Implementation on a high-performance platform of a hybrid parallel solver for DG-MOSFETs

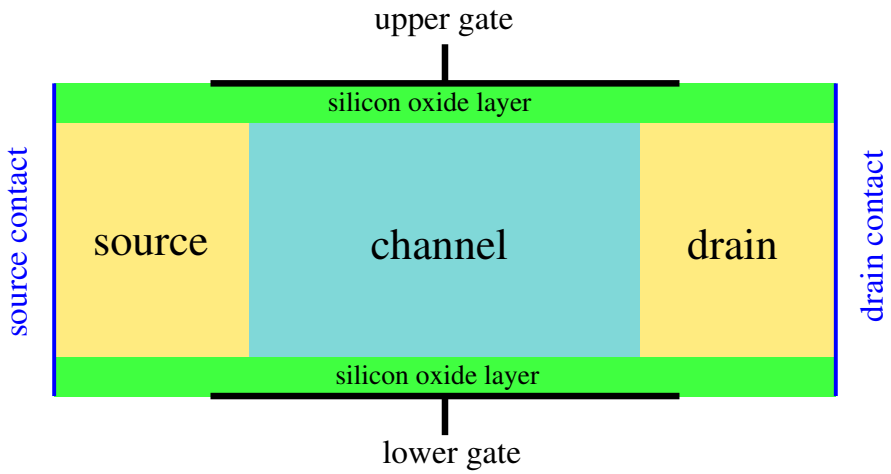
F. Vecil, J.M. Mantas, M.J. Cáceres, C. Sampedro, A. Godoy, F. Gámiz

Granada, 19 de junio de 2017

Outline

Outline

Geometry



About the scaling

In 1971, the Intel 4004 processor had 1000 transistors, whose channel length was 10000 nm. In 2003 the Intel Pentium IV had 50 million. Nowadays, for instance, Intel's i7-4650U has 1.3 billion transistors, whose channel is 22 nm long. The shortest transistor in the market is 14 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 voltages needed to switch on or off the transistor.

Outline

The confinement

Dimensional coupling

Electrons are **particles** along the x-dimension, **waves** along the z-dimension.

Description of the confinement

A set of 1D Schrödinger eigenvalue problems describe the electrons along z.

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

Subbands and wave functions

The eigenvalues $\{\epsilon_{\nu,p}\}_{(\nu,p)\in\{1,2,3\}\times\mathbb{Z}_{>0}}$ represent the energy levels, called *subbands* in physics.
The eigenfunctions $\{\psi_{\nu,p}(\cdot)\}_{(\nu,p)\in\{1,2,3\}\times\mathbb{Z}_{>0}}$ are called *wave functions* in physics.

Electron population

The subbands decompose the electron population of the ν^{th} valley into independent populations. The densities are indexed on the pair (ν, p).

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The unconfined dimension

BTE

The Boltzmann Transport Equation (one for each pair (ν, p)) reads

$$\frac{\partial f_{\nu,p}}{\partial t} + \overbrace{\frac{1}{\hbar}\frac{\partial \epsilon_\nu^{\mathrm{kin}}}{\partial k_x}\frac{\partial f_{\nu,p}}{\partial x}}^{\text{free motion}} - \overbrace{\frac{1}{\hbar}\frac{\partial \epsilon_{\nu,p}}{\partial x}\frac{\partial f_{\nu,p}}{\partial k_x}}^{\text{force field}} = \overbrace{\mathcal{Q}_{\nu,p}[f]}^{\text{scatterings}} \quad ,$$

$$f_{\nu,p}(t=0,x,\boldsymbol{k}) = \underbrace{\varrho_{\nu,p}^{\mathrm{eq}}(x)}_{\text{equil. dens.}} \underbrace{M_\nu(\boldsymbol{k})}_{\text{Maxw.}} .$$

The model

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Schrödinger-Poisson block

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

$$-\operatorname{div}_{x,z}\left[\varepsilon_R \nabla_{x,z} V\right] = -\frac{q}{\varepsilon_0}\left(N[V] - N_D\right), \qquad N[V] = 2\sum_{\nu,p} \varrho_{\nu,p}\left|\psi_{\nu,p}[V]\right|^2$$

These equations cannot be decoupled because we need the eigenfunctions to compute the potential, and we need the potential to compute the eigenfunctions.

