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# D1.8 Public Report (b) on Simulation methods for coupled problems

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## **Abstract**

This document contains the Public Report on the simulation of coupled problems in the area of electromagnetic field and circuit simulation. The in-house circuit simulators MECS (HUB) and LinzFrame (FHO) were coupled with the device/electro-magnetic field solver devEM from Magwel (MAG), for which as well netlist extraction techniques were proposed (TUD). Since electronic components behave both linear and nonlinear, two interfaces were established. The former include most passive devices and on-chip inductors, transmission lines, baluns, MEMS etc. The latter include semiconductor devices, memristors etc. The devEM simulator provides the space discretization of the 3D device whereas the circuit simulators MECS and LinzFrame provide the models for lumped devices (e.g. Spice models, BSIMxxx, Simkit etc.) and the numerical tools for time (transient) and multirate integration as well as linear and nonlinear solvers.

## Introduction

This document covers the R&D activities in WP1 and mainly the tasks T1.1 "Coupled EM-Device-Circuit and coupled EM-Heat Simulation" and T1.2 "Multirate methods EM-Device-Circuit Simulation and electro-thermal power switches". Moreover, the tasks cover the couplings between the device/EM simulators devEM and PTM-ET from partner MAGWEL (MAG) with the circuit simulators MECS from Humboldt University (HUB) and LinzFrame from FHO and SPICE netlist export from TUD. The MECS and LinzFrame simulators, respectively, serve as master and the devEM simulator correspondingly as slave. The latter performs the numeric space discretization of the EM/field equations, whereas MECS and LinzFrame provide the lumped device models for the surrounding circuit and the numerical simulation engines. The netlist extraction case is similar, however, there is no interaction after space discretization.

The numerical simulation tools comprise standard techniques such as AC, DC and transient, based on the well-known BDF techniques with variable step size control and moreover novel methods such as transient analysis based on spline/wavelet approximations and multirate methods for radio frequency circuits. Two interfaces for linear devices, such as capacitors, inductors, baluns, transmission lines etc., and for semiconductors were developed. For the former the time varying magnetic fields are essential for their functionality whereas for the latter they can be ignored (when no special devices such as semiconductor Hall sensors are simulated). Magnetic fields are captured by the vector potentials. Their time variations give rise to induced electric fields. However in semiconductors the induced electric field is negligible since the rate of change of the magnetic field is weak. This is because the conductivity in semiconductors is relatively low in comparison with metals and, moreover, the typical distances at the nanoscale are too small to give rise to an appreciable voltage drop. Hence, the magnetic field contributions can be usually ignored in semiconductors, leading to much smaller systems of equations. Moreover linear devices must be evaluated through the simulator interface only once which simplifies the coupling.

We presuppose basic knowledge on Maxwell's equations and semiconductor device modeling.

## 1 3D modeling of devices

### 1.1 Maxwell's equation

The four Maxwell's equations read

$\nabla \times \mathbf{E} = -\dot{\mathbf{B}}$	Induction law, Maxwell-Faraday's law
$\nabla \times \mathbf{H} = \mathbf{J} + \dot{\mathbf{D}}$	Maxwell-Ampère's law
$\nabla \cdot \mathbf{D} = \rho$	Gauss' law
$\nabla \cdot \mathbf{B} = 0$	Gauss' law for magnetism

where  $\mathbf{E}$ ,  $\mathbf{D}$  are the electric field strength and the displacement, and  $\mathbf{H}$ ,  $\mathbf{B}$  the magnetic field strength and induction, respectively. Moreover  $\rho$  and  $\mathbf{J}$  are the electric charge density and current density, respectively. A dot on a variable denotes the partial derivative with respect to time :  $\dot{X} = \partial_t X$ . From Maxwell's equation one obtains the continuity law

$$\nabla \cdot \mathbf{J} + \dot{\rho} = 0 \quad \text{continuity law} \quad (1)$$

