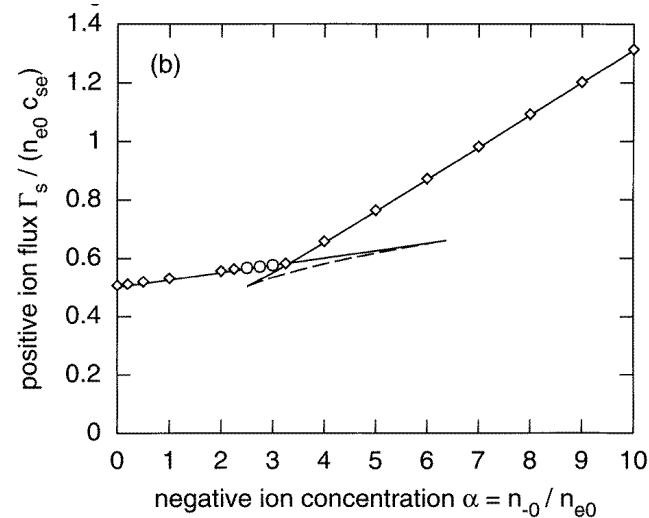


## MODELING CHALLENGES

- Non-local transport (Due to geometry and magnetic field)
  - ✗ Global models cannot describe the discharge
- Non-Maxwellian EEDF
  - ✗ Domain is too big for PIC simulation
- **Anomalous transport**
  - Presence of magnetic field

# Motivation: Plasma Propulsion with Electronegative gases

## Electronegative plasma transport theory\*



## MODELING CHALLENGES

This talk

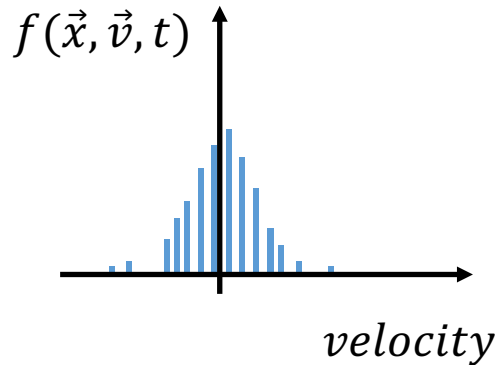
- Non-local transport (Due to geometry and magnetic field)
  - ✗ Global models cannot describe the discharge
- Non-Maxwellian EEDF
  - ✗ Domain is too big for PIC simulation
- Anomalous transport
  - Presence of magnetic field
- **Negative Ions**
  - Change transport, produce instabilities, and double layers

# PART I:

## From the microscopic description to the macroscopic description

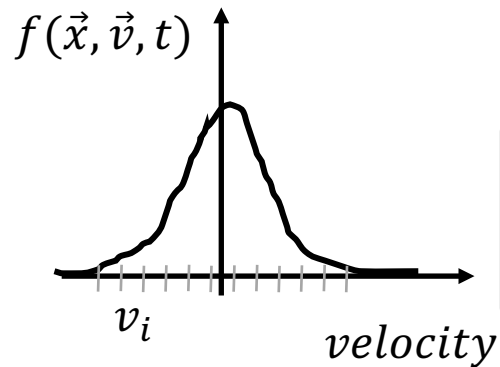


# Modeling plasmas: from microscopic to macroscopic



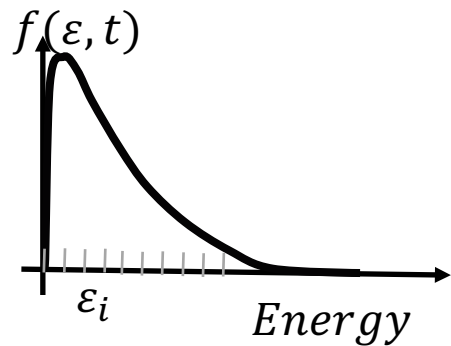
More info:

Birdsall, A.B. Langdon (1998)  
Benchmarks: Turner et al. (2012), Charoy et al. (2019)



More info:

K. Hara, PhD thesis (2015)  
V. Kolobov, R. Arslanbekov and D. Levko (2018)



More info:

Hagelaar & Pitchford (2005)  
A Tejero-del-Caz et al (2019)  
Kortshagen, Busch and Tsendin (1996)  
Igor D. Kaganovich and Oleg Polomarov (2003)

## Microscopic description

Hamiltonian dynamics for N-particle system

## Kinetic Equation

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

## Resolution methods:

1. PIC (stochastic resolution)
  - ✓ 2D “realistic” simulations
  - ✗ Numerical noise and cost
2. Direct resolution of Boltzmann
  - ✓ No noise
  - ✗ More expensive and difficult
3. Local and non-local (two-term) Boltzmann solvers
  - ✓ No noise and efficient
  - ✗ “Local” or 1D



# Modeling plasmas: from microscopic to macroscopic

## Plasma

|                    |            |                 |
|--------------------|------------|-----------------|
| $n_{gas}$          | $n_{ions}$ | $n_{electrons}$ |
| $v_{gas}$          | $v_{ions}$ | $v_{electrons}$ |
| $T_{gas}$          | $T_{ions}$ | $T_{electrons}$ |
| $\vec{E}, \vec{B}$ |            |                 |

Which model to use in weakly collisional conditions?

## Microscopic description

Hamiltonian dynamics for N-particle system

## Kinetic Equation

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

## Fluid Equations

We take moments (weighted average in the velocity space)

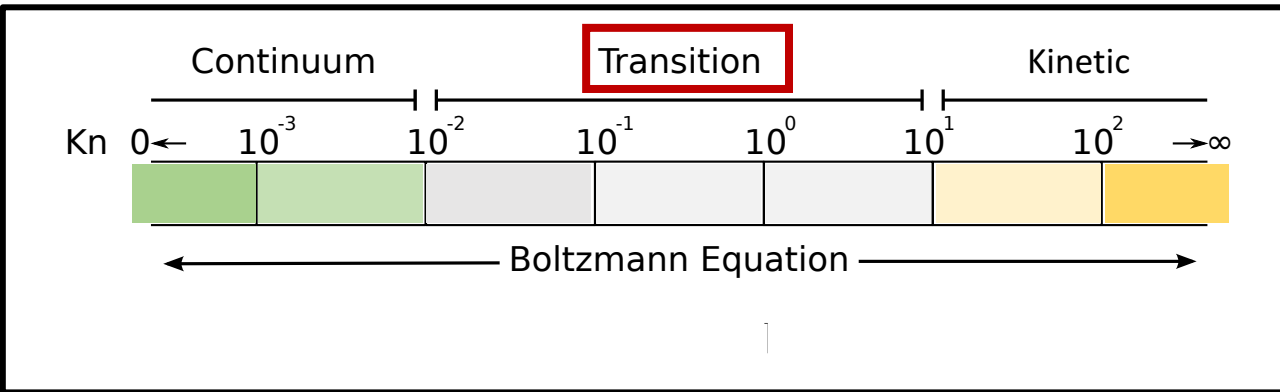
$$\frac{\partial \mathbf{M}_{\alpha}}{\partial t} + \vec{\nabla} \cdot \langle \vec{v} \mathbf{V}_{\alpha} f_{\alpha} \rangle = - \left\langle \mathbf{V}_{\alpha} \frac{\vec{F}_{\alpha}}{m_{\alpha}} \cdot \vec{\nabla}_{\vec{v}} f_{\alpha} \right\rangle + \left\langle \mathbf{V}_{\alpha} \left( \frac{\delta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

- ✓ 2D/3D with complex geometries
- ✗ Closure and pure kinetic effects

## Closure models:

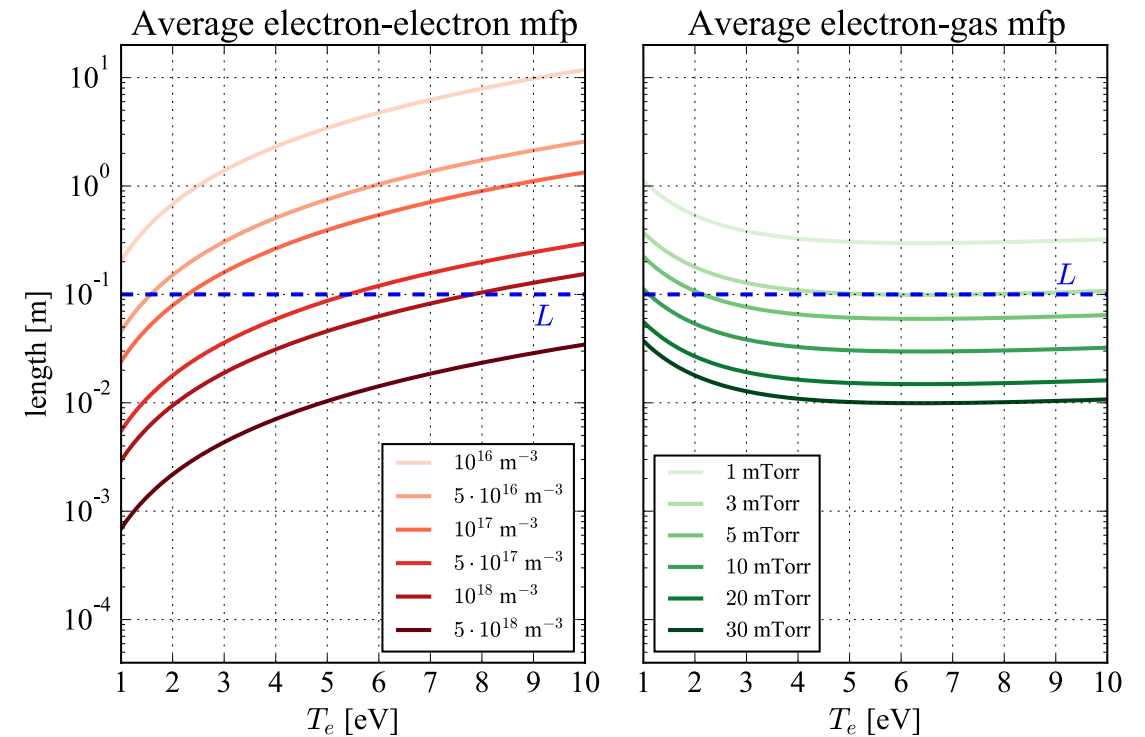
- Moments methods (Grad's, max-entropy)
- Chapman-Enskog expansion
- Hybrid models (kinetic-fluid)
- Euler (MHD) equations

# Regime of validity of each model

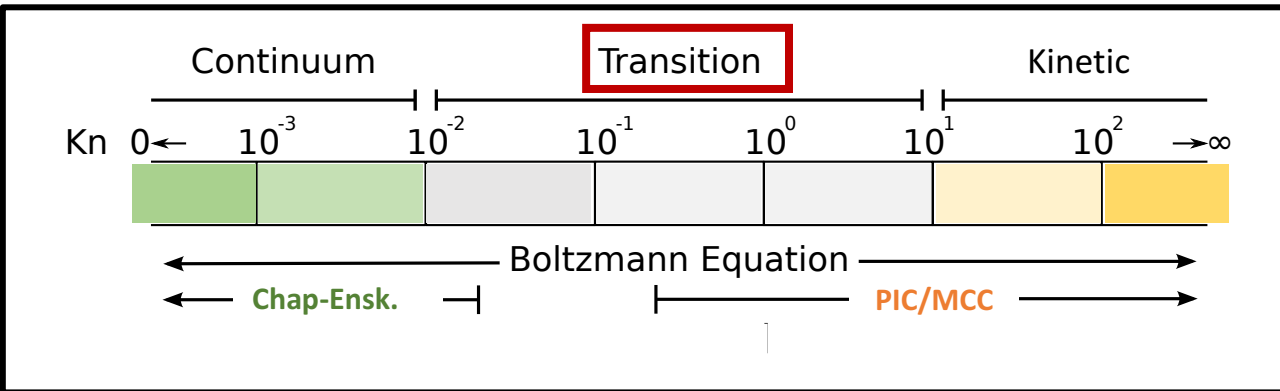


$$Kn = \frac{\text{mean free path}}{\text{characteristic length}}$$

## Electron collisional mean free path in argon

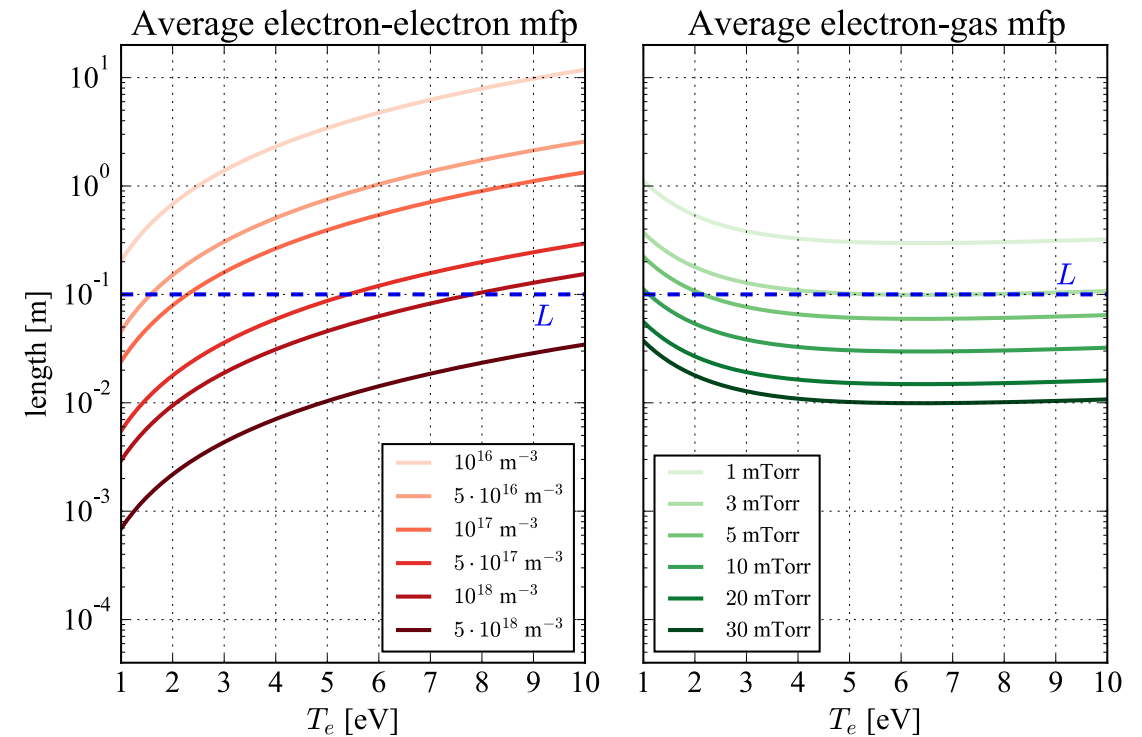


# Regime of validity of each model

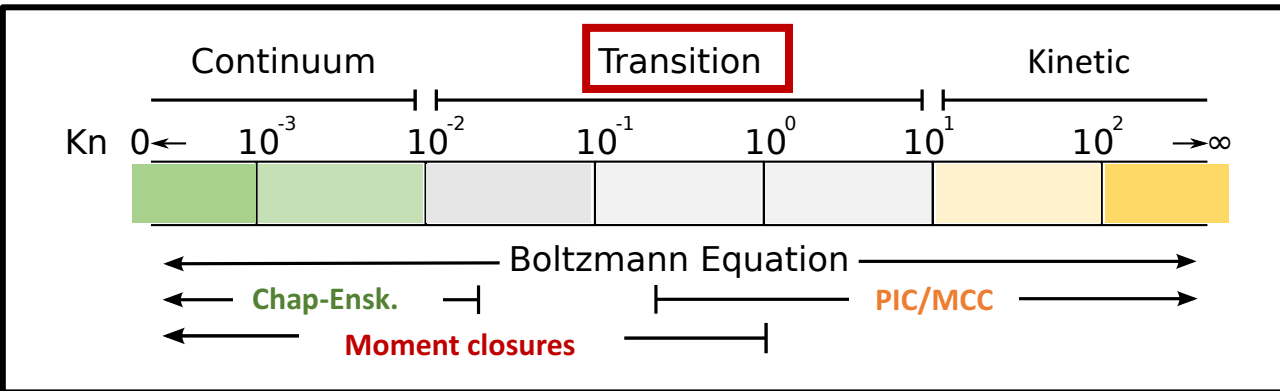


- **Chapman Enskog:** for moderate collisional plasmas.
  - Ferziger & Kaper (1972)
    - Multi-component (Boltzmann)
  - Braginskii (1965)
    - Magnetized and fully-ionized (Landau)
  - Zhdanov (2002)
    - Magnetized and partially ionized (Boltzmann)
  - Graille, Magin, Massot (2009)
    - Magnetized and partially-ionized (Boltzmann)

