Kinetic model and numerical scheme for electrons in glow discharge plasmas

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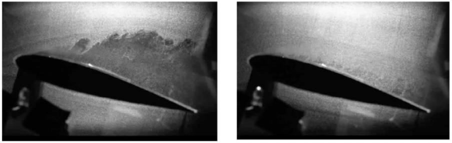
Physical context

Cold plasmas in industry:

- Deicing
- Airflow control
- Components cleaning

Plasma actuators :

- enhances lift
- prevents flow separation



(a) (b)

Physical context

Cold plasma parameters (glow discharge) :

- atmospheric pressure
- partially ionized : $\delta_e = 10^{-6}$ to 10^{-4}
- several species : neutral particles, electrons and ions
- low temperature : 1eV for electrons and room temperature for heavy species
- Debye length $\approx 10^{-6} m$

Multiscale problem : velocities between particles are very different

Drift diffusion system

Equations for electrons

$$\partial_t \rho + \nabla_x \cdot \Gamma = S$$
$$\partial_t \rho_W + \nabla_x \cdot \Gamma_W + E \cdot \Gamma = S_W$$
$$\Gamma = -\frac{1}{\rho_n}[E\mu\rho + \nabla_x(D\rho)]$$

ρ density, ρ_W internal energy, E electric field, μ mobility, D diffusion, S ionization source term

- if T depends only on $E/\rho_n \Rightarrow$ mass eq only

Kinetic approach :

- Two term approximation (used in BOLSIG+[1])

Goal : Use Lattice Boltzmann method to solve DD system

[1] G J M Hagelaar, 2015

Lattice Boltzmann method

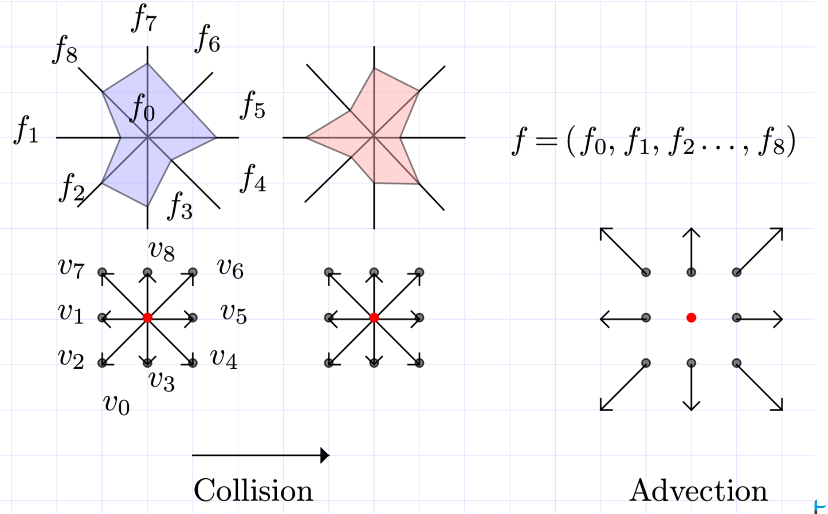
Goal : Use Lattice Boltzmann method to solve DD system

Lattice Boltzmann method

- solve a Boltzmann equation - like
- cartesian grid in space
- velocity variable belongs to a speed lattice $\{v_i\}_{1\leq i\leq n}$
- computing advection and collision separately
- compute moments by summing over $\{v_i\}_{1\leq i\leq n}$

$$f_i(t+\Delta t, x+v_i\Delta t) = f_i(t,x) + \frac{\Delta t}{\tau}(Mf_i - f_i)$$

Lattice Boltzmann method



Lattice Boltzmann method

- Lattices D_nQ_m : n = dimension, m = number of velocities
- Some lattices correspond to Gauss-Hermite nodes ($D1Q3$, $D2Q9$...)
- f is expanded in terms of Hermite polynomials
- $\rho, \rho u$... are then computed with Gauss-Hermite quadrature

Advantages of LBM

- simple calculation procedure
- easy and efficient implementation for parallel computation
- simple and robust handling of complex geometries

Lattice Boltzmann method

- Which collision operator in order to solve DD ?
- What kind of boundary conditions ?

