A contribution to the simulation of Vlasov-based models

Francesco Vecil

Universitat Autònoma de Barcelona

Universitat Autònoma de Barcelona, 17/12/07

Outline

Outline

Objects of the simulations

The goal of this work is a contribution to the numerical simulation of kinetic models for electronic engineering and plasma physics.

- **Plasmas** are ionized gases: positive, negative and neutral charges dissociate.
- **Electronic devices** are physical solid state devices, like semiconductors, which exploit the electronic properties of semiconductor materials (e. g. silicon) by manipulating their conductivity via the *doping*.

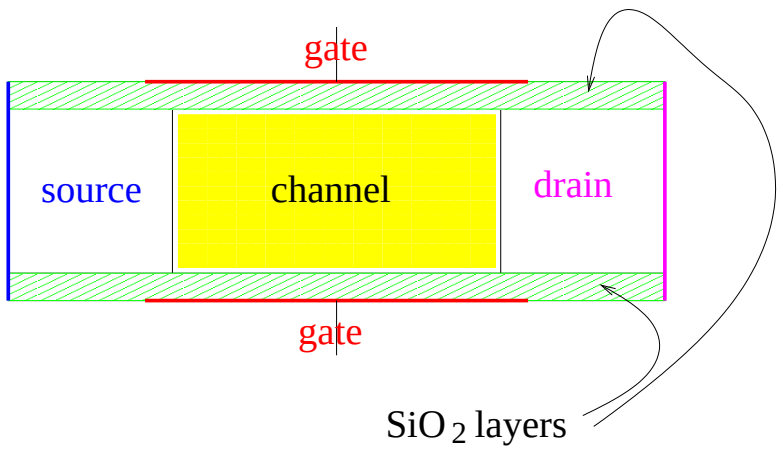


Figure: A **M**etal **O**xide **S**emiconductor **F**ield **E**ffect **T**ransistor.

Objects of the simulations

The goal of this work is a contribution to the numerical simulation of kinetic models for electronic engineering and plasma physics.

- **Plasmas** are ionized gases: positive, negative and neutral charges dissociate.
- **Electronic devices** are physical solid state devices, like semiconductors, which exploit the electronic properties of semiconductor materials (e. g. silicon) by manipulating their conductivity via the *doping*.

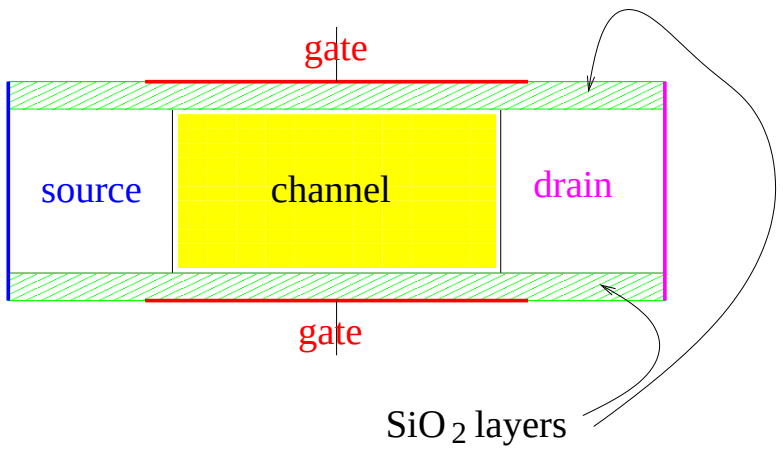


Figure: A **M**etal **O**xide **S**emiconductor **F**ield **E**ffect **T**ransistor.

Objects of the simulations

The goal of this work is a contribution to the numerical simulation of kinetic models for electronic engineering and plasma physics.

- **Plasmas** are ionized gases: positive, negative and neutral charges dissociate.
- **Electronic devices** are physical solid state devices, like semiconductors, which exploit the electronic properties of semiconductor materials (e. g. silicon) by manipulating their conductivity via the *doping*.

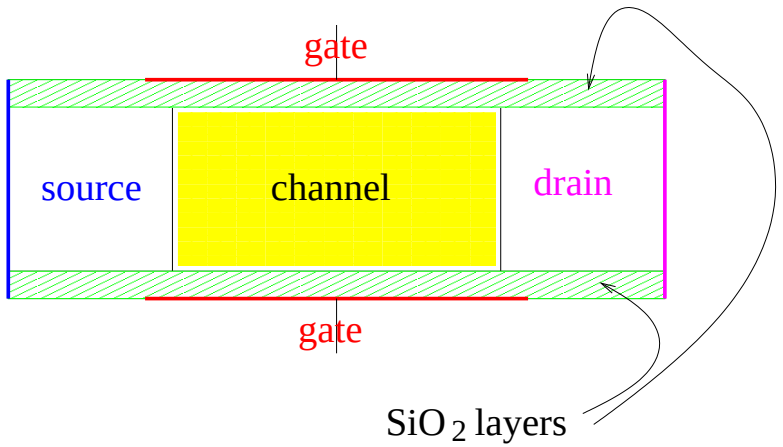


Figure: A **M**etal **O**xide **S**emiconductor **F**ield **E**ffect **T**ransistor.

Aspects of the modelling

Transport.

The Boltzmann Transport Equation (BTE) describes, at microscopic level, how the charge carriers move inside the object of study:

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f + \frac{F(t,x)}{m} \cdot \nabla_v f = \mathcal{Q}[f].$$

Force field.

Apart from the free motion, the charge carriers may be driven by the effect of a force field, usually of three categories:

- self-consistent Poisson equation, in semiconductors;
- coupled Schrödinger-Poisson equation, in nanostructures;
- Lorentz force (Maxwell equations), in plasmas.

Collisions.

The charge carriers may have collisions with other carriers, with the fixed lattice or with phonons (pseudo-particles describing the vibration of the lattice).

Aspects of the modelling

Transport.

The Boltzmann Transport Equation (BTE) describes, at microscopic level, how the charge carriers move inside the object of study:

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f + \frac{F(t,x)}{m} \cdot \nabla_v f = \mathcal{Q}[f].$$

Force field.

Apart from the free motion, the charge carriers may be driven by the effect of a force field, usually of three categories:

- self-consistent Poisson equation, in semiconductors;
- coupled Schrödinger-Poisson equation, in nanostructures;
- Lorentz force (Maxwell equations), in plasmas.

Collisions.

The charge carriers may have collisions with other carriers, with the fixed lattice or with phonons (pseudo-particles describing the vibration of the lattice).

Aspects of the modelling

Transport.

The Boltzmann Transport Equation (BTE) describes, at microscopic level, how the charge carriers move inside the object of study:

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f + \frac{F(t,x)}{m} \cdot \nabla_v f = \mathcal{Q}[f].$$

Force field.

Apart from the free motion, the charge carriers may be driven by the effect of a force field, usually of three categories:

- self-consistent Poisson equation, in semiconductors;
- coupled Schrödinger-Poisson equation, in nanostructures;
- Lorentz force (Maxwell equations), in plasmas.

Collisions.

The charge carriers may have collisions with other carriers, with the fixed lattice or with phonons (pseudo-particles describing the vibration of the lattice).

Transport

Two categories of transport equations are used.

Microscopic models.

At kinetic level the motion is described by a probabilistic magnitude f defined in the phase space (x, v), (x, p) or (x, k): the choice of the problem may make more suitable the use of the velocity v instead of the impulsion p or the wave vector k.

Macroscopic models.

The system does not depend on v or p or k; the magnitude describing the evolution just depends on time and position. Starting from the BTE, hydrodynamics or diffusion limits give Euler, Navier-Stokes, Spherical Harmonics Expansion, Energy-Transport or Drift-Diffusion systems.

Transport

Two categories of transport equations are used.

Microscopic models.

At kinetic level the motion is described by a probabilistic magnitude f defined in the phase space (x, v), (x, p) or (x, k): the choice of the problem may make more suitable the use of the velocity v instead of the impulsion p or the wave vector k.

Macroscopic models.

The system does not depend on v or p or k; the magnitude describing the evolution just depends on time and position. Starting from the BTE, hydrodynamics or diffusion limits give Euler, Navier-Stokes, Spherical Harmonics Expansion, Energy-Transport or Drift-Diffusion systems.

Transport

Two categories of transport equations are used.

Microscopic models.

At kinetic level the motion is described by a probabilistic magnitude f defined in the phase space (x, v), (x, p) or (x, k): the choice of the problem may make more suitable the use of the velocity v instead of the impulsion p or the wave vector k.

Macroscopic models.

The system does not depend on v or p or k; the magnitude describing the evolution just depends on time and position. Starting from the BTE, hydrodynamics or diffusion limits give Euler, Navier-Stokes, Spherical Harmonics Expansion, Energy-Transport or Drift-Diffusion systems.

Outline

Motivation

We need a **Pointwise** interpolation method which does not add spurious oscillations when high gradients appear, e.g. when a jump has to be transported.

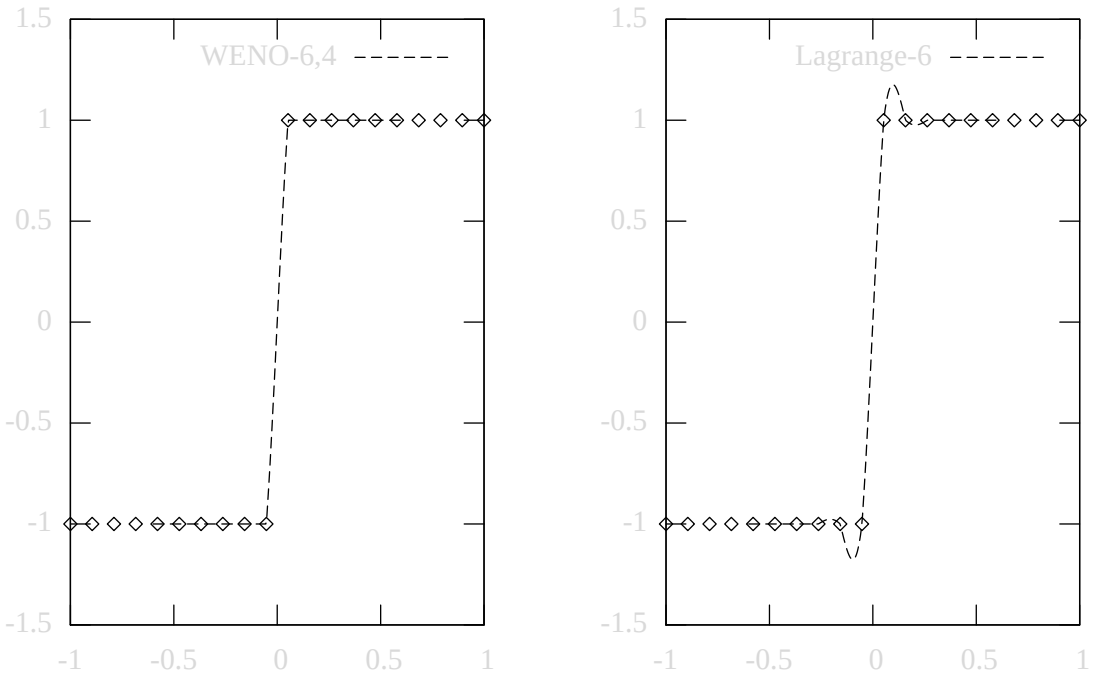


Figure: Left: PWENO interpolation. Right: Lagrange interpolation.

Motivation

We need a **Pointwise** interpolation method which does not add spurious oscillations when high gradients appear, e.g. when a jump has to be transported.

