Development of high order Discontinuous Galerkin fluid solver for argon plasma flows

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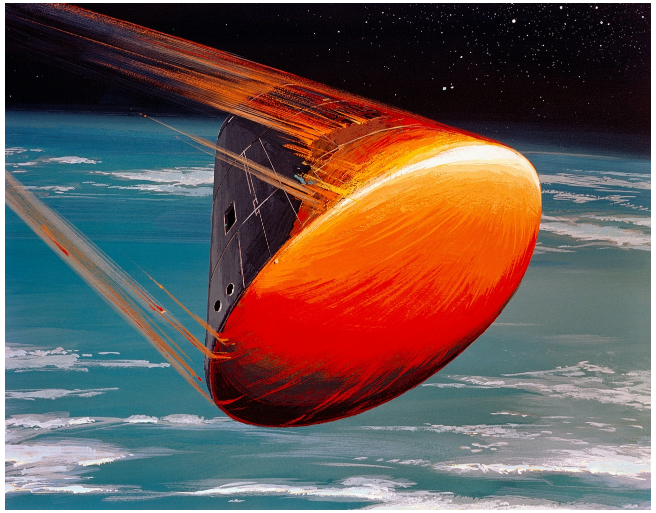
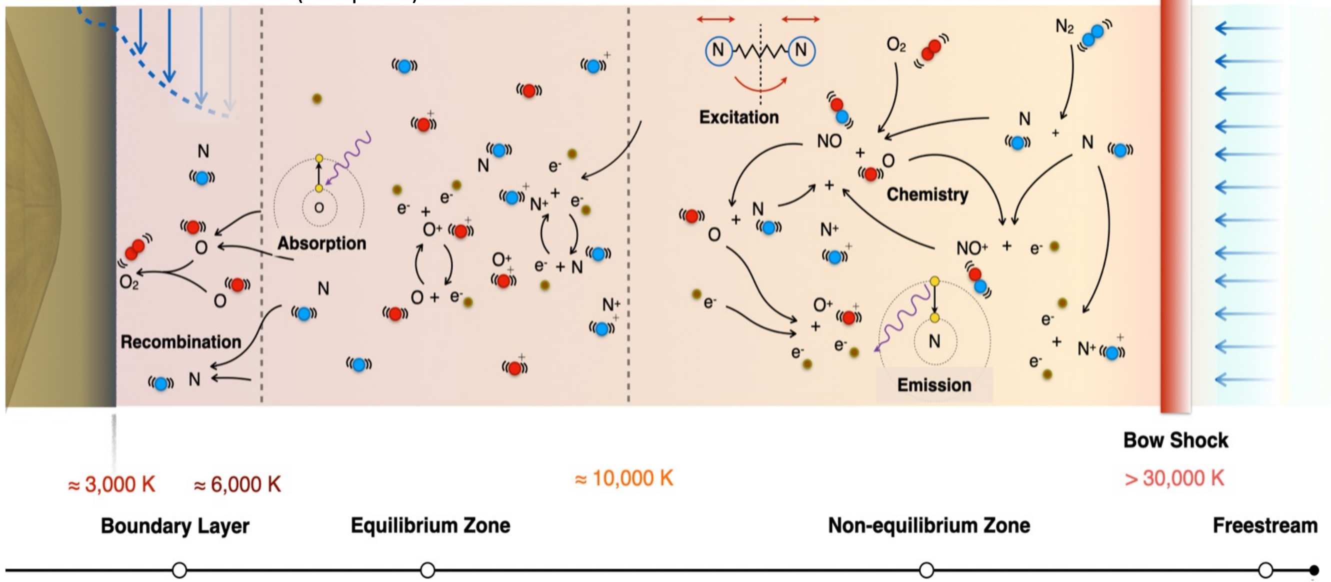
Hypersonic Flight



Artistic impression of Apollo capsule reentry (Wikipedia)

$$M_\infty > 5$$

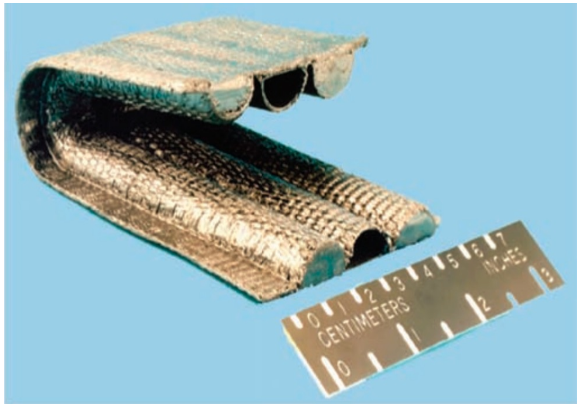
Concept art of an hypersonic vehicle (Raytheon)



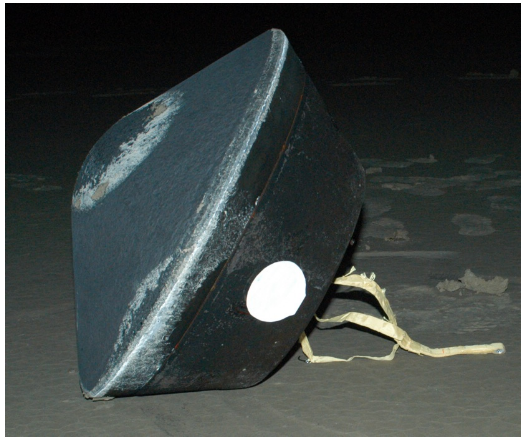
Chemistry and plasma formation behind an hypersonic shock (A. Del Val)

- High temperatures
- Formation of new species:
  - Molecules (Ions + Neutrals)
  - Atoms (Ions + Neutrals)
  - Electrons

Thermal protection systems (TPS) for hypersonic cruise flight

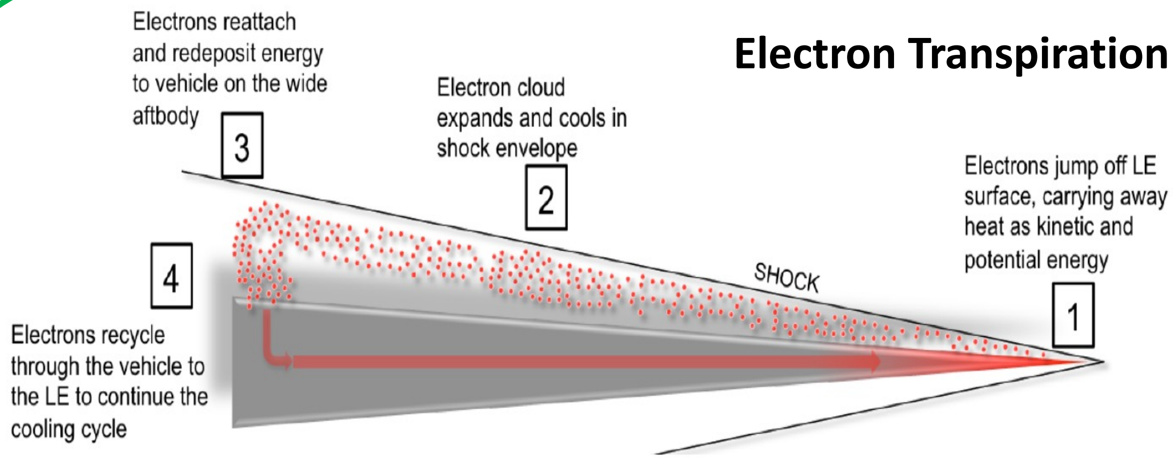


Heat-pipe-cooled leading edge (NASA)

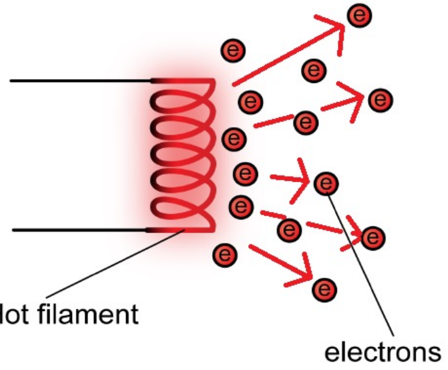


Stardust: utilized ablation thermal protection system (NASA)

Electron Transpiration Cooling



Schematics of ETC for **hypersonic leading edges** (Uribarri, Allen 2015)



Schematic of **thermionic emission** (Adapted from [Hanquist,2017])

$$J_e \propto T_w^2 \exp\left(\frac{-W_F}{T_w}\right)$$

- ✓ Preserves shape of the component
- ✓ No excessive weight added
- Materials must have low work function W_F
- Subjected to corrosion