Idea : construct a lattice Boltzmann scheme from a kinetic model giving drift diffusion system at hydrodynamic limit

Summary

- Kinetic model and hydrodynamic limit
- Approximated model for 2D
- 1D Problem and numerical tests

Kinetic model

- Starting from previous work [2] : scaling parameter $\varepsilon = \sqrt{\frac{m_e}{m_n}}$
- Considering electrons f_e, neutral particles f_n and ions f_i
- Coupled scaled dimensionless system :

$$\partial_t f_e + \frac{1}{\varepsilon}(v \cdot \nabla_x f_e + F_e \cdot \nabla_v f_e) = \frac{1}{\varepsilon^2} Q_e^\varepsilon(f_e, f_i, f_n)$$
$$\partial_t f_i + v \cdot \nabla_x f_i + F_i \cdot \nabla_v f_i = \frac{1}{\varepsilon^2} Q_i^\varepsilon(f_e, f_i, f_n)$$
$$\partial_t f_n + v \cdot \nabla_x f_n + F_n \cdot \nabla_v f_n = \frac{1}{\varepsilon^2} Q_n^\varepsilon(f_e, f_i, f_n)$$

- Boltzmann, Fokker-Planck and special ionization operator
- Euler equations for heavy particles
- Energy Transport system for electrons

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[2] I Choquet, P Degond, B Lucquin-Desreux, 2007

Kinetic model

Electrons distribution function f satisfies

$$\partial_t f + \frac{1}{\varepsilon}(v\cdot\nabla_x f - E\cdot\nabla_v f) = \frac{1}{\varepsilon^2} Q_{en}^0(f) + \frac{1}{\varepsilon} Q_{ee}(f) + Q_{en}^2(f) + Q_{ion}(f) + \mathcal{O}(\varepsilon)$$

- $Q_{en}^0 + \varepsilon^2 Q_{en}^2$: expansion of Boltzmann operator
- Q_{ee} : BGK operator
- Q_{ion} : simplified ionization operator

Result : With $f_{i,n}$ = isotropic Maxwellians and simplified operators
$\rightarrow$ drift diffusion model

Method : Hilbert expansion

$$f = f_0 + \varepsilon f_1 + \varepsilon^2 f_2 + \mathcal{O}(\varepsilon^3)$$

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Terms of order ε^{-2}

Find f_0 st $Q^0_{en}(f_0) = 0$

$$Q^0_{en}(f) = \rho_n \sigma_{en} \int_{\mathbb{S}^2_+} ||v||[f(v - 2(v,\omega)\omega) - f(v)]d\omega$$

Properties[3]

- $\text{Ker}(Q_{en}) =$ isotropic functions
- Self adjoint in $L^2_{f_n}(\mathbb{R}^3)$
- ψ st $Q^0_{en}(\psi) = \phi$ have a solution $\Leftrightarrow \phi \in \text{Ker}(Q^0_{en})^\perp \Leftrightarrow$ for all $W = \frac{v^2}{2}$, $S_W = \{v \quad \text{st} \quad v^2/2 = W\}$

$$\int_{S_W} \phi(v) dN(v) = 0$$

This implies that f_0 is isotropic

[3] I Choquet, P Degond, B Lucquin-Desreux, 2007

Terms of order ε^{-1}

Find f_1 st :

$$Q^0_{en}(f_1) = v \cdot \nabla_x f_0 - E \cdot \nabla_v f_0 - Q_{ee}(f_0) \qquad (1)$$

where

$$Q_{ee}(f) = M(f) - f$$

$M(f)$: Maxwellian associated to f

Equation (1) has a solution iff $Q_{ee}(f_0) = 0 \Leftrightarrow f_0$ is Maxwellian

$$f_1 = -\frac{1}{2\nu_{en}\rho_n||v||}[v \cdot \nabla_x f_0 - E \cdot \nabla_v f_0] + \tilde{f}_1$$

where $\tilde{f}_1 \in \mathrm{Ker}(Q^0_{en})$

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Terms of order ε^0

$$Q_{en}^0(f_2) = \partial_t f_0 + v \cdot \nabla_x f_1 - E \cdot \nabla_v f_1 - Q_{en}^2(f_0) - Q_{ee}(f_1) - Q_{ion}(f_0)$$

has a solution if and only if

$$\int_{S_W} (\partial_t f_0 + v \cdot \nabla_x f_1 - E \cdot \nabla_v f_1) dN(v) = \int_{S_W} (Q_{en}^2(f_0) + Q_{ee} + Q_{ion}(f_0)) dN(v)$$