## Electron collisional mean free path in argon

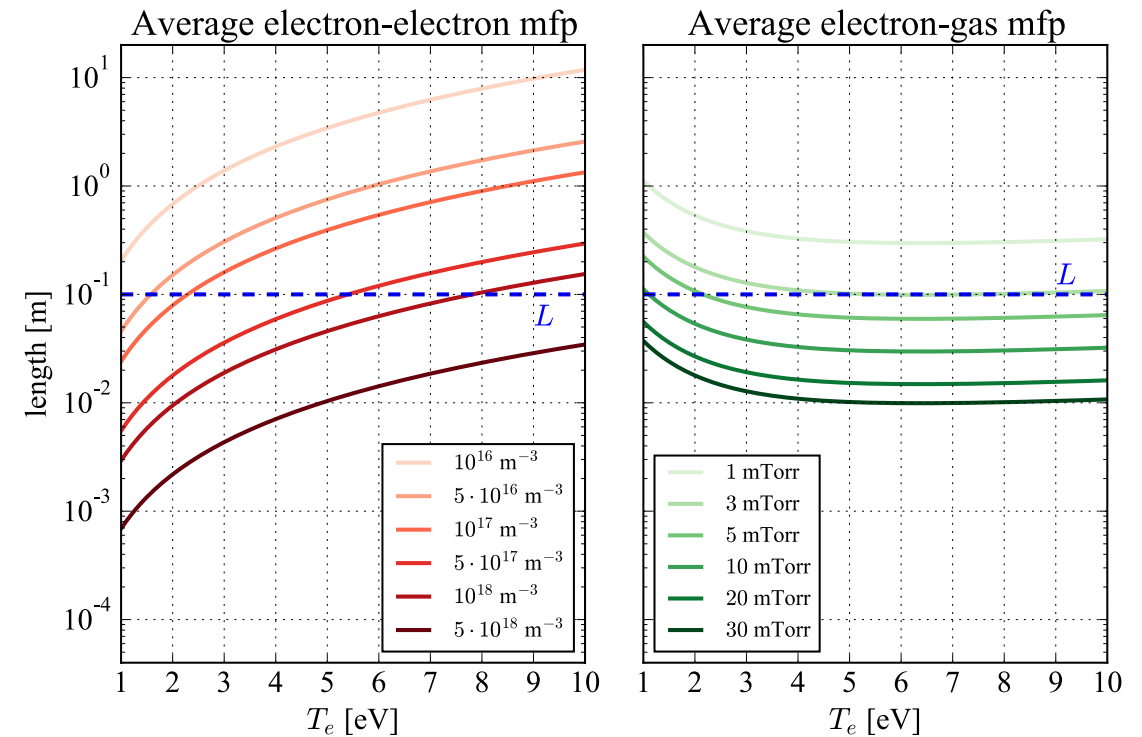


# Regime of validity of each model



- **Moment methods:** for weakly collisional plasmas
  - Grad's method (1949)
    - Landau and Boltzmann operators.
  - Landau Fluids (1997)
    - Landau damping
  - Levermore's Maximum Entropy (1996)
    - Mostly BGK operator
  - Pearson IV, angular moments, other closures...

## Electron collisional mean free path in argon



# Moment (multi-fluid) hierarchies: closure problem

## Microscopic description

### Boltzmann equation

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

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

Average in velocity space

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

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

## Multi-fluid description

### Moment hierarchy

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

Macroscopic variables

$$\begin{pmatrix} \text{Mass} \\ \text{Momentum} \\ \text{Energy} \\ \text{Heat flux} \end{pmatrix} \begin{pmatrix} \rho \\ \rho u_i \\ \frac{1}{2} \rho u_i u_j + \frac{1}{2} P_{ij} \\ \rho u_i u_j u_k + P_{ij} u_k + P_{jk} u_i + P_{ik} u_j + Q_{ijk} \\ \vdots \end{pmatrix}$$

Fluxes

$$\begin{pmatrix} \rho u_i \\ \rho u_i u_j + P_{ij} \\ \rho u_i u_j u_k + 3P_{(ij} u_{k)} + Q_{ijk} \\ \rho u_i u_j u_k u_l + 6u_{(i} u_j P_{kl)} + 4u_{(i} Q_{jkl)} + R_{ijkl} \\ \vdots \end{pmatrix}$$

Electromagnetic forces

$$\begin{pmatrix} 0 \\ q_\alpha n E_i \\ 2q_\alpha n u_{(j} E_{i)} \\ 3q_\alpha \left( n E_{(i} u_j u_{k)} + \frac{E_{(i} P_{jk)}}{m} \right) \\ \vdots \end{pmatrix}$$

Collisional terms

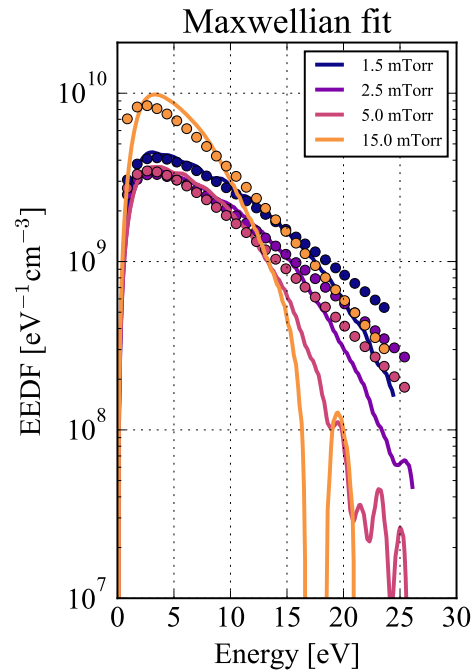
Closure problem:

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

Collisional integrals:

- Depend on cross-section data and VDF

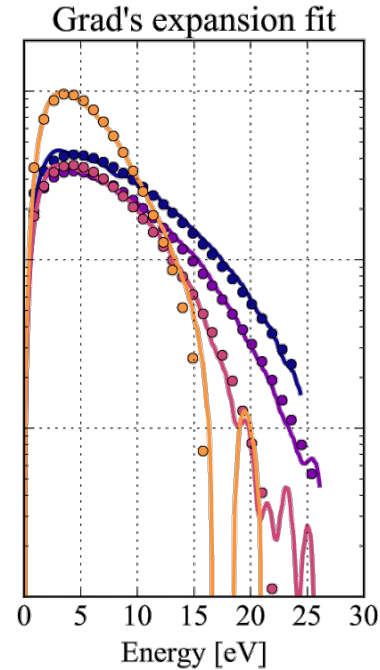
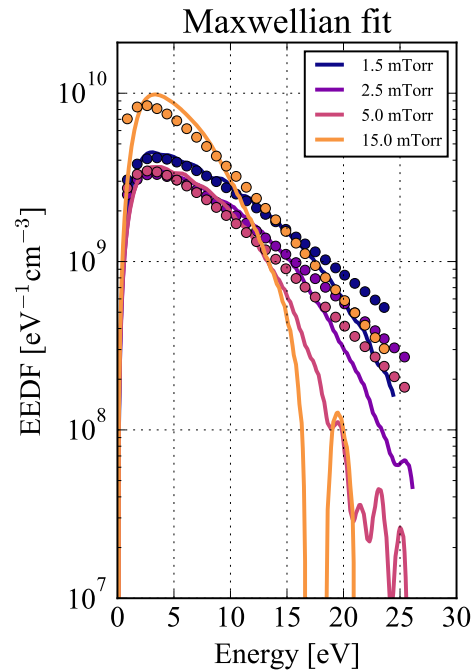
# Different distribution functions for moment models



$$f_{\epsilon}^{(M)}(\mathbf{c}_{\epsilon}, \mathbf{x}, t) = n_{\epsilon} \left( \frac{\beta_{\epsilon}}{\pi} \right)^{3/2} \exp(-\beta_{\epsilon} c_{\epsilon}^2)$$

- **Not able to capture depletion at the tails**

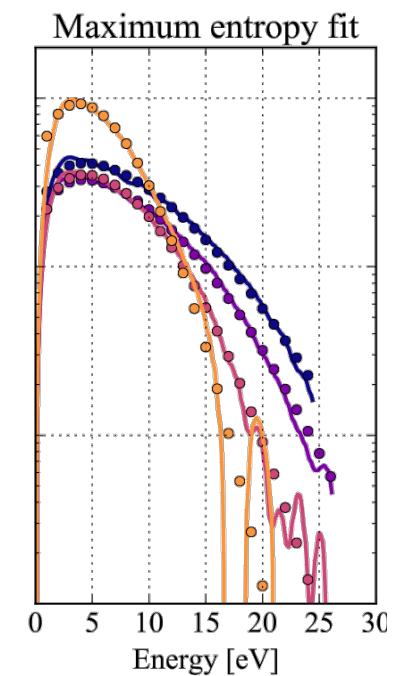
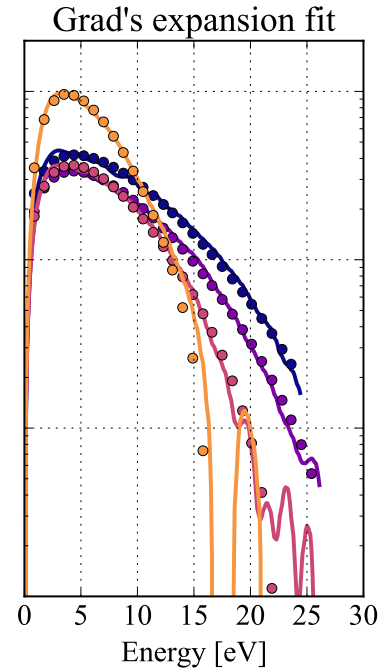
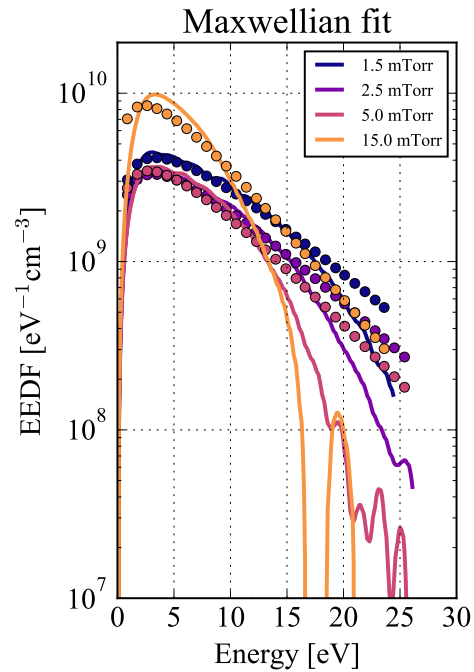
# Different distribution functions for moment models



$$f_e^{(Grad)}(\mathbf{x}, \mathbf{v}, t) = f^{(M)} \left( 1 + a + A_i c_{e_i} + B_{ij} c_{e_i} c_{e_j} + D_{ijk} c_{e_i} c_{e_j} c_{e_k} + \dots \right)$$

- Is able to capture well the both low and high-energies.
- ✓ **Advantages:** Fast to compute the closure. Can be used with Boltzmann and Landau collisional operators.
- ✗ **Disadvantages:** Positivity of distribution function, problems at high Mach numbers (loss of hyperbolicity)

# Different distribution functions for moment models

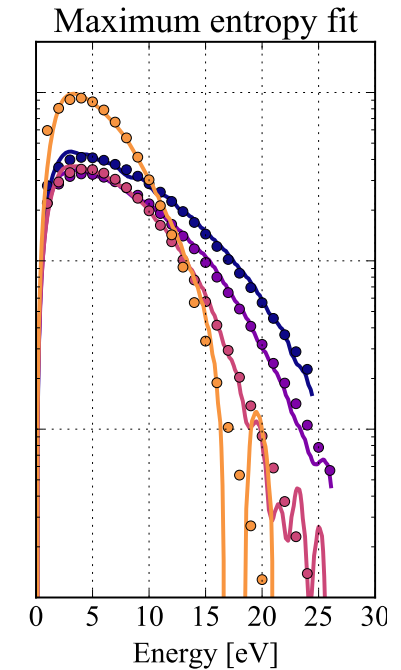
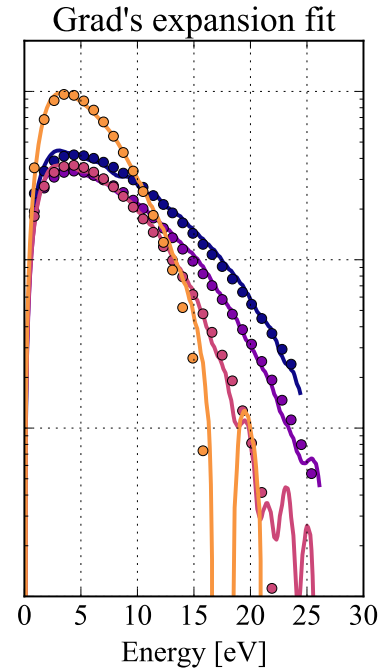
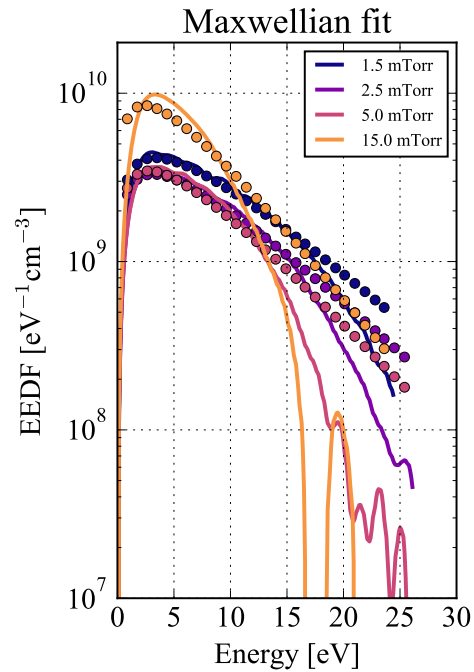


$$f_{\epsilon}^{(MaxEnt)}(\mathbf{x}, \mathbf{v}, t) = f^{(M)} \exp \left( a + A_i c_{\epsilon_i} + B_{ij} c_{\epsilon_i} c_{\epsilon_j} + D_{ijk} c_{\epsilon_i} c_{\epsilon_j} c_{\epsilon_k} + \dots \right)$$

- Is able to capture well the both low and high-energies.
- ✓ **Advantages:** **Positivity.** **Druyvesteyn** is a particular case. Good at supersonic speeds (to represent shocks).
- ✗ **Disadvantages:** **Difficult and slow** to compute closure. Collisional terms mostly based on **BGK** operator.



# Different distribution functions for moment models



- **Moment distribution seem to be able to capture depletion at high energies:**
  - **Need to go for higher moments (> heat flux).**
  - **What is the simplest model capturing the excess kurtosis?**
  - **How do we obtain the closure of fluxes and collisional terms?**

## PART II:

# Grad's closure with heat-flux and EEDF perturbations

# Grad's method: Derivation of the equations

**Step 1:** Choose number of moments and assume a distribution function shape

Moment weights:

$$\psi = \left( m_{\epsilon}, m_{\epsilon} \mathbf{v}, \frac{m_{\epsilon}}{2} c_{\epsilon}^2, \frac{m_{\epsilon}}{2} c_{\epsilon}^2 \mathbf{c}_{\epsilon}, \frac{m_{\epsilon}}{2} c_{\epsilon}^4 \right)^T \quad \text{Total} = (9 \text{ eqs.})$$

$\downarrow$   
 Mass  
(1 eq.)

$\downarrow$   
 Momentum  
(3 eq.)

$\downarrow$   
 Energy  
(1 eq.)

$\downarrow$   
 Heat Flux  
(3 eq.)

$\downarrow$   
 Contracted fourth-  
moment  
(1 eq.)