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The model

The electron-phonon interactions

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

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

Structure of the S^s

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

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

$$\frac{1}{W_{(\nu,p)\leftrightarrow(\nu',p')}} = \int_0^{L_z} |\psi_{\nu,p}|^2 |\psi_{\nu',p'}|^2 \,\mathrm{d}z, \qquad [W] = m.$$

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The Newton scheme

The functional

Solving the Schrödinger-Poisson block

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

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

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

The scheme

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

$$\mathrm{d}P(V^{(k)},V^{(k+1)}-V^{(k)})=-P[V^{(k)}],\qquad \mathrm{d}=\text{directional derivative.}$$

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Newton-Raphson

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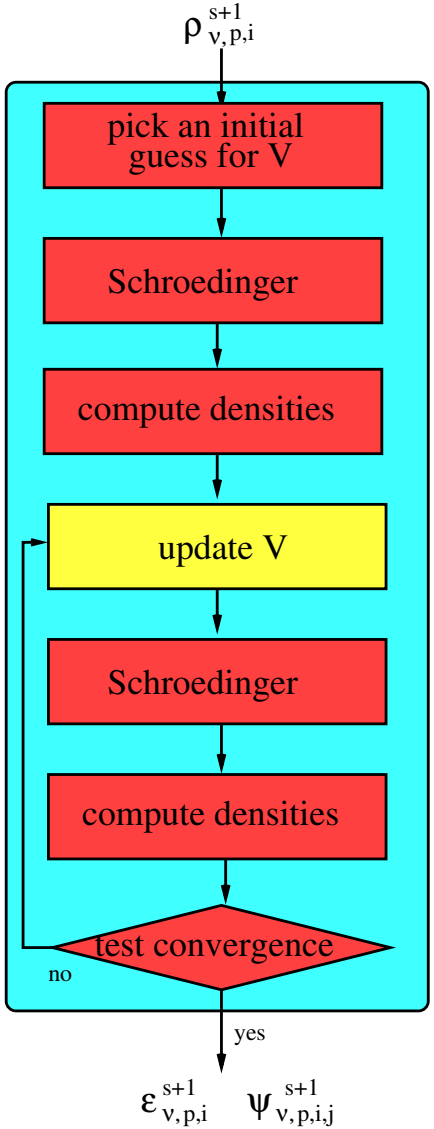
$$
\begin{aligned}
&- \operatorname{div}_{x,z}\left[\varepsilon_{\mathrm{R}}(x,z)\,\nabla V^{(k+1)}(x,z)\right] + \int \mathcal{A}^{(k)}(x,z,\zeta)\,V^{(k+1)}(x,\zeta)\,\mathrm{d}\zeta \\
&= -2\sum_{\nu,p} \varrho_{\nu,p}\left|\psi^{(k)}_{\nu,p}[V]\right|^2 + \int \mathcal{A}^{(k)}(x,z,\zeta)\,V^{(k)}(x,\zeta)\,\mathrm{d}\zeta.
\end{aligned}
$$

with

$$
\begin{aligned}
\mathcal{A}^{(k)}(x,z,\zeta) = 2\sum_{\nu,p}\sum_{p'\neq p} &\frac{\varrho_{\nu,p}(x) - \varrho_{\nu,p'}(x)}{\epsilon^{(k)}_{\nu,p'}(x) - \epsilon^{(k)}_{\nu,p}(x)} \\
&\times \psi^{(k)}_{\nu,p}(x,\zeta)\,\psi^{(k)}_{\nu,p'}(x,\zeta)\,\psi^{(k)}_{\nu,p'}(x,z)\,\psi^{(k)}_{\nu,p}(x,z).
\end{aligned}
$$

Framework


$\rho^{s+1}_{\nu,p,i}$
pick an initial guess for V
Schroedinger
compute densities
update V
Schroedinger
compute densities
test convergence
no
yes
$\varepsilon^{s+1}_{\nu,p,i}$
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Numerical methods

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

The Schrödinger equation

Equation

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

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

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

The derivatives are discretized by finite differences in alternate directions, the integral is computed via trapezoid rule. The system is preconditioned by the Crout version of the Incomplete LU factorization. Then, the system is solved by the IDRs method.

