Coupling of Quantum and Electrothermal Effects in Semiconductor Device Simulation

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Outline of The Talk

1. **Motivations**
2. **Matematical Modeling Of Electrothermal Effects**
   - Classical ThEB Model
   - Reduced Model: SThEB
   - Quantum Correction
3. **Iterative Solution Algorithm**
4. **Discretization Method**
5. **Validation Of The QSThEB Model**
6. **Device Mutual Heating**
7. **Concluding Remarks**

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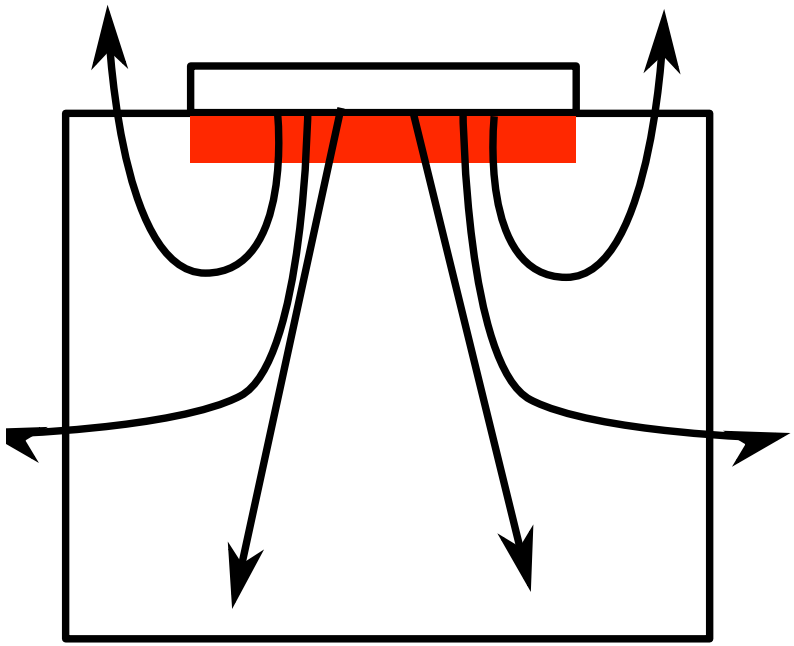
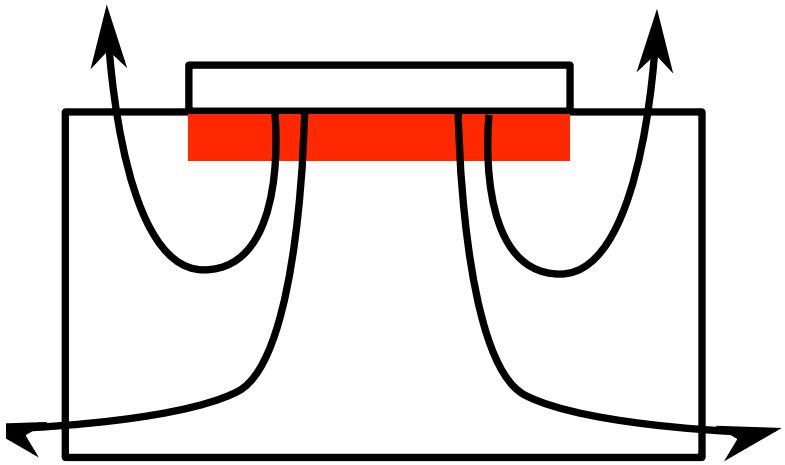
Electro-Thermal Effects

- **self-heating** and **mutual-heating** effects will gain increasing importance in the near future
- In emerging **SOI** and **thin-film** CMOS technologies single device cooling is going to become a serious limitation





