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Numerical coupling of electric circuit equations with the transient energy-transport equations for semiconductors

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1 Modelling

1.1 The energy-transport model for semiconductors

For semiconductor devices smaller than $1\mu m$ thermal effects get significant influence. The energy-transport (ET) model for semiconductors takes into account carrier heating. We consider the ET-model for electrons coupled to the drift-diffusion (DD) model for holes as minority carriers. The ET-model for electrons consists of conservation laws for electron density n and energy density $\epsilon = \frac{3}{2}nT$ with electron temperature T. These are coupled to Poisson's equation for the electrostatic potential. With electron current density J_n and energy current density J_ϵ the scaled transient ET-model reads

$$\lambda^2 \Delta V = n - p - C(x), \tag{1.1}$$

$$\partial_t n - \operatorname{div} J_n = -R, \tag{1.2}$$

$$\partial_t \epsilon - \operatorname{div} J_\epsilon = -J_n \nabla V + W(n,T) - \frac{3}{2}TR, \tag{1.3}$$

where p denotes the hole density and R is the recombination term. λ designates the scaled Debye-length and $C(x)$ the doping profile of the device. For the energy-relaxation term $W(n,T)$ we use the Fokker-Planck approximation

$$W = -\frac{3}{2}\frac{n(T-T_0)}{\tau_0} \tag{1.4}$$

with lattice temperature T_0 and energy relaxation time τ_0. Under the assumption of nondegenerated Boltzmann statistics and parabolic band structure the specifying current relations are given in the DD-formulation

$$J_n = \mu_n \left(\nabla n - \frac{n}{T}\nabla V\right), \quad J_\epsilon = \mu_n \left(\nabla \epsilon - \frac{\epsilon}{T}\nabla V\right). \tag{1.5}$$

Here μ_n denotes the electron mobility. The DD-model for holes reads

$$\partial_t p + \operatorname{div} J_p = -R, \quad J_p = -\mu_p \left(\nabla p + p\nabla V\right) \tag{1.6}$$

with hole mobility μ_p. For recombination we use the Shockley-Read-Hall approximation. The model is completed by initial and boundary values for n, p, V and T.

1.2 Coupling to circuit equations

For modelling a semiconductor device as part of an electric circuit we couple the ET-model with equations from modified nodal analysis (MNA), which consist of the Kirchhoff current law and specifying current-voltage characteristics of resistors, capacitors and inductors. The coupling between device and surrounding circuit happens through the current leaving the device and the potential in the circuit nodes adjacent to the device. The total current in the device consists of electron current, hole current and displacement current

$$J_{tot} = J_n + J_p + J_{disp} \quad \text{with} \quad J_{disp} = -\lambda^2 \left(\partial_t V\right)_x .$$

We denote by j_S the vector containing the current leaving all terminals except for one reference terminal and introduce the semiconductor incidence matrix A_S. Thus we get the coupled system for an electric circuit containing a semiconductor device connected to circuit nodes number i and j. It consists of the differetial-algebraic equation (DAE) achieved by MNA where the semiconductor current has been added

$$\begin{aligned} \frac{1}{\overline{t}} A_C \frac{dq(A_C^T e)}{dt} + A_R g(A_R^T e) + A_L i_L + A_V i_V + A_S j_S &= -A_I i_s, \\ \frac{1}{\overline{t}} \frac{d\Phi(i_L)}{dt} - A_L^T e &= 0, \\ A_V^T e &= v_s, \end{aligned}$$

with incidence matrices A_α and current in the corresponding branches i_α. Charge, conductivity and flux are denoted by q, g and Φ. Voltage sources and current sources are denoted by v_s and i_s. We add the equations describing the coupling via the semiconductor current

$$j_S^D - \lambda^2 V_x = 0 \quad \text{and} \quad j_S - \beta \left[J_n + J_p - \partial_t j_S^D\right]_{x=0} = 0,$$

and the equations for the semiconductor model (1.1) - (1.6). β and $\overline{t}$ denote scaling constants. The boundary conditions for the potential V read

$$V|_{x=0} = e_i + V_{bi}|_{x=0} \quad \text{and} \quad V|_{x=1} = e_j + V_{bi}|_{x=1},$$

where V_{bi} denotes the built-in potential of the device. Thus the complete system is described by a partial differential-algebraic equation (PDAE). It will be completed by boundary and initial conditions and has to be solved for $e, i_L, i_V, n, \epsilon, p, V$.

