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INDEX-2 ELLIPTIC PARTIAL DIFFERENTIAL-ALGEBRAIC MODELS FOR CIRCUITS AND DEVICES

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Abstract. We consider a system of partial differential-algebraic equations which model an electric network containing semiconductor devices. We introduce a topological condition which permits to give a notion of tractability index for this kind of nonlinear coupled system, and prove an existence result for index-2 systems.

Key words. RLC networks, semiconductors, steady-state drift-diffusion, coupled systems, elliptic partial differential-algebraic equations (PDAEs), tractability index

AMS subject classifications. 35J60, 34M15

1. Introduction. Commonly in circuit simulation, network designs are simulated on the basis of lumped network equations. These equations are usually derived from Modified Nodal Analysis (MNA). Generally, this modeling yields a system of differential algebraic equations (DAEs). So-called index concepts [7] are used to classify these equations. The index roughly determines the number of inherent differentiations, which are needed to derive an ordinary differential equation.

For the classical MNA equations, various index cases can be distinguished solely by structural means. That is, the network topology determines the index, see e.g. [4, 5, 12]. Using for instance the tractability index [9], one decomposes the set of variables accordingly and projects parts of the equations.

Nowadays, downscaling as in semiconductor devices demands to include more and more former secondary effects in the electric circuit simulation. This leads directly to coupled systems of differential algebraic equations (DAEs) for the electric network and partial differential equations (PDEs) for the semiconductor devices. The coupling has two parts. On the one hand, an additional source term occurs in the current balance of the electric network. On the other hand, the boundary conditions of the device equations depend on the time-dependent node potentials, which are genuine unknowns of the electric network.

The scope of the work at hand is twofold. In first place, we wish to generalize the index concept available for DAEs to the setting above described, with coupled DAEs and PDEs. Our approach is to determine additional topological conditions on the coupling matrices which relate the DAE and PDE parts, such that the known results keep their validity for the enlarged system. This system will be viewed as electric network with a nonlinear controlled source (for the semiconductor device). And we will need to determine conditions under which the additional source terms has no further structural consequences. The second aim of this paper, is to establish an existence result for an index-2 system, according to the generalization above described. This is the main result of this paper, since to our knowledge no existence results are available in literature for index-2 systems in the class of our study.

The work is organized as follows. Section 2 covers the modeling of the coupled system; both subsystems are described in details and the coupling terms are defined. In Section 3 we recapitulate the tractability index concepts. We describe its application to the MNA equations and we give also a topological interpretation of the index conditions. In Section 4 we state the main result, whose

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proof is presented in the following Section 5. First, we establish necessary a priori estimates for the network equations, next we define an iteration map for the device equation. It will be used later to define an iteration map for the coupled problem, which allows to conclude the proof of the main theorem by applying Schauder's fixed point theorem.

2. Coupled circuit-device model. We consider electric networks which include some components described by distributed equations. The specific application we have in mind is a model for an integrated circuit with semiconductor devices. Nevertheless, this model is susceptible of different generalizations and extensions.

In this section we present the general coupled model, while we postpone the clarification of the needed mathematical assumptions to a later section.

An electric network is described by the electrical potentials at the nodes and by the currents through the branches. Using the approach of Modified Nodal Analysis (MNA) [6, 11], the electric network equations can be obtained by the Kirchhoff current law, replacing the constitutive equations for the currents through branches with capacitors and resistances, and by the constitutive equations for the remaining components. We consider a linear RLC network, that is, a network which connects linear capacitors, inductors and resistors, and independent voltage and current sources. We refer to the respective number of elements as n_C , n_L , n_R , n_V , and n_I . We assume that the network additionally connects semiconductor devices. Let the network has m nodes plus the ground node, where the potential is zero. We denote by $e(t) \in \mathbb{R}^m$ the node potentials, by $i_L(t) \in \mathbb{R}^{n_L}$ the currents through inductors, by $i_V(t) \in \mathbb{R}^{n_V}$ the currents through voltage sources, by $v_V(t) \in \mathbb{R}^{n_V}$ the given input of independent voltage sources, and by $i_I(t) \in \mathbb{R}^{n_I}$ the input of independent current sources. The resulting MNA equations can be written in the form

(2.1)
$$E\dot{x} = Ax + \sigma + b(t).$$

This is a differential-algebraic equation for the unknown

 $x^{\top} = \begin{bmatrix} e^{\top}, & i_L^{\top}, & i_V^{\top} \end{bmatrix} \in \mathbb{R}^n, \quad n = m + n_L + n_V,$

where the matrices $E, A \in \mathbb{R}^{n \times n}$ and the input data $b \in \mathbb{R}^n$ are given by

$$E = \begin{bmatrix} A_C C A_C^{\top} & O & O \\ O & L & O \\ O & O & O \end{bmatrix}, A = - \begin{bmatrix} A_R G A_R^{\top} & A_L & A_V \\ -A_L^{\top} & O & O \\ -A_V^{\top} & O & O \end{bmatrix}, b(t) = - \begin{bmatrix} A_I i_I(t) \\ O \\ v_V(t) \end{bmatrix}$$

Here, $A_C \in \mathbb{R}^{n \times n_C}$, $A_R \in \mathbb{R}^{n \times n_R}$, $A_L \in \mathbb{R}^{n \times n_L}$, $A_V \in \mathbb{R}^{n \times n_V}$, $A_I \in \mathbb{R}^{n \times n_I}$, are incidence matrices, which describe the topology of the network. Moreover $C \in \mathbb{R}^{n_C \times n_C}$, $G \in \mathbb{R}^{n_G \times n_G}$ and $L \in \mathbb{R}^{n_L \times n_L}$ denote the capacitance matrix, the conductance matrix and the inductance matrix, respectively, which are regular. The term σ in (2.1) represents the coupling with the devices which we treat below.

We need to supplement equation (2.1) with consistent initial data

(2.2)
$$x(t_0) = x_0.$$

The consistency of the initial data will be discussed in the next section.

For a detailed expression of σ , we need to introduce the device model. For simplicity we consider a network containing only one semiconductor device. The case of circuits with many devices can be dealt using the same arguments, but the notation would be much heavier. We assume that the device occupies a bounded domain $\Omega \subset \mathbb{R}^d$, and has $n_D + 1$ terminals. In other words, the boundary $\partial \Omega$ of Ω contains $n_D + 1$ open (in \mathbb{R}^{d-1}), disjoint, nonempty subsets Γ_i , $i = 0, 1, \ldots, n_D$, which represent the terminals of the device, and we can write

$$\partial \Omega = \Gamma \cup \Gamma_N, \quad \Gamma = \bigcup_{i=0}^{n_D} \Gamma_i, \quad \Gamma_N = \partial \Omega \setminus \Gamma.$$

We neglect all thermal effects, and assume that two carriers are responsible for the device's output current, that is, electrons with negative charge -q, and holes with positive charge q. The behavior of the device is described in terms of quasi-Fermi potentials for electron and holes, denoted by $\phi_n(\mathbf{x},t)$ and $\phi_p(\mathbf{x},t)$ and electrostatic potential, denoted by $\phi(\mathbf{x},t)$, with $(\mathbf{x},t) \in \Omega \times [t_0,t_1]$. The unknown $u = (\phi, \phi_n, \phi_p)$ satisfies the drift-diffusion equations [8]:

(2.3)
$$-\nabla \cdot (\epsilon \nabla \phi) = \rho, \qquad -\nabla \cdot (a_n \nabla \phi_n) = H, \qquad -\nabla \cdot (a_p \nabla \phi_p) = -H.$$

Here $\epsilon(\mathbf{x})$ is the dielectric constant, $\rho(\mathbf{x}, u)$ is the total charge density, $a_n(\mathbf{x}, u)$ and $a_p(\mathbf{x}, u)$ are the product of the mobilities times the respective carrier densities, and $H(\mathbf{x}, u)$ is the generationrecombination term. A more detailed description of these functions will be given later. The driftdiffusion equations are supplemented with Dirichlet boundary conditions on Γ , and homogeneous Neumann conditions on Γ_N :

(2.4a)
$$\phi - \phi_{\text{bi}} = \phi_n = \phi_p = e_{D,k}(t), \text{ on } \Gamma_{D,k}, \quad k = 0, \dots, n_D,$$

(2.4b)
$$\frac{\partial \phi}{\partial \nu} = \frac{\partial \phi_n}{\partial \nu} = \frac{\partial \phi_p}{\partial \nu} = 0, \quad \text{on} \quad \Gamma_N$$

where $\phi_{\rm bi}(\mathbf{x})$ is the built-in potential [8] (defined by $\rho(\mathbf{x}, u_{\rm bi}) = 0$, $u_{\rm bi} = (\phi_{\rm bi}, 0, 0)$), $e_{D,k}(t)$ is the applied potential at Γ_k , $k = 0, 1, \ldots, n_D$, and $\partial/\partial \nu = \nu \cdot \nabla$ is the normal derivative along the external unit normal to the boundary, ν . The time dependence of the device's unknown is caused by the time dependence of the external applied potentials, $e_D^{\top} = [e_{D,0}, e_{D,1}, \ldots, e_{D,n_D}]$.