In what follows we assume linear isotropic materials, i.e.,

$$\begin{aligned}\mathbf{D} &= \epsilon \mathbf{E} \\ \mathbf{B} &= \mu \mathbf{H}\end{aligned}\quad (2)$$

where  $\epsilon$  is the dielectric constant and  $\mu$  the permeability. It should be noted that materials of different types can be stacked or blocks of different materials can be placed next to each other. This results into abrupt jumps in the overall permittivity  $\epsilon$  and permeability  $\mu$ . However, generally we assume that the parameters depend on the space coordinate. Magwel's simulator devEM employs as unknowns the scalar potential  $\mathbf{E} = -(\nabla V + \dot{\mathbf{A}})$  and vector potentials  $\mathbf{B} = \nabla \times \mathbf{A}$ . To avoid second order partial differential equations (PDEs) in time, one may introduce the so called quasi-canonical momentum  $\mathbf{\Pi} = \dot{\mathbf{A}} = \partial_t \mathbf{A}$ .

## 1.2 Maxwell's equations and full 3D device models

### 1.2.1 Maxwell's equation in metals

With the Ohmic law  $\mathbf{J} = \sigma \mathbf{E}$ ,  $\mathbf{D} = \epsilon \mathbf{E}$  and the Maxwell-Ampère law one obtains

$$\frac{1}{\mu} \nabla \times \nabla \times \mathbf{A} = \frac{1}{\mu} (\nabla \nabla \cdot \mathbf{A} - \Delta \mathbf{A}) = -\sigma (\nabla V + \mathbf{\Pi}) - \epsilon \frac{\partial}{\partial t} (\nabla V + \mathbf{\Pi}) \quad (3)$$

From the continuity law (1) we get a second equation

$$-\nabla \cdot \mathbf{J} - \dot{\rho} = -\nabla \cdot \mathbf{J} - \nabla \cdot \dot{\mathbf{D}} = \sigma \nabla \cdot (\nabla V + \mathbf{\Pi}) + \epsilon \frac{\partial}{\partial t} (\nabla \cdot (\nabla V + \mathbf{\Pi})) = 0 \quad (4)$$

From the equations (3) and (4) one obtains 4 equations for the scalar and vector potentials ( $V, \mathbf{A}$ ).

### 1.2.2 Maxwell's equations in isolators

Since in ideal isolators  $\mathbf{J} = 0$  and  $\rho = 0$  is valid and moreover linearity of the materials can be assumed, i.e.,  $\mathbf{D} = \epsilon \mathbf{E}$  and  $\mathbf{B} = \mu \mathbf{H}$ , we obtain with  $\nabla \cdot \mathbf{D} = 0$

$$\begin{aligned}\epsilon \nabla \cdot (\nabla V + \mathbf{\Pi}) &= 0 \\ \frac{1}{\mu} \nabla \times \nabla \times \mathbf{A} &= \frac{1}{\mu} (\nabla \nabla \cdot \mathbf{A} - \Delta \mathbf{A}) = -\epsilon \frac{\partial}{\partial t} (\nabla V + \mathbf{\Pi})\end{aligned}\quad (5)$$

From the equations (5) one obtains 4 equations for the scalar and vector potentials ( $V, \mathbf{A}$ ).

## 1.3 Maxwell's equations in semiconductors

As already discussed above, the induction can be neglected in most cases, i.e.,  $\mathbf{\Pi} \approx 0$ . However, we write the equations here without simplification. From Gauss' law we get

$$-\epsilon \nabla \cdot (\nabla V + \mathbf{\Pi}) = \rho, \quad \rho = q(p - n + N_D - N_A) \quad (6)$$

where  $n, p$  are the concentrations of free electrons/holes, respectively, and  $N_D, N_A$  the donator/exceptor concentrations. From the Maxwell-Ampère law one obtains

$$\frac{1}{\mu} \nabla \times \nabla \times \mathbf{A} = \mathbf{J}_p + \mathbf{J}_n - \epsilon \frac{\partial}{\partial t} (\nabla V + \mathbf{\Pi}) \quad (7)$$

where  $\mathbf{J}_n$ ,  $\mathbf{J}_p$  are the currents densities of electrons/holes, respectively. The current densities of the electrons  $\mathbf{J}_n$  and holes  $\mathbf{J}_p$  are given by

$$\begin{aligned}\mathbf{J}_n &= -q\mu_n \left( n (\nabla V + \mathbf{\Pi}) - \frac{kT}{q} \cdot \nabla n \right) \\ \mathbf{J}_p &= -q\mu_p \left( p (\nabla V + \mathbf{\Pi}) + \frac{kT}{q} \cdot \nabla p \right)\end{aligned}\quad (8)$$

Herein  $q$  is the elementary charge,  $\mu_n$ ,  $\mu_p$  the mobilities of electrons and holes,  $k$  the Boltzmann constant and  $T$  the absolute temperature. Finally  $V_T = \frac{kT}{q}$  is the thermal voltage.

