Lattice Boltzmann schemes for multi-temperature plasmas

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Macroscopic Model for Multi-temperature Plasmas

Expansion of equations and solutions

- Species distribution functions

Electrons

$$f_e = f_e^0(1+\varepsilon\phi_e + \varepsilon^2\phi_e^2 + \varepsilon^3\phi_e^3) + \mathcal{O}(\varepsilon^4),$$

Heavy particles $i \in H$

$$f_i = f_i^0(1+\varepsilon\phi_i + \varepsilon^2\phi_i^2) + \mathcal{O}(\varepsilon^3).$$

- Boltzmann equations

Electrons

$$\varepsilon^{-2}\mathscr{D}_e^{-2}(f_e^0) + \varepsilon^{-1}\mathscr{D}_e^{-1}(f_e^0, \phi_e) + \mathscr{D}_e^0(f_e^0, \phi_e, \phi_e^2) + \varepsilon\mathscr{D}_e^1(f_e^0, \phi_e, \phi_e^2, \phi_e^3) = \varepsilon^{-2}\mathcal{J}_e^{-2} + \varepsilon^{-1}\mathcal{J}_e^{-1} + \mathcal{J}_e^0 + \varepsilon\mathcal{J}_e^1 + \mathcal{O}(\varepsilon^2),$$

Heavy particles $i \in H$

$$\mathscr{D}_i^0(f_i^0) + \varepsilon\mathscr{D}_i^1(f_i^0, \phi_i) = \varepsilon^{-1}\mathcal{J}_i^{-1} + \mathcal{J}_i^0 + \varepsilon\mathcal{J}_i^1 + \mathcal{O}(\varepsilon^2).$$

- Constraints

Electrons

$$\langle\langle f_e^0, \hat\psi_e^l\rangle\rangle_e = \langle\langle f_e, \hat\psi_e^l\rangle\rangle_e, \quad l \in \{1,2\},$$

Heavy particles $i \in H$

$$\langle\langle f_h^0, \hat\psi_h^l\rangle\rangle_h = \langle\langle f_h, \hat\psi_h^l\rangle\rangle_h, \quad l \in \{1,\dots,n^H+4\}.$$

Resume of the Chapman-Enskog steps

Order	Time	Heavy particles	Electrons
ε^{-2}	t_e^0		Expression of f_e^0 Thermalization (T_e)
ε^{-1}	t_h^0	Expression of f_i^0, $i \in H$ Thermalization (T_h)	Equation for ϕ_e Zero-order momentum relation
ε^0	t^0	Equation for ϕ_i, $i \in H$ Euler	Equation for ϕ_e^2 Drift-diffusion First-order momentum relation
ε	$\frac{t^0}{\varepsilon}$	Navier-Stokes	Second-order Drift-diffusion

Order ε^{-2} — Electron thermalization

Proposition

The zero-order electron distribution function f_e^0, solution to the Boltzmann equation at order ε^{-2}, *i.e.*, $\mathscr{D}_e^{-2}(f_e^0) = \mathcal{J}_e^{-2}$, that satisfies the scalar constraints is a Maxwell-Boltzmann distribution function at the electron temperature

$$f_e^0 = n_e \left(\frac{1}{2\pi T_e}\right)^{3/2} \exp\left(-\frac{1}{2T_e}\mathbf{C}_e\cdot\mathbf{C}_e\right).$$

Order ε^{-1} — Heavy particles thermalization

Proposition

The zero-order family of heavy-particle distribution functions f_h^0 solution to the Boltzmann equation at order ε^{-1}, *i.e.*, $\mathcal{J}_i^{-1} = 0$, $i \in \mathrm{H}$, that satisfies the scalar constraints is a family of Maxwell-Boltzmann distribution functions at the heavy-particle temperature

$$f_i^0 = n_i \left(\frac{m_i}{2\pi T_h} \right)^{3/2} \exp\left(-\frac{m_i}{2T_h} \mathbf{C}_i \cdot \mathbf{C}_i \right), \quad i \in \mathrm{H}.$$

