A Deterministic Solver for a Hybrid Quantum-Classical Transport Model in NanoMOSFETs

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in collaboration with
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Outline

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Main Objective

The goal of this work is a contribution to the numerical simulation of kinetic models for nowadays transistors.

Here we sketch the typical architecture of a **MOSFET**.

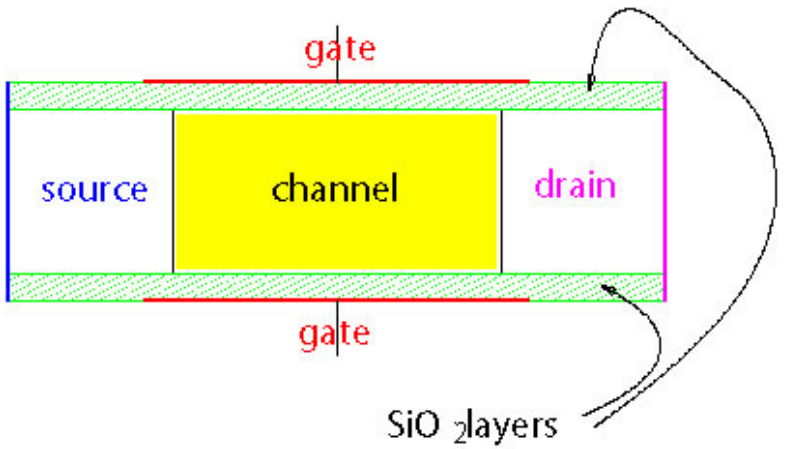

Figure: A **M**etal **O**xide **S**emiconductor **F**ield **E**ffect **T**ransistor.

Mesoscale Modelling

Transport.

The Boltzmann Transport Equation (BTE) describes, at mesoscopic 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: self-consistent Poisson equation.

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).

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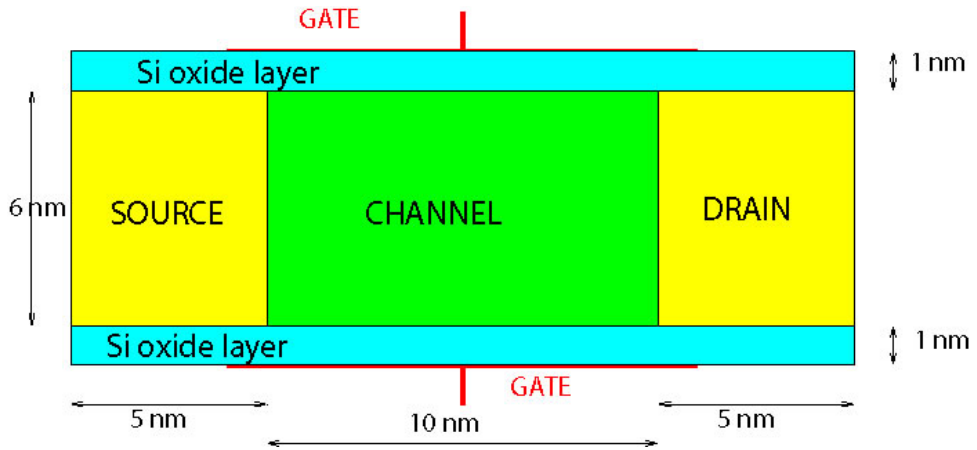
The model

We afford the simulation of a nanoscaled MOSFET.



Dimensional coupling

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 confined in a potential well behave like waves, moreover they are supposed to be at equilibrium, therefore their state is given by the stationary-state Schrödinger equation.

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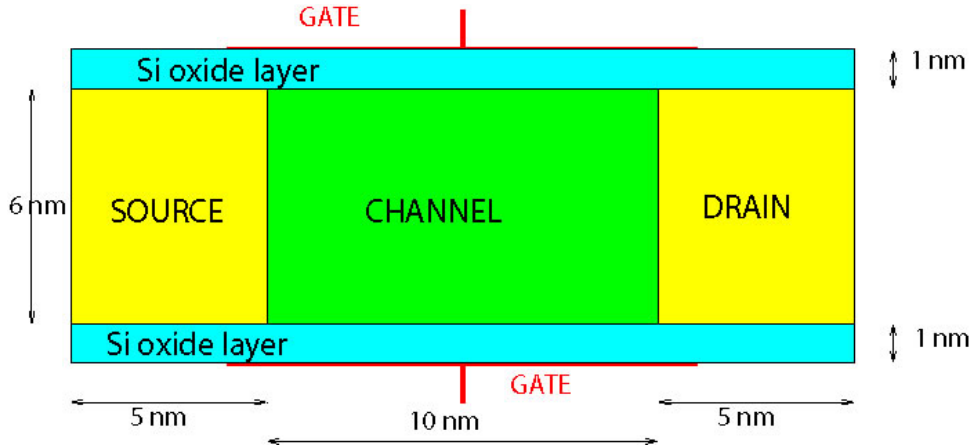

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Subband decomposition

Electrons in different energy levels, also called *sub-bands*, another name for the eigenvalues of the Schrödinger equation, 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.

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Subbands are also coupled in the scattering operator, where the carriers are allowed to jump from an energy level to another one.