The external potentials e_D coincide with the electric potentials at the nodes of the network which correspond to the terminals. The identification between external potential and node potential can be accomplished by using a selection matrix $S_D = (s_{D,kh}) \in \mathbb{R}^{m \times m_D}$, where $m_D = n_D + 1$ is the total number of device terminals connected to the network, and $s_{D,kh}$ is equal to 1 if the node k is connected to the terminal h, and equal to 0 otherwise. We can write

(2.5)
$$e_D = S_D^{\top} e = \hat{S}^{\top} x \quad \text{with} \quad \hat{S} = \begin{bmatrix} S_D \\ O \\ O \end{bmatrix} \in \mathbb{R}^{n \times m_D}$$

Notice the typographic difference to the space variable x. This coupling relation will be called *network-to-device coupling*, since it says how the network variables x affect the device variables u.

On the other hand, once we know a solution u to the drift-diffusion equations we can compute the currents through the terminals of the device (Ohmic contacts). At the terminal Γ_k $(k = 0, 1, \ldots, n_D)$, we define (e.g. [2])

$$j_{D,k}(t) = \int_{\Gamma_k} \nu \cdot j(\mathbf{x}, t) \, \mathrm{d}\Sigma(\mathbf{x}), \quad \text{with } j = -a_n \nabla \phi_n - a_p \nabla \phi_p.$$

For our purpose, this terminal currents can also be computed via space integrals. To this end, we introduce the auxiliary functions ψ_k , $k = 0, 1, ..., n_D$, defined by the unique solution of the following elliptic boundary value problem:

(2.6)
$$\begin{cases} -\nabla \cdot (\epsilon \nabla \psi_k) = 0, & \text{in } \Omega, \\ \psi_k = \delta_{ik}, & \text{on } \Gamma_i, \quad i = 0, 1, \dots, n_D, \qquad \frac{\partial \psi_k}{\partial \nu} = 0, \text{ on } \Gamma_N, \end{cases}$$

where δ_{ik} is Kronecker's delta ($\delta_{ik} = 1$ if i = k, $\delta_{ik} = 0$ if $i \neq k$). Then, the electric current $j_{D,k}$ through Γ_k is also given by

(2.7)
$$j_{D,k} = -\int_{\Omega} \nabla \psi_k \cdot (a_n \nabla \phi_n + a_p \nabla \phi_p) \,\mathrm{dx}$$

This is indeed compatible with the first definition above: from (2.3) we have $\nabla \cdot (a_n \nabla \phi_n + a_p \nabla \phi_p) = 0$; using Gauss' divergence theorem and recalling the boundary values of ψ_k , we recover the former definition (if ϕ_n , ϕ_p are sufficiently regular on the boundary). The device currents $j_{D,k}$ (2.7) then enter the current balances of the network. Thus the term σ in (2.1) takes the form

(2.8)
$$\sigma = -\hat{S}j_D, \quad j_D^{\top} = [j_{D,0}, \ j_{D,1}, \ \dots, \ j_{D,n_D}] \in \mathbb{R}^{m_D}$$

This coupling relation will be called *device-to-network coupling*, since it says how the device variable u affect the network variable x.

The network-to-device coupling condition and the device-to-network coupling condition can be relaxed. First, we observe that the current j_D is unchanged if the electric potential ϕ is shifted by a constant in space, possibly depending on time. Thus, we can modify the boundary values for u, replacing the applied potentials $e_{D,k}$ with the applied voltages $v_{D,k} = e_{D,k} - e_{D,0}, k = 0, 1, \ldots, n_D$, with respect to the ground terminal 0,

(2.9a)
$$\phi - \phi_{\text{bi}} = \phi_n = \phi_p = v_{D,k}(t), \text{ on } \Gamma_{D,k}, k = 0, \dots, n_D,$$

(2.9b)
$$\frac{\partial \phi}{\partial \nu} = \frac{\partial \phi_n}{\partial \nu} = \frac{\partial \phi_p}{\partial \nu} = 0, \quad \text{on} \quad \Gamma_N$$

We have $v_{D,0} = 0$, and we introduce the vector of applied voltages

$$v_D = \begin{bmatrix} v_{D,1} \\ \vdots \\ v_{D,n_D} \end{bmatrix} = \begin{bmatrix} e_{D,1} - e_{D,0} \\ \vdots \\ e_{D,n_D} - e_{D,0} \end{bmatrix}.$$

In compact form we can write

(2.10)
$$v_D = \hat{A}_D^\top e_D, \quad \hat{A}_D = \begin{bmatrix} -1 & \cdots & -1 \\ 1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 1 \end{bmatrix} \in \mathbb{R}^{m_D \times n_D}.$$

The applied voltages v_D depend on the node potentials of the network by means of an incidence matrix A_D , defined by using the selection matrix S_D ,

(2.11)
$$v_D = A_D^\top e, \quad A_D = S_D \hat{A}_D.$$

We introduce also the matrix

(2.12)
$$\hat{A} = \begin{bmatrix} A_D \\ O \\ O \end{bmatrix} \in \mathbb{R}^{n \times m_D}$$

Then we can write

(2.13)
$$v_D = A_D^\top e = \hat{A}^\top x.$$

This modified *network-to-device coupling* relation will be used throughout this paper.

Next, for any electric network element the sum of currents leaving it is zero. Of course this can also be proven for the considered semiconductor device, that is,

$$\sum_{i=0}^{n_D} j_{D,i} = 0.$$

Hence we can express $j_{D,0}$ as a linear combination of the current through the other terminals, so that we can write

(2.14)
$$j_D = \hat{A}_D i_D, \quad i_D = [j_{D,1}, \dots, j_{D,n_D}] \in \mathbb{R}^{n_D}.$$

Then we can recast (2.8) in the form

(2.15)
$$\sigma = -\hat{A}i_D.$$

This modified *device-to-network coupling* relation will be used throughout this paper.

In the following section we investigate the structure of the coupled problem (2.1), (2.2), (2.3), (2.9), (2.13), (2.15) from the viewpoint of the tractability index.

3. Tractability index. The full coupled problem presented in the previous section has the following general structure:

(3.1a) $\begin{cases} E\dot{x} = Ax + \sigma + b(t), & t \in [t_0, t_1], \\ x(t_0) = x_0, \end{cases}$

(3.1b)
$$\begin{cases} \mathcal{F}(\mathbf{x}, u, \nabla u, \nabla^2 u) = 0, & \mathbf{x} \in \Omega \subset \mathbb{R}^d \\ \mathcal{B}(\mathbf{x}, u, \partial u/\partial \nu, \eta) = 0, & \mathbf{x} \in \partial\Omega, \end{cases}$$

x

$$\left(\begin{array}{c} \mathcal{D}(\mathbf{x}, u, \partial u / \partial \nu, \eta) = 0, \end{array} \right)$$

(3.1c)
$$\sigma = U s(u)$$

(3.1d)
$$\eta = V^{\top}$$

for the unknown (x, σ, u, η) . In the following we explain all ingredients and their relation to the special case of an electric network with a distributed semiconductor device as described in the previous section.

(a) The first subproblem (3.1a) is a system of differential algebraic equations (DAE) for the unknown $x : [t_0, t] \to \mathbb{R}^n$, in a functional space \mathcal{W}_x , with initial data x_0 . The vector function $b(t) \in \mathbb{R}^n$ is a given input, while $\sigma \in \mathbb{R}^n$ expresses the coupling with the remaining part of the problem. — This system represents the electric network equations.

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- (b) The subproblem (3.1b) is a boundary value problem for a system of elliptic partial differential equations (PDE), for the unknown u in a functional space \mathcal{W}_u (see below). The boundary data in (3.1b) depend on a vector $\eta \in \mathbb{R}^k$. — This system gives the relation for a distributed, static device (semiconductor), where $\eta \in \mathbb{R}^k$ expresses the coupling with the first part of the problem.
- (c) The condition (3.1c) is the PDE-to-DAE coupling condition, which represents how the PDE unknown u affects the DAE problem. We assume $U \in \mathbb{R}^{n \times \ell}$ is a fixed matrix and s is a vector valued function $s : \mathcal{W}_u \to \mathbb{R}^{\ell}$. The term σ represents the device currents (through its terminals) padded with zeros.
- (d) The condition (3.1d) is the DAE-to-PDE coupling condition, which represents how the DAE unknown x affects the PDE problem. We assume $V \in \mathbb{R}^{n \times k}$ to be a given matrix. The term η represents the applied node potential.

In the following, we will use that the matrices E and $A \in \mathbb{R}^{n \times n}$ are positive and negative semidefinite, respectively. Moreover, we assume that the matrix pencil $A - \lambda E \in \mathbb{R}^{n \times n}[\lambda]$ is regular.