Proposition

the first-order conservation equations of heavy-particle mass, momentum, and energy read

$$\partial_t \rho_i + \boldsymbol{\partial}_{\mathbf{x}}\cdot(\rho_i \mathbf{v}_h + \tfrac{\varepsilon}{M_h}\rho_i \mathbf{V}_i) = 0, \quad i \in \mathrm{H},$$

$$\partial_t(\rho_h \mathbf{v}_h) + \boldsymbol{\partial}_{\mathbf{x}}\cdot(\rho_h \mathbf{v}_h \otimes \mathbf{v}_h + \tfrac{1}{M_h^2} p\mathbb{I}) = -\tfrac{\varepsilon}{M_h^2}\boldsymbol{\partial}_{\mathbf{x}}\cdot\boldsymbol{\Pi}_h + \tfrac{1}{M_h^2} nq\mathbf{E} + \mathbf{I}\wedge\mathbf{B},$$

$$\partial_t(\rho_h e_h) + \boldsymbol{\partial}_{\mathbf{x}}\cdot(\rho_h e_h \mathbf{v}_h) = -(p_h\mathbb{I} + \varepsilon\boldsymbol{\Pi}_h):\boldsymbol{\partial}_{\mathbf{x}}\mathbf{v}_h - \tfrac{\varepsilon}{M_h}\boldsymbol{\partial}_{\mathbf{x}}\cdot\mathbf{q}_h + \tfrac{\varepsilon}{M_h}\mathbf{J}_h\cdot\mathbf{E}' + \Delta E_h^0 + \varepsilon\Delta E_h^1.$$

Order ε^1 — Electrons   Drift-diffusion

Proposition

the first-order conservation equations of electron mass and energy read

$$\partial_t \rho_e + \boldsymbol{\partial}_{\mathbf{x}} \cdot \left[\rho_e \left(\mathbf{v}_h + \frac{1}{M_h} (\mathbf{V}_e + \varepsilon \mathbf{V}_e^2) \right) \right] = 0,$$

$$\partial_t (\rho_e e_e) + \boldsymbol{\partial}_{\mathbf{x}} \cdot (\rho_e e_e \mathbf{v}_h) = -p_e \boldsymbol{\partial}_{\mathbf{x}} \cdot \mathbf{v}_h - \frac{1}{M_h} \boldsymbol{\partial}_{\mathbf{x}} \cdot (\mathbf{q}_e + \varepsilon \mathbf{q}_e^2) + \frac{1}{M_h} (\mathbf{J}_e + \varepsilon \mathbf{J}_e^2) \cdot \mathbf{E}' + \delta_{b0} \varepsilon M_h \mathbf{J}_e \cdot \mathbf{v}_h \wedge \mathbf{B} + \Delta E_e^0 + \varepsilon \Delta E_e^1 .$$

LB scheme with Source Terms

LB scheme with Source Terms

Let us first introduce the framework of the scheme.

- Space x lives in a Lattice $\alpha \subset \mathbb{R}^d$
- Velocities belong to a finite set $\nu = \{v_j,\ 0 \leqslant j \leqslant J\}$
- The distribution of particles f is denoted by $f_j(x,t)$, $0 \leqslant j \leqslant J$
- Momenta vector $m = (m_k)_{0 \leqslant k \leqslant j}$, is defined by the momenta matrix
$$m_k = \sum_{0 \leqslant j \leqslant J} M_{kj} f_j$$
- The conserved momenta are mass $\rho = m_0$ and directional momenta $q_\alpha = m_\alpha$, $1 \leqslant \alpha \leqslant d$
$$\rho = \sum_{0 \leqslant j \leqslant J} f_j, \qquad q_\alpha = \sum_{0 \leqslant j \leqslant J} v_j^\alpha f_j$$
- The source terms are given by $\varphi = (\varphi_k)_{0 \leqslant k \leqslant J}$, with $\varphi_k = 0$ for $d+1 \leqslant k \leqslant J$