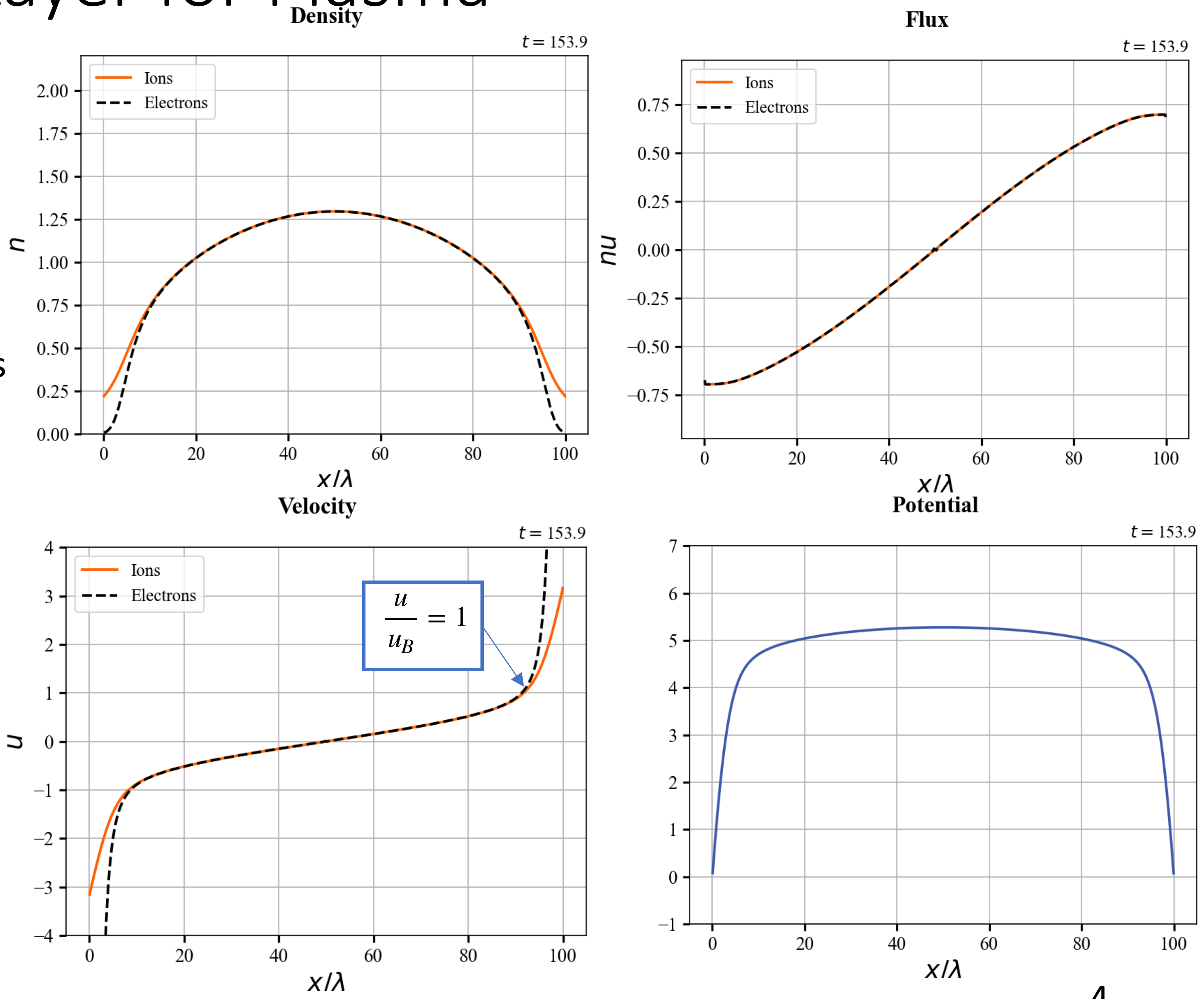
Sheath: a Boundary Layer for Plasma

- **Bulk**
  - Quasi-neutrality $n_e \sim n_i$
  - Production of particles through of ionization ($\propto n_e(x)$)
- **Sheath**
  - The electron thermal flux to the wall is higher than the ion ones due to the **disparity of inertia**

$$J_e = n_e\sqrt{\frac{8k_B T_e}{\pi m_e}} \gg J_h = n_i\sqrt{\frac{8k_B T_h}{\pi m_h}}$$

  - At **steady state** a potential gradient develops in order to guarantee the equivalence of fluxes
  - The ions are accelerated at the so called **Bohm speed** (only collisionless)

$$u_B = \sqrt{\frac{k_B T_e}{m_i}}$$



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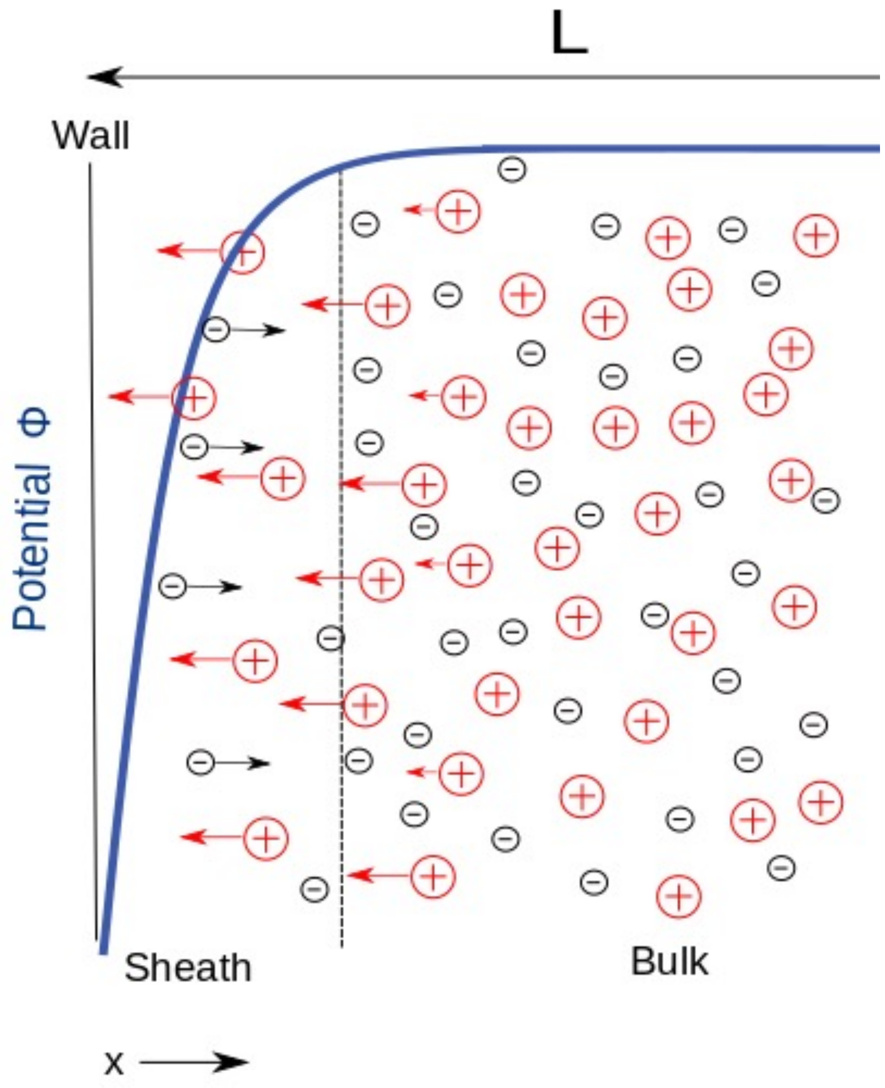

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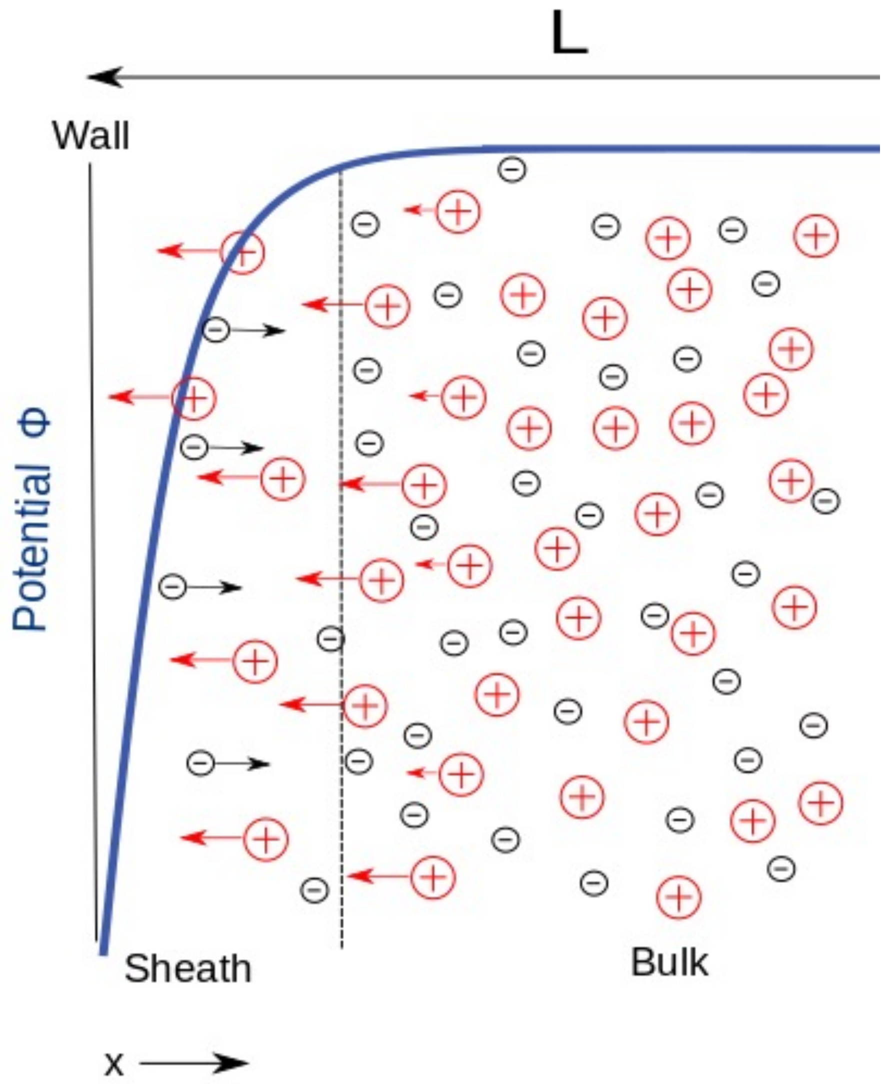
- Simulating Plasma
  - Fluid Modeling of plasma-sheath
- Numerical method
- Results
- Conclusions and Future Works

