The model
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Numerical methods for the Schrödinger-Poisson block
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Solvers for the BTE block
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Experiments
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Simulation of sub-band model for ultra-short DG MOSFET devices

Naoufel Ben Abdallah, María José Cáceres, José Antonio Carrillo, Francesco Vecil

Kinetic models of classical and quantum particle systems, Toulouse, 14 March 2011

The model
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Numerical methods for the Schrödinger-Poisson block
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Solvers for the BTE block
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Experiments
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Outline

The model	Numerical methods for the Schrödinger-Poisson block	Solvers for the BTE block	Experiments
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Geometry

Outline

The model

We afford the simulation of a nanoscaled MOSFET.
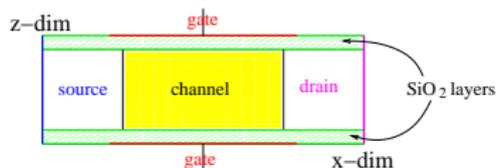
About the scaling

In 1971, the Intel 4004 processor had 1000 transistors, whose channel length was 10000 nm. In 1974, the Intel 8008 processor had 6-7 thousand. In 2003 the Intel Pentium IV had 50 million. Nowadays processors may have 400 million transistors, whose channel is 28 nm long.

Why is it important?

Smaller MOSFETs allow for the construction of smaller devices with better performances; moreover, they allow silicon and energy saving, due to the lower source-drain potential drop needed to switch on or off the transistor.

Geometry

The model
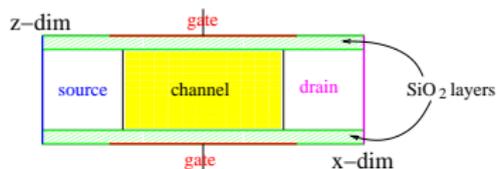
Dimensional coupling

x-dimension is unconfined unlike z-dimension, therefore we adopt a different description:

- along x-dimension the electrons behave like particles, their movement being described by the Boltzmann Transport Equation;

- along z-dimension the electrons, confined in a potential well, behave like waves; the equilibrium being reached much faster than transport (quasi-static phenomenon), their state is given by the stationary-state Schrödinger equation.

The model

Subband decomposition

Due to the confinement, different *sub-bands* (another name for the eigenvalues of the Schrödinger equation) identify independent populations, which have to be transported 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.

The model

Subband decomposition

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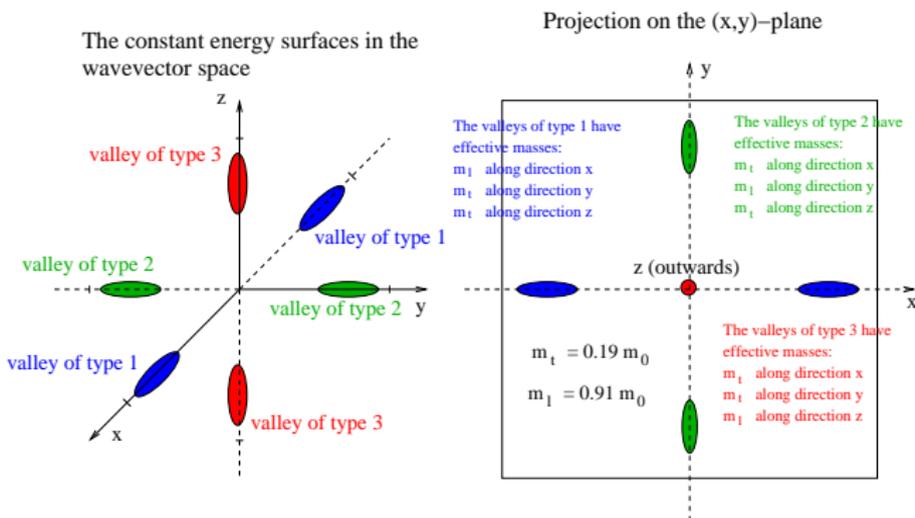
Coupling between dimensions

