Numerical Analysis of DAEs from Coupled Circuit and Semiconductor Simulation ⋆

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Abstract

In this work we are interested in the numerical solution of a coupled model of differential algebraic equations (DAEs) and partial differential equations (PDEs). The DAEs describe the behavior of an electrical circuit that contains semiconductor devices and the partial differential equations constitute drift-diffusion equations modeling the semiconductor devices in the circuit.

After space discretization using a finite element method, the coupled system results in a differential-algebraic system with a properly stated leading term. We investigate the structure and the properties of this DAE system. In particular, we develop structural criteria for the DAE index. This is of basic interest since DAE properties like stability, existence and uniqueness of solutions depend strongly on its index.

Key words: differential algebraic equation, partial differential equation, tractability index, modified nodal analysis, drift-diffusion equations

1 Introduction

Nowadays semiconductor devices in an electrical circuit are modeled by small circuits containing basic network elements (capacitors, resistors, inductors, voltage and current sources) described by algebraic and ordinary differential equations. But these equivalent circuits may depend on hundreds of parameters and its correct adjustment has become a very difficult task for the network design. This has motivated the idea of using distributed device models, represented by a system of partial differential equations, to describe the behavior

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of the semiconductor devices within the circuit [1]. The resulting mathematical models couple the differential algebraic equations (DAEs) describing the behavior of circuit and the partial differential equations (PDEs) modeling semiconductor devices.

In this work we are interested in the numerical solution of the system that is obtained when high frequency devices in an electrical circuit are modeled via drift-diffusion equations. In section 2 the equations resulting from the Modified Nodal Analysis (MNA) of the circuit are explained. The drift-diffusion equations are presented in section 3 as well as its discretization by a finite element method.

Finally, in section 4 the DAE that results from the coupling of the MNA equations and the discrete drift-diffusion equations is constructed and its index is studied. The knowledge about the DAE index allows us to determine the conditions that consistent initial values must satisfy and which numerical methods are feasible for its solution.

2 Circuit Equations

The mathematical model that results from modified nodal analysis applied to an electrical network containing resistors, capacitors, inductors and independent voltage and current sources[1] has the form [3]

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

$$\frac{\mathrm{d}}{\mathrm{d}t} \phi(j_L, t) - A_L^T e = 0, \tag{2}$$

$$A_V^T e - v_S(t) = 0. \tag{3}$$

The unknowns $e(t) : \mathbb{R} \to \mathbb{R}^{n_N}$, $j_L(t) : \mathbb{R} \to \mathbb{R}^{n_L}$ and $j_V(t) : \mathbb{R} \to \mathbb{R}^{n_V}$ represent the node potentials, excepting the mass node, the currents through inductors and the currents through voltage sources respectively. The matrices A_C, A_R, A_L, A_V and A_I are the element-related (reduced) incidence matrices, they have entries from $\{-1, 0, 1\}$. Let the following assumptions on the circuit equations be satisfied in the forthcoming sections:

(1) the input functions $v_S(t)$ and $i_S(t)$, associated to the independent voltage and current sources respectively, are continuous,

[1] Controlled sources have been neglected to simplify matters.

(2) the functions $q_C(u,t)$, $\phi(j,t)$ and $g(u,t)$ are continuously differentiable and have positive definite partial Jacobians

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

(3) and the circuit contains neither loops of voltage sources only nor cut sets of current sources only. These two conditions hold if and only if the matrices A_V and $(A_C\ A_R\ A_L\ A_V)^T$ have full column rank, respectively.

The second assumption concerning the Jacobians reflects local passivity of capacitances, inductances and resistances [4]. The third assumption is necessary from the electric point of view in order to prevent short-circuits.

Under these assumptions it was shown [17,3] that the index of the circuit equations (1)-(3) does not exceed two. More precisely, the index equals two if and only if the circuit contains LI-cut sets (cut sets of inductors and current sources) or CV-loops (loops of capacitors and voltage sources) with at least one voltage source.

Additionally, the previous assumptions allow the circuit equation systems to be formulated as DAEs with a properly stated leading term [14].

3 Drift-Diffusion Equations

We will consider the non-stationary drift-diffusion model of a semiconductor device. For convenience, we formulate the model equations in only one spatial dimension. The segment $\bar{\Omega} = [0,\, l] \subset \mathbb{R}$ describes the range of the device, including its contacts and $t \in [t_a, t_b]$ represents the time. The model equations are given by the Poisson equation

$$-\frac{\partial}{\partial x}\left(\varepsilon \frac{\partial \psi}{\partial x}\right) = q(C + p - n), \quad \forall x \in \Omega \tag{4a}$$

for the electrostatic potential $\psi = \psi(x,t)$ and the continuity equations

$$-q\frac{\partial n}{\partial t} + \frac{\partial J_n}{\partial x} = q\, R, \qquad q\frac{\partial p}{\partial t} + \frac{\partial J_p}{\partial x} = -q\, R, \quad \forall x \in \Omega \tag{4b}$$

for the densities of electrons $n = n(x,t)$ and holes $p = p(x,t)$. In (4a)-(4b) ε represents the dielectric constant and q is the elementary charge. The current densities caused by electrons and holes, J_n and J_p respectively, can be described as a composition of a drift and a diffusion current,

$$J_n = q\, \mu_n \left(U_T \frac{\partial n}{\partial x} - n\frac{\partial \psi}{\partial x}\right), \qquad J_p = -q\, \mu_p \left(U_T \frac{\partial p}{\partial x} + p\frac{\partial \psi}{\partial x}\right). \tag{4c}$$

In the previous expressions U_T is the thermal voltage, it depends on the Boltzmann constant, the elementary charge and the temperature T of the semiconductor. Here we will consider T as a constant. The electrons and holes mobilities, μ_n and μ_p respectively, are assumed to be nonnegative, bounded functions of x.

In (4a) $C = C(x)$ is the doping profile of the semiconductor. The function R in (4b) describes the balance of generation and recombination of electrons and holes. Frequently used models for R are the Shockley-Read-Hall recombination R_{SHR} and the Auger recombination R_{Au},

$$
\begin{aligned}
&R_{SRH} = \frac{np - \eta_i^2}{\tau_n(p + \eta_i) + \tau_p(n + \eta_i)}, \quad R_{Au} = (np - \eta_i^2)(C_n n + C_p p), \\
&R = R_{SHR} + R_{Au},
\end{aligned}
$$

where τ_n and τ_p reflect the average lifetimes of electrons and holes. The so-called intrinsic concentration η_i is the geometric average of the carrier concentrations in a semiconductor in equilibrium and C_n and C_p are the Auger coefficients.

For a more detailed description of mathematical models for semiconductors and results about existence and uniqueness of solutions of these models see e.g. [15,16,5,12,6,8].

The electric currents

$$
\begin{pmatrix} j_0(t) \\ j_l(t) \end{pmatrix} = \begin{pmatrix} J(0,t) \\ -J(l,t) \end{pmatrix} \text{ with } J(x,t) = J_n(x,t) + J_p(x,t) - \varepsilon \frac{\partial}{\partial t}\frac{\partial \psi}{\partial x}(x,t),
$$

represent the semiconductor's output to the potentials applied to its boundary. The values of $j_0(t)$ and $j_l(t)$ satisfy $j_l(t) = -j_0(t),\ \forall t \in [t_a,\, t_b]$ [2]. This means that we may choose one of the terminals of the semiconductor device as reference terminal, let us say the terminal at $x = l$, the current through it may be calculated in terms of the current leaving the other terminal. In what follows we will refer to $j_0(t)$ as the semiconductor's current.