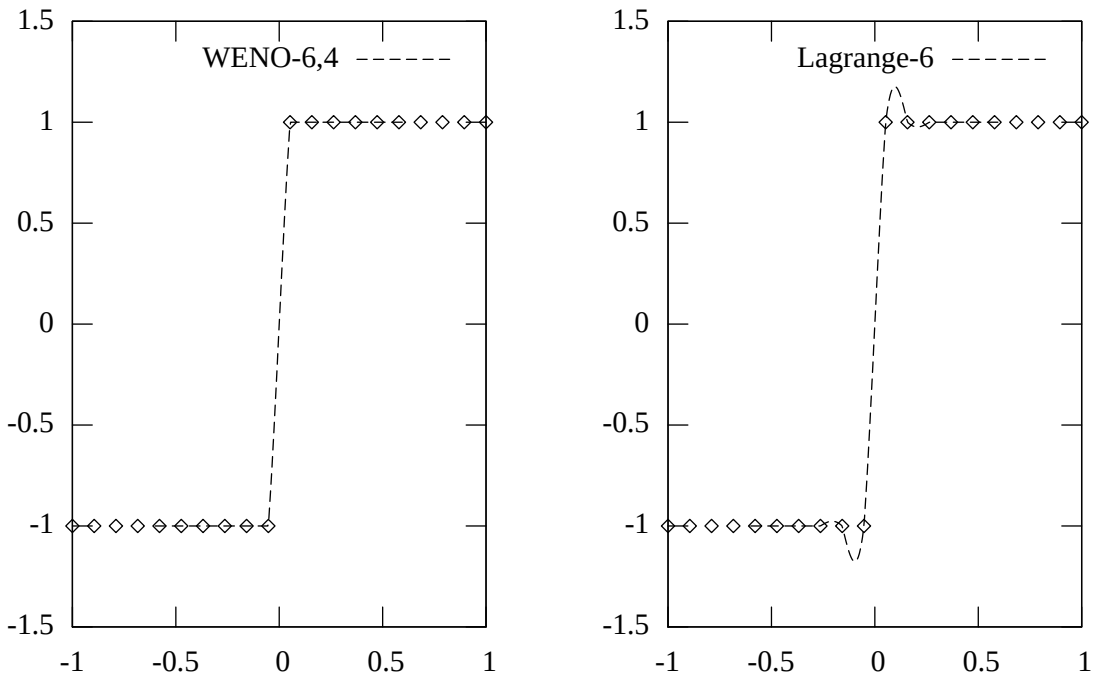
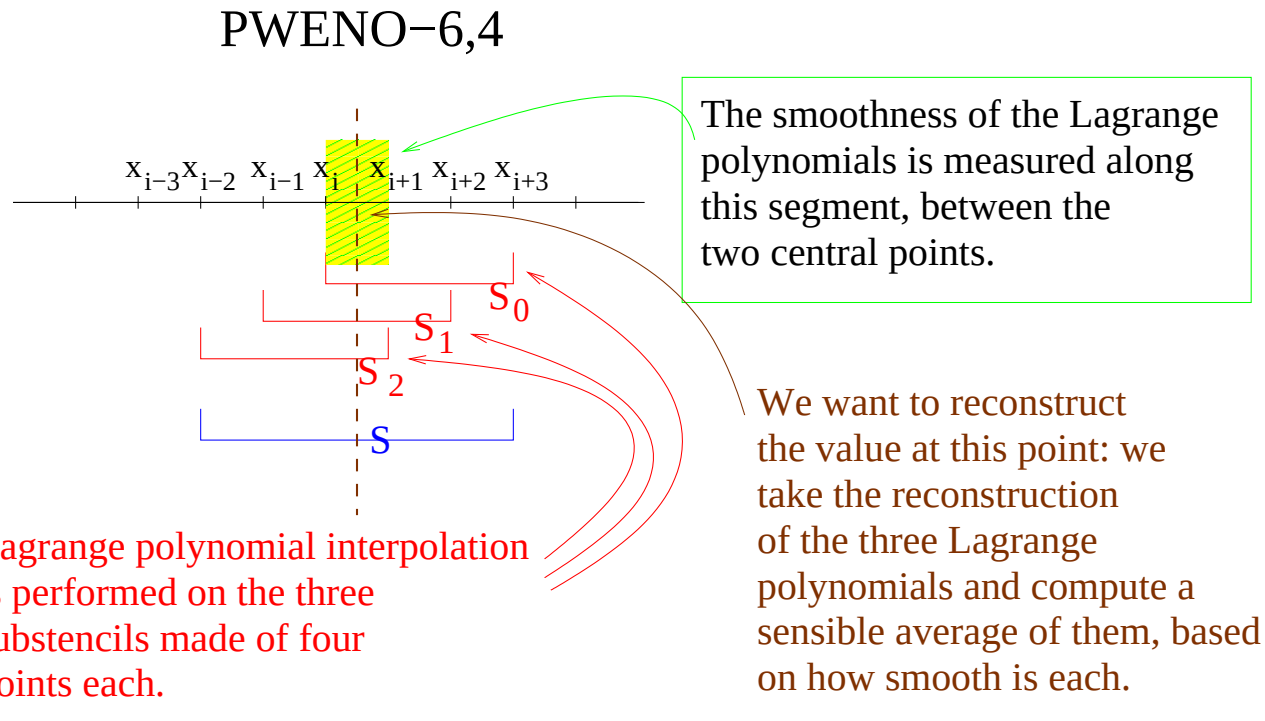


Figure: Left: PWENO interpolation. Right: Lagrange interpolation.

Non-oscillatory properties

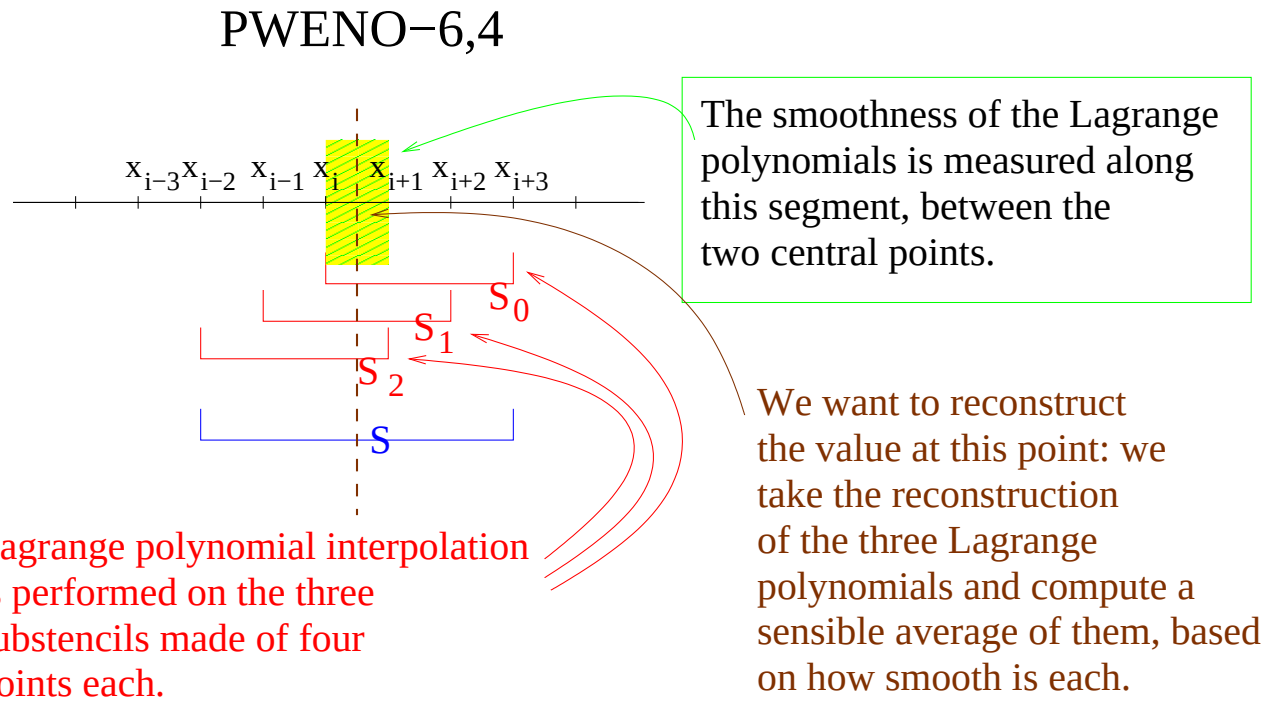
Essentially Non Oscillatory (ENO) methods are based on on a sensible average of Lagrange polynomial reconstructions.

We describe the case of PWENO-6,4: we take a stencil of six points and divide it into three substencils of four points:



Non-oscillatory properties

Essentially Non Oscillatory (ENO) methods are based on on a sensible average of Lagrange polynomial reconstructions.
We describe the case of PWENO-6,4: we take a stencil of six points and divide it into three substencils of four points:



The average

If we note $p_r(x)$ the Lagrange polynomials, PWENO reconstruction reads

$$p_{PWENO}(x) = \omega_0(x)p_0(x) + \omega_1(x)p_1(x) + \omega_2(x)p_2(x).$$

Convex combination.

The convex combination $\{\omega_r(x)\}_r$ must penalize the substencils $\mathcal{S}_r$ in which the $p_r(x)$ have high derivatives.

Smoothness indicators

In order to decide which substencils $\mathcal{S}_r$ are "regular" and which ones are not, we have to introduce the smoothness indicators: we use a weighted sum of the L^2-norms of the Lagrange polynomials $p_r(x)$ to measure their regularity close to the reconstruction point x. The following smoothness indicators have been proposed by Jiang and Shu:

$$\beta_r = \Delta x \left\| \frac{dp_r}{dx} \right\|_{L^2_{(x_i,x_{i+1})}} + \Delta x^3 \left\| \frac{d^2p_r}{dx^2} \right\|_{L^2_{(x_i,x_{i+1})}} + \Delta x^5 \left\| \frac{d^3p_r}{dx^3} \right\|_{L^2_{(x_i,x_{i+1})}}.$$

The average

If we note $p_r(x)$ the Lagrange polynomials, PWENO reconstruction reads

$$p_{PWENO}(x) = \omega_0(x)p_0(x) + \omega_1(x)p_1(x) + \omega_2(x)p_2(x).$$

Convex combination.

The convex combination $\{\omega_r(x)\}_r$ must penalize the substencils $\mathcal{S}_r$ in which the $p_r(x)$ have high derivatives.

Smoothness indicators

In order to decide which substencils $\mathcal{S}_r$ are "regular" and which ones are not, we have to introduce the smoothness indicators: we use a weighted sum of the L^2-norms of the Lagrange polynomials $p_r(x)$ to measure their regularity close to the reconstruction point x. The following smoothness indicators have been proposed by Jiang and Shu:

$$\beta_r = \Delta x \left\| \frac{dp_r}{dx} \right\|_{L^2_{(x_i,x_{i+1})}} + \Delta x^3 \left\| \frac{d^2p_r}{dx^2} \right\|_{L^2_{(x_i,x_{i+1})}} + \Delta x^5 \left\| \frac{d^3p_r}{dx^3} \right\|_{L^2_{(x_i,x_{i+1})}}.$$

The average

If we note $p_r(x)$ the Lagrange polynomials, PWENO reconstruction reads

$$p_{PWENO}(x) = \omega_0(x)p_0(x) + \omega_1(x)p_1(x) + \omega_2(x)p_2(x).$$

Convex combination.

The convex combination $\{\omega_r(x)\}_r$ must penalize the substencils $\mathcal{S}_r$ in which the $p_r(x)$ have high derivatives.

Smoothness indicators

In order to decide which substencils $\mathcal{S}_r$ are "regular" and which ones are not, we have to introduce the smoothness indicators: we use a weighted sum of the L^2-norms of the Lagrange polynomials $p_r(x)$ to measure their regularity close to the reconstruction point x. The following smoothness indicators have been proposed by Jiang and Shu:

$$\beta_r = \Delta x \left\| \frac{dp_r}{dx} \right\|_{L^2_{(x_i,x_{i+1})}} + \Delta x^3 \left\| \frac{d^2p_r}{dx^2} \right\|_{L^2_{(x_i,x_{i+1})}} + \Delta x^5 \left\| \frac{d^3p_r}{dx^3} \right\|_{L^2_{(x_i,x_{i+1})}}.$$

High order reconstruction

Admit for now that the convex combination is given by the normalization $\omega_r(x) = \frac{\tilde{\omega}_r(x)}{\sum_{s=0}^{2} \tilde{\omega}_s(x)}$ of the protoweights $\tilde{\omega}_r(x)$ defined this way:

$$\tilde{\omega}_r(x) = \frac{d_r(x)}{(\epsilon + \beta_r)^2}.$$

Regular reconstruction

Suppose that all the β_r are equal; then we have

$$\omega_r(x) = d_r(x).$$

The optimal order is achieved by Lagrange reconstruction $p_{Lagrange}(x)$ in the whole stencil $\mathcal{S}$, so if we define $d_r(x)$ to be the polynomials such that

$$p_{Lagrange}(x) = d_0(x)p_0(x) + d_1(x)p_1(x) + d_2(x)p_2(x),$$

then we have achieved the optimal order because $p_{PWENO}(x) = p_{Lagrange}(x)$.