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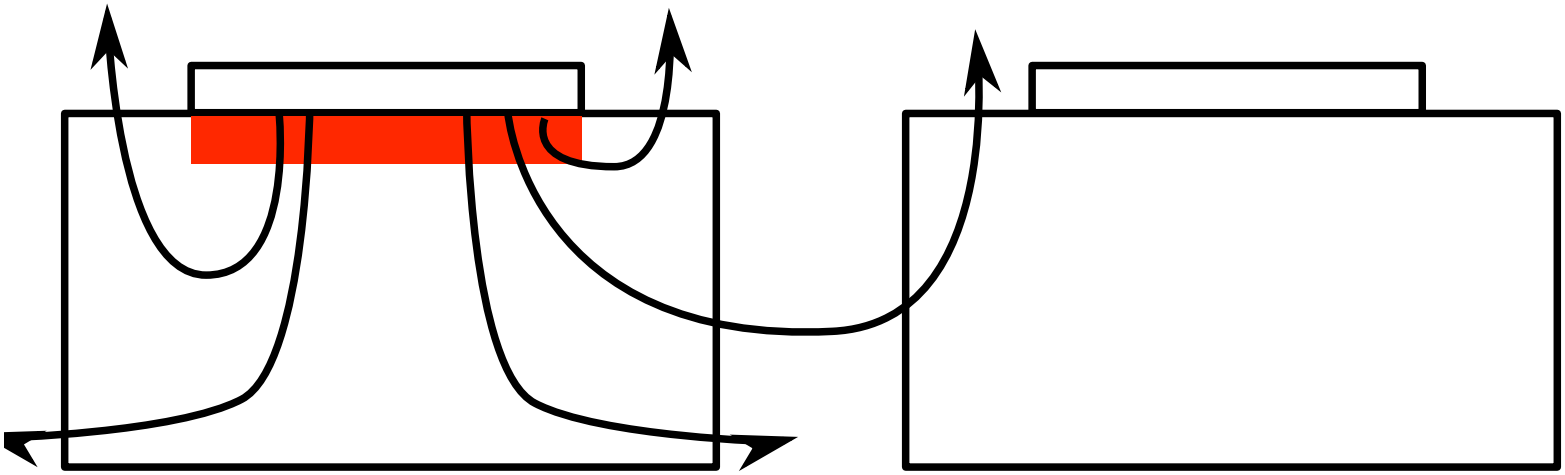
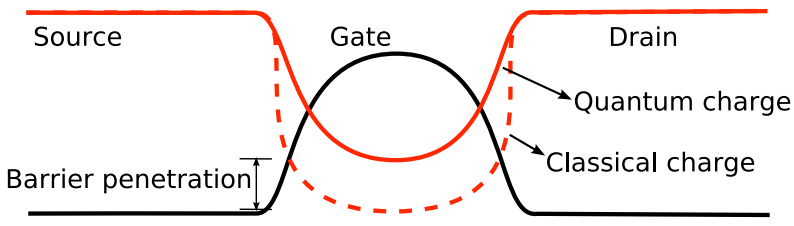
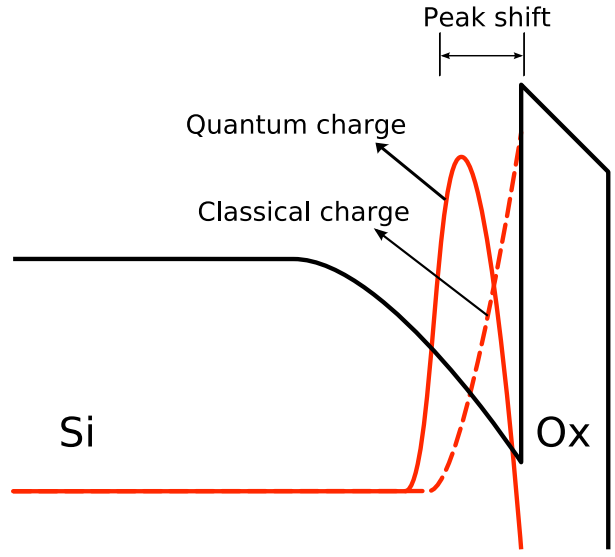


Quantum Effects

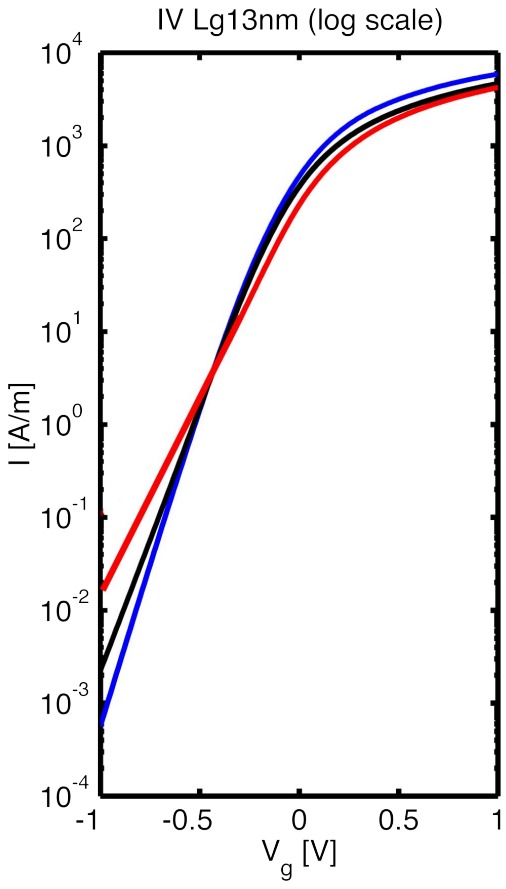
Quantum Electrostatic (QE) effects: source-to-drain tunneling, energy quantization effects due to strong confinement, equivalent oxide thickness

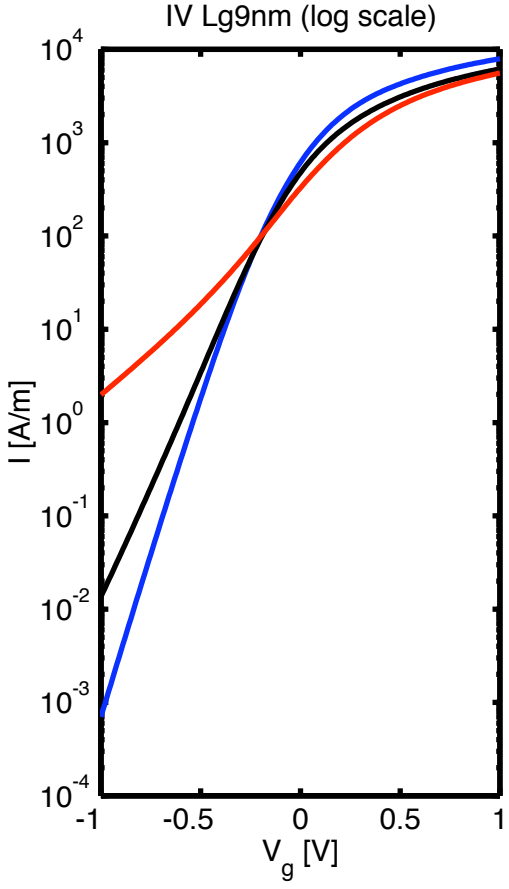




Quantum Effects

Due to **off-state leakage currents** caused by QE effects, **steady-state power consumption** will become an important factor