Description of the scheme

The scheme is composed by 4 steps that take into account successively the different terms of the Boltzmann equation

- relaxation towards equilibrium
- first part of the source terms
- free motion
- second part of the source terms

Let us introduce relaxation parameters s_k, $0 \leqslant k \leqslant J$, with $s_k = 0$ for $0 \leqslant k \leqslant d$. The momenta m_k^* after collision satisfy

$$m_k^* = m_k + s_k(m_k^{eq} - m_k), \quad 0 \leqslant k \leqslant J$$

Description of the scheme

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- relaxation towards equilibrium
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Let us introduce the parameter $a \in [0, 1]$ that ponders the first and second part of the source terms. The momenta $\tilde{m}_k$ after this step are given by

$$\tilde{m}_k = m_k^* + a\Delta t \varphi_k, \quad 0 \leqslant k \leqslant J$$

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The free motion step mimics at the discrete level the free evolution through characteristics

$$\bar{f}_j(x, t + \Delta t) = \tilde{f}_j(x - v_j \Delta t, t), \quad 0 \leqslant j \leqslant J$$

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The momenta $\hat{m}_k$ after this step are given by

$$\hat{m}_k = \bar{m}_k + (1-a)\Delta t \varphi_k, \quad 0 \leqslant k \leqslant J$$

Description of the scheme

The scheme is composed by 4 steps that take into account successively the different terms of the Boltzmann equation

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- first part of the source terms
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The global scheme can be reduced to

$$m_k(x, t+\Delta t) = \sum_{0\leqslant j,l\leqslant J} M_{kj} M_{jl}^{-1} \Big[m_l^*(x - v_j \Delta t, t) + a \Delta t \varphi_l(x - v_j \Delta t, t) \Big] + (1-a)\Delta t \varphi_k(x, t+\Delta t)$$

for $0 \leqslant k \leqslant J$

Formal Expansion – zeroth-order

We investigate the Taylor expansion method proposed previously by F. Dubois to LB scheme with source term.
The goal is to establish the equivalent partial differential equations at second-order in the asymptotic limit Δt goes to 0.

Proposition – zeroth-order

The momenta yield to equilibrium state

$$m_k = m_k^{\text{eq}} + \mathcal{O}(\Delta t), \qquad 0 \leqslant k \leqslant J$$
$$m_k^* = m_k^{\text{eq}} + \mathcal{O}(\Delta t), \qquad 0 \leqslant k \leqslant J$$

Formal Expansion – first-order

Let us introduce

- $F^{\text{eq}}_{\alpha\beta} = \sum_{0\leqslant j\leqslant J} v_j^\alpha v_j^\beta f_j^{\text{eq}}$ $\qquad 1 \leqslant \alpha, \beta \leqslant d$
- $\theta_k = \sum_{0\leqslant j\leqslant J} M_{kj}\big(\partial_t f_j^{\text{eq}} + \sum_{\alpha=1}^{d} v_j^\alpha \partial_\alpha f_j^{\text{eq}}\big)$ $\qquad d{+}1 \leqslant k \leqslant J$

Proposition – first-order equations

Mass conservation

$$\partial_t \rho + \sum_{\alpha=1}^{d} \partial_\alpha q_\alpha = \varphi_0 + \mathcal{O}(\Delta t)$$

Momenta conservation for $1 \leqslant \alpha \leqslant d$

$$\partial_t q_\alpha + \sum_{\beta=1}^{d} \partial_\beta F^{\text{eq}}_{\alpha\beta} = \varphi_\alpha + \mathcal{O}(\Delta t)$$

Expansion of the unconserved momenta

$$m_k = m_k^{\text{eq}} - \frac{\Delta t}{s_k}\theta_k + \mathcal{O}(\Delta t^2), \qquad d{+}1 \leqslant k \leqslant J$$

$$m_k^* = m_k^{\text{eq}} - \big(\tfrac{1}{s_k} - 1\big)\Delta t\, \theta_k + \mathcal{O}(\Delta t^2), \qquad d{+}1 \leqslant k \leqslant J$$