High order reconstruction

Admit for now that the convex combination is given by the normalization $\omega_r(x) = \frac{\tilde{\omega}_r(x)}{\sum_{s=0}^{2} \tilde{\omega}_s(x)}$ of the protoweights $\tilde{\omega}_r(x)$ defined this way:

$$\tilde{\omega}_r(x) = \frac{d_r(x)}{(\epsilon + \beta_r)^2}.$$

Regular reconstruction

Suppose that all the β_r are equal; then we have

$$\omega_r(x) = d_r(x).$$

The optimal order is achieved by Lagrange reconstruction $p_{Lagrange}(x)$ in the whole stencil $\mathcal{S}$, so if we define $d_r(x)$ to be the polynomials such that

$$p_{Lagrange}(x) = d_0(x)p_0(x) + d_1(x)p_1(x) + d_2(x)p_2(x),$$

then we have achieved the optimal order because $p_{PWENO}(x) = p_{Lagrange}(x)$.

High order reconstruction

Admit for now that the convex combination is given by the normalization $\omega_r(x) = \frac{\tilde{\omega}_r(x)}{\sum_{s=0}^{2} \tilde{\omega}_s(x)}$ of the protoweights $\tilde{\omega}_r(x)$ defined this way:

$$\tilde{\omega}_r(x) = \frac{d_r(x)}{(\epsilon + \beta_r)^2}.$$

High gradients

Otherwise, suppose for instance that β_0 is high order than the other ones: in this case $\mathcal{S}_0$ is penalized and most of the reconstruction is carried by the other more "regular" substencils.

Outline

Motivation

In this work, splitting techniques are used at different levels, namely:

- to split the Boltzmann Transport Equation into the solution of the transport part and the collisional part for separate, i.e. the **Time Splitting**:

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f + F \cdot \nabla_v f = \mathcal{Q}[f]$$

splits into

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f + F \cdot \nabla_v f = 0, \qquad \frac{\partial f}{\partial t} = \mathcal{Q}[f];$$

- to split the (x, v)-phase space in a collisionless context (**Dimensional Splitting**):

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f + F \cdot \nabla_v f = 0$$

splits into

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f = 0, \qquad \frac{\partial f}{\partial t} + F \cdot \nabla_v f = 0.$$

Motivation

In this work, splitting techniques are used at different levels, namely:

- to split the Boltzmann Transport Equation into the solution of the transport part and the collisional part for separate, i.e. the **Time Splitting**:

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f + F \cdot \nabla_v f = \mathcal{Q}[f]$$

splits into

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f + F \cdot \nabla_v f = 0, \qquad \frac{\partial f}{\partial t} = \mathcal{Q}[f];$$

- to split the (x, v)-phase space in a collisionless context (**Dimensional Splitting**):

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f + F \cdot \nabla_v f = 0$$

splits into

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f = 0, \qquad \frac{\partial f}{\partial t} + F \cdot \nabla_v f = 0.$$

Motivation

In this work, splitting techniques are used at different levels, namely:

- to split the Boltzmann Transport Equation into the solution of the transport part and the collisional part for separate, i.e. the **Time Splitting**:

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f + F \cdot \nabla_v f = \mathcal{Q}[f]$$

splits into

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f + F \cdot \nabla_v f = 0, \qquad \frac{\partial f}{\partial t} = \mathcal{Q}[f];$$

- to split the (x, v)-phase space in a collisionless context (**Dimensional Splitting**):

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f + F \cdot \nabla_v f = 0$$

splits into

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f = 0, \qquad \frac{\partial f}{\partial t} + F \cdot \nabla_v f = 0.$$

General framework

The (formal) exact solution of the linear PDE

$$\frac{\partial f}{\partial t} = Lf, \qquad f(t=0) = f^0$$

is

$$f(t) = e^{Lt} f^0.$$

If we can write the linear operator L as the sum of two linear operators,

$$L = L_1 + L_2,$$

then we may approximate the exact solution by solving for separate

$$\frac{\partial f}{\partial t} = L_1 f \qquad \text{and} \qquad \frac{\partial f}{\partial t} = L_2 f.$$

Several schemes are proposed for reconstructing the solution of the original PDE from the solution of either blocks; a first order (in time) scheme is given by

$$\tilde{f}(t+\Delta t) = e^{L_2 \Delta t} e^{L_1 \Delta t} f(t),$$

while a second order (in time) scheme is given by

$$\tilde{f}(t+\Delta t) = e^{L_1 \frac{\Delta t}{2}} e^{L_2 \Delta t} e^{L_1 \frac{\Delta t}{2}} f(t).$$

General framework

The (formal) exact solution of the linear PDE

$$\frac{\partial f}{\partial t} = Lf, \qquad f(t=0) = f^0$$

is

$$f(t) = e^{Lt} f^0.$$

If we can write the linear operator L as the sum of two linear operators,

$$L = L_1 + L_2,$$

then we may approximate the exact solution by solving for separate

$$\frac{\partial f}{\partial t} = L_1 f \qquad \text{and} \qquad \frac{\partial f}{\partial t} = L_2 f.$$

Several schemes are proposed for reconstructing the solution of the original PDE from the solution of either blocks; a first order (in time) scheme is given by

$$\tilde{f}(t+\Delta t) = e^{L_2 \Delta t} e^{L_1 \Delta t} f(t),$$

while a second order (in time) scheme is given by

$$\tilde{f}(t+\Delta t) = e^{L_1 \frac{\Delta t}{2}} e^{L_2 \Delta t} e^{L_1 \frac{\Delta t}{2}} f(t).$$

General framework

The (formal) exact solution of the linear PDE

$$\frac{\partial f}{\partial t} = Lf, \qquad f(t=0) = f^0$$

is

$$f(t) = e^{Lt} f^0.$$

If we can write the linear operator L as the sum of two linear operators,

$$L = L_1 + L_2,$$

then we may approximate the exact solution by solving for separate

$$\frac{\partial f}{\partial t} = L_1 f \qquad \text{and} \qquad \frac{\partial f}{\partial t} = L_2 f.$$

Several schemes are proposed for reconstructing the solution of the original PDE from the solution of either blocks; a first order (in time) scheme is given by

$$\tilde{f}(t+\Delta t) = e^{L_2 \Delta t} e^{L_1 \Delta t} f(t),$$

while a second order (in time) scheme is given by

$$\tilde{f}(t+\Delta t) = e^{L_1 \frac{\Delta t}{2}} e^{L_2 \Delta t} e^{L_1 \frac{\Delta t}{2}} f(t).$$

General framework

The (formal) exact solution of the linear PDE

$$\frac{\partial f}{\partial t} = Lf, \qquad f(t=0) = f^0$$

is

$$f(t) = e^{Lt} f^0.$$

If we can write the linear operator L as the sum of two linear operators,

$$L = L_1 + L_2,$$

then we may approximate the exact solution by solving for separate

$$\frac{\partial f}{\partial t} = L_1 f \qquad \text{and} \qquad \frac{\partial f}{\partial t} = L_2 f.$$

Several schemes are proposed for reconstructing the solution of the original PDE from the solution of either blocks; a first order (in time) scheme is given by

$$\tilde{f}(t+\Delta t) = e^{L_2 \Delta t} e^{L_1 \Delta t} f(t),$$

while a second order (in time) scheme is given by

$$\tilde{f}(t+\Delta t) = e^{L_1 \frac{\Delta t}{2}} e^{L_2 \Delta t} e^{L_1 \frac{\Delta t}{2}} f(t).$$

Outline

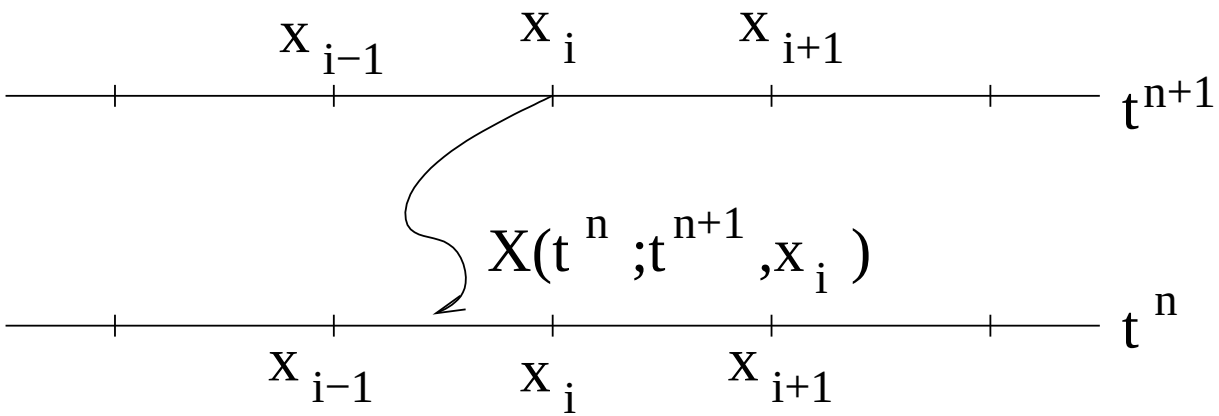
Linear advection

We propose two schemes for solving the linear advection

$$\frac{\partial f}{\partial t} + v\frac{\partial f}{\partial x} = 0 :$$

Semi-Lagrangian:

Directly integrate backward in the characteristic



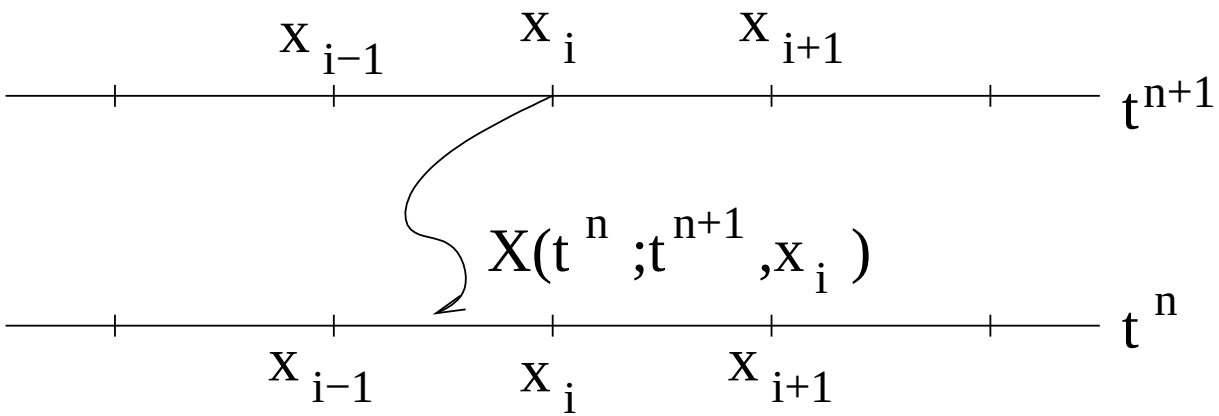
Linear advection

We propose two schemes for solving the linear advection

$$\frac{\partial f}{\partial t} + v\frac{\partial f}{\partial x} = 0 :$$

Semi-Lagrangian:

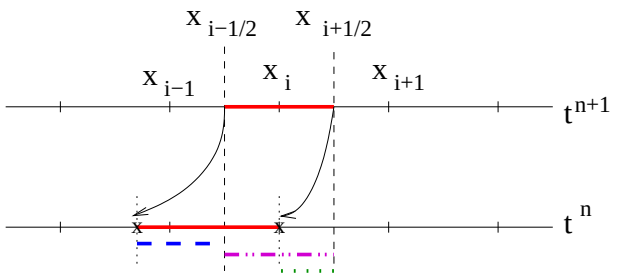
Directly integrate backward in the characteristic



Linear advection

Flux Balance Method:

Total mass conservation is forced. It is based on the idea of following backward the characteristics, but integral values are taken instead of point values:



The averages along the red segments are the same, because we have followed the characteristics backward.