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The Thermo–Energy-Balance (ThEB) Model

$$
\begin{cases}
\mathrm{div}\mathbf{D} = q\left(p - n + N_D^+ - N_A^-\right) \\
\dfrac{\partial n}{\partial t} - \dfrac{1}{q}\mathrm{div}\mathbf{J}_n = -U \\
\dfrac{\partial p}{\partial t} + \dfrac{1}{q}\mathrm{div}\mathbf{J}_p = -U \\
\dfrac{\partial (n\, w_n)}{\partial t} + \mathrm{div}\mathbf{S}_n = \mathbf{E}\cdot\mathbf{J}_n - n\, w_n\, U + \left(\dfrac{\partial (n\, w_n)}{\partial t}\right)_{coll} \\
\dfrac{\partial (p\, w_p)}{\partial t} + \mathrm{div}\mathbf{S}_p = \mathbf{E}\cdot\mathbf{J}_p - p\, w_p\, U + \left(\dfrac{\partial (p\, w_p)}{\partial t}\right)_{coll} \\
\dfrac{\partial (\rho_L\, c_L\, T_L)}{\partial t} + \mathrm{div}\mathbf{S}_L = H_L.
\end{cases}
$$

[Baccarani et al., 1986-1993; Bosisio, 1996; Grasser, 1999; Medina, Pagani, S., 2006]

Constitutive Equations for Vector Fields

$$
\begin{cases}
\mathbf{D} = \varepsilon \mathbf{E} = -\varepsilon \, \boldsymbol{\nabla} \, \varphi \\
\mathbf{J}_n = -q \, \mu_n \, n \, \boldsymbol{\nabla} \left(\varphi - \dfrac{K_B \, T_n}{q} \right) + q \, D_n \, \boldsymbol{\nabla} \, n \\
\mathbf{J}_p = -q \, \mu_p \, p \, \boldsymbol{\nabla} \left(\varphi + \dfrac{K_B \, T_p}{q} \right) - q \, D_p \, \boldsymbol{\nabla} \, p \\
\mathbf{S}_n = -\dfrac{\mathbf{J}_n}{q} \left(w_n + K_B \, T_n \right) - \kappa_n \, \boldsymbol{\nabla} \, T_n \\
\mathbf{S}_p = \dfrac{\mathbf{J}_p}{q} \left(w_p + K_B \, T_p \right) - \kappa_p \, \boldsymbol{\nabla} \, T_p \\
\mathbf{S}_L = -\kappa_L \, \boldsymbol{\nabla} \, T_L
\end{cases}
$$

- **Quasi–static approximation** for the electric field
- **Generalized DD** laws for current densities and carrier energy flows
- **Fourier law** for lattice heat flow

Constitutive Equations for Scalars

$$D_\nu = \mu_\nu \left(K_B T_\nu / q\right) \qquad \nu = n, p$$

$$U = (p\, n - n_{eq}^2) F(n, p)$$

$$\kappa_\nu = 3/2 (K_B/q)^2 \sigma_\nu T_\nu, \qquad \kappa_L = \kappa_{L,0} \left(T_L / T_0\right)^{-4/3}$$

$$w_\nu = \left(3/2 K_B\, T_\nu\right),$$

$$\left(\frac{\partial \left(\nu\, w_\nu\right)}{\partial\, t}\right)_{coll} = -\nu \left(w_\nu - w_\nu^{eq}\right) / \tau_{w,\nu}$$

$$H_L = E_G\, U - \left(\frac{\partial (n\, w_n)}{\partial t}\right)_{coll} - \left(\frac{\partial (p\, w_p)}{\partial t}\right)_{coll}$$

- **Generalized** Einstein relations
- **Convective terms are neglected** in the energy density
- **Relaxation approximation** in the energy collision terms
- The last relation expresses the fact that the **system is closed**

Physical Simplifications and SThEB Model

To reduce the computational complexity of the ThEB model,

the carrier energy flow balance equations are dropped out by:

- neglecting energy outflow and recombination/generation
- assuming steady-state conditions
- enforcing the condition that the system is closed

$$\begin{cases} \mathrm{div}\mathbf{D} = \rho \\ \mathrm{div}\mathbf{J}_n - q\dfrac{\partial n}{\partial t} = qU \\ \mathrm{div}\mathbf{J}_p + q\dfrac{\partial p}{\partial t} = -qU \\ \dfrac{\partial W_L}{\partial t} + \mathrm{div}\mathbf{S}_L = H \end{cases}$$

Constitutive Equations

$$
\begin{cases}
\mathbf{J}_n = -q\,\mu_n\,n\,\boldsymbol{\nabla}\left(\varphi - \dfrac{K_B\,T_L}{q}\right) + q\,D_n\,\boldsymbol{\nabla}\,n \\
\mathbf{J}_p = -q\,\mu_p\,p\,\boldsymbol{\nabla}\left(\varphi + \dfrac{K_B\,T_L}{q}\right) - q\,D_p\,\boldsymbol{\nabla}\,p \\
D_{n,p} = \mu_{n,p}\dfrac{K_B\,T_L}{q} \\
H = \mathbf{J}\cdot\mathbf{E} + E_G\,U
\end{cases}
$$

- **Only one temperature** to describe non-isothermal conditions
- Heat source term:

1. Joule heat dissipation
2. Energy loss/gain to the lattice through rec./gen.

Post-Processing of Carrier Temperatures

Once the SThEB system is solved, carrier temperatures can be computed by post-processing

$$T_\nu = T_L \left(1 + \frac{\tau_{w_\nu} \, \mathbf{E} \cdot \mathbf{J}_\nu}{\frac{3}{2} K_B \, T_L \, \nu} \right) \qquad \nu = n, p.$$