2 Numerical discretisation

For numerical solution we firstly discretise in time by use of the 2 stage backward difference formula BDF2. We consider the onedimensional model for the semiconductor device with the partition $0 = x_0 < x_1 < ... < x_N = 1$ with $I_i = (x_{i-1}, x_i)$ and $h = x_i - x_{i-1}$ for $i = 1, ..., N$. For space discretisation of Poisson's equation we use a P1 finite element scheme. For (1.2) and (1.3) after time discretisation we have to solve a boundary value problem in each timestep of type

$$-J_x + \sigma g = f \tag{2.1}$$

with $g = \mu_n n$ or $g = \mu_n \epsilon$, respectively. For space discretisation we employ the mixed hybrid finite element approach introduced by Marini and Pietra as it ensures current continuity across interelement boundaries and positivity of the electron density. We introduce the finite dimensional spaces:

$$\begin{aligned} V_h &= \left\{\psi \in L^2(\Omega) : \psi(x) = a_i + b_i P_i(x) \text{ in } I_i, i = 1, ..., N\right\}, \\ W_h &= \left\{\phi \in L^2(\Omega) : \phi \text{ is constant in } I_i, i = 1, ..., N\right\}, \\ \Lambda_{h,\zeta} &= \{\xi \text{ is defined at the nodes } x_0, ...x_N : \xi(x_0) = \zeta(0), \xi(x_N) = \zeta(1)\}, \end{aligned}$$

with a degree 2 polynomial $P_i(x)$. With these we get for the approximation J^h for the current, the piecewise constant approximation for the density $\overline{g}^h$ and the approximation for the density in the nodes g^h the weak hybrid mixed formulation

Find $J^h \in V_h, \overline{g}^h \in W_h, g^h \in \Lambda_{h,g_D}$ such that:

$$\sum_{i=1}^{N} \left(\int_{I_i} K_i J^h \psi dx + \int_{I_i} S_i \overline{g}^h \psi_x dx - \left[e^{-\frac{V}{T}} g^h \psi \right]_{x_{i-1}}^{x_i} \right) = 0, \tag{2.2}$$

$$\sum_{i=1}^{N} \left(- \int_{I_i} J_x^h \phi dx + \int_{I_i} \sigma \overline{g}^h \phi dx \right) - \sum_{i=1}^{N} \left(\int_{I_i} f \phi dx \right) = 0, \tag{2.3}$$

$$\sum_{i=1}^{N} \left(\left[\xi J^h \right]_{x_{i-1}}^{x_i} \right) = 0, \tag{2.4}$$

for all $\psi \in V_h, \phi \in W_h, \xi \in \Lambda_{h,0}$, with K_i and S_i as constant approximations for $\exp(\frac{-V}{T})$. Equation (2.2) is the weak form of (1.5) after exponential fitting and (2.4) is the weak formulation of the current continuity. This can be written as

$$\begin{pmatrix} A & \tilde{B}^T & -\tilde{C}^T \\ -B & D & 0 \\ C & 0 & 0 \end{pmatrix} \begin{pmatrix} J^h \\ \overline{g}^h \\ g^h \end{pmatrix} = \begin{pmatrix} 0 \\ F \\ 0 \end{pmatrix}$$

with matrices A, B, C, D, which are (mixed) stiffness matrices to the spaces defined above. A static condensation procedure can be employed to eliminate J^h and $\overline{g}^h$. This finally leads to the system

$$Mg^h = G, \tag{2.5}$$

where M is a tridiagonal M-matrix. For the electron equation (1.2) G is positive for adequate time step size. The eliminated variabes J^h and $\overline{g}^h$ can be computed afterwards from g^h.

After time and space discretisation we solve the complete discretised system by a quasi Newton-method.

As numerical example we will consider a simple test circuit containing a pn-diode. We perform simulations for operational voltage with a frequency of 1GHz and 10GHz, respectively. Furtheron the results will be compared to those achieved by usage of the transient DD-model and the stationary ET-model.

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test circuit