Formal Expansion – second-order

Let us introduce

- $\Lambda^k_{\alpha\beta} = \sum_{0\leqslant j\leqslant J} M^{-1}_{jk} v_j^\alpha v_j^\beta \qquad 1 \leqslant \alpha, \beta \leqslant d,\ 0 \leqslant k \leqslant J$

Proposition – second-order equations

Mass conservation

$$\partial_t \rho + \sum_{\alpha=1}^{d} \partial_\alpha q_\alpha = \varphi_0 + (\tfrac{1}{2} - a)\Delta t \Big(\partial_t \varphi_0 + \sum_{\alpha=1}^{d} \partial_\alpha \varphi_\alpha\Big) + \mathcal{O}(\Delta t^2)$$

Momenta conservation for $1 \leqslant \alpha \leqslant d$

$$\partial_t q_\alpha + \sum_{\beta=1}^{d} \partial_\beta F^{eq}_{\alpha\beta} = \varphi_\alpha + (\tfrac{1}{2} - a)\Delta t \Big(\partial_t \varphi_\alpha + \sum_{\beta,\gamma=1}^{d} \Lambda^\gamma_{\alpha\beta} \partial_\beta \varphi_\gamma\Big)$$

$$+ \Delta t \sum_{k=d+1}^{J} \sum_{\beta=1}^{d} \Lambda^k_{\alpha\beta} \big(\tfrac{1}{s_k} - \tfrac{1}{2}\big) \partial_\beta \theta_k + \mathcal{O}(\Delta t^2)$$

LB scheme for Electrons and Heavy Particles

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Framework for two species (electrons–heavy particles)

- Space x lives in a Lattice $\alpha \subset \mathbb{R}^d$
- Velocities belong to a finite set $\nu = \{v_j,\ 0 \leqslant j \leqslant J\}$
- The distribution of electrons f^e (resp. heavy particles f^h) is denoted by $f_j^e(x,t)$ (resp. $f_j^h(x,t)$), $0 \leqslant j \leqslant J$
  We define $F = (f_0^h, \ldots, f_J^h, f_0^e, \ldots, f_J^e)$
- The momenta $m = (\rho^h, \rho^e, q_1^h, \ldots, q_d^h, q_1^e, \ldots, q_d^e, E, \delta E)$ are linked with F by the momenta matrix M, such that $m = MF$ with

$$M = \begin{bmatrix} 1 & \ldots & 1 & 0 & \ldots & 0 \\ 0 & \ldots & 0 & 1 & \ldots & 1 \\ v_0^1 & \ldots & v_J^1 & 0 & \ldots & 0 \\ \vdots & & \vdots & \vdots & & \vdots \\ v_0^d & \ldots & v_J^d & 0 & \ldots & 0 \\ 0 & \ldots & 0 & v_0^1 & \ldots & v_J^1 \\ \vdots & & \vdots & \vdots & & \vdots \\ 0 & \ldots & 0 & v_0^d & \ldots & v_J^d \\ |v_0|^2/2 & \ldots & |v_J|^2/2 & |v_0|^2/2 & \ldots & |v_J|^2/2 \\ |v_0|^2/2 & \ldots & |v_J|^2/2 & -|v_0|^2/2 & \ldots & -|v_J|^2/2 \end{bmatrix}$$

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  We define $F = (f_0^h, \ldots, f_J^h, f_0^e, \ldots, f_J^e)$
- The momenta $m = (\rho^h, \rho^e, q_1^h, \ldots, q_d^h, q_1^e, \ldots, q_d^e, E, \delta E)$ are linked with F by the momenta matrix M, such that $m = MF$
- The masses ρ^h, ρ^e, the heavy particles momenta $q_1^h, \ldots, q_d^h$, and the global energy E are conserved during the collision
- The electron momenta $q_1^e, \ldots, q_d^e$ relax towards equilibrium states defined by $(q_\alpha^e)^{\text{eq}} = q_\alpha^h (\rho^e/\rho^h)^2$
- The exchanged energy term δE relaxes towards equilibrium state defined by $\delta E^{\text{eq}} = 0$