Property[4]

for $\phi = \phi_0 + \mathcal{O}(\varepsilon)$ and $f = f_0 + \mathcal{O}(\varepsilon)$ isotropic

$$\frac{64\pi^2}{3\sigma_{en}\rho_n T_n} \int_0^\infty \partial_W [W^2(\frac{f_0}{T_n} + \partial_W f_0)] \phi_0 dW = \int_{\mathbb{R}^3} Q_{en}^2(f_0) \phi_0 dv$$

[4] P Degond, A Nouri, C Schmeiser, 2000

Terms of order ε^0

Ionization recombination reaction

$$N + e^- \rightleftharpoons N^+ + e^- + e^-$$

$$Q_{ion}(f) = \int_{\mathbb{R}^3} \rho_n \sigma_{ion} [2\delta' f(v') - \delta f(v)] dv'$$

where $\delta = \delta(v^2 - 2v'^2 - 2\Delta)$ with Δ : threshold energy

Property[5]

Q_{ion} collisional invariant is

$$\psi = 1 + \frac{v^2}{2}$$

$$\int_{\mathbb{R}^3} Q^0_{ion}(f) \begin{pmatrix} 1 \\ \frac{v^2}{2} \end{pmatrix} dv = \begin{pmatrix} R \\ -\Delta R \end{pmatrix}$$

[5] I Choquet, P Degond, B Lucquin-Desreux, 2007

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Fluid equations

Drift diffusion system

$$\begin{cases} \partial_t \rho + \nabla_x \cdot \Gamma = S \\ \partial_t (\rho T^{\frac{3}{2}}) + \nabla_x \cdot \Gamma_w + E \cdot \Gamma = S_W \end{cases}$$

$$\Gamma = -\frac{1}{\rho_n}[E\mu\rho + \nabla_x(D\rho)]$$

$$\Gamma_W = -\frac{3}{2\rho_n}[E\mu_W \rho T + \nabla_x(D_W \rho T)]$$

$$D = \frac{2\sqrt{T}}{3\nu_{en}\sqrt{\pi}}, \quad \mu = \frac{2}{3\nu_{en}\sqrt{T\pi}}$$

$$D_W = \frac{2}{3}D, \quad \mu_W = \frac{2}{3}\mu$$

Approached model (2D case)

$x, v \in \mathbb{R}^2$, projecting on the following space[6]

$$D = \{f \in L^2_{\frac{1}{w}}(\mathbb{R}^2) | f = \sum_{n=0}^{2} a^n H^n(v)\}$$

where H^n are Hermite polynomials, $w = \frac{1}{2\pi} exp(-\frac{v^2}{2})$ and

$$a^n = \int_{\mathbb{R}^2} f(v) H^n(v) dv, \quad a^0 = \rho, \quad a^1 = \rho u ...$$

- for $f \in D$: projection on D of $Q_\alpha(f)$, $\alpha = en, ee, ion$
- Allows to have collision terms depending only on a^n

[6] X Shan, X-F Yuan, H Chen, 2006

Fluid equations (2D case)

Approached drift diffusion system

$$\begin{cases} \partial_t \rho + \nabla_x \cdot \Gamma = S \\ \partial_t(\rho(T-1)) + \nabla_x \cdot \Gamma + E \cdot \Gamma = S_W \end{cases}$$

where

$$-\Gamma = \frac{2\sqrt{2}}{3\pi^{3/2}\sigma_{en}\rho_n}[\rho E + \nabla_x(\rho T)]$$

$$D = \frac{2\sqrt{2}T}{3\pi^{3/2}\sigma_{en}} \qquad \mu = D/T$$

- Good approx for mass equation but not for energy

1D Problem : Setting of the problem

- We focus on density equation
- Temperature is supposed to be constant $= 1$
- No ionization processes

