Kinetic model and numerical scheme for electrons in glow discharge plasmas

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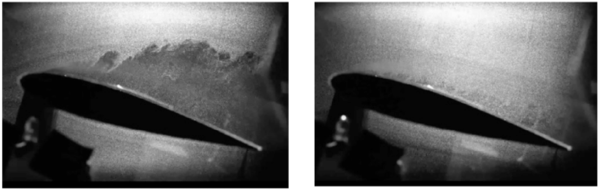
Physical context

Cold plasmas applications in the industry:

- Deicing
- Airflow control
- Components cleaning

Plasma actuators :

- generate a plasma discharge around the wing
- prevent flow separation
- enhancing lift



(a) (b)

Physical context

Cold plasma parameters (glow discharge) :

- atmospheric pressure discharges
- partially ionized gas : ionization degree $\delta_e = 10^{-6}$ 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 (or ions) :

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

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

- if the temperature depends only on $E/\rho_n \Rightarrow$ only mass equation (local field approximation)

Goal : Use Lattice Boltzmann method to solve DD

Summary

- A little reminder of lattice Boltzmann method
- Kinetic model for plasmas
- Derivation of a LB scheme
- Numerical results
- Conclusion and prospects

Lattice Boltzmann method

The classical form of a LB scheme is

$$f_i(t + \Delta t, x + \lambda_i \Delta t) = f_i(t, x) + \omega(M_i(t, x) - f_i(t, x))$$

- f_i : function of a of spatial points $x \in \mathbb{R}^m$ (forming a Cartesian grid) and time t
- $\{\lambda_i\}_{i=0,\dots n}$: discrete set of velocities such that $x + \lambda_i \Delta t$ belongs to the spatial
- ω is a parameter depending on Δt and other parameters

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Lattice Boltzmann method

The classical form of a LB scheme is

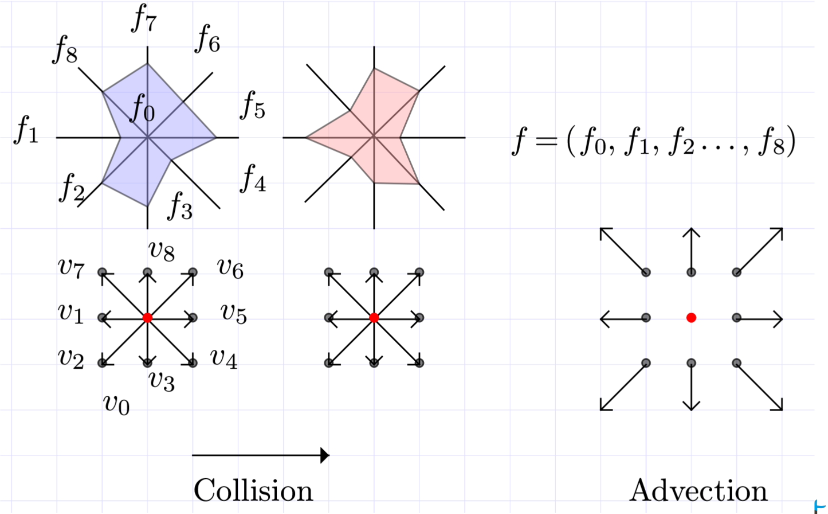
$$f_i(t+\Delta t, x+\lambda_i \Delta t) = f_i(t,x) + \omega(M_i(t,x) - f_i(t,x))$$

- discrete moments of f are computed by

$$\sum_i f_i, \quad \sum_i f_i \lambda_i \ldots$$

- M_i is a function defined with the moments of f
- the scheme consists in a relaxation step and a streaming step

Lattice Boltzmann method



Lattice Boltzmann method

Lattice Boltzmann equation

$$\partial_t f_i + v_i \partial_x f_i = \frac{1}{\tau}(M_i - f_i)$$

can be rewritten in the characteristics variable $\xi = (t + l, x + \lambda_i l)$