Physical Interpretation

$$\boxed{\text{local increase of } T_\nu \text{ w.r.t. } T_L = \frac{\mathcal{E}_{Joule}}{\mathcal{E}_{Th,\nu}}}$$

- $\mathcal{E}_{Joule}$: energy density dissipated through Joule effect
- $\mathcal{E}_{Th,\nu}$: thermal energy density of electron/hole gas assumed in equilibrium with the lattice

First Order Quantum Correction

- Quantum correction to the electrostatic potential (cf. QCDD model general framework, [de Falco, Gatti, Lacaita, S., JCP 2005])

$$\varphi \qquad \rightarrow \qquad (\varphi + G_\nu),\ \nu = n, p$$

- Models for the correction term:
  - Improved Modified Local Density Approach [Jungermann et al. 2001]
  - Density-Gradient model [Ancona et al. 1989]
  - Direct solution of the Schrödinger equation [Pirovano et al 2002]
- Corrections to energy and energy fluxes are neglected (cf. [Romano, JCP 2007])

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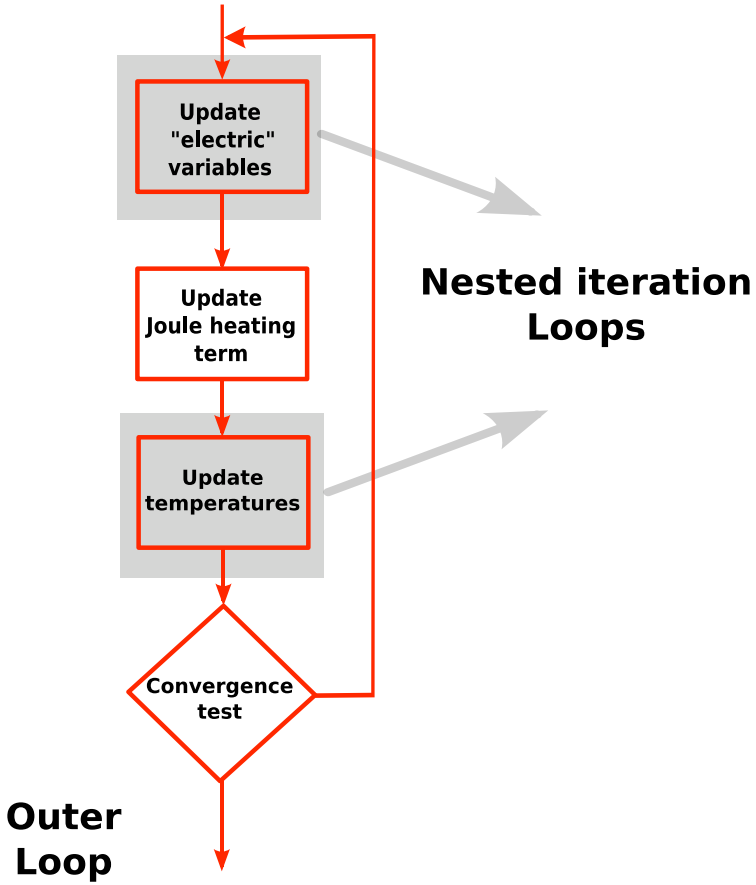
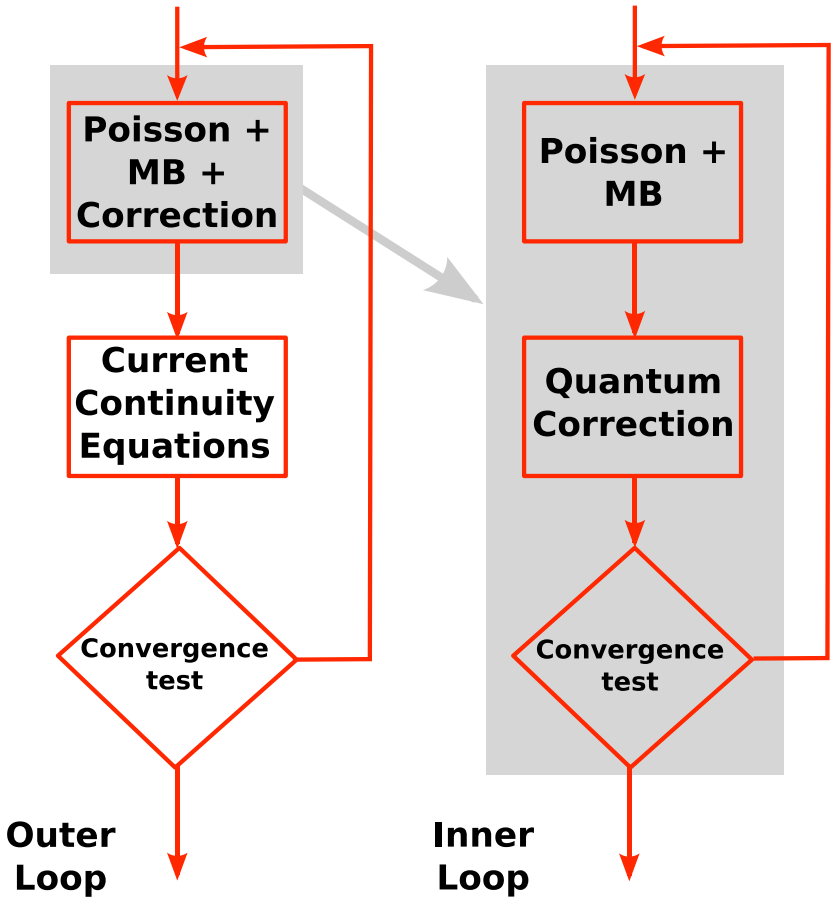
Outer Iteration Loop