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

Bandstructure

The three valleys

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

The constant energy surfaces in the wavevector space

valley of type 3

valley of type 1

valley of type 2

valley of type 2

valley of type 1

valley of type 3

Projection on the (x,y)–plane

The valleys of type 1 have effective masses:
m_l along direction x
m_t along direction y
m_t along direction z

The valleys of type 2 have effective masses:
m_t along direction x
m_l along direction y
m_t along direction z

z (outwards)

The valleys of type 3 have effective masses:
m_t along direction x
m_t along direction y
m_l along direction z

$m_t = 0.19\, m_0$

$m_l = 0.91\, m_0$

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

Coupling between subbands and valleys

The sub-bands as well as the valleys are coupled by the Poisson equation in the expression of the total density and, if the case, by the scattering operator.

Non-parabolicity

The bandstructure around the three minima can be expanded following the Kane non-parabolic approximation (ν indexes the valley):

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

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

The model · Numerical methods for the Schrödinger-Poisson block · Solvers for the BTE block · Experiments
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Geometry

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Outline

The model | Numerical methods for the Schrödinger-Poisson block | Solvers for the BTE block | Experiments
○○○○○○○○●○○ | ○○○○○○○ | ○○○○○ | ○○○○○○○○○○

Mathematical model

The model

BTE

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

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

Schrödinger-Poisson block

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

$$\langle\chi_{\nu,p}[V], \chi_{\nu,p'}[V]\rangle = \delta_{p,p'}$$

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

$$N[V] = \sum_{\nu,p}\rho_{\nu,p}|\chi_{\nu,p}[V]|^2$$

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.

The model

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

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The model

The collision operator

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

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

every S^s represents a different interaction.

Structure of the S^s

The missing dimension of the wave-vector $k \in \mathbb{R}^2$, instead of $k \in \mathbb{R}^3$, is replaced by an overlap integral $W_{(\nu,p),(\nu',p')}$:

$$
S^s_{(\nu,p,k)\to(\nu',p',k')} = C_{\nu\to\nu'} \frac{1}{W_{(\nu,p),(\nu',p')}} \delta\left(\epsilon^{tot}_{\nu',p'}(k') - \epsilon^{tot}_{\nu,p}(k) \pm \text{some energy} \right)
$$

$$
\frac{1}{W_{(\nu,p),(\nu',p')}} = \int_0^{l_z} |\chi_{\nu,p}|^2 |\chi_{\nu',p'}|^2 dz, \qquad [W] = m.
$$

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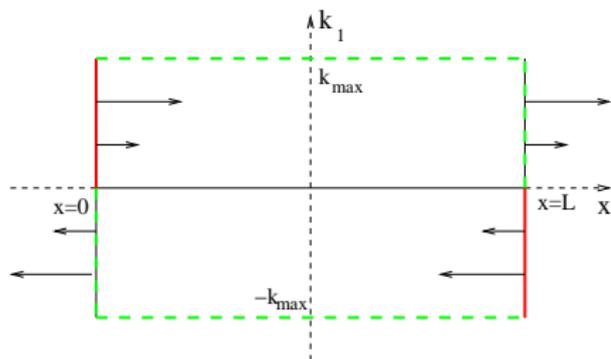$$

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The model
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Numerical methods for the Schrödinger-Poisson block
○○○○○○○
Solvers for the BTE block
○○○○○
Experiments
○○○○○○○○○○
Mathematical model

Boundary conditions

= force the density to stay close to the equilibrium density

- - - - - = Homogeneous Neumann
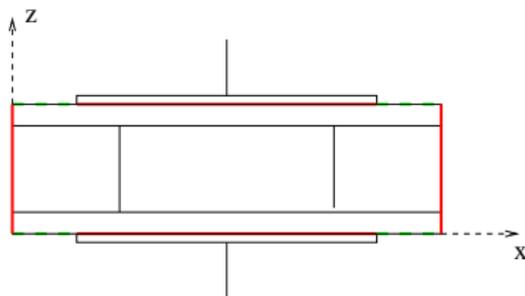
= Dirichlet