- LBE is integrated between $l = 0$ and $l = \Delta t$:

$$f_i(t + \Delta t, x + v_i \Delta t) - f_i(t, x)$$

- relaxation term is approximated with rectangle method or with trapezoidal rule :

$$\frac{\Delta t}{2\tau}(M_i - f_i)(t + \Delta t, x + \lambda_i \Delta t) + \frac{\Delta t}{2\tau}(M_i - f_i)(t, x)$$

The scheme is then

$$f_i(t+\Delta t, x+v_i\Delta t) = f_i(t,x) + \frac{\Delta t}{2\tau}[(M_i - f_i)(t+\Delta t, x+\lambda_i\Delta t) + (M_i - f_i)(t,x)]$$

A change of variable is performed to obtain an explicit scheme

$$g_i(t,x) = f_i(t,x) - \frac{\Delta t}{2\tau}(M_i - f_i)(t,x)$$

Finally we obtain

$$g_i(t+\Delta t, x+v_i\Delta t) = g_i(t,x) + \omega(M_i - g_i)(t,x)$$

with $\omega = \frac{\Delta t}{\tau+\Delta t/2}$

Lattice Boltzmann method

A classical approach in LBM is to use Hermite polynomials :

$$w(\lambda) = \frac{1}{(2\pi)^{\frac{1}{2}}} \exp(-\frac{\lambda_i^2}{2})$$

$$1, \quad \lambda, \quad \lambda \otimes \lambda - I_m ...$$

In this case the lattice velocities λ_i are Gauss-Hermite points and M_i is expressed in terms of Hermite polynomials

$$M_i = w(\lambda_i)\rho[1 + u\lambda_i + \ ...]$$

with

$$\rho = \sum_i f_i, \quad u = \sum_i f_i \lambda_i / \rho, \quad ...$$

Lattice Boltzmann method

We want to solve drift diffusion equations, several questions arise :

- Which collision operator to solve DD ?
- Which lattice is adapted to this problem ?
- What kind of boundary conditions ?

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

Kinetic model

- Starting from previous work [1] : 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 :

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

- Collisions considered : ellastic inter/intra-species collisions, inellastic ionization-recombination collisions

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

Kinetic model

Simplifications : $f_{i,n}$ = isotropic Maxwellians, simplified Q_{ion}, Q_{ee}

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

This equation gives at hydrodynamic limit drift diffusion model

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Kinetic model

Hilbert expansion of f

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

- Q_{en}^0 collisions will cause f_0 to be isotropic
- $Q_{ee} \Rightarrow f_0$ is also maxwellian
- f_1 will give the form of the flux in DD equation :

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

  where $\tilde{f}_1 \in \mathrm{Ker}(Q_{en}^0)$
- Q_{en}^2 : relaxation term on electronic temperature
- Q_{ion} : source term taking into account ionization processes

Fluid equations

By integrating the kinetic equation against 1 and $v^2/2$ we obtain :

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

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

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

Two possibilities depending on the cross section chosen :

- Hard spheres : $D \propto \sqrt{T}$, $\mu \propto \sqrt{T}^{-1}$
- Maxwellian molecules : $D \propto T$, $\mu \propto 1$

Derivation of a LB scheme

We start with a $D1Q3$ lattice $v = +1, 0, -1$. Ionization collisions are omitted. We define :

$$\sum_i f_i = \rho, \sum_i f_i v_i = \rho u, \sum_i f_i v_i^2 = \mathcal{E}$$

Collision operators are projected onto the 3 first polynomials of Hermit basis

$$Q_{en}^0(f)(v) \approx -2\sigma_{en}\rho_n \rho u w(v) \frac{v}{3}$$

$$Q_{en}^2(f)(v) \approx -4\sqrt{2\pi}\rho_n \sigma_{en} \left(\mathcal{E} - T_n \rho\right) w(v) \left(\frac{v^2}{3^2} - \frac{1}{3}\right)$$

$$F(f)(v) \approx -w(v)E\left(\rho\frac{v}{3} + \rho u \left(\frac{v^2}{3^2} - \frac{1}{3}\right)\right)$$

$$Q_{ee}(f)(v) \approx w(v)\left(\rho + \rho u v + \frac{1}{2}\rho\left(T - 1\right)\left(v^2 - 1\right)\right) - f$$