The structure of the coupling term σ depends on the solution of the PDE system, in the following sense. If the system (3.1b) admits a solution uniquely determined from given boundary data η , then applying the coupling condition (3.1d) we can write

$$u = \tilde{u}(V^{\top}x),$$

i.e., u as function of the DAE (3.1a) unknown x. Thus in the perspective of the DAE, the coupling to the PDE can be written as the following relation:

(3.2)
$$\sigma = \varrho(x), \quad \varrho(x) := Ur(V^{\top}x),$$

using the coupling condition (3.1c) and $r(V^{\top}x) := s(\tilde{u}(V^{\top}x))$. On the other hand, if the solution u is not uniquely determined by the boundary data η , then the PDE system (3.1b) defines a multivalued function $u = \tilde{u}(\eta)$, which leads to a multivalued version of (3.2). We can give meaning to this coupled problem also in the case of a multivalued function $\varrho(x)$. We say that (x, u) is a solution of the PDAE (3.1) if x belongs to \mathcal{W}_x , u belongs to $C([t_0, t_1]; \mathcal{W}_u)$ and they satisfy, respectively, the DAE (3.1a), the PDE (3.1b) and the coupling conditions (3.1c), (3.1d). The PDE variable u depends parametrically on time through the boundary data η , that is, through x(t). The concept of solution to (3.1) will be clarified in details when we will specialize the generic system for application to electric networks containing semiconductor devices.

3.1. Tractability index of DAEs with a nonlinear term. In the following we investigate the index of the coupled problem from the electric network perspective, by using a perturbative approach. The main idea is that the nonlinearity is confined only to the PDE part of the equations and, thus, to the PDE-to-DAE coupling term. The impact of the nonlinearity to the DAE is controlled by the matrix U, so we wish to find additional conditions on this matrix so that the nonlinearity does not alter the structure of the DAE in terms of differential and algebraic variables splitting.

From the viewpoint of the tractability index [9] of the PDAE system (3.1) we will concentrate formally on the DAE system (3.1a), with σ given by (3.2). Thus, given a regular matrix pencil $A - \lambda E$, we consider the nonlinear system

(3.3)
$$E\dot{x} = Ax + \varrho(x) + b(t), \quad \varrho(x) = Ur(V^{\top}x).$$

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for the sole unknown x. We will not derive a general theory of tractability index of a nonlinear system of the form (3.3). Instead we will follow a different approach: we wish to determine additional structural conditions, depending on the coupling matrices U, V, which allow to *extend* the tractability index from the matrix pencil $A - \lambda E$ to the nonlinear problem (3.3) only.

3.1.1. Basics of the tractability index and related projectors. Thus our starting point is the notion of tractability index of the matrix pencil $A - \lambda E$. There are several ways of defining this concept. We follow the approach described in [9], which is based on the construction of an appropriate sequence of matrices. We proceed by induction. The basis are the initial matrices

$$E_0 := E, \quad A_0 := A.$$

Assuming that the matrices E_i , A_i are already defined up to $k-1 \ge 0$, we need to define the matrices corresponding to k. To this end, we denote by Q_i a projector onto the ker E_i , and by $P_i = I - Q_i$, its complementary projector for $i = 0, \ldots, k-1$. Thereby we assume that it holds

(3.4)
$$Q_i Q_j = O, \quad j = 0, \dots, i-1,$$

which is indeed always feasible. Then the matrices E_k , A_k are defined by

(3.5)
$$E_k = E_{k-1} - A_{k-1}Q_{k-1}, \quad A_k = A_{k-1}P_{k-1}.$$

This procedure (3.5) can be continued indefinitely, but after a finite number of μ iterations, we will end up with a nonsingular matrix E_{μ} with E_k singular for $k < \mu$ (unless the matrix pencil $A - \lambda E$ was singular). Then, of course, the sequence will stagnate: $E_{\mu+i} = E_{\mu}$ for all $i \ge 0$. The number μ is called tractability index of the matrix pencil $A - \lambda E$.

The sequence of matrices (matrix chain) (3.5) derived for the matrix pencil $A - \lambda E$ has an immediate application to the system (3.3) of DAEs. Using the matrix chain properties, one can show that (3.3) is equivalent to

$$E_k(P_{k-1}\cdots P_0\dot{x} + Q_0x + \cdots + Q_{k-1}x) = A_kx + \varrho(x) + b(t)$$

for any k. In particular for $k = \mu$, we have E_{μ} is nonsingular and we can write

(3.6)
$$P_{\mu-1}\cdots P_0\dot{x} + Q_0x + \ldots + Q_{\mu-1}x = E_{\mu}^{-1}(A_{\mu}x + \varrho(x) + b(t)).$$

This equation enables us to decouple the original system into a differential equation for the variable $P_0 \cdots P_\mu x$, and algebraic equations for the variables [9]

$$P_0 \cdots P_{\mu-1}Q_{\mu}x, \dots, P_0Q_1x, Q_0x$$

if $\rho(x)$ were not present.

Furthermore we introduce \hat{Q}_i as a projector onto ker (E_i^{\top}) and its complementary version $\hat{P}_i = I - \hat{Q}_i$, for i = 0, 1. Next, we wish to find additional conditions, depending on the coupling matrices U, V, such that this decoupling is preserved also for the nonlinear equation (3.3). A general discussion can be found in [3]. In the following we derive appropriate additional conditions for index-1 and index-2 matrix pencils with a nonlinear coupling term.

3.1.2. Index-1 matrix pencil $A - \lambda E$. Let us assume that the matrix pencil $A - \lambda E$ has index 1 ($\mu = 1$), that is,

$$(3.7) E_0 ext{ is singular, } E_1 ext{ is nonsingular.}$$

Then (3.6) reads $P_0 \dot{x} + Q_0 x = E_1^{-1} (A_1 x + \rho(x) + b(t))$. Applying the projectors P_0 , Q_0 , and observing that $A_1 Q_0 = O$, we get the following projected equations

(3.8a)
$$\dot{y} := P_0 \dot{x} = P_0 E_1^{-1} \left(A_1 y + \varrho(x) + b(t) \right)$$

(3.8b)
$$z := Q_0 x = Q_0 E_1^{-1} \left(A_1 y + \varrho(x) + b(t) \right)$$

for the components $y = P_0 x$ and $z = Q_0 x$. The original unknown can be recovered by the relation x = y + z.

In absence of the nonlinear term $\varrho(x)$ we could solve the first equation for y and use the solution to determine z from the second equation. Now, we wish to find a condition which ensures the same behavior also in the presence of $\varrho(x)$. The unknown x can be expressed in terms of y, b and $\varrho(x)$ only, by inserting (3.8b):

$$\begin{aligned} x &= y + z = y + Q_0 E_1^{-1} (A_1 y + \varrho(x) + b) = (I + Q_0 E_1^{-1} A_1) y + Q_0 E_1^{-1} b + Q_0 E_1^{-1} \varrho(x) \\ &= M_1^* y + M_1 b + M_1 \varrho(x), \end{aligned}$$

with $M_1 = Q_0 E_1^{-1}$, $M_1^* = I + M_1 A_1$. Recalling that $\rho(x) = Ur(V^{\top}x)$, we have

$$r(V^{\top}x) = r\left(V^{\top}M_1^*y + V^{\top}M_1b + V^{\top}M_1Ur(V^{\top}x)\right)$$

Thus, to avoid recursion in z, it is sufficient to assume the condition

(3.9)
$$V^{\top} M_1 U \equiv V^{\top} Q_0 E_1^{-1} U = O$$

Under this condition, the system (3.8) becomes

(3.10a)
$$\dot{y} = P_0 E_1^{-1} \left[A_1 y + \rho (M_1^* y + M_1 b) + b \right].$$

(3.10b)
$$z = Q_0 E_1^{-1} \left[A_1 y + \rho (M_1^* y + M_1 b) + b \right]$$

and we find that (3.8) has an index-1 structure.

We notice that (3.9) is implied by either of the following conditions:

$$(3.11) V^{\top} Q_0 = O,$$

(3.12)
$$Q_0 E_1^{-1} U = O.$$

PROPOSITION 3.1. Let $A - \lambda E \in \mathbb{R}^{n \times n}[\lambda]$ be an index-1 matrix pencil, and let $U \in \mathbb{R}^{n \times \ell}$. Then the condition (3.12) is equivalent to:

$$(3.13)\qquad \qquad \hat{Q}_0^\top U = O.$$

for any projector \hat{Q}_0 onto ker E_0^{\top} .

Proof. From (3.12) we have that $Q_0U' = O$ with $U' = E_1^{-1}U$, that is, there exists a matrix $U' \in \mathbb{R}^{n \times \ell}$ such that $U = E_1U' = E_0U'$. Multiplying from the left-hand side by the transpose of the projector onto the ker E_0^{-1} , we obtain immediately (3.13).