- - - - - = homogeneous Neumann

Outline

The model | Numerical methods for the Schrödinger-Poisson block | Solvers for the BTE block | Experiments
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Iterative schemes

The Newton scheme

The functional

Solving the Schrödinger-Poisson block

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

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

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

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

The scheme

which is achieved by means of a Newton-Raphson iterative scheme

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

The model | Numerical methods for the Schrödinger-Poisson block | Solvers for the BTE block | Experiments
0000000000 | 0●00000 | 00000 | 000000000

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The iterations

Derivatives

The Gâteaux-derivatives of the eigenproperties are needed:

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\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 developping calculations, we are led to a Poisson-like equation

$$
-\mathrm{div}\,(\varepsilon_R \nabla V^{new}) + \int_0^{l_z} \mathcal{A}[V^{old}](z, \zeta)V^{new}(\zeta)d\zeta
$$

$$
= -\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,
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where $\mathcal{A}[V]$ is essentially the Gâteaux-derivative of the functional $P[V]$.

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The model   Numerical methods for the Schrödinger-Poisson block   Solvers for the BTE block   Experiments
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Iterative schemes

The Gummel scheme

The iteration

Solving the Schrödinger-Poisson block

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

Comparison with Newton

We here repeat the Newton iteration:

$$-\text{div}\,(\varepsilon_R \nabla V^{new}) + \int_0^{l_z} \mathcal{A}[V^{old}](z, \zeta) V^{new}(\zeta) d\zeta$$
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The model | Numerical methods for the Schrödinger-Poisson block | Solvers for the BTE block | Experiments
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Framework

The model   Numerical methods for the Schrödinger-Poisson block   Solvers for the BTE block   Experiments
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Solvers for Schrödinger and Poisson

Outline

The model   Numerical methods for the Schrödinger-Poisson block   Solvers for the BTE block   Experiments
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Solvers for Schrödinger and Poisson

Numerical methods

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

The Schrödinger equation

Equation

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

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.

The model	Numerical methods for the Schrödinger-Poisson block	Solvers for the BTE block	Experiments
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Outline

Wave-vector space

The wave-vector space is adimensionalized by a change of variables into ellipsoidal variables, in order to better integrate the scattering operator and to have a simple expression for the kinetic energy and related magnitudes.

Ellipsoidal coordinated

The wave-vector for the νth valley reads:

$$(\tilde{k}_x, \tilde{k}_y) = \frac{\sqrt{m_e \kappa_B T_L}}{\hbar} \sqrt{2w(1 + \alpha_\nu w)} \left(\sqrt{m_{x,\nu}} \cos(\phi), \sqrt{m_{y,\nu}} \sin(\phi) \right).$$

The model   Numerical methods for the Schrödinger-Poisson block   Solvers for the BTE block   Experiments
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Adimensionalizations

Wave-vector space

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BTE in ellipsoidal coordinates

Let the flux coefficients

$$
\begin{aligned}
a^1_\nu(w,\phi) &= C^V \frac{\sqrt{2w(1+\alpha_\nu w)}\cos(\phi)}{\sqrt{m_{x,\nu}}} \frac{1}{1+2\alpha_\nu w} \\
a^2_{\nu,p}(x,w,\phi) &= -C^V \frac{\partial \epsilon_{\nu,p}}{\partial x}(x) \frac{1}{1+2\alpha_\nu w} \frac{\sqrt{2w(1+\alpha_\nu w)}\cos(\phi)}{\sqrt{m_{x,\nu}}} \\
a^3_{\nu,p}(x,w,\phi) &= C^V \frac{\partial \epsilon_{\nu,p}}{\partial x}(x) \frac{\sin(\phi)}{\sqrt{m_{x,\nu}}\sqrt{2w(1+\alpha_\nu w)}}.
\end{aligned}
$$