Derivation of a LB scheme

We consider the lattice Boltzmann equation with these operators :

$$\partial_t f_i + \frac{v_i}{\varepsilon}\partial_x f_i = \frac{1}{\varepsilon^2} Q^0_{en}(f_i)(v_i) + Q^2_{en}(f_i)(v_i) + \frac{1}{\varepsilon} F(f_i)(v_i) + \frac{1}{\varepsilon} Q_{ee}(f_i)(v_i)$$

As previously, by taking the Hilbert expansion of f we can obtain equations on the moments of f :

$$\begin{aligned} f_i &= f_i^0 + \varepsilon f_i^1 + \mathcal{O}\left(\varepsilon^2\right) \\ \rho &= \rho^0 + \varepsilon \rho^1 + \mathcal{O}\left(\varepsilon^2\right) \\ \rho u &= (\rho u)^0 + \varepsilon (\rho u)^1 + \mathcal{O}\left(\varepsilon^2\right) \\ \rho T &= (\rho T)^0 + \varepsilon (\rho T)^1 + \mathcal{O}\left(\varepsilon^2\right) \end{aligned}$$

Derivation of a LB scheme

The system obtained is

$$\partial_t \rho^0 + \partial_x (\rho u)^1 = 0$$
$$\partial_t (\rho T)^0 + \partial_x (\rho u)^1 + \frac{1}{9} E (\rho u)^1 = -\frac{4}{9}\sqrt{2\pi}\rho_n \sigma_{en}((\rho T)^0 - T_n \rho^0)$$

with

$$(\rho u)^1 = -\frac{E\rho^0}{2\sigma_{en}\rho_n} - \frac{\partial_x (\rho T)^0}{2\sigma_{en}\rho_n}$$

- this is not consistent with the DD system
- the quadrature is probably not accurate enough
- in order to have the right equation it would be mandatory to have at least 5 Gauss points (for example $D1Q5$)
- for 2D in space that would require a lot of points

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LB scheme for advection diffusion problem

- We focus on density equation
- D and μ are assumed to be constant and equal
- No ionization processes

1D Drift diffusion equation

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

This time we choose to use D1Q2[2] scheme

- two LB schemes proposed for convection-diffusion problems
- results of L^2 and L^∞ stability

[2] S Dellacherie, 2012

LB scheme for advection diffusion problem

Scheme

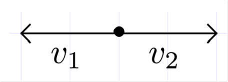
We use the change of variable with the trapezoidal rule

$$g_i(t+\Delta t, x + \frac{v_i}{\varepsilon}\Delta t) = g(t,x) + \Delta t(Q_i(f) + F_i(f))(t,x)$$

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

- $Q_i(f) = -\frac{\sigma_{en}}{2\varepsilon^2} q v_i$
- $F_i(f) = -\frac{1}{2\varepsilon} E \rho v_i$

Here $q = \rho u$



LB scheme for advection diffusion problem

Lattice Boltzmann equation :

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

Again, by using the Hilbert expansion of f in ε we can show that the fluid limit of the LBE is

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

with

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

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LB scheme for advection diffusion problem

Link with finite differences schemes

For $\Delta t = \varepsilon \Delta x$ LB scheme is equivalent to

$$\rho_j^{n+1} = \frac{1}{2}(\rho_{j+1}^n + \rho_{j-1}^n) + \frac{1}{2}\left(1 - \frac{\Delta x}{2\varepsilon}(2+\sigma_{en})\right)(q_{j-1}^n - q_{j+1}^n) + \frac{\Delta x}{4}(E_{j+1}^n \rho_{j+1}^n - E_{j-1}^n \rho_{j-1}^n)$$

$$q_j^{n+1} = \frac{1}{1+\frac{\Delta x \sigma_{en}}{2\varepsilon}}\Big(\frac{1}{2}(\rho_{j-1}^n - \rho_{j+1}^n) - \frac{\Delta x}{2}E_j^{n+1}\rho_j^{n+1} + \frac{1}{2}\left(1 - \frac{\sigma_{en}\Delta x}{2\varepsilon}\right)(q_{j-1}^n + q_{j+1}^n) - \frac{\Delta x}{4}(E_{j+1}^n \rho_{j+1}^n + E_{j-1}^n \rho_{j-1}^n)\Big)$$