The first term in (8) is the drift term whereas the second term corresponds to the diffusion current. IN homogeneously doped semiconductors one may say that the drift current is an Ohmic current corresponding to a conductance  $\sigma = q(\mu_p p + \mu_n n)$ .

The densities of electrons and holes read

$$\begin{aligned}n &= n_i \exp \frac{V - \Phi^n}{V_T} \\ p &= n_i \exp \frac{\Phi^p - V}{V_T}\end{aligned}\quad (9)$$

where  $\Phi^n$ ,  $\Phi^p$  are the quasi-Fermi potentials for electrons/holes, respectively. The continuity equation holds for the electrons and holes separately, i.e.,

$$\begin{aligned}\nabla \cdot \mathbf{J}_n - q \frac{\partial n}{\partial t} &= -q(G - R) = -qU(n, p), \\ \nabla \cdot \mathbf{J}_p + q \frac{\partial p}{\partial t} &= q(G - R) = qU(n, p)\end{aligned}\quad (10)$$

with generation/recombination terms  $G$ ,  $R$ . Often the net generation rate  $U(n, p) = G - R$  is introduced. The unknown physical quantities are the concentrations of electrons and holes ( $n$ ,  $p$ ) and the scalar potential  $V$  and vector potential  $A$ , i.e., 6 scalar unknowns. Alternatively, one can choose as unknowns the quasi-Fermi potentials  $\Phi^n$ ,  $\Phi^p$  instead of the carriers concentrations. The latter formulation is of practical advantage since the carrier concentration can vary by orders of magnitude.

Since the equations are underdetermined, the gauge conditions are required, i.e., it should be noted that the Maxwell-Ampère equation is complete with the following gauge condition

$$\frac{1}{\mu} \nabla(\nabla \cdot \mathbf{A}) + \xi \epsilon \nabla(\partial_t V) = 0 \quad (11)$$

However this is usually implemented by demanding

$$\frac{1}{\mu} \nabla \cdot \mathbf{A} + \xi \epsilon \partial_t V = 0 \quad (12)$$

For  $\xi = 0$  one obtains the Coulomb and for  $\xi = 1$  the Lorenz gauge. The system of PDEs is of second order in time. Introducing the quasi-canonical momentum  $\mathbf{\Pi} = \partial_t \mathbf{A}$ , a first order system is obtained. For the coupling of a circuit with a device simulator it is preferred to have a first order system, since circuit simulators are typically based on first order ordinary differential-algebraic equations in time. The interfaces presuppose therefore a first order system.

## 1.4 Boundary conditions

**Metal-semiconductor (Schottky-) contact.** Employing the short hand  $N = N_D - N_A$  and (10) we get the abrupt voltage drop at the contact  $\delta V = \Phi - V = V_{metal} - V$

$$\delta V = V_T \ln \left( -\frac{N}{2n_i} \left( 1 + \sqrt{1 - \frac{4n_i^2}{N^2}} \right) \right) \quad p - \text{dope}, \quad N < 0$$
$$\delta V = -V_T \ln \left( \frac{N}{2n_i} \left( 1 + \sqrt{1 - \frac{4n_i^2}{N^2}} \right) \right) \quad n - \text{dope}, \quad N > 0$$

**Isolator-semiconductor contact.** The continuity of the scalar potential  $V$  is assumed. The continuity equation for electrons and holes at the semiconductor side determines the potentials uniquely.

**Metal-isolator contact.** The scalar potential  $V$  is the sole unknown. The surface charge at the contact is obtained from the gradient in normal direction.

## 2 Coupled EM/device/circuit systems

In the section before, the partial differential equations (PDEs) have been presented, resulting from Maxwell's equations and the full 3D device models. The PDEs are discretized in the space coordinates by the device simulator devEM from MAG. Therefore the devEM device simulator delivers a huge set of ordinary differential equations in time.

