A SOLVER FOR A COUPLED QUANTUM-CLASSICAL MODEL FOR NANOMOSFETS

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- 2002, graduated at the Universitas Studii Paduani (Padua), Italy, with a graduation thesis about “Asynchronus exponential growth in an age-structured cell population”
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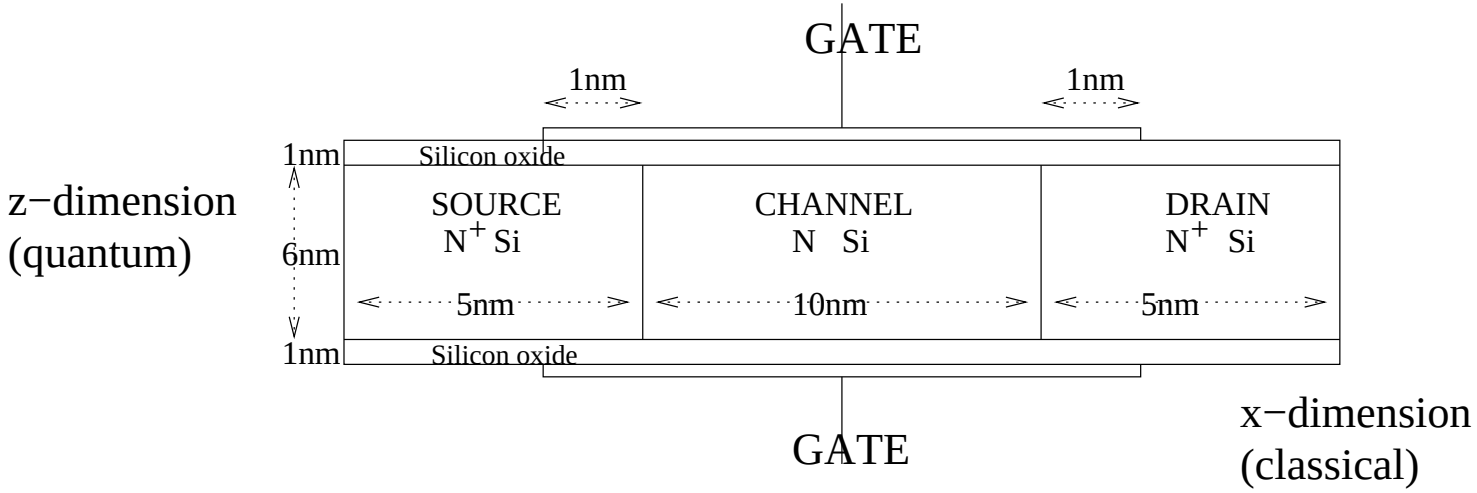
SCHEME OF THE PRESENTATION

- The MOSFET
- The model
- Numerical schemes
- (Partial) results

The MOSFET

The MOSFET is a transistor in which the conductivity can be altered by varying the voltage between the gates and the source,



which induces a potential penetrating inside the channel and making the device be turned off, on, or work as a resistor.

The model

x-dimension is 20 nm, therefore we adopt a classical description, supposing that the carriers behave like ballistic particles, driven by the effects of the free motion and the force field, while their collisions are taken into account by the right hand side (Boltzmann Transport Equation):

$$\frac{\partial f_p}{\partial t} + \frac{1}{\hbar}\nabla_k \epsilon_p \cdot \nabla_x f_p - \frac{1}{\hbar}\nabla_x \epsilon_p \cdot \nabla_k f_p = \mathcal{Q}[f]_p,$$

plus an initial datum

$$f_p(t = 0, x, k_1, k_2) = f_{p,0}(x, k_1, k_2)$$

and some boundary conditions.

z-dimension

The z-dimension (6 nm) is confined, therefore the carriers behave like waves, their energy levels become discretized and a quantum description is proper. Therefore we use a steady-state Schrödinger equation to compute their energy levels and distribution for any position x (which acts only as parameter), under the effects of the self-consistent electric field and the confining potential :

$$-\frac{\hbar^2}{2m_e}\frac{d}{dz}\left(\frac{1}{m_*(z)}\frac{d\chi^p[V]}{dz}\right) - q\left(V + V_c\right)\chi^p[V] = \epsilon^p[V]\chi^p[V]$$

$\{\chi^p[V]\}_p \subseteq H_0^1$ orthonormal basis.