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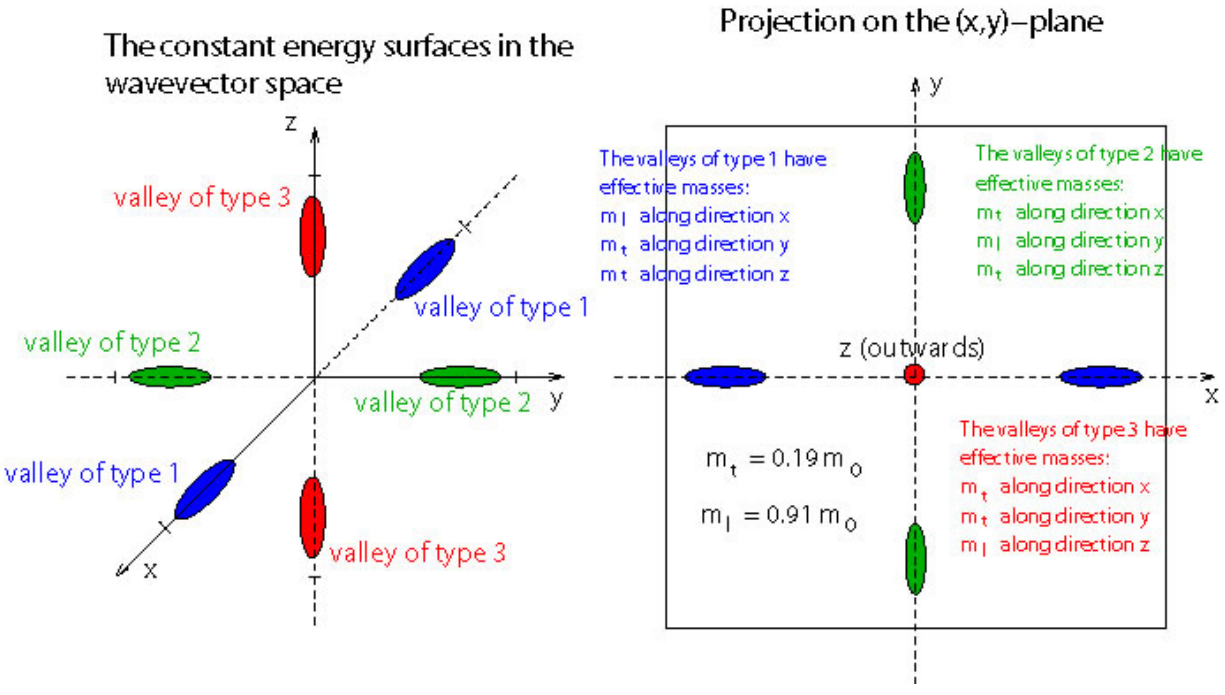
Bandstructure

The three valleys

The Si bandstructure presents six minima in the first Brillouin zone:



The axes of the ellipsoids are disposed along the x, y and z axes of the reciprocal lattice. The three minima have the same value, therefore there is no gap.

Bandstructure

Non-parabolicity

The bandstructure around the three minima can be expanded following the Kane non-parabolic approximation:

$$\epsilon_\nu^{kin} = \frac{\hbar^2}{1+\sqrt{1+2\tilde{\alpha}_\nu\hbar^2\left(\frac{k_x^2}{m_\nu^x}+\frac{k_y^2}{m_\nu^y}\right)}}\left(\frac{k_x^2}{m_\nu^x}+\frac{k_y^2}{m_\nu^y}\right),$$

where $m_\nu^{\{x,y\}}$ are the axes of the ellipsoids (called *effective masses*) of the ν^{th} valley along x and y directions, and the $\tilde{\alpha}_\nu$ are known as Kane dispersion factors.

The simplest case: one-valley, parabolic

$$\epsilon^{kin} = \frac{\hbar^2|k|^2}{2m_*},$$

with m_* an average value between the effective masses.

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The Boltzmann Transport Equation (one for each band and for each valley) reads

$$\frac{\partial f_{\nu,p}}{\partial t} + \frac{1}{\hbar}\nabla_k \epsilon_\nu^{kin} \cdot \nabla_x f_{\nu,p} - \frac{1}{\hbar}\nabla_x \epsilon_{\nu,p}^{pot} \cdot \nabla_k f_{\nu,p} = \mathcal{Q}_{\nu,p}[f], \qquad f_{\nu,p}(t=0) = \rho_{\nu,p}^{eq} M.$$

Schrödinger-Poisson block

$$-\frac{\hbar^2}{2}\frac{d}{dz}\left[\frac{1}{m_\nu}\frac{d\chi_{\nu,p}[V]}{dz}\right] - q\left(V + V_c\right)\chi_{\nu,p}[V] = \epsilon_{\nu,p}^{pot}[V]\chi_{\nu,p}[V]$$

$\{\chi_{\nu,p}\}_p \subseteq H_o^1(0, l_z)$ orthonormal basis in $L^2(0, l_z)$

$$-\text{div}\left[\varepsilon_R \nabla V\right] = -\frac{q}{\varepsilon_0}\left(\sum_{\nu,p} \rho_{\nu,p}|\chi_{\nu,p}[V]|^2 - N_D\right)$$

plus boundary conditions.