In contrary, circuit simulators require lumped models, i.e., the terminal currents, voltages, magnetic fluxes and electric charges. Their relations exhibit often nonlinear dependencies. Circuits based on lumped device are formulated by the modified nodal analysis, resulting in systems of ordinary differential algebraic equations (DAEs) in time. After space discretization of the 3D device model, devEM provides to circuit simulators also a huge system of DAEs. The circuit simulator provides therefore the time integration, also referred to as transient simulation or initial value problem.

First, we briefly describe the well-known modified nodal analysis for the lumped modeling of circuits, see Section 2.0.1. Then we discuss the coupling relations for including EM models into the circuit simulation systems and combine them with the spatially discretized Maxwell equations. Finally, we apply an adaptive time stepping scheme to the resulting coupled differential-algebraic equation system.

### 2.0.1 Lumped circuit modeling

The common approach for simulating circuits is the modified nodal analysis (MNA). It bases on Kirchhoff's laws described by

$$A_i = 0, \quad v = A^T e \quad (13)$$

with the incidence matrix  $A$ , mapping branches to nodes of the circuit. The circuit variables consists of all branch currents  $i$ , of all branch voltages  $v$  and of all nodal potentials  $e$ . They are completed by the constitutive element/device equations

$$i_{[1]} = \frac{d}{dt}q(v_{[1]}) + g(v_{[1]}, t), \quad v_{[2]} = \frac{d}{dt}\phi(i_{[2]}) + r(i_{[2]}, t) \quad (14)$$

for terminal current and voltage controlling elements, respectively. Notice, all basic types as capacitances, inductances, resistances and sources are covered by a suitable choice of the functions  $q$ ,  $g$ ,  $\phi$  and  $r$ . Performing the modified nodal analysis, we get the following reduced equation system having only the nodal potentials  $e$  and the currents  $i_2$  of the voltage controlling elements, see [2]:

$$A_{[11]}\frac{d}{dt}q(A_{[11]}^T e) + A_{[11]}g(A_{[11]}^T e, t) + A_{[2]}i_{[2]} = 0, \quad (15)$$

$$\frac{d}{dt}\phi(i_{[2]}) + r(i_{[2]}, t) - A_{[2]}^T e = 0, \quad (16)$$

where the incidence matrix  $A = (A_{[11]}, A_{[2]})$  is split with respect to the current and voltage controlling elements. The equations (15)-(16) are generated automatically from netlists providing the node to branch element relation (for entries of  $A_{[11]}$  and  $A_{[2]}$ ) as well as the element related functions  $\tilde{q}$ ,  $g$ ,  $\phi$  and  $r$ .

## 2.0.2 Modeling the coupling

We assume that the contacts between the electromagnetic field model and the lumped circuit model to be perfectly electric conducting such that  $\mathbf{B} \cdot n_{\perp} = 0$  and  $e \cdot n_{\parallel} = 0$  with  $n_{\perp}$  and  $n_{\parallel}$  being the outer unit normal vectors transversal and parallel to the contact boundary. This motivates the boundary conditions, cf. [1],

$$(\nabla \times \mathbf{A}) \cdot n_{\perp} = 0, \quad (\nabla V + \mathbf{\Pi}) \cdot n_{\parallel} = 0. \quad (17)$$

Denoting by  $\Gamma_k$  the  $k$ -th contact of the electromagnetic field model element with  $\Gamma_0$  being the reference contact we get the current through  $\Gamma_k$  as

$$i_k = \int_{\Gamma_k} [\mathbf{J} - \partial_t(\epsilon(\nabla V + \mathbf{\Pi}))] \cdot n_{\perp} d\sigma \quad (18)$$

with  $\mathbf{\Pi} = \partial_t \mathbf{A}$  the canonical momentum introduced in chapter 1.2. Note that the equation for  $\mathbf{J}$  in section 1.2 and the boundary condition (17) guarantee that the sum of all contact currents equals zero, that means

$$\sum_k i_k = 0.$$

This model property is necessary for all lumped element descriptions in order to preserve the Kirchhoff's current law. In order to reveal the relation to the voltages  $v_k$  between the contact  $\Gamma_k$  and the reference contact  $\Gamma_0$ , we express the scalar potential  $V$  as

$$V(x, t) = V_{bi}(x) + V_c(x, t) \quad (19)$$

with the contact potential

$$V_c(x, t) = \begin{cases} v_k & \text{if } x \in \Gamma_k \\ 0 & \text{else.} \end{cases}$$

Here, we assumed the reference contact  $\Gamma_0$  to be the ground node for simplicity. The potential  $V_{bi}$  describes the position dependent built-in potential arising by varying doping concentrations and bonding different materials.