Conservation-law form

$$
\frac{\partial \Phi_{\nu,p}}{\partial t} + \frac{\partial}{\partial x}\left[a^1_\nu \Phi_{\nu,p}\right] + \frac{\partial}{\partial w}\left[a^2_{\nu,p}\Phi_{\nu,p}\right] + \frac{\partial}{\partial \phi}\left[a^3_{\nu,p}\Phi_{\nu,p}\right] = \mathcal{Q}_{\nu,p}[\Phi]s(w)
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Adimensionalizations

BTE in ellipsoidal coordinates

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\begin{aligned}
a_\nu^1(w, \phi) &= C^V \frac{\sqrt{2w(1 + \alpha_\nu w)} \cos(\phi)}{\sqrt{m_{x,\nu}}} \frac{1}{1 + 2\alpha_\nu w} \\
a_{\nu,p}^2(x, w, \phi) &= -C^V \frac{\partial \epsilon_{\nu,p}}{\partial x}(x) \frac{1}{1 + 2\alpha_\nu w} \frac{\sqrt{2w(1 + \alpha_\nu w)} \cos(\phi)}{\sqrt{m_{x,\nu}}} \\
a_{\nu,p}^3(x, w, \phi) &= C^V \frac{\partial \epsilon_{\nu,p}}{\partial x}(x) \frac{\sin(\phi)}{\sqrt{m_{x,\nu}} \sqrt{2w(1 + \alpha_\nu w)}}.
\end{aligned}
$$

Conservation-law form

$$
\frac{\partial \Phi_{\nu,p}}{\partial t} + \frac{\partial}{\partial x}\left[a_\nu^1 \Phi_{\nu,p}\right] + \frac{\partial}{\partial w}\left[a_{\nu,p}^2 \Phi_{\nu,p}\right] + \frac{\partial}{\partial \phi}\left[a_{\nu,p}^3 \Phi_{\nu,p}\right] = \mathcal{Q}_{\nu,p}[\Phi] s(w)
$$

Outline

Runge-Kutta

We propose a Runge-Kutta time discretization.

Runge-Kutta

If the BTE is written in conservation-law form, then we advance in time by the third order Total Variation Diminishing Runge-Kutta scheme: if the evolution equation reads $\dfrac{df}{dt} = H(t,f)$, then

1. $f^{(1)} = \Delta t H^n(t^n, f^n)$

2. $f^{(2)} = \frac{3}{4}f^n + \frac{1}{4}f^{(1)} + \frac{1}{4}\Delta t H^{(1)}(t^n + \Delta t, f^{(1)})$

3. $f^{n+1} = \frac{1}{3}f^n + \frac{2}{3}f^{(2)} + \frac{2}{3}H^{(2)}\left(t^n + \frac{1}{2}\Delta t, f^{(2)}\right)$