Because the dependent variables in (4) are of highly different orders of magnitude and show a strongly different behavior in regions with small and large space charge, two scalings are recommended in [16]. The scaled one-dimensional

[2] This is a consequence of charge conservation. Differentiating (4a) with respect to time and adding (4b) yields $\dfrac{\partial J}{\partial x} \equiv 0$.

Poisson equation [3] reads

$$-\frac{\partial}{\partial x}\left(\lambda^2\frac{\partial\psi}{\partial x}\right) = C - n + p, \quad \lambda^2 = \frac{\varepsilon U_T}{qC_0x_s^2}. \tag{5a}$$

The constants C_0 and x_s depend on the scaling. The continuity equations change to

$$-\frac{\partial n}{\partial t} + \frac{\partial J_n}{\partial x} = R, \qquad J_n = \mu_n\left(\frac{\partial n}{\partial x} - n\frac{\partial\psi}{\partial x}\right) \tag{5b}$$

$$\frac{\partial p}{\partial t} + \frac{\partial J_p}{\partial x} = -R, \qquad J_p = -\mu_p\left(\frac{\partial p}{\partial x} + p\frac{\partial\psi}{\partial x}\right) \tag{5c}$$

and the boundary and initial conditions for the scaled model are

$$\psi(0,t) = \frac{1}{U_T}\left(\psi_{bi}(0) + \omega_0(e(t))\right), \quad \psi(l,t) = \frac{1}{U_T}\left(\psi_{bi}(l) + \omega_l(e(t))\right), \tag{5d}$$

$$n(0,t) = \frac{C(0) + \sqrt{C(0)^2 + 4\eta_i^2}}{2}, \quad n(l,t) = \frac{C(l) + \sqrt{C(l)^2 + 4\eta_i^2}}{2}, \tag{5e}$$

$$p(0,t) = \frac{-C(0) + \sqrt{C(0)^2 + 4\eta_i^2}}{2}, \quad p(l,t) = \frac{-C(l) + \sqrt{C(l)^2 + 4\eta_i^2}}{2}, \tag{5f}$$

$$n(x,t_a) = n_a(x), \quad p(x,t_a) = p_a(x). \tag{5g}$$

The function $\psi_{bi}(x)$ is the built-in potential and ω_0, ω_l are the externally applied biases. In this work we want to consider the semiconductor devices as part of an electrical circuit modeled by (1)-(3). Then the biases applied to the semiconductor boundaries depend on the node potentials of the circuit, that is why in (5d) we have written ω_0 and ω_l as functions of e.

The current of the semiconductor in terms of the scaled variables is

$$j_0(t) = \frac{q\mu_0U_TC_0}{x_s}J(0,t) = \frac{q\mu_0U_TC_0}{x_s}\left(J_n(0,t) + J_p(0,t) - \lambda^2\frac{\partial}{\partial x}\frac{\partial\psi}{\partial t}(0,t)\right),$$

where μ_0 is a constant that also depends on the scaling.

In [7] it is pointed out that not only for the numerical solution of this problem, but also for the study of its analytical properties, it is convenient to replace the Poisson equation (5a) by the energy conservation equation

$$\frac{\partial J}{\partial x} = \frac{\partial}{\partial x}\left(J_n + J_p - \lambda^2\frac{\partial}{\partial x}\frac{\partial\psi}{\partial t}\right) = 0, \tag{6}$$

[3] The scaled variables and constants have been named as the original ones.

that is obtained after differentiation of the Poisson equation with respect to time and elimination of $\dfrac{\partial n}{\partial t}$ and $\dfrac{\partial p}{\partial t}$ from the continuity equations. If the initial value for $\psi(x, t_a) = \psi_a(x)$ is chosen such that the functions $\psi_a(x), n_a(x)$ and $p_a(x)$ satisfy the Poisson equation,

$$-\frac{\partial}{\partial x}\left(\lambda^2 \frac{\partial\, \psi_a}{\partial\, x}\right) = q(C + p_a - n_a) \tag{7}$$

the equivalence between (5a) and (6) is guaranteed [7].

3.1 Finite Element Method for the Numerical Solution of the Drift-Diffusion Equations

The functions $(\psi(x,t), n(x,t), p(x,t))$ are a weak solution of (5) if

$$\psi(x,t), n(x,t), p(x,t) \in L_2\left((t_a, t_b), H^1(\Omega)\right),$$

have generalized derivatives $\dfrac{\partial n}{\partial t}, \dfrac{\partial p}{\partial t} \in L_2\left((t_a, t_b), L_2(\Omega)\right)$ and satisfy the equations

$$\lambda^2 \int_0^l \frac{\partial\psi}{\partial x}\frac{\partial\varphi}{\partial x}\mathrm{d}x = \int_0^l (C - n + p)\,\varphi \mathrm{d}x, \tag{8a}$$

$$-\int_0^l \frac{\partial n}{\partial t}\varphi\, \mathrm{d}x - \int_0^l J_n \frac{\partial\varphi}{\partial x}\,\mathrm{d}x = \int_0^l R\varphi\,\mathrm{d}x, \tag{8b}$$

$$\int_0^l \frac{\partial p}{\partial t}\varphi\, \mathrm{d}x - \int_0^l J_p \frac{\partial\varphi}{\partial x}\,\mathrm{d}x = -\int_0^l R\varphi\,\mathrm{d}x, \tag{8c}$$

for all functions $\varphi \in H_0^1(\Omega)$ and almost all $t \in [t_a, t_b]$ as well as the boundary and initial conditions in (5d)-(5g).

An approximation $(\psi_h(x,t), n_h(x,t), p_h(x,t))$ of the weak solution of this problem can be determined by the finite element method. For sake of simplicity, let us divide the interval $[0,\, l]$ into equally-spaced subintervals $[x_{i-1},\, x_i]$ with $h = x_i - x_{i-1}$, $x_1 = 0$, $x_m = l$ for $i = 2, \ldots, m$. Using the Galerkin ansatz

$$\psi_h(x,t) = \sum_{j=1}^{m} \psi_j(t)\varphi_j(x),$$

the function $\psi_h(x,t)$ is obtained by solving the system consisting of the equation (8a) for all basis functions $\varphi_i(x), i = 2, \ldots, m-1$ as well as the boundary and initial conditions in (5d)-(5g). As basis functions $\varphi_i(x)$ we choose the polynomials of degree one satisfying

$$\varphi_i(x_j) = \begin{cases} 1, & \text{if } i = j, \\ 0, & \text{else.} \end{cases}$$

for all $j = 1, 2, \ldots, m$. The integral in the right-hand-side of (8a) is approximated with the trapezoidal rule.

3.1.1 Discretization of the Continuity Equations

To obtain the approximations $n_h(x,t)$ and $p_h(x,t)$ equations (8b) and (8c) are not discretized in the usual way, but by the so-called Scharfetter-Gummel discretization [15]. This way, the area of convergence is usually larger than that one for the standard discretization. The Scharfetter-Gummel discretization is based on the assumption that $J_n(x,t)$ and $J_p(x,t)$ can be approximated by constant functions on each subinterval $(x_{j-1},\, x_j], j = 2, \ldots, m$.