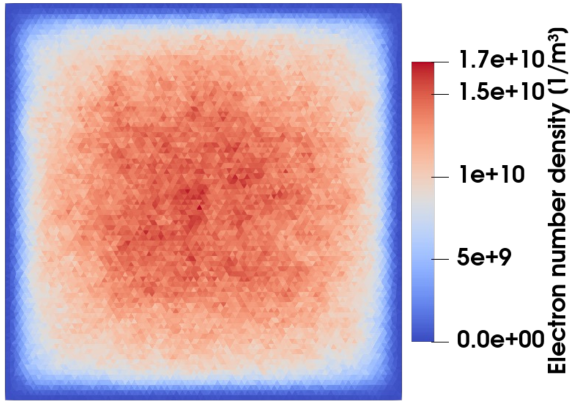


Simulating Plasma

Rarefied — Continuum

Increasing pressure (and so number of particles!)

Particle methods



Particle-In-Cell - Direct Simulation Monte Carlo (PIC-DSMC) (Credit P. Parodi)

- More accurate
- More computational expensive (suited for rarefied gases)

Fluid models

- Multifluid
- Multicomponent

- Governing equations of macroscopic quantities
- Less accurate but less computational expensive

Fluid modeling Challenges

MULTIFLUID (MF)

State-of-the-Art

- Each species treated as a single fluid

n_k	Species number density
u_k	**Species** velocity
T_k	Species temperature

✗ Air11 **44**

MULTICOMPONENT (MC)

Proposed Approach

- The plasma is treated as a single fluid (**Bulk**), with species diffusing inside

n_k	Species number density
u	**Bulk** velocity
T_h, T_e	Heavy/electron temperature

✓ Air11 **16**

$$\mathrm{Air11} = \{\mathrm{N_2}, \mathrm{O_2}, \mathrm{N}, \mathrm{O}, \mathrm{NO}, \mathrm{N_2^+}, \mathrm{O_2^+}, \mathrm{N^+}, \mathrm{O^+}, \mathrm{NO^+}, \mathrm{e^-}\}$$

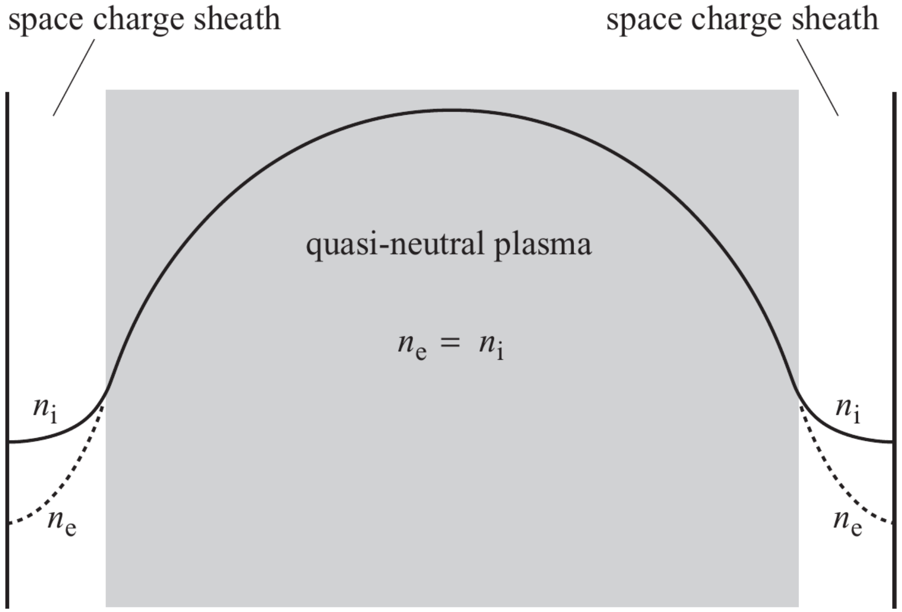
MF:

- **Poisson equation** for charge conservation
- **Plasma physics** community

MC:

- **Poisson equation** for charge conservation
- **Re-entry** and **Combustion** community

Simulating the sheath



One-dimensional discharge [Chabert & Braithwaite, 2011]

Pressure [Pa]	$n_n = {p_n}/{k_B T_h}$	$\eta = \frac{n^0_{charges}}{n^0_{neutr}}$
1	$1.25 \cdot 10^{20}\ m^{-3}$	$\sim 10^{-4}$
10	$1.25 \cdot 10^{21}\ m^{-3}$	$\sim 10^{-5}$
100	$1.25 \cdot 10^{22}\ m^{-3}$	$\sim 10^{-6}$
1000	$1.25 \cdot 10^{23}\ m^{-3}$	$\sim 10^{-7}$

DC Discharge

- S = {Ar^+, e^-} in an uniform thermal bath of neutrals
- **Isothermal** mixture
- Floating walls
  - Incident particles are **absorbed** and "reinjected" in the domain (proportional to $n_e(x)$)

Challenges

- Strong **disparity of inertia** of the simulated species (electrons vs. heavies)
- Small sheath width ($\sim 10\ \lambda_D$)

$$\lambda_D = \sqrt{\frac{\epsilon_0 k_B T_e}{n_e e^2}} \sim 10^{-4}\mathrm{m}$$

- Thermal non-equilibrium ($T_e = 23209.08\ K \gg T_h = 580.22\ K$)

Governing Equations – Multifluid*

$$\partial_t n_e + \partial_x \left(n_e u_e\right) = n_e \nu^{iz},$$ Electron Density

$$\partial_t n_i + \partial_x \left(n_i u_i\right) = n_e \nu^{iz},$$ Ion Density

$$\partial_t \left(n_e u_e\right) + \partial_x \left[n_e \left(u_e^2 + \varepsilon^{-1}\right)\right] = \varepsilon^{-1} n_e \partial_x \phi - n_e u_e \nu_{en},$$ Electron Momentum

$$\partial_t \left(n_i u_i\right) + \partial_x \left[n_i \left(u_i^2 + \kappa\right)\right] = - n_i \partial_x \phi - n_i u_i \nu_{in}$$ Ion Momentum

$$\partial_{xx}^2 \phi = \chi^{-1} \left(n_e - n_i\right)$$ Poisson

Ionization (red)

Elastic collisions (green)

Argon Testcase

$$\varepsilon = \frac{m_e}{m_i} = 1.36 \cdot 10^{-5}, \quad \kappa = \frac{T_i}{T_e} = 0.025, \quad \chi = \frac{\lambda_D^2}{L_0^2} = 10^{-4}$$

*Alvarez Laguna et al.(2020)

Governing Equations - Multicomponent

$$\partial_t n_e + \partial_x (n_e u) + \partial_x (n_e V_e) = n_e \nu^{iz},$$

$$\partial_t n_i + \partial_x (n_i u) + \partial_x (n_i V_i) = n_e \nu^{iz},$$

$$\partial_t (\rho u) + \partial_x (\rho u^2 + p) = - n q \partial_x \phi - \sum_{j \in \mathscr{C}} \rho_j u_j \nu_{jn}$$

$$\partial^2_{xx} \phi = \chi^{-1} (n_e - n_i)$$

Electron Density

Ion Density

Momentum (Fluid)

Poisson

$$n q = n_e q_e + n_i q_i$$

$$\rho u = \sum_j \rho_j u_j = \sum_{j \in \mathscr{S}} \int m_j c_j f_j d c_j$$

$$p = \sum_{j \in \mathscr{S}} p_j$$

$$V_k = \frac{1}{n_k} \int C_k f_k d c_k, \quad C_k = c_k - u$$

Binary Diffusion

$$V_k = \left(- \frac{D_k}{n_k} \partial_x n_k - \mu_k \partial_x \phi \right) \quad D_k = \frac{k_B T_k}{m_k \nu_k} \quad \mu_k = \frac{e}{m_k \nu_k}$$