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On the other hand, given $\hat{Q}_0^{\top}U = O$, thus $\hat{P}_0^{\top}U = U$. Then we have $E_1P_0 = E_0 = \hat{P}_0^{\top}\hat{E}_1$, with $\hat{E}_1 = E_0 + \hat{Q}_0^{\top}\hat{Q}_0$. Then $E_1^{-1}\hat{P}_0^{\top} = P_0\hat{E}_1^{-1}$. From (3.13) we have $E_1^{-1}U = E_1^{-1}\hat{P}_0^{\top}U = P_0E_1^{-1}U$ that, multiplied by Q_0 , gives (3.12). \Box

If ρ is a function, it is possible to apply the notion of tractability index for nonlinear DAEs, introduced by März [10]. It is possible to prove that the additional condition (3.11), together with the index-1 conditions for the matrix pencil $A - \lambda E$, imply that (3.8), with algebraic ρ , is an index-1 system [3]. Condition (3.12), or equivalently condition (3.13), is in general different from (3.11), even when U = V, unless we can choose $\hat{Q}_0 = Q_0$. This is possible only if ker $E_0 = \ker E_0^{\top}$.

3.1.3. Index-2 matrix pencil $A - \lambda E$. Let us assume that the matrix pencil $A - \lambda E$ has index 2 ($\mu = 2$), that is,

(3.14) E_0 is singular, E_1 is singular, E_2 is nonsingular.

Then equation (3.6) becomes

$$P_1 P_0 \dot{x} + Q_1 x + Q_0 x = E_2^{-1} \left(A_2 x + \varrho(x) + b(t) \right).$$

Using the projectors P_0P_1 , P_0Q_1 and Q_0P_1 on equation (3.6), we obtain the three projected equations

(3.15a)
$$\dot{y} = P_0 P_1 E_2^{-1} \left(A_2 y + \varrho(x) + b(t) \right)$$

(3.15b)
$$w = P_0 Q_1 E_2^{-1} \left(A_2 y + \varrho(x) + b(t) \right),$$

(3.15c)
$$z = Q_0 Q_1 \dot{w} + Q_0 P_1 E_2^{-1} \left(A_2 y + \varrho(x) + b(t) \right),$$

for the components of the unknown $y = P_0 P_1 x$, $w = P_0 Q_1 x$, and $z = Q_0 x$. The original unknown x can be recovered from the relation x = y + w + z.

In absence of the nonlinear term $\varrho(x)$ this is an index-2 system, since we can solve the equation (3.15a) for y, then compute w by (3.15b), and finally compute z by (3.15c). We see that in the solution appears the time derivative of the source term b(t), because of the term \dot{w} in (3.15c). To keep the same structure also when $\varrho(x)$ is present, we proceed as before. We can compute

$$\begin{aligned} x &= y + w + z \\ &= y + P_0 Q_1 E_2^{-1} \left(A_2 y + \varrho(x) + b \right) + \left[Q_0 Q_1 \dot{w} + Q_0 P_1 E_2^{-1} \left(A_2 y + \varrho(x) + b(t) \right) \right] \\ &= M_2^* y + M_2 b + M_2 \varrho(x) + Q_0 Q_1 \dot{w}, \end{aligned}$$

with

(3.16)
$$M_2 = (P_0Q_1 + Q_0P_1)E_2^{-1}, \quad M_2^* = I + M_2A_2.$$

To avoid recursion in z and w as in the index-1 case, it is sufficient to have:

$$(3.17a) V^{\top} Q_0 Q_1 = O,$$

(3.17b)
$$V^{\top} M_2 U \equiv V^{\top} (P_0 Q_1 + Q_0 P_1) E_2^{-1} U = O.$$

Under these conditions, system (3.15) becomes

(3.18a)
$$\dot{y} = P_0 P_1 E_2^{-1} \left[A_2 y + \varrho (M_2^* y + M_2 b) + b \right],$$

(3.18b)
$$w = P_0 Q_1 E_2^{-1} \left[A_2 y + \varrho (M_2^* y + M_2 b) + b \right]$$

(3.18c)
$$z = Q_0 Q_1 \dot{w} + Q_0 P_1 E_2^{-1} \left[A_2 y + \varrho (M_2^* y + M_2 b) + b \right].$$

We notice that (3.17b) is implied by either of the following conditions:

(3.19)
$$V^{\top}(P_0Q_1 + Q_0P_1) = O,$$

$$(3.20) (P_0Q_1 + Q_0P_1)E_2^{-1}U = O$$

The first condition is equivalent to [3]

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(3.21)
$$V^{\top}Q_0 = V^{\top}Q_1 = O.$$

Thus, (3.19) implies both (3.17a) and (3.17b). Moreover, if ρ is a nonlinear function and $A - \lambda E$ is an index-2 matrix pencil, then the additional condition (3.19) implies that (3.18) is an index-2 system according to the definition given in [10] (see [3]).

The following Proposition 3.4 explores the topological implications of condition (3.20). This proposition requires as prerequisite the following two lemmas.

LEMMA 3.2. Let $A - \lambda E \in \mathbb{R}^{n \times n}[\lambda]$ be an index-2 matrix pencil, and let $U \in \mathbb{R}^{n \times \ell}$. Then the following conditions are equivalent:

(i) There exist a matrix $U' \in \mathbb{R}^{n \times \ell}$ such that

(3.22)
$$(I - P_0 P_1) E_2^{-1} U = Q_0 Q_1 U'.$$

(ii) There exist a matrix $U' \in \mathbb{R}^{n \times \ell}$ such that

$$(3.23) U = E_0 U'$$

that is, for any projector \hat{Q}_0 onto ker E_0^{\top} we have

$$\hat{Q}_0^{\dagger} U = O.$$

(iii) There exist a matrix $U' \in \mathbb{R}^{n \times \ell}$ such that

(3.25)
$$Q_0 E_2^{-1} U = Q_0 Q_1 U',$$

and we have

(3.26)
$$Q_1 E_2^{-1} U = O.$$

Proof. First we prove that (i) implies (ii). Let $(I - P_0P_1)E_2^{-1}U = Q_0Q_1U'$. Since $Q_0Q_1 = -(I - P_0P_1)P_1P_0$, we find

$$(I - P_0 P_1)(E_2^{-1}U + P_1 P_0 U') = O,$$

that is, $(I - P_0P_1)U'' = O$, with $U'' = E_2^{-1}U + P_1P_0U'$. Hence, $U = E_2(-P_1P_0U' + U'') = E_2(-P_1P_0U' + P_0P_1U'')$. And since $(P_1P_0)(P_0P_1) = P_0P_1$, we get $U = E_2P_1P_0(-U' + P_0P_1U'') = E_0(-U' + P_0P_1U'')$, that is, (3.23).

To prove that (*ii*) implies (*iii*), we note that $E_2P_1P_0 = E_0 = \hat{P}_0^{\top}\hat{E}_1$, with $\hat{E}_1 = E_0 + \hat{Q}_0^{\top}\hat{Q}_0$ and $\hat{P}_0 = I - \hat{Q}_0$. Since \hat{E}_1 is invertible, we get the identity

$$P_1 P_0 \hat{E}_1^{-1} = E_2^{-1} \hat{P}_0^{\top}.$$

Then we find from (3.23) in (ii):

$$E_2^{-1}U = E_2^{-1}E_0U' = E_2^{-1}\hat{P}_0^{\top}E_0U' = P_1P_0\hat{E}_1^{-1}E_0U',$$

where the last equality follows from (3.27). Multiplying this identity by Q_0 and Q_1 , observing that $Q_0P_1P_0 = -Q_0Q_1$, we find (3.25) and (3.26).

Finally, to prove that (*iii*) implies (*i*) it is sufficient to note that $I - P_0P_1 = Q_0 + Q_1 - Q_0Q_1$. This concludes the proof of the lemma. \Box

LEMMA 3.3. Let $A - \lambda E \in \mathbb{R}^{n \times n}[\lambda]$ be an index-2 matrix pencil, and let $U \in \mathbb{R}^{n \times \ell}$. Then the following conditions are equivalent:

(i) It holds

(3.28)
$$Q_1 E_2^{-1} U = O$$

(ii) It holds

(3.29)
$$U = E_1 E_2^{-1} U$$

(iii) There exist a matrix $U' \in \mathbb{R}^{n \times \ell}$ such that

$$(3.30) U = E_1 U',$$

that is, for any projector \hat{Q}_1 onto ker E_1^{\top} , we have

$$\hat{Q}_1^\top U = O.$$

Proof. If U satisfies (3.28), then $E_2^{-1}U = P_1E_2^{-1}U$. Then, $U = E_2P_1E_2^{-1}U$, and (3.29) follows from $E_2P_1 = E_1$. Thus, (i) implies (ii). Moreover (ii) implies trivially (iii). It remains to show that (iii) implies (i). For \hat{Q}_1 and $\hat{P}_1 = I - \hat{Q}_1$, we have $E_2P_1 = E_1 = \hat{P}_1^{\top}\hat{E}_2$ with the invertible matrix $\hat{E}_2 = E_1 + \hat{Q}_1^{\top}\hat{Q}_1$. Then it holds $E_2^{-1}\hat{P}_1^{\top} = P_1\hat{E}_2^{-1}$. Now using $\hat{Q}_1^{\top}U = O$, it follows

$$E_2^{-1}U = E_2^{-1}\hat{P}_1^\top U = P_1 E_2^{-1} U.$$

Multiplying by Q_1 we obtain (3.28), which concludes the proof. \Box

PROPOSITION 3.4. Let $A - \lambda E \in \mathbb{R}^{n \times n}[\lambda]$ be an index-2 matrix pencil, and let $U \in \mathbb{R}^{n \times \ell}$. Then the following conditions are equivalent:

(i) The matrix U satisfies the condition (3.20).