Let us denote by $J_{n,h}(x,t)$, $J_{p,h}(x,t)$, $\mu_{n,h}$ and $\mu_{p,h}$ the piecewise constant functions that approximate $J_n(x,t)$, $J_p(x,t)$, μ_n and μ_p, respectively,

$$\begin{aligned} J_{n,h}(x,t) &= J_n^j(t), \quad J_{p,h}(x,t) = J_p^j(t), \\ \mu_{n,h}(x) &= \mu_n^j \;=\; \mu_n(x_{j-1} + h/2), \\ \mu_{p,h}(x) &= \mu_p^j \;=\; \mu_p(x_{j-1} + h/2) \end{aligned}$$

for $x \in (x_{j-1},\, x_j]$. The relation

$$\mu_n^j \left(\frac{\partial n_h}{\partial x} - n_h \frac{\partial \psi_h}{\partial x} \right) = J_n^j,$$

with $x \in [x_{j-1},\, x_j]$ and initial value $n_h(x_{j-1}, t) = n_{j-1}$ is an initial value problem (IVP) that can be solved for $n_h(x,t)$. Its solution is

$$n_h(x,t) = \begin{cases} e^{(\psi_j - \psi_{j-1})(x - x_{j-1})/h} \left(n_{j-1} + \frac{J_n^j}{\mu_n^j} \left(\frac{h}{\psi_j - \psi_{j-1}} \right) \right) - \frac{J_n^j}{\mu_n^j} \left(\frac{h}{\psi_j - \psi_{j-1}} \right) & \text{if } \psi_j \neq \psi_{j-1} \\ n_{j-1} + \frac{J_n^j}{\mu_n^j} (x - x_{j-1}) & \text{else.} \end{cases}$$

Evaluating $n_h(x,t)$ at $x = x_j$, an expression for J_n^j in terms of ψ_{j-1}, ψ_j, n_{j-1} and n_j is obtained. In a similar way, J_p^j can be calculated in terms of ψ_{j-1}, ψ_j, p_{j-1} and p_j.

Replacing φ by the basis functions φ_j in (8b)-(8c) yields

$$
\begin{aligned}
-\int_{x_{j-1}}^{x_{j+1}} \frac{\partial n}{\partial t}\varphi_j \,\mathrm{d}x - J_n^j \int_{x_{j-1}}^{x_j} \frac{\partial \varphi_j}{\partial x}\,\mathrm{d}x - J_n^{j+1}\int_{x_j}^{x_{j+1}} \frac{\partial \varphi_j}{\partial x}\,\mathrm{d}x &= \int_{x_{j-1}}^{x_{j+1}} R\varphi_j \,\mathrm{d}x,\\
\int_{x_{j-1}}^{x_{j+1}} \frac{\partial p}{\partial t}\varphi_j \,\mathrm{d}x - J_p^j \int_{x_{j-1}}^{x_j} \frac{\partial \varphi_j}{\partial x}\,\mathrm{d}x - J_p^{j+1}\int_{x_j}^{x_{j+1}} \frac{\partial \varphi_j}{\partial x}\,\mathrm{d}x &= -\int_{x_{j-1}}^{x_{j+1}} R\varphi_j \,\mathrm{d}x
\end{aligned}
$$

for $j = 2, 3, \ldots, m-1$. Inserting the expressions obtained above for J_n^j and J_p^j into the last equations and approximating the integrals that contain partial derivatives with respect to time and those in the right-hand-sides by the trapezoidal rule we obtain an IVP for the coefficients that define $n_h(x,t)$ and $p_h(x,t)$

$$
\begin{aligned}
-h\frac{\mathrm{d}}{\mathrm{d}t}n_j + \frac{1}{h}\mu_n^{j+1}f(z_{j+1})n_{j+1} - \frac{1}{h}\left(\mu_n^{j+1}f(-z_{j+1}) + \mu_n^j f(z_j)\right)n_j&\\
+\frac{1}{h}\mu_n^j f(-z_j)n_{j-1} - hR_j &= 0, \quad (9)\\
h\frac{\mathrm{d}}{\mathrm{d}t}p_j - \frac{1}{h}\mu_p^{j+1}f(-z_{j+1})p_{j+1} + \frac{1}{h}\left(\mu_p^{j+1}f(z_{j+1}) + \mu_p^j f(-z_j)\right)p_j&\\
-\frac{1}{h}\mu_p^j f(z_j)p_{j-1} + hR_j &= 0, \quad (10)
\end{aligned}
$$

$$
\begin{aligned}
&n_1 = n(0,t),\; n_m = n(l,t),\; p_1 = p(0,t),\; p_m = p(l,t),\\
&n_j(t_a) = n_a(x_j),\; p_j(t_a) = p_a(x_j), \qquad \text{for } j = 2, 3, \ldots, m-1.
\end{aligned}
$$

In the first two equations, $z_j = \psi_j - \psi_{j-1}$ and

$$
f(z) = \begin{cases} \frac{z}{e^z - 1}, & \text{if } z \neq 0,\\ 1, & \text{else.}\end{cases}
$$

The function $n_h(x,t)$ has the form, for $x \in (x_{j-1},\, x_j]$ and $t \in [t_a,\, t_b]$,

$$
n_h(x,t) = \begin{cases} n_j\left(\frac{e^{z_j(x-x_{j-1})/h}-1}{e^{z_j}-1}\right) - n_{j-1}\left(\frac{e^{z_j(x-x_{j-1})/h}-e^{z_j}}{e^{z_j}-1}\right), & \text{if } z_j \neq 0,\\ n_{j-1} + (n_j - n_{j-1})\frac{x-x_{j-1}}{h}, & \text{else.}\end{cases} \quad (11)
$$

The current of the semiconductor can be approximated by

$$
j_0(t) \approx \frac{q\mu_0 U_T C_0}{x_s}\left(J_{n,h}(0,t) + J_{p,h}(0,t) - \lambda^2 \frac{\partial}{\partial t}\frac{\partial \psi_h(0,t)}{\partial x}\right) = j_S^c - \frac{\mathrm{d}}{\mathrm{d}t}j_S^d,
$$

where j_S^c denotes the conduction current and the derivative of j_S^d with respect to the time, the displacement current,

$$j_S^c = \alpha \left(J_{n,h}(0,t) + J_{p,h}(0,t) \right), \quad \alpha = \frac{q\mu_0 U_T C_0}{x_s}$$
$$j_S^d = \beta \left(\psi_2(t) - \psi_1(t) \right) = \beta \left(\psi_2(t) - \frac{1}{U_T} \left(\psi_{bi}(0) + \omega_0(e,t) \right) \right), \quad \beta = \alpha \frac{\lambda^2}{h}.$$

If standard finite elements are used to obtain the approximations $n_h(x,t)$ and $p_h(x,t)$, i.e., if $n_h(x,t) = \sum_{j=1}^{m} n_j(t)\varphi_j(x)$ instead of (11), the equations that define the coefficients $n_j(t)$ and $p_j(t)$ have the same form as (9) and (10), but $f(z) = 1 - \frac{z}{2}$. Note that only when $z_j = 0$ one obtains the same approximation to $n(x,t)$ and $p(x,t)$, $x \in (x_{j-1}, x_j]$.

For the proof of convergence of the discretization scheme presented here we refer to [15].