These 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.

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The collision operator

The collision operator takes into account the electron-optical phonon scattering mechanism. It reads

$$\mathcal{Q}_{\nu,p}[f] = \sum_{s} \sum_{\nu',p'} \int_{\mathbb{R}^2} \left[S^{s}_{(\nu',p',k') \to (\nu,p,k)} f_{\nu',p'}(k') - S^{s}_{(\nu,p,k) \to (\nu',p',k')} f_{\nu,p}(k) \right] dk' :$$

every S^s represents a different interaction, which may be elastic or inelastic, intra-valley or inter-valley. Each of them is inter-band.

Structure of the S^s

Each of the S^s consists of a constant, an overlap integral and a delta for the exchange of energy:

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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**):

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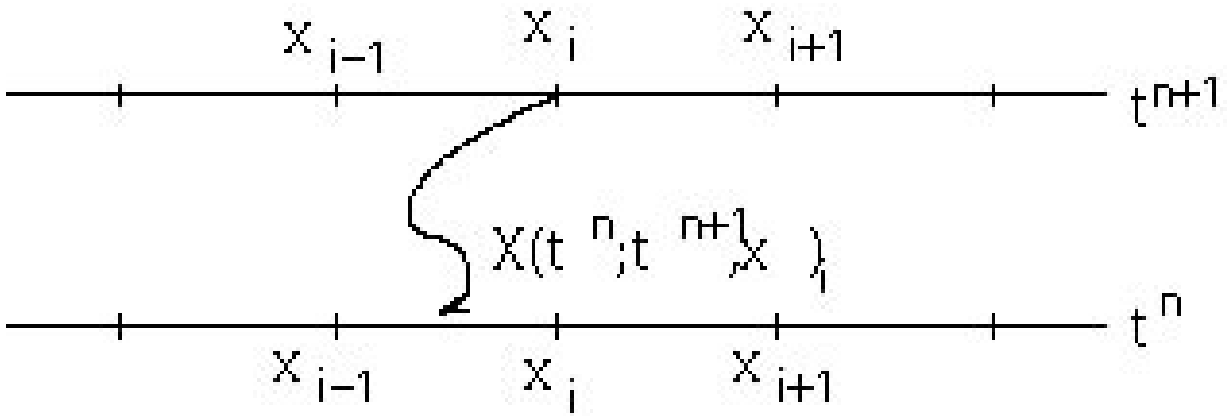
Linear advection

We propose two schemes for solving the linear advection

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

Semi-Lagrangian:

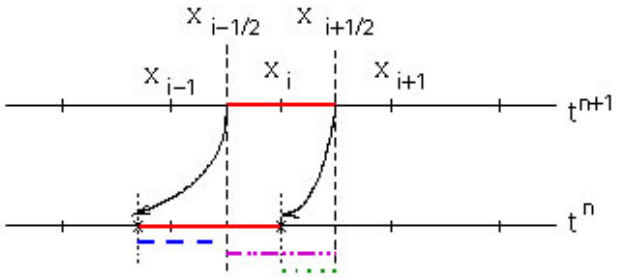
Directly integrate backward in the characteristic



Linear advection 2

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

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J.A. Carrillo, F. Vecil, SIAM J. Sci. Computing 2007

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.