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Adimensionalization of the 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 ν^{th} 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 Jacobian

The magnitude $s_\nu(w)$ represents the dimensionless Jacobian of the change of variables in the wave-vector space:

$$s_\nu(w) = \left| \det \frac{\partial (k_x, k_y)}{\partial (w, \phi)} \right| = \sqrt{m_{x,\nu} m_{y,\nu}} (1 + 2\alpha_\nu w).$$

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BTE in ellipsoidal coordinates

Let the flux coefficients

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

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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Runge-Kutta time integration

We use a Runge-Kutta time discretization.

Runge-Kutta

We advance in time by the third order Total Variation Diminishing Runge-Kutta scheme: if the evolution equation reads

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

(no explicit time-dependency), then

1. $\Phi^{(1)}_{\nu,p} = \Delta t H_{\nu,p}(\Phi^n)$
2. $\Phi^{(2)}_{\nu,p} = \frac{3}{4}\Phi^n_{\nu,p} + \frac{1}{4}\Phi^{(1)}_{\nu,p} + \frac{1}{4}\Delta t H_{\nu,p}(\Phi^{(1)})$
3. $\Phi^{n+1} = \frac{1}{3}\Phi^n_{\nu,p} + \frac{2}{3}\Phi^{(2)}_{\nu,p} + \frac{2}{3}H_{\nu,p}(\Phi^{(2)})$

Integrating the scattering operator

Here go the formulae for the integration of the collisional operator in the ellipsoidal dimensionless variables.

Inelastic phenomena

$$
\begin{aligned}
&\mathcal{Q}_{\nu,p}[\Phi]s_\nu(w) \\
=&C^{\mathcal{Q}}s_\nu(w)\sum_{\nu',p'}\frac{\gamma_{\nu'\to\nu}N_{\nu'\to\nu}}{W_{(\nu',p')\leftrightarrow(\nu,p)}}\mathbb{I}_{\{\Gamma_-\geq 0\}}\int_{\phi'=0}^{2\pi}\Phi_{\nu',p'}\left(\Gamma'_-,\phi'\right)\,\mathrm{d}\phi' \\
+&C^{\mathcal{Q}}s_\nu(w)\sum_{\nu',p'}\frac{\gamma_{\nu'\to\nu}\left(N_{\nu'\to\nu}+1\right)}{W_{(\nu',p')\leftrightarrow(\nu,p)}}\mathbb{I}_{\{\Gamma_+\geq 0\}}\int_{\phi'=0}^{2\pi}\Phi_{\nu',p'}\left(\Gamma_+,\phi'\right)\,\mathrm{d}\phi' \\
-&C^{\mathcal{Q}}2\pi\Phi_{\nu,p}(w,\phi)\sum_{\nu',p'}\frac{\gamma_{\nu\to\nu'}N_{\nu\to\nu'}}{W_{(\nu,p)\leftrightarrow(\nu',p')}}\mathbb{I}_{\{\Gamma_+\geq 0\}}s_{\nu'}\left(\Gamma_+\right) \\
-&C^{\mathcal{Q}}2\pi\Phi_{\nu,p}(w,\phi)\sum_{\nu',p'}\frac{\gamma_{\nu\to\nu'}\left(N_{\nu\to\nu'}+1\right)}{W_{(\nu,p)\leftrightarrow(\nu',p')}}\mathbb{I}_{\{\Gamma_-\geq 0\}}s_{\nu'}\left(\Gamma_-\right)
\end{aligned}
$$