The coupling

x-dimension and z-dimension are coupled through the Poisson equation for computing the electrostatic field, which has the contribution of the free electrons density moving in the device and the doping profile, i.e. the injected impurities which form part of the MOSFET:

$$-\text{div}_{x,z}\left(\varepsilon_R \text{grad}_{x,z} V\right) = -\frac{q}{\varepsilon_0}(N[V] - N_D),$$

plus some boundary conditions.

Numerical schemes

The fundamental numerical techniques are relative to:

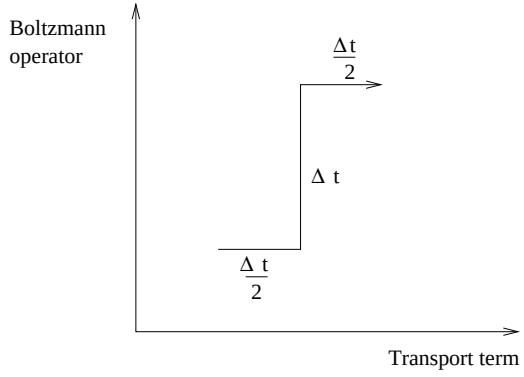
- splitting methods (Strang's splitting)
- Newton iteration for the Schrödinger-Poisson block.

Time splitting

The time step Δt is fixed: the method is implicit and we hope we can achieve the equilibrium in few steps.
The BTE is solved through a second order time splitting scheme (Strang's splitting). Solving the complete Boltzmann equation

$$\frac{\partial f_p}{\partial t} + \frac{1}{\hbar}\left\{\epsilon_p^{tot}, f_p\right\} = \mathcal{Q}[f]_p$$

reduces to solving for separate the advection problem and the collision operator and then recombine them.

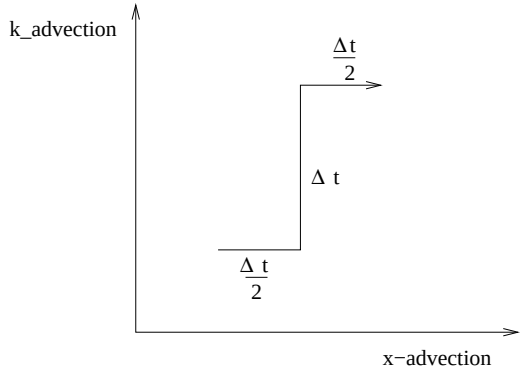


(x, k_1)-advection problem

In order to solve problem

$$\frac{\partial f_p}{\partial t} + \frac{1}{\hbar}\frac{\partial \epsilon_p^{kin}}{\partial k_1}\frac{\partial f_p}{\partial x} - \frac{1}{\hbar}\frac{\partial \epsilon_p^{pot}}{\partial x}\frac{\partial f_p}{\partial k_1} = 0$$

we adopt the same scheme as to split the advection problem from the collision problem:



We are thus led to solving for separate two linear advection problems.

The linear transport problem

The linear transport

$$\begin{cases} \frac{\partial f}{\partial t} + v\frac{\partial f}{\partial x} = 0 \\ f(t^n, x) = f^n(x) \end{cases}$$

is the building block for the Boltzmann part. Three solvers are proposed:

- direct Semi Lagrangian: following backward the characteristics we obtain a good control of the total variation (when applied to the proper PWENO interpolator), therefore no spurious oscillations appear. Drawback: it is not conservative.

The linear transport problem

- Flux Balance Method: conservative method based on a similar idea as the SL; its drawback is that it does not control oscillations as good as SL does.
- Positive Flux Conservative-3: conservative method, controls oscillations by means of some slope correctors; its drawback: it is low order.

Collisions

By now, a simple relaxation time operator is used:

$$\frac{\partial f_p}{\partial t} = \frac{1}{\tau} \sum_q \left[M \rho_q - f_p \right],$$

whose analytic solution is straightforward. The complete Boltzmann operator has to be written for a detailed description: works in progress...