Fluid variables

$$n_{\epsilon} = \int_{\infty} f_{\epsilon} d\mathbf{v}, \quad \rho_{\epsilon} u_{\epsilon i} = \int_{\infty} m_{\epsilon} v_i f_{\epsilon} d\mathbf{v}, \quad p_{\epsilon} = \frac{1}{3} \int_{\infty} m_{\epsilon} c_{\epsilon}^2 f_{\epsilon} d\mathbf{v},$$

$$q_{\epsilon i} = \frac{1}{2} \int_{\infty} m_{\epsilon} c_{\epsilon}^2 c_{\epsilon i} f_{\epsilon} d\mathbf{v}, \quad \text{and} \quad p_{\epsilon iijj} = \frac{1}{2} \int_{\infty} m_{\epsilon} c_{\epsilon}^4 f_{\epsilon} d\mathbf{v}.$$

Deviation of fourth mom from Maxwellian (excess kurtosis)

$$\Delta_{\epsilon} = \frac{p_{\epsilon iijj} - p_{\epsilon iijj}^{(M)}}{p_{\epsilon iijj}^{(M)}} = \frac{2}{15} \frac{\rho_{\epsilon}}{p_{\epsilon}^2} \int_{\infty} m_{\epsilon} c_{\epsilon}^4 (f_{\epsilon} - f_{\epsilon}^{(M)}) d\mathbf{v}$$

Distribution function:  $f^{(9M)}(c_i)$   
(Grad's (1949))

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

Coefficients?  
 $a, A_i, B, D_i, E$

# Grad's method: Derivation of the equations

**Step 1:** Choose number of moments and assume a distribution function shape

**Step 2:** Compute distribution function coefficients with the definition of the moments

$$f^{(9M)}(c_i) = f_{\epsilon}^{(M)}(c_i) \left( 1 + a + A_i c_{\epsilon i} + B c_{\epsilon}^2 + D_i c_{\epsilon}^2 c_{\epsilon i} + E c_{\epsilon}^4 \right)$$

Flux definition:  $0 = \frac{1}{2} \int_{\infty} dv^3 C_i f_{\alpha}^{(8M)} = A_i \langle C_i C_i f_{\alpha}^{(0)} \rangle + D_i \langle C_i C_j C^2 f_{\alpha}^{(0)} \rangle = A_i + D_i \frac{5 p_{\alpha}}{\rho_{\alpha}}$

Heat Flux definition:  $q_{i\alpha} = \frac{1}{2} \int_{\infty} dv^3 C_i C^2 f_{\alpha}^{(8M)} = A_i \frac{5}{2} \frac{p^2}{\rho} + D_i \frac{35}{2} \frac{p_{\alpha}^3}{\rho_{\alpha}^2}$

$$A_i = -\frac{\rho_e}{p_e^2} q_{ei}$$

$$D_i = \frac{1}{5} \frac{\rho_e^2}{p_e^3} q_{ei}$$

Mass, energy and fourth moment:

$$a = \frac{15}{8} \Delta_e \quad B = -\frac{5 m_e}{4 e T_e} \Delta_e$$

$$E = -\frac{m_e^2}{8 e^2 T_e^2} \Delta_e$$

Obtained distribution:  $f_{\epsilon}(\mathbf{x}, \mathbf{c}_{\epsilon}, t) = f_{\epsilon}^{(M)} \left\{ 1 + \frac{8 \beta_{\epsilon}^2}{5 \rho_{\epsilon}} q_{ei} c_{\epsilon i} \left( \beta_{\epsilon} c_{\epsilon}^2 - \frac{5}{2} \right) + \left( \frac{15}{8} - \frac{5 \beta_{\epsilon}}{2} c_{\epsilon}^2 + \frac{\beta_{\epsilon}^2}{2} c_{\epsilon}^4 \right) \Delta_{\epsilon} \right\}$

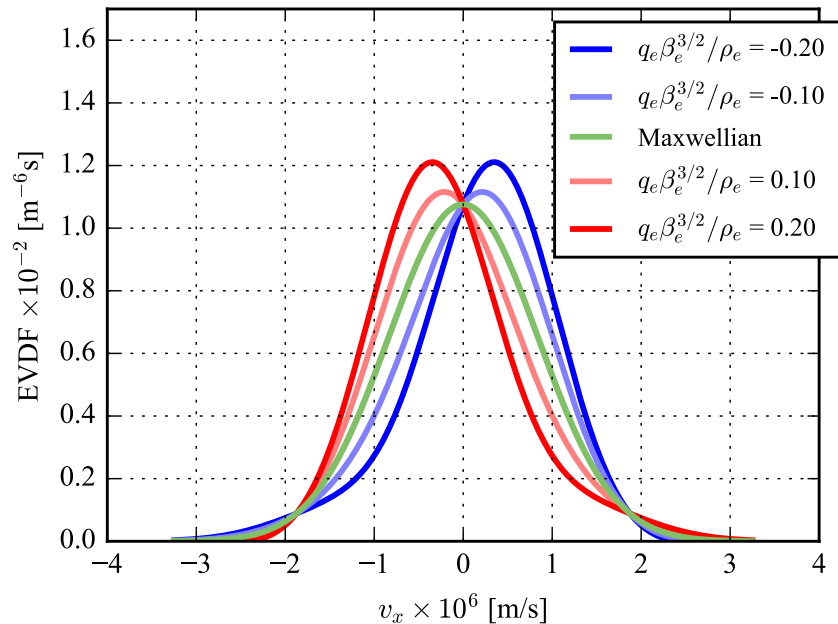
Perturbation depends on fluid quantities<sup>13</sup>

# Analysis of non-equilibrium distribution function

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

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

Skewness modification



# Analysis of non-equilibrium distribution function

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

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

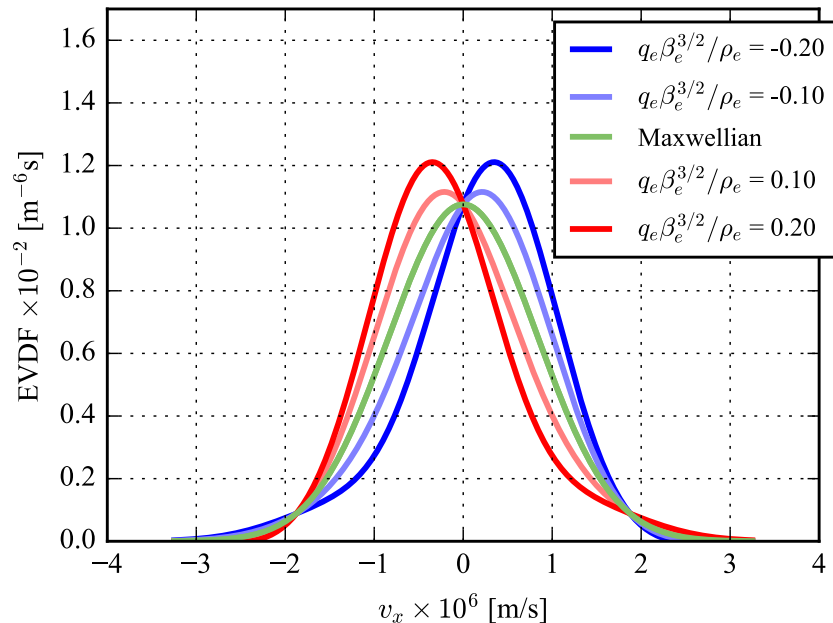
**The VDF depends on 5 fluid quantities**

|                 |             |                    |             |
|-----------------|-------------|--------------------|-------------|
| <b>Density</b>  | $n_e$       | <b>Temperature</b> | $T_e$       |
| <b>Velocity</b> | $\vec{u}_e$ | <b>Heat Flux</b>   | $\vec{q}_e$ |

**4<sup>th</sup>-moment**

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

Skewness modification



# Analysis of non-equilibrium distribution function

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

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

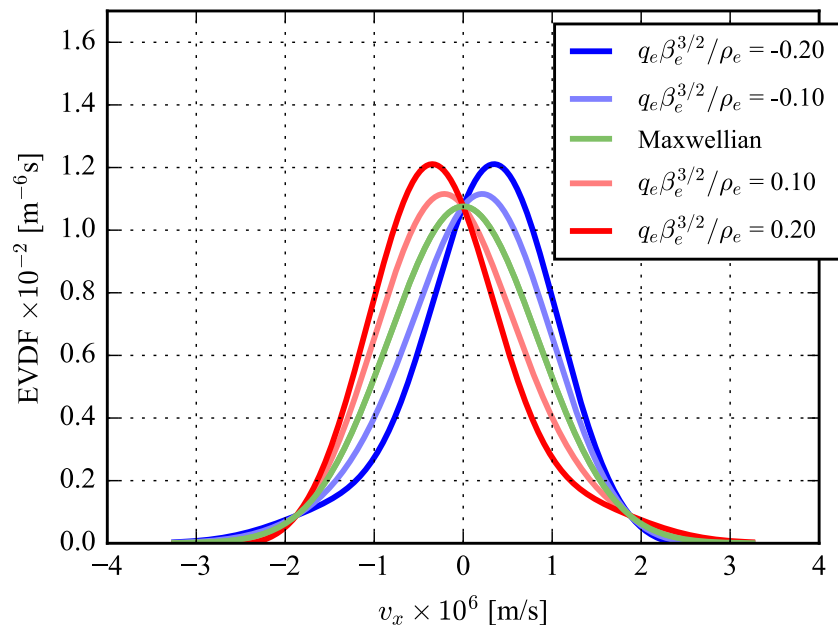
**The VDF depends on 5 fluid quantities**

|                 |             |                    |             |
|-----------------|-------------|--------------------|-------------|
| <b>Density</b>  | $n_e$       | <b>Temperature</b> | $T_e$       |
| <b>Velocity</b> | $\vec{u}_e$ | <b>Heat Flux</b>   | $\vec{q}_e$ |

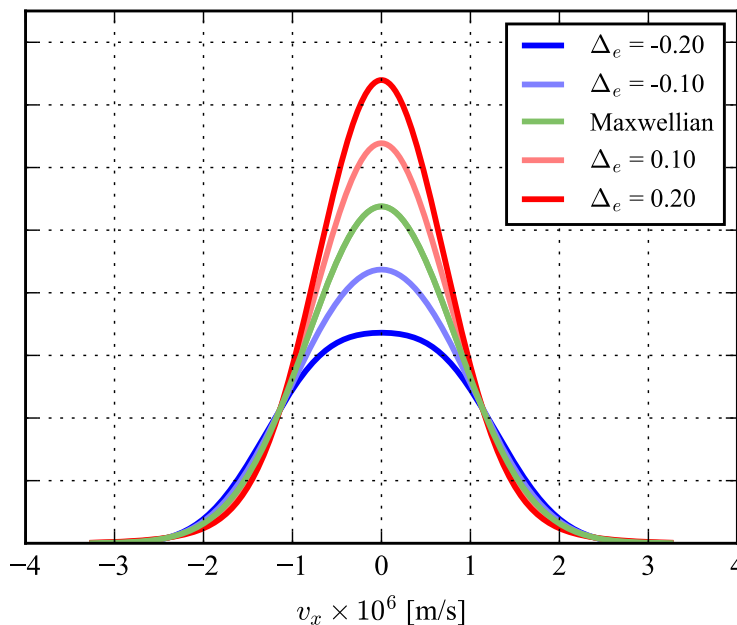
**4<sup>th</sup>-moment**

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

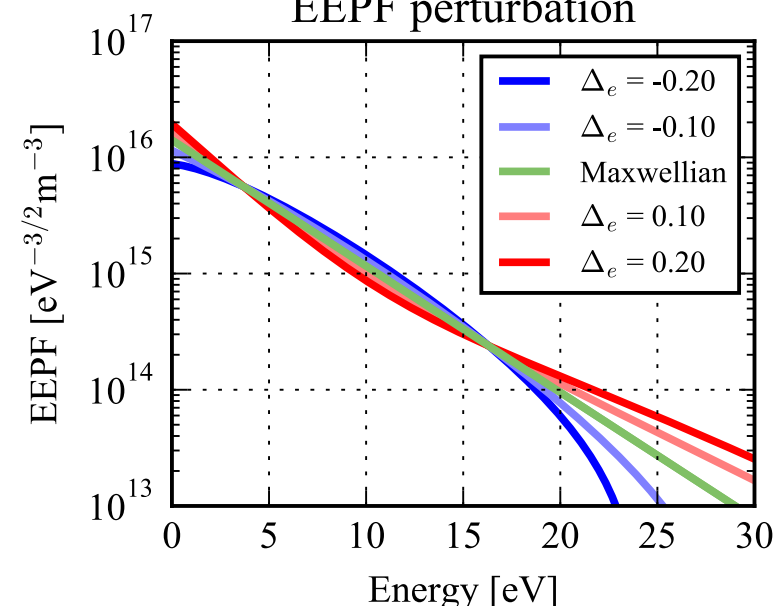
Skewness modification



Kurtosis modification

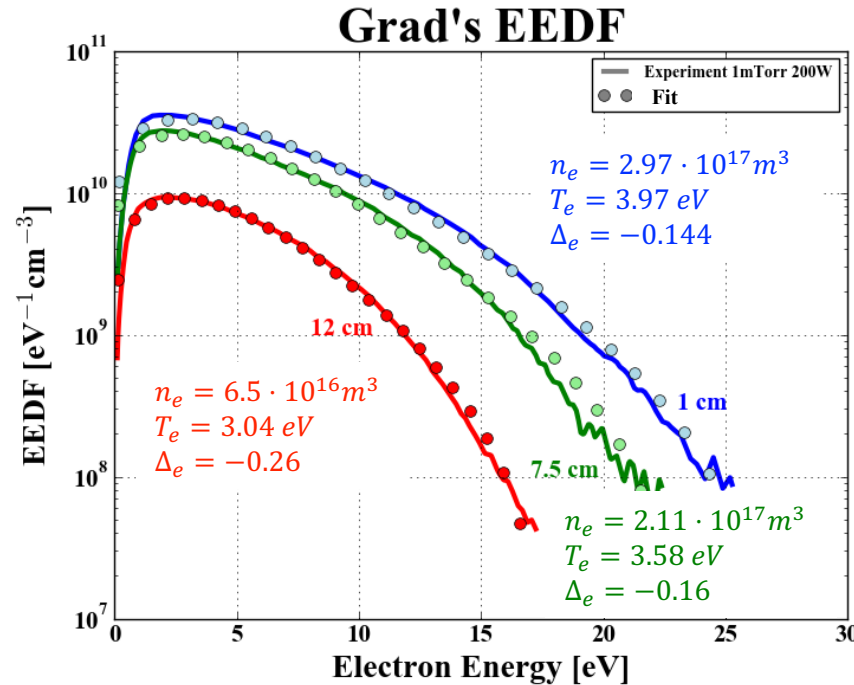
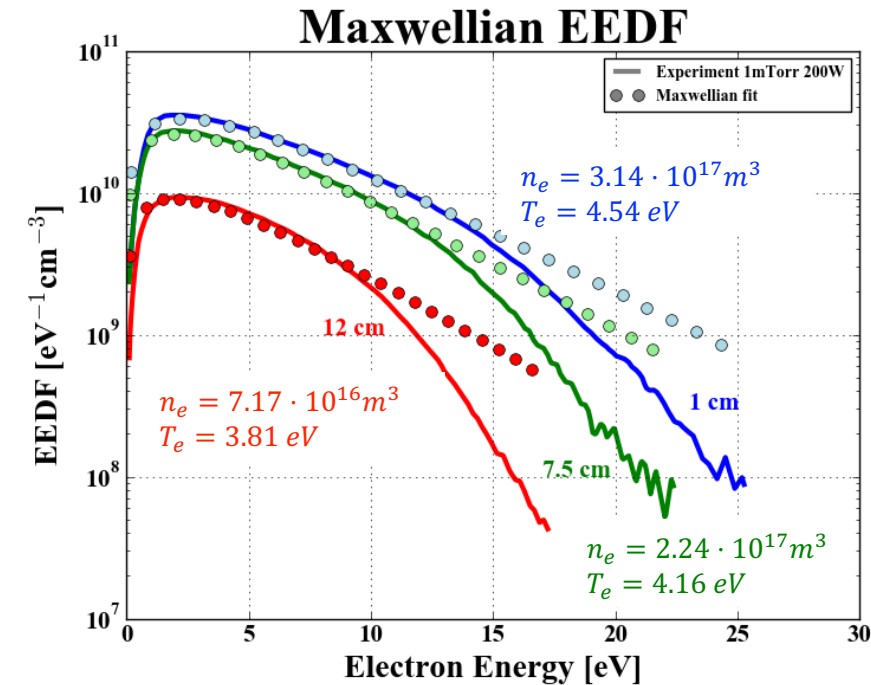


EEPF perturbation



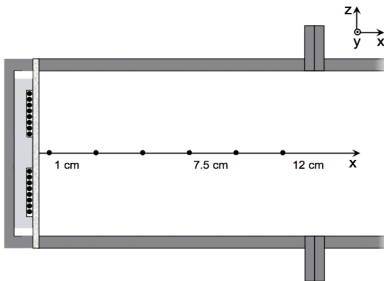
# Comparison with experiments: Different positions

We compare the Grad's EEDF to the experiments:



Inductive Argon discharge

- $p = 1 \text{ mTorr}$
- $P = 200 \text{ W}$



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



# Grad's method: Derivation of the equations

**Step 1:** Choose number of moments and assume a distribution function shape

**Step 2:** Compute distribution function coefficients with the definition of the moments.

**Step 3:** With the computed distribution function, we obtain the closure flux

The flux of the heat flux is:

$$r_{\epsilon_{ij}} = \frac{1}{2} \int_{\infty} m_{\epsilon} c_{\epsilon}^2 c_{\epsilon_i} c_{\epsilon_j} f_{\epsilon} d\mathbf{v} = \frac{5 p_{\epsilon}^2}{2 \rho_{\epsilon}} (1 + \Delta_{\epsilon}) \delta_{ij}$$