(*ii*) It holds

$$(3.32) Q_0 E_2^{-1} U = O, Q_1 E_2^{-1} U = O$$

(iii) It holds

$$(3.33) U = E_0 E_2^{-1} U = E_1 E_2^{-1} U.$$

Proof. First, we prove that (i) is equivalent to (ii). Given (i) for U, then U satisfies (3.22) with $U' = E_2^{-1}U$, since $P_0Q_1 + Q_0P_1 = I - P_0P_1 - Q_0Q_1$. Hence all statements of Lemma 3.2 hold, in particular, we have $Q_1E_2^{-1}U = O$. Together with (3.20), this implies $Q_0E_2^{-1}U = O$, and thus holds (3.32). On the other hand, (i) follows immediately from (ii).

Next, we prove that (*ii*) is equivalent to (*iii*). First, using Lemma 3.3 we observe that the equality $Q_1 E_2^{-1} U = O$, is equivalent to $U = E_1 E_2^{-1} U$. In a similar way, the equality $Q_0 E_2^{-1} U = O$ is equivalent to $U = E_2 P_0 E_2^{-1} U = E_0 E_2^{-1} U - A_1 Q_1 E_2^{-1} U$. It follows that (3.32) is equivalent to

$$U = E_1 E_2^{-1} U, \quad U = E_0 E_2^{-1} U - A_1 Q_1 E_2^{-1} U.$$

Using the equivalence of $Q_1 E_2^{-1} U = O$ and $U = E_1 E_2^{-1} U$, the above equalities are equivalent to (3.33). \Box

In conclusion, condition (3.19) is equivalent to $V^{\top}Q_0 = V^{\top}Q_1 = O$, while condition (3.20) is equivalent to $\hat{Q}_0^{\top}U = \hat{Q}_1^{\top}U = O$. Thus, even if U = V, the two conditions are equivalent only if $\ker E_i^{\top} = \ker E_i$, which is not true in general.

In the following we will assume the conditions

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$$(3.34a) V^{\top} Q_0 Q_1 = O,$$

(3.34b)
$$(P_0Q_1 + Q_0P_1)E_2^{-1}U = O,$$

which imply (3.17). By Prop. 3.4, the conditions (3.34b) and (3.32) are equivalent. Thus by (3.34b), the split equations (3.18) simplify as follows: (since $\rho = Ur$)

(3.35a)
$$\dot{y} = P_0 P_1 E_2^{-1} [A_2 y + \varrho(M_2^* y + M_2 b) + b],$$

(3.35b)
$$w = P_0 Q_1 E_2^{-1} \left[A_2 y + b \right],$$

(3.35c)
$$z = Q_0 Q_1 \dot{w} + Q_0 P_1 E_2^{-1} [A_2 y + b].$$

3.2. Application to MNA equations and topological interpretation of the index conditions. Here we go back to problem (3.3) and we discuss the additional conditions and their topological interpretation for the MNA equations in both index-1 and index-2 case. Thus we consider matrices E and A as in equation (2.1).

To make explicit the additional condition we also need the coupling matrices U, V. In the MNA case both U and V coincide with the matrix \hat{A} , introduced in (2.12),

(3.36)
$$U = V = \hat{A} = \begin{bmatrix} A_D \\ O \\ O \end{bmatrix}.$$

where A_D is defined in (2.11).

3.2.1. Topological interpretation of the index-1 conditions. In our index-1 case, E_0 is singular while $E_1 = E_0 - A_0 Q_0$ is nonsingular and the additional condition (3.12) is satisfied. It is simple to see that ker $E_0 = \ker A_C^{\top} \times \{0\} \times \mathbb{R}^{n_V} = \ker E_0^{\top}$ (since E_0 is symmetric). Thus it is possible to choose $\hat{Q}_0 \equiv Q_0$. Let Q_C be a projector onto the kernel of A_C^{\top} and $P_C = I - Q_C$. Then we can choose

(3.37)
$$Q_0 = \begin{bmatrix} Q_C & O & O \\ O & O & O \\ O & O & I \end{bmatrix}, \quad P_0 = \begin{bmatrix} P_C & O & O \\ O & I & O \\ O & O & O \end{bmatrix}.$$

Furthermore the matrix chain is continued by

(3.38)
$$E_{1} = \begin{bmatrix} A_{C}CA_{C}^{\top} + A_{R}GA_{R}^{\top}Q_{C} & O & A_{V} \\ -A_{L}^{\top}Q_{C} & L & O \\ -A_{V}^{\top}Q_{C} & O & O \end{bmatrix}, \quad A_{1} = -\begin{bmatrix} A_{R}GA_{R}^{\top}P_{C} & A_{L} & O \\ -A_{L}^{\top}P_{C} & O & O \\ -A_{V}^{\top}P_{C} & O & O \end{bmatrix}.$$

The text proposition, which is derived from [5, 12], characterizes the kernel of E_1 .

PROPOSITION 3.5. Let E_1 be the matrix defined in (3.38). Then

$$\operatorname{ker} E_1 = \left\{ [e^\top, i_L^\top, i_V^\top]^\top \in \mathbb{R}^n : Q_C e \in \operatorname{ker}(A_C, A_V, A_R)^\top, i_V \in \operatorname{ker}(Q_C^\top A_V), \\ P_C e = -M_C^{-1} A_V i_V, \ i_L = L^{-1} A_L^\top Q_C e \right\},$$

where $M_C = P_C^{\top} A_C C A_C^{\top} P_C + Q_C^{\top} Q_C$, and

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$$\ker E_1^{\top} = \left\{ [e, i_L, i_V]^{\top} \in \mathbb{R}^n : Q_C e \in \ker(A_C, A_V, A_R)^{\top}, P_C e = 0, \\ i_L = 0, i_V \in \ker(Q_C^{\top} A_V) \right\}.$$

Using this proposition, we find [12, 5, 1]:

PROPOSITION 3.6. For the nonlinear problem (3.3), the index-1 conditions (3.7) and the additional condition (3.12) are satisfied if and only if all of the following topological conditions hold:

(3.39)
$$\ker(A_C, A_V, A_R)^{\top} = \{0\}, \quad \ker(Q_C^{\top} A_V) = \{0\}, \quad Q_C^{\top} A_D = O.$$

Proof. By Proposition 3.5, the first two conditions are equivalent to ker $E_1 = \{0\}$, i.e., to the index-1 condition (3.7). Then by Proposition 3.1 and the symmetry of E_0 , (3.12) is equivalent to the last condition. \Box

REMARK 1. The topological conditions (3.39) have simple physical interpretations [1, 5, 12]. The first condition forbids cutsets composed of independent current sources and inductors. The second condition states that loops containing at least one voltage source and any number of capacitors and diodes are forbidden. The third conditionstates that any device terminal is connected to ground by a path of capacitors.

For an index-1 MNA system, using the projector Q_0 defined in (3.37), the differential and algebraic variables are:

$$y = P_0 x = \begin{bmatrix} P_C e \\ i_L \\ O \end{bmatrix}, \quad z = Q_0 x = \begin{bmatrix} Q_C e \\ O \\ i_V \end{bmatrix}.$$

Under the conditions in Proposition 3.6, they satisfy equations (3.10).

3.2.2. Topological interpretation of the index-2 conditions. The pencil $A - \lambda E$ has tractability index-2 if and only if E_1 is singular and E_2 is nonsingular. Thus, system (3.3) is index-2 if ker $E_1 \neq \{0\}$, ker $E_2 = \{0\}$, and the additional conditions in (3.34) are satisfied. Due to Lemma 3.2 and Lemma 3.3, the additional conditions are equivalent to (3.34a), (3.24), (3.31).

We render explicit the index-2 conditions for the MNA equations using the following proposition [12, 5].