1D Drift diffusion equation

$$\partial_t \rho - \partial_x (D \partial_x \rho + E \mu \rho) = 0$$

In this case $D = \mu$

Lattice chosen : D1Q2[7]

[7] S Dellacherie, 2012

1D Problem : Scheme

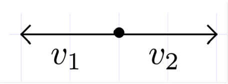
Scheme

$$f_i(t+\Delta t, x+\frac{v_i}{\varepsilon}\Delta t) = f_i(t,x) + \Delta t(Q(f_i(t,x)) + F(f_i(t,x)))$$

Two velocities : $v_i = (-1)^i \varepsilon \frac{\Delta x}{\Delta t}, \; i = 1, 2$

- $Q(f_i(t,x)) = -\frac{\sigma_{en}}{2\varepsilon^2} q v_i + \frac{1}{\varepsilon}(\frac{\rho + q v_i}{2} - f_i)$
- $F(f_i(t,x)) = -\frac{1}{2\varepsilon} E \rho v_i$

Here $q = \rho u$



1D Problem : discrete kinetic equation

Kinetic equation with discrete velocity :

$$\partial_t f_i + \frac{v_i}{\varepsilon} \partial_x f_i = Q(f_i) + F(f_i)$$

Proposition :

The hydrodynamic limit is exactly

$$\partial_t \rho - \partial_x (D \partial_x \rho + E \mu \rho) = 0$$

with

$$D = \mu = \frac{1}{\sigma_{en}}$$

1D Problem : link with fluid schemes

$$\underbrace{f_i(t+\Delta t, x+\frac{v_i}{\varepsilon}\Delta t)}_{\text{advection}} = \underbrace{f_i(t,x) + \Delta t(Q(f_i(t,x)) + F(f_i(t,x)))}_{\textbf{collision}}$$

Timestep for moments :

$$\rho(t+\Delta t, x) = f_1^\star(t, x+\frac{v}{\varepsilon}\Delta t) + f_2^\star(t, x-\frac{v}{\varepsilon}\Delta t)$$
$$q(t+\Delta t, x) = v f_2^\star(t, x-\frac{v}{\varepsilon}\Delta t) - v f_1^\star(t, x+\frac{v}{\varepsilon}\Delta t)$$

Where $v = |v_{1,2}|$ and $f^\star$ is f after the collision

1D Problem : link with fluid schemes

Moments after the collision :

$$\rho^\star = \rho$$
$$q^\star = q\left(1 - \frac{\sigma_{en}}{\varepsilon^2}\Delta t\right) - E\rho\frac{\Delta t}{\varepsilon}$$

We know :

$$\underbrace{\begin{pmatrix} 1 & 1 \\ v_1 & v_2 \end{pmatrix}}_{M} \underbrace{\begin{pmatrix} f_1 \\ f_2 \end{pmatrix}}_{f} = \underbrace{\begin{pmatrix} \rho \\ q \end{pmatrix}}_{m}$$

Thus [8]

$$f^\star = M^{-1} m^\star$$

[8] F Dubois 2008

Fluid schemes

$$\rho_j^{n+1} = \frac{1}{2}(\rho_{j+1}^n + \rho_{j-1}^n) + \left(\frac{1}{2v} - \frac{\sigma_{en}\Delta t}{2v\varepsilon^2}\right)\Delta t(q_{j-1}^n - q_{j+1}^n) + \frac{\Delta t}{2v\varepsilon}(E_{j+1}^n\rho_{j+1}^n - E_{j-1}^n\rho_{j-1}^n)$$

$$q_j^{n+1} = \frac{v}{2}(\rho_{j-1}^n - \rho_{j+1}^n) + \left(\frac{1}{2} - \frac{\sigma_{en}\Delta t}{2\varepsilon^2}\right)(q_{j-1}^n + q_{j+1}^n) - \frac{\Delta t}{2\varepsilon}(E_{j+1}^n\rho_{j+1}^n + E_{j-1}^n\rho_{j-1}^n)$$