The Schrödinger-Poisson block

In order to compute the equilibrium states, the potential, the eigenproperties (potential band-energy, z-charge distribution, Fermi levels) and the band occupations, we need to be able to solve three main problems:

- 1D Newton iteration for the border potential
- stationary-state Schrödinger equation
- 2D Newton iteration for the Schrödinger-Poisson problem (potential)

Numerics for the Schrödinger equation

The Schrödinger equation

$$\frac{\hbar^2}{2m_e}\frac{d}{dz}\left(\frac{1}{m_*(z)}\frac{d\chi^p[V]}{dz}\right) - q\left(V + V_c\right)\chi^p[V] = \epsilon^p[V]\chi^p[V]$$

$\{\chi^p[V]\}_p \subseteq H_0^1$ orthonormal basis.

is discretized through finite differences, then the diagonalization is performed through a LAPACK routine called DSTEQR.
As a remark, another routine, DSTEGR, had been tried before, but it did not work properly. Why?

Newton schemes

The building block for the computation of the potential is the solution os the 1D and 2D Schrödinger-Poisson problems

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

completed by the boundary conditions for the potential V and, most of all, provided with an expression for the density $N[V]$; changing the density, we shall obtain and solve different problems.

Technical point. In order to perform the Newton iteration, we must be able to compute the Gâteaux derivative of the density with respect to V, in direction U: $dN(V,U)$. It is here that the Schrödinger equation plays a rôle.

Border potential

It is the 1D Schrödinger-Poisson problem where the density is defined by

$$N[V_b] = \frac{\int N_D(0,\zeta)d\zeta}{\sum_q e^{-\frac{\epsilon_p[V_b]}{k_B T_L}}} \sum_p e^{-\frac{\epsilon_q[V_b]}{k_B T_L}} |\chi_p[V_b](z)|^2$$

and homogeneous Neumann conditions are imposed at $z = 0$ and $z = l_z$.

Equilibrium state

In order to initialize the solver of the kinetic equation, we need to compute the equilibrium state when no drain-source voltage is applied. It is the 2D Schrödinger-Poisson problem where the density is defined by

$$N[V^{eq}] = \frac{\int N_D(0,\zeta)d\zeta}{\sum_q e^{-\frac{\epsilon_q[V_b]}{k_B T_L}}} \sum_p e^{-\frac{\epsilon_p[V^{eq}]}{k_B T_L}} |\chi_p[V^{eq}](z)|^2,$$

plus the boundary conditions.

Computation of the potential

We propose two versions for the computation of the potential:

- **explicit version:** given the band occupations $\{\rho_p\}_p$, the density is just defined as

$$N[V] = \sum_p \rho_p |\chi_p[V]|^2$$

Computation of the potential

- **semi-implicit version:** given the band occupations $\{\rho_p\}_p$ and the potential band-energies (i.e. the Schrödinger eigenvalues) $\{\epsilon_p\}$ the density is just defined as

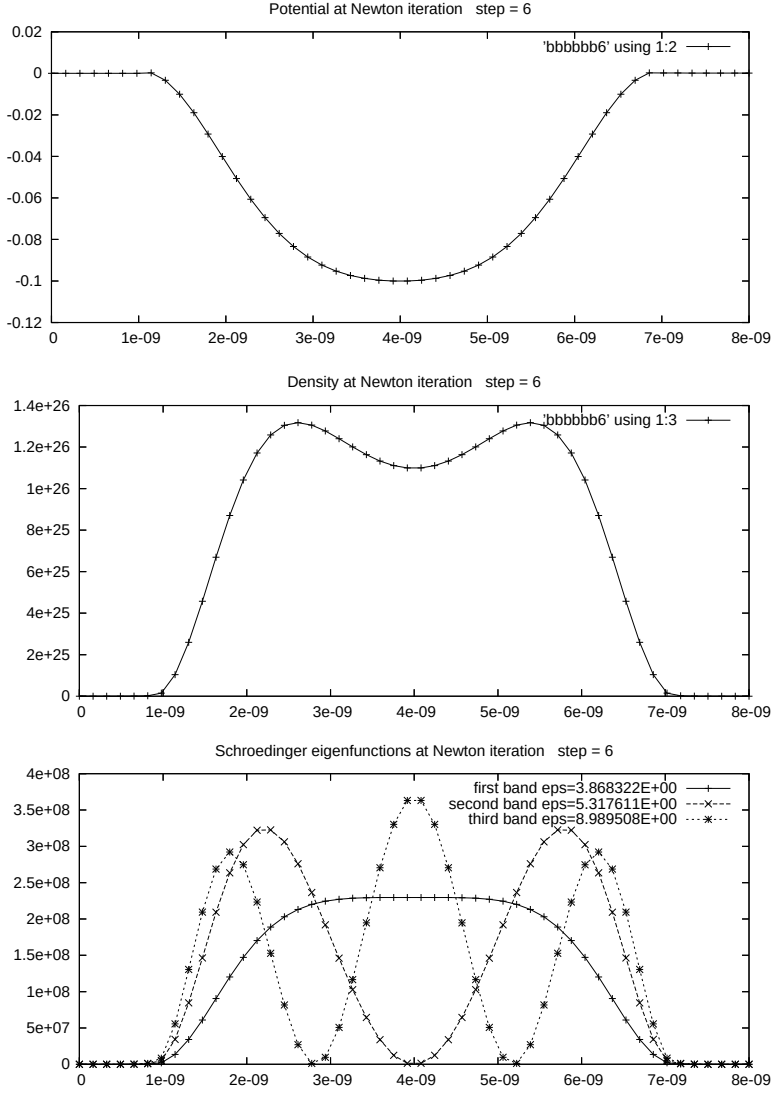
$$N[V] = \sum_p e^{\epsilon_p} \rho_p e^{-\epsilon_p[V]} |\chi_p[V]|^2.$$