LEMMA 3.7. Let Q_{CVR} denote a projector onto the ker $(A_C, A_V, A_R)^{\top}$ (with $Q_{CVR} = Q_C Q_{CVR}$) and Q_{CV}^* denote a projector onto the ker $(Q_C^{\top}A_V)$). Then

$$Q_1^* = \begin{bmatrix} Q_{CVR} & O & -P_C M_C^{-1} A_V Q_{CV}^* \\ L^{-1} A_L^\top Q_{CVR} & O & O \\ O & O & Q_{CV}^* \end{bmatrix},$$

with $M_C = P_C^{\top} A_C C A_C^{\top} P_C + Q_C^{\top} Q_C$, is a projector onto ker E_1 . Moreover, (3.40) $Q_1 = -Q_1^* (E_1 - A_1 Q_1^*)^{-1} A_1$, G. Alì, A. Bartel, N. Rotundo

is a projector onto ker E_1 , which satisfies condition (3.4).

Proof. First we observe that $Q_1^{*2} = Q_1^*$, since $Q_{CVR}P_C = 0$. Moreover, since $P_CQ_{CVR} = O$, we have also $E_1Q_1^* = O$, thus Q_1^* is a projector onto ker E_1 . Next, using $A_1Q_1^* = -(E_1 - A_1Q_1^*)Q_1^*$, it holds

$$Q_1^2 = -Q_1^{*2}(E_1 - A_1Q_1^*)^{-1}A_1 = Q_1.$$

Since $E_1Q_1 = O$, Q_1 is also a projector onto ker E_1 , and recalling that $A_1 = A_0P_0$, we immediately have that it satisfy the condition (3.4). \Box

It remains to see which are the additional conditions for the MNA equations. By the results from Section 3.1, the conditions to be satisfied are

$$\hat{A}^{\top}Q_0Q_1 = O, \quad \hat{Q}_0^{\top}\hat{A} = O, \quad \hat{Q}_1^{\top}\hat{A} = O.$$

As noted above, we can choose $\hat{Q}_0 = Q_0$, so the first condition is implied by the second one, i.e., we have the conditions $Q_0^{\top} \hat{A} = O$, $\hat{Q}_1^{\top} \hat{A} = O$. Using the characterization of ker E_1^{\top} in Proposition 3.5, it follows that we can choose

$$\hat{Q}_1 = \begin{bmatrix} Q_{CVR} & O & O \\ O & O & O \\ O & O & Q_{CV}^* \end{bmatrix}.$$

Summing up, we have only to assume the following additional topological conditions:

PROPOSITION 3.8. Given the DAE (3.3), such that E and A are symmetric and condition

$$Q_C^+ A_D = C$$

holds. Then this DAE is index-2 if and only if one of the following conditions hold:

$$\ker(A_C, A_V, A_R)^\top \neq \{0\}, \qquad \ker(Q_C^\top A_V) \neq \{0\}$$

Proof. We notice $Q_C^{\top}A_C = 0$ implies $Q_{CVR}^{\top}Q_C^{\top}A_D = 0$ and this implies $Q_{CVR}^{\top}A_D = 0$ (since $Q_{CVR} = Q_C Q_{CVR}$). \Box

This completes the more abstract index and matrix investigations. We now come to the a priori estimates for the coupled system.

4. Main result. Next we tackle a core result of this paper, which is an existence result of the above introduced coupled system of a linear network DAE with a semiconductor (3.1). This problem is restated with more model details for the semiconductor device in the box below (4.1-4.4)

The main assumptions on the coupled problem are as follows: The MNA equation behind (4.1) employs positive definite matrices:

(4.5) the matrices C, L and G are symmetric and positive definite.

This assumption implies that E is positive semi-definite and A is negative semi-definite. Moreover, we assume that our electric networks is connected. Then for $\sigma = 0$ the pencil $A - \lambda E$ is regular and the tractability index is at most 2 [5]. Thus we assume the topological conditions (Prop. 3.8):

(4.6)
$$Q_C^{\top} A_D = O, \quad \ker(A_C, A_V, A_R)^{\top} \neq \{0\}, \quad \ker(Q_C^{\top} A_V) \neq \{0\}$$

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Device equations for $u(\mathbf{x},t) = (\phi, \phi_n, \phi_p)(\mathbf{x},t)$:

(4.2)
$$\begin{cases} -\nabla \cdot (\epsilon(\mathbf{x})\nabla\phi) = \rho(\mathbf{x}, u), & \text{in } \Omega, \\ -\nabla \cdot (a_n(\mathbf{x}, u)\nabla\phi_n) = H(\mathbf{x}, u), & \text{in } \Omega, \\ -\nabla \cdot (a_p(\mathbf{x}, u)\nabla\phi_p) = -H(\mathbf{x}, u), & \text{in } \Omega, \\ \phi - \phi_{\mathrm{bi}} = \phi_n = \phi_p = e_{D,k}(t), & \text{on } \Gamma_k \ (k = 0, 1, \dots, n_D), \\ \frac{\partial \phi}{\partial \nu} = \frac{\partial \phi_n}{\partial \nu} = \frac{\partial \phi_p}{\partial \nu} = 0, & \text{on } \Gamma_N, \end{cases}$$

Network-to-device coupling conditions:

(4.3)
$$e_D = V^{\top} x,$$

Device-to-network coupling conditions: $(k = 0, 1, ..., n_D)$

4.4)
$$\sigma = -Ui_D$$
, with $i_{D,k} = -\int_{\Omega} \nabla \psi_k \cdot (a_n \nabla \phi_n + a_p \nabla \phi_p) \, \mathrm{dx}.$

(i.e., the existence of an LI-cutset or a CV-loop [5]), such that by Prop. 3.8 $A - \lambda E$ has tractability index 2. As regards the independent voltage source $v_V(t)$ and current source $i_I(t)$, we assume that

(4.7)
$$v_V(t) \in C^1([t_0, t_1]; \mathbb{R}^{n_V}), \quad i_I(t) \in C^1([t_0, t_1]; \mathbb{R}^{n_I}),$$

i.e., the source term b(t) is continuously differentiable.

For the drift-diffusion problem (4.2) with unknown $u = (\phi, \phi_n, \phi_p)$, The source term $\rho(\mathbf{x}, u)$ represents the total charge density,

(4.8)
$$\rho(\mathbf{x}, u) = qN(\mathbf{x}) - qn(u) + qp(u),$$

where $N(\mathbf{x})$ is the doping profile and n(u), p(u) are the electron and hole number densities. They are given by the Maxwell-Boltzmann relations

$$n(u) = n_{\rm i} \exp\left(\frac{\phi - \phi_n}{\phi_{\rm th}}\right), \quad p(u) = n_{\rm i} \exp\left(\frac{\phi_p - \phi}{\phi_{\rm th}}\right),$$

with n_i intrinsic concentration, and ϕ_{th} thermal potential. For the doping profile $N(\mathbf{x})$ in ρ , and for the dielectric constant $\epsilon(\mathbf{x})$, we assume

(4.9)
$$N, \epsilon \in L^{\infty}(\Omega), \quad \epsilon(\mathbf{x}) \ge \epsilon > 0 \quad \text{for all } \mathbf{x} \in \Omega,$$

for a real constant $\underline{\epsilon}$. The functions $a_n(\mathbf{x}, u)$ and $a_p(\mathbf{x}, u)$ are related to the mobilities μ_n, μ_p by

(4.10)
$$a_n(\mathbf{x}, u) = qn(u)\mu_n(\mathbf{x}, n(u)), \quad a_p(\mathbf{x}, u) = qp(u)\mu_p(\mathbf{x}, p(u)),$$

where the mobilities are continuous functions of the space and of the carrier concentration. Commonly, the mobilities are assumed to be strictly positive and continuous functions. This leads to the model assumptions:

(i)
$$a_n(\mathbf{x}, u), a_p(\mathbf{x}, u)$$
 are continuous functions,

(4.11) (ii) for any compact set
$$K \subset \mathbb{R}^3$$
 there exist a constant \underline{a}_K such that $a_n(\mathbf{x}, u), a_p(\mathbf{x}, u) \geq \underline{a}_K > 0$ for all $\mathbf{x} \in \Omega, u \in K$.

The generation-recombination term $H(\mathbf{x}, u)$ is assumed to take the form

(4.12)
$$H(\mathbf{x}, u) = H'(\mathbf{x}, n(u), p(u)) \left(n(u)p(u) - n_{\mathbf{i}}^2 \right) =: h(\mathbf{x}, u) \left(n(u)p(u) - n_{\mathbf{i}}^2 \right),$$

for some regular function $H'(\mathbf{x}, n, p)$. This expression covers the most common generation-recombination mechanisms with the exception of impact ionization. We note that

$$n(u)p(u) - n_{i}^{2} = n_{i}^{2} \exp\left(\frac{\phi_{p} - \phi_{n}}{\phi_{th}}\right) - n_{i}^{2} =: g(\phi_{p} - \phi_{n}).$$

Based on these considerations, we assume that

(4.13) (i) $H(\mathbf{x}, u) = h(\mathbf{x}, u)g(\phi_p - \phi_n),$ (ii) $h(\mathbf{x}, u), g(v)$ are continuous functions, (iii) g(v)v > 0 for all $v \in \mathbb{R},$ (vi) $h(\mathbf{x}, u) \ge 0$ for all $\mathbf{x} \in \Omega, \ u \in \mathbb{R}^3.$

To introduce our existence result for the coupled problem, we need the spaces

$$\mathcal{W}_{x} := \{ x \in C^{0}([t_{0}, t_{1}]; \mathbb{R}^{n}) : P_{0}x \in C^{1}([t_{0}, t_{1}]; \mathbb{R}^{n}\}, \\ \mathcal{W}_{u} := (H^{1}(\Omega) \cap L_{\infty}(\Omega))^{3},$$

and we employ in \mathbb{R}^m the Euclidean vector norm $|\cdot|$.