1D Problem : test case

Numerical tests

$$\partial_t \rho - \partial_x (D \partial_x \rho + E \mu \rho) = 0$$

$$\partial_x^2 \phi = \frac{1}{\lambda^2}(\rho - 1)$$

Where $E = -\partial_x \phi$

Stationary problem with Dirichlet boundary conditions, assuming :

$$D \partial_x \rho + E \mu \rho = 0$$

We test near approximated solution

$$\rho(x) = 1 + \phi(x)/T$$

$$\phi(x) = \frac{\delta T(\exp(\alpha x) - \exp(-\alpha x))}{\rho_i(\exp(\alpha) - \exp(-\alpha))}$$

1D Problem : test case

- Domain : $x \in [0, 1]$
- Tests for $\Delta x \in [0.1, 5.10^{-4}]$
- Parameters : $\lambda = 0.5$, $\varepsilon = \sqrt{\Delta x}$, $\Delta t = \varepsilon \Delta x$
- Initial condition :

$$\rho(t = 0, x) = 1 + \phi(x)/T + \beta sin(2\pi x)$$
$$\phi(t = 0, x) = \frac{\delta T(\exp(\alpha x) - \exp(-\alpha x))}{\exp(\alpha) - \exp(-\alpha)}$$
$$f_i(t = 0, x) = \rho(0, x)/2$$

- Boundary conditions :

$$f_i = \frac{\rho_0}{2}$$

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Numerical Results

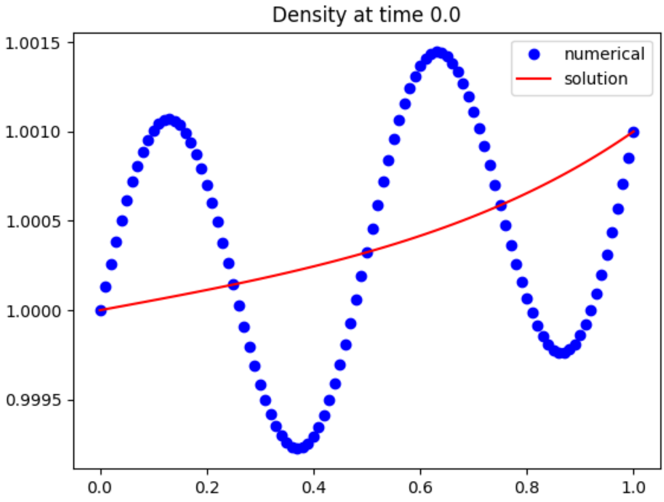
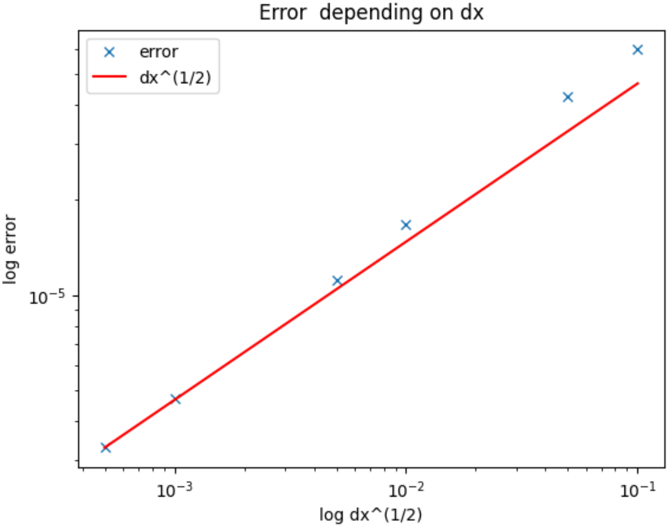


Figure: Test for $\Delta x = 0.001$

Numerical Results



Conclusion

Work in progress

- gain one order by changing the scheme
- working on D1Q3 scheme with hermite polynomials

Prospects

- add positive ions collisions, and recombination reaction
- Scaling for $T = T(E/\rho_n)$ asymptotic
- 2D lattice Boltzmann

Thank you for your attention

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