We expect this scheme to be more stable.

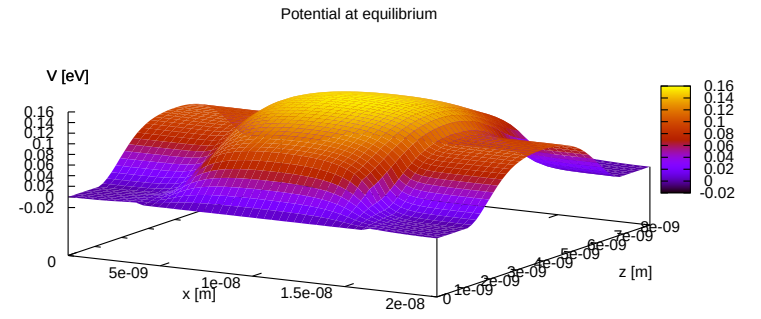
Numerical results

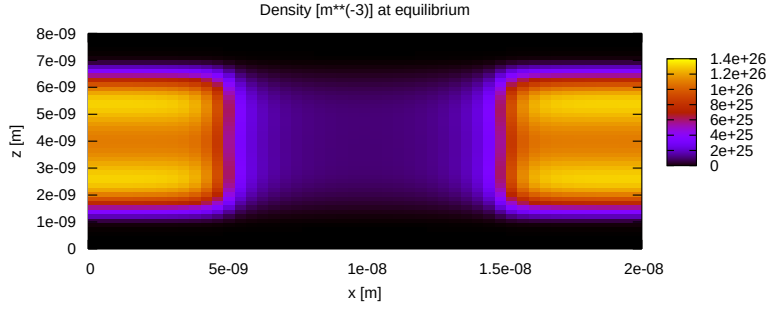
Up to now, we have the results for the border potential and for the equilibrium state. Still the code does not provide correct results for the kinetic equation.

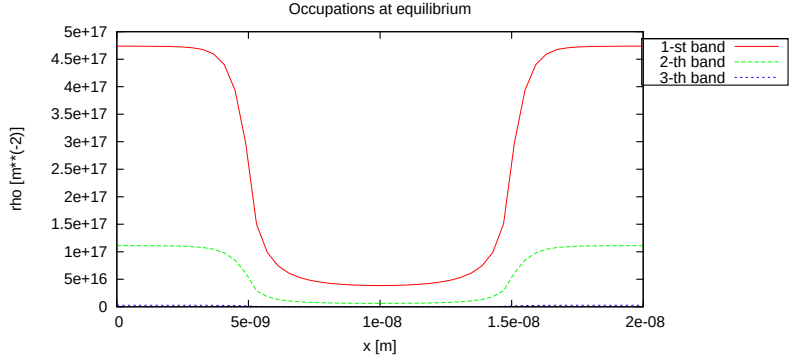
Border potential



Equilibrium







Conclusions and perspectives

Some improvements to the code have to be made:

- get results fro the dynamics
- electrons have six configurations
- add one dimension