3.1.2 Resulting Initial Value Problem

Let us denote by $\Psi(t), N(t)$ and $P(t)$ the unknowns of the discretized problem, i.e., $\Psi(t) = (\psi_2(t), \ldots, \psi_{m-1}(t))^T$, $N(t) = (n_2(t), \ldots, n_{m-1}(t))^T$ and $P(t) = (p_2(t), \ldots, p_{m-1}(t))^T$ for $t \in [t_a, t_b]$. The resulting initial value problem for Ψ, N and P can be written as an index-1 semi-explicit DAE

$$T\Psi - \left(\frac{h}{\lambda}\right)^2 (C - N + P) - \Psi_0(e,t) = 0, \tag{12a}$$
$$\frac{\mathrm{d}}{\mathrm{d}t} N - \frac{1}{h^2} g_1(e, \Psi, N, t) + R(N,P) = 0, \tag{12b}$$
$$\frac{\mathrm{d}}{\mathrm{d}t} P + \frac{1}{h^2} g_2(e, \Psi, P, t) + R(N,P) = 0, \tag{12c}$$

$$\Psi(t_a) = \Psi_a, \quad N(t_a) = N_a, \quad P(t_a) = P_a \tag{12d}$$

where $\Psi_0(e,t)$ has the components[4] $\Psi_0(e,t) = (\psi_1(t)\ 0\ \ldots\ 0\ \psi_m(t))^T$ and $T \in \mathbb{R}^{(m-2)\times(m-2)}$ is the tridiagonal matrix with elements

$$T(i,i) = 2, \quad T(i+1,i) = T(i,i+1) = -1 \quad i = 1, 2, \ldots, m-2.$$

The vectors C and R have components $C(x_{i+1})$ and $R(N(i), P(i))$ for $i = 1, 2, \ldots, m-2$. The functions g_1 and g_2 are vector-valued functions easily identifiable from the discretized equations. Since their expressions depend on the node potentials of the circuit, we have written them as functions of e too. The vectors N_a and P_a represent the initial values for $N(t)$ and $P(t)$, $N_a = (n_a(x_2), \ldots, n_a(x_{m-1}))^T$, $P_a = (p_a(x_2), \ldots, p_a(x_{m-1}))^T$. If the initial

[4] $\psi_1(t) = \psi(0,t)$ and $\psi_m(t) = \psi(l,t)$. They depend on the node potentials of the circuit.

value for $\Psi(t)$ is such that

$$\Psi_a = T^{-1}\left(\frac{h}{\lambda}\right)^2 (C - N_a + P_a) + T^{-1}\Psi_0(e_a, t_a), \tag{12e}$$

then (12) has a locally unique solution and is equivalent to the ODE

$$\frac{\mathrm{d}}{\mathrm{d}t}\Psi + T^{-1}\frac{1}{\lambda^2}\left(g_1(e,\Psi,N,t) + g_2(e,\Psi,P,t)\right) - T^{-1}\frac{\mathrm{d}}{\mathrm{d}t}\Psi_0(e,t) = 0, \tag{13a}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}N - \frac{1}{h^2}g_1(e,\Psi,N,t) + R(N,P) = 0, \tag{13b}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}P - \frac{1}{h^2}g_2(e,\Psi,P,t) + R(N,P) = 0. \tag{13c}$$

This ODE is obtained when the model consisting of the continuity equations and the energy conservation equation is discretized using a finite element method as described above.

4 Coupling of the Network and Space-Discretized Drift-Diffusion Equations

In [18], the partial differential algebraic equation that results from the coupling between the circuit equations and drift-diffusion equations for the semiconductor devices was studied as abstract differential algebraic system [11]. There it was proved that the coupled system has an index not greater than two if the assumptions in section 2 are satisfied. More precisely, it has index 2 if and only if the circuit contains LI-cut sets or CVS-loops (loops of capacitors, voltage sources and semiconductor devices) with at least one voltage source or one semiconductor device.

In this work we study the coupling between the circuit equations and discretized drift-diffusion equations for the semiconductor devices in the circuit and prove that this system has the same index under the same conditions on the circuit as the system considered in [18].

Suppose we want to couple n_S semiconductor devices, described by discretized drift-diffusion models, to an electrical circuit. The vector $j_S = (j_{01}, \ldots, j_{0n_S})^T$ represents the current through the semiconductors. The incidence of these currents in the circuit may be described by $A_S j_S$ where $A_S \in \mathbb{R}^{n_N \times n_S}$ is such that

$$A_S(i,k) = \begin{cases} -1, & \text{if the reference terminal of the semiconductor } k \\ & \text{is connected to node } i, \\ 1, & \text{if the other terminal of the semiconductor } k \\ & \text{is connected to node } i, \\ 0, & \text{else.} \end{cases}$$

If δ_{i,n_S} represents the i-th unitary vector of dimension n_S and the k-th semiconductor device is connected to nodes i_k and j_k of the circuit with the reference terminal connected to node j_k, the k-th column of A_S is equal to the difference between the i-th and the j-th unitary vectors, i.e., $A_S\delta_{k,n_S} = \delta_{i_k,n_N} - \delta_{j_k,n_N}$. The biases applied to the semiconductor terminals can also be described in terms of A_S

$$\begin{pmatrix} \omega_{0_k}(e,t) \\ \omega_{l_k}(e,t) \end{pmatrix} = \begin{pmatrix} e_{i_k}(t) \\ e_{j_k}(t) \end{pmatrix} = \begin{pmatrix} \delta^T_{i_k,n_N} e \\ \delta^T_{j_k,n_N} e \end{pmatrix} = \begin{pmatrix} \delta^T_{i_k,n_N} e \\ \delta^T_{i_k,n_N} e - \delta^T_{k,n_S} A_S^T e \end{pmatrix}.$$

Since the t variable in the semiconductor equations was scaled, the circuit equations must also be scaled before coupling the discretized drift-diffusion equations to them. With

$$\begin{aligned} &\hat{t} = \frac{1}{t_s} t,\ \hat{e}(\hat{t}) = e(t),\ \hat{j}_L(\hat{t}) = j_L(t),\ \hat{j}_V(\hat{t}) = j_V(t), \\ &\hat{i}_S(\hat{t}) = i_S(t),\ \hat{v}_S(\hat{t}) = v_S(t), \\ &\hat{q}(A_C^T\hat{e},\hat{t}) = \frac{1}{t_s} q(A_C^T e,t),\ \hat{\phi}(\hat{j}_L,\hat{t}) = \frac{1}{t_s}\phi(j_L,t),\ \hat{g}(A_R^T\hat{e},\hat{t}) = g(A_R^T e,t), \end{aligned}$$

the scaled circuit equations have the same form as (1)-(3).

The system that describes the behavior of the circuit containing n_S semiconductor devices is formed by the scaled modified nodal analysis equations [5], where the first one changes to [19]

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

in order to include the incidence of the semiconductor devices currents into the circuit and the discretized drift-diffusion models of the n_S semiconductor devices we want to couple to the circuit.

[5] The scaled variables have been renamed as the original ones.

Let us connect one semiconductor device to the circuit, suppose it is located between the nodes i and j with its reference terminal connected to node j. In this case, the DAE that results from the coupling of the circuit equations with the discretized semiconductor equations reads

$$
\begin{aligned}
A_C \frac{\mathrm{d}}{\mathrm{d}t} q_C(A_C^T e, t) + A_R g(A_R^T e, t) + A_L j_L + A_V j_V + A_I i_S(t) & \\
+ A_S j_S &= 0, && \text{(14a)}\\
\frac{\mathrm{d}}{\mathrm{d}t}\phi(j_L, t) - A_L^T e &= 0, && \text{(14b)}\\
A_V^T e - v_S(t) &= 0, && \text{(14c)}\\
j_S^d - \beta\left(\delta_{1,m-2}^T \Psi - \tfrac{1}{U_T}\psi_{bi}(0) - \frac{1}{U_T} e_i\right) &= 0, && \text{(14d)}\\
j_S(t) - j_S^c(e, \Psi, N, P, t) + \frac{\mathrm{d}}{\mathrm{d}t} j_S^d &= 0, && \text{(14e)}\\
T\Psi - \left(\tfrac{h}{\lambda}\right)^2 (C - N + P) - \Psi_0(e) &= 0, && \text{(14f)}\\
\frac{\mathrm{d}}{\mathrm{d}t} N - \frac{1}{h^2} g_1(e, \Psi, N, t) + R(N, P) &= 0, && \text{(14g)}\\
\frac{\mathrm{d}}{\mathrm{d}t} P + \frac{1}{h^2} g_2(e, \Psi, P, t) + R(N, P) &= 0, && \text{(14h)}
\end{aligned}
$$