Description of the scheme

Extending the velocities by periodicity $v_j = v_{j-J-1}$ for $J+1 \leqslant j \leqslant 2J+1$, the global scheme can be reduced to

$$m_k(x, t+\Delta t) = \sum_{j,l=0}^{2J+1} M_{kj} M_{jl}^{-1} m_l^*(x - v_j \Delta t, t)$$

where the momenta after collision are defined by

- $m_k^* = m_k$ for $k \in \{0, 1, 2, \ldots, d+1, 2d+2\}$
- $m_k^* = m_k + s_k(m_k^{\text{eq}} - m_k)$ for $k \in \{d+2, \ldots, 2d+1, 2d+3\}$

Second-order mass conservation

Let us introduce

- $v_\alpha^h = q_\alpha^h / \rho^h$, $1 \leqslant \alpha \leqslant d$
- $\theta_\alpha^e = \sum_{0 \leqslant j \leqslant J} v_j^\alpha \big(\partial_t (f_j^e)^{\mathrm{eq}} + \sum_{\beta=1}^d v_j^\beta \partial_\beta (f_j^e)^{\mathrm{eq}} \big) \qquad 1 \leqslant \alpha \leqslant d$

Proposition – heavy particles mass conservation

$$\partial_t \rho^h + \sum_{\alpha=1}^d \partial_\alpha q_\alpha^h = \mathcal{O}(\Delta t^2)$$

Proposition – electron mass conservation

$$\partial_t \rho^e + \sum_{\alpha=1}^d \partial_\alpha (\rho^e v_\alpha^h) = \Delta t \sum_{\alpha=1}^d \big(\tfrac{1}{s_\alpha} - \tfrac{1}{2}\big) \partial_\alpha \theta_\alpha^e + \mathcal{O}(\Delta t^2)$$

Second-order momentum conservation

Let us introduce

- $p^h = \frac{1}{d} \sum_{0\leqslant j\leqslant J} |v_j - v^h|^2 (f_j^h)^{\text{eq}}$
- $\Pi_{\alpha\beta} = -\sum_{\gamma=1}^{d} \Lambda_{\alpha\beta}^{\gamma}(\frac{1}{s_\gamma} - \frac{1}{2})\theta_\gamma^e - \Lambda_{\alpha\beta}^{E}(\frac{1}{s_E} - \frac{1}{2})\theta_E \quad 1 \leqslant \alpha, \beta \leqslant d$
- $\Lambda_{\alpha\beta}^{\gamma} = \sum_{0\leqslant j\leqslant J} v_j^\alpha v_j^\beta M_{j\gamma+d+1}^{-1}, \; \Lambda_{\alpha\beta}^{E} = \sum_{0\leqslant j\leqslant J} v_j^\alpha v_j^\beta M_{j2J+1}^{-1}$
- $\theta_E = \sum_{0\leqslant j\leqslant J} \frac{1}{2}|v_j|^2 \Big[\partial_t\big((f_j^h)^{\text{eq}} - (f_j^e)^{\text{eq}}\big) + \sum_{\beta=1}^{d} v_j^\beta \partial_\beta\big((f_j^h)^{\text{eq}} - (f_j^e)^{\text{eq}}\big)\Big]$

Proposition – heavy particles momentum conservation

$$\partial_t q_\alpha^h + \sum_{\beta=1}^{d} \partial_\beta(q_\alpha^h v_\beta^h + p^h \delta_{\alpha\beta}) = -\Delta t \sum_{\beta=1}^{d} \partial_\beta \Pi_{\alpha\beta} + \mathcal{O}(\Delta t^2)$$

