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A Concept for Classification of Partial Differential Algebraic Equations in Nanoelectronics

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Summary. The design of electronic circuits is based on numerical simulation of corresponding mathematical models. Systems of differential algebraic equations (DAEs) reproduce the time behaviour of idealised electric networks. In nanoelectronics, miniaturisation causes parasitic effects, which can not be neglected any longer. These spatial phenomena yield models consisting of partial differential equations (PDEs). Thus the circuit's behaviour is given by partial differential algebraic equations (PDAEs), which couple DAEs in time and PDEs in time/space. We present a rough concept for classifying existing PDAE models in nanoelectronics. The categorisation rests primarily upon the physical background in each model.

Key words: partial differential algebraic equations, differential algebraic equations, partial differential equations, index, chip design, nanoelectronics.

1 Introduction

The mathematical model of dynamical systems often results from some network approach, which yields time-dependent systems of differential algebraic equations (DAEs). That is, we consider ideally joint lumped elements, without spatial coordinate, but with the topology information given by the incidences of these elements. In contrast, spatial physical effects are described by partial differential equations (PDEs) in space or time/space. Thus an enhanced model requires a coupling of DAEs and PDEs, which yields systems of so-called partial differential algebraic equations (PDAEs). Such systems of PDAEs arise in many technologies like mechanical engineering as coupled multibody systems with sole or flexible/plastic systems, see [5], in nanoelectronics (see below) and others.

Furthermore the wording PDAE is also used for singular implicit PDEs, i.e., where singular matrices arise in front of partial derivatives, see [8], for

example. In case of electronic circuits, a specific multivariate model yields an efficient representation of amplitude and/or frequency modulated signals including widely separated time scales. The introduction of different time variables (for the occurring scales) transforms the circuit's DAE into a PDAE in the sense of a singular PDE, see [9].

In this paper, we focus on PDAE models in nanoelectronics setting with PDE-enhancement of DAE models, rather than singular PDEs. Modified nodal analysis yields large systems of DAEs for ideal circuits, see [7]. We write such a system in the general form

$$\mathbf{f} : \mathbb{R}^k \times \mathbb{R}^k \times I \to \mathbb{R}^k, \quad \mathbf{f}(\mathbf{y}, \dot{\mathbf{y}}, t) = \mathbf{0}, \quad t \in I := [0, T], \tag{1}$$

where $\mathbf{y} : I \to \mathbb{R}^k$ denotes unknown node voltages and branch currents. A consistent initial value $\mathbf{y}(0) = \mathbf{y}_0$ completes the usual electric network model. In addition, we formulate schematically a system of PDEs corresponding to a parasitic effect via an operator

$$\mathcal{L} : D \times I \times V \to \mathbb{R}^m, \;\; \mathcal{L}(\mathbf{x}, t, \mathbf{v}) = \mathbf{0}, \quad \mathbf{x} \in D \subset \mathbb{R}^d, \quad t \in I \tag{2}$$

with a solution $\mathbf{v} : D \times I \to \mathbb{R}^m$ in some function space V. Initial and/or boundary conditions have to be specified appropriately. Coupling the systems (1) and (2) using some variables/functions results in a PDAE. The coupling can be done via artificial variables, source terms, boundary conditions (BCs) or even more sophisticated constructions.

Since the mathematical structure of PDAEs is rather complex, we can not derive a universal classification of all existing PDAE models. Alternatively, we introduce a rough concept to categorise some important models arising in ongoing research within the field of nanoelectronics.

2 PDAE Models

Each spatial physical phenomenon requires a corresponding modelling via a PDE. The following aspects arise due to miniaturisation in chip design. We distinguish two general types of coupling:

i) Refined Modelling: Usually semiconductors, transmission lines and other components with spatial distribution are given by subcircuits of lumped electric elements (companion models). To obtain a somewhat more precise model (also considering down-scaling phenomena), we replace one or several of these subcircuit descriptions by a PDE model for the corresponding electric effect in the network. These can be one or several semiconductor elements, which behave critical in an electronic network, and where it makes sense to simulate these elements more detailed. Another possibility is to replace a transmission line model based on DAEs by an according PDE. This is a natural way, which bypasses a huge number of more or less artifical parameters of the companion model.