- Diffusion Velocity (yellow)
- Elastic collisions (green)
- Ionization (red)

Momentum equation

$$\partial_t(\rho u) + \partial_x(\rho u^2 + p) = -nq\partial_x\phi - \sum_{j\in\mathscr{C}} \rho_j u_j \nu_{jn}$$

$$\rho u = \rho_e u_e + \rho_i u_i + \rho_n u_n = n_e m_e u_e + n_i m_i u_i + n_n m_n u_n$$

$$p = p_e + p_i + p_n = n_e k_B T_e + n_i k_B T_h + n_n k_B T_h$$

$$nq = n_e q_e + n_i q_i$$

Neutrals at rest as background gas

$$n_{e,i} = n^0_{charges}\bar{n}_{e,i}$$

$$u_0 = u_B = \sqrt{\frac{k_B T_e}{m_i}}$$

$$\varepsilon = \frac{m_e}{m_i} \sim 10^{-5}$$

$$\kappa = \frac{T_h}{T_e} \sim 10^{-2}$$

$$\bar{\rho}\,\bar{u} = n^0_{charges} u_0 m_h (\varepsilon \bar{n}_e \bar{u}_e + \bar{n}_i \bar{u}_i)$$

$$\bar{p} = n^0_{charges} u_0^2 (\bar{n}_e + \kappa \bar{n}_i)$$

$$\bar{n}\,\bar{q} = n^0_{charges} e\,[(\bar{n}_e - \bar{n}_i)]$$

$$\bar{\rho}\,\bar{u} \sim \bar{n}_i \bar{u}_i$$

Electron pressure

Lorentz force

Updated MC
momentum equation

$$\partial_t(n_i u_i) + \partial_x[n_i(u_i^2 + \kappa) + n_e] = (n_e - n_i)\partial_x\phi - n_i u_i \nu_{in}$$

Ion MF
momentum equation

$$\partial_t(n_i u_i) + \partial_x[n_i(u_i^2 + \kappa)] = -n_i\partial_x\phi - n_i u_i \nu_{in}$$

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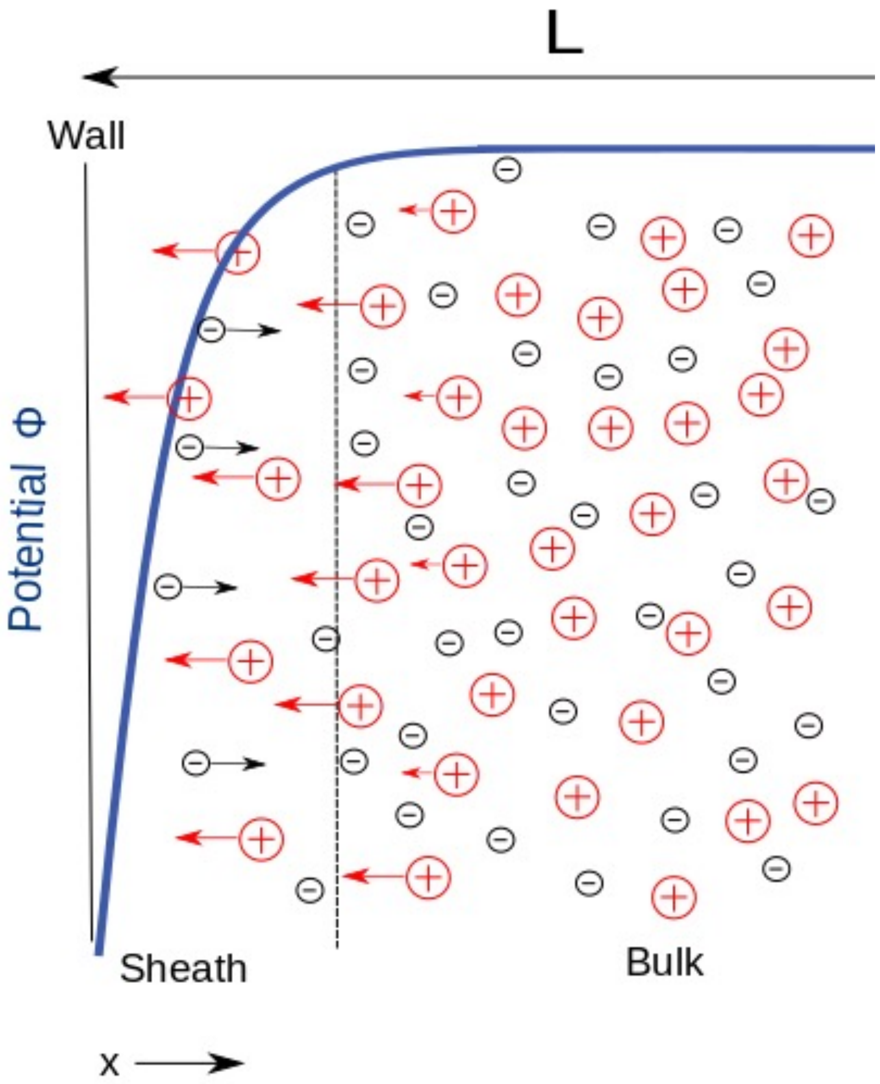
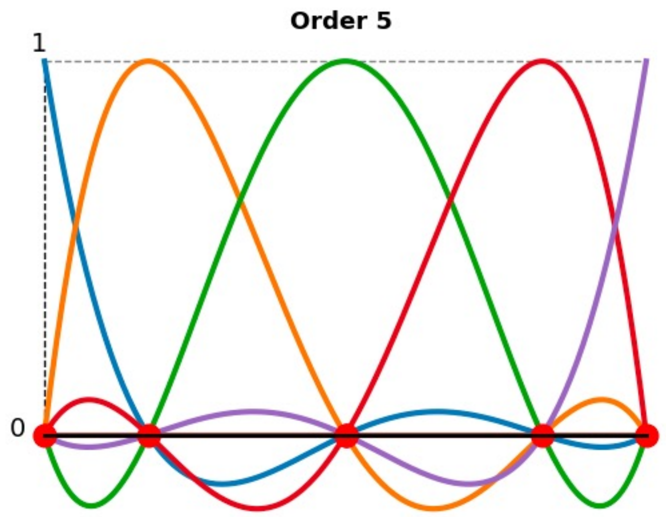
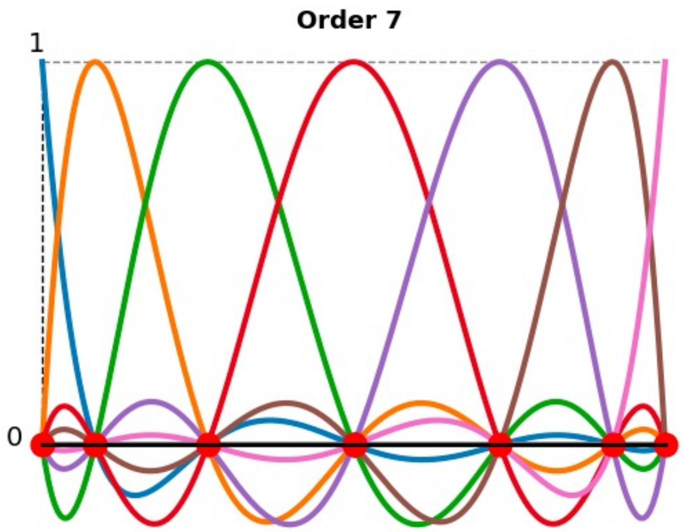


Numerical Methods

- **Reference Solution**
  - **Multifluid**
  - Roe, Lax Friedrichs
  - ESDIRK64

- **Binary Diffusion**
  - **Multicomponent**
  - Roe, Lax Friedrichs
  - Incomplete Penalty Method (IPM)
  - ESDIRK64





An adapted Explicit first stage Single Diagonally Implicit Runge-Kutta (ESDIRK64) scheme

$$\mathcal{B} = \begin{array}{c|c} \mathbf{c}^T & \mathbf{A} \\ \hline 0 & \mathbf{b} \end{array} \quad \Rightarrow \quad \begin{array}{c|cccc} 0 & a_{11} & a_{1,2} & \cdots & a_{1s} \\ c_2 & a_{21} & a_{22} & \cdots & a_{2s} \\ \vdots & \vdots & & \ddots & \cdots \\ c_s & a_{s,1} & a_{s,2} & \cdots & a_{s,s} \\ \hline 0 & b_1 & b_2 & \cdots & b_s \end{array}$$

Residual vector

$$\hat{\mathbf{u}}^k = \beta\,\mathbf{u}^n + \Delta t \sum_{j=1}^{s} a_{ij}\mathbf{M}^{-1}\mathbf{R}\left(\hat{\mathbf{u}}^j\right), \quad k = 1,\ldots,s$$

$$\mathbf{u}^{n+1} = \mathbf{u}^n + \Delta t \sum_{j=1}^{k} b_j \mathbf{M}^{-1}\mathbf{R}\left(\hat{\mathbf{u}}^j\right)$$