Second-order global energy conservation

Let us introduce

- $H = E + p^h + p^e$
- $p^e = \frac{1}{d} \sum_{0 \leqslant j \leqslant J} |v_j - v^h|^2 (f_j^e)^{\text{eq}}$
- $Q_\beta^e = - \sum_{\gamma=1}^{d} \Lambda_{2J\beta}^{\gamma} (\frac{1}{s_\gamma} - \frac{1}{2}) \theta_\gamma^e \qquad 1 \leqslant \beta \leqslant d$
- $\Lambda_{2J\beta}^{\gamma} = \sum_{0 \leqslant j \leqslant J} \frac{1}{2} |v_j|^2 v_j^\beta (M^{-1}_{j\gamma+d+1} + M^{-1}_{J+1+j\gamma+d+1})$

Proposition – global energy conservation

$$\partial_t E + \sum_{\beta=1}^{d} \partial_\beta (H v_\beta^h) = -\Delta t \sum_{\beta=1}^{d} \partial_\beta Q_\beta^e + \mathcal{O}(\Delta t^2)$$

Numerical Simulations

Framework

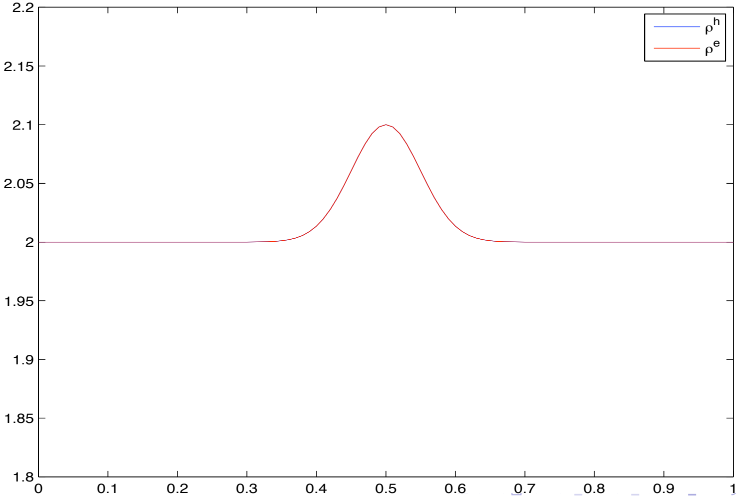
- D1Q3 scheme with 2 species (h for ions and e for electrons)
- Momenta matrix

$$M = \begin{bmatrix} 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 \\ -1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 1 \\ 1/2 & 0 & 1/2 & 1/2 & 0 & 1/2 \\ 1/2 & 0 & 1/2 & -1/2 & 0 & -1/2 \end{bmatrix} \begin{array}{l} \longleftarrow \text{heavy particle mass is conserved} \\ \longleftarrow \text{electron mass is conserved} \\ \longleftarrow \text{heavy particle momentum is conserved} \\ \longleftarrow (q^e)^* = q^e + s_v(q^h\rho^e/\rho^h - q^e) \\ \longleftarrow \text{global energy is conserved} \\ \longleftarrow (\delta E)^* = \delta E + s_E(0 - \delta E) \end{array}$$

- The distribution of charge induces internal electric force acting on each species

Numerical Simulations

- Weak electron diffusion velocity
- Weak relaxation for temperatures
- Initial condition : thermal non equilibrium



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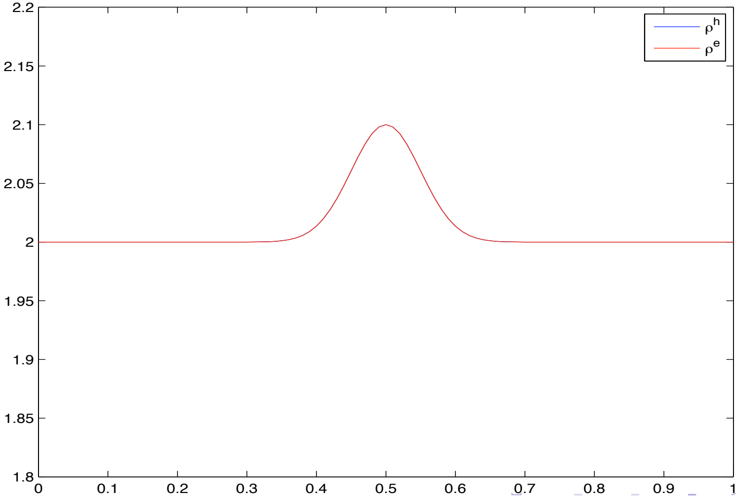