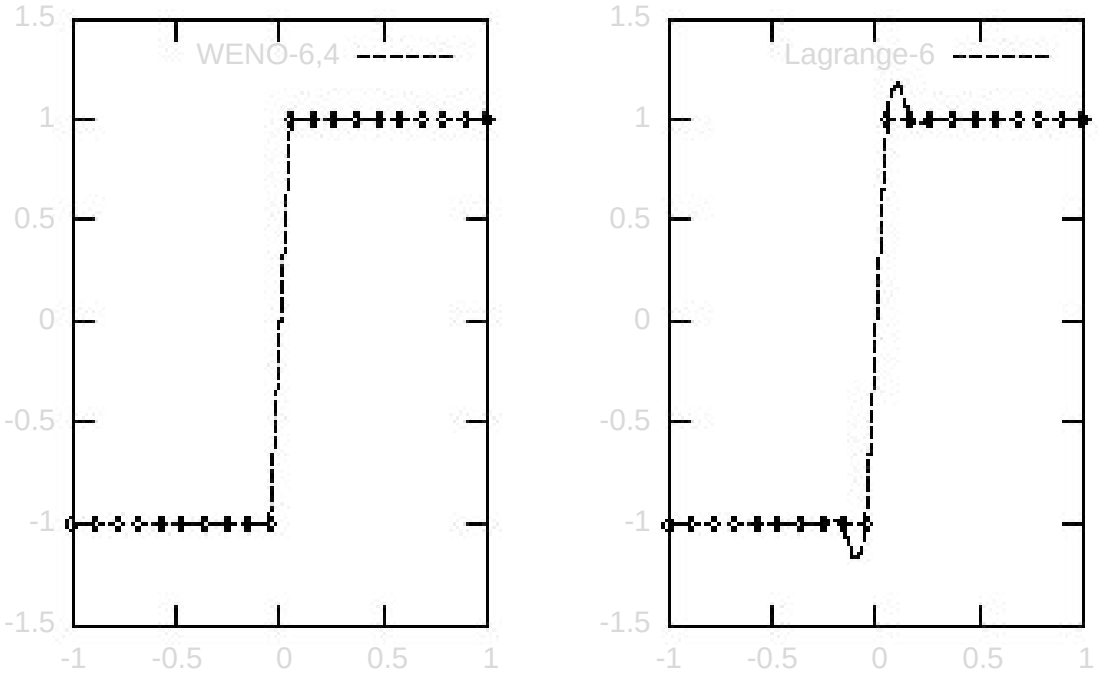

Figure: Left: PWENO interpolation. Right: Lagrange interpolation.

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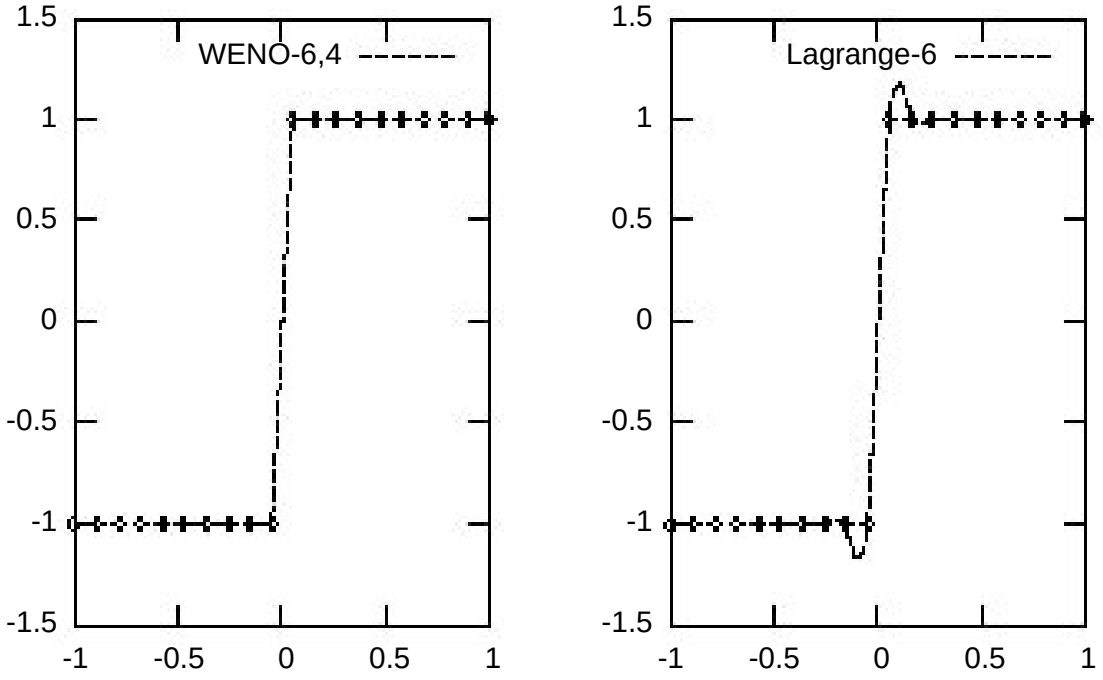
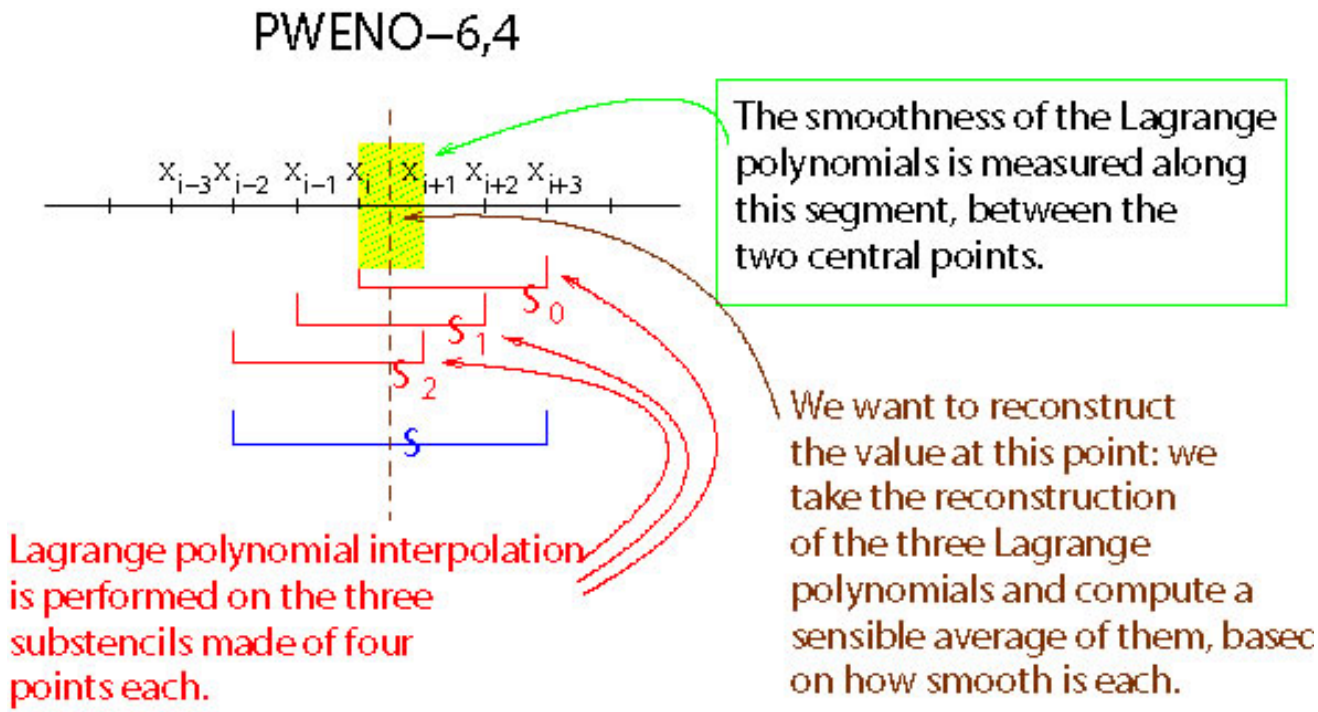