Mass matrix

$$\beta = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 0 \end{pmatrix}$$

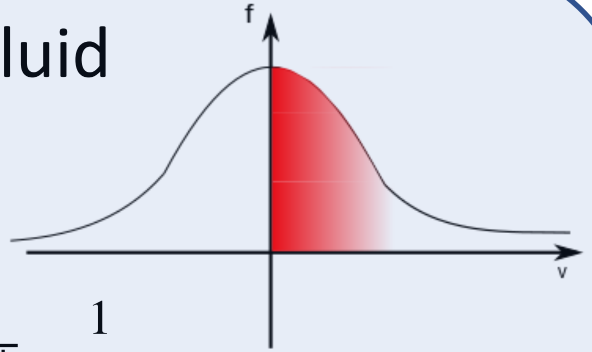
Fluid equations

Poisson

$$\begin{pmatrix} 1 \\ 1 \\ 1 \\ 0 \end{pmatrix} = \beta^{MC}$$

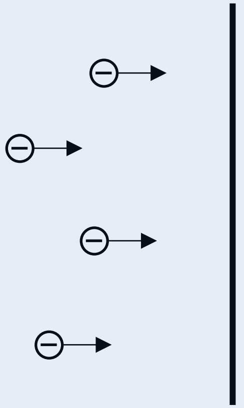
Boundary conditions

Multifluid



- **Electrons (Subsonic)**

$$\left(u_e\right)^{L,R} = \mp \frac{1}{\sqrt{2\pi\varepsilon}}$$



- **Ions (Supersonic)**

$$n_e^G = n_e^{int}$$

$$n_i^G = n_i^{int}$$

$$u_i^G = u_i^{int}$$

- **Potential (Floating wall)**

$$V_W = 0$$

Multicomponent

- **Electrons**

$$\Gamma_e^{L,R} = F^C + F^D = \left(n_e u_e + n_e V_e\right)^{L,R} = \mp \frac{n_e}{\sqrt{2\pi\varepsilon}}$$

- **Ions**

$$n_i^G = n_i^{int}$$

$$u_i^G = u_i^{int}$$

- **Potential (Floating wall)**

$$V_W = 0$$

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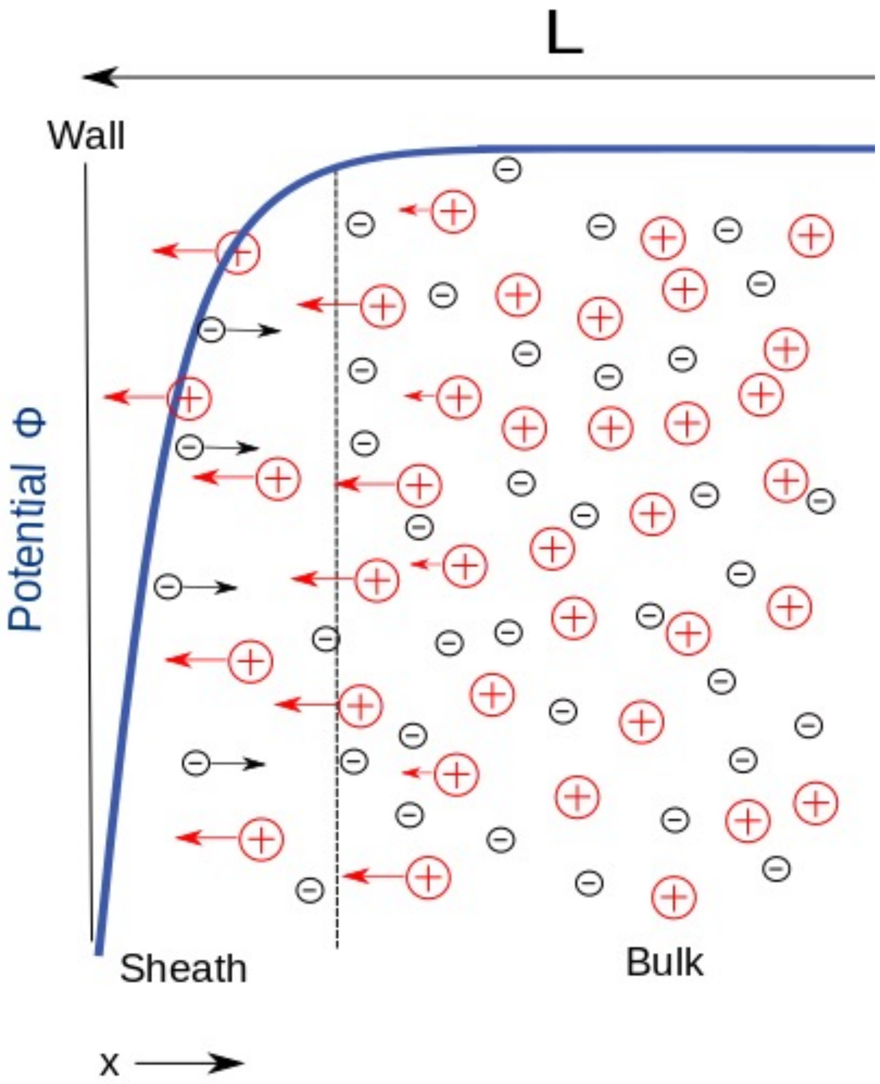


Collisionality and asymptotic behaviour*

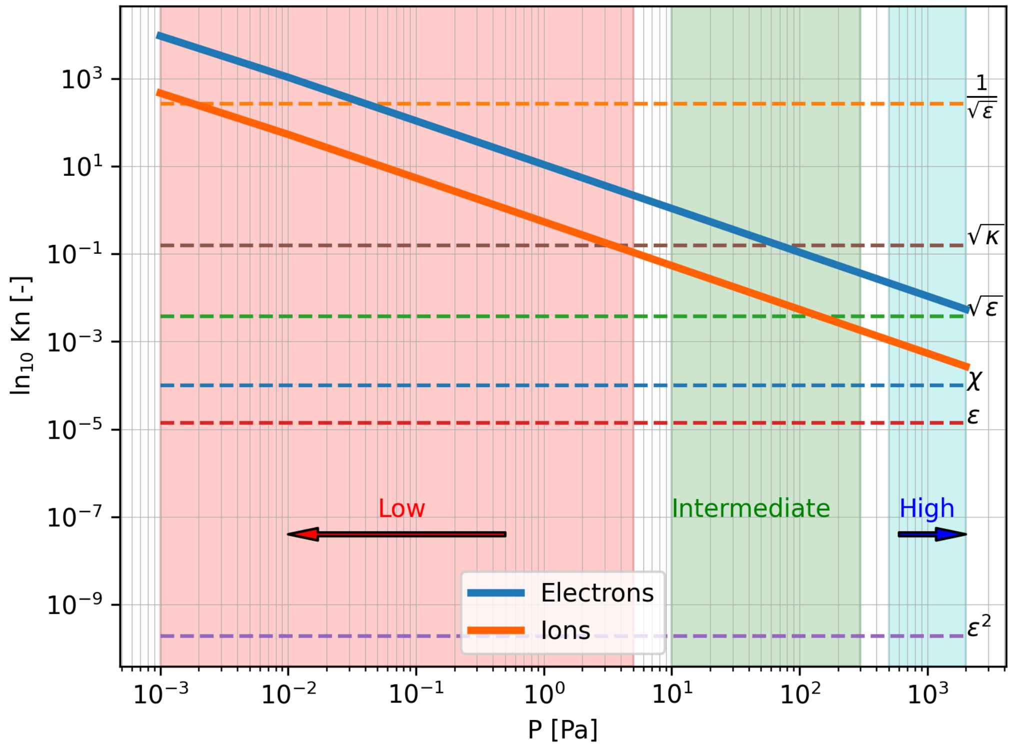
$$\nu_{en} = \left[\frac{1}{t_0}\right] \underbrace{\frac{16}{3\sqrt{2\pi}} \frac{1}{\sqrt{\varepsilon}\mathrm{Kn}_{en}}}_{\bar{\nu}_{en}}$$

$$\nu_{in} = \left[\frac{1}{t_0}\right] \underbrace{\frac{8}{3\sqrt{\pi}} \frac{\sqrt{\kappa}}{\mathrm{Kn}_{in}}}_{\bar{\nu}_{in}}$$