Summary

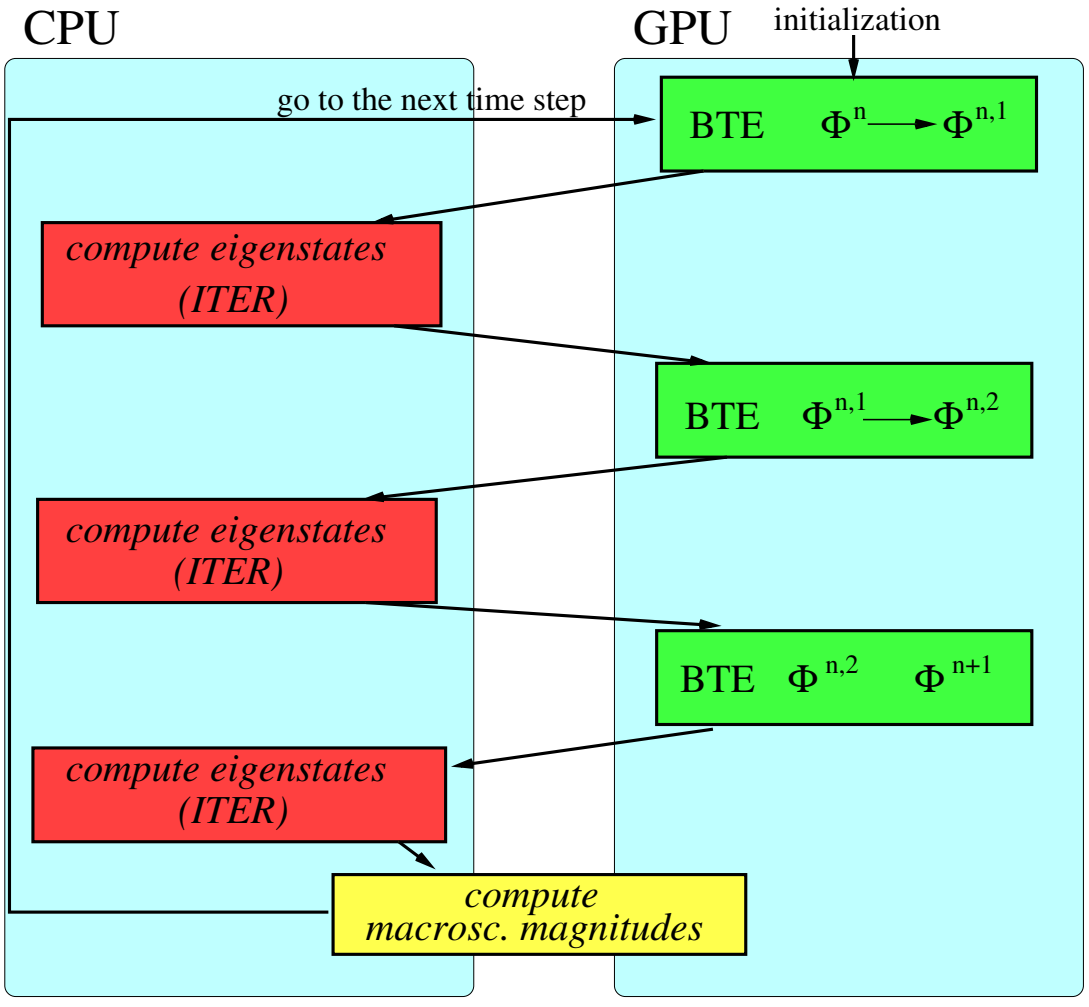
Up to some constants here omitted, the system rewrites in dimensionless form:

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

$$\begin{cases} \textbf{(Schrödinger)} & -\dfrac{\mathrm{d}}{\mathrm{d}z}\left[\dfrac{1}{m_{z,\nu}}\dfrac{\mathrm{d}\psi_{\nu,p}[V]}{\mathrm{d}z}\right] - (V + V_c)\,\psi_{\nu,p}[V] = \epsilon_{\nu,p}[V]\,\psi_{\nu,p}[V] \\ \textbf{(Poisson)} & -\mathrm{div}\left[\varepsilon_R \nabla V\right] = -\left(N[V] - N_D\right) \end{cases}$$