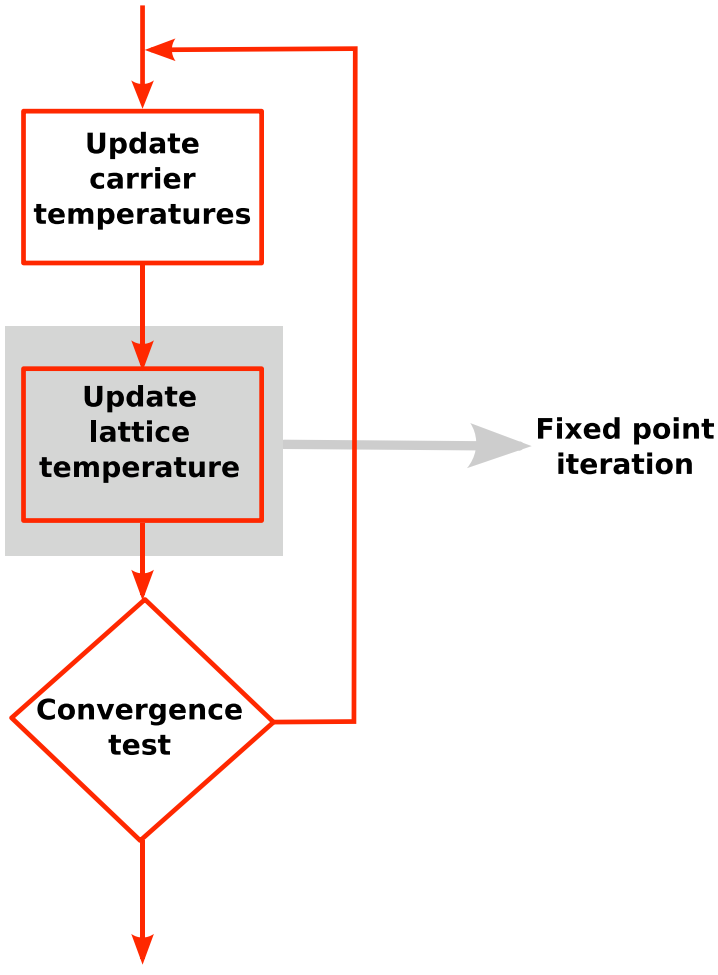
- Superior performance with respect to other approaches was demonstrated in [Baccarani et al. '96]
- Complete decoupling allows for high flexibility in implementing different models and discretization schemes
- Vector extrapolation techniques improve speed (RRE, Anderson)

Electric Iteration Loop



- Introduced in [de Falco, Gatti, Lacaita, S. 2005]
- Analysis in [de Falco, Jerome, S. 2007]

Thermal Iteration Loop



- If the simplified model is used, the first step can be skipped
- Iteration is needed because of the dependence $\kappa = \kappa(T)$

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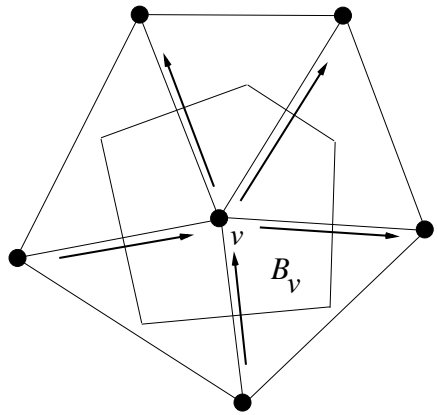
Discretization scheme



Diffusion-Advection-Reaction (DAR) Pb.:

$$\begin{cases} \mathcal{L}(u) = -\mathrm{div}\mathbf{F}(u) + c\,u = f \\ \mathbf{F}(u) = \alpha\,\gamma\,(\eta\,\boldsymbol{\nabla}\,u - \boldsymbol{\beta}\,u)\,, \end{cases}$$

- FVSG discretization scheme
- Flux conservation across the Voronoi cell associated with every node of $\mathcal{T}_h$
- $F_i^K = \alpha^K < \gamma\,\eta >_i^K < \eta >_i^K \dfrac{u_k\,B(\Delta\psi_i^K) - u_j\,B(-\Delta\psi_i^K)}{|e_i^K|}$,
- Weakly acute triangulation should be used in practical computations
- (Primal Mixed) Galerkin interpretation simplifies imposing complex transmission conditions at interfaces