FLUX BALANCE METHOD means evualuating the flux at time t^{n+1} from a balance of fluxes at previous time t^n :

- the average along the purple segment
- plus the average along the blue segment
- minus the average along the green segment

Outline

The system

We solve a Vlasov equation with given potential and a linear relaxation-time operator as collision operator by time (linear) splitting to decouple the Vlasov part and the Boltzmann part, and recursively dimensional splitting to divide the x-advection from the v-advection:

$$\frac{\partial f}{\partial t} + v\frac{\partial f}{\partial x} - \frac{d\left(\frac{x^2}{2}\right)}{dx}\frac{\partial f}{\partial v} = \frac{1}{\tau}\left[\frac{1}{\pi}e^{-\frac{v^2}{2}}\rho - f\right], \qquad f(0,x) = f_0(x).$$

We expect the solution to rotate (due to the Vlasov part and the potential) and to converge to an equilibrium (due to collisions) given by

$$f_s = \frac{\text{mass}(f)}{\pi^2}\exp\left(-\frac{x^2+v^2}{2}\right).$$

Setting up initial conditions

We perform tests with three initial conditions, more or less close to the equilibrium; the relaxation time is set $\tau = 3.5$:

$$
\begin{aligned}
f_0^{(1)} &= Z_1 \sin^2\left(\frac{x}{2}\right) e^{-\frac{x^2+v^2}{2}} \\
f_0^{(2)} &= Z_2 \sin^2\left(\frac{x}{2}\right) \sin^2\left(\frac{v}{2}\right) e^{-\frac{x^2+v^2}{2}} \\
f_0^{(3)} &= Z_3 \left[1 + 0.05 \sin^2\left(\frac{x}{2}\right)\right] e^{-\frac{x^2+v^2}{2}}.
\end{aligned}
$$

Entropies

The global and local relative entropies are defined this way:

$$
\begin{aligned}
H[f; f_s] &= \int_{\mathbb{R}} \int_{\mathbb{R}} \frac{|f - f_s|^2}{f_s} dv dx \\
\tilde{H}[f; \rho M_1] &= \int_{\mathbb{R}} \int_{\mathbb{R}} \frac{|f - \rho M_1|^2}{f_s} dv dx.
\end{aligned}
$$

Outline

Two-stream instability

The problem

We set the problem in a collisionless context. The force field is self-consistently computed through a Poisson equation. Equations are normalized, periodic boundary conditions are taken for both the transport and the potential.

$$\frac{\partial f}{\partial t} + v\frac{\partial f}{\partial x} - \frac{\partial \Phi}{\partial x}\frac{\partial f}{\partial v} = 0$$

$$\frac{\partial^2 \Phi}{\partial x^2} = 1 - \int_{\mathbb{R}} f dv$$

$$f(t=0,x,v) = f_{eq}(v)\left[1 + 0.01\left(\frac{\cos(2kx)+\cos(3kx)}{1.2} + \cos(kx)\right)\right].$$

As initial condition, we perturb the equilibrium-state given by

$$f_{eq}(v) = K(1+v^2)e^{-\frac{v^2}{2}},$$

K being a normalization factor.

Outline

The model

We describe via the Boltzmann Transport Equation the transport/collision in an electronic device

$$\frac{\partial f}{\partial t} + \frac{1}{\hbar}\nabla_k \varepsilon \cdot \nabla_x f - \frac{q}{\hbar} E \cdot \nabla_k f = \mathcal{Q}[f]$$
$$\Delta \Phi = \frac{q}{\epsilon_0}\left[\rho[f] - N_D\right], \qquad E = -\nabla_x \Phi$$
$$f_0(x,k) = N_D(x) M(k),$$

where the band structure is given in the parabolic approximation

$$\varepsilon(k) = \frac{\hbar^2 |k|^2}{2 m_*},$$

m_* being the Silicon effective mass.

The collision operator

The collision operator takes into account the scattering of the carriers with acoustic phonons, in the elastic approximation, and with optical phonons, with a single frequency ω. Therefore the operator reads, in the low-density approximation:

$$\mathcal{Q}[f] = \int_{\mathbb{R}^3} \left[S(k',k) f(t,x,k') - S(k,k') f(t,x,k) \right] dk',$$

where the scattering rate is given by

$$\begin{aligned} S(k,k') &= K \left[(n_q+1)\delta(\epsilon(k') - \epsilon(k) + \hbar\omega) + n_q \delta(\epsilon(k') - \epsilon(k) - \hbar\omega) \right] \\ &+ K_0 \delta(\epsilon(k') - \epsilon(k)). \end{aligned}$$

Outline

Adimensionalization

The system is reduced to dimensionless magnitudes in order to improve numerical results by making the computer perform calculations on numbers of order 1. Then splitting schemes are applied to solve for separate transport and collision, and dimensional splitting is applied to separate x-dimension from k_1-dimension.

adim.	parameter	400 nm device	50 nm device
$\tilde{k} = k^* k$	$k^* = \frac{\sqrt{2m^* k_B T_L}}{\hbar}$	$4.65974 \times 10^8 m^{-1}$	$4.65974 \times 10^8 m^{-1}$
$\tilde{x} = l^* x$	$l^* =$ device length	$1\ \mu m$	$250\ nm$
$\tilde{t} = t^* t$	$t^* =$ typical time	$1\ ps = 10^{-12} s$	$1\ ps = 10^{-12} s$
$\tilde{V}(\tilde{x}) = V^* V(x)$	$V^* =$ typical Vbias	$1V$	$1V$
$\tilde{E}(\tilde{x}) = E^* E(x)$	$E^* = \frac{1}{10}\frac{V^*}{l^*}$	$100000 V m^{-1}$	$400000 V m^{-1}$
$\tilde{\varepsilon}(\tilde{k}) = \varepsilon^* \varepsilon(k)$	$\epsilon^* = \frac{\hbar^2 k^{*2}}{2m^*}$	$4.14195e-21$	$4.14195e-21$
$\tilde{\rho}(\tilde{x}) = \rho^* \rho(x)$	$\rho^* = \left(\frac{2m^* k_B T_L}{\hbar}\right)^{3/2}$	1.01178×10^{26}	1.01178×10^{26}
$\tilde{j}(\tilde{x}) = j^* j(x)$	$j^* = \frac{1}{l^{*2} t^*}$	10^{24}	1.6×10^{25}
$\tilde{u}(\tilde{x}) = u^* u(x)$	$u^* = \frac{l^*}{t^*}$	10^6	250000
$\tilde{W}(\tilde{x}) = W^* W(x)$	$W^* = (l^*/t^*)^2$	10^{12}	6.25×10^{10}

Collision integraion

The solution of the collisions is achieved when we are able to solve the following integrals (in dimensionless units):

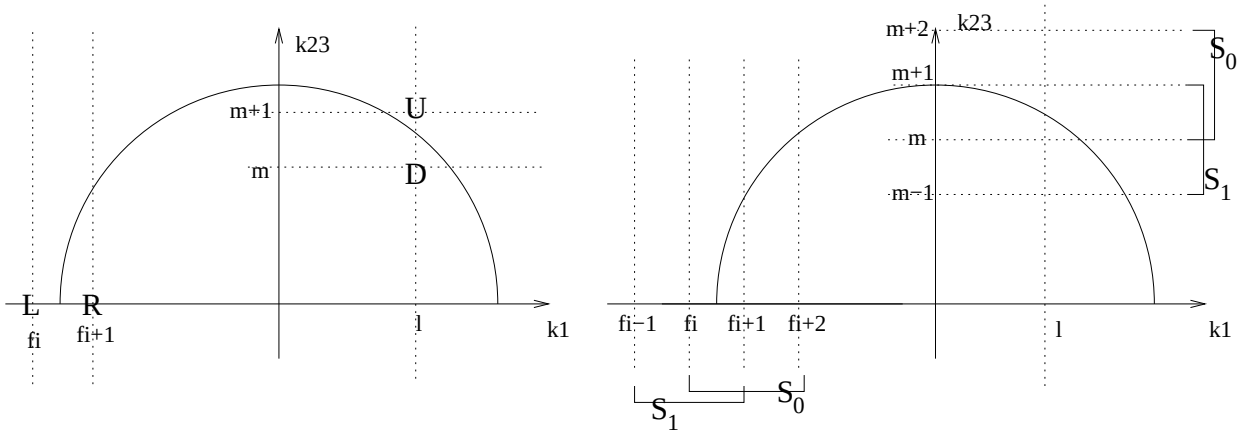
$$\begin{aligned}
\mathcal{Q}^{+}[f] &= c_0\pi \int_{-\sqrt{\gamma_0(k)}}^{\sqrt{\gamma_0(k)}} f\left(k'_1, \sqrt{\gamma_0(k) - k'^2_1}\right) dk'_1 \\
&+ c_+\pi \int_{-\sqrt{\gamma_+(k)}}^{\sqrt{\gamma_+(k)}} f\left(k'_1, \sqrt{\gamma_+(k) - k'^2_1}\right) dk'_1 \\
&+ \chi_{\{\gamma_-(k)>0\}} c_-\pi \int_{-\sqrt{\gamma_-(k)}}^{\sqrt{\gamma_-(k)}} f\left(k'_1, \sqrt{\gamma_-(k) - k'^2_1}\right) dk'_1
\end{aligned}$$

with $\gamma_0(k) = \varepsilon(k)$, $\gamma_+(k) = \varepsilon(k) + \dfrac{\hbar\omega}{\varepsilon^*}$, $\gamma_-(k) = \varepsilon(k) - \dfrac{\hbar\omega}{\varepsilon^*}$, and

$$\mathcal{Q}^{-}[f] = c_0 2\pi\sqrt{\gamma_0(k)} f(k) + \chi_{\{\gamma_-(k)>0\}} c_+ 2\pi\sqrt{\gamma_-(k)} f(k) + c_- 2\pi\sqrt{\gamma_+(k)} f(k).$$

Collision integraion

For integrating along the $[-\sqrt{\gamma}, \sqrt{\gamma}]$-segment following a semicircle in the $\left(k_1, \sqrt{k_2^2 + k_3^2}\right)$-plane, we have adopted as strategy a plain linear interpolation using the values of the two nearest points along the vertical lines. Other more sofisticated strategies have not significantly improved the results.



Outline

Multifrequency phonons

We present the results relative to a device where phonons are not single-frequency: the structure of the solver allows an easy implementation of such model.

Outline

Setting the problem

Kinetic equation.

Consider the following problem: take the **transport equation**

$$\varepsilon \frac{\partial f_\varepsilon}{\partial t} + v \frac{\partial f_\varepsilon}{\partial x} = \frac{1}{\varepsilon} \left(\frac{1}{2} \int_{-1}^{1} f_\varepsilon dv - f_\varepsilon \right)$$

with $(t, x, v) \in [0, T] \times \mathbb{R} \times [-1, 1]$, completed by initial and boundary conditions.

Diffusive limit.

As $\varepsilon \to 0$, f_ε relaxes to the **heat equation**

$$\frac{\partial \rho}{\partial t} - \frac{1}{3} \frac{\partial^2 \rho}{\partial x^2} = 0.$$

Drawbacks.

- The heat equation is not v-dependent: no microscopic feature.
- The heat equation transport information at infinite velocity, the transport equation at $\mathcal{O}\left(\frac{1}{\varepsilon}\right)$ velocity.

Setting the problem

Kinetic equation.

Consider the following problem: take the **transport equation**

$$\varepsilon \frac{\partial f_\varepsilon}{\partial t} + v \frac{\partial f_\varepsilon}{\partial x} = \frac{1}{\varepsilon} \left(\frac{1}{2} \int_{-1}^{1} f_\varepsilon dv - f_\varepsilon \right)$$

with $(t, x, v) \in [0, T] \times \mathbb{R} \times [-1, 1]$, completed by initial and boundary conditions.

Diffusive limit.

As $\varepsilon \to 0$, f_ε relaxes to the **heat equation**

$$\frac{\partial \rho}{\partial t} - \frac{1}{3} \frac{\partial^2 \rho}{\partial x^2} = 0.$$

Drawbacks.

- The heat equation is not v-dependent: no microscopic feature.
- The heat equation transport information at infinite velocity, the transport equation at $\mathcal{O}\left(\frac{1}{\varepsilon}\right)$ velocity.