THEOREM 4.1. Under the assumptions (4.5)–(4.13), the index-2 coupled problem (4.1)–(4.4) admits a solution, $(x, u) \in \mathcal{W}_x \times C^0([t_0, t_1]; \mathcal{W}_u)$. Moreover, any solution satisfies the estimates:

(4.14)
$$|P_0P_1x(t)|^2 \le c_y e^{k(t-t_0)} \left(|y_0|^2 + |b_0|^2 + \|b\|_{H^1([t_0,t_1])}\right).$$

(4.15)
$$|P_0Q_1x(t)|^2 \le c_w e^{k(t-t_0)} \left(|y_0|^2 + |b_0|^2 + ||b||_{H^1([t_0,t_1])} \right)$$

(4.16)
$$|Q_0 x(t)|^2 \le c_z \left(|y(t)| + |\dot{y}(t)| + |b(t)| + |\dot{b}(t)| \right),$$

(4.17)
$$\inf_{\Gamma_D} \phi_{\mathrm{bi}} + \min_i e_{D,i} \le \phi \le \sup_{\Gamma_D} \phi_{\mathrm{bi}} + \max_i e_{D,i},$$

(4.18)
$$\min_{i} e_{D,i} \le \phi_n \le \max_{i} e_{D,i}, \qquad \min_{i} e_{D,i} \le \phi_p \le \max_{i} e_{D,i},$$

for some positive constants c_y , c_w , c_z and k depending only on E_0 , A_0 .

5. Proof of the main theorem. The proof of Thm. 4.1 is based on an iteration map argument and it is an extension of the proof used in [2], where an index-1 coupled network-device systems is studied. The derivation requires several steps: passivity of the semiconductor device, a priori estimates and an iteration map. Most preliminary results are common in the index-1 and the index-2 case, thus we report on all needed lemmas and present full details of index-2 specific aspects.

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Passivity. The following a priori estimates rely essentially on the passivity of the semiconductor model (i.e., the coupling term σ):

LEMMA 5.1. Let the assumption (4.13) for the generation-recombination term hold. Given $x \in W_x$, let $u \in W_u$ satisfy the boundary value problem (4.2)–(4.3), Then the coupling term σ (4.4) satisfies the passivity condition

$$(5.1) x^{\top} \sigma \le 0$$

This lemma was proven in [2]. The dissipativity condition (5.1) is equivalent to the usual passivity condition, since it holds:

$$e_D^\top j_D = x^\top V j_D = x^\top U i_D = -x^\top \sigma \ge 0.$$

A priori estimates for the network equation. Passivity (5.1) allows us to obtain estimates for the network variables, independently of the device variables.

PROPOSITION 5.2 (A priori estimates for the network). Let the network assumptions (4.5)–(4.7) be given and let $x \in W_x$ satisfy the network equation (4.1) with consistent initial value x_0 . Let σ be given such that the passivity condition (5.1) holds. Then, for all $t \in [t_0, t_1]$, the differential part $y = P_0P_1x$, and the algebraic parts $w = P_0Q_1x$, $z = Q_0x$ of the solution, satisfy the estimates

(5.2)
$$|y(t)|^2 \le c_y e^{k(t-t_0)} \left(|y_0|^2 + |b_0|^2 + \|b\|_{H^1([t_0, t_1])} \right),$$

(5.3)
$$|w(t)|^2 \le c_w e^{k(t-t_0)} \left(|y_0|^2 + |b_0|^2 + \|b\|_{H^1([t_0,t_1])} \right),$$

(5.4)
$$|z(t)| \le c_z \left(|y(t)| + |\dot{y}(t)| + |b(t)| + |\dot{b}(t)| \right),$$

for some positive constants c_y , c_w , c_z and k depending only on E, A.

Proof. Multiplying (4.1) by x^{\top} , using the passivity condition (5.1) and the assumption (4.5), we obtain

$$x^{\top}E\dot{x} \leq x^{\top}b(t).$$

Due to the symmetry of E, we have $Q_0^{\top} E = O$. Then the inequality becomes

 $(P_0 x)^\top E(P_0 \dot{x}) \le x^\top b(t).$

since $x = P_0 x + Q_0 x$. Integrating this result on $[t_0, t]$ with $t \le t_1$, we find

(5.5)
$$\frac{1}{2}(P_0x)^{\top}E(P_0x) \le \frac{1}{2}(P_0x_0)^{\top}E(P_0x_0) + \int_{t_0}^t x^{\top}(\tau)b(\tau)\,\mathrm{d}\tau$$

(using also $E^{\top} = E$). On the one hand, E is positive definite when restricted to $P_0 \mathbb{R}^n$. Recalling $P_0 x = P_0 P_1 x + P_0 Q_1 x$, we can find a positive constant c_E such that

(5.6)
$$\frac{1}{2}(P_0x)^{\top} E(P_0x) \ge c_E |P_0x|^2 \ge c_E(|y|^2 + |w|^2).$$

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On the other hand, the hypothesis (4.6) and the decomposition (3.35) imply

$$\begin{aligned} x^{\top}b &= y^{\top}b + w^{\top}b + z^{\top}b \\ &= y^{\top}b + [P_0Q_1E_2^{-1}(A_2y + b)]^{\top}b + [Q_0Q_1\dot{w} + Q_0P_1E_2^{-1}(A_2y + b)]^{\top}b \\ &= y^{\top}M_2^{*\top}b + b^{\top}M_2^{\top}b - w^{\top}(Q_0Q_1)^{\top}\dot{b} + \frac{d}{dt}[w^{\top}(Q_0Q_1)^{\top}b] \end{aligned}$$

with M_2 and M_2^* defined in (3.16). The last equality contains no quadratic terms in the terms of x. Then, using the Schwarz inequality, we obtain

$$\begin{split} &\int_{t_0}^t x^\top(\tau)b(\tau)\,\mathrm{d}\tau\\ &\leq c \int_{t_0}^t (|y(\tau)|^2 + |b(\tau)|^2 + |w(\tau)|^2 + |\dot{b}(\tau)|^2)\,\mathrm{d}\tau + w^\top(Q_0Q_1)^\top b - w_0^\top(Q_0Q_1)^\top b_0\\ &\leq c \int_{t_0}^t (|y(\tau)|^2 + |w(\tau)|^2)\,\mathrm{d}\tau + c \|b\|_{H^1([t_0,t_1])}^2 + \delta|w(t)|^2 + c(\delta)|b(t)|^2 - w_0^\top(Q_0Q_1)^\top b_0 \end{split}$$

where δ is a small positive real number which will be chosen later. Using the previous inequality, (5.5), (5.6) and choosing $\delta = \frac{c_E}{2}$, we get

$$\frac{1}{2}c_E(|y|^2 + |w|^2) \le \frac{1}{2}(P_0x_0)^\top E(P_0x_0) - w_0^\top (Q_0Q_1)^\top b_0 + c||b||_{H^1([t_0,t_1])}^2 + c \int_{t_0}^t (|y(\tau)|^2 + |w(\tau)|^2) \,\mathrm{d}\tau$$

From Gronwall's lemma, we find the inequality

$$|y(t)|^{2} + |w(t)|^{2} \le C_{0}e^{c(t-t_{0})}$$

with $C_0 = c(|y_0|^2 + |b_0|^2 + ||b||_{H^1([t_0, t_1])})$, which proves both (5.2) and (5.3). Finally, we have

$$z = Q_0 Q_1 \dot{w} + Q_0 P_1 E_2^{-1} [A_2 y + b] Q_0 Q_1 E_2^{-1} \left[A_2 \dot{y} + \dot{b} \right] + Q_0 P_1 E_2^{-1} [A_2 y + b].$$

which proves (5.4).