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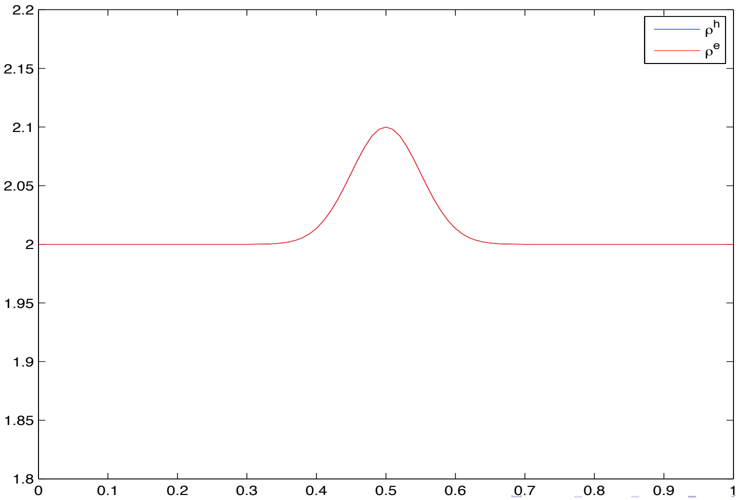

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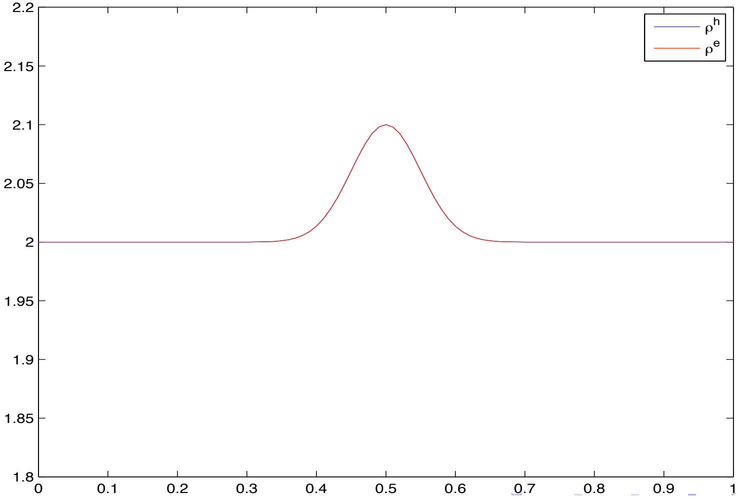
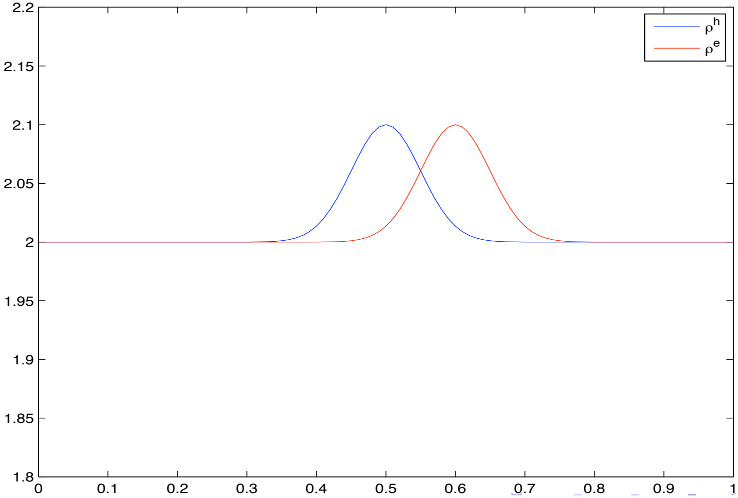


Numerical Simulations

- Weak electron diffusion velocity
- Weak relaxation for temperatures
- Initial condition : electric dipole