This approach is called refined modelling. It has a special type of coupling. Boundary conditions for the Ohmic contacts of the PDE model are the node potentials of the connect network nodes (Dirichlet condition). At the remaining boundaries in multiple dimensions, where there is no electric contract, one may have von-Neumann conditions with no flux or field conditions at insulated contacts. On the other hand, the output of the PDE model is an electric current, which is eventually a source term to the network's DAE. Abstractly, we obtain systems of the type

$$\begin{aligned} A\mathbf{u}_t + \mathcal{L}_D\mathbf{u} - \mathbf{h}(\mathbf{u},t) &= \mathbf{0} && \text{(PDE in } I \times D\text{)} \\ \mathbf{u}|_{\Gamma_1} &= \mathbf{g}(\mathbf{y}) && \text{(Dirichlet BC)} \\ \tfrac{\partial}{\partial \mathbf{n}}\mathbf{u}\big|_{\Gamma_2} &= \mathbf{h}(\mathbf{y}) && \text{(von-Neumann BC)} \\ \mathbf{f}(\mathbf{y},\dot{\mathbf{y}},t) &= \boldsymbol{\lambda}(\mathbf{u}) && \text{(DAE in } I\text{)}, \end{aligned} \tag{3}$$

where $\mathcal{L}_D$ represents a differential operator with respect to space. The involved PDE can be of mixed type (elliptic, hyperbolic, parabolic). Thereby, the coupling is performed via the input $\boldsymbol{\lambda}$ and the boundary conditions $\mathbf{g}$ and $\mathbf{h}$ (where we have a decomposition of the boundary: $\partial D = \Gamma_1 \cup \Gamma_2$). Furthermore, analysing complex systems (3) may yield simpler but still highly accurate companion models for the underlying component.

In nanoelectronics, the PDAE systems, which have been considered in the literature or are part of ongoing research, can principally be categorised into the following cases:

Semiconductors: Here transistors are described by drift-diffusion or quantum mechanical equations coupled with the electric network. Existence and uniqueness results for nonstationary and stationary drift-diffusion network systems are found in [1, 2], for an index analysis of the arising PDAE, we refer to [4]. Currently, efficient numerical codes are being developed.

Transmission line effects: Also down-scaling causes a decreasing distance of transmission lines and thus an undesired interaction arises. Telegrapher's equation describes the underlying physical effect. The coupling of PDEs and DAEs accords to the form (3). Now the involved PDE is exclusively of hyperbolic type, which implies a specific numerical treatment, see [6] for details.

Electromagnetic fields: The DAEs (1) result from a network approach to avoid a simulation of the complete circuit using Maxwell's equations. However, if some crucial parts of the circuit demand a refined model, a separation from the network can be done. Thus we apply Maxwell's equations to represent the small part, whereas we use the network DAEs for the major part.

ii) Multiphysical Extension: This modelling is much more complex, since we do not add a physical dimension to the electric network, but have a distributed additional effect:

Thermal aspects: The increase of the clock rate in chips causes a higher power loss in the electronic network. Thus we have to consider heat distribution and conduction between the circuit's elements. In contrast to the effects

described above, the heat evolution runs in parallel to the time-dependence of voltages and currents. Thus a thermal network can be associated to the electric network. In the thermal part, specific 0D elements can be refined into elements with spatial distribution or elements can be located in macro structures. Combining the heat equation for the spatial elements with the network yields

$$\begin{aligned} A\mathbf{u}_t + \mathcal{L}_D\mathbf{u} - \mathbf{h}(\mathbf{u},t) &= \mathbf{s}(\mathbf{x}) \quad && \text{(PDE in } I\times D\text{)} \\ \mathbf{u}|_{\partial D} &= \mathbf{g}(\mathbf{x}) && \text{(BC)} \\ \mathbf{f}(\mathbf{y},\dot{\mathbf{y}},t,\boldsymbol{\mu}(\mathbf{u})) &= \mathbf{0} && \text{(DAE in } I\text{)}\,. \end{aligned} \tag{4}$$