where the function $\Psi_0(e)$ is

$$
\Psi_0(e) = \left(\tfrac{1}{U_T}\left(\psi_{bi}(0) + e_i\right),\ 0,\ \ldots,\ 0,\ \tfrac{1}{U_T}\left(\psi_{bi}(l) + e_j\right)\right)^T
$$

and A_S is a column vector, $A_S = \delta_{i,n_N} - \delta_{j,n_N}$. In order to study the properties of (14), we will rewrite it as a DAE of the form

$$
A \frac{\mathrm{d}}{\mathrm{d}t} d(y, t) + b(y, t) = 0 \tag{15}
$$

with unknowns $y = \left(e, j_L, j_V, j_S, j_S^d, \Psi, N, P\right)^T \in \mathbb{R}^{n_N + n_L + n_V + 1 + 1 + 3(m-2)}$. The matrix A and the vectors d and b are

$$
A = \begin{pmatrix} A_C & 0 & 0 & 0 & 0 \\ 0 & I & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & I & 0 \\ 0 & 0 & 0 & 0 & I \end{pmatrix}, \quad d(y, t) = \begin{pmatrix} q_C(A_C^T e, t) \\ \phi(j_L, t) \\ j_S^d \\ N \\ P \end{pmatrix}, \tag{16a}
$$

$$
b(y,t) = \begin{pmatrix} A_R g(A_R^T e,t)+A_L j_L+A_V j_V+A_I i_S(t)+A_S j_S \\ -A_L^T e \\ A_V^T e - v_S(t) \\ j_S^d - \beta\left(\delta_{1,m-2}^T \Psi - \frac{1}{U_T}\psi_{bi}(0) - \frac{1}{U_T} e_i\right) \\ j_S - j_S^c(e,\Psi,N,P,t) \\ T\Psi - \left(\frac{h}{\lambda}\right)^2 (C-N+P) - \Psi_0(e,t) \\ -\frac{1}{h^2} g_1(e,\Psi,N,t)+R(N,P) \\ \frac{1}{h^2} g_2(e,\Psi,P,t)+R(N,P) \end{pmatrix}. \tag{16b}
$$

The null space of A is given by $\ker A = \ker A_C \times \{0\} \times \{0\} \times \{0\} \times \{0\}$. The image space of

$$
D(y,t) := \frac{\partial d(y,t)}{\partial y} = \begin{pmatrix} C(A_C^T e,t)A_C^T & 0 & 0\ 0\ 0\ 0\ 0\ 0 \\ 0 & L(j_L,t) & 0\ 0\ 0\ 0\ 0\ 0 \\ 0 & 0 & 0\ 0\ 1\ 0\ 0\ 0 \\ 0 & 0 & 0\ 0\ 0\ 0\ I\ 0 \\ 0 & 0 & 0\ 0\ 0\ 0\ 0\ I \end{pmatrix}
$$

is $\operatorname{im} D(y,t) = \operatorname{im} C(A_C^T e,t)A_C^T \times \mathbb{R}^{n_L} \times \mathbb{R} \times \mathbb{R}^{m-2} \times \mathbb{R}^{m-2}$. The positive definiteness of $C(A_C^T e,t)$ implies that $\ker A_C \cap \operatorname{im} C(A_C^T e,t)A_C^T = \{0\}$ and $\dim(\ker A_C) + \dim(\operatorname{im} C(A_C^T e,t)A_C^T) = n_C$. Then, A and $D(y,t)$ satisfy

$$
\ker A \oplus \operatorname{im} D(y,t) = \mathbb{R}^{n_C+n_L+1+2(m-2)}. \tag{17}
$$

The DAE (15) with A, d and b as in (16) has a properly stated leading term [10] if, besides (17), the spaces $\ker A$ and $\operatorname{im} D(y,t)$ are independent of y and have bases that are continuously differentiable in t and $d(y,t) \in \operatorname{im} D(y,t)$, $\forall y$, $\forall t \in [t_a,\, t_b]$. In (16), $\ker A$ is constant, but $\operatorname{im} D(y,t)$ depends on y, with $\tilde{R} = A^+ A$ it can be reformulated as [6]

$$
A \frac{\mathrm{d}}{\mathrm{d}t}\left(\tilde{R} d(y,t)\right) + b(y,t) = 0 \tag{18}
$$

that has a properly stated leading term [14]. Due to $A\tilde{R} = A$, Backward Differentiation Formulas (BDF) and Runge–Kutta (RK) methods applied to (15) and (18) are equivalent and there is no need to compute $\tilde{R}$ in practice.

Lemma 1 *If the assumptions in section 2 are satisfied and the circuit contains neither LI-cut sets nor CVS-loops with at least one voltage source or one semiconductor device, the DAE (18) has index one.*

PROOF. For the index determination, we use the tractability index concept. It allows us to compute the index checking the rank of certain matrices only. Let

$$
G_0(y,t) = A\tilde{R}D = AD,\ B_0(y,t) = \frac{\partial b}{\partial y}(y,t),\ N_0(y,t) = \ker G_0(y,t),
$$

[6] A^+ denotes the Moore-Penrose pseudo inverse of A.

Q_0 be a projector onto N_0 and $G_1 = G_0 + B_0 Q_0$. If G_0 is singular with constant rank and G_1 is non-singular, the DAE has tractability index one. Note that

$$N_0(y,t) = N_0 = \left\{ y \mid y_e \in \ker A_C^T,\ y_L = y_S^d = y_N = y_P = 0 \right\}$$

and, if Q_C denotes a projector onto $\ker A_C^T$, the matrix

$$Q_0 = \begin{pmatrix} Q_C & 0&0&0&0&0&0&0 \\ 0 & 0&0&0&0&0&0&0 \\ 0 & 0&I&0&0&0&0&0 \\ 0 & 0&0&1&0&0&0&0 \\ 0 & 0&0&0&0&0&0&0 \\ 0 & 0&0&0&0&I&0&0 \\ 0 & 0&0&0&0&0&0&0 \\ 0 & 0&0&0&0&0&0&0 \end{pmatrix}$$

is a projector onto N_0. Then

$$G_1 = \begin{pmatrix} A_C C(A_C^T e,t) A_C^T + A_R G(A_R^T e,t) A_R^T Q_C & 0 & A_V & A_S & 0 & 0 & 0 & 0 \\ -A_L^T Q_C & L(j_L,t) & 0 & 0 & 0 & 0 & 0 & 0 \\ A_V^T Q_C & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{\beta}{U_T} \delta_{i,n_N}^T Q_C & 0 & 0 & 0 & 0 & -\beta \delta_{1,m-2}^T & 0 & 0 \\ -\frac{\partial j_S^c}{\partial e} Q_C & 0 & 0 & 1 & 1 & -\frac{\partial j_S^c}{\partial \Psi} & 0 & 0 \\ -\frac{1}{U_T}\left(\delta_{i,n_N}\ 0 \ldots \delta_{j,n_N}\right)^T Q_C & 0 & 0 & 0 & 0 & T & 0 & 0 \\ -\frac{1}{h^2}\frac{\partial g_1}{\partial e} Q_C & 0 & 0 & 0 & 0 & -\frac{1}{h^2}\frac{\partial g_1}{\partial \Psi} & I & 0 \\ \frac{1}{h^2}\frac{\partial g_2}{\partial e} Q_C & 0 & 0 & 0 & 0 & \frac{1}{h^2}\frac{\partial g_2}{\partial \Psi} & 0 & I \end{pmatrix}.$$