The flux of the Fourth moment:

$$r_{\epsilon_{ii jj k}} = \frac{1}{2} \int_{\infty} m_{\epsilon} c_{\epsilon}^4 c_{\epsilon_k} f_{\epsilon} d\mathbf{v} = 14 \frac{p_{\epsilon}}{\rho_{\epsilon}} q_{\epsilon_k}$$

# Grad's method: Derivation of the equations

**Step 1:** Choose number of moments and assume a distribution function shape

**Step2:** Compute distribution function coefficients with the definition of the moments.

**Step 3:** With the computed distribution function, we obtain the closure flux

**Step 4:** Compute collisional integrals (Moments of the Boltzmann collisional operator)

# Derivation of collisional source terms: Elastic Collisions

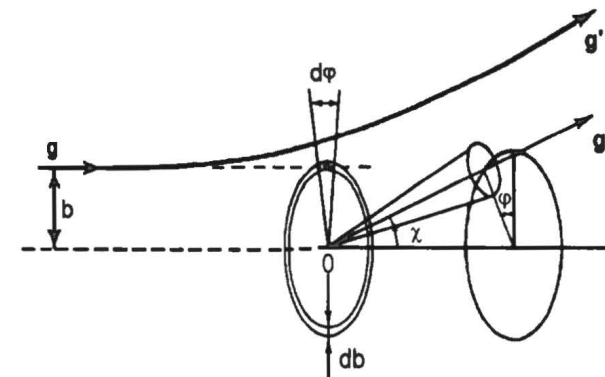
Boltzmann operator

$$\left. \frac{\delta f_e}{\delta t} \right|_{coll} = \int_{\infty} \int (f'_e f'_g - f_e f_g) g \sigma_{eg}(g, \chi) d\Omega d^3 \vec{v}_g$$

Weak version of Boltzmann operator

$$\left\langle \psi(\vec{v}_e) \left. \frac{\delta f_e}{\delta t} \right|_{coll} \right\rangle = \int_{\infty} \int_{\infty} \int (\psi(\vec{v}'_e) - \psi(\vec{v}_e)) f_e f_g g \sigma_{eg}(g, \chi) d\Omega d^3 \vec{v}_g d^3 \vec{v}_e$$

$$\vec{g} = \vec{v}_e - \vec{v}_g \quad \text{and} \quad d\Omega = \sin \chi d\varphi d\chi$$



## Mechanics of the collision

Conservation properties in a scattering collision:

$$\begin{aligned} m_e \vec{v}_e + m_g \vec{v}_g &= m_e \vec{v}'_e + m_g \vec{v}'_g \\ \frac{1}{2} m_e v_e^2 + \frac{1}{2} m_g v_g^2 &= \frac{1}{2} m_e v_e'^2 + \frac{1}{2} m_g v_g'^2 \end{aligned}$$

## Pre- and after-collision relations

$$\begin{aligned} \vec{v}_e &= \vec{G} + \frac{\mu_{eg}}{m_e} \vec{g} & \text{and} & & \vec{v}_g &= \vec{G} - \frac{\mu_{eg}}{m_g} \vec{g} \\ \vec{v}'_e &= \vec{G} + \frac{\mu_{eg}}{m_e} \vec{g}' & \text{and} & & \vec{v}'_g &= \vec{G} - \frac{\mu_{eg}}{m_g} \vec{g}' \end{aligned}$$

In the reference frame of the vector  $\vec{g}$

$$\vec{g}' = g \left( \cos \chi \vec{i} + \sin \chi \cos \varphi \vec{j} + \sin \chi \sin \varphi \vec{k} \right)$$

## Definitions in center-of-mass (Jacobi variables)

$$\begin{aligned} \vec{G} &= \frac{m_e \vec{v}_e + m_g \vec{v}_g}{m_e + m_g} \\ \vec{g} &= \vec{v}_e - \vec{v}_g \\ \vec{g}' &= \vec{v}'_e - \vec{v}'_g \\ |\vec{g}| &= |\vec{g}'| \\ \vec{G} &= \vec{G}' \end{aligned} \quad \mu_{eg} = \frac{m_e m_g}{m_e + m_g}$$

We can see that we can write :

$$\vec{v}_e(\vec{G}, \vec{g}, \chi, \varphi), \quad \vec{v}_g(\vec{G}, \vec{g}, \chi, \varphi), \quad \vec{v}'_e(\vec{G}, \vec{g}, \chi, \varphi), \quad \vec{v}'_g(\vec{G}, \vec{g}, \chi, \varphi)$$

# Derivation of collisional source terms: Elastic Collisions

We write the integrals as function of Jacobi variables and averaged cross sections  $(\vec{G}, \vec{g}, \chi, \varphi)$

**Momentum  
and viscosity cross-section**

$$Q^{(1)}(g) = 2\pi \int_0^\pi (1 - \cos \chi) \sigma_{eg}(g, \chi) \sin \chi d\chi$$
$$Q^{(2)}(g) = 2\pi \int_0^\pi (1 - \cos^2 \chi) \sigma_{eg}(g, \chi) \sin \chi d\chi$$

Momentum exchange:

$$\vec{R}_{eg} = \left\langle m_e \vec{v}_e \frac{\delta f_e}{\delta t} \right|_{coll} \rangle = -\mu_{eg} \int_\infty d^3 \vec{g} \int_\infty d^3 \vec{G} \vec{g} Q^{(1)} f_e f_g g$$

Energy exchange:

$$Q_{eg} = \left\langle \frac{m_e}{2} v_e^2 \frac{\delta f_e}{\delta t} \right|_{coll} \rangle = -\mu_{eg} \int_\infty d^3 \vec{g} \int_\infty d^3 \vec{G} (\vec{G} \cdot \vec{g}) Q^{(1)} f_e f_g g$$

Heat-Flux exchange:

$$\vec{R}_{eg}^{hF} = \left\langle \frac{m_e}{2} v_e^2 \vec{v}_e \frac{\delta f_e}{\delta t} \right|_{coll} \rangle = -\frac{\mu_{eg}}{2} \int_\infty d^3 \vec{g} \int_\infty d^3 \vec{G} \left\{ \left[ (\vec{G} \cdot \vec{g}) \vec{G} + G^2 \vec{g} + \left( \frac{\mu_{eg}}{m_e} \right)^2 g^2 \vec{g} \right] Q^{(1)} - 2 \left( \frac{\mu_{eg}}{m_e} \right) \left[ \frac{1}{2} g^2 \vec{G} - \frac{3}{2} (\vec{G} \cdot \vec{g}) \vec{g} \right] Q^{(2)} \right\} f_e f_g g$$

Fourth-moment exchange:

$$Q_{eg}^{(4)} = \left\langle \frac{m_e}{2} v_e^4 \frac{\delta f_e}{\delta t} \right|_{coll} \rangle = -2\mu_{eg} \int_\infty d^3 \vec{g} \int_\infty d^3 \vec{G} \left\{ \left[ G^2 + \left( \frac{\mu_{eg}}{m_e} \right)^2 g^2 \right] (\vec{G} \cdot \vec{g}) Q^{(1)} + \left( \frac{\mu_{eg}}{m_e} \right) \left[ \frac{3}{2} (\vec{G} \cdot \vec{g})^2 - \frac{1}{2} g^2 G^2 \right] Q^{(2)} \right\} f_e f_g g$$

# Derivation of collisional source terms: Elastic Collisions

**Boltzmann operator**  $\left. \frac{\delta f_e}{\delta t} \right|_{e_g} = \int \int (f'_e f'_g - f_e f_g) g \sigma d\Omega d\mathbf{v}_g$

Momentum exchange:

$$\mathbf{R}_{eg}^{(el)} = \underbrace{-m_e n_e \nu_{eg}^{(fr,1)} \mathbf{u}_e}_{\text{Frictional force}} - \underbrace{n_e \nu_{eg}^{(skew,1)} \frac{\mathbf{q}_e}{p_e}}_{\text{Soret effect}}$$

Energy exchange:

$$Q_{eg}^{(el)} = \underbrace{\frac{m_e}{m_g} n_e \nu_{eg}^{(fr,2)} e (T_g - T_e)}_{\text{Temp. relaxation}} + \underbrace{\frac{m_e}{m_g} n_e \nu_{eg}^{(kurt,2)} \Delta_e e T_g}_{\text{Kurtosis correction}} - \underbrace{n_e \nu_{eg}^{(skew,2)} \frac{\mathbf{q}_e}{p_e} \cdot \mathbf{u}_e}_{\text{Effect of skewness}}$$

Heat-Flux exchange:

$$\mathbf{R}_{eg}^{hF,(el)} = \underbrace{-n_e \nu_{eg}^{(fr,3)} e T_e \mathbf{u}_e}_{\text{Dufour effect}} - \underbrace{\nu_{eg}^{(skew,3)} \mathbf{q}_e}_{\text{Skewness relaxation}}$$

Fourth-moment exchange:

$$Q_{eg}^{(el,4)} = \underbrace{n_g \frac{m_e}{m_g} \nu_{eg}^{(fr,4)} \frac{p_e^2}{\rho_e} \left( \frac{T_g}{T_e} - 1 \right)}_{\text{Kurtosis relaxation}} + \underbrace{n_g \frac{m_e}{m_g} \nu_{eg}^{(kurt,4)} \frac{p_e^2}{\rho_e} \frac{T_g}{T_e}}_{\text{Additional correction}} + \underbrace{4 \nu_{eg}^{(skew,3)} \mathbf{q}_e \cdot \mathbf{u}_e}_{\text{Effect of skewness}}$$

**BGK operator**  $\left. \frac{\delta f_e}{\delta t} \right|_{e_g} = -\nu_m f_e$

Momentum exchange:

$$\mathbf{R}_{eg}^{(el)} = -m_e n_e \nu_m \mathbf{u}_e$$

Energy exchange:

$$Q_{eg}^{(el)} = -3 \frac{m_e}{m_g} n_e \nu_m e T_e$$

Heat-Flux exchange:

$$\mathbf{R}_{eg}^{hF,(el)} = -\nu_m \mathbf{q}_e$$

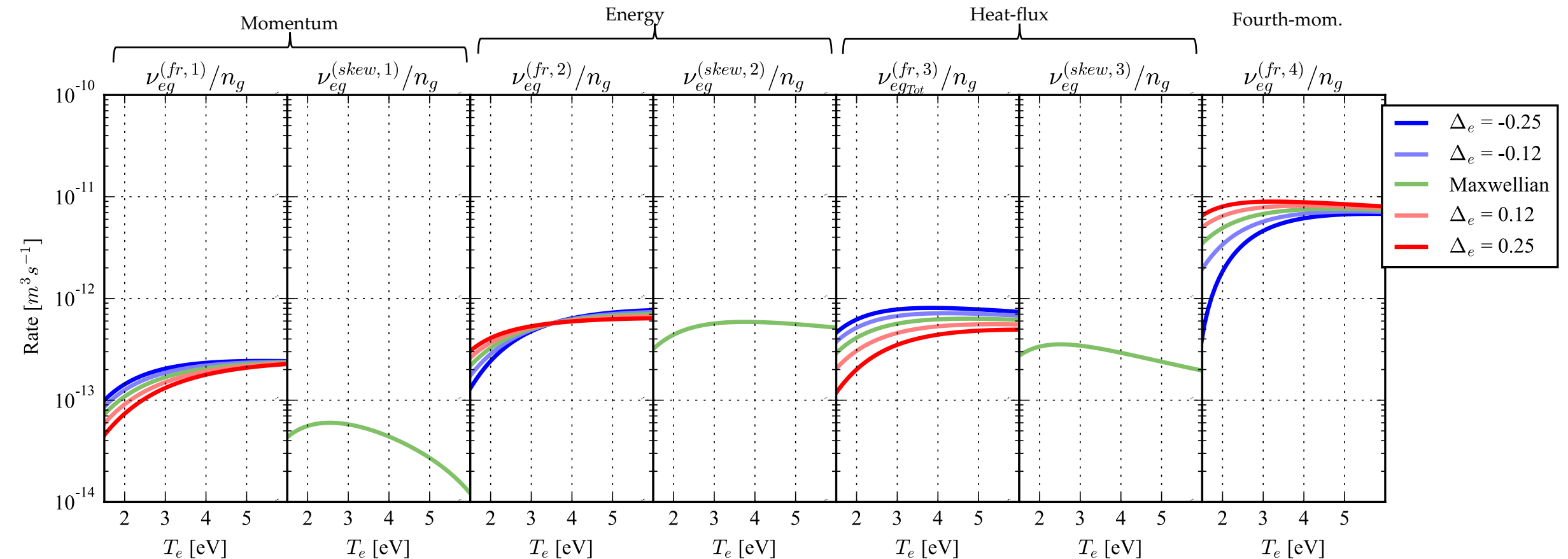
Fourth-moment exchange:

$$Q_{eg}^{(el,4)} = -\frac{m_e}{m_g} \nu_m \frac{p_e^2}{\rho_e} \Delta_e$$

# Derivation of collisional source terms: Elastic Collisions

We write the integrals as function of Jacobi variables and averaged cross sections

The friction terms depend on the kurtosis perturbation:



The frequencies depend on the Chapman-Cowling integrals:  $\Omega_{\text{eg}}^{(l,r)}(T_e) = \frac{1}{2} \left( \frac{1}{\pi \beta_e} \right)^{1/2} \int_0^\infty \xi^{2r+3} e^{-\xi^2} Q^{(l)} d\xi$  with  $\xi = \sqrt{\beta_e} g$

# Derivation of collisional source terms: Electron-electron & Ionization

Mass exchange:

$$\dot{n}_e^{(iz)} = n_e n_g K_{iz}^{(0)}$$

Momentum exchange:

Conserved in electron-electron and neglected in inelastic

Energy exchange:

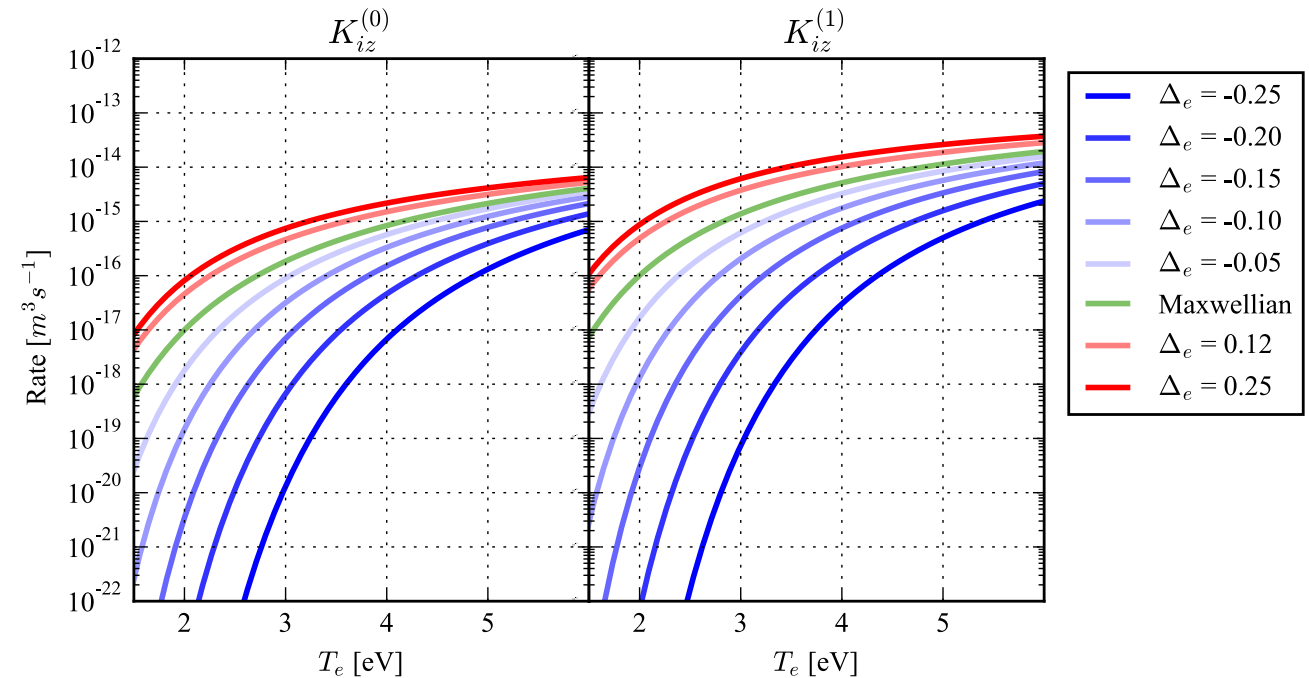
$$Q_{eg}^{(inel)} = - \sum_{k=0}^{excit,iz} n_e n_g K_{inel,k}^{(0)} n_g \phi_k^*$$

Heat-Flux exchange:

$$R_{ee}^{hF} = -n_e \nu_{ee}^{(skew)} q_e$$

Fourth-moment exchange:

$$Q_{ee}^{(4)} = -n_e \nu_{ee}^{(kurt)} \frac{p_e^2}{\rho_e} \Delta_e \quad Q_{eg}^{(inel,4)} = -2 \sum_{k=0}^{excit,iz} \left( \frac{p_e^2}{\rho_e} \right) K_{inel,k}^{(1)} \left( \frac{\phi_k^*}{T_e} \right)$$



Ionization and inelastic rate largely depend on the kurtosis!