In this case, the included PDE is of parabolic type (Fourier Law). The coupling is present in the source terms and boundary conditions $\mathbf{s}$, $\boldsymbol{\mu}$, $\mathbf{g}$: Here dissipated power is not only entering the boundary conditions, but is also a source term for the evolution equation; on the other hand, the temperature enters the electric network as parameter and thus causes a more general dependence. For further details, we refer to [3].

Electromagnetics: In principle, one can interpret an electromagnetic field influencing the complete circuit as a multiphysical case, too. Consequently, the contribution of the field to each component has to be modelled appropriately.

3 Illustrative Example

We consider the electric circuit given in Fig. 1. In the refined description, where the diode is modelled by semiconductor equations, we have:
a) electric network: (current through voltage source j_V, node potential u_1, u_2)

$$j_V + \frac{u_1-u_2}{R} = 0, \quad \frac{u_2-u_1}{R} + j_d + C\frac{\mathrm{d}}{\mathrm{d}t}u_2 = 0, \quad u_1 - v(t) = 0. \tag{5a}$$

b) 1D drift-diffusion: (electron/hole density n/p, electrostatic potential V – currents j_p, j_n)

$$-q\partial_t n + \partial_x j_n = qR, \qquad j_n = -q\left\{-D_n\partial_x n + \mu_n n\partial_x V\right\}, \tag{5b}$$

$$q\partial_t p + \partial_x j_p = -qR, \qquad j_p = q\left\{-D_p\partial_x p - \mu_p p\partial_x V\right\}, \tag{5c}$$

$$-\epsilon\partial_x^2 V - q(C+p-n) = 0, \qquad j_d = \frac{\epsilon}{l}\frac{\mathrm{d}}{\mathrm{d}t}u_2 + \frac{1}{l}\int_0^l \{j_n + j_p\}\mathrm{d}x, \tag{5d}$$

$$\begin{pmatrix} V(0,t)-V_{\mathrm{bi}} \\ V(l,t)-V_{\mathrm{bi}} \end{pmatrix} = \begin{pmatrix} u_2 \\ 0 \end{pmatrix}, \quad n(0,t) = n(l,t) = n_0, \quad p(0,t) = p(l,t) = p_0. \tag{5e}$$

This involves parameters: resistance R, capacity C, input $v(t)$ for the network equations; the diode is defined on a 1D-line segment ($[0,l]$) with mobilities μ_n, μ_p, diffusivities D_n, D_p, unit of charge q, permittivity ϵ, doping profile $C : [0,l] \to \mathbb{R}$ and according built-in potential $V_{\mathrm{bi}} : [0,l] \to \mathbb{R}$. Furthermore, j_d specifies the output current of the diode and therefore our coupling quantity.

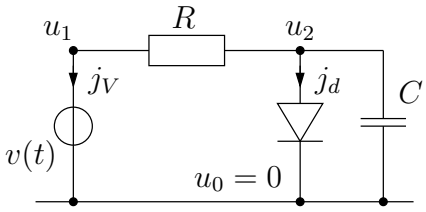

Fig. 1 : Example circuit.

The boundary conditions for the carrier densities (n_0, p_0) are obtained from equilibrium assumptions, see [1] for more details. As a further refinement of this example, one could image telegrapher's equation for the parallel connection of the diode and the capacitor.

4 Conclusions

In nanoelectronics, a sophisticated modelling of physical effects leads to systems of PDAEs. An elementary classification of some crucial models has been presented, which considers the type of the underlying PDEs and especially the physical nature of the coupling: models can be (i) refined, replacing simple (0D) descriptions by (more advanced) spatial models, or (ii) multiphysically extended, adding a new layer of effects.

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