The vector $y = \left(y_e\ y_L\ y_V\ y_S\ y_S^d\ y_\Psi\ y_N\ y_P\right)^{\mathrm{T}}$ belongs to $\ker G_1$ if and only if it satisfies

$$y_L = L(\cdot)^{-1} A_L^T Q_C y_e, \quad y_N = \tfrac{1}{h^2}\left(\tfrac{\partial g_1}{\partial e} Q_C y_e + \tfrac{\partial g_1}{\partial \Psi} y_\Psi\right) \tag{19a}$$

$$y_P = -\tfrac{1}{h^2}\left(\tfrac{\partial g_2}{\partial e} Q_C y_e + \tfrac{\partial g_2}{\partial \Psi} y_\Psi\right), \quad y_S^d = \tfrac{\partial j_S^c}{\partial e} Q_C y_e - y_S + \tfrac{\partial j_S^c}{\partial \Psi} y_\Psi, \tag{19b}$$

$$y_\Psi = \tfrac{1}{U_T} T^{-1} \left(\delta_{i,n_N}\ 0\ \cdots\ 0\ \delta_{j,n_N}\right)^T Q_C y_e, \tag{19c}$$

$$A_C C(\cdot) A_C^T y_e + A_R G(\cdot) A_R^T Q_C y_e + A_V y_V + A_S y_S = 0, \tag{19d}$$

$$A_V^T Q_C y_e = 0, \tag{19e}$$

$$\tfrac{1}{U_T} \delta_{i,n_N}^T Q_C y_e - \delta_{1,m-2}^T y_\Psi = 0. \tag{19f}$$

Inserting y_Ψ from (19c) into (19f) yields $A_S^T Q_C y_e = 0$ because T satisfies[7] $T^{-1}(1,1) + T^{-1}(1,m-2) = 1$.

[7] The matrix T of size $k \in \mathbb{N}$ is a symmetric matrix of the form

$$T_k = \begin{pmatrix} \alpha_{k+1} + \alpha_k & -\alpha_k \delta_{1,k-1}^T \\ -\alpha_k \delta_{1,k-1} & T_{k-1} \end{pmatrix}.$$

This means that its inverse is also a symmetric matrix that can be written as $T_k^{-1} = \left(\begin{smallmatrix} a & b^T \\ b & C \end{smallmatrix}\right)$ with b a $(k-1)$-dimensional vector and C a $(k-1)\times(k-1)$ matrix, the scalar a and the vector b must then satisfy the k relations $(\alpha_{k+1} + \alpha_k)\, a - \alpha_k \delta_{1,k-1}^T b = 1$ and $-\alpha_k \delta_{1,k-1} a + T_{k-1} b = 0$, adding the last $k-1$ equations one

Let Q_{VS} be a projector onto $\ker \begin{pmatrix} A_V^T Q_C \\ A_S^T Q_C \end{pmatrix}$, then $Q_{VS} y_e = y_e$ and

$$Q_{VS}^T Q_C^T A_V = Q_{VS}^T Q_C^T A_S = 0.$$

Multiplying equation (19d) by $Q_{VS}^T Q_C^T$ one obtains that y_e must also satisfy $A_R^T Q_C y_e = 0$ (remember that $G(\cdot)$ is positive definite). Consequently, $Q_C y_e$ belongs to $\ker \left(A_C\ A_V\ A_R\ A_S\right)^T$ if we regard the previous conditions for $Q_C y_e$ and take into account that $A_C^T Q_C y_e = 0$.

Since Q_{CRVS} is a projector onto $\ker \left(A_C\ A_R\ A_V\ A_S\right)^T$, it holds that

$$Q_{CRVS}\, Q_C\, y_e = Q_C\, y_e.$$

Then, equation (19d) implies that y_e, y_L, y_V satisfy

$$A_C C(\cdot) A_C^T Q_C y_e + A_V y_V + A_S y_S = 0.$$

Multiplying this relation by Q_C^T one obtains that y_V, y_S fulfill

$$Q_C^T A_V y_V + Q_C^T A_S y_S = 0,$$

i.e., $\left(y_V\ y_S\right)^T \in \ker \left(Q_C^T A_V\ Q_C^T A_S\right)$.

If the circuit does not have LI-cut sets, the matrix $\left(A_C\ A_R\ A_V\ A_S\right)^T$ has full column rank and $Q_C y_e = 0$. If the circuit does not contain CVS-loops with at least one voltage source or one semiconductor device, the matrix $\left(Q_C^T A_V\ Q_C^T A_S\right)$ has full column rank and then $\left(y_V\ y_S\right)^T = 0$. Hence, condition (19d) implies $y_e \in \ker A_C C(\cdot) A_C^T = \ker A_C^T$, i.e., $y_e = Q_C y_e = 0$. Finally, $y_L = y_\Psi = y_N = y_P = y_S^d = 0$ and G_1 is a non-singular matrix. $\square$

Due to the results in [10] it can be assured that, under the assumptions of Lemma 1, the system (18) has also perturbation index one. Furthermore, if the initial value $y_a = (e_a, j_{La}, j_{Va}, j_{Sa}, j_{Sa}^d, \Psi_a, N_a, P_a)^T$ satisfies

$$Q_C^T(A_R g(A_R^T e_a, t_a) + A_L j_{La} + A_V j_{Va} + A_I i_S(t_a) + A_S j_{Sa}) = 0, \tag{20a}$$

$$A_V^T e_a - v_S(t_a) = 0, \tag{20b}$$

$$T\Psi_a - \left(\tfrac{h}{\lambda}\right)^2 (C - N_a + P_a) - \Psi_0(e_a, t_a) = 0, \tag{20c}$$

$$j_{Sa}^d - \beta\left(\delta_{1,m-2}^T \Psi_a - \tfrac{1}{U_T}\left(\psi_{bi}(0) + \delta_{i,n_N}^T e_a\right)\right) = 0 \tag{20d}$$

the DAE (18) is uniquely solvable. In addition, BDF and RK methods applied to its numerical solution, are convergent.

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obtains that $\alpha_k b_1 + \alpha_1 b_{k-1} = \alpha_k a$ that together with the first relation implies that $\alpha_{k+1} a + \alpha_1 b_{k-1} = 1$.

Suppose the circuit contains LI-cut sets or CVS-loops with at least one voltage source or one semiconductor device. Let Q_{C-VS} denote a projector onto $\ker Q_C^T\,(A_V\ A_S)$. Then, the vector y belongs to $\ker G_1$ if conditions (19a)-(19c) are satisfied and

$$A_C C(\cdot) A_C^T P_C y_e + A_V y_V + A_S y_S = 0,\ Q_C y_e = Q_{CRVS} Q_C y_e,\ \left(\begin{smallmatrix} y_V \\ y_S \end{smallmatrix}\right) = Q_{C-VS} \left(\begin{smallmatrix} y_V \\ y_S \end{smallmatrix}\right).$$

Since $\operatorname{im} Q_{CRVS} \subseteq \operatorname{im} Q_C$, the projector Q_{CRVS} may be constructed such that $\ker Q_C \subseteq \ker Q_{CRVS}$. The vector $y \in \ker G_1$ may then be described by conditions (19a)-(19c) and

$$P_C y_e = -H_C(\cdot)^{-1}\,(A_V\ A_S)\,Q_{C-VS}\,(y_V\ y_S)^T\,, \tag{21a}$$

$$Q_C y_e = Q_{CRVS}\,(y_e + Q_C y_e - y_e) = Q_{CRVS} y_e,\ \left(\begin{smallmatrix} y_V \\ y_S \end{smallmatrix}\right) = Q_{C-VS} \left(\begin{smallmatrix} y_V \\ y_S \end{smallmatrix}\right), \tag{21b}$$

where the matrix $H_C(\cdot) = A_C C(\cdot) A_C^T + Q_C^T Q_C$ is positive definite. Because of $P_C^T H_C(\cdot) = H_C(\cdot) P_C$, we get

$$Q_C H_C(\cdot)^{-1}\,(A_V\ A_S)\,Q_{C-VS} = H_C(\cdot)^{-1}\left(Q_C^T A_V\ Q_C^T A_S\right) Q_{C-VS} = 0$$

and $P_C H_C(\cdot)^{-1}\,(A_V\ A_S)\,Q_{C-VS} = H_C(\cdot)^{-1}\,(A_V\ A_S)\,Q_{C-VS}$.

