Consistent initialization for coupled circuit-device simulation

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Abstract For a coupled circuit device simulation in the time domain, consistent initial values have to be calculated. We study the structure and properties of the differential-algebraic equations (DAEs) that arise after space discretization of the partial differential equation part coming from the device modelling. Exploiting the special DAE structure, we show that a consistent inital value can be computed within two steps: firstly determines an operation point. Secondly a linear system is solved which corrects the operation point such that the hidden constraints are also satisfied. Finally, an algorithm for the calculation of such values is proposed.

1 Introduction

Nowadays semiconductor devices in an electrical circuit are modeled via equivalent circuits containing only basic elements that can be described by algebraic and ordinary differential equations. With the rapid development of chip technology these equivalent circuits have become more and more complex. This has motivated the idea of using distributed device models, represented by a system of Partial Differential Equations (PDE), to describe the behavior of the semiconductor devices in the circuit [1, 2]. The resulting mathematical model couples the differential algebraic equations (DAEs) describing the circuit and the partial differential equations (PDEs) modeling the semiconductor devices.

In order to numerically simulate electrical circuits described by such a model, we discretize the partial differential equations in space first. This results in a DAE for the coupled simulation problem. The numerical simulation of this DAE involves the problems of finding consistent initial values for the integration. DAEs are known for the fact that solutions have to fulfill certain contraints. Correspondingly, initial values have to be found that satisfy these constraints.

The main objective of this article is the determination of appropriate initial values for the DAE arising after space discretization. We study which conditions initial values should satisfy in order to be consistent and present an algorithm for their calculation. This algorithm is based on the ideas presented in [3, 4]. Due to the

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special properties of this DAE, discussed later on in this paper, a consistent initial value for it can be calculated in two steps: in the first one an operating point is computed and in the second one this point is corrected by solving a linear system of equations.

This paper is organized as follows. First we describe briefly the coupled DAE-PDE model of the coupled circuit device system as well as the DAE system that is obtained after spatial discretization. Section 3 is devoted to the properties of this DAE. In section 4, the conditions for consistent initial values are studied and an algorithm for the calculation of such values is proposed. This algorithm has been implemented in MATLAB.

2 Coupled system for the circuit and device simulation

For simplicity and shorter description, we restrict to the case of coupling only one semiconductor device to an electrical circuit. Assume this semiconductor device to have n_S metal semiconductor contacts and let n_N be the number of nodes in the graph associated to the circuit. Each contact of the semiconductor device is joined to a node of the electrical circuit. The contacts of the semiconductor joined to the same node of the electrical circuit define a terminal. Let n_T be the number of terminals of the semiconductor device. We define the following incidence matrix $A_S \in \mathbb{R}^{(n_N-1)\times(n_T-1)}$ by

$$A_S(i,j) = \begin{cases} 1, & \text{if terminal } j \text{ is joined to the node } i \\ -1, & \text{if the reference terminal is attached to node } i \\ 0, & \text{else} \end{cases}$$

The system proposed in [2] couples the modified nodal analysis (MNA) equations for electrical circuits to the drift diffusion (DD) equations for semiconductor devices. The MNA equations have the form

$$A_C \frac{\mathrm{d}\, q_C(A_C^T e,t)}{\mathrm{d}t} + A_R g_R(A_R^T e,t) + A_L j_L + A_V j_V + A_S j_S + A_I i_S(t) = 0, \tag{1a}$$

$$\frac{\mathrm{d}\, \phi(j_L,t)}{\mathrm{d}t} - A_L^T e = 0, \tag{1b}$$

$$A_V^T e - v_S(t) = 0 \tag{1c}$$

with $t \in [t_0, t_F]$. The matrices A_C, A_R, A_L, A_V, A_S and A_I describe the element related reduced incidence matrices. The functions $v_S(t)$, $i_S(t)$, $q_C(u,t)$, $g(u,t)$ and $\phi(j,t)$ describe the constitutive relations for the circuit elements. As unknowns we have the node potentials $e(t) : \mathbb{R} \to \mathbb{R}^{n_N-1}$, except of the mass node, as well as the currents $j_L(t) : \mathbb{R} \to \mathbb{R}^{n_L}$ through inductors, the currents $j_V(t) : \mathbb{R} \to \mathbb{R}^{n_V}$ through voltage sources and the currents $j_S : \mathbb{R} \to R^{n_T-1}$through semiconductor devices. Note that the term $A_S j_S$ within the Kirchoff's current law equation (1a) involves a coupling to

the DD model since the current j_S at the semiconductor's contacts depends on the DD variables.