Figure: Left: PWENO interpolation. Right: Lagrange interpolation.

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:



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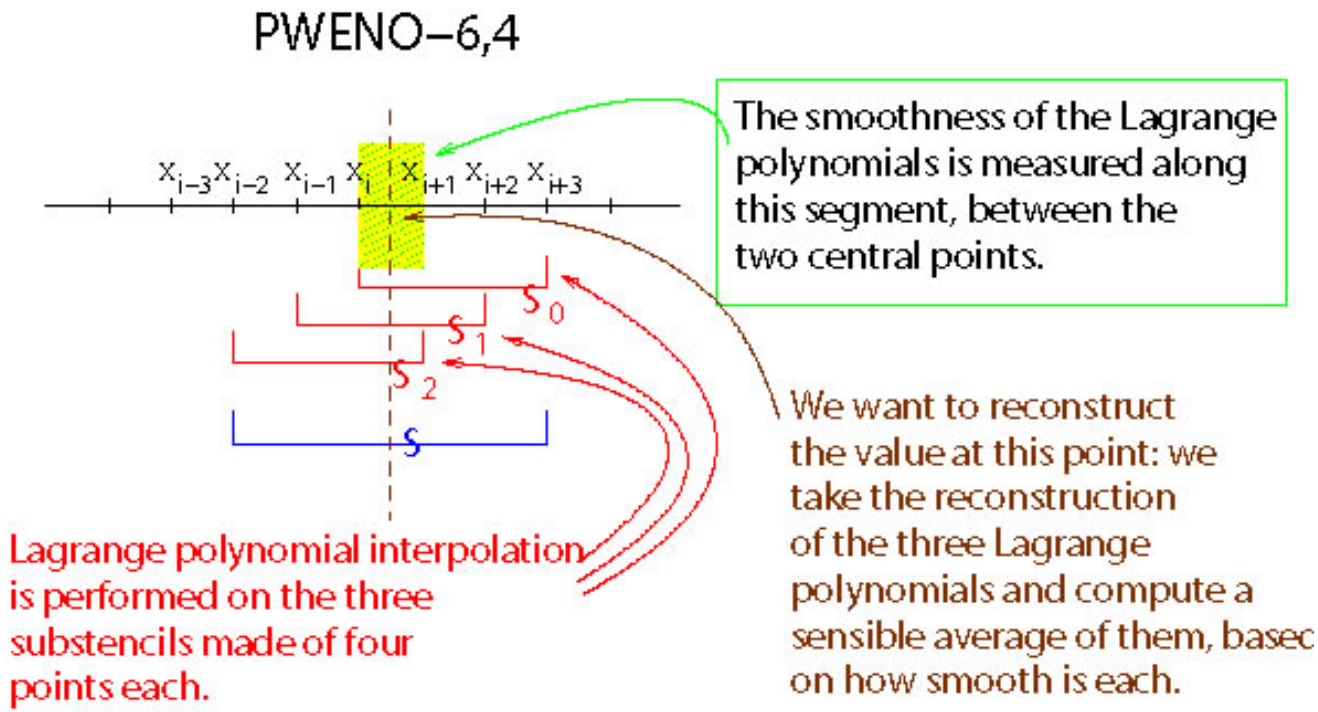

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Vlasov with confining potential

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 two initial conditions, more or less close to the equilibrium; the relaxation time is set $\tau = 3.5$:

$$f_0^{(1)} = Z_1 \sin^2\left(\frac{x}{2}\right) e^{-\frac{x^2+v^2}{2}}$$
$$f_0^{(2)} = Z_2 \sin^2\left(\frac{x}{2}\right) \sin^2\left(\frac{v}{2}\right) e^{-\frac{x^2+v^2}{2}}$$

Entropies

The global and local relative entropies are defined this way:

$$H[f; f_s] = \int_{\mathbb{R}} \int_{\mathbb{R}} \frac{|f - f_s|^2}{f_s} dvdx$$
$$\tilde{H}[f; \rho M_1] = \int_{\mathbb{R}} \int_{\mathbb{R}} \frac{|f - \rho M_1|^2}{f_s} dvdx.$$

Vlasov-Poisson: Two-stream instability

The problem

We set the problem in a collision-less 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.