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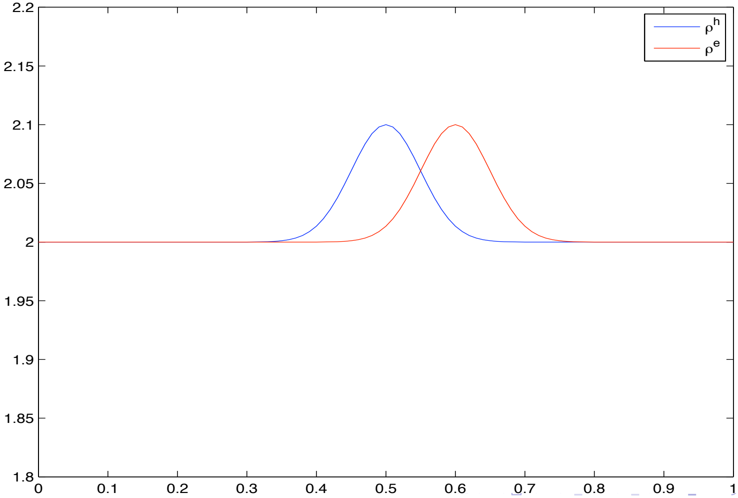

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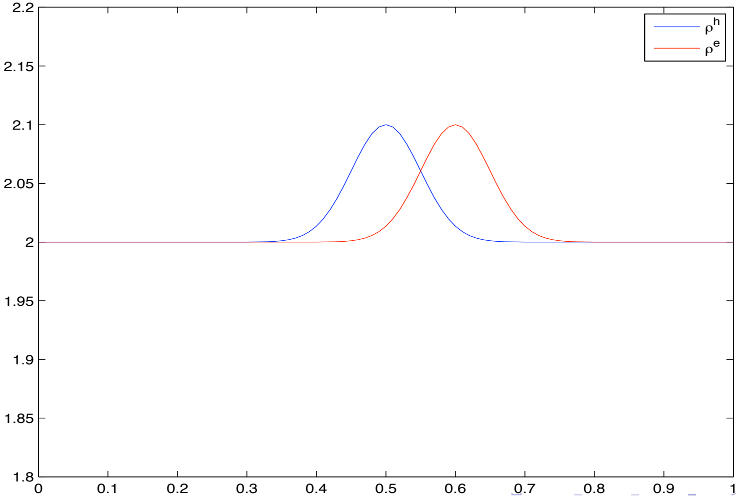

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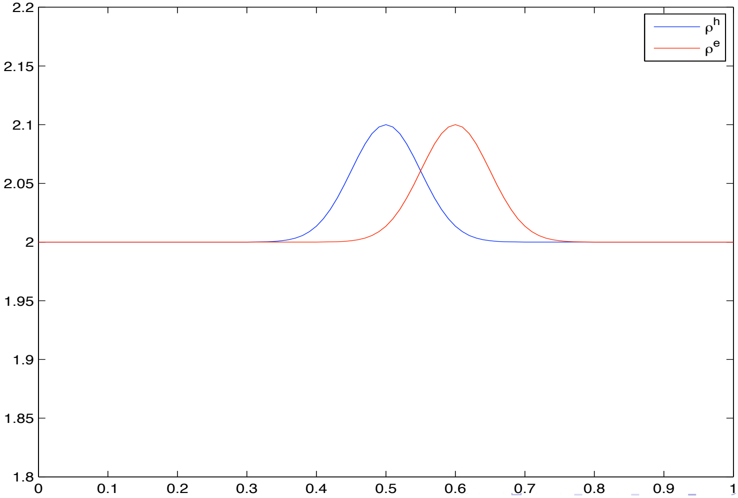

In prospect

- A more accurate calculus of the viscous stress tensor for heavy particles. In particular, it seems to have a good agreement with the model for symmetric mesh
- Numerical simulations for three species (neutral, ions and electron)
- Add a chemistry term in the model because plasmas are strongly reactive gas mixtures