Setting the problem

Kinetic equation.

Consider the following problem: take the **transport equation**

$$\varepsilon \frac{\partial f_\varepsilon}{\partial t} + v \frac{\partial f_\varepsilon}{\partial x} = \frac{1}{\varepsilon} \left(\frac{1}{2} \int_{-1}^{1} f_\varepsilon dv - f_\varepsilon \right)$$

with $(t, x, v) \in [0, T] \times \mathbb{R} \times [-1, 1]$, completed by initial and boundary conditions.

Diffusive limit.

As $\varepsilon \to 0$, f_ε relaxes to the **heat equation**

$$\frac{\partial \rho}{\partial t} - \frac{1}{3} \frac{\partial^2 \rho}{\partial x^2} = 0.$$

Drawbacks.

- The heat equation is not v-dependent: no microscopic feature.
- The heat equation transport information at infinite velocity, the transport equation at $\mathcal{O}\left(\frac{1}{\varepsilon}\right)$ velocity.

Setting the problem

Kinetic equation.

Consider the following problem: take the **transport equation**

$$\varepsilon \frac{\partial f_\varepsilon}{\partial t} + v \frac{\partial f_\varepsilon}{\partial x} = \frac{1}{\varepsilon} \left(\frac{1}{2} \int_{-1}^{1} f_\varepsilon dv - f_\varepsilon \right)$$

with $(t, x, v) \in [0, T] \times \mathbb{R} \times [-1, 1]$, completed by initial and boundary conditions.

Diffusive limit.

As $\varepsilon \to 0$, f_ε relaxes to the **heat equation**

$$\frac{\partial \rho}{\partial t} - \frac{1}{3} \frac{\partial^2 \rho}{\partial x^2} = 0.$$

Drawbacks.

- The heat equation is not v-dependent: no microscopic feature.
- The heat equation transport information at infinite velocity, the transport equation at $\mathcal{O}\left(\frac{1}{\varepsilon}\right)$ velocity.

Approximations

The $\mathbb{P}1$-approximation

By truncating the Hilbert expansion in ε of f_ε

$$f_\varepsilon = F_0 + \varepsilon F_1 + \varepsilon^2 F_2 + \ldots$$

at first order we obtain the $\mathbb{P}1$-approximation:

$$f_\varepsilon \approx \rho(t,x) - \varepsilon v \frac{\partial \rho}{\partial x}.$$

Drawbacks

- The $\mathbb{P}1$-approximation is not non-negative.
- As well as in heat equation, information is transported at infinite velocity.

Approximations

The $\mathbb{P}1$-approximation

By truncating the Hilbert expansion in ε of f_ε

$$f_\varepsilon = F_0 + \varepsilon F_1 + \varepsilon^2 F_2 + \ldots$$

at first order we obtain the $\mathbb{P}1$-approximation:

$$f_\varepsilon \approx \rho(t,x) - \varepsilon v \frac{\partial \rho}{\partial x}.$$

Drawbacks

- The $\mathbb{P}1$-approximation is not non-negative.
- As well as in heat equation, information is transported at infinite velocity.

Approximations

The $\mathbb{P}1$-approximation

By truncating the Hilbert expansion in ε of f_ε

$$f_\varepsilon = F_0 + \varepsilon F_1 + \varepsilon^2 F_2 + \ldots$$

at first order we obtain the $\mathbb{P}1$-approximation:

$$f_\varepsilon \approx \rho(t,x) - \varepsilon v \frac{\partial \rho}{\partial x}.$$

Drawbacks

- The $\mathbb{P}1$-approximation is not non-negative.
- As well as in heat equation, information is transported at infinite velocity.

Moment equations

Moments

Define the zeroth, first and second moment by

$$\begin{pmatrix} \rho_\varepsilon \\ J_\varepsilon \\ \mathbb{P}_\varepsilon \end{pmatrix} = \frac{1}{2} \int_{-1}^{1} \begin{pmatrix} 1 \\ v/\varepsilon \\ v^2 \end{pmatrix} f_\varepsilon dv.$$

Moment equations

Integrating the kinetic equation, we obtain the moment equations

$$\begin{aligned} \frac{\partial \rho_\varepsilon}{\partial t} + \frac{\partial J_\varepsilon}{\partial x} &= 0 \\ \varepsilon^2 \frac{\partial J_\varepsilon}{\partial t} + \frac{\partial \mathbb{P}_\varepsilon}{\partial x} &= -J_\varepsilon, \end{aligned}$$

which need some **closure strategy**, the k^{th}-moment equation being dependent on the $(k+1)^{th}$-moment.

Moment equations

Moments

Define the zeroth, first and second moment by

$$\begin{pmatrix} \rho_\varepsilon \\ J_\varepsilon \\ \mathbb{P}_\varepsilon \end{pmatrix} = \frac{1}{2} \int_{-1}^{1} \begin{pmatrix} 1 \\ v/\varepsilon \\ v^2 \end{pmatrix} f_\varepsilon dv.$$

Moment equations

Integrating the kinetic equation, we obtain the moment equations

$$\begin{aligned} \frac{\partial \rho_\varepsilon}{\partial t} + \frac{\partial J_\varepsilon}{\partial x} &= 0 \\ \varepsilon^2 \frac{\partial J_\varepsilon}{\partial t} + \frac{\partial \mathbb{P}_\varepsilon}{\partial x} &= -J_\varepsilon, \end{aligned}$$

which need some **closure strategy**, the k^{th}-moment equation being dependent on the $(k+1)^{th}$-moment.

Closures

Two closures were proposed, one at zero-th order and one at first order.

Zero-th order closure

By truncating the modified Hilbert expansion

$$f_\varepsilon = \exp\left(a_0 + \varepsilon a_1 + \varepsilon^2 a_2 + \ldots\right)$$

at first order, and injecting the obtained approximation

$$\tilde{f}_\varepsilon(t,x,v) = \frac{\rho(t,x)}{Z(t,x)} e^{-\varepsilon v \frac{\frac{\partial \rho}{\partial x}}{\rho}(t,x)}$$

into the zero-th moment equation, we obtain the following system:

$$\frac{\partial \rho}{\partial t} - \frac{\partial}{\partial x}\left[\frac{\rho}{\varepsilon}\mathbb{G}\left(\varepsilon \frac{\frac{\partial \rho}{\partial x}}{\rho}\right)\right] = 0,$$

where

- $Z(t,x)$ is a normalizing factor for the density $\rho(t,x)$;
- $\mathbb{G}(x) = \coth(x) - \frac{1}{x}$.

Closures

Two closures were proposed, one at zero-th order and one at first order.

Zero-th order closure

By truncating the modified Hilbert expansion

$$f_\varepsilon = \exp\left(a_0 + \varepsilon a_1 + \varepsilon^2 a_2 + \ldots\right)$$

at first order, and injecting the obtained approximation

$$\tilde{f}_\varepsilon(t,x,v) = \frac{\rho(t,x)}{Z(t,x)} e^{-\varepsilon v \frac{\frac{\partial \rho}{\partial x}}{\rho}(t,x)}$$

into the zero-th moment equation, we obtain the following system:

$$\frac{\partial \rho}{\partial t} - \frac{\partial}{\partial x}\left[\frac{\rho}{\varepsilon}\mathbb{G}\left(\varepsilon \frac{\frac{\partial \rho}{\partial x}}{\rho}\right)\right] = 0,$$

where

- $Z(t,x)$ is a normalizing factor for the density $\rho(t,x)$;
- $\mathbb{G}(x) = \coth(x) - \frac{1}{x}$.

Closures

First order closure

The first order closure comes from an Entropy Minimization Principle; it leads to the following system:

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \frac{\partial J}{\partial x} &= 0 \\ \varepsilon^2 \frac{\partial J}{\partial t} + \frac{\partial}{\partial x}\left[\rho \psi\left(\frac{\varepsilon J}{\rho}\right)\right] &= -J \end{aligned}$$

and the microscopic approximation is reconstructed by

$$\tilde{f}_\varepsilon(t,x,v) = \rho(t,x)\frac{\exp\left[v\mathbb{G}^{(-1)}\left(\frac{\varepsilon J}{\rho(t,x)}\right)\right]}{\mathbb{F}\circ\mathbb{G}^{(-1)}\left(\frac{\varepsilon J}{\rho(t,x)}\right)},$$

where

- $\mathbb{F}(x) = \frac{\sinh(x)}{x}$;
- $\psi(x) = \frac{\mathbb{F}''}{\mathbb{F}}\left(\mathbb{G}^{(-1)}(x)\right)$.

Outline

Kinetic equation

We propose a splitting scheme for solving the kinetic equation

$$\frac{\partial f_\varepsilon}{\partial t} + v\frac{\partial f_\varepsilon}{\partial x} = \frac{1}{\varepsilon}\left(\frac{1}{2}\int_{-1}^{1} f_\varepsilon dv - f_\varepsilon\right)$$

without need of mesh-resolving parameter ε as it tends to zero.

Decomposition

Split f_ε into its mean value plus fluctuations:

$$\begin{aligned} f_\varepsilon &= \rho_\varepsilon + \varepsilon g_\varepsilon \\ &= \frac{1}{2}\int_{-1}^{1} f_\varepsilon dv + \varepsilon g_\varepsilon . \end{aligned}$$

Splitting

Step (i) $$\frac{\partial f_\varepsilon}{\partial t} = \frac{1}{\varepsilon^2}(\rho_\varepsilon - f_\varepsilon) - \frac{v}{\varepsilon}\frac{\partial \rho_\varepsilon}{\partial x}, \qquad \frac{\partial g_\varepsilon}{\partial t} = -\frac{1}{\varepsilon^2}\left(g_\varepsilon + v\frac{\partial \rho_\varepsilon}{\partial x}\right)$$

Step (ii) $$\frac{\partial f_\varepsilon}{\partial t} + v\frac{\partial g_\varepsilon}{\partial x} = 0, \qquad \frac{\partial g_\varepsilon}{\partial t} = 0.$$

Kinetic equation

We propose a splitting scheme for solving the kinetic equation

$$\frac{\partial f_\varepsilon}{\partial t} + v\frac{\partial f_\varepsilon}{\partial x} = \frac{1}{\varepsilon}\left(\frac{1}{2}\int_{-1}^{1} f_\varepsilon dv - f_\varepsilon\right)$$

without need of mesh-resolving parameter ε as it tends to zero.

Decomposition

Split f_ε into its mean value plus fluctuations:

$$\begin{aligned} f_\varepsilon &= \rho_\varepsilon + \varepsilon g_\varepsilon \\ &= \frac{1}{2}\int_{-1}^{1} f_\varepsilon dv + \varepsilon g_\varepsilon. \end{aligned}$$

Splitting

Step (i) $\dfrac{\partial f_\varepsilon}{\partial t} = \dfrac{1}{\varepsilon^2}(\rho_\varepsilon - f_\varepsilon) - \dfrac{v}{\varepsilon}\dfrac{\partial \rho_\varepsilon}{\partial x}, \qquad \dfrac{\partial g_\varepsilon}{\partial t} = -\dfrac{1}{\varepsilon^2}\left(g_\varepsilon + v\dfrac{\partial \rho_\varepsilon}{\partial x}\right)$

Step (ii) $\dfrac{\partial f_\varepsilon}{\partial t} + v\dfrac{\partial g_\varepsilon}{\partial x} = 0, \qquad \dfrac{\partial g_\varepsilon}{\partial t} = 0.$

Kinetic equation

We propose a splitting scheme for solving the kinetic equation

$$\frac{\partial f_\varepsilon}{\partial t} + v\frac{\partial f_\varepsilon}{\partial x} = \frac{1}{\varepsilon}\left(\frac{1}{2}\int_{-1}^{1} f_\varepsilon dv - f_\varepsilon\right)$$

without need of mesh-resolving parameter ε as it tends to zero.