Suppose Ω to be a bounded domain in $\mathbb{R}^d$, $d \in \{1,2,3\}$ and let $x \in \Omega$ represent the space variable. The DD equations are given by the following set of PDEs for the electrostatic potential $\psi(x,t)$ and the electrons and holes densities, $n(x,t)$ and $p(x,t)$ respectively.

$$\nabla \cdot (-\varepsilon \nabla \psi) - q(C - n + p) = 0, \tag{1d}$$

$$-\frac{\partial n}{\partial t} + \frac{1}{q}\mathrm{div} J_n - R(n,p) = 0, \qquad J_n - q\mu_n(U_T \nabla n - n\nabla\psi) = 0, \tag{1e}$$

$$\frac{\partial p}{\partial t} + \frac{1}{q}\mathrm{div} J_p + R(n,p) = 0, \qquad J_p + q\mu_p(U_T \nabla p + p\nabla\psi) = 0. \tag{1f}$$

For simplicity, we consider the mobilities μ_n and μ_p as well as the material quantities ε and U_T as constants. The elementary charge q is always constant.

The boundary of the semiconductor device is here divided into two disjoint parts $\Gamma = \Gamma_D \cup \Gamma_N$. The first one includes the metal semiconductor contacts (Ohmic contacts) where the external potentials are applied and can divided into n_T disjoints contacts. The contact n_T is chosen as reference contact. The corresponding boundary conditions have the form

$$n = n_D(x), \quad p = p_D(x), \quad \psi = \psi_{bi}(x) + \psi_{ext}(x, A_S^{\mathrm{T}} e) \tag{1g}$$

for all $x \in \Gamma_D$ and $t \in [t_0, t_F]$. On Γ_N homogeneous Neumann boundary conditions are imposed, i.e.

$$\nabla\psi \cdot \nu = 0, \quad J_n \cdot \nu = 0, \quad J_p \cdot \nu = 0 \tag{1h}$$

for all $x \in \Gamma_N$ and $t \in [t_0, t_F]$ with ν being the unit vector pointing in the outer normal direction of Ω. In (1g), $\psi_{ext}(x, A_S^{\mathrm{T}} e)$ denotes the externally applied voltage[1] and $\psi_{bi}(x)$, $n_D(x)$ as well as $p_D(x)$ are given functions that do not depend on time.

The currents $j_{S_1}, j_{S_2}, \ldots, j_{S_{n_T-1}}$ at the semiconductor terminals can be calculated as

$$j_{S_i} = -\int_\Omega (J_n + J_p) \cdot \nabla w_i \, \mathrm{d}x - \frac{\mathrm{d}}{\mathrm{d}t} q_{S_i}, \quad q_{S_i} = -\int_\Omega \varepsilon \nabla\psi \cdot \nabla w_i \, \mathrm{d}x, \tag{1i}$$

where the functions w_i, $i = 1, 2, \ldots, n_T - 1$ are chosen such that

$$\nabla \cdot (-\varepsilon \nabla w_i) = 0, \quad \text{in } \Omega, \tag{2a}$$

$$w_i|_{\Gamma_j \subset \Gamma_D} = \delta_{ij},\ j = 1, 2, \ldots, n_T \quad \text{and} \quad \nabla w_i \cdot \nu = 0, \ \text{on } \Gamma_N. \tag{2b}$$

This way, we may express $\psi_{ext}(x, A_S^{\mathrm{T}} e)$ as

$$\psi_{ext}(x, A_S^{\mathrm{T}} e) = (w_1 \ w_2 \ \cdots \ w_{n_T-1}) \cdot A_S^{\mathrm{T}} e.$$

[1] Since we consider the semiconductor device as part of an electrical circuit, ψ_{ext} is not an independent function to be assigned, but it is to be determined by the electrical network