### 2.0.3 Holistic DAE system

The circuit DAE system (15) - (16) is extended by currents  $i_M$  through the contact of the EM-element and summarized as a DAE of the form

$$A_C \frac{d}{dt} d_C(y_C) + b_C(y_C, t) + B_{CM} i_M = 0, \quad (20)$$

where  $y_C = (e, i_{[2]})^\top$  collects the circuit variables. The spatially discretized Maxwell system together with the coupling boundary condition (17) are summarized into the system

$$A_M \frac{d}{dt} d_M(y_M, y_C) + b_M(y_M, y_C, t) = 0 \quad (21)$$

where  $y_M = (V, n, p, \mathbf{A}, \mathbf{\Pi})^\top$  are the Maxwell system variables from the 3D device equations and

$$d_M(y_M, y_C) = \begin{pmatrix} y_M \\ (B_{CM}^\top, 0)y_C \end{pmatrix} = \begin{pmatrix} y_M \\ B_{CM}^\top e \end{pmatrix} = \begin{pmatrix} y_M \\ v_{app} \end{pmatrix}$$

$$b_M(y_M, y_C, t) = \beta_M(y_M, v_{app}, t)$$

with  $v_{app}$  describing the voltages at the EM device contacts. Analogously to the discretization of the Maxwell-Ampère equation and we discretize the coupling condition (18) and summarize it to

$$A_{MC} \frac{d}{dt} d_{MC}(y_M, y_C) + b_{MC}(y_M, y_C, t) = i_M \quad (22)$$

with  $d_{MC}(y_M, y_C) = d_M(y_M, y_C)$  and  $b_{MC}(y_M, y_C, t) = \beta_{MC}(y_M, v_{app}, t)$ .

Collecting (20), (21) and (22), we obtain the coupled DAE system

$$\underbrace{\begin{bmatrix} A_M & 0 & 0 \\ 0 & A_{MC} & 0 \\ 0 & 0 & A_C \end{bmatrix}}_{=:A} \frac{d}{dt} \underbrace{\begin{pmatrix} d_M(y_M, y_C) \\ d_{MC}(y_M, y_C) \\ d_C(y_C) \end{pmatrix}}_{=:d} + \underbrace{\begin{pmatrix} b_M(y_M, y_C, t) \\ b_{MC}(y_M, y_C, t) - i_M \\ b_C(y_C, t) - B_{CM} i_M \end{pmatrix}}_{=:b} = 0. \quad (23)$$

### 2.0.4 Time Discretization

The resulting DAE system (23)

$$A \frac{d}{dt} d(x) + b(x, t) = 0$$

is solved by the backward differentiation (BDF) methods (cf. [3]), i.e., we solve the nonlinear systems

$$\frac{1}{h_n} \sum_{i=0}^k \alpha_{ni} A d(x_{n-i}, t_{n-i}) + b(x_n, t_n) = 0 \quad (24)$$

at each time point  $t_n$ . Here,  $h_n := t_n - t_{n-1}$  is the time stepsize,

$$\alpha_{ni} = \frac{t_n - t_{n-1}}{t_n - t_{n-i}} \prod_{j=1, j \neq i}^k \frac{t_n - t_{n-j}}{t_{n-i} - t_{n-j}}, \quad i = 1, \dots, k,$$

$$\alpha_{n0} = - \sum_{i=1}^k \alpha_{ni},$$

are the BDF coefficients and  $x_{n-i}$  are the numerical approximations of the exact solution  $x(t_{n-i})$  at the time points  $t_{n-i}$ . The implemented time integration scheme has the option to switch to a Runge Kutta scheme (Radau IIa), for starting and restarting the integration.