Outline

1. The model
   - Geometry
   - Mathematical model

2. Numerical methods for the Schrödinger-Poisson block
   - Iterative schemes
   - Solvers for Schrödinger and Poisson

3. Solvers for the BTE block
   - Adimensionalizations
   - Time discretization

4. Experiments
   - Newton vs. Gummel
   - Equilibria
   - Time-dependent simulations
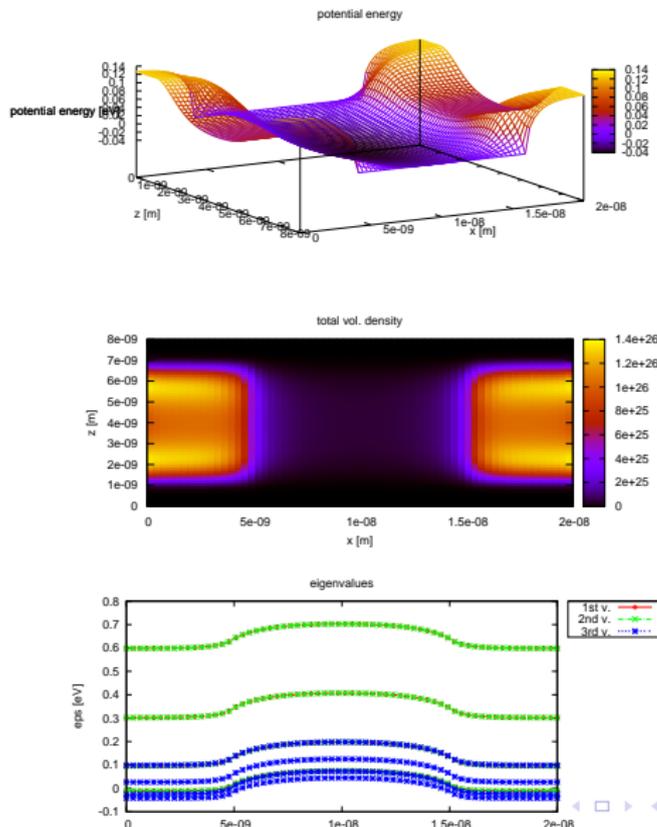   - Plasma oscillations

Number of iterations

Newton schemes require much less iterations than Gummel in order to compute the thermodynamical equilibrium and any update of the potential; the results are the same up to machine error.
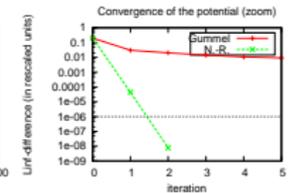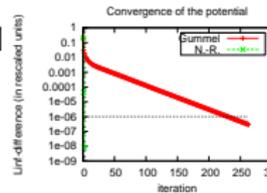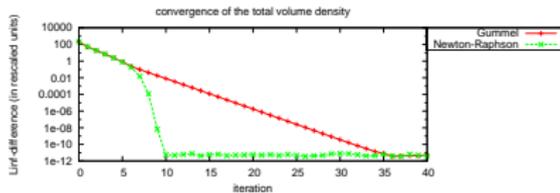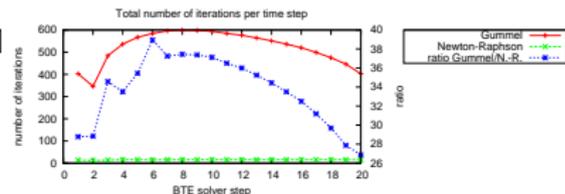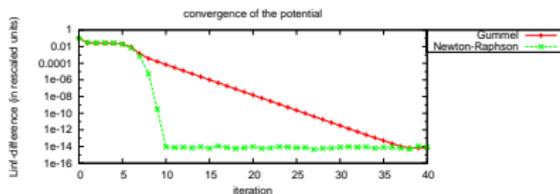
Outline

Thermodynamical equilibrium: three-valley case

The model Numerical methods for the Schrödinger-Poisson block Solvers for the BTE block Experiments
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Time-dependent simulations

Outline

1. The model
   - Geometry
   - Mathematical model

2. Numerical methods for the Schrödinger-Poisson block
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   - Adimensionalizations
   - Time discretization