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The Newton scheme

The PDE to solve

Solving the Schrödinger-Poisson block

$$-\frac{\hbar^2}{2}\frac{d}{dz}\left[\frac{1}{m_\nu}\frac{d\chi_{\nu,p}[V]}{dz}\right]-q\left(V+V_c\right)\chi_{\nu,p}[V]=\epsilon^{pot}_{\nu,p}[V]\chi_{\nu,p}[V]$$

$$-\mathrm{div}\left[\varepsilon_R\nabla V\right]=-\frac{q}{\varepsilon_0}\left(\sum_{\nu,p}\rho_{\nu,p}|\chi_{\nu,p}[V]|^2-N_D\right)$$

is equivalent to minimizing, under the constraints of the Schrödinger equation, the functional associated to $P[V]$

$$P[V]=-\mathrm{div}\left(\varepsilon_R\nabla V\right)+\frac{q}{\varepsilon_0}\left(\sum_{\nu,p}\rho_{\nu,p}|\chi_{\nu,p}[V]|^2-N_D\right),$$

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which is achieved by means of a Newton scheme

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

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The iterations

Derivatives

The Gâteaux-derivatives of the eigenproperties are needed:

$$\begin{aligned} d\epsilon_{\nu,p}(V,U) &= -q\int U(\zeta)|\chi_{\nu,p}[V](\zeta)|^2 d\zeta \\ d\chi_{\nu,p}(V,U) &= -q\sum_{p'\neq p}\frac{\int U(\zeta)\chi_{\nu,p}[V](\zeta)\chi_{\nu,p'}[V](\zeta)d\zeta}{\epsilon_{\nu,p}[V]-\epsilon_{\nu,p'}[V]}\chi_{\nu,p'}[V](z). \end{aligned}$$

Iterations

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

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

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The Schrödinger equation

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$$-\frac{\hbar^2}{2}\frac{d}{dz}\left[\frac{1}{m_\nu}\frac{d\chi_{\nu,p}}{dz}\right]-q\left(V+V_c\right)\chi_{\nu,p}=\epsilon_{\nu,p}\chi_{\nu,p}$$

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 equations 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 (full) is solved by means of a LAPACK routine called DGESV.

Numerical methods

The Schrödinger equation

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We need to solve equations 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 (full) is solved by means of a LAPACK routine called DGESV.

Three Schrödinger-Poisson Problems

Boundary potential

$V_{bp}(0) = V_{bp}(L_z) = 0$ and

$$N[V_{bp}](0,z) = \frac{\int_0^{L_z} N_D(0,\zeta)d\zeta}{\mathcal{Z}[V_{bp}](0)} \sum_{p=1}^{\infty} e^{-\frac{\epsilon_p[V_{bp}](0)}{k_B T_L}} |\chi_p[V_{bp}](0,z)|^2,$$

where the repartition function has the general expression:

$$\mathcal{Z}[V](x) = \sum_{q=1}^{\infty} e^{-\frac{\epsilon_q[V](x)}{k_B T_L}}.$$

The Thermodynamical equilibrium

$$N[V_{eq}] = \frac{\int_0^{L_z} N_D(0,\zeta)d\zeta}{\mathcal{Z}[V_{bp}](0)} \sum_{p=1}^{\infty} e^{-\frac{\epsilon_p[V_{eq}](x)}{k_B T_L}} |\chi_p[V_{eq}](x,z)|^2.$$

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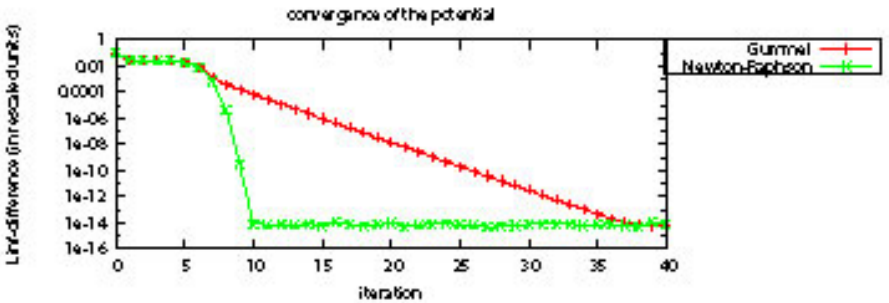
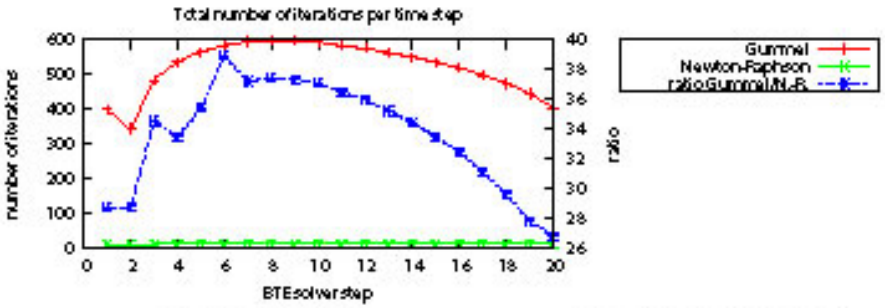
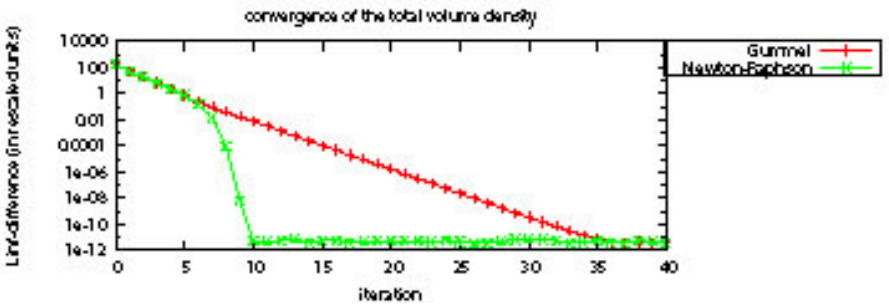
Efficiency versus Gummel