The discretization of (1d)-(1f) in space results in a DAE system [5] for

$$y(t) = (e, j_L, j_V, j_S, q_S, \Psi, N, P)^{\mathrm{T}} : \mathbb{R} \to \mathbb{R}^m$$

with $m = n_N - 1 + n_L + n_V + 2(n_T - 1) + 3M$. Here M denotes the number of interior and Neumann nodes in the spatial mesh used to discretize the PDEs in the system. For each $t \in [t_0, t_F]$, the vector $\Psi(t)$ contains the approximations to the values of ψ at the mesh points or mesh elements. The same holds for $N(t)$ and $P(t)$. The resulting DAE has the form

$$A \frac{\mathrm{d}}{\mathrm{d}t} d(y,t) + b(y,t) = 0 \tag{3a}$$

with

$$A = \begin{pmatrix} A_C & 0 & 0 & 0 & 0 \\ 0 & I & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & I & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & M_h & 0 \\ 0 & 0 & 0 & 0 & M_h \end{pmatrix}, \qquad d = \begin{pmatrix} A_C^+ A_C q_C(A_C^{\mathrm{T}} e(t), t) \\ \phi(j_L(t), t) \\ q_S(t) \\ N(t) \\ P(t) \end{pmatrix} \tag{3b}$$

and

$$b = \begin{pmatrix} A_R g_R(A_R^{\mathrm{T}} e, t) + A_L j_L + A_V j_V + A_S j_S + A_I i_S(t) \\ -A_L^{\mathrm{T}} e \\ A_V^{\mathrm{T}} e - v_S(t) \\ q_S + f(A_S^{\mathrm{T}} e, \Psi) \\ j_S + g(A_S^{\mathrm{T}} e, \Psi, N, P) \\ T_h \Psi + h(A_S^{\mathrm{T}} e, N, P) \\ r_1(A_S^{\mathrm{T}} e, \Psi, N) \\ r_2(A_S^{\mathrm{T}} e, \Psi, P) \end{pmatrix}. \tag{3c}$$

The matrix A_C^+ above denotes the Moore-Penrose inverse of A_C. All functions of the system above are assumed to be continuously differentiable with respect to all their components. Suppose further the matrices T_h and M_h to be symmetric and positive definite.[2] The partial derivatives

$$C(u,t) = \frac{\partial q_C(u,t)}{\partial u}, \quad L(j,t) = \frac{\partial \phi(j,t)}{\partial j}, \quad G(u,t) = \frac{\partial g_R(u,t)}{\partial u}$$

[2] This is always true for Galerkin approximations with basis functions $\varphi_i(x)$ that provide independent functions $\frac{d}{dx}\varphi_i(x)$.

are also assumed to be positive definite, that means, we consider all capacitors, inductors and resistors to be passive.[3] Finally, suppose that

$$J_h = \frac{\partial f(u,\Psi)}{\partial u} - \frac{\partial h(u,N,P)}{\partial u} T_h^{-1} \frac{\partial f(u,\Psi)}{\partial \Psi}$$

is a symmetric and positive definite matrix[4].

In what follows we assume that the circuit contains neither loops of voltage sources only nor cut sets of current sources only. It is a natural assumption since a violation would lead to a short circuit in reality.

3 Properties of the DAE obtained after spatial discretization

Let $D(y,t) = \frac{\partial d(y,t)}{\partial y}$. Note that it is such that $\operatorname{im} D(y,t)$ is constant. The DAE (3) also has a properly stated leading term, that means,

$$\operatorname{im} D(y,t) \oplus \ker A = \mathbb{R}^k \tag{4}$$

with $k = n_C + n_L + n_T - 1 + 2M$ is satisfied and there exists a projector $R \in \mathbb{R}^{k\times k}$ that realizes the decomposition (4), i.e. $R^2 = R$, $\operatorname{im} D(y,t) = \operatorname{im} R$ and $\ker A = \ker R$. One possible choice is $R = A^+A$, where A^+ denotes the Moore-Penrose inverse of A.

Since the network equations usually do not fulfill high smoothness conditions, we use the tractability index concept [6] for the index determination. Additionally, this concept leads us easily to network topological conditions characterizing the index of the discretized coupled DAE system. The DAE-index depends on the regularity of certain matrices $G_i, i = 0,1,2,\ldots$ that are recursively constructed.

1. Since the matrix $G_0(y,t) = AD(y,t)$ is singular for all $(y,t) \in \mathbb{R}^m \times \mathbb{R}$, the DAE has always an index greater than zero [5, 7].
2. The DAE index is one if and only if the matrix $G_1(y,t) = G_0(y,t) + \frac{\partial b(y,t)}{\partial y} Q_0$ is nonsingular with Q_0 being a projector onto $\ker G_0$. It is shown that this is the case if the circuit contains neither loops of capacitors, voltage sources and semiconductor devices with at least one semiconductor device or one voltage source (CVS-loops) nor cut sets of inductors and currents sources (LI-cut sets)

[3] We need passivity of resistors only if they are not connected by a capacitive path.