4. Experiments
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   - Equilibria
   - Time-dependent simulations
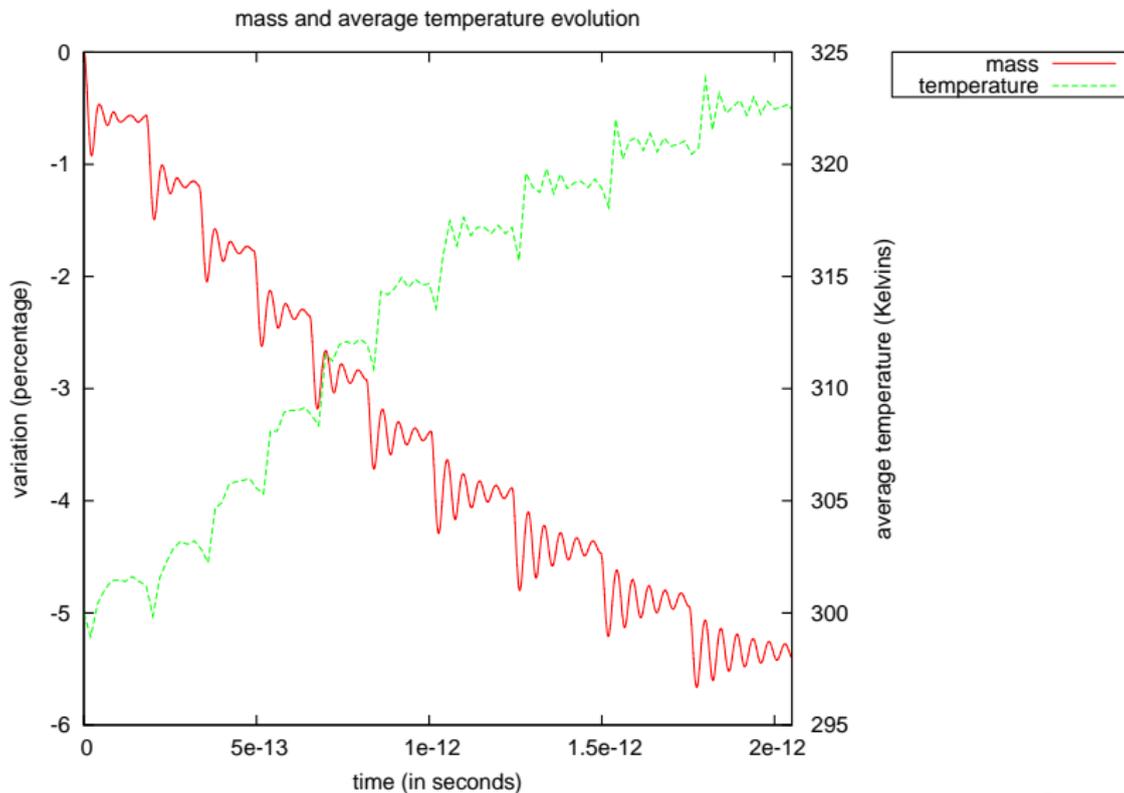   - Plasma oscillations

The model | Numerical methods for the Schrödinger-Poisson block | Solvers for the BTE block | Experiments
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Time-dependent simulations

Long-time behavior

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

The model
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Numerical methods for the Schrödinger-Poisson block
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Solvers for the BTE block
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Experiments
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Plasma oscillations

Outline

Mass and temperature oscillations

mass and average temperature evolution

The model Numerical methods for the Schrödinger-Poisson block Solvers for the BTE block Experiments
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Plasma oscillations

Numerically-computed oscillations

The plasma frequency is given by

$$\omega_p = \sqrt{\frac{q^2 N_e}{\varepsilon_R \varepsilon_0 m_*}}.$$

N_D^{high} ($\times 10^{26} m^{-3}$)	ε_R	$m_\star$	N_e ($\times 10^{26} m^{-3}$)	ω_{num} ($\times 10^{14} s^{-1}$)	ω_p ($\times 10^{14} s^{-1}$)	Ratio $\frac{\omega_{num}}{\omega_{ref}}$	Expected Ratio
1	11.7	0.5	.400	$\omega_{ref} = 1.344$	1.475	1	/
2	11.7	0.5	.783	2.051	2.064	1.52	$\sqrt{2}$
4	11.7	0.5	1.544	2.813	2.899	2.09	2
1	5.85	0.5	.400	1.848	2.086	1.37	$\sqrt{2}$