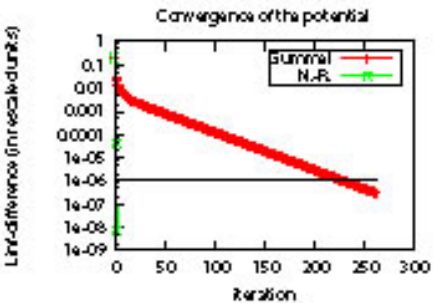
Gummel iteration

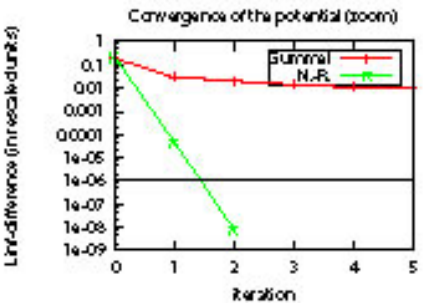
$$-\mathrm{div}\left(\varepsilon_R \nabla V^{new}\right) + \frac{q}{\varepsilon_0} N[V^{old}] \frac{q}{k_B T_L}(V^{new} - V^{old}) = -\frac{q}{\varepsilon_0}\left(N[V^{old}] - N_D\right),$$











Outline

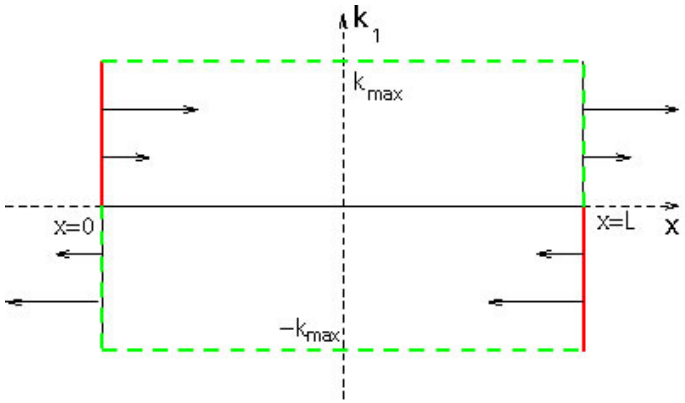
Collision operator

Results are presented for the the DG MOSFET in the one-valley, parabolic-band approximation. Moreover, the complete collision operator is substituted by a simple relaxation-time operator:

$$\mathcal{Q}_p f = \frac{1}{\tau}\left(\rho_p M - f_p\right).$$

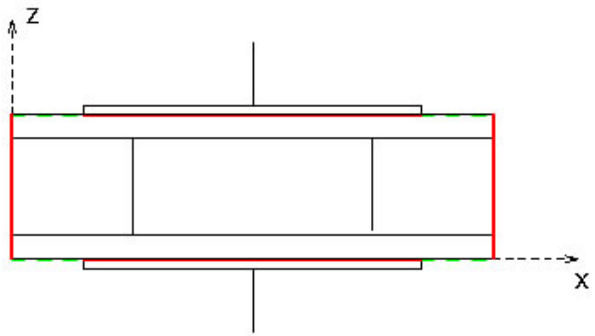
The goal of this work is just the setting up of numerical tools for a more profound and realistic simulation.
A parallel code in the most realistic case is being implemented.

