Numerical Coupling of Circuit Equations with Energy-Transport equations

M. Brunk and A. Jüngel
Johannes Gutenberg-Universität Mainz
55099 Mainz, Germany
brunk@math.uni-mainz.de

***Abstract*— Due to miniaturization of integrated circuits it becomes preferable to simulate electric circuits including distributed models of semiconductors. We present the coupling of the transient energy-transport equations with circuit modelling equations achieved by modified nodal analysis (MNA). The coupled system is space discretised by use of an exponential fitting mixed hybrid finite element method in one space dimension and time discretised by use of the 2 step backward difference formula (BDF2). Numerical simulations are performed for a rectifier circuit containing four pn-diodes as semiconductor devices.**

Keywords—Mixed finite elements, exponential fitting, Energy-Transport, semiconductors, modified nodal analysis, electric circuits

I. Semiconductor Device Modelling

For semiconductor devices smaller than $1\mu m$ thermal effects get significant influence. The energy-transport model for semiconductors takes into account carrier heating. We consider the energy-transport model for electrons coupled to the drift-diffusion model for holes. As they occur as minority carriers the drift-diffusion model provides satisfying accuracy. The energy-transport 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 energy-transport model reads

$$\lambda^2 \Delta V = n - p - C(x), \tag{1}$$

$$\partial_t n - \operatorname{div} J_n = -R, \tag{2}$$

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

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

$$W = -\frac{3}{2}\frac{n(T-T_0)}{\tau_0} \tag{4}$$

with lattice temperature T_0 and energy relaxation time τ_0. Under the assumption of non degenerated Boltzmann statistics for electron density and parabolic band structure the specifying current relations are given in the drift-diffusion formulation

$$J_n = \mu_n \left(\nabla n - \frac{n}{T}\nabla V\right), \quad J_\epsilon = \mu_n \left(\nabla \epsilon - \frac{\epsilon}{T}\nabla V\right) \tag{5}$$

as introduced in [1]. Here μ_n denotes the electron mobility. The drift-diffusion model for holes reads

$$\partial_t p + \operatorname{div} J_p = -R, \quad J_p = -\mu_p \left(\nabla p + p \nabla V\right) \tag{6}$$

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.

In one-dimensional case we consider the interval $I = [0,1]$ 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 $i = 1, ..., N$. We firstly discretise in time by use of the 2 stage backward difference formula BDF2. For space discretisation of Poisson's equation we use a P1 finite element scheme. For (2) and (3) after time discretisation we have to solve a boundary value problem in each time step of type

$$-J_x + \sigma g = f \tag{7}$$

with $g = \mu_n n$ or $g = \mu_n \epsilon$, respectively. For space discretisation we employ the mixed hybrid finite element approach introduced in [2] as it ensures current continuity across interelement boundaries and positivity of the electron density.

We introduce the finite dimensional spaces:

$$V_h = \left\{\psi \in L^2(\Omega) : \psi(x) = a_i + b_i P_i(x) \text{ in } I_i, i = 1, ..., N\right\},$$

$$W_h = \left\{\phi \in L^2(\Omega) : \phi \text{ is constant in } I_i, i = 1, ..., N\right\},$$

$$\Lambda_{h,\zeta} = \{\xi \text{ is defined at the nodes } x_0, ...x_N : \xi(x_0) = \zeta(0), \xi(x_N) = \zeta(1)\}.$$

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 mixed hybrid formulation

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

$$\sum_{i=1}^{N} \left(\int_{I_i} K_i J^h \psi dx + \int_{I_i} S_i \overline{g}^h \psi_x dx - \left[e^{-\frac{V}{T}} g^h \psi \right]_{x_{i-1}}^{x_i} \right) = 0, \tag{8}$$

$$\sum_{i=1}^{N} \left(-\int_{I_i} J_x^h \phi dx + \int_{I_i} \sigma \overline{g}^h \phi dx \right) - \sum_{i=1}^{N} \left(\int_{I_i} f \phi dx \right) = 0, \tag{9}$$

$$\sum_{i=1}^{N} \left(\left[\xi J^h \right]_{x_{i-1}}^{x_i} \right) = 0, \tag{10}$$

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 (8) is

the weak form of (5) after exponential fitting and (10) 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

$$Mg^h = G, \tag{11}$$

where M is a tridiagonal M-matrix. For the electron equation (2) G is positive for adequate time step size. The eliminated variables J^h and $\overline{g}^h$ can be computed afterwards from g^h.

II. Coupling to Circuit Equations

For modelling a semiconductor device as part of an electric circuit we couple the energy-transport 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. This determines the boundary values for the potential in the device. If terminal k of the device (denoted by Γ_k) is connected to circuit node number i we get

$$V(t) = e_i(t) + V_{bi}|_{\Gamma_k} \qquad \text{on } \Gamma_k, \tag{12}$$

where e_i denotes the potential in the circuit node and V_{bi} the built in potential of the device. The total current in the device consists of electron current, hole current and displacement current

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

Denoting by j_S the vector containing the current leaving all terminals beside one reference terminal and introducing the semiconductor incidence matrix A_S as introduced in [3], 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 MNA-equations 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

$$\begin{aligned} j_S^D - \lambda^2 V_x &= 0, \\ j_S - \beta \left[J_n + J_p - \partial_t j_S^D \right]_{x=0} &= 0, \end{aligned}$$

and the equations for the semiconductor model (1) - (6). β and $\overline{t}$ denote scaling constants. The boundary conditions for the potential V read

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

The system will be completed by boundary and initial conditions and has to be solved for $e, i_L, i_V, n, \epsilon, p, V$.

III. Numerical Solution

For solving the complete system we proceed as we do for the device simulation. Firstly we employ time discretisation. Thereafter we proceed with space-discretisation including static condensation for electron, energy and hole equations. For the spatial derivative of V we use a simple difference quotient.

The finally achieved system is solved by use of full Newton method. For the temperature that is given via the piecewise constant approximation

$$\overline{T} = \frac{2}{3} \frac{\overline{\epsilon}}{\overline{n}} \tag{13}$$

we start with values at the previous time step and update according to (13) during Newton method only if the semiconductor variables $(n, \epsilon, p, V)^T$ between two iterations differ less than the potentially updated temperature from the old one, what for we use the test

$$\|(n, \epsilon, p, V)^T - (n, \epsilon, p, V)^T_{old}\|_2 \leq \max\left(10^{-6}, 0.01 \|T_{new} - T\|_2^{0.8}\right).$$

Here the variables denote the vectors containing the coefficients for the corresponding ansatz functions.

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. Further on the results will be compared to those achieved by usage of the transient drift-diffusion model and the stationary energy-transport model.

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