# Set of equations with the fourth moment (1D)

## Electrons (9 eqs in 3D):

|                         |                                                                                                                                                                                                                                                                                                                                                       |
|-------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Density                 | $\frac{\partial n_e}{\partial t} + \frac{\partial}{\partial x_i} n_e u_{ei} = \dot{n}_e,$                                                                                                                                                                                                                                                             |
| Momentum                | $m_e \frac{\partial}{\partial t} n_e u_{ei} + \frac{\partial}{\partial x_j} (m_e n_e u_{ei} u_{ej} + p_e \delta_{ij}) = -en_e E_i + R_i,$                                                                                                                                                                                                             |
| Energy                  | $\frac{3}{2} \frac{\partial p_e}{\partial t} + \frac{\partial}{\partial x_k} \left( q_{ek} + \frac{3}{2} p_e u_{ek} \right) + p_e \frac{\partial u_{ek}}{\partial x_k} = Q,$                                                                                                                                                                          |
| Heat flux               | $\frac{\partial q_{ei}}{\partial t} + \frac{\partial}{\partial x_j} (r_{eij} + q_{ei} u_{ej}) + r_{eijk} \frac{\partial u_{ek}}{\partial x_j} + q_{ej} \frac{\partial u_{ei}}{\partial x_j} - \frac{5}{2} \frac{p_e}{\rho_e} \frac{\partial p_e}{\partial x_j} \delta_{ij} = R_i^{hf} - \frac{5}{2} \frac{p_e}{\rho_e} (R_i - m_e \dot{n}_e u_{ei}),$ |
| 4 <sup>th</sup> -moment | $\frac{\partial p_{eijj}}{\partial t} + \frac{\partial}{\partial x_k} (r_{eijjk} + p_{eijj} u_{ek}) + 4r_{eij} \frac{\partial u_{ei}}{\partial x_j} - 4 \frac{q_{ei}}{\rho_e} \frac{\partial p_e}{\partial x_j} \delta_{ij} = Q^{(4)} - 4 \frac{q_{ei}}{\rho_e} (R_i - m_e \dot{n}_e u_{ei}).$                                                        |

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



# Intermediate ideas to take with you

1. In ICP discharges we measure kurtosis perturbations in the EEDF, this can be obtained by the resolution of the contracted fourth moment.
2. By taking **higher moments**, the **distribution function is more perturbed** (less Maxwellian), but the mathematical complexity increases.
3. Most of multi-fluid models assume BGK-like operators (all the moments have the same collision frequency).
4. Deviations from the Maxwellian can lead to “**unexpected terms**” in the equations. These terms are usually disregarded in simple fluid models.

## Literature

Classical books: Grad's (1949), Chapman & Cowling (1970), Balescu (1988)

Modern books: Gombosi (2003), Struchtrup (2005), Kremer (2010)

Plasma physics: Braginskii (1965), Zhdanov (2002)

Rigorous Chapman-Enskog: Ern & Giovangigli (1994), Magin et al. (2009)

Collisionless Landau Fluids: Hunana (2019)

Courses: Clinton Groth (UTIAS)

## PART III:

# Numerical resolution of the moment equations

# 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**

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

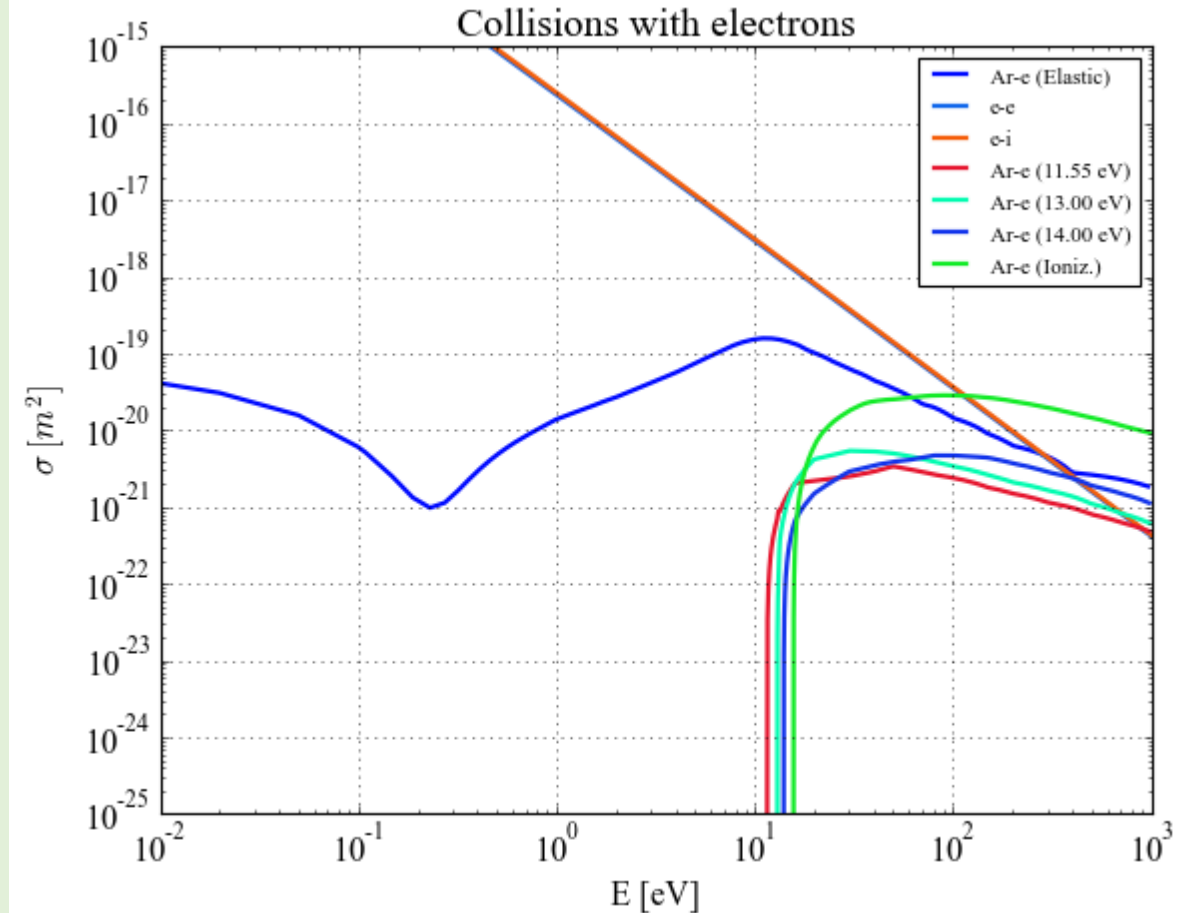
$$\frac{dT_e}{dt} = \text{Inel. losses} + \text{El. losses}$$

- **High-order moment**

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

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

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



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

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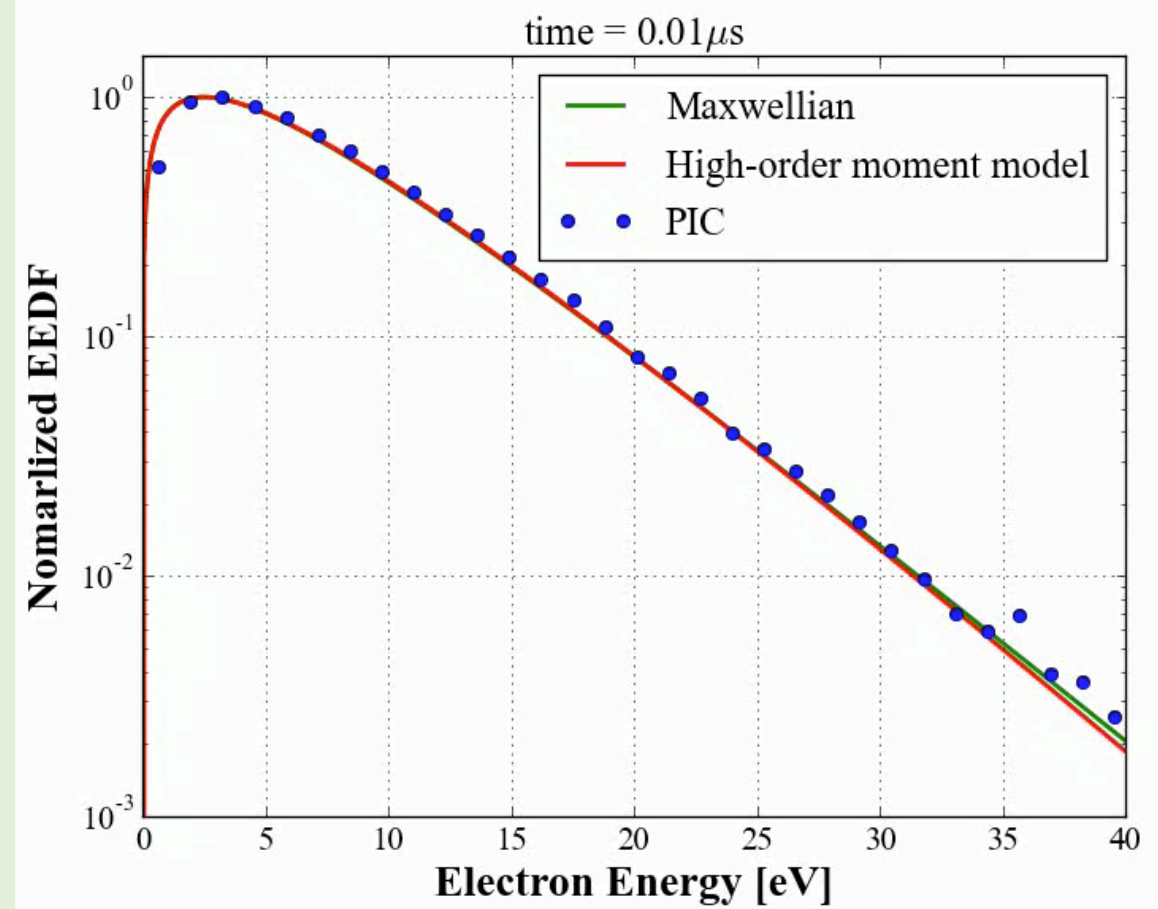
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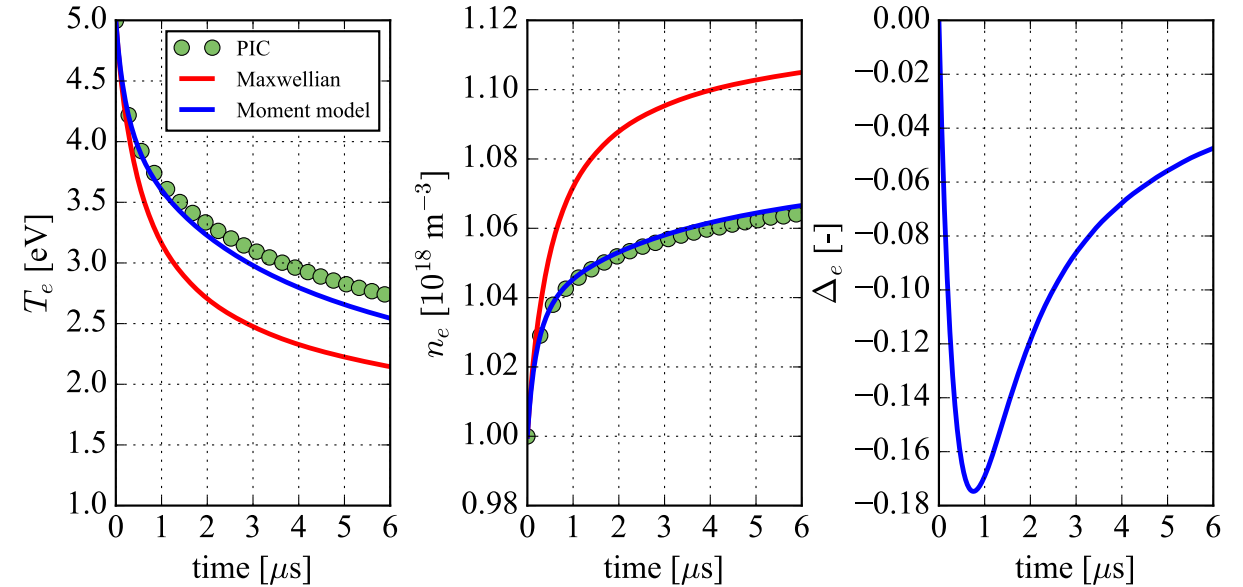
$$\frac{d\Delta_e}{dt} = -(\text{Inel. losses} + \text{El. Losses}) + (e - e \text{ colls.})$$



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

- The resolution of the higher moment seems to capture better the relaxation as compare to a model solving for a Maxwellian distribution.
- The collisional coefficients depend on the shape of the EEDF ( $\Delta_e$ )

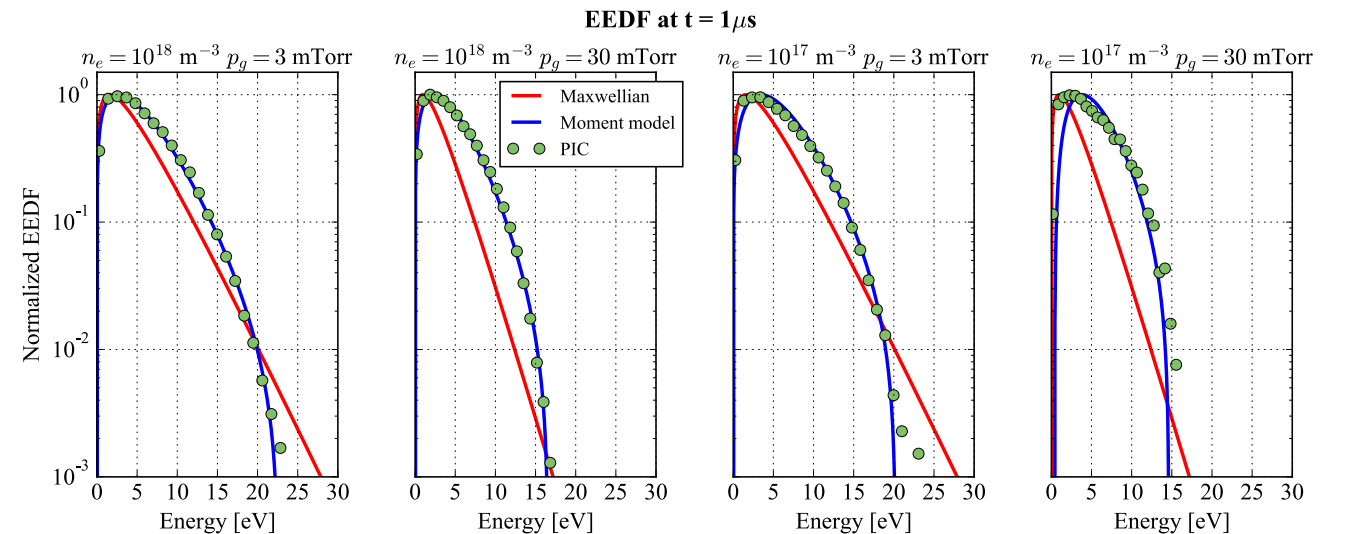
Case 1:  $n_e = 10^{18} \text{ m}^{-3}$  and  $p_g = 3 \text{ mTorr}$



- We tried different conditions:

- $n_e = 10^{17}, 10^{18} \text{ m}^{-3}$
- $p_g = 3, 30 \text{ mTorr}$

- The moment model captures the deviation of the EEDF from Maxwellian.