The adaptive time step control estimates the error for the dynamic components  $d(x_n, t_n)$ . Such a control is more stable and reliable for higher index DAE systems. The error is estimated by the difference of  $d(x_n, t_n)$  and  $d(x_n^p, t_n)$  with  $x_n^p$  being the predictor

$$x_n^p := \sum_{i=1}^{k+1} \gamma_{ni} x_{n-i}$$

and

$$\gamma_{ni} := \prod_{j=1, j \neq i}^{k+1} \frac{t_n - t_{n-j}}{t_{n-i} - t_{n-j}}, \quad i = 1, \dots, k + 1.$$

## 2.0.5 Implementation issues and results

The construction of the coupled simulation is shown in Fig. 1. It is realized in a Python framework combining a Python implementation of the HUB circuit solver MECS with a C++ implementation of the MAGWEL's field solver devEM.

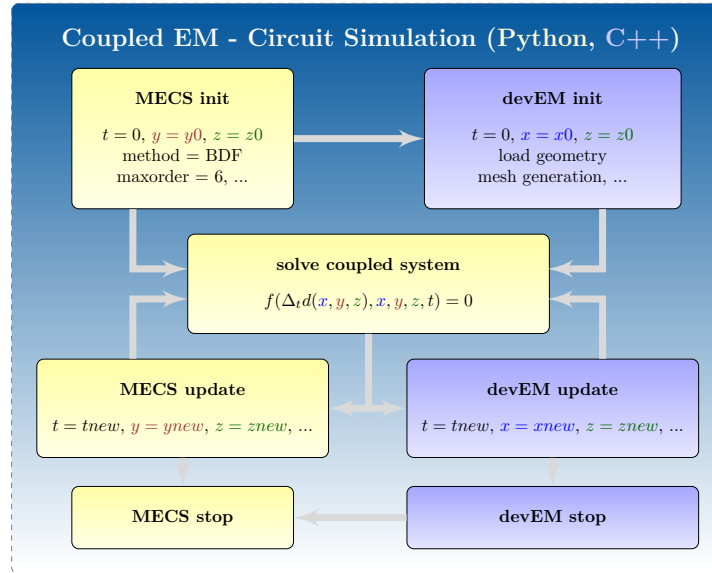


Figure 1: Flow diagram for the coupled field circuit simulation. It is realized in a Python framework including C++ implementations of the field solver devEM.

A typical design is shown in Fig. 2 where the balun is modeled in full 3D and the surrounding circuitry as lumped devices. The figures 3-5 depict the simulation results after time integration for the magnetic field strength  $B$ .

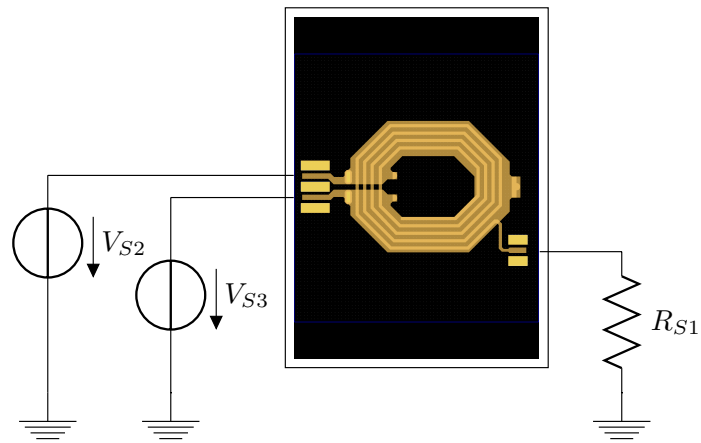
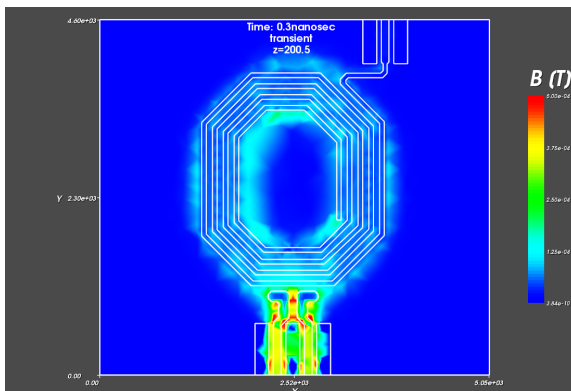
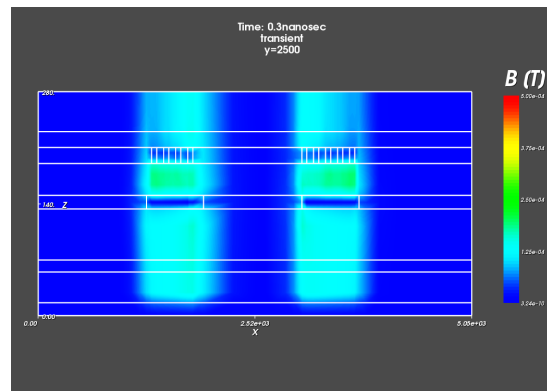