LB scheme for advection diffusion problem

- Finite difference schemes allows us to compute equivalent equations[3]
- We want a diffusive scaling $\Delta t \sim \Delta x^2$ to recover diffusion
- One possible choice is $\varepsilon = \frac{\sigma_{en}\Delta x}{2}$, this gives :

$$\partial_t \rho = \left(C\partial_x^2 \rho + C\partial_x(E\rho)\right) + O(\Delta x)$$

with $C = \left(\frac{1}{\sigma_{en}} - \frac{2}{\sigma_{en}^2}\right)$

- then σ_{en} can be used to fit the value of $D = \mu$ that is wanted
- in this case there is a condition : $\sigma_{en} > 2$

[3] F Dubois, 2008

1D Problem : numerical results

Stability 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

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

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

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

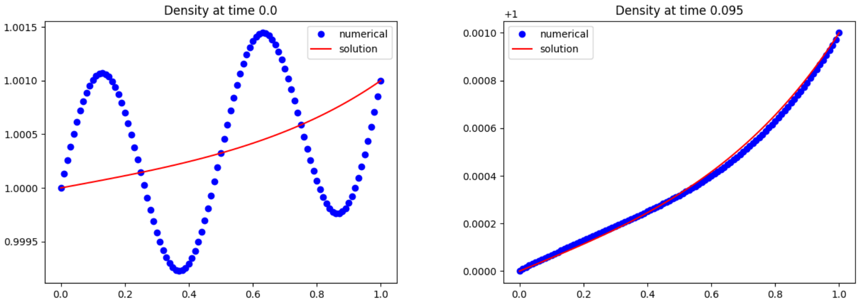
$$\rho(t = 0, x) = 1 + \phi(x)/T + \beta sin(2\pi x)$$
$$\phi(t = 0, x) = \frac{\delta T(\exp(\alpha x) - \exp(-\alpha x))}{\exp(\alpha) - \exp(-\alpha)}$$
$$f_i(t = 0, x) = \rho(0, x)/2$$

- Boundary conditions :

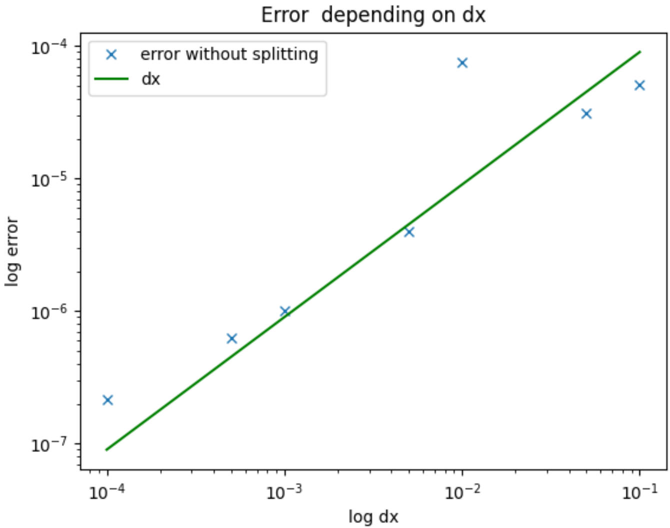
$$f_i = \frac{\rho_0}{2}$$

Numerical Results

Test for $\Delta x = 0.01$



Numerical Results



Conclusion

Work in progress

- using two $D1Q2$ schemes to recover diffusion coefficient that could be different from mobility coefficient
- ionization process was added

Prospects

- physical test case in $2D$
- L^{∞} or L^2 stability results ?

Thank you for your attention