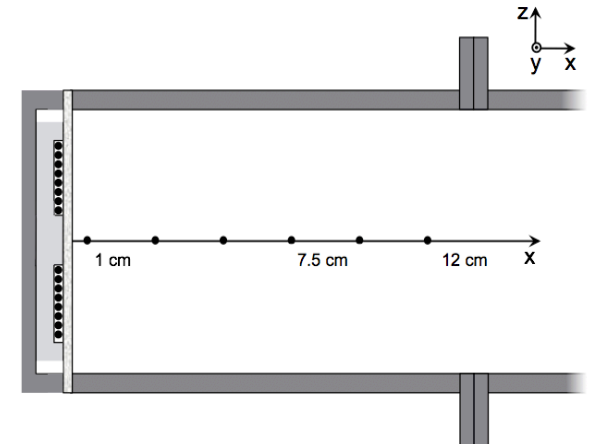
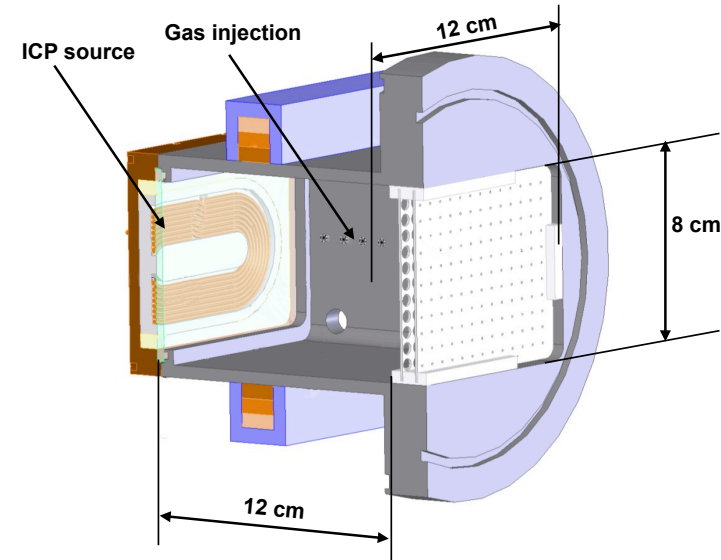


# Case 2: 1D simulation of an ICP reactor

We study a 1D slab along the axis of the ICP reactor working on argon.

The model has the following assumptions:

- Plasma is quasi-neutral.
- The plasma is assumed to be ambipolar in the  $x$ -direction
- The gas is assumed to be at constant temperature.
- We assume a 2D edge-to-center plasma density ration as proposed by Lucken et al. (2018).
- We solve for the following variables:
  - Plasma density
  - Velocity in the  $x$ -direction
  - Electron temperature
  - Electron heat-flux in the  $x$ -direction
  - Fourth moment (electron kurtosis)

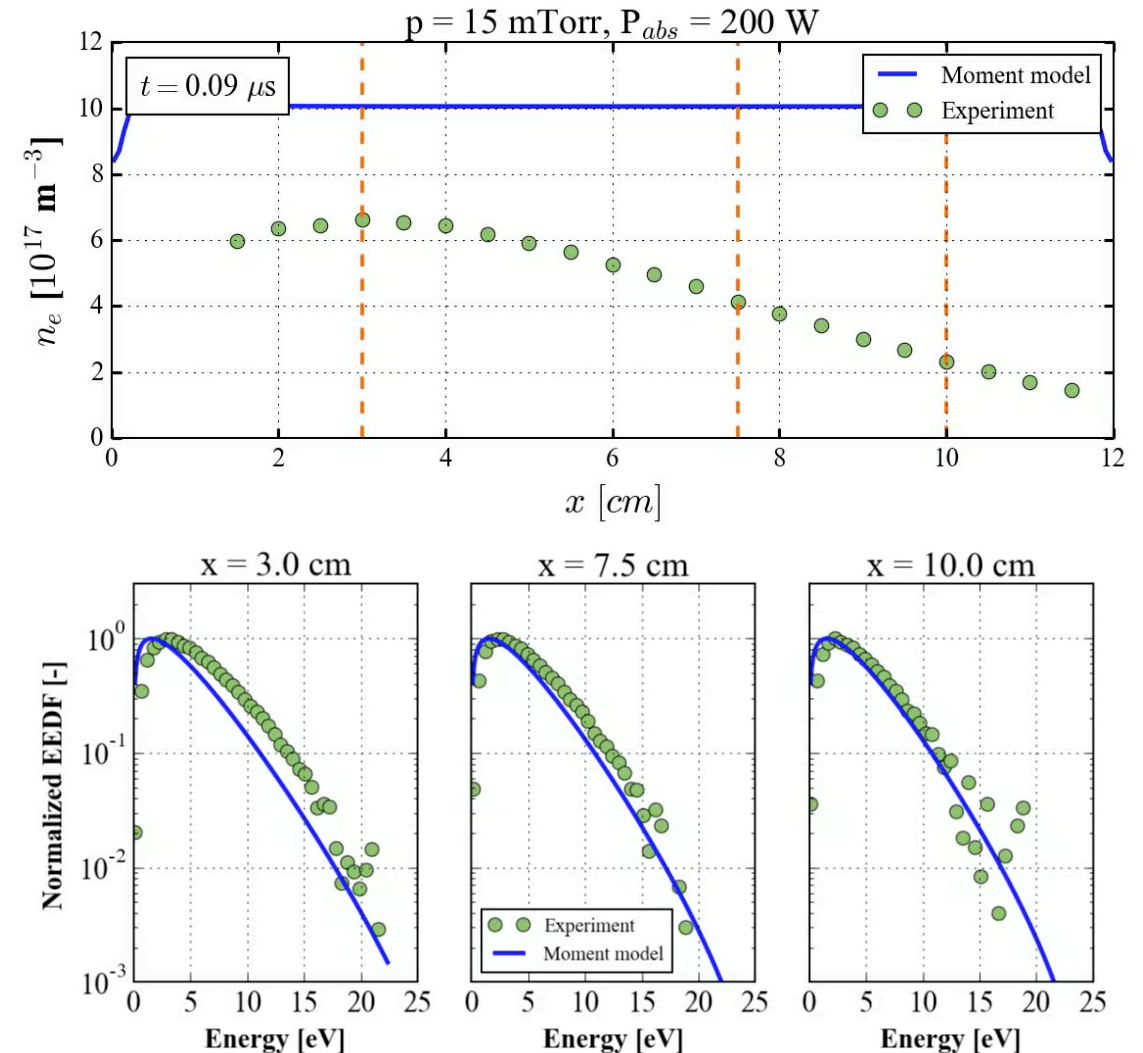


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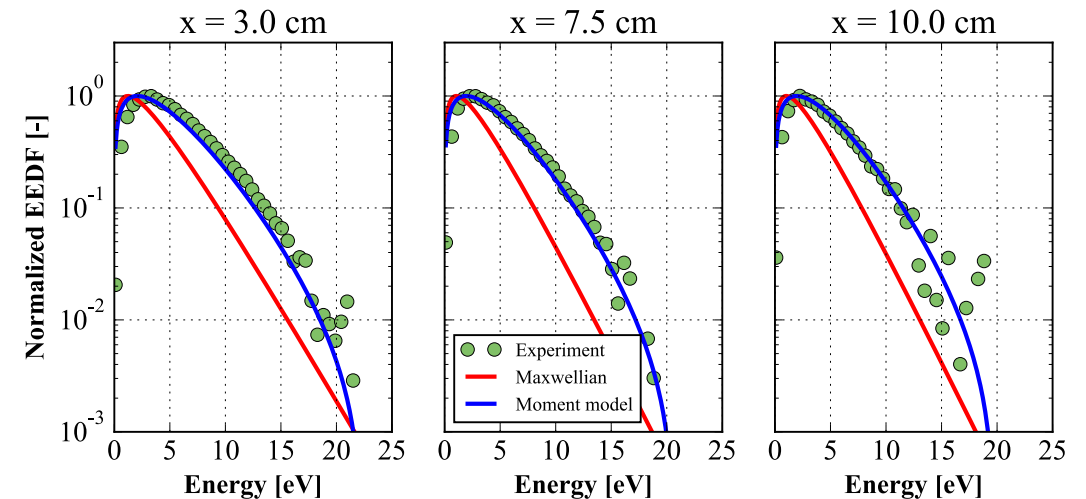
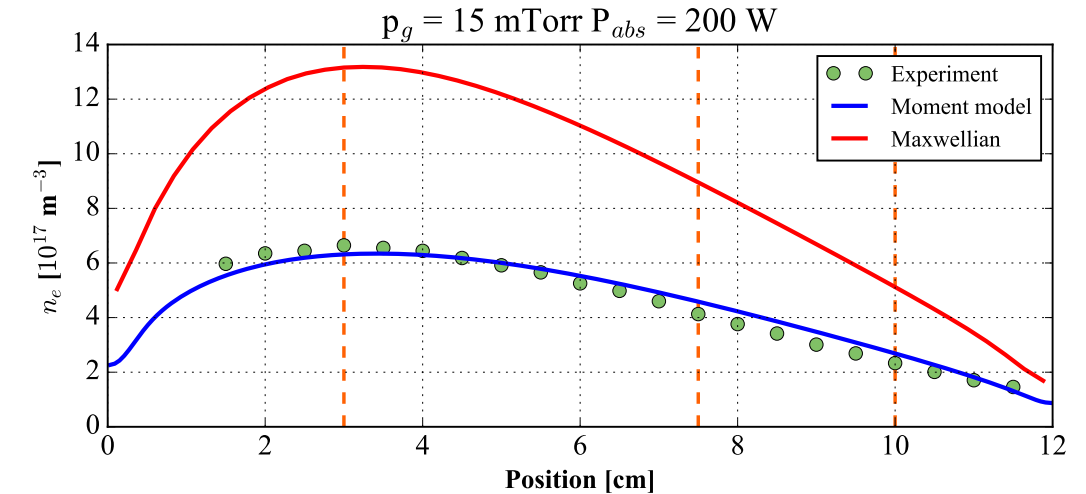


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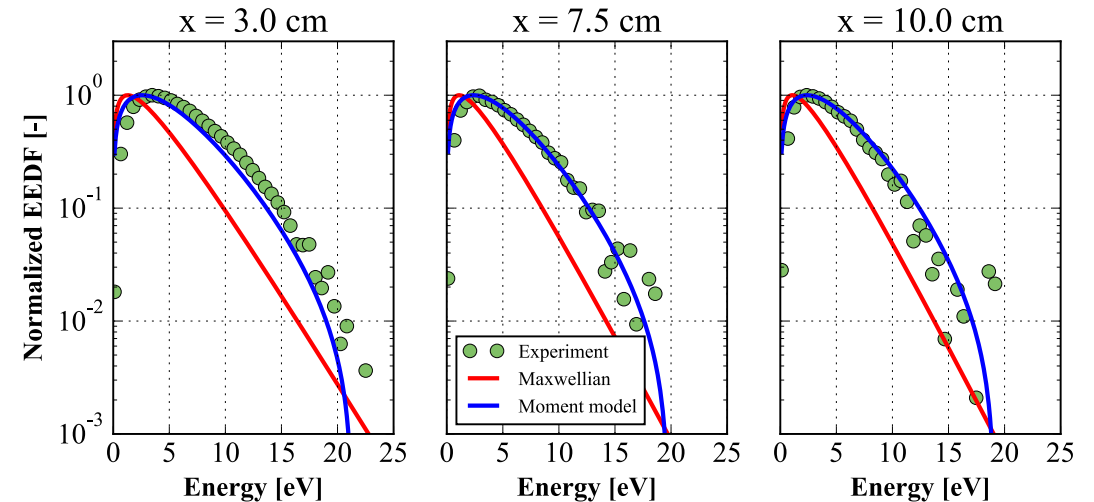
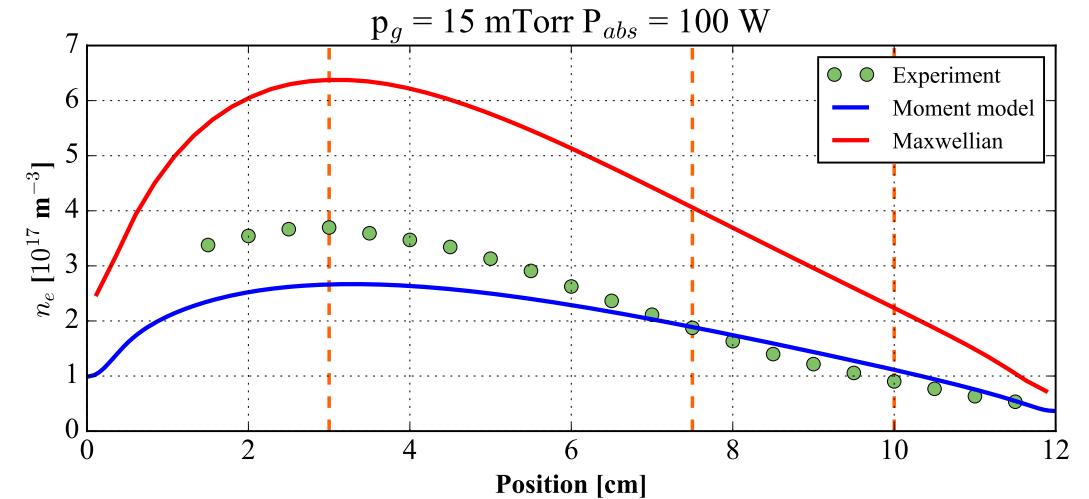


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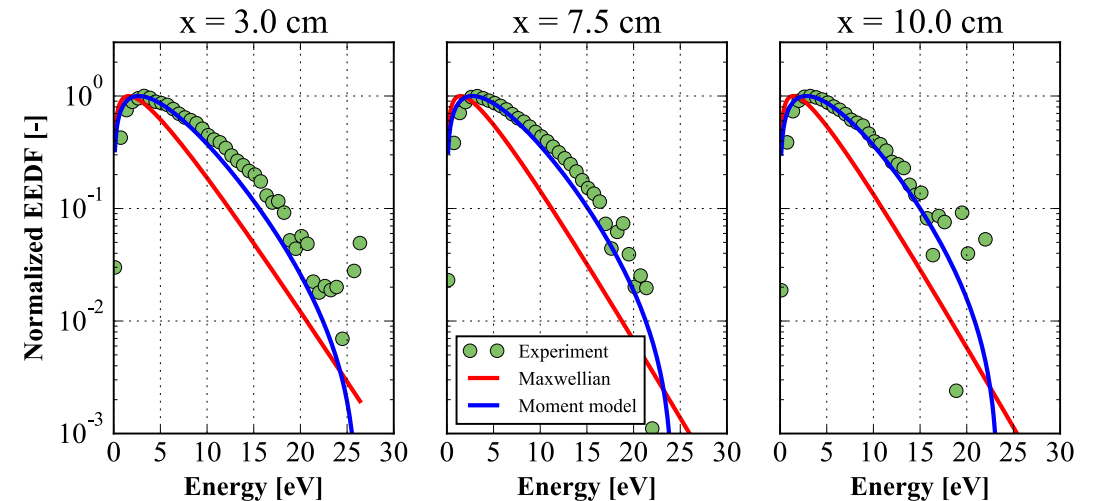
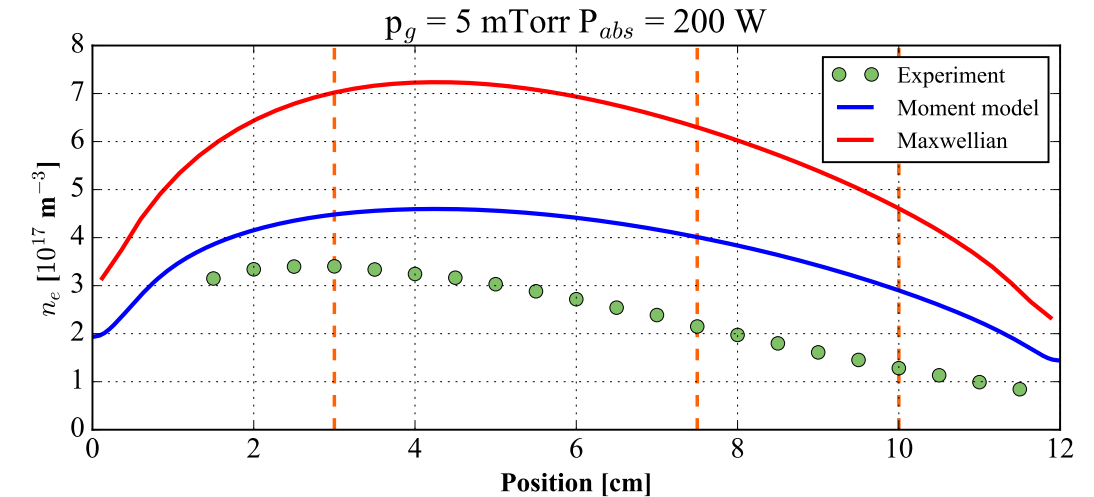


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# Intermediate ideas to take with you

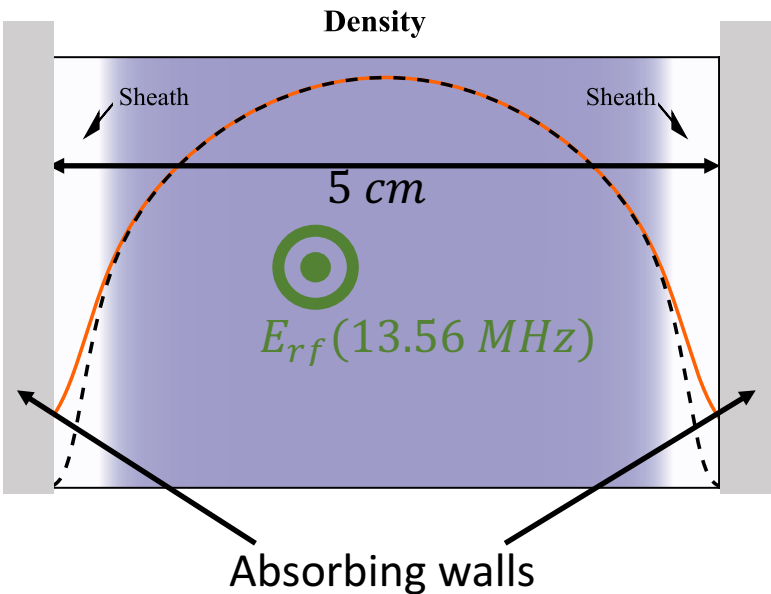
1. The model seems to capture the EEDF as measured in experiments and simulated by kinetic solvers
2. The model is very efficient as the transport coefficients are parametrized with the local excess kurtosis.
3. The 1D reduction seems to provide interesting results, **particularly in the comparison of the EEDF**.  
However, the reduction of the dimensionality adds additional simplifications.