Decomposition

Split f_ε into its mean value plus fluctuations:

$$\begin{aligned} f_\varepsilon &= \rho_\varepsilon + \varepsilon g_\varepsilon \\ &= \frac{1}{2}\int_{-1}^{1} f_\varepsilon dv + \varepsilon g_\varepsilon. \end{aligned}$$

Splitting

Step (i) $$\frac{\partial f_\varepsilon}{\partial t} = \frac{1}{\varepsilon^2}(\rho_\varepsilon - f_\varepsilon) - \frac{v}{\varepsilon}\frac{\partial \rho_\varepsilon}{\partial x}, \qquad \frac{\partial g_\varepsilon}{\partial t} = -\frac{1}{\varepsilon^2}\left(g_\varepsilon + v\frac{\partial \rho_\varepsilon}{\partial x}\right)$$

Step (ii) $$\frac{\partial f_\varepsilon}{\partial t} + v\frac{\partial g_\varepsilon}{\partial x} = 0, \qquad \frac{\partial g_\varepsilon}{\partial t} = 0.$$

Kinetic equation

We drop the notation of the ε-dependency and resume the scheme in the following steps: knowing f^n, g^n and ρ^n

Step (i)

- update[**Step (i)a**] f:

$$f_{i,j}^{n+1/2} = e^{-\frac{\Delta t}{\varepsilon^2}} f_{i,j}^n + \left(1 - e^{-\frac{\Delta t}{\varepsilon^2}}\right) \rho_i^n$$

- update[**Step (i)b**] g:

$$g_{i,j}^{n+1/2} = e^{-\frac{\Delta t}{\varepsilon^2}} g_{i,j}^n + \left(1 - e^{-\frac{\Delta t}{\varepsilon^2}}\right) \bar{\mathbb{D}}_j \rho_i^n$$

- update[**Step (i)c**] ρ:

$$\rho_i^{n+1/2} = \rho_i^n$$

Kinetic equation

Step (ii)

- update[**Step (ii)a**] f:

$$f_{i,j}^{n+1} = f_{i,j}^{n+1/2} + \Delta t \mathbb{D}_j g_{i,j}^{n+1/2}$$

- update[**Step (ii)b**] g:

$$g_{i,j}^{n+1} = g_{i,j}^{n+1/2}$$

- update[**Step (iii)c**] ρ by a right-rectangluar rule:

$$\rho_i^{n+1} = \frac{\Delta v}{2} \sum_{j=0}^{j-2} f_{i,j}^{n+1}$$

Kinetic equation

Derivatives

The discrete derivatives are defined in alternate direction under the upwinding constraint, for the sake of stability (for rescuing the usual three-point centered scheme of the Laplacian):

$$\left[\mathbb{D}_j\varphi\right]_i = \frac{1}{\Delta x}\begin{cases} -v_j\left(\varphi_i - \varphi_{i-1}\right) & \text{if } v_j > 0 \\ -v_j\left(\varphi_{i+1} - \varphi_i\right) & \text{if } v_j < 0 \end{cases}$$

$$\left[\bar{\mathbb{D}}_j\varphi\right]_i = \frac{1}{\Delta x}\begin{cases} -v_j\left(\varphi_{i+1} - \varphi_i\right) & \text{if } v_j > 0 \\ -v_j\left(\varphi_i - \varphi_{i-1}\right) & \text{if } v_j < 0 \end{cases}$$

Numerics for the first order closure

We recall the first order closure (dropping ε-dependency):

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \frac{\partial J}{\partial x} &= 0 \\ \varepsilon^2 \frac{\partial J}{\partial t} + \frac{\partial}{\partial x}\left[\rho \psi\left(\frac{\varepsilon J}{\rho}\right)\right] &= -J \end{aligned}$$

Strategy

We introduce a new unknown $z(t,x)$ and two new parameters λ and α; the non-linear equation for the first moment is now an advection equation and the non-linearities only appear at a right hand side:

$$\begin{pmatrix} \frac{\partial}{\partial t} & \frac{\partial}{\partial x} & 0 \\ 0 & \varepsilon^2 \frac{\partial}{\partial t} & \frac{\partial}{\partial x} \\ 0 & \varepsilon^2 \lambda^2 \frac{\partial}{\partial x} & \frac{\partial}{\partial t} \end{pmatrix} \begin{pmatrix} \rho \\ J \\ z \end{pmatrix} = \begin{pmatrix} 0 \\ -J \\ \frac{1}{\alpha}\left(\rho\psi(u) - z\right) \end{pmatrix},$$

with $u = \frac{\varepsilon J}{\rho}$. As $\alpha \to 0$, this system relaxes towards the original system.

Numerics for the first order closure

We recall the first order closure (dropping ε-dependency):

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \frac{\partial J}{\partial x} &= 0 \\ \varepsilon^2 \frac{\partial J}{\partial t} + \frac{\partial}{\partial x}\left[\rho \psi\left(\frac{\varepsilon J}{\rho}\right)\right] &= -J \end{aligned}$$

Strategy

We introduce a new unknown $z(t,x)$ and two new parameters λ and α; the non-linear equation for the first moment is now an advection equation and the non-linearities only appear at a right hand side:

$$\begin{pmatrix} \frac{\partial}{\partial t} & \frac{\partial}{\partial x} & 0 \\ 0 & \varepsilon^2 \frac{\partial}{\partial t} & \frac{\partial}{\partial x} \\ 0 & \varepsilon^2 \lambda^2 \frac{\partial}{\partial x} & \frac{\partial}{\partial t} \end{pmatrix} \begin{pmatrix} \rho \\ J \\ z \end{pmatrix} = \begin{pmatrix} 0 \\ -J \\ \frac{1}{\alpha}\left(\rho\psi(u) - z\right) \end{pmatrix},$$

with $u = \frac{\varepsilon J}{\rho}$. As $\alpha \to 0$, this system relaxes towards the original system.

Numerics for the first order closure

We recall the first order closure (dropping ε-dependency):

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \frac{\partial J}{\partial x} &= 0 \\ \varepsilon^2 \frac{\partial J}{\partial t} + \frac{\partial}{\partial x}\left[\rho \psi\left(\frac{\varepsilon J}{\rho}\right)\right] &= -J \end{aligned}$$

Strategy

We introduce a new unknown $z(t,x)$ and two new parameters λ and α; the non-linear equation for the first moment is now an advection equation and the non-linearities only appear at a right hand side:

$$\begin{pmatrix} \frac{\partial}{\partial t} & \frac{\partial}{\partial x} & 0 \\ 0 & \varepsilon^2 \frac{\partial}{\partial t} & \frac{\partial}{\partial x} \\ 0 & \varepsilon^2 \lambda^2 \frac{\partial}{\partial x} & \frac{\partial}{\partial t} \end{pmatrix} \begin{pmatrix} \rho \\ J \\ z \end{pmatrix} = \begin{pmatrix} 0 \\ -J \\ \frac{1}{\alpha}\left(\rho\psi(u) - z\right) \end{pmatrix},$$

with $u = \frac{\varepsilon J}{\rho}$. As $\alpha \to 0$, this system relaxes towards the original system.

Numerics for the first order closure

Diagonalization

We diagonalize it by means of a linear transformation of its unknowns ($\mu = \varepsilon\lambda$)

$$\begin{pmatrix} \rho \\ J \\ z \end{pmatrix} = \begin{pmatrix} \frac{1}{\mu^2} & \frac{1}{\mu^2} & \frac{1}{\mu^2} \\ 0 & \frac{1}{\varepsilon\mu} & -\frac{1}{\varepsilon\mu} \\ 0 & 1 & 1 \end{pmatrix} \begin{pmatrix} f_0 \\ f_+ \\ f_- \end{pmatrix},$$

Splitting

then apply splitting technique between the α-relaxations and the ε-relaxations:

$$\begin{pmatrix} \frac{\partial}{\partial t} & 0 & 0 \\ 0 & \frac{\partial}{\partial t} + \frac{\mu}{\varepsilon}\frac{\partial}{\partial x} & 0 \\ 0 & 0 & \frac{\partial}{\partial t} - \frac{\mu}{\varepsilon}\frac{\partial}{\partial x} \end{pmatrix} \begin{pmatrix} f_0 \\ f_+ \\ f_- \end{pmatrix} = \begin{pmatrix} -\frac{1}{\alpha}\left(\rho\psi(u) - z\right) \\ -\frac{f_+}{\varepsilon^2} + \frac{z}{2\varepsilon^2} + \frac{1}{2\alpha}\left(\rho\psi(u) - z\right) \\ -\frac{f_-}{\varepsilon^2} + \frac{z}{2\varepsilon^2} + \frac{1}{2\alpha}\left(\rho\psi(u) - z\right) \end{pmatrix}.$$

Numerics for the first order closure

Diagonalization

We diagonalize it by means of a linear transformation of its unknowns ($\mu = \varepsilon\lambda$)

$$\begin{pmatrix} \rho \\ J \\ z \end{pmatrix} = \begin{pmatrix} \frac{1}{\mu^2} & \frac{1}{\mu^2} & \frac{1}{\mu^2} \\ 0 & \frac{1}{\varepsilon\mu} & -\frac{1}{\varepsilon\mu} \\ 0 & 1 & 1 \end{pmatrix} \begin{pmatrix} f_0 \\ f_+ \\ f_- \end{pmatrix},$$

Splitting

then apply splitting technique between the α-relaxations and the ε-relaxations:

$$\begin{pmatrix} \frac{\partial}{\partial t} & 0 & 0 \\ 0 & \frac{\partial}{\partial t} + \frac{\mu}{\varepsilon}\frac{\partial}{\partial x} & 0 \\ 0 & 0 & \frac{\partial}{\partial t} - \frac{\mu}{\varepsilon}\frac{\partial}{\partial x} \end{pmatrix} \begin{pmatrix} f_0 \\ f_+ \\ f_- \end{pmatrix} = \begin{pmatrix} -\frac{1}{\alpha}\left(\rho\psi(u) - z\right) \\ -\frac{f_+}{\varepsilon^2} + \frac{z}{2\varepsilon^2} + \frac{1}{2\alpha}\left(\rho\psi(u) - z\right) \\ -\frac{f_-}{\varepsilon^2} + \frac{z}{2\varepsilon^2} + \frac{1}{2\alpha}\left(\rho\psi(u) - z\right) \end{pmatrix}.$$

Numerics for the first order closure

Stiffness in **Step 1.**

Step 1 is again stiff as $\varepsilon \to 0$:

$$\frac{\partial f_\pm}{\partial t} \pm \frac{\mu}{\varepsilon}\frac{\partial f_\pm}{\partial x} = -\frac{1}{\varepsilon^2}\left[f_\pm - \frac{z}{2}\right],$$

which means that $f_\pm$ is relaxed towards $\frac{z}{2}$, so we apply the same strategy as before and split $f_\pm$ into the following sum:

$$f_\pm = \frac{z}{2} + \varepsilon g_\pm$$

and follow the same calculations as before.