Knudsen number

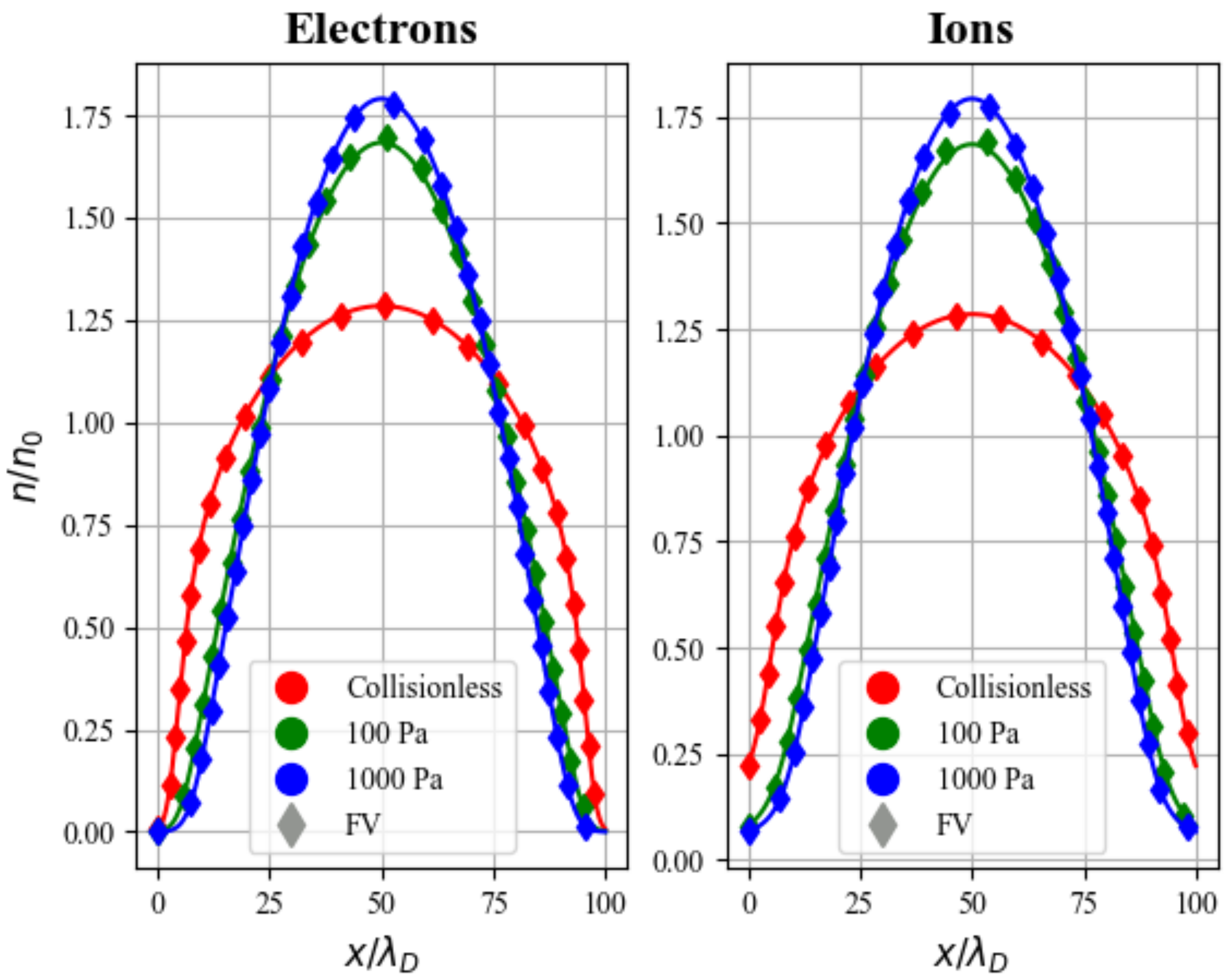
$$\mathrm{Kn}_{kn} = \frac{\lambda_{kn}\left(n^0, \Omega_{kn}\right)}{L_0}$$

Bulk $L_0 = L$



How different models behave with Knudsen number varying?

Comparison FV-DG



Finite Volume

- Roe Flux with third order solution reconstruction
- Third Order explicit Runge-Kutta
- 602 cells (more refined close to the wall)

Discontinuous Galerkin

- Roe Flux
- Adapted 4th order six-stage Explicit first stage Single Diagonally Implicit Runge-Kutta (ESDIRK64) scheme
- 4th order Interpolation Gauss-Lobatto-Legendre
- 100 cells

Low and High pressure regimes*

Multifluid

$$\partial_t n_e + \partial_x (n_e u_e) = n_e \nu^{iz}$$
$$\partial_t n_i + \partial_x (n_i u_i) = n_e \nu^{iz}$$
$$\partial_t (n_e u_e) + \partial_x \left[n_e \left(u_e^2 + \frac{1}{\varepsilon} \right) \right] = \frac{n_e}{\varepsilon} \partial_x \phi - n_e u_e \left(\frac{16}{3\sqrt{2\pi}} \frac{1}{\sqrt{\varepsilon} \mathrm{Kn}_{en}} \right)$$
$$\partial_t (n_i u_i) + \partial_x [n_i (u_i^2 + \kappa)] = - n_i \partial_x \phi - n_i u_i \left(\frac{8}{3\sqrt{\pi}} \frac{\sqrt{\kappa}}{\mathrm{Kn}_{in}} \right)$$
$$\partial_{xx}^2 \phi = \frac{n_e - n_i}{\chi}$$

Multicomponent

$$\partial_t n_e + \partial_x (n_e u_i) + \frac{3\sqrt{2\pi}}{16} \frac{\mathrm{Kn}_{en}}{\sqrt{\varepsilon}} \partial_x [-\partial_x n_e + n_e \partial_x \phi] = n_e \nu^i z$$
$$\partial_t n_i + \partial_x (n_i u_i) = n_e \nu^{iz}$$
$$\partial_t (n_i u_i) + \partial_x [n_e + n_i (u_i^2 + \kappa)] = (n_e - n_i) \partial_x \phi - n_i u_i \left(\frac{8}{3\sqrt{\pi}} \frac{\sqrt{\kappa}}{\mathrm{Kn}_{in}} \right)$$
$$\partial_{xx}^2 \phi = \frac{n_e - n_i}{\chi}$$

Procedure:

1. Identify the correct value of the Knudsen number
2. Expand quantities as power series of small parametes ε (and χ in the Bulk region)
$$f^{(\varepsilon,\chi)} = f^{(0,\chi)} + \varepsilon f^{(1,\chi)} + O(\varepsilon^2)$$
3. Let $\varepsilon \to 0$ (and $\chi \to 0$ independently)
4. Obtain the asymptotic limit of the two models

*Multicomponent diffusion to be completed

High Collisionality

$$\mathrm{Kn}_{en} \sim \sqrt{\varepsilon}, \quad \mathrm{Kn}_{in} < \sqrt{\varepsilon}$$

Multifluid

$$\partial_t n_e + \partial_x (n_e u_e) = n_e \nu^{iz}$$

$$\partial_t n_i = n_e \nu^{iz}$$

$$n_e u_e = n_e V_e = \frac{3\sqrt{2\pi}}{16} (-\partial_x n_e + n_e \partial_x \phi)$$

$$u_i = 0$$

$$n_e = n_i$$

Multicomponent

$$\partial_t n_e + \frac{3\sqrt{2\pi}}{16} \partial_x (-\partial_x n_e + n_e \partial_x \phi) = n_e \nu^{iz}$$