# PART IV:

## Non-ambipolar models and future perspectives



# Non quasi-neutral model: ICP Discharge at low-pressure



We study a 1D ICP Xenon discharge:

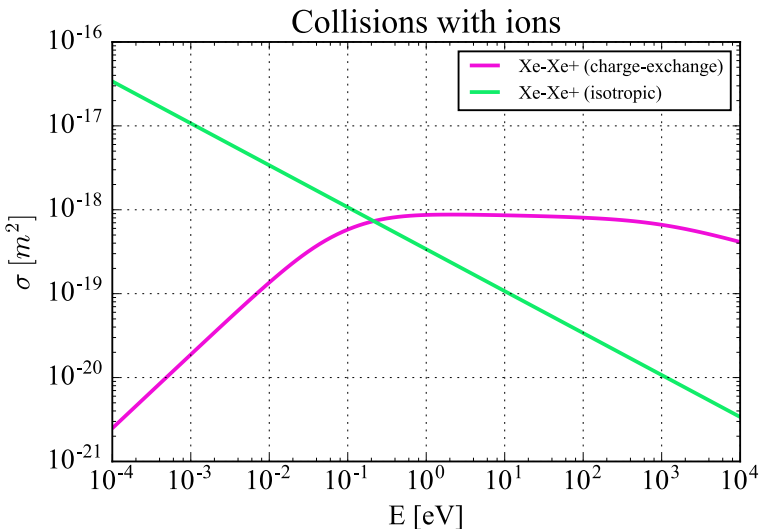
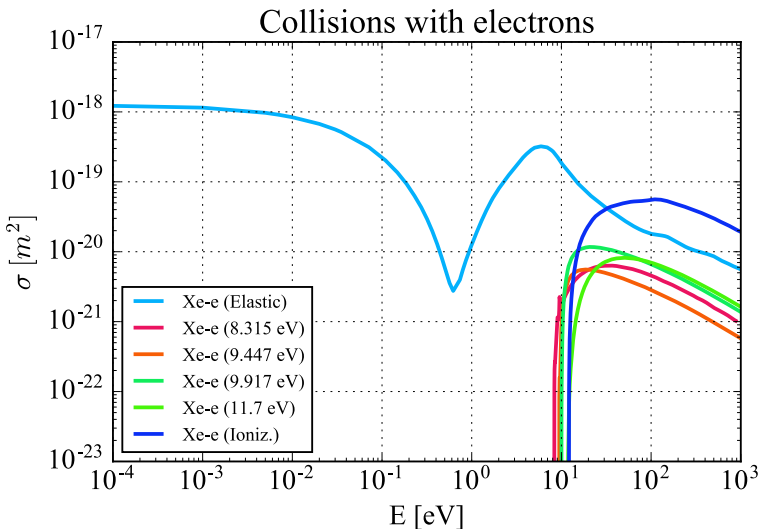
- $p_{\text{gas}} \sim 3 \text{ mTorr}$
- $n_e \sim 10^{15} \text{ m}^{-3}$
- 4 excitation collisions + single ionization + elastic + backscattering

We consider a model solving for:

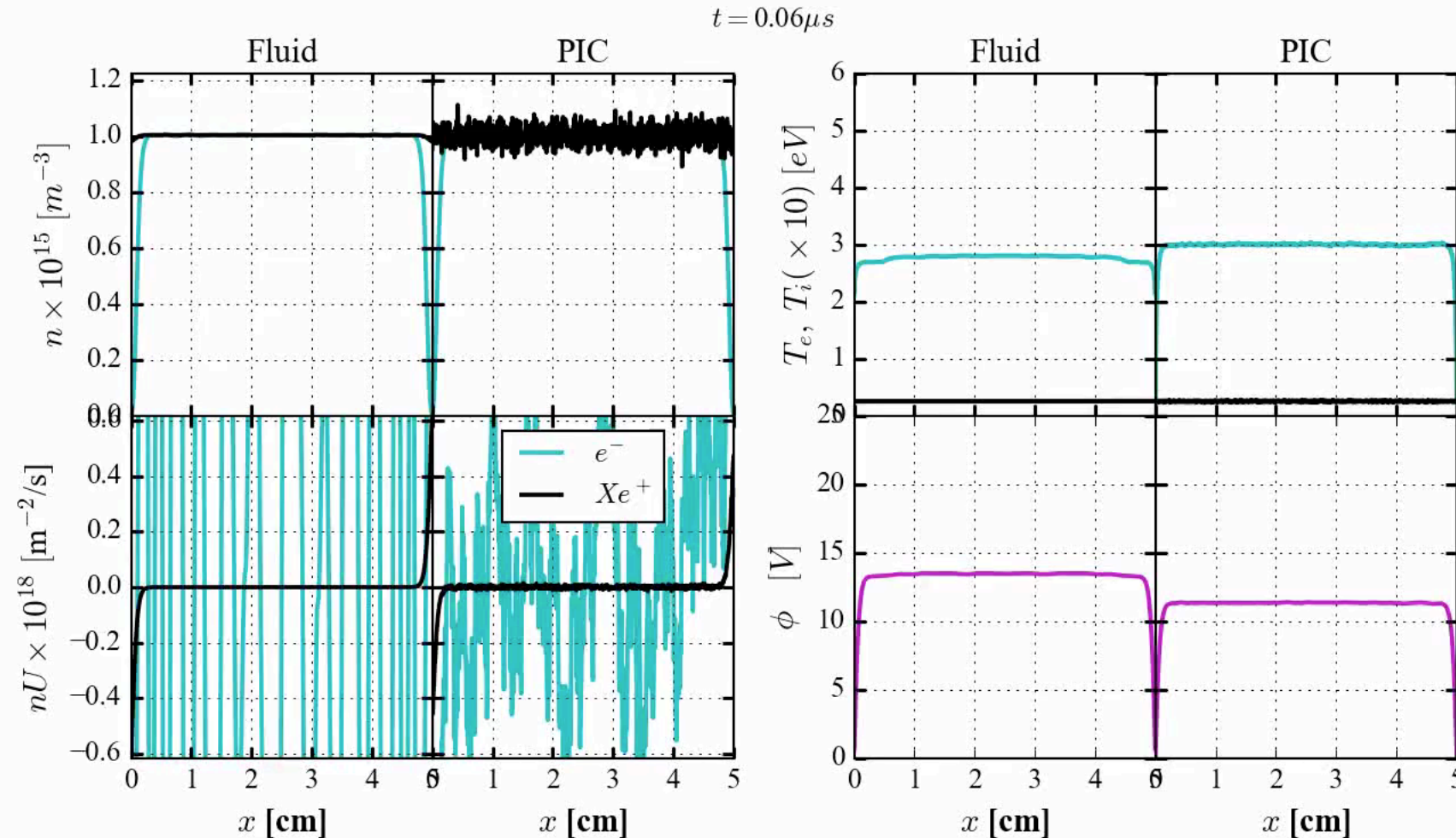
- 5 moments for electrons
- 3 moments for ions
- Poisson equation

| Reaction                                                       | Process             | Thresh. [eV] |
|----------------------------------------------------------------|---------------------|--------------|
| <i>Electron impact Xe</i>                                      |                     |              |
| $e + \text{Xe} \rightarrow e + \text{Xe}$                      | Elastic             | 0            |
| $e + \text{Xe} \rightarrow e + \text{Xe}^* (8.315 \text{ eV})$ | Excitation          | 8.315 eV     |
| $e + \text{Xe} \rightarrow e + \text{Xe}^* (9.447 \text{ eV})$ | Excitation          | 9.477 eV     |
| $e + \text{Xe} \rightarrow e + \text{Xe}^* (9.917 \text{ eV})$ | Excitation          | 9.917 eV     |
| $e + \text{Xe} \rightarrow e + \text{Xe}^* (11.7 \text{ eV})$  | Excitation          | 11.7 eV      |
| $e + \text{Xe} \rightarrow \text{Xe}^+ + 2e$                   | Elec. impact ioniz. | 12.13 eV     |
| <i>Scattering of ions</i>                                      |                     |              |
| $\text{Xe}^+ + \text{Xe} \rightarrow \text{Xe}^+ + \text{Xe}$  | Elastic             | 0            |
| $\text{Xe}^+ + \text{Xe} \rightarrow \text{Xe} + \text{Xe}^+$  | Charge exch.        | 0            |

Table : Collisional processes



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



## Model

### Electrons:

- Mass
- Momentum (with inertia)
- Energy
- Heat Flux
- **4<sup>th</sup>-moment**

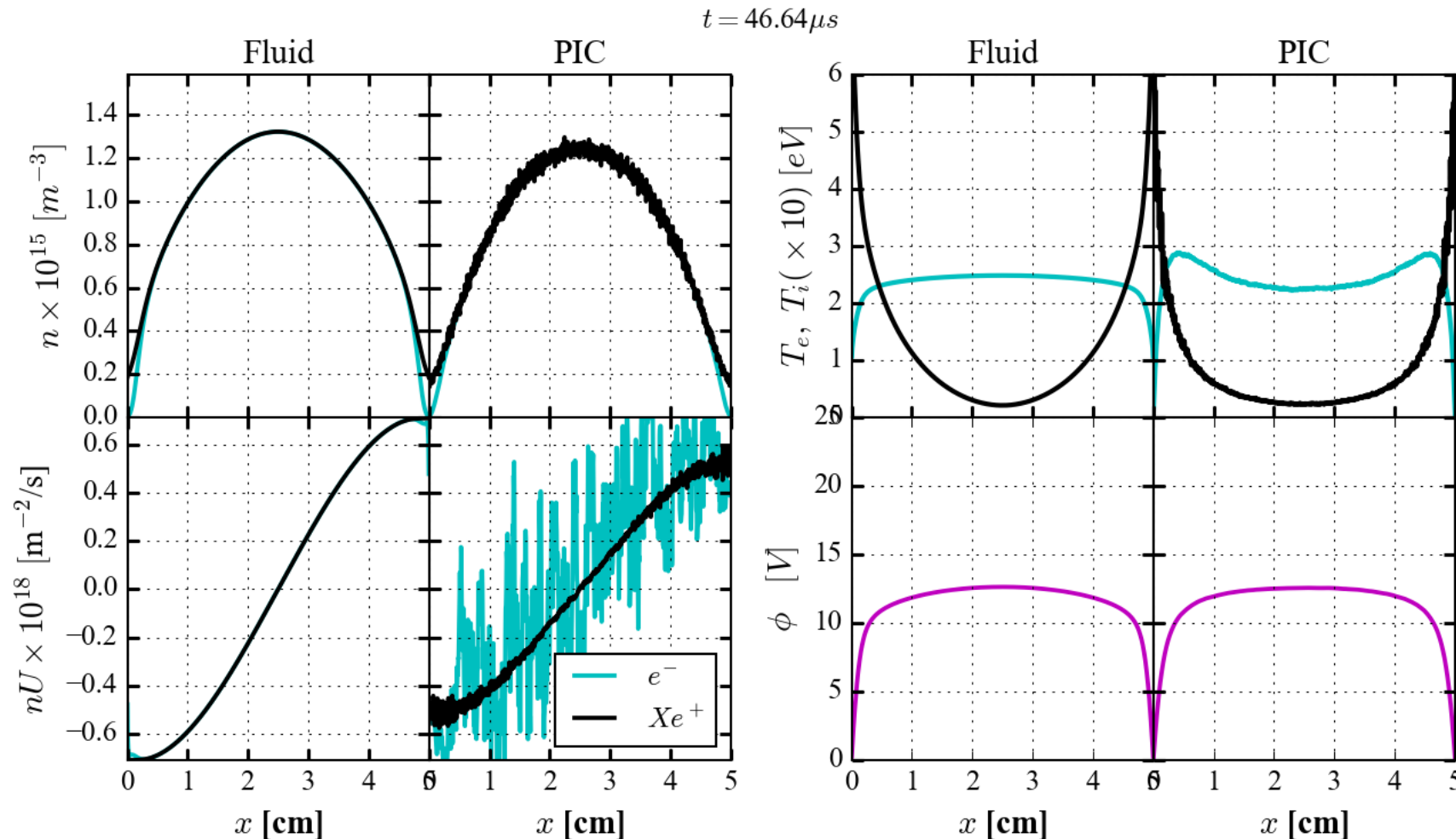
### Ions:

- Mass
  - Momentum
  - Energy
- } Collisions follow Benilov (1998)

### Poisson Eq.

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

## Converged solution



## Comparison

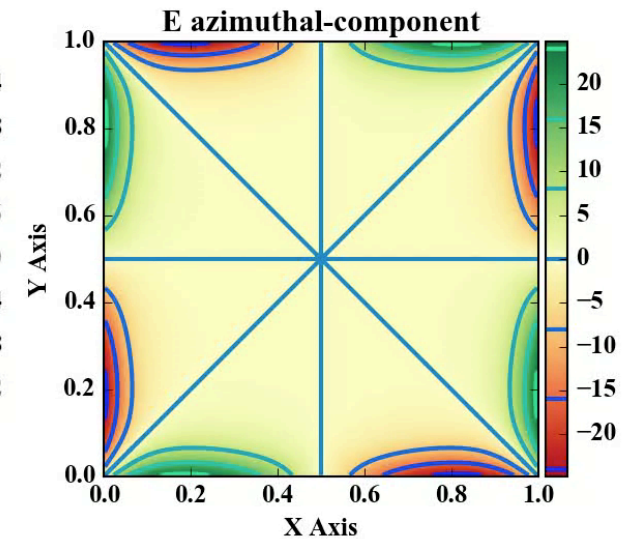
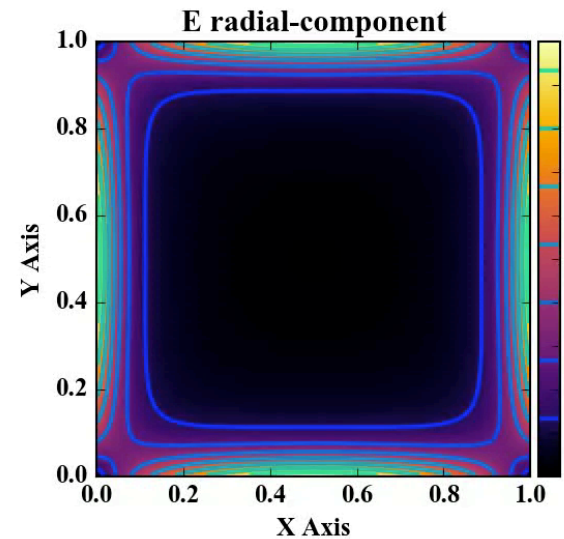
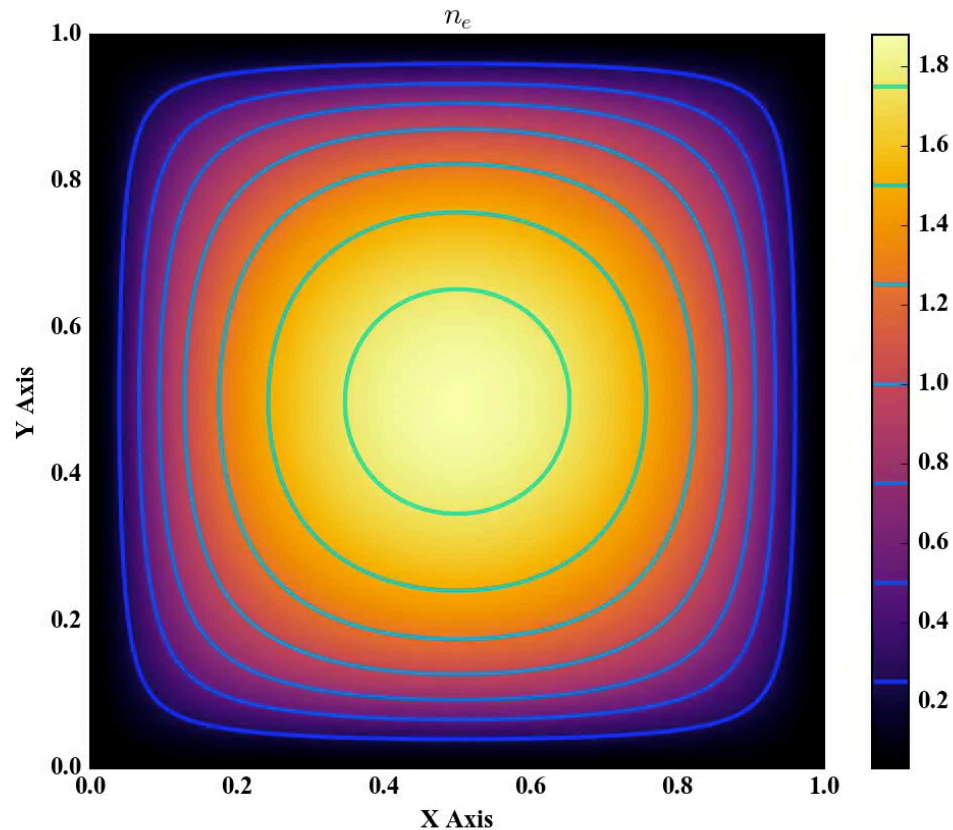
- Density is closer
- Temperature drops at the seath
- Ion temperature is well captured
- Flux at the wall is overestimated
- The potential drop is identical