Numerics for the first order closure

Solving **Step 1.**

Developping all the computations and rewriting the system in the original variables we get:

$$
\begin{aligned}
z^{n+1/2} &= z^n + \frac{\varepsilon(1-e^{-\Delta t/\varepsilon^2})}{2}\left(\bar{\mathbb{D}}_+(z^n)+\bar{\mathbb{D}}_-(z^n)\right) + \Delta t\left[\mathbb{D}_+\left(e^{-\Delta t/\varepsilon^2}\frac{\mu J^n}{2}\right.\right.\\
&\left.\left.+(1-e^{-\Delta t/\varepsilon^2})\frac{\bar{\mathbb{D}}_+(z^n)}{2}\right)+\mathbb{D}_-\left(e^{-\Delta t/\varepsilon^2}\frac{(-\mu J^n)}{2}+(1-e^{-\Delta t/\varepsilon^2})\frac{\bar{\mathbb{D}}_-(z^n)}{2}\right)\right]\\
J^{n+1/2} &= e^{-\Delta t/\varepsilon^2}J^n + \frac{1-e^{-\Delta t/\varepsilon^2}}{2\mu}\left(\bar{\mathbb{D}}_+(z^n)-\bar{\mathbb{D}}_-(z^n)\right) + \frac{\Delta t}{\varepsilon\mu}\left[\mathbb{D}_+\left(e^{-\Delta t/\varepsilon^2}\frac{\mu J^n}{2}\right.\right.\\
&\left.\left.+(1-e^{-\Delta t/\varepsilon^2})\frac{\bar{\mathbb{D}}_+(z^n)}{2}\right)-\mathbb{D}_-\left(e^{-\Delta t/\varepsilon^2}\frac{(-\mu J^n)}{2}+(1-e^{-\Delta t/\varepsilon^2})\frac{\bar{\mathbb{D}}_-(z^n)}{2}\right)\right]\\
\rho^{n+1/2} &= \rho^n + \frac{\Delta t}{\mu^2}\left(\mathbb{D}_+\left(e^{-\Delta t/\varepsilon^2}\frac{\mu J^n}{2}+(1-e^{-\Delta t/\varepsilon^2})\frac{\bar{\mathbb{D}}_+(z^n)}{2}\right)\right.\\
&\left.+\mathbb{D}_-\left(e^{-\Delta t/\varepsilon^2}\frac{(-\mu J^n)}{2}+(1-e^{-\Delta t/\varepsilon^2})\frac{\bar{\mathbb{D}}_-(z^n)}{2}\right)\right).
\end{aligned}
$$

Numerics for the first order closure

Solving **Step 2.**

Step 2 just involves relaxations, and no more details are given; after reconstructing the original variables we obtain

$$\begin{aligned} z^{n+1} &= e^{-\Delta t/\alpha} z^{n+1/2} + (1 - e^{-\Delta t/\alpha}) \rho^{n+1/2} \psi^{n+1/2} \\ J^{n+1} &= J^{n+1/2} \\ z^{n+1} &= z^{n+1/2}. \end{aligned}$$

Numerics for the first order closure

Derivatives

Discretized derivatives are subjected to upwinding and are taken in alternate directions, in order to rescue the classical three-points centered scheme for the Laplacian of the heat equation in the $(\alpha \to 0, \varepsilon \to 0)$-scheme:

$$
\begin{aligned}
\left(\bar{\mathbb{D}}_+(\varphi)\right)_i &= -\frac{\mu}{\Delta x}\left(\varphi_{i+1} - \varphi_i\right) \\
\left(\mathbb{D}_+(\varphi)\right)_i &= -\frac{\mu}{\Delta x}\left(\varphi_i - \varphi_{i-1}\right) \\
\left(\bar{\mathbb{D}}_-(\varphi)\right)_i &= \frac{\mu}{\Delta x}\left(\varphi_i - \varphi_{i-1}\right) \\
\left(\mathbb{D}_-(\varphi)\right)_i &= \frac{\mu}{\Delta x}\left(\varphi_{i+1} - \varphi_i\right).
\end{aligned}
$$

Outline

Comparison between closures

We plot here the $L^2_{t,x,v}$-difference between the $f_\varepsilon(t,x,v)$ given by the kinetic scheme and the $\tilde{f}_\varepsilon(t,x,v)$ reconstructed from heat equation or closure schemes. As initial datum we choose a symmetric f_0 and an asymmetric f_0:

$$f_0(x,v) = \begin{cases} 2 & -0.5 \le x \le 0.5 \text{ and } -0.75 \le v \le 0.25 \quad \text{for the asymmetric i. d.} \\ 2 & -0.5 \le x \le 0.5 \text{ and } -0.5 \le v \le 0.5 \quad \text{for the symmetric i. d.} \\ 1 & \text{otherwise} \end{cases}$$

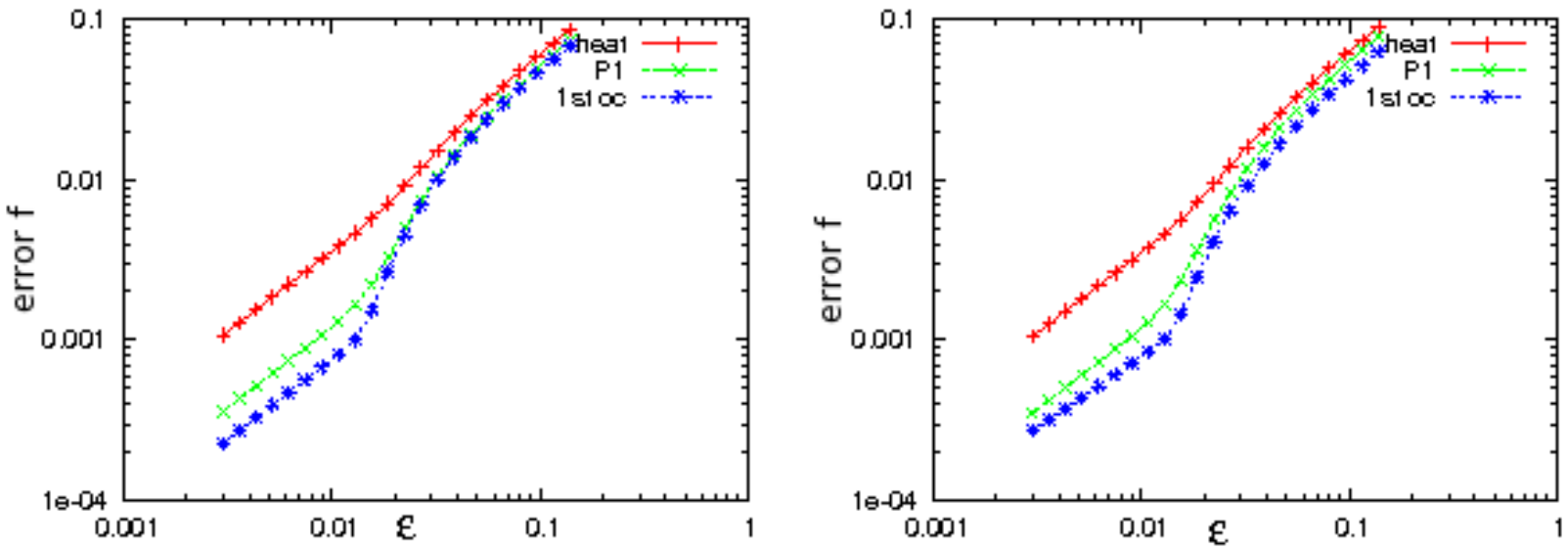
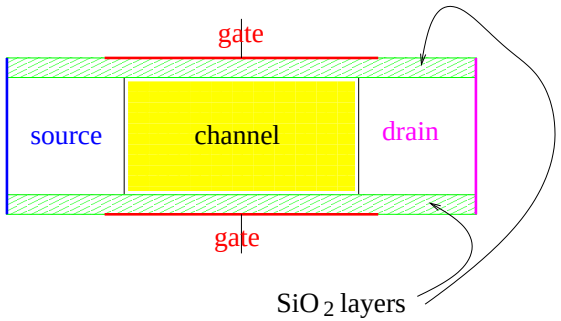


Figure: Left: symmetric initial datum. Right: asymmetric initial datum.

Outline

The model

We afford now the simulation of a nanoscaled MOSFET.



Hybridity

x-dimension is longer than *z*-dimension, therefore we adopt a different description:

- along *x*-dimension electrons behave like particles, their movement being described by the Boltzmann Transport Equation;
- along *z*-dimension electrons behave like waves, moreover they are supposed to be at equilibrium, therefore their state is given by the stationary-state Schrödinger equation.

The model

Subband decomposition

Electrons in different energy levels, also called *subbands*, which corresponding to eigenvalues of the Schrödinger equation describing their state along the z-dimension, have to be considered independent populations, so that we have to transport them for separate.

Coupling between dimensions

Dimensions and subbands are coupled in the Poisson equation for the computation of the electrostatic field in the expression of the total density.

Coupling between subbands

Subbands are coupled also in the scattering operator, depending on whether we allow inter-band scattering or not.

The model

BTE

The Boltzmann Transport Equation (one for each band) reads

$$\frac{\partial f_p}{\partial t} + \frac{1}{\hbar}\nabla_k \epsilon_p^{kin} \cdot \nabla_k f_p - \frac{1}{\hbar}\nabla_x \epsilon_p^{pot} \cdot \nabla_k f_p = \mathcal{Q}_p f_p, \qquad f_p(t=0,x,k) = f_0(x,k).$$

Schrödinger-Poisson

The Schrödinger-Poisson block reads

$$-\frac{\hbar^2}{2}\frac{d}{dz}\left[\frac{1}{m_*}\frac{d\chi_p}{dz}\right] - q\left(V + V_c\right)\chi_p = \epsilon_p^{pot}\chi_p$$

$$\{\chi_p\}_p \subseteq H_o^1(0, l_z) \text{ orthonormal basis}$$

$$-\text{div}\left[\varepsilon_R \nabla V\right] = \frac{q}{\varepsilon_0}\left(N[V] - N_D\right)$$

plus boundary conditions.

These two equations cannot be decoupled because we need the eigenfunctions to compute the potential (in the expression of the total density), and we need the potential to compute the eigenfunctions.

The model

The collision operator

For the scope of this work, we are just using a linear relaxation-time inter-band operator; a more detailed description has not been tested yet:

$$\mathcal{Q}_p f_p(t,x,k) = \frac{1}{\tau}\left[\frac{\sum_q \rho_q(t,x)}{\sum_r e^{-\frac{\epsilon_r(t,x)}{k_B T_L}}}\mathcal{M}(k)e^{-\frac{\epsilon_p(t,x)}{k_B T_L}} - f_p(t,x,k)\right],$$

where $\mathcal{M} = \frac{\hbar^2}{2\pi k_B T_L m_*}\exp\left(\frac{\hbar^2|k|^2}{2k_B T_L m_*}\right)$ is the Maxwellian and the relaxation time comes from the mobility μ from formula $\tau = \frac{\mu m_*}{q}$.

Band structure

The kinetic contribution to the energy-band function is taken in the parabolic approximation, therefore it does not depend on the band nor on position, which makes computations quite easier:

$$\epsilon^{kin}(k) = \frac{\hbar^2|k|^2}{2m_* k_B T_L}.$$

Outline

Numerical methods

We need to solve the Schrödinger eigenvalue problem and Poisson equations.

The Schrödinger equation

Equation

$$-\frac{\hbar^2}{2}\frac{d}{dz}\left[\frac{1}{m_*}\frac{d\chi_p}{dz}\right]-q\left(V+V_c\right)\chi_p=\epsilon_p\chi_p$$

is discretized by alternate finite differences for the derivatives then the symmetric matrix is diagonalized by a LAPACK routine called DSTEQR.

The Poisson equation

We need to solve 1D and 2D equation like

$$-\mathrm{div}\left[\varepsilon_R\nabla V\right]+\int_0^{l_z}\mathcal{A}(z,\zeta)V(\zeta)d\zeta=\mathcal{B}(z).$$

The derivatives are discretized by finite differences in alternate directions, the integral is computed via trapezoid rule and the linear system is solved by means of a LAPACK routine called DGESV.

Numerical methods

We need to solve the Schrödinger eigenvalue problem and Poisson equations.

The Schrödinger equation

Equation

$$-\frac{\hbar^2}{2}\frac{d}{dz}\left[\frac{1}{m_*}\frac{d\chi_p}{dz}\right]-q\left(V+V_c\right)\chi_p=\epsilon_p\chi_p$$

is discretized by alternate finite differences for the derivatives then the symmetric matrix is diagonalized by a LAPACK routine called DSTEQR.

The Poisson equation

We need to solve 1D and 2D equation like

$$-\mathrm{div}\left[\varepsilon_R\nabla V\right]+\int_0^{l_z}\mathcal{A}(z,\zeta)V(\zeta)d\zeta=\mathcal{B}(z).$$

The derivatives are discretized by finite differences in alternate directions, the integral is computed via trapezoid rule and the linear system is solved by means of a LAPACK routine called DGESV.

Numerical methods

We need to solve the Schrödinger eigenvalue problem and Poisson equations.

The Schrödinger equation

Equation

$$-\frac{\hbar^2}{2}\frac{d}{dz}\left[\frac{1}{m_*}\frac{d\chi_p}{dz}\right] - q\left(V + V_c\right)\chi_p = \epsilon_p \chi_p$$

is discretized by alternate finite differences for the derivatives then the symmetric matrix is diagonalized by a LAPACK routine called DSTEQR.

The Poisson equation

We need to solve 1D and 2D equation like

$$-\text{div}\left[\varepsilon_R \nabla V\right] + \int_0^{l_z} \mathcal{A}(z,\zeta)V(\zeta)d\zeta = \mathcal{B}(z).$$

The derivatives are discretized by finite differences in alternate directions, the integral is computed via trapezoid rule and the linear system is solved by means of a LAPACK routine called DGESV.