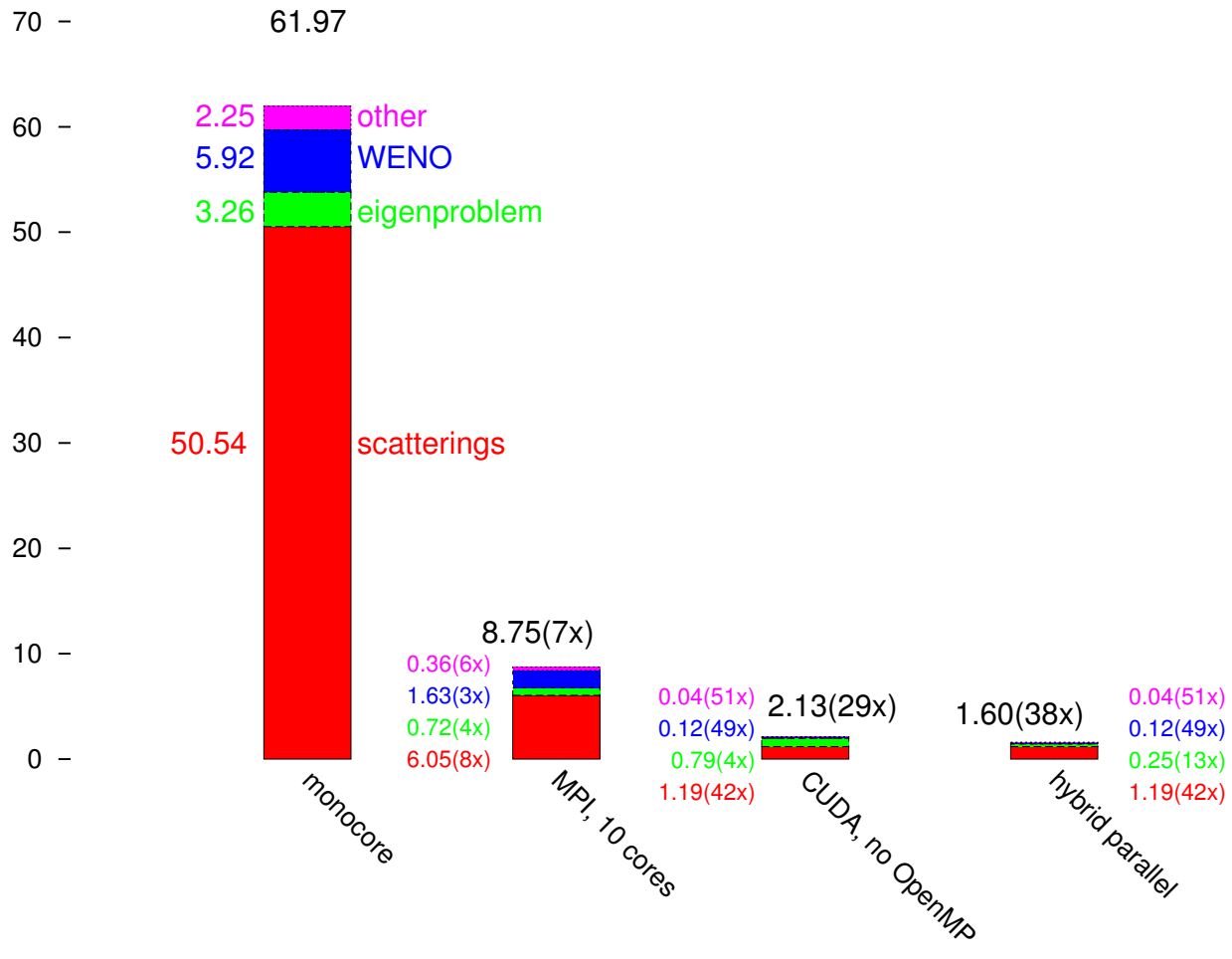
Outline

Overall design of the solver



Outline

Parallel performances on GPU

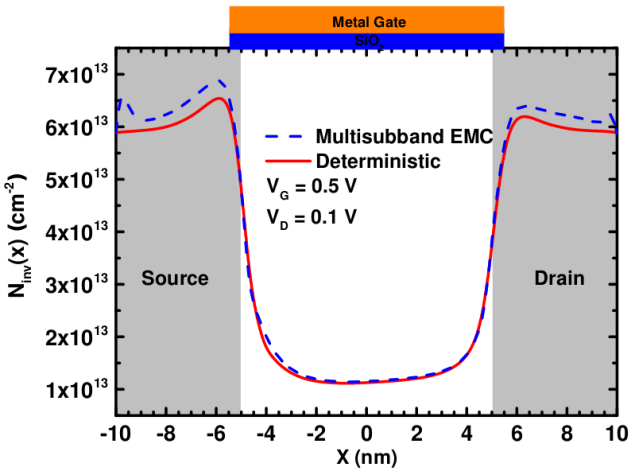


Parallel performances on GPU

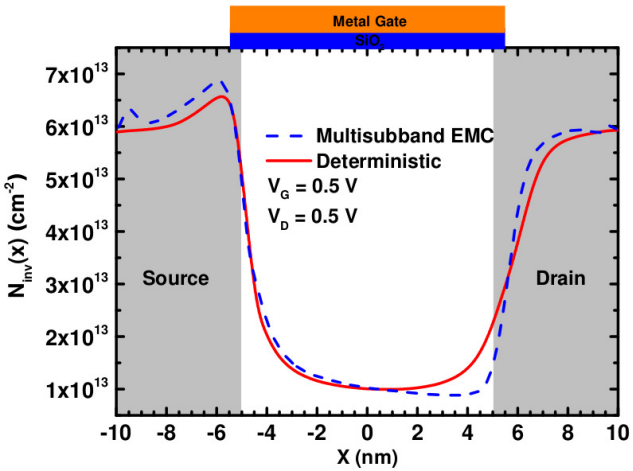
The bottleneck is, at the state of the art, the integration of the scattering operator.