Figure 2: Test Benchmark: Simple circuit with the balun device. The RF input signals  $V_{S2}$  and  $V_{S3}$  are sinusoidal ones operating with 1GHz frequency. The RF output is given as current through the resistance  $R_{S1}$ .

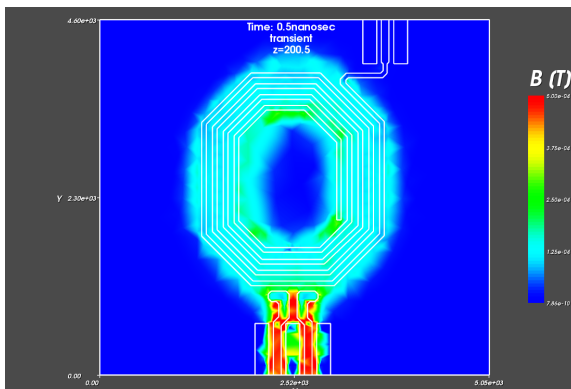


(a) Balun device top are view. Showing the magnetic inductance  $B$ .

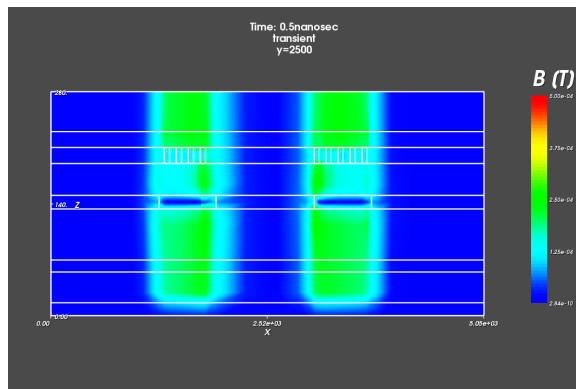


(b) Balun device cross-sectional area view. Showing the magnetic inductance  $B$ .

Figure 3: **10GHz** benchmark of Balun device at time point  $t = 0.3$  nanoseconds.



(a) Balun device top are view. Showing the magnetic inductance  $B$ .



(b) Balun device cross-sectional area view. Showing the magnetic inductance  $B$ .

Figure 4: **10GHz** benchmark of Balun device at time point  $t = 0.5$  nanoseconds.

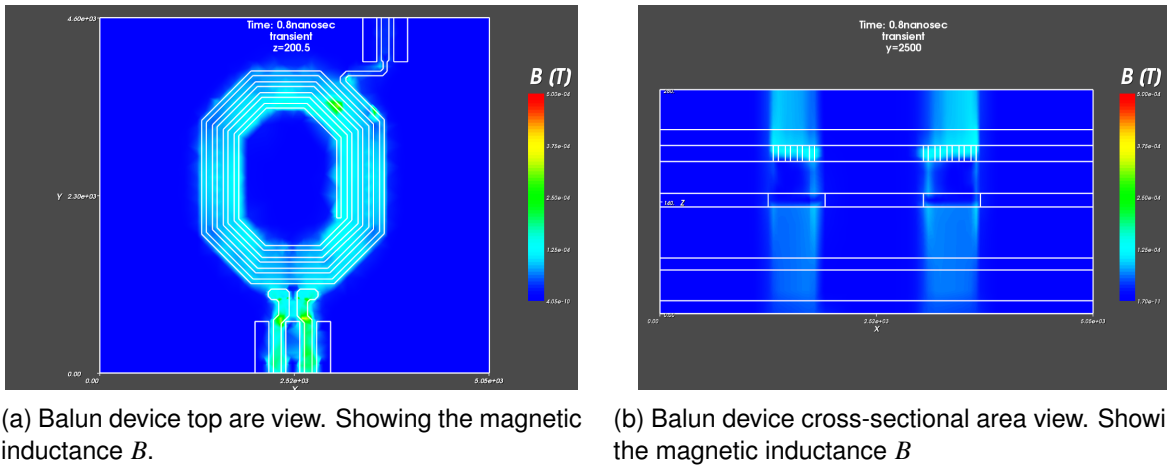


Figure 5: **10GHz** benchmark of Balun device at time point  $t = 0.8$  nanoseconds.