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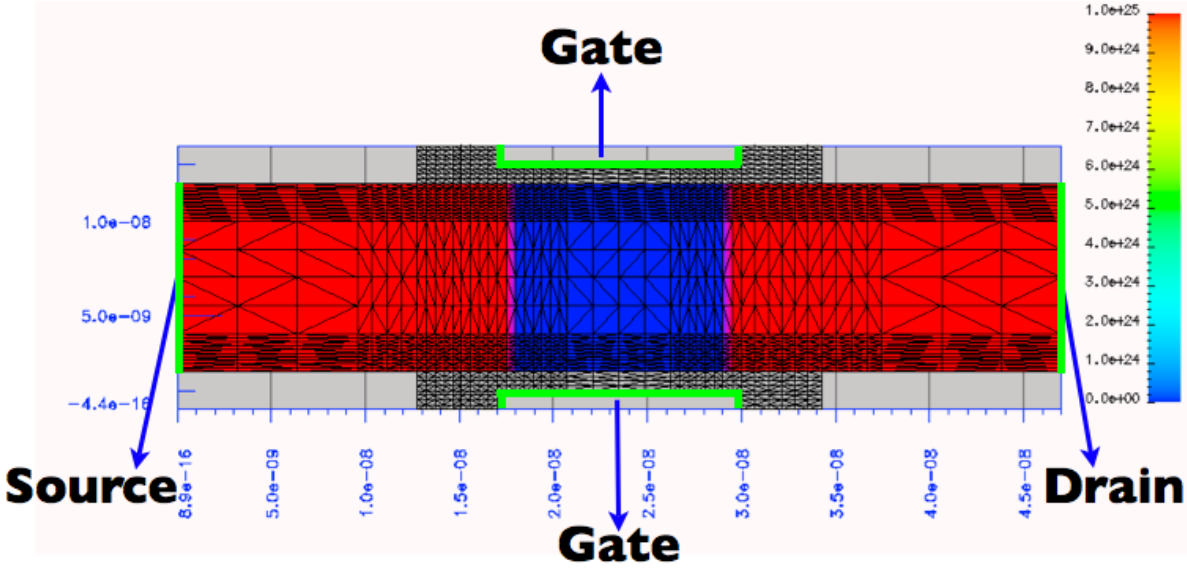
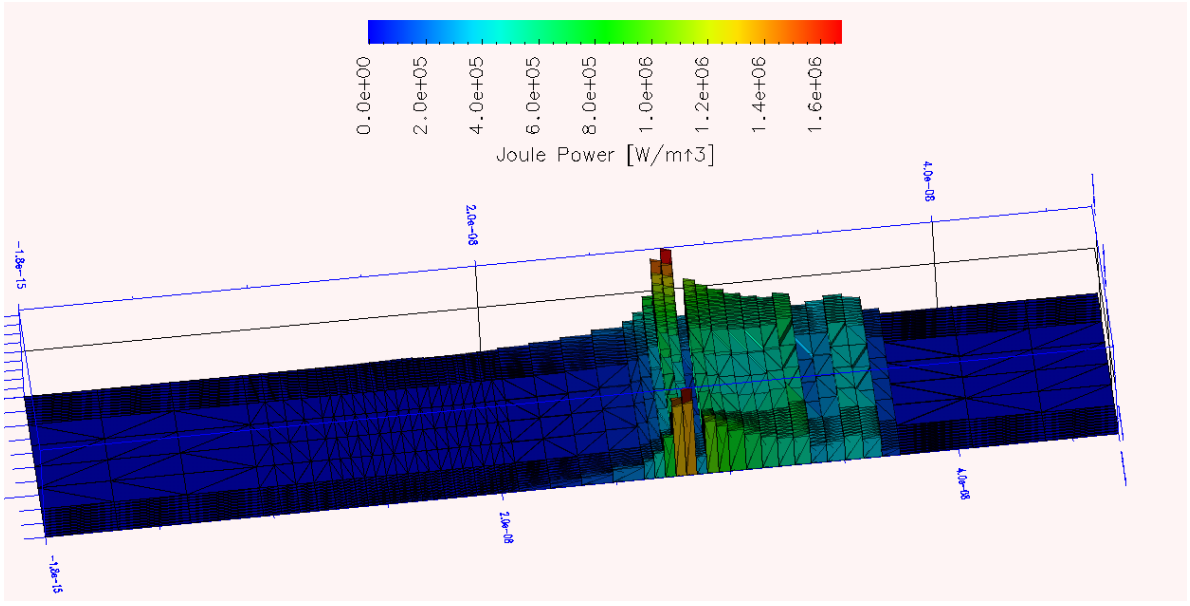
Double-Gate MOSFET



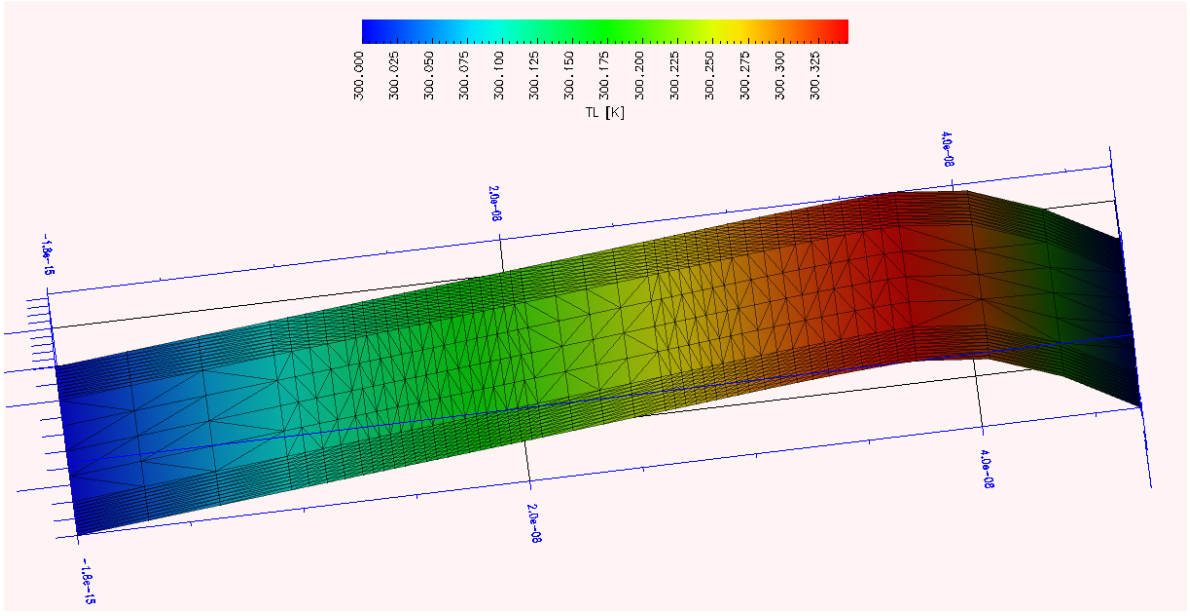
- Channel length $13nm$
- Source, Drain doping $10^{25} m^{-3}$
- Channel doping $10^{20} m^{-3}$