If we denote $C_L = L(\cdot)^{-1} A_L^T$, $C_N = \frac{1}{h^2}(\frac{\partial g_1}{\partial e} + \frac{\partial g_1}{\partial \Psi} C_\Psi)$, $C_P = -\frac{1}{h^2}(\frac{\partial g_2}{\partial e} + \frac{\partial g_2}{\partial \Psi} C_\Psi)$, $C_{j_S^d} = (\frac{\partial j_S^c}{\partial e} + \frac{\partial j_S^c}{\partial \Psi} C_\Psi)$ and $C_\Psi = \frac{1}{U_T} T^{-1}(\delta_{i,n_N}\ 0\ \cdots\ 0\ \delta_{j,n_N})^T$, a projector Q_1 onto $\ker G_1$ can be written as

$$Q_1 = \begin{pmatrix} Q_{CRVS} & 0 & -H_C(\cdot)^{-1}(A_V\ A_S)Q_{C-VS} & 0\ 0\ 0\ 0 \\ C_L\, Q_{CRVS} & 0 & 0 & 0\ 0\ 0\ 0 \\ 0 & 0 & Q_{C-VS} & 0\ 0\ 0\ 0 \\ C_{j_S^d} Q_{CRVS} & 0 & (0 ... 0 - 1) Q_{C-VS} & 0\ 0\ 0\ 0 \\ C_\Psi Q_{CRVS} & 0 & 0 & 0\ 0\ 0\ 0 \\ C_N Q_{CRVS} & 0 & 0 & 0\ 0\ 0\ 0 \\ C_P Q_{CRVS} & 0 & 0 & 0\ 0\ 0\ 0 \end{pmatrix}.$$

Lemma 2 *If the assumptions in section 2 are satisfied, the circuit contains LI-cut sets or CVS-loops with at least one voltage source or one semiconductor device and N and P are always greater than zero, the DAE (18) has index 2.*

PROOF. Again, we use the tractability index concept for the index determination. The DAE has tractability index two if the matrix G_1 is singular and has constant rank and $G_2 = G_1 + B_0 P_0 Q_1$ is non-singular. It can be proved that if N and P are always greater than zero the matrix G_1 has constant rank [8]. It remains to show that G_2 is non-singular.

[8] By looking at the structure of Q_1 one sees that it has constant rank if the products $C_N Q_{CRVS}$, $C_P Q_{CRVS}$ and $C_{j_S^d} Q_{CRVS}$ have constant rank. Using that $\dim(\operatorname{im} AB) = \dim(\operatorname{im} B) - \dim(\operatorname{im} B \cap \ker A)$ the desired result is obtained.

In $B_0P_0Q_1$, only the first, third and fourth columns are different to zero, they are

$$\begin{pmatrix} A_LC_LQ_{CRVS} \\ 0 \\ 0 \\ C_{j_S^d}Q_{CRVS} \\ -\left(\frac{\partial j_S^c}{\partial N}C_N+\frac{\partial j_S^c}{\partial P}C_P\right)Q_{CRVS} \\ \left(\frac{h}{\lambda}\right)^2(C_N-C_P)Q_{CRVS} \\ \left(\left(-\frac{1}{h^2}\frac{\partial g_1}{\partial N}+\frac{\partial R}{\partial N}\right)C_N+\frac{\partial R}{\partial P}C_P\right)Q_{CRVS} \\ \left(\left(\frac{1}{h^2}\frac{\partial g_2}{\partial P}+\frac{\partial R}{\partial P}\right)C_P+\frac{\partial R}{\partial N}C_N\right)Q_{CRVS} \end{pmatrix}, \begin{pmatrix} -A_RG(\cdot)A_R^TH_C(\cdot)^{-1}(A_V\ A_S)Q_{C-VS} \\ A_L^TH_C(\cdot)^{-1}(A_V\ A_S)Q_{C-VS} \\ -A_V^TH_C(\cdot)^{-1}(A_V\ A_S)Q_{C-VS} \\ -\frac{\beta}{U_T}\delta_{i,n_C}^TH_C(\cdot)^{-1}(A_V\ A_S)Q_{C-VS}+(0\cdots 0\ -1)Q_{C-VS} \\ \frac{\partial j_S^c}{\partial e}H_C(\cdot)^{-1}(A_V\ A_S)Q_{C-VS} \\ \frac{1}{U_T}\left(\delta_{i,n_N}\ 0\cdots 0\ \delta_{j,n_N}\right)^TH_C(\cdot)^{-1}(A_V\ A_S)Q_{C-VS} \\ \frac{1}{h^2}\frac{\partial g_1}{\partial e}H_C(\cdot)^{-1}(A_V\ A_S)Q_{C-VS} \\ -\frac{1}{h^2}\frac{\partial g_2}{\partial e}H_C(\cdot)^{-1}(A_V\ A_S)Q_{C-VS} \end{pmatrix}.$$

Suppose the vector $y = (y_e\ y_L\ y_V\ y_S\ y_{S^d}\ y_\Psi\ y_N\ y_P)^T$ belongs to the null space of G_2. Multiplying the first equation of $G_2y = 0$ by Q_{CRVS}^T one obtains $Q_{CRVS}^TA_LL(\cdot)^{-1}A_L^TQ_{CRVS}y_e = 0$. Since $L(\cdot)$ is positive definite, this is equivalent to $A_L^TQ_{CRVS}y_e = 0$. Due to the assumption that the circuit does not contain cut sets of current sources only, the matrix $(A_C\ A_L\ A_R\ A_V\ A_S)^T$ has full column rank and, consequently, $A_L^TQ_{CRVS}y_e = 0 \Leftrightarrow Q_{CRVS}y_e = 0$.

Inserting y_Ψ from the sixth equation of $G_2y = 0$ into the fourth and taking into account that the matrix T satisfies that $T^{-1}(1,1) + T^{-1}(1,m-2) = 1$, the components y_e, y_V and y_S of y must satisfy

$$\delta A_S^T\left(Q_Cy_e - H_C(\cdot)^{-1}(A_V\ A_S)\,Q_{C-VS}\left(\begin{smallmatrix} y_V \\ y_S \end{smallmatrix}\right)\right) = \left(0\ \cdots\ 0\ \tfrac{1}{\beta}\right)Q_{C-VS}\left(\begin{smallmatrix} y_V \\ y_S \end{smallmatrix}\right)$$

where $\delta = \frac{T^{-1}(1,m-2)}{U_T}$. The last condition and the third equation of $G_2y = 0$ may be written as

$$\begin{pmatrix} A_V^T \\ A_S^T \end{pmatrix}Q_Cy_e - \begin{pmatrix} A_V^T \\ A_S^T \end{pmatrix}H_C(\cdot)^{-1}(A_V\ A_S)\,Q_{C-VS}\left(\begin{smallmatrix} y_V \\ y_S \end{smallmatrix}\right) = \begin{pmatrix} 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & 0 & \frac{1}{\beta\delta} \end{pmatrix}Q_{C-VS}\left(\begin{smallmatrix} y_V \\ y_S \end{smallmatrix}\right).$$