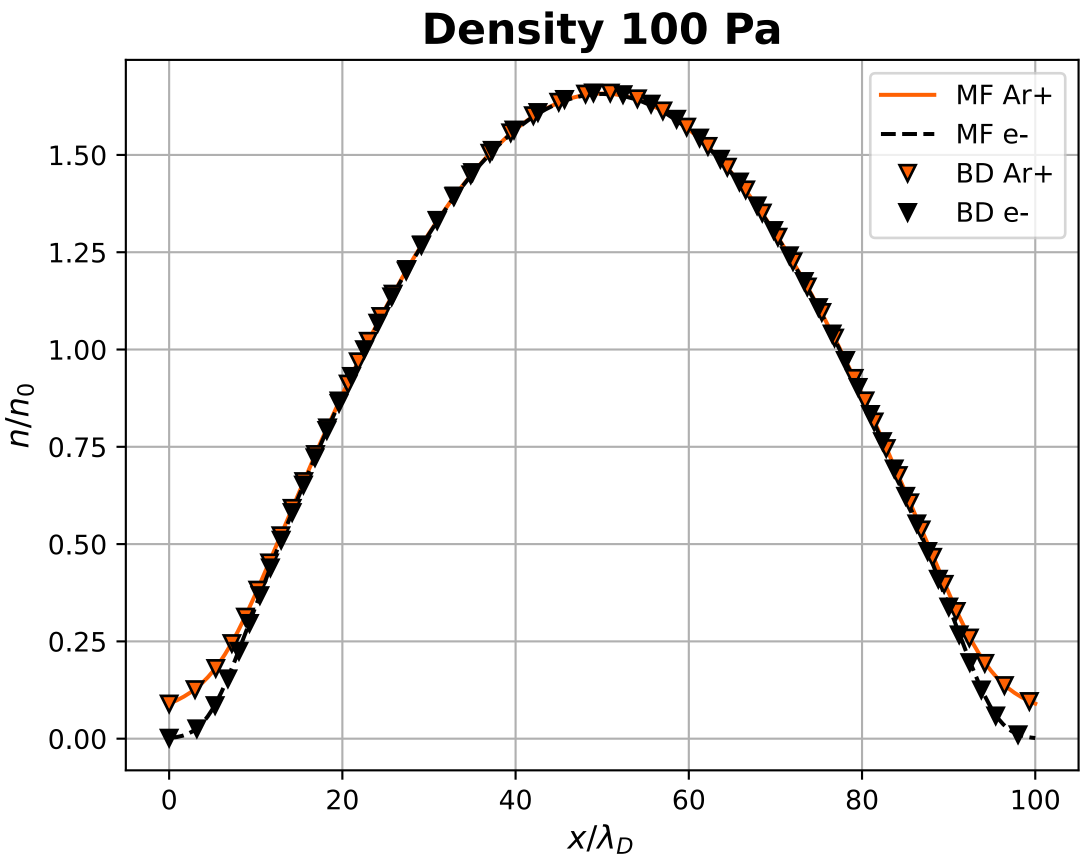
$$\partial_t n_i = n_e \nu^{iz}$$

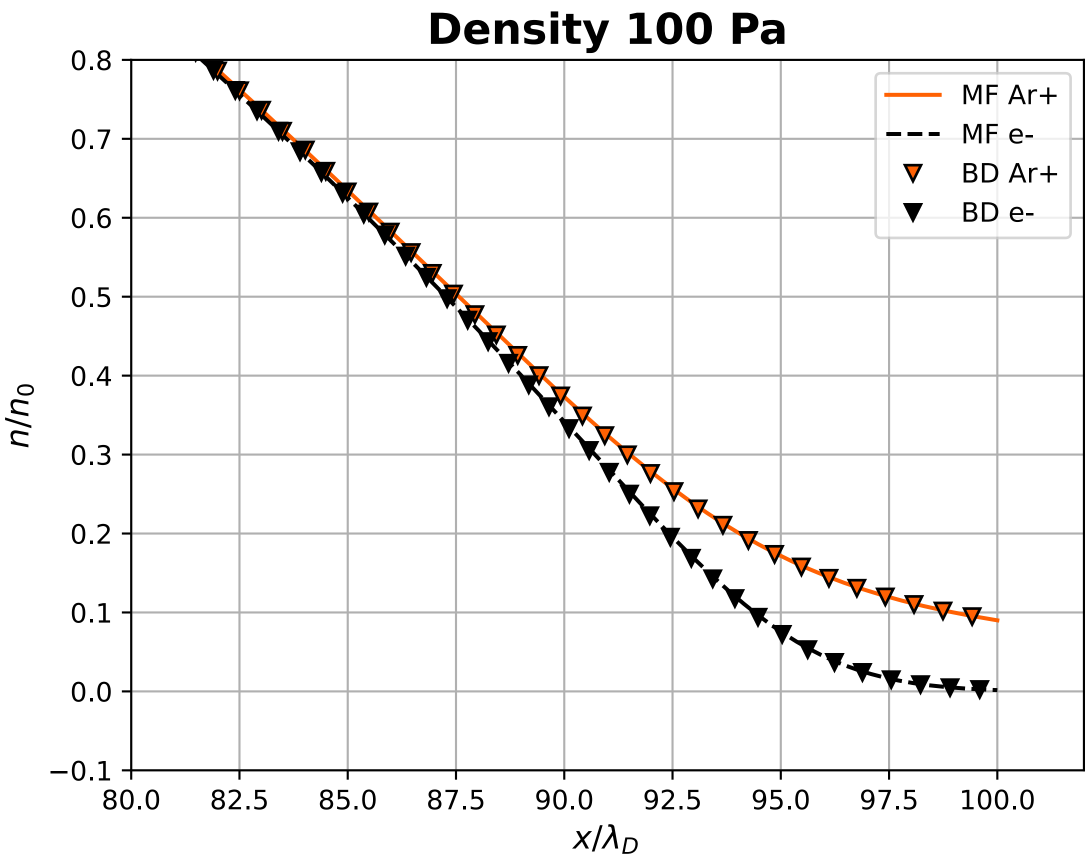
$$u_i = 0$$

$$n_e = n_i$$

- As expected the two models tend to same governing equations for collisional level.
- The electron momentum reduces to the binary diffusion expression of the diffusion velocity
- The Poisson equation expresses the **quasineutrality constraint** (Bulk)

High Pressure – 100 Pa





Low Collisionality

$$\mathrm{Kn}_{en} > \frac{1}{\sqrt{\varepsilon}}, \quad \mathrm{Kn}_{in} \sim \frac{1}{\sqrt{\varepsilon}}$$

Multifluid

$$\partial_t n_e + \partial_x (n_e u_e) = n_e \nu^{iz}$$
$$\partial_t n_i + \partial_x (n_i u_i) = n_e \nu^{iz}$$
$$\partial_t (n_e u_e) + \partial_x \left[n_e \left(u_e^2 + \frac{1}{\varepsilon} \right) \right] = \frac{n_e}{\varepsilon} \partial_x \phi - n_e u_e \left(\frac{16}{3\sqrt{2\pi}} \frac{1}{\sqrt{\varepsilon} \mathrm{Kn}_{en}} \right)$$
$$\partial_t (n_i u_i) + \partial_x \left[n_i \left(u_i^2 + \kappa \right) \right] = - n_i \partial_x \phi - n_i u_i \left(\frac{8}{3\sqrt{\pi}} \frac{\sqrt{\kappa}}{\mathrm{Kn}_{in}} \right)$$
$$\partial_{xx}^2 \phi = \frac{n_e - n_i}{\chi}$$

Multicomponent

$$\partial_t n_e + \partial_x (n_e u_i) + \frac{3\sqrt{2\pi}}{16} \frac{\mathrm{Kn}_{en}}{\sqrt{\varepsilon}} \partial_x \left[-\partial_x n_e + n_e \partial_x \phi \right] = n_e \nu^i z$$
$$\partial_t n_i + \partial_x (n_i u_i) = n_e \nu^{iz}$$
$$\partial_t (n_i u_i) + \partial_x \left[n_e + n_i \left(u_i^2 + \kappa \right) \right] = (n_e - n_i) \partial_x \phi - n_i u_i \left(\frac{8}{3\sqrt{\pi}} \frac{\sqrt{\kappa}}{\mathrm{Kn}_{in}} \right)$$
$$\partial_{xx}^2 \phi = \frac{n_e - n_i}{\chi}$$

Multifluid:

$$\partial_t n_e + \partial_x (n_e u_e) = n_e \nu^{iz}$$
$$\partial_t n_i + \partial_x (n_i u_i) = n_e \nu^{iz}$$
$$\boxed{\partial_x n_e = n_e \partial_x \phi}$$
$$\partial_t (n_i u_i) + \partial_x \left[n_i \left(u_i^2 + \kappa \right) \right] = - n_i \partial_x \phi$$
$$\boxed{n_e = n_i}$$