Device iteration map. As known results for the device equations indicate [8], we consider for the unknown function $\Phi := (\phi_n, \phi_p)$ the following set:

$$\mathcal{M}(e_D) = \{ \psi \in L^2(\Omega) \mid \min_i e_{D,i} \le \psi \le \max_i e_{D,i} \text{ a.e. in } \Omega \}^2$$

given any applied voltage $e_D \in \mathbb{R}^{m_D}$. For any $e_D^* \in \mathbb{R}^{m_D}$ and $\Phi^* = (\phi_n^*, \phi_p^*) \in \mathcal{M}(e_D^*)$ we partly linearize the device equations (4.2) as follows. First the PDE for the electric potential is solved:

(5.7)
$$\begin{cases} -\nabla \cdot (\epsilon \nabla \phi^*) = \rho(\phi, \phi_n^*, \phi_p^*), & \text{in } \Omega, \\ \phi - \phi_{\text{bi}} = e_{D,i}^*, & \text{on } \Gamma_{D,i}, & \frac{\partial \phi}{\partial \nu} = 0, & \text{on } \Gamma_N \end{cases}$$

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It solution is denoted as $\phi^* = \phi^*(e_D^*, \Phi^*)$. Then the the remaining PDEs for the device equations are solved:

(5.8)
$$\begin{cases} -\nabla \cdot (a_n^* \nabla \phi_n) = H_1^* H_2, \\ -\nabla \cdot (a_p^* \nabla \phi_p) = -H_1^* H_2, & \text{in } \Omega \\ \phi_n = \phi_p = e_{D,i}, & \text{on } \Gamma_{D,i}, & \frac{\partial \phi_n}{\partial \nu} = \frac{\partial \phi_p}{\partial \nu} = 0, & \text{on } \Gamma_N \end{cases}$$

where superscript * denotes evaluation at $u = u^* = (\phi^*, \phi_n^*, \phi_p^*)$. This gives rise to consider the map

(5.9)
$$\Phi^{\sharp}(e_D; e_D^*) : \Phi^* \mapsto \Phi = \Phi^{\sharp}(e_D; e_D^*)(\Phi^*) =: \Phi^{\sharp}(e_D; e_D^*, \Phi^*).$$

The well-posedness of $\Phi^{\sharp}(e_D; e_D^*)$ has been proven in [2]. In summary, it holds:

LEMMA 5.3. Given $e_D^* \in \mathbb{R}^{m_D}$ and $\Phi^* \in \mathcal{M}(e_D^*)$.

a) Problem (5.7) has a unique solution $\phi^* \in H^1(\Omega)$ satisfying

$$\inf_{\Gamma_D} \phi_{\mathrm{bi}} + \min_i e_{D,i}^* \le \phi^* \le \sup_{\Gamma_D} \phi_{\mathrm{bi}} + \min_i e_{D,i}^*, \quad a.e. \ in \ \Omega.$$

b) For $\phi^* = \phi^*(e_D^*, \Phi^*)$ solution of (5.7), problem (5.8) has a unique solution $\Phi = (\phi_n, \phi_p) \in (H^1(\Omega)^2)$, which satisfies

 $\min_{i} e_{D,i} \le \phi_n \le \max_{i} e_{D,i}, \quad \min_{i} e_{D,i} \le \phi_p \le \max_{i} e_{D,i} \quad a.e. \ in \ \Omega.$

Thus given also $e_D \in \mathbb{R}^{m_D}$, the map

$$\Phi^{\sharp}(e_D; e_D^*) : \mathcal{M}(e_D^*) \to \mathcal{M}^{\sharp}(e_D) := \mathcal{M}(e_D) \cap H^1(\Omega),$$

stated in (5.9), is well-defined. We note this Lemma gives also the estimates for the electric potential, which appear in Theorem 4.1. — The map $\Phi^{\sharp}(e_D; e_D^*)$ defines also a modified terminal current $i_D^{\sharp}(e_D; e_D^*, \Phi^*) \in \mathbb{R}^{m_D}$ with components

$$j_{D,k}^{\sharp}(e_D; e_D^*, \Phi^*) = -\int_{\Omega} \nabla \psi_k \cdot (a_n^* \nabla \phi_n + a_p^* \nabla \phi_p) \,\mathrm{dx}$$

for $(\phi_n, \phi_p) = \phi^{\sharp}(e_D; e_D^*, \Phi^*)$ and auxiliary function ψ_k (2.6), $k = 0, \ldots, n_D$. In [2], it was proven:

LEMMA 5.4. Given $e_D^* \in \mathbb{R}^{m_D}$ and $\Phi^* \in \mathcal{M}(e_D^*)$, the map $e_D \mapsto i_D^{\sharp}(e_D; e_D^*, \Phi^*)$ $(\mathbb{R}^{n_D} \to \mathbb{R}^{n_D})$ is Lipschitz-continuous with respect to the applied voltage e_D and i_D^{\sharp} satisfies the passivity condition

$$v_D^{\top} i_D^{\sharp}(e_D; e_D^*, \Phi^*) \ge 0, \quad v_D = \hat{A}^{\top} e_D.$$

Iteration map for the coupled problem. Due to Lemma 5.4, we can consider a modified coupled problem with the modified current i_D^{\sharp} to construct an iteration map for the coupled on an appropriate subset for e_D^* . Since in the coupled problem the unknown function (e_D, Φ) is time dependent, we need to consider

$$C^{0}_{CP}([t_0, t_1]) := C^{0}([t_0, t_1], \mathbb{R}^{m_D}) \times \left(C^{0}([t_0, t_1], L^2(\Omega))\right)^2$$

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as the function space and we need to extend the set $\mathcal{M}(e_D)$ to

$$\mathcal{M}_{t_0,t_1}(e_D) = \{ \psi \in C^0([t_0,t_1], L^2(\Omega)) \mid \\ \min_i e_{D,i} \le \psi \le \max_i e_{D,i} \text{ a.e. in } \Omega, \ \forall t \in [t_0,t_1] \}^2$$

and consider boundary data $e_D^* \in C([t_0, t_1], \mathbb{R}^{m_D})$. In fact, Lemma 5.3 can be extended to this setting [2].

If x satisfies the a priori estimate (5.2)–(5.4), then the applied potentials $e_D = S^{\top} x$ are bounded:

(5.10)
$$|e_D(t)| \le C_D(t_0, t_1), \quad \forall t \in [t_0, t_1],$$

where $C_D(t_0, t_1)$ depends on the time interval $[t_0, t_1]$. Thus we can consider the subset M of $C_{CP}^0([t_0, t_1])$:

$$\mathsf{M} = \{ (e_D, \Phi) \in C^0_{\mathrm{CP}}([t_0, t_1]) : |e_D| \le C_D(t_0, t_1) \ \forall t \in [t_0, t_1], \ \Phi \in \mathcal{M}(e_D) \}.$$

Given $(e_D^*, \Phi^*) \in \mathsf{M}$, we solve the modified coupled problem

(5.11)
$$E\dot{x} = Ax + \sigma^{\sharp} + b(t), \quad \text{in} [t_0, t_1]$$

(5.12)
$$P_0 P_1 x(t_0) = y_0$$

$$(5.13) e_D = V^\top x$$

(5.14)
$$\sigma^{\sharp} = -U \, i_D^{\sharp}(e_D; e_D^*, \Phi^*),$$

where the current $i_D^{\sharp}(e_D; e_D^*, \Phi^*)$ is defined from the quasi-Fermi potentials $\Phi = \Phi^{\sharp}(e_D; e_D^*, \Phi^*)$, which solve the system (5.7)–(5.8).

The modified coupled problem (5.11)-(5.14) admits a unique solution, because of the Lipschitz continuity of $\sigma^{\sharp} = -U i_D^{\sharp}(e_D; e_D^*, \Phi^*)$ with respect to e_D (Lemma 5.4). Moreover, Lemma 5.3 applies, because passivity is given (Lemma 5.4), and the uniquely defined solution x satisfies the estimates (5.2)-(5.4), and thus estimate (5.10). Hence, the coupled system (5.11)-(5.14) defines a map from M to itself,

$$T : (e_D^*, \Phi^*) \mapsto (e_D, \Phi) = (V^{\top} x, \Phi^{\sharp}(e_D; e_D^*, \Phi^*))$$

and it holds:

LEMMA 5.5 (Fixed-point map). The set M is a nonempty, bounded, closed, convex subset of $C^0([t_0, t_1], \mathbb{R}^{n_D+1}) \times C^0([t_0, t_1], L^2(\Omega))$. The map T is a compact automorphism of M.

The proof from [2] applies also to our index-2 case. Hence by Schauder's fixed point theorem, T admit a fixed point (x, Φ, ϕ) , which solves the original problem (4.1)–(4.4). Thus Theorem 4.1 is proven.

REMARK 2. Notice, the coupling term $\varrho(x)$ (3.2) does not occur explicitly in the a priori estimates nor in the discussion of the fixed point map. This is due to the fact of the passivity, which we maintain also in the modified problem for the fixed point argument. Also the algebraic variables w and z do not occur in the fixed point argument, since we restrict ourselves to the inherent ODEpart. And in fact, having found the differential solution y and the device solution ϕ , ϕ_n , ϕ_p , y is also differentiable and we obtain bounds for the remaining terms (w and z).

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6. Conclusions. We have investigated a coupled problem of elliptic partial differential equations (PDE) and differential algebraic equations (DAE). Such systems occur in circuit simulation, for example. Due to certain conditions, we are able to give meaning to the tractability index in this setting. Furthermore, we were able to prove an existence result for the related index-2 coupled system by using Schauder's fixed point theorem and using previous results for coupled systems of index-1.

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