Outline

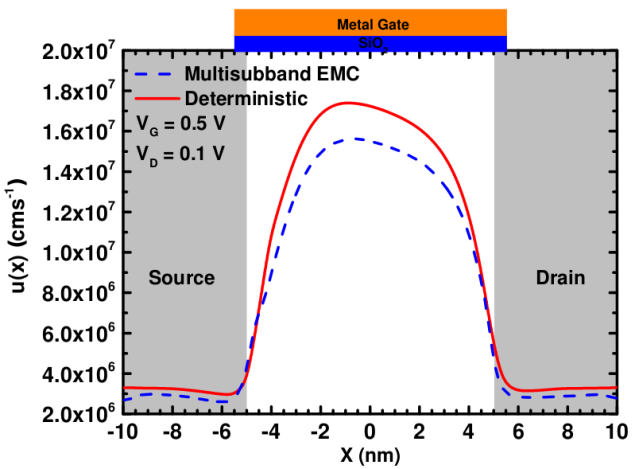
Comparison to Monte-Carlo



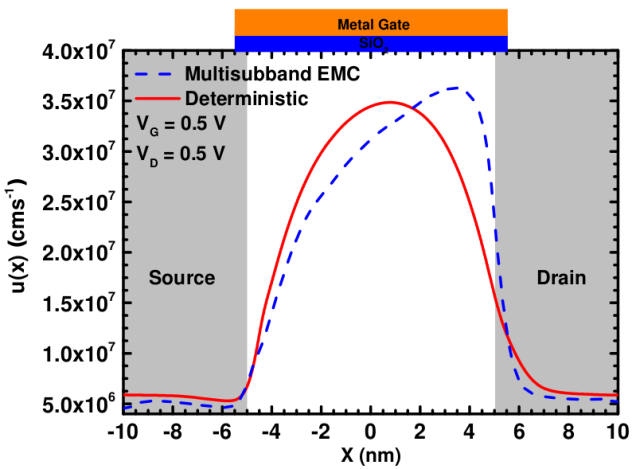
(a) For a $V_{\mathrm{D}} = 0.1$ V bias



(b) For a $V_{\mathrm{D}} = 0.5$ V bias

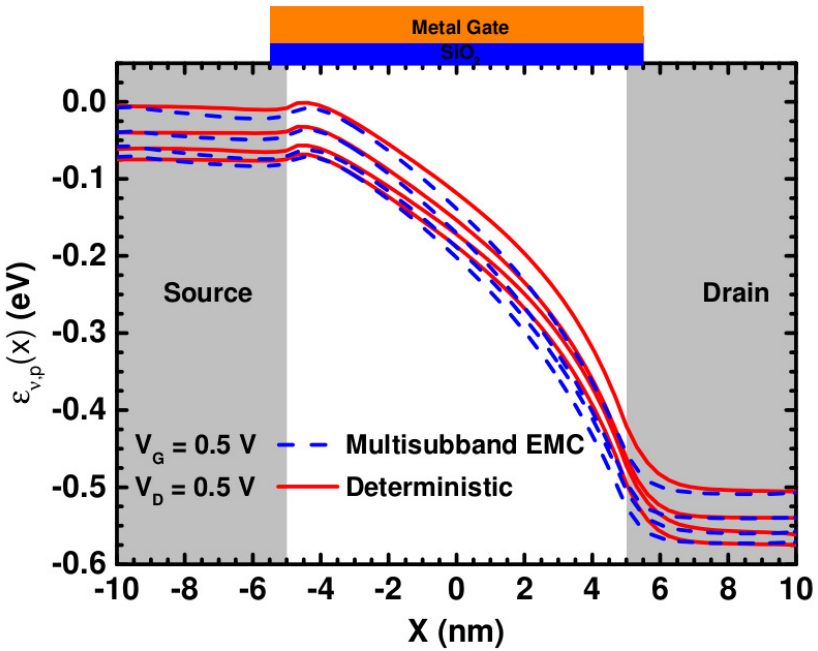


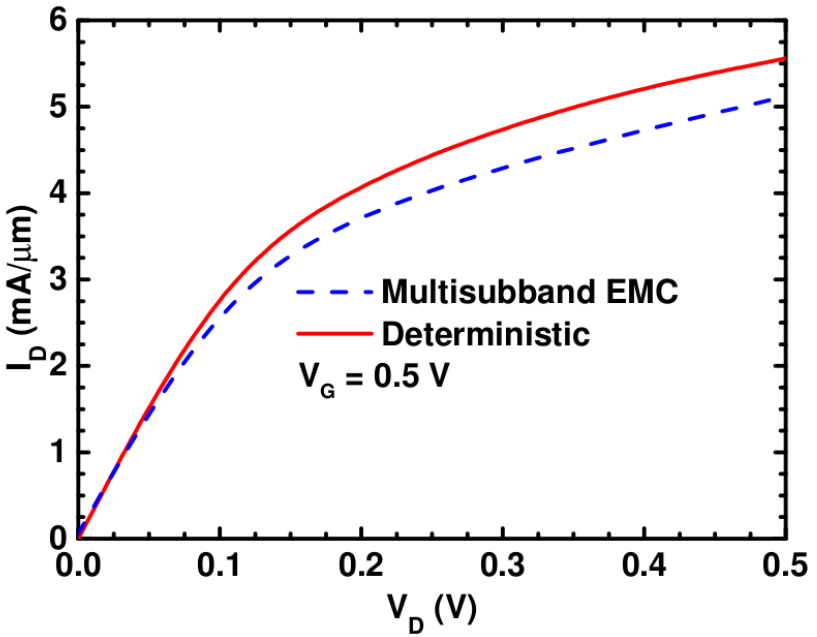
(c) For a $V_{\mathrm{D}} = 0.1$ V bias



(d) For a $V_{\mathrm{D}} = 0.5$ V bias

Comparison to Monte-Carlo





Comparison to Monte-Carlo

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