[4] Let $w_{i,h}$ denote the approximations to the functions $w_i(x)$ defined in (2) with a Galerkin method. If they are written as linear combination of the same functions as the approximations to ψ and $\frac{d}{dx} w_{i,h}(x)$ are linearly independent (this is e.g. the case if the spatial mesh is sufficiently fine), then it holds that J_h is symmetric and positive definite, since

$$J_h(i,j) = \int_\Omega \nabla w_{i,h} \cdot \nabla w_{j,h} \, \mathrm{d}x, \quad i,j = 1,2,\ldots,n_T - 1.$$

[5, 7]. Since $\operatorname{im} D(y,t)$ is constant, the DAE is also numerically qualified [8] in this case.

3. In all other cases the matrix $G_2 = G_1 + \frac{\partial b(y,t)}{\partial y} P_0 Q_1$ with $Q_1(y,t)$ being a projector onto $\ker G_1(y,t)$ is nonsingular, i.e. the DAE index equals to two [5, 7].

4 Consistent initial values for the DAE associated to the coupled system

One of the difficult parts in solving DAEs numerically is to determine a consistent set of initial conditions in order to start the integration. In order to calculate consistent initial values for the DAE system (3), we exploit its special structure.

If (3) has index one, its flow is restricted to

$$\mathscr{M}_0(t) = \left\{ y \in \mathbb{R}^m | \exists z \in \mathbb{R}^k : Az + b(y,t) = 0 \right\}.$$

and $\mathscr{M}_0(t)$ is completely filled by this flow [6].

Theorem 1. *If the DAE (3) satisfies the conditions in section 2 and the circuit contains neither CVS-loops nor LI-cut sets, then the system*

$$\begin{aligned} Az_0 + b(y_0, t_0) &= 0, \\ (I-R)z_0 + d(y_0, t_0) - Ry^0 &= 0 \end{aligned}$$

is locally uniquely solvable for z_0, y_0 and provides a consistent initial value y_0 for (3). The vector y^0 can be arbitrarily chosen. [6, 7]

Speaking in terms of electrical variables, if the circuit contains neither CVS-loops nor LI-cut sets, initial values for the inductive currents, the capacitive branch voltages $A_C^{\mathrm{T}} e$, the charges at the semiconductor contacts q_S and the concentrations of electrons and holes on the mesh nodes can be arbitrarily chosen.

The flow of index-two DAEs is additionally restricted by so-called hidden constraints and the set of consistent values at t_0 is a proper subset of $\mathscr{M}_0(t_0)$. In this case, we can compute a consistent initial value for (3) as follows [3, 7]

- Describe the hidden constraints.
- Compute a value y_0 that satisfies the explicit equation of the DAE system with $y_0 \in \mathscr{M}_0(t_0)$.
- Correct this value in order to fulfill the hidden constraints, i.e. calculate a value $y_* \in \mathscr{M}_1(t_0) \subset \mathscr{M}_0(t_0)$.

To describe the hidden constraints we follow the idea in [3, 4, 7] and reduce the index of the DAE system. For this reason, we introduce the DAE

$$(A \quad W_1) \frac{\mathrm{d}}{\mathrm{d}t} \begin{pmatrix} d(y,t) \\ W_1 b(y,t) \end{pmatrix} + (I - W_1) b(y,t) = 0 \tag{5}$$

where W_1 is a projector along $\operatorname{im} G_1(y,t)$. It holds $W_1 W_0 = W_1$ for any projector W_0 along $\operatorname{im} G_0(y,t) = \operatorname{im} A$. The DAE (5) has been obtained by replacing $W_1 b(y,t)$ in the original DAE (3) by its differentiated form. The DAE (5) has also a properly stated leading term and index one. It is clear that every solution of (3) is also a solution of (5). Conversely, every solution y of (5) that satisfies $W_1 b(y(t),t) = 0$ at least at one point $t \in [t_0, t_F]$, is also a solution of original DAE (3).