Multiplying it by Q_{C-VS}^T, we get

$$Q_{C-VS}^T\left((A_V\ A_S)^TH_C(\cdot)^{-1}(A_V\ A_S) + \begin{pmatrix} 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & 0 & 0 \\ 0 & \cdots & 0 & \frac{1}{\beta\delta} \end{pmatrix}\right)Q_{C-VS}\left(\begin{smallmatrix} y_V \\ y_S \end{smallmatrix}\right) = 0.$$

Because the matrices in this sum are positive definite, it is zero if and only if

$$(A_V\ A_S)\,Q_{C-VS}\left(\begin{smallmatrix} y_V \\ y_S \end{smallmatrix}\right) = 0 \quad \text{and} \quad Q_{C-VS}\left(\begin{smallmatrix} y_V \\ y_S \end{smallmatrix}\right) \in \ker\begin{pmatrix} 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & 0 & 0 \\ 0 & \cdots & 0 & \frac{1}{\beta\delta} \end{pmatrix}.$$

If $(v_1\ v_2)^T = Q_{C-VS}\left(\begin{smallmatrix} y_V \\ y_S \end{smallmatrix}\right)$, the above conditions imply $v_2 = 0$ and $A_V\,v_1 + A_S\,v_2 = 0$. Since A_V has full column rank we find $v_1 = 0$. Regarding. $Q_{CRVS}y_e = Q_{C-VS}\left(\begin{smallmatrix} y_V \\ y_S \end{smallmatrix}\right) = 0$, it holds that $B_0P_0Q_1y = 0$. Thus, y belongs to $\ker G_2$ if and only if it belongs to $\ker G_1$, i.e., if $y = Q_1 y$. This implies $Q_{CRVS} y_e = Q_{C-VS} \left(\begin{smallmatrix} y_V \\ y_S \end{smallmatrix} \right) = 0$ and $y = Q_1 y = 0$. $\square$

Due to the results in [13], it can be assured that, under the assumptions of Lemma 2, the DAE (18) has also perturbation index two.

Following the steps in lemmata 1 and 2, it is easy to prove that the results remain the same for a nonuniform spatial mesh and circuits containing more than one semiconductor device. Furthermore, the index results do not change when standard finite elements are used to approximate the functions $n(x,t)$ and $p(x,t)$.

Lemma 3 *The DAE that originates from the coupling of the ODE (13) to the circuit equations can also be written as a DAE with properly stated leading term and has the same index as the DAE previously analyzed.*

PROOF. This DAE can be written as a DAE of the form $\bar{A}\frac{\mathrm{d}}{\mathrm{d}t}\bar{d}(y,t)+\bar{b}(y,t) = 0$ with

$$\bar{A} = \begin{pmatrix} A_C & 0 & 0 & 0 & 0 & 0 \\ 0 & I & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & I & 0 & 0 \\ 0 & 0 & 0 & 0 & I & 0 \\ 0 & 0 & 0 & 0 & 0 & I \end{pmatrix}, \ \bar{d}(y,t) = \begin{pmatrix} q_C(A_C^T e,t) \\ \phi(j_L,t) \\ j_S^d \\ T\Psi-\Psi_0 \\ N \\ P \end{pmatrix},$$

$$\bar{b}(y,t) = \begin{pmatrix} A_R g(A_R^T e,t)+A_L j_L+A_V j_V+A_I i_S(t)+A_S j_S \\ -A_L^T e \\ A_V^T e-v_S(t) \\ j_S^d-\beta\left(\delta_{1,m-2}^T\Psi-\frac{1}{U_T}(\psi_{bi}(0)-e_i)\right) \\ j_S-j_S^c(e,\Psi,N,P,t) \\ \frac{1}{\lambda^2}(g_1(e,\Psi,N,t)+g_2(e,\Psi,N,t)) \\ -\frac{1}{h^2}g_1(e,\Psi,N,t)+R(N,P) \\ \frac{1}{h^2}g_2(e,\Psi,P,t)+R(N,P) \end{pmatrix}.$$

In this case, $\ker \bar{A} \oplus \operatorname{im} \bar{D}(y,t) = \mathbb{R}^{n_C+n_L+3(m-2)+1}$. The null space $\bar{N}_0$ of $\bar{G}_0$ is

$$\bar{N}_0 = N_0 \cap \left\{ y \mid y_\Psi = \frac{1}{U_T} T^{-1} \left(\delta_{i,n_N}\ 0\ \ldots\ 0\ \delta_{j,n_N}\right)^T y_e \right\}$$

and a projector $\bar{Q}_0$ onto $\bar{N}_0$ can then be written as

$$\bar{Q}_0 = Q_0 + \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{U_T}T^{-1}\left(\delta_{i,n_N}\ 0\cdots 0\ \delta_{j,n_N}\right)^T Q_C & 0 & 0 & 0 & 0 & -I & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}.$$

Following the steps in the proof of lemma 1 it can be proved that the DAE has index one if the circuit contains neither LI-cut sets nor CVS-loops with at least one voltage source or one semiconductor device. A projector $\bar{Q}_1$ onto the null space of $\bar{G}_1$ is now

$$\bar{Q}_1 = \begin{pmatrix} Q_{CRVS} & 0 & -H_C(\cdot)^{-1}(A_V\ A_S)Q_{C-VS} & 0\ 0\ 0\ 0 \\ C_L\, Q_{CRVS} & 0 & 0 & 0\ 0\ 0\ 0 \\ 0 & 0 & Q_{C-VS} & 0\ 0\ 0\ 0 \\ C_{j_S^d} Q_{CRVS} & 0 & (0...0{-}1)Q_{C-VS} & 0\ 0\ 0\ 0 \\ \bar{C}_\Psi Q_{CRVS} & 0 & -C_\Psi H_C(\cdot)^{-1}(A_V\ A_S)Q_{C-VS} & 0\ 0\ 0\ 0 \\ C_N Q_{CRVS} & 0 & 0 & 0\ 0\ 0\ 0 \\ C_P Q_{CRVS} & 0 & 0 & 0\ 0\ 0\ 0 \end{pmatrix}$$

with $\bar{C}_\Psi = C_\Psi - \left(\frac{h}{\lambda}\right)^2 T^{-1}\,(C_N - C_P)$.

In a very similar way as in lemma 2 it can be proved that also in this case the DAE has tractability index two if the circuit contains LI-cut sets or CVS-loops with at least one voltage source or one semiconductor device. $\square$

5 Summary

Electrical circuits containing semiconductor devices can be modeled as a coupled system of differential algebraic and partial differential equations. An approximate solution of such a system can be obtained, as proposed here, by discretizing the partial differential equations in space and solving numerically the resulting DAE. In order to gain information about how to choose consistent initial values, what type of numerical methods may be used for the solution of this DAE, etc., it is important to determine its index.

In the lemmata 1 and 2, the special case of an electrical circuit containing only one semiconductor device modeled by one-dimensional drift-diffusion equations was studied. We proved that the resulting DAE has always index smaller or equal to two. It can be determined by topological conditions on the circuit only. These results can easily be generalized to circuits with more semiconductor devices. We expect that if drift-diffusion equations in two or three spatial dimensions are used to model the semiconductor devices in the circuit the index conditions will be very similar.

Because for the numerical solution of the drift-diffusion equations it is sometimes recommended to replace the Poisson equation by the energy conservation equation we also studied the DAE resulting from the coupling of the circuit equations and the ODE (13). In lemma 3 it was proved that the results about the tractability index are also valid for this DAE.

For the numerical solution of the coupled system we have made some experiments with a coupling between the device simulator TeSCA [9] developed at

Weierstrass Institute in Berlin and DASSL [2]. It is our intention now to implement a software for the solution of the whole DAE that is not based on the coupling of the two simulators. Comparisons between both approaches will be the subject of a future work.

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