Double-Gate MOSFET (without QC)



- $V_{DS} = 0.5V$
- $V_{GS} = 0V$
- Joule power density $(\vec{J}_n + \vec{J}_p) \cdot \vec{E}$

Double-Gate MOSFET (without QC)



- $V_{DS} = 0.5V$
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- Lattice temperature T_L

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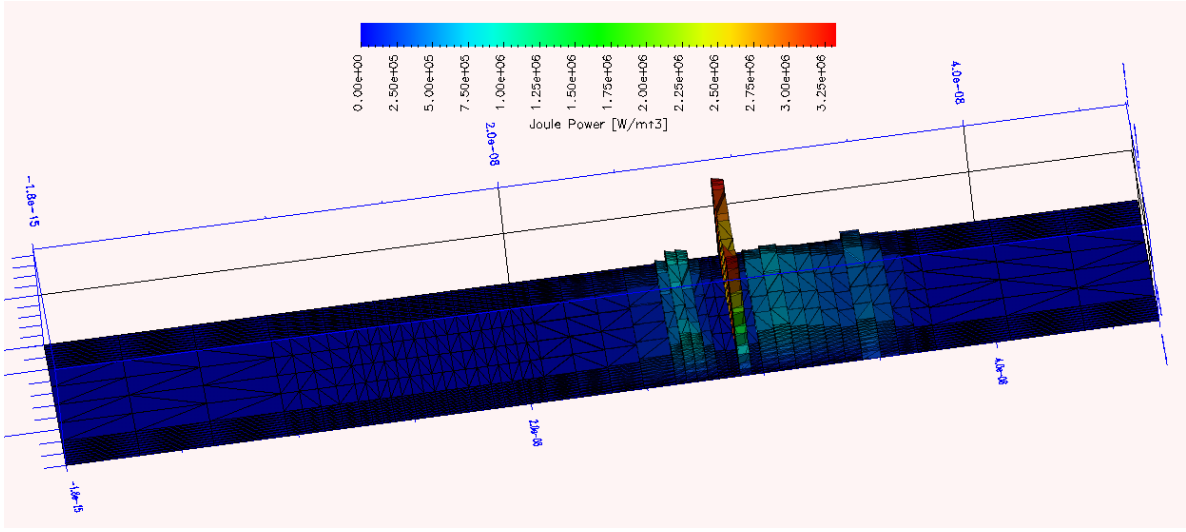

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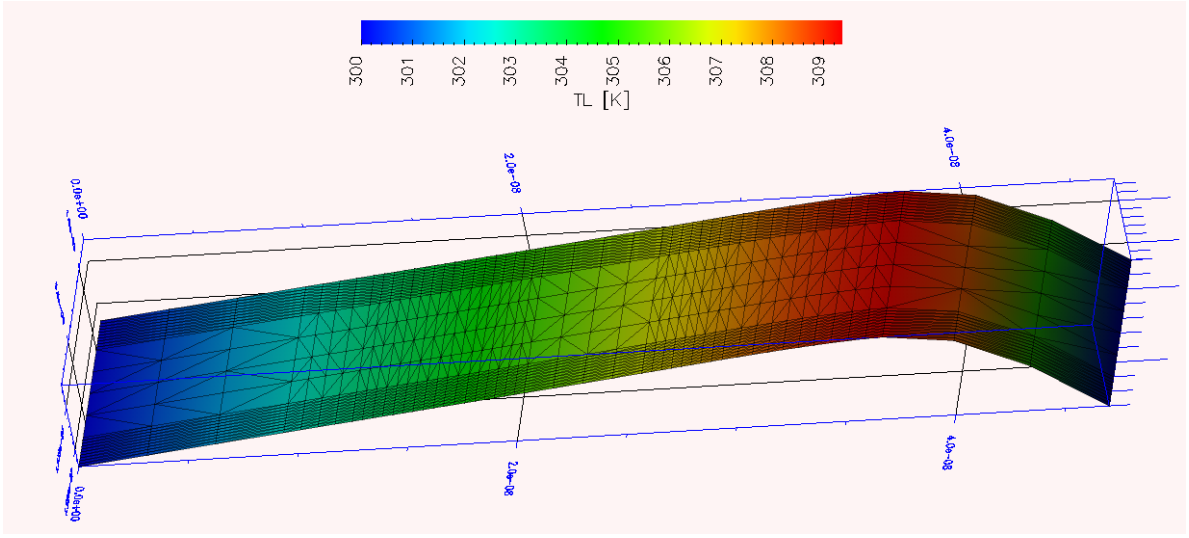

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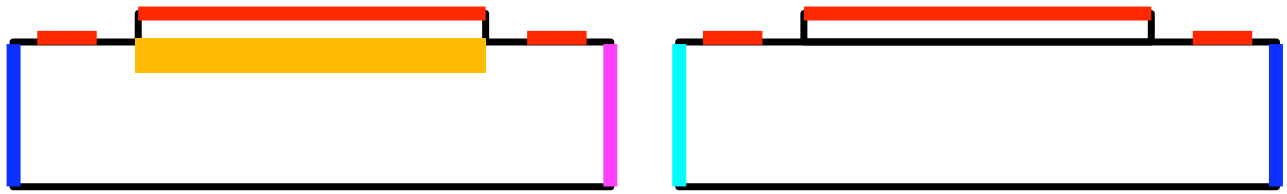
0D Thermal elements