Overview

The Newton scheme

We seek to find the minimum of the functional $P[V]$ leading to the Poisson equation

$$-\text{div}\,(\varepsilon_R \nabla V) + \frac{q}{\varepsilon_0}\,(N[V] - N_D) = 0$$

by means of a Newton scheme

$$dP(V^{old}, V^{new} - V^{old}) = -P[V^{old}].$$

After computing the Gâteaux-derivative of the density and developping calculations, we are led to a Poisson-like equation

$$\begin{aligned} & -\text{div}\,(\varepsilon_R \nabla V^{new}) + \frac{q}{\varepsilon_0}\int_0^{l_z} \mathcal{A}[V^{old}](z,\zeta)V^{new}(\zeta)d\zeta \\ = \quad & -\frac{q}{\varepsilon_0}\,(N[V] - N_D) + \frac{q}{\varepsilon_0}\int_0^{l_z} \mathcal{A}[V^{old}](z,\zeta)V^{new}(\zeta)d\zeta. \end{aligned}$$

Discretization for the transport

Once we have developped the method for updating the band-potential energies, we can focus the attention on solving the transport. Two discretization are proposed.

Runge-Kutta

FDWENO evaluates via dimension-by-dimension approximation the derivatives $\frac{\partial f_p}{\partial x}$ and $\frac{\partial f_p}{\partial k_1}$ and is coupled with the TVD (Total Variation Diminishing) **Runge-Kutta-3** for the time discretization.

Time- & dimensional-splitting

The BTE is split into the solution of the transport and the collisions, then inside the transport we split dimensions and solve linear advection problems:

$$\begin{aligned} \frac{\partial f_p}{\partial t} + \frac{1}{\hbar}\frac{\partial \epsilon^{kin}}{\partial k_1}\frac{\partial f_p}{\partial x} - \frac{1}{\hbar}\frac{\partial \epsilon_p^{pot}}{\partial x}\frac{\partial f_p}{\partial k_1} &= 0 \\ \frac{\partial f_p}{\partial t} &= \mathcal{Q}_p f_p. \end{aligned}$$

Discretization for the transport

Once we have developped the method for updating the band-potential energies, we can focus the attention on solving the transport. Two discretization are proposed.

Runge-Kutta

FDWENO evaluates via dimension-by-dimension approximation the derivatives $\frac{\partial f_p}{\partial x}$ and $\frac{\partial f_p}{\partial k_1}$ and is coupled with the TVD (Total Variation Diminishing) **Runge-Kutta-3** for the time discretization.

Time- & dimensional-splitting

The BTE is split into the solution of the transport and the collisions, then inside the transport we split dimensions and solve linear advection problems:

$$\begin{aligned} \frac{\partial f_p}{\partial t} + \frac{1}{\hbar}\frac{\partial \epsilon^{kin}}{\partial k_1}\frac{\partial f_p}{\partial x} - \frac{1}{\hbar}\frac{\partial \epsilon_p^{pot}}{\partial x}\frac{\partial f_p}{\partial k_1} &= 0 \\ \frac{\partial f_p}{\partial t} &= \mathcal{Q}_p f_p. \end{aligned}$$

Discretization for the transport

Once we have developped the method for updating the band-potential energies, we can focus the attention on solving the transport. Two discretization are proposed.

Runge-Kutta

FDWENO evaluates via dimension-by-dimension approximation the derivatives $\frac{\partial f_p}{\partial x}$ and $\frac{\partial f_p}{\partial k_1}$ and is coupled with the TVD (Total Variation Diminishing) **Runge-Kutta-3** for the time discretization.

Time- & dimensional-splitting

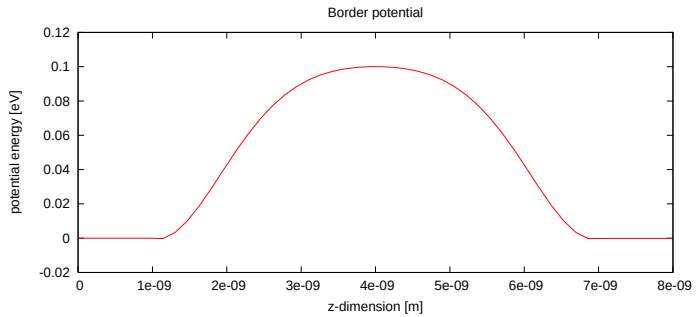
The BTE is split into the solution of the transport and the collisions, then inside the transport we split dimensions and solve linear advection problems:

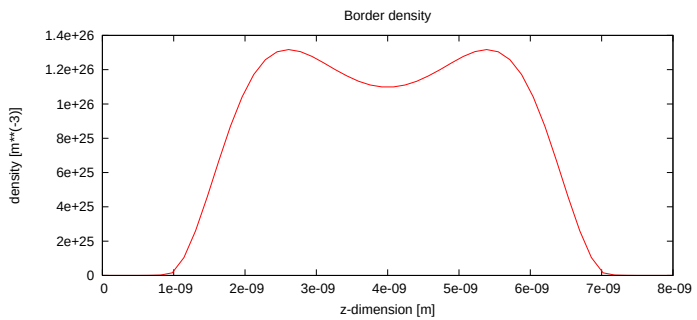
$$\begin{aligned} \frac{\partial f_p}{\partial t} + \frac{1}{\hbar}\frac{\partial \epsilon^{kin}}{\partial k_1}\frac{\partial f_p}{\partial x} - \frac{1}{\hbar}\frac{\partial \epsilon_p^{pot}}{\partial x}\frac{\partial f_p}{\partial k_1} &= 0 \\ \frac{\partial f_p}{\partial t} &= \mathcal{Q}_p f_p. \end{aligned}$$

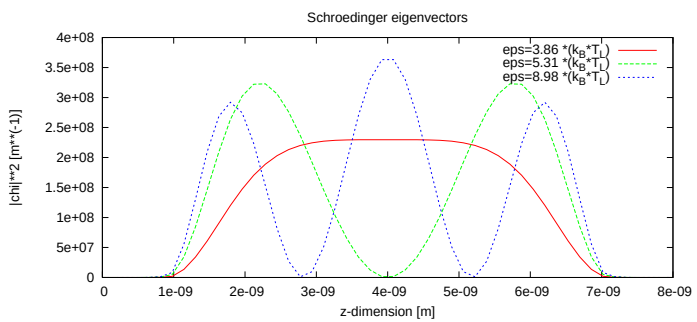
Outline

Border potential

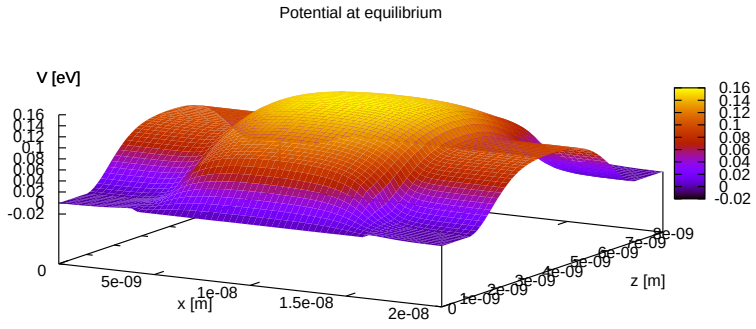
First of all we have to compute the border potential respecting the electrical neutrality, to use it for the border values in 1D-Schrödinger-2D-Poisson equations.

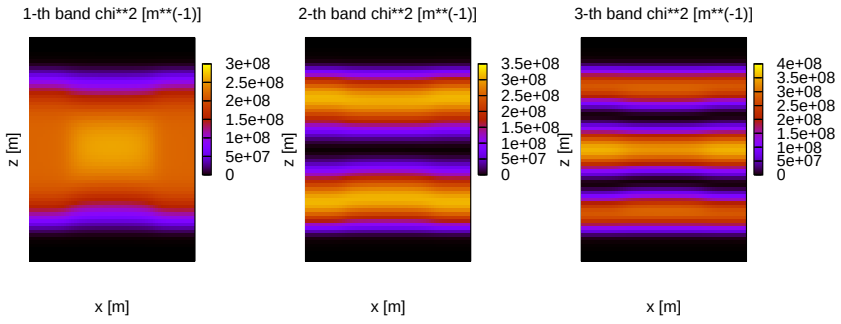


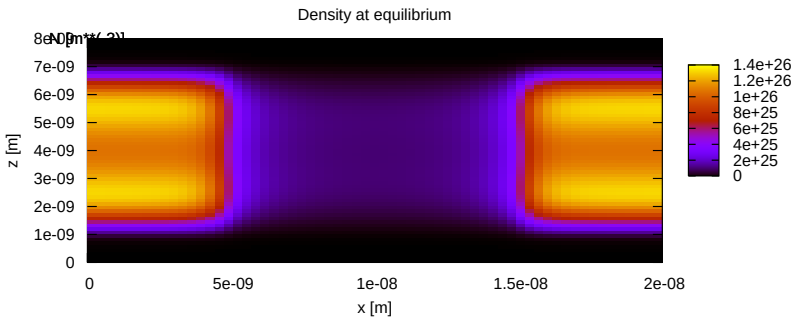


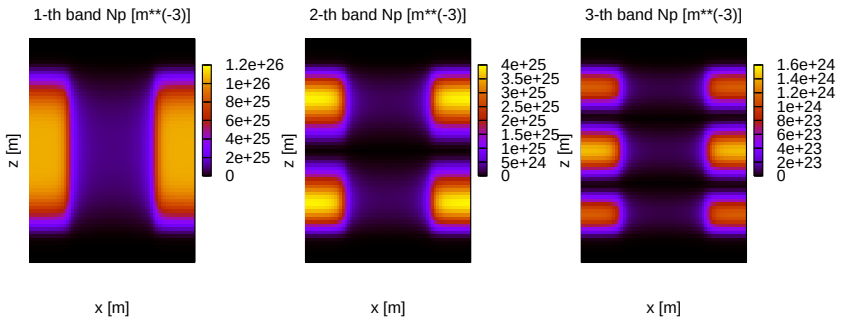


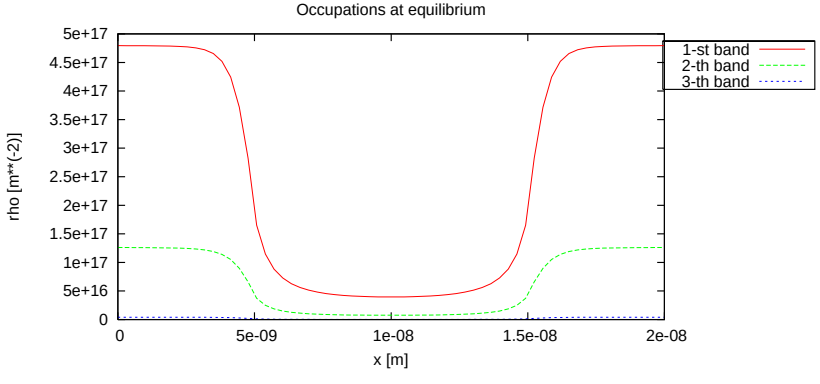
Thermodynamical equilibrium

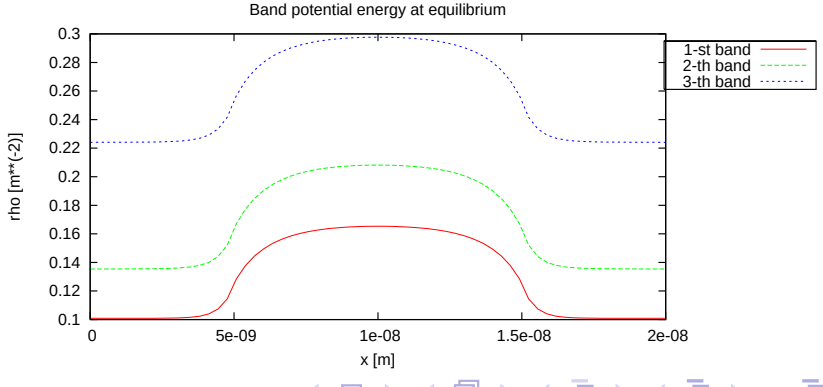












Long-time behavior

We propose now some results relative to the long-time behavior of the system.