Boundary Conditions



= force the density to stay close to the equilibrium density

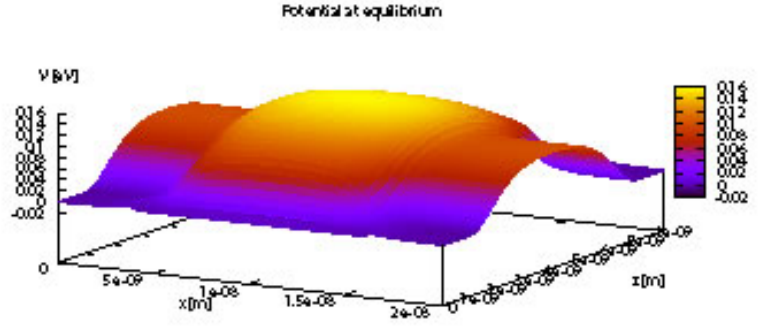
= Homogeneous Neumann

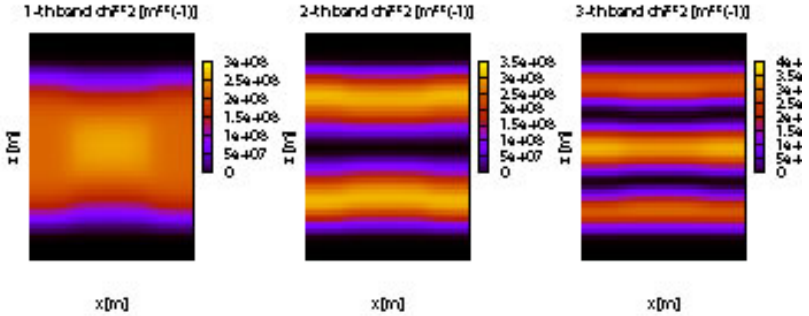


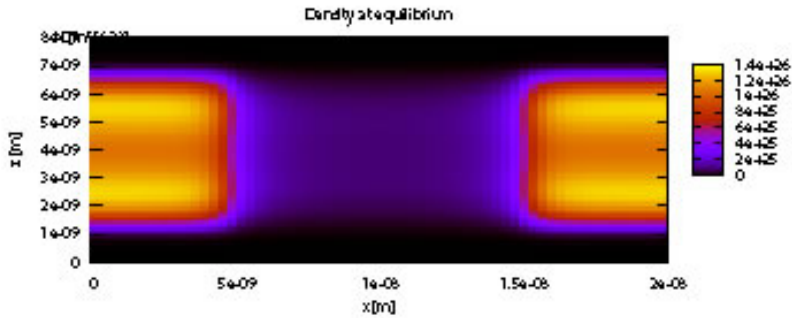
= Dirichlet

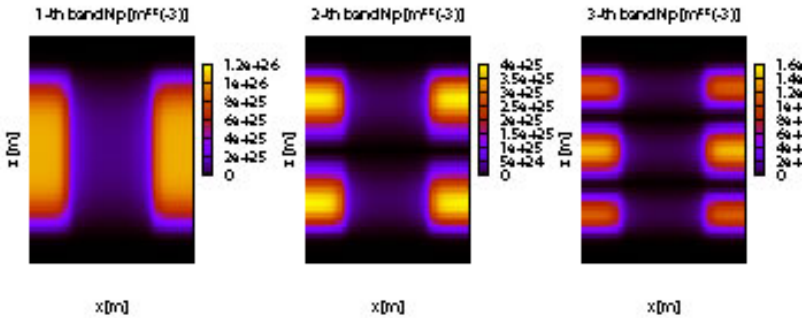
= homogeneous Neumann

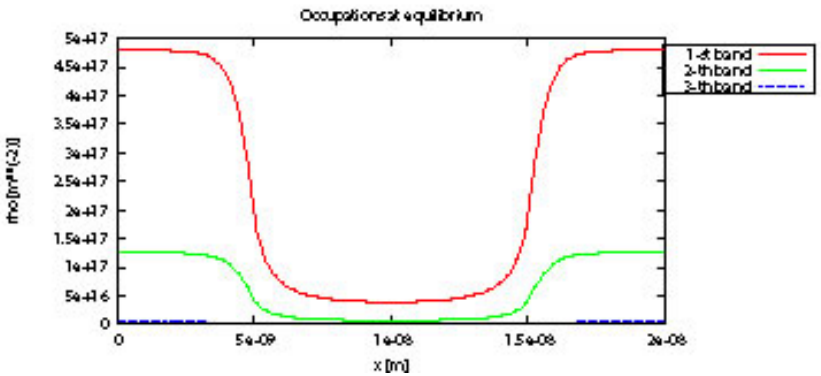
Thermodynamical equilibrium: one-valley case

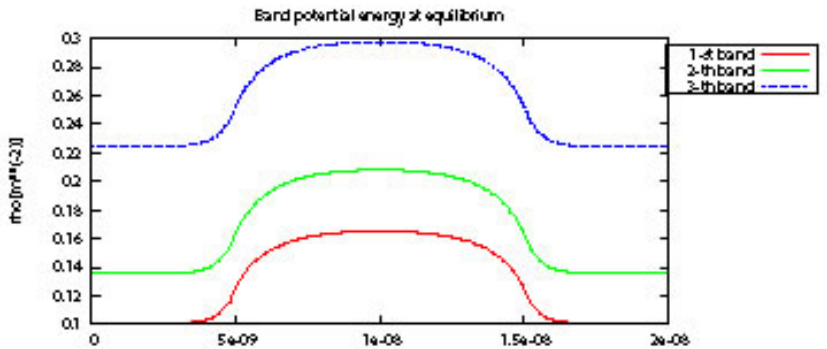












Transient states