## Conclusion

This Public Report summarizes the research results on "Simulation methods for coupled problems" from the fp7 project nanoCOPS. The EM/field/device simulator devEM has been coupled with the circuit simulators MECS from Humboldt University and LinzFrame from University of Applied Sciences of Upper Austria. The two latter simulators employ the well-known Modified Nodal Analysis and the industry standards for the lumped circuit models RLCG, MOS and bjt semiconductors, such as the BSIMxxx models from the University of California at Berkeley and the Simkit library from NXP Semiconductors. The device simulator serves for the spatial discretization of the partial differential equations and provides via an interface a system of ordinary differential-algebraic equations in time, whereas the circuit simulators perform the numerical time integration and serve as the master.

The simulators were coupled holistically, i.e., strong coupling where full Newton-Raphson methods are applicable. This contrasts to co-simulation approaches, where only iterative relaxation based methods are applicable. Co-simulation, though easy to implement, suffer from poor convergence speed or even fail to converge when the underlying physical problem, e.g., a system of ordinary or partial differential equations, does not fulfill special requirements such as a diagonal dominance after space and time discretization. In contrary, holistic simulations with full (damped) Newton-Raphson iterative solvers for the resulting discretized equations normally converge rapidly. Failure of convergence are mainly caused by an inappropriate physical modeling, initialization, or space discretization of the underlying partial differential equations.

Section 1 summarizes basic electro-magnetic field theory, corresponding gauge equations and semiconductor theory. Moreover the spatial discretization of the electro-magnetic field and device equations are derived, with emphasis on semiconductor devices. Section 2 deals with the holistic coupling of a circuit simulator with a device simulator. Since we treat both linear and nonlinear devices, two interfaces were established. Linear devices must be evaluated only once, since the Jacobian matrices of the algebraic and dynamic contributions are independent of the state variables, and the device simulator provides via the linear interface sparse matrix stamps for the algebraic and dynamic contributions of the device separately. This can be achieved by a preprocessing step. In contrary, the Jacobians and the right-hand-sides of nonlinear (semiconductor) devices depend on the current values

of the state variables. A holistic approach requires therefore a permanent exchange via the nonlinear interface. Therefore the nonlinear interface is significantly more complex than the linear one and it requires refined validation techniques.

The circuit simulators provide on the one hand the models for the lumped devices and on the other the classical analysis tools DC, AC and transient (time integration). Time integration is performed by the Backward Differentiation Formulas (BDF) or Gear's formulas, multistep methods which are stiffly stable and also A-stable for orders smaller than two, for the start up Runge-Kutta methods of higher order such as the RADAU techniques; and novel spline/wavelet based integration formulas are employed. Since the nanoCOPS project has also a focus on radio frequency circuits, classical time integration is prohibitively slow, since the signal waveforms of radio frequency circuits exhibit bandpass characteristic, i.e., the spectrum is centered at the vicinity of a carrier frequency. The multirate method decouples the slowly varying envelope from the carrier waveform which makes the holistic device/circuit simulation possible even for radio frequency circuits operating in the GHz range.

## References

- [1] S. Baumanns. Coupled Electromagnetic Field/Circuit Simulation. Modeling and Numerical Analysis. PhD thesis, Universität zu Köln, 2012.
- [2] D. Estévez Schwarz and C. Tischendorf. Structural analysis of electric circuits and consequences for mna. *Internat. J. Circ. Theor. Appl.*, 28(2):131–162, 2000.
- [3] C. W. Gear. Simultaneous numerical solution of differential-algebraic equations. *Circuit Theory, IEEE Transactions on*, CT-18(1):89–95, 1971.