This approach suggests that the solution $y(t)$ of the index-two DAE should satisfy $y(t) \in \mathscr{M}_1(t)$, $\forall t \in [t_0, t_F]$ with

$$\mathscr{M}_1(t) = \left\{ y \in \mathscr{M}_0(t) \mid \exists z \in \mathbb{R}^m : W_1 \left(\frac{\partial b(y,t)}{\partial y} z + \frac{\partial b(y,t)}{\partial t} \right) = 0 \right\}.$$

The next step is to compute a value $y_0 \in \mathscr{M}_0(t_0)$. This can be done by solving the system $b(y_0, t_0) = 0$. For general DAEs, one can not expect that this system is always solvable. However, if the circuit-device system is well posed then the system has a unique equilibrium solution for physical reasons.

For DAE systems of the form (3) it has been shown [7] that the index-two components[5] of the solution can be described by Ty with

$$T = \begin{pmatrix} Q_{CRVS} & 0 & 0 & 0 \\ 0 & 0_{n_L} & 0 & 0 \\ 0 & 0 & Q_{C-VS} & 0 \\ 0 & 0 & 0 & 0_{n_T-1+3M} \end{pmatrix},$$

if Q_{CRVS} denotes a projector onto $\ker (A_C\, A_R\, A_V\, A_S)^{\mathrm{T}}$, Q_{C-VS} a projector onto $\ker Q_C^{\mathrm{T}} (A_V\, A_S)$ and Q_C is a projector onto $\ker A_C^{\mathrm{T}}$. In (3) these components occur only linearly, i.e. with $U = I - T$ it can be written as

$$A \frac{\mathrm{d}}{\mathrm{d}t} d(y,t) + \tilde{b}(Uy,t) + \mathscr{B} T y = 0.$$

Theorem 2. *If the DAE (3) satisfies the conditions in section 2 and the circuit contains either CVS-loops or LI-cut sets, then the following linear system provides a consistent initialization (z_*, y_*):*

$$\begin{pmatrix} A & \mathscr{B}T \\ 0 & U \\ W_1 B_0 D_0^- & 0 \\ (I-R) & 0 \end{pmatrix} \begin{pmatrix} z^* \\ y^* \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ W_1 B_0 D_0^- d_0 - W_1 b_0 \\ 0 \end{pmatrix}$$

with $z_* := z^*$, $y_* := y^* + y_0$, y_0 being any value belonging to $\mathscr{M}_0(t_0)$ and

$$B_0 := \tfrac{\partial b(Uy_0,t_0)}{\partial Uy}, \quad D_0 := \tfrac{\partial d(Uy_0,t_0)}{\partial Uy}, \quad b_0 := \tfrac{\partial b(Uy_0,t_0)}{\partial t}, \quad d_0 := \tfrac{\partial d(Uy_0,t_0)}{\partial t}.$$

[5] By index-two components we mean those components that depend on derivatives of the input functions.

The matrix D_0^- denotes a generalized inverse of D_0 satisfying $D_0 D_0^- = R$.

Proof. It is shown [7] that this linear system is uniquely solvable. In order to prove that (z_*, y_*) is a consistent initialization for (3), we have to check that the hidden constraints are fulfilled. With $z = D_0^- z_* - D_0^- d_0$ it holds that

$$W_1 \left(\frac{\partial b(y_0, t_0)}{\partial y} z + \frac{\partial b(y_0, t_0)}{\partial t} \right) = 0$$

The explicit equations are fulfilled with $Uy^* = 0$, $Az_* + \mathscr{B}Ty_* = 0$ and $b(y_0, t) = 0$.

5 Conclusions

It has been shown that the differential-algebraic equations arising from a monolithic coupled circuit device simulation have the special structure that the higher index components, i.e. here the index-two components, appear only linearly in the systems. This result extends the knowledge from circuit simulation [3] to the coupled circuit device simulation.

Uniquely solvable equation systems have been presented that allow a computation of consistent initial values. Starting from an initial solution that satisfies the index-1 constraint, e.g. from an operating point, only a linear system has to be solved in order to get a consistent initialization.

As known already for circuits [3], the special structure implies that two Euler integration steps yield always a consistent value. However, this value is a consistent one at the timepoint $t_0 + 2h$ supposed the system is integrated by a stepsize h. The systems presented here provide a consistent initialization at the initial time point t_0.

Following our approach, a non-linear system of equations must be solved in order to obtain an initial solution that satisfies the index-1 constraints, e.g. an operating point. By solving then a linear system of equations, a consistent initialization at the time point t_0 is obtained. However, in order to construct the linear system of equations constant projectors must be computed.

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