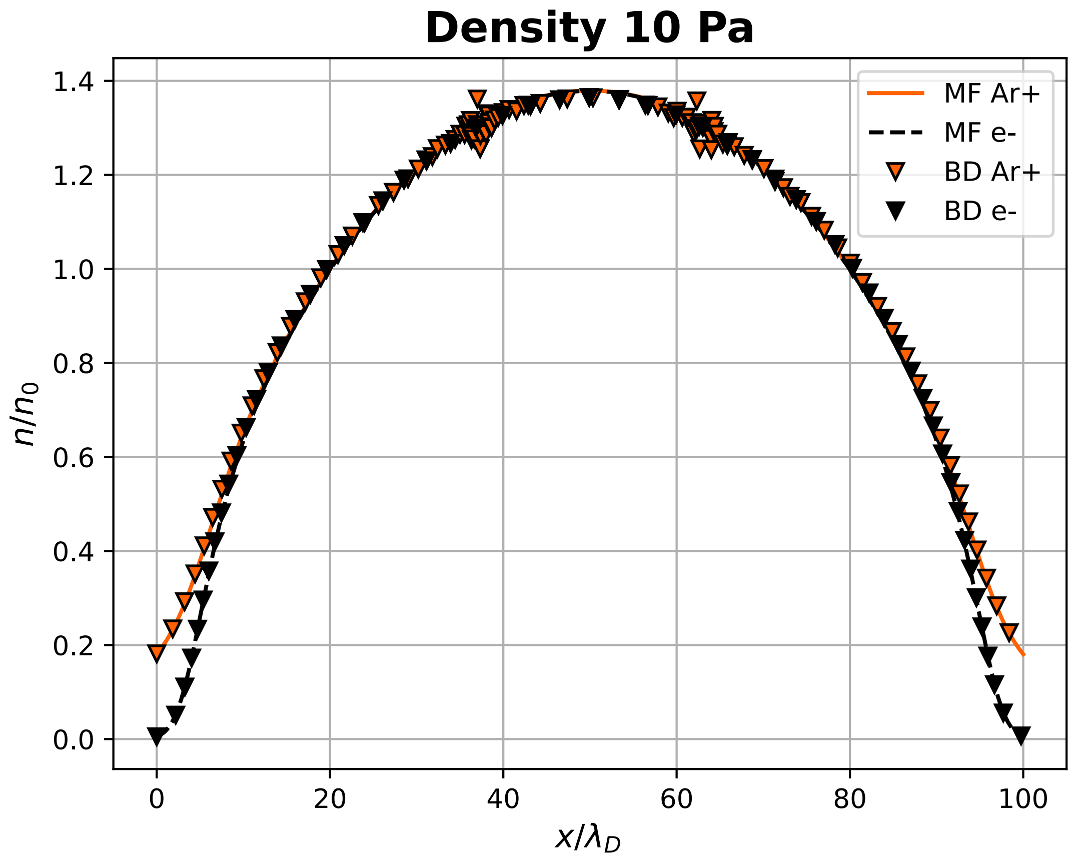
Boltzmann Relation

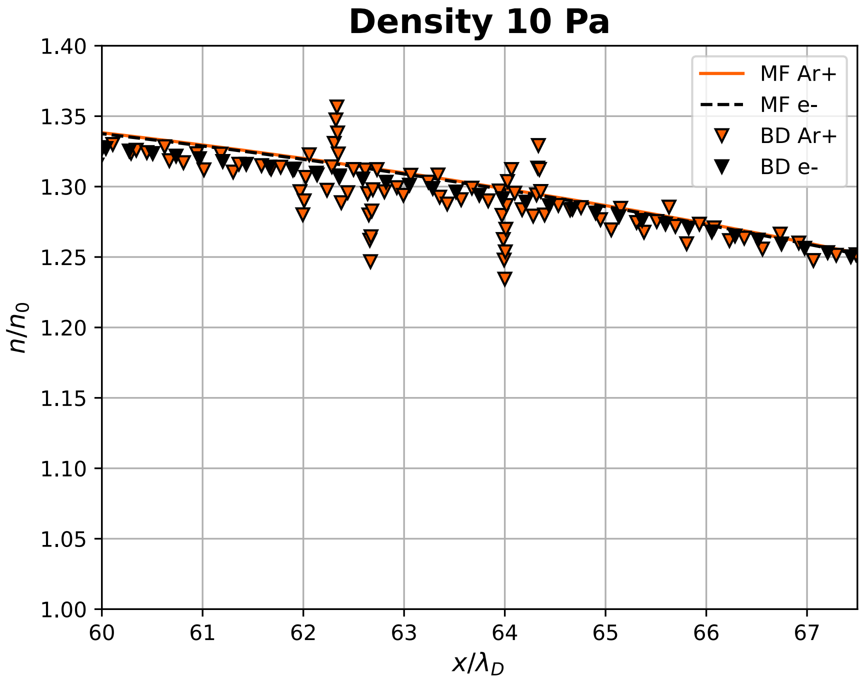
Quasineutrality

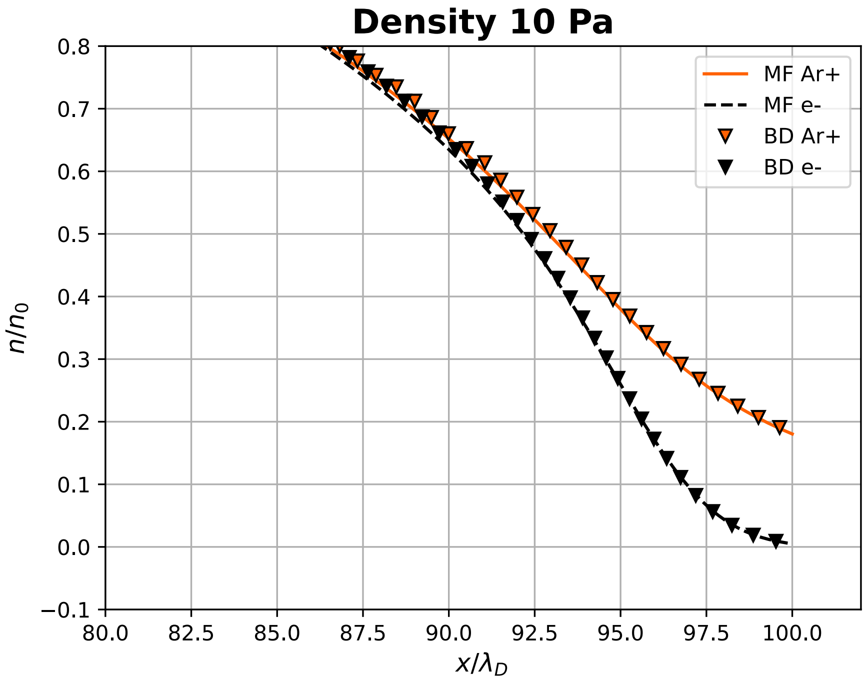
Multicomponent:

$$\boxed{\partial_x n_e = n_e \partial_x \phi}$$
$$\partial_t n_i + \partial_x (n_i u_i) = n_e \nu^{iz}$$
$$\partial_t (n_i u_i) + \partial_x \left[n_i \left(u_i^2 + \kappa \right) \right] = - n_i \partial_x \phi$$
$$\boxed{n_e = n_i}$$

Low Pressure – 10 Pa







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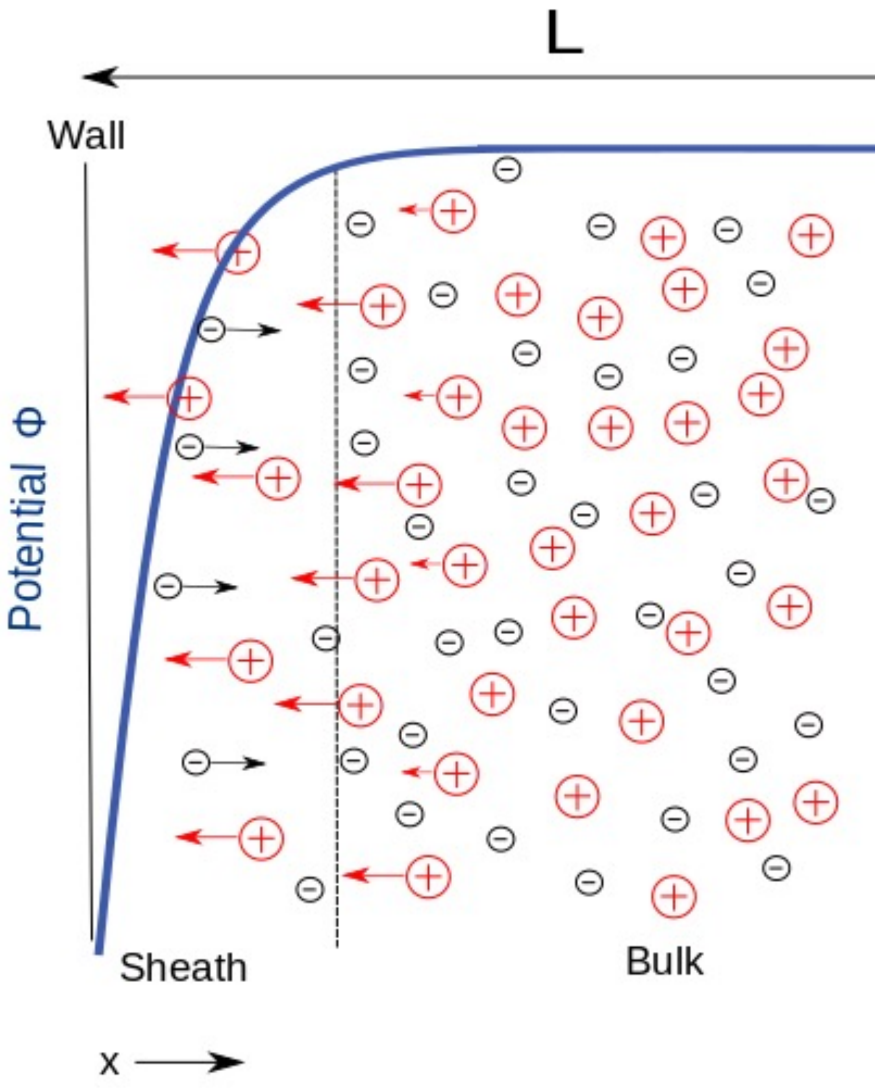

Conclusions

- We developed a Discontinuous Galerkin fluid solver for argon plasma flows
- Results have been validated both against Finite volume reference solution
- A multicomponent Binary Diffusion modeling has been proposed and detailed
  - The model, although simple, is able to converge satifyingly at high pressures
  - At low pressures some instabilities appear, probably due to numerical unbalanced diffusion
  - This source of instabilities will be furtherly investigated
- Next steps will involve:
  - Implementing Multicomponent Diffusion modeling in order to simulate more complex mixtures (approach validated in Finite Volumes)
  - Developing Asymptotic Preserving schemes in order to overcome the intrinsic stiffness of the problem

Development of high order Discontinuous Galerkin fluid solver for argon plasma flows

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