- Dirichlet condition at the contacts implies an **infinite cooling capacity** which is unphysical
- A $0D$ model of heat flow through the contact can be defined via the **thermal resistance** $R_{th} \propto \kappa_{metal}^{-1} L$
- A $0D$ thermal resistance can also be used to take into account mutual heating among devices on the same CHIP (cf. [Medina, Pagani, S., 2006])
- More generally devices could be coupled via a **thermal network** [Grasser et al.]
- Details on FEM implementation of $0D$ coupling conditions in [Culpo, de Falco, Substructuring Methods for Coupled PDE/DAE Systems]

Mutual heating of devices integrated on the same CHIP



- Γ_r, Γ_s, Γ_{i1}, Γ_{i2}, Γ_n, Ω_P
- $-\frac{\theta(\vec{x})-T_0}{R_r} = H(\vec{x})$ on Γ_r
- $-\frac{\theta(\vec{x})-T_0}{R_s} = H(\vec{x})$ on Γ_s
- $P(\vec{x}) > 0$ in Ω_P
- Transmission conditions:
  - $H_1(\vec{x}) = -\left(\frac{1}{R_i}\right)\left(\theta_1(\vec{x}) - \langle\theta_2\rangle_{\Gamma_{i2}}\right)$ on Γ_{i1}
  - $H_2(\vec{x}) = -\left(\frac{1}{R_i}\right)\left(\theta_2(\vec{x}) - \langle\theta_1\rangle_{\Gamma_{i1}}\right)$ on Γ_{i1}
  - $\langle H_1\rangle_{\Gamma_{i1}} + \langle H_2\rangle_{\Gamma_{i2}} = 0$

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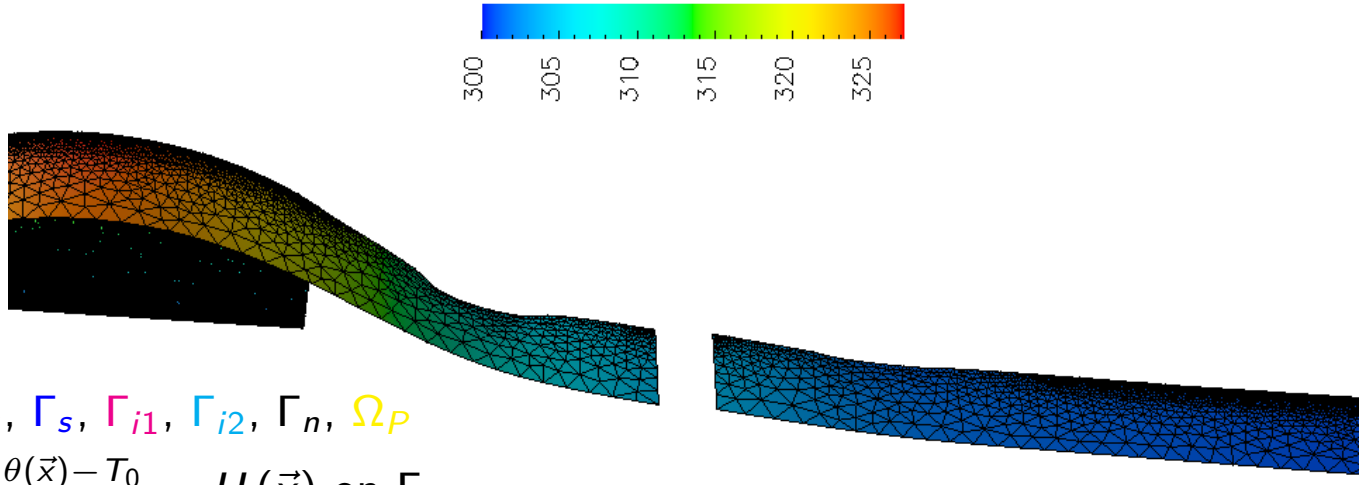

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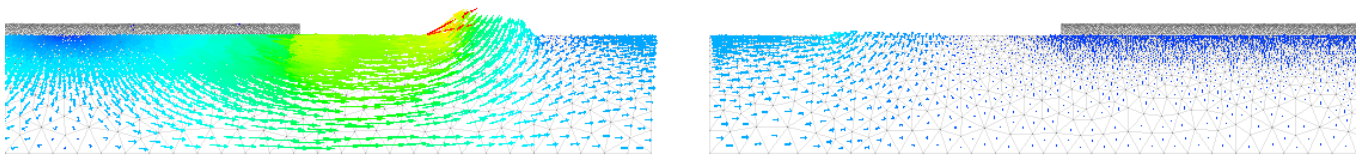

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Conclusions and Future Perspectives

Conclusions:

- A **Quantum Simplified Thermal Energy Balance (QSThEB)** model for a consistent description of **local self–heating and quantum effects** has been discussed
- An **Iterative Solution Map** for the QSThEB model has been developed within the framework of Gummel's decoupled algorithm
- A **Reduced-Order Thermal Coupling Model** has been proposed to allow heat flux exchange between neighbouring devices
- Models and computational techniques have been extensively validated on **realistic** devices under different working conditions

Future work:

- Development of a **parallel implementation** for the Domain-Decomposition iterative solution of the QSThEB model
- **3D simulations** (and corresponding 3D/0D coupling)