# Perspectives: extension to multi-dimensions

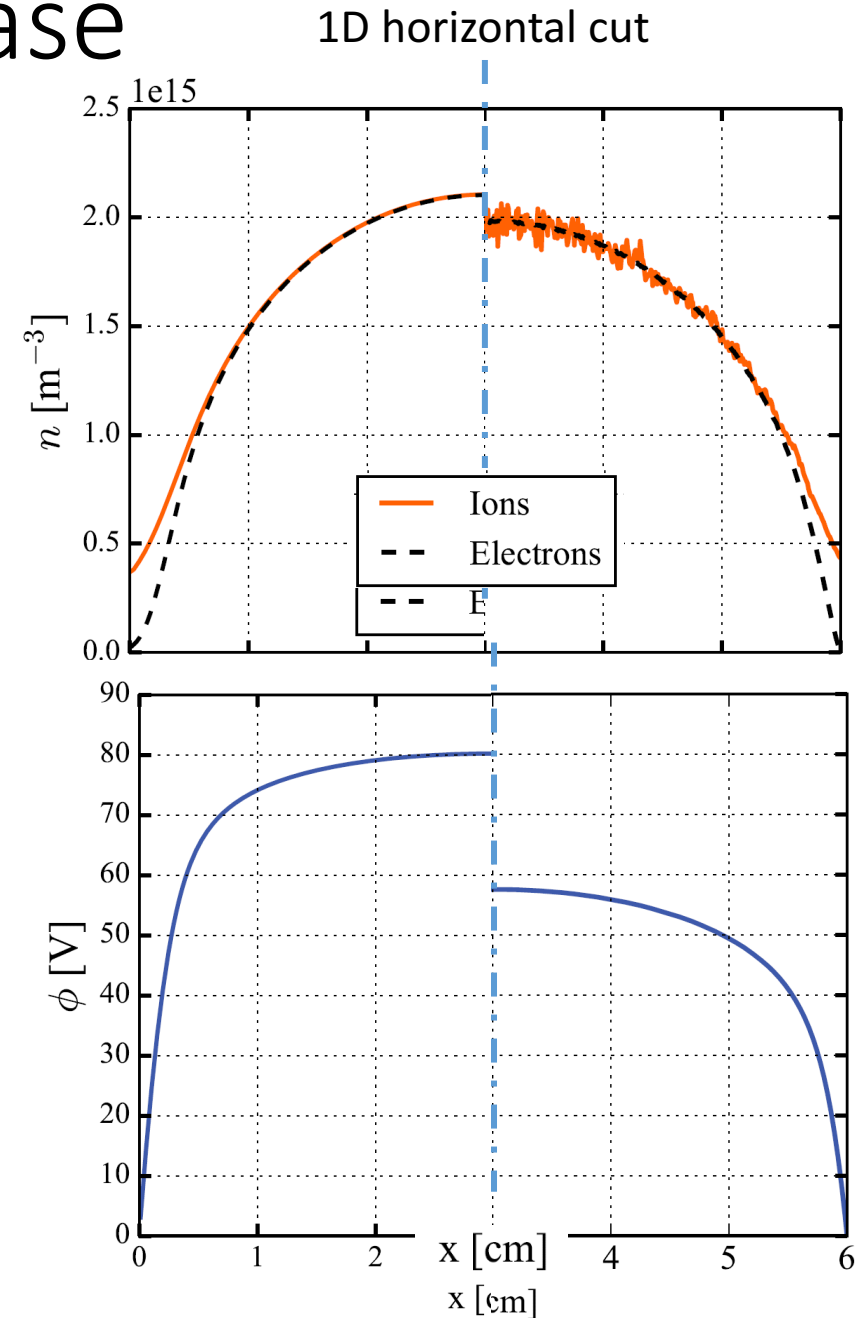
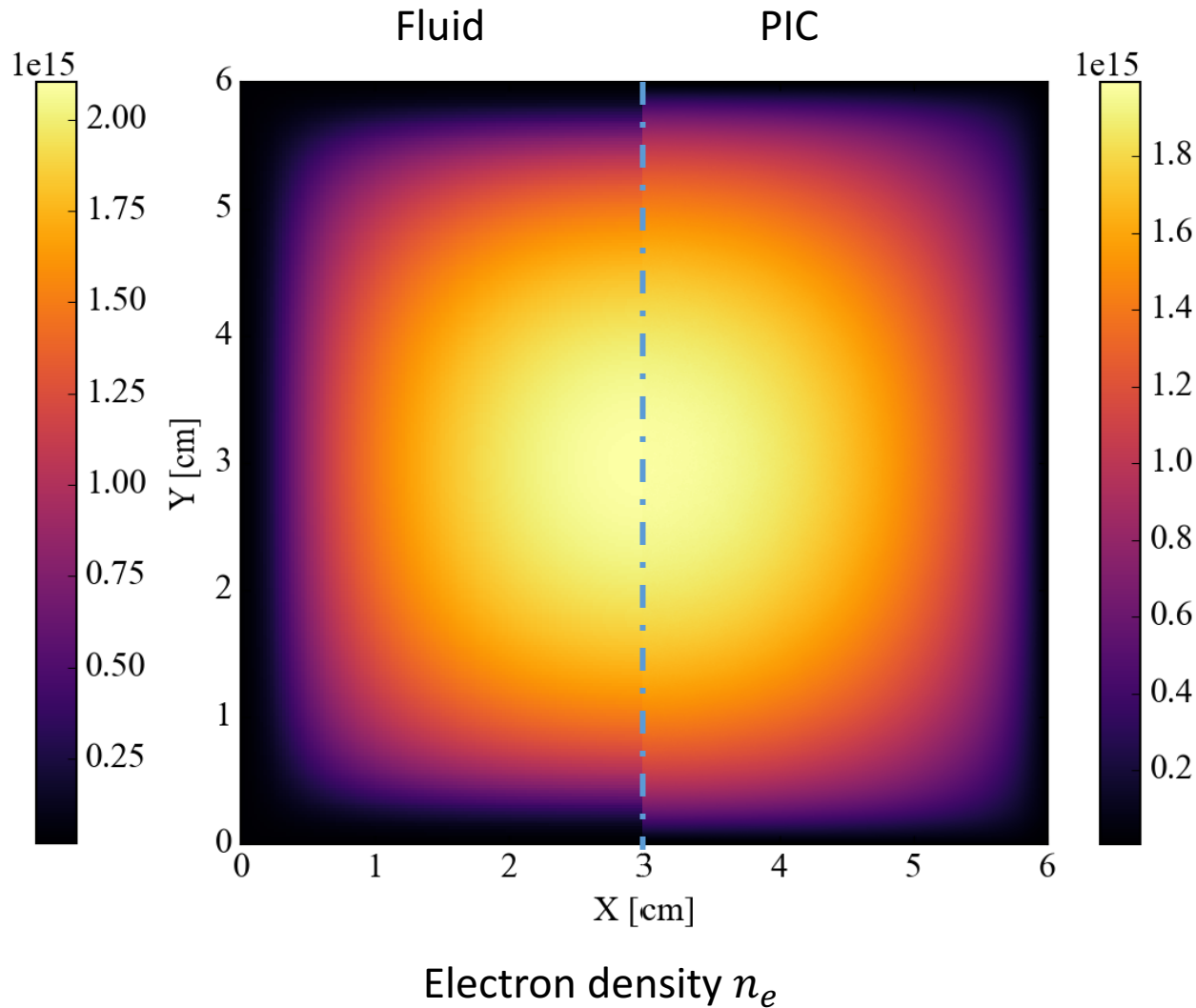
1. **An isothermal moment model (including electron inertia)** is implemented in a 2D code for magnetized discharges. The set of equations allows for representing instabilities and situations with non-ambipolar diffusion.

Work of Louis Reboul's PhD thesis.

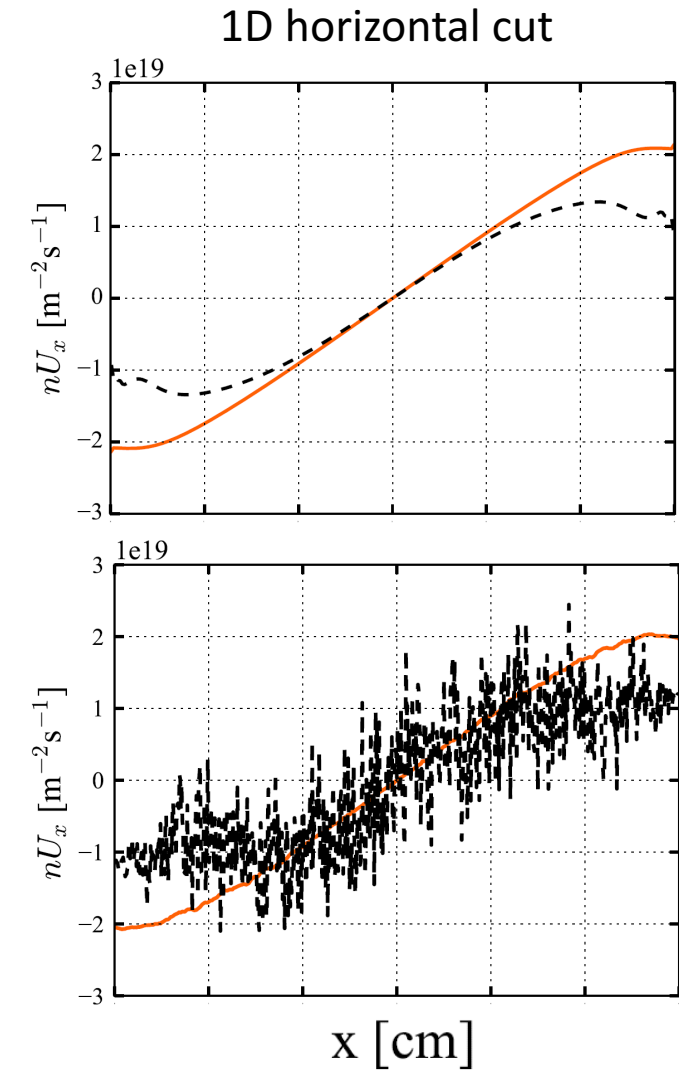
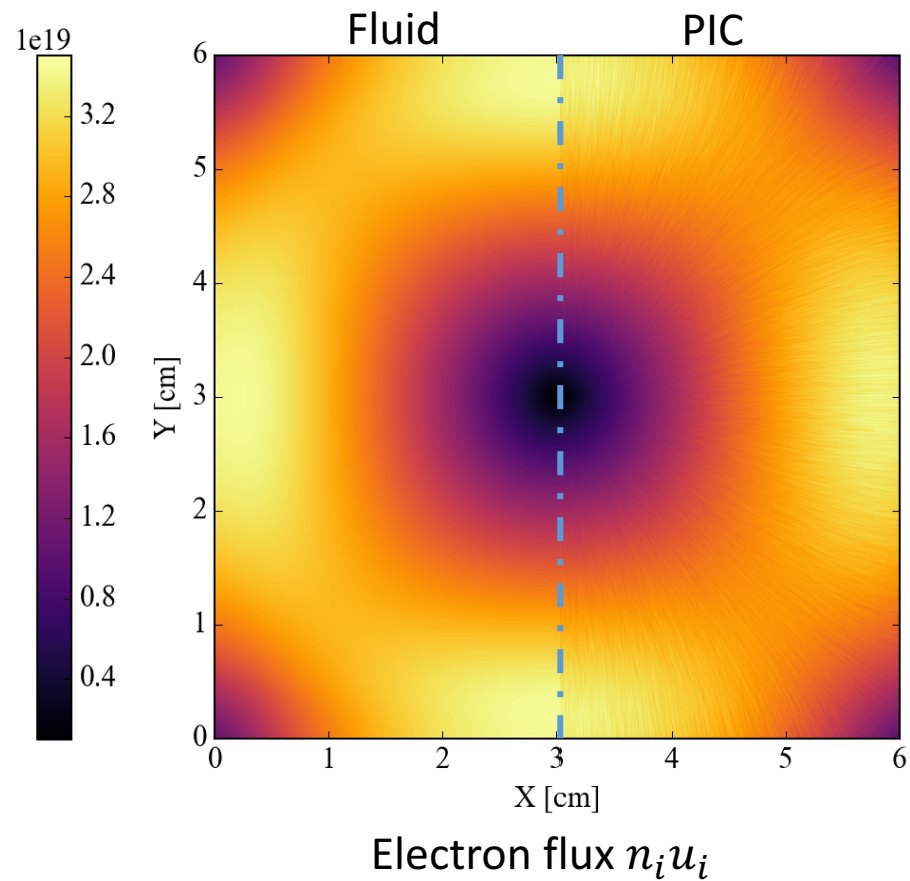
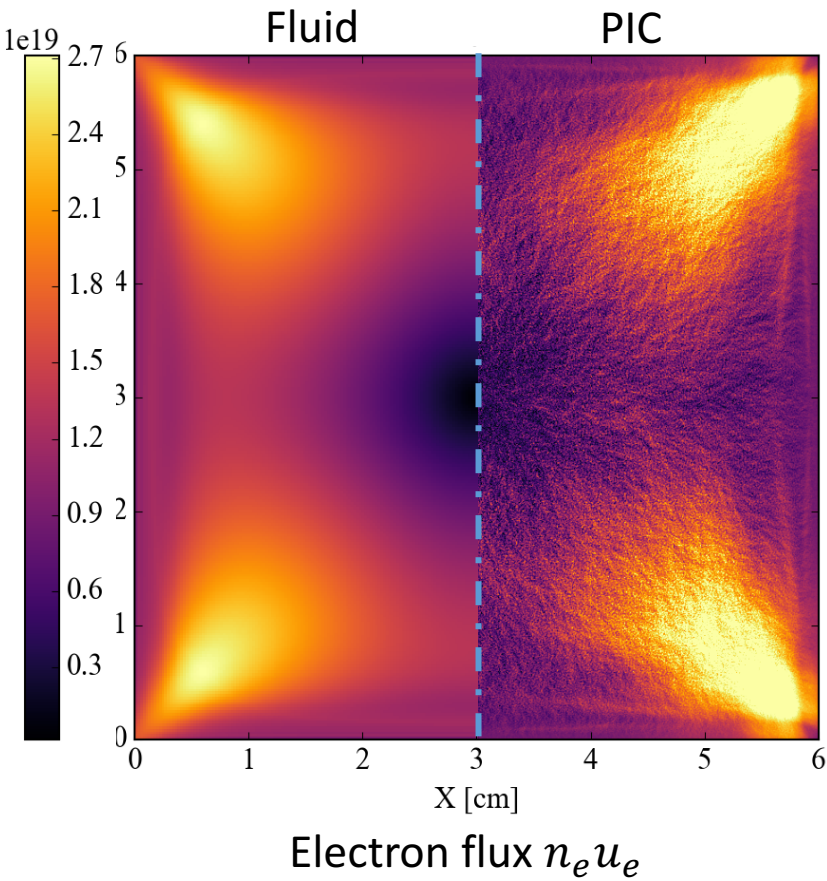




# Isothermal non-magnetized case



# Isothermal non-magnetized case



# Summary and conclusions

1. The model seems promising for capturing the non-equilibrium processes under the conditions of interest of ICP discharges (high-density plasmas in large systems)
2. The comparison with PIC is also promising and shows the improvement due to the fourth moment
3. The model would help to study 2D/3D effects that might be important (especially in the presence of a magnetic field)
4. Paper with derivation of the model and comparison to experiments in preparation.

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