# A Multilevel Error-Correction Scheme for the Electro-Thermal Modelling of Device Structures

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**Device design in nano-electronics generally yields strongly coupled problems in time-domain. The solution of such problems formally entails a monolithic approach that is characterised by a large system matrix. In this paper, a error correction scheme is proposed within the context of electro-thermal coupling in device structures. The scheme avoids the computational burden of a monolithic implementation and retains the convergence order in time by conveniently solving an error equation in a recursive fashion. The method can also be integrated with sub-problem-wise order reduction technique.**

***Index Terms*—Differential algebraic equations, Electro-thermal coupling , Error correction, Fractional time step.**

## I. Introduction

In this paper an approach for solving electro-thermal problems encountered in device structure is described. The approach is built upon the finite integration technique (FIT) [1], [2] and aims at avoiding the computational burden of a monolithic solution. This paper is organised as follows: In Section 2, the electro-thermal problem is formulated, and numerically solved. In Section 3 a simple numerical example is provided.

## II. Dynamical Electro-Thermal Modelling of Devices Structures

### A. Problem Statement

We depict a structure of interest in Fig. 1. Typically, these structures comprise dielectric materials, vias, contacts, and metal interconnects. We want to compute the temperature in such configurations resulting from an applied voltage. The governing equations are

$$\nabla \cdot \mathbf{J} = -\frac{\partial \varrho_\mathrm{e}}{\partial t};\ \varrho_\mathrm{e} = -\nabla \cdot (\varepsilon \mathbf{E})\,;\ \mathbf{J} = \sigma \mathbf{E};\ \mathbf{E} = -\nabla\phi - \frac{\partial \mathbf{A}}{\partial t}; \tag{1}$$

$$\rho c_\mathrm{e} \frac{\partial T}{\partial t} = \nabla \cdot (\kappa \nabla T) + \dot{q}_\mathrm{i}, \tag{2}$$

where $\mathbf{J}$ is the current density, $\mathbf{A}$ the magnetic potential, $\mathbf{E}$ the electric field, $\phi$ the electric potential, $\varepsilon$ and $\sigma$ the permittivity and conductivity of the medium, $\varrho_\mathrm{e}$ the electric charge density, $\rho c_\mathrm{e}$ the thermal capacitance, $\kappa$ the thermal conductivity, $T$ the temperature, and $\dot{q}_\mathrm{i}$ an impressed heat source. The system (1)–(2) is coupled through $\dot{q}_\mathrm{i} = \mathbf{E} \cdot \mathbf{J}$ and the temperature dependence of $\sigma$, $\rho c_\mathrm{e}$, and $\kappa$.

### B. Numerical Solution

We attain the numerical solution of (1)–(2) by means of FIT [1], [2]. The grid counterpart of (1)–(2) reads

$$\tilde{\mathbf{S}}\mathbf{M}_\sigma\tilde{\mathbf{S}}^\top\Phi = 0, \qquad \mathbf{M}_\mathrm{c}\frac{\partial}{\partial t}\mathbf{T} = -\tilde{\mathbf{S}}\mathbf{M}_\kappa\tilde{\mathbf{S}}^\top\mathbf{T} + \mathbf{Q}_\mathrm{i}, \tag{3}$$

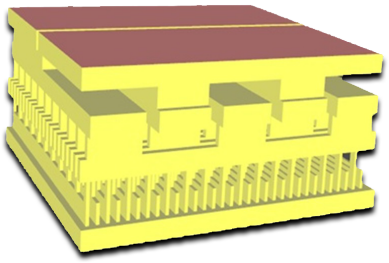

Fig. 1. Typical layout (stretched along the vertical direction) of a power transistor. Image from [3].

where $\Phi$ and $\mathbf{T}$ are the potential and temperature vectors, $\mathbf{M}_\sigma$, $\mathbf{M}_\mathrm{c}$, and $\mathbf{M}_\kappa$ are *diagonal* material matrices representing conductivity, thermal capacitance, and thermal conductivity, respectively; the grid heat source $\mathbf{Q}_\mathrm{i}$ is given by

$$\mathbf{Q}_\mathrm{i} \equiv \sum_i \mathbf{P}\left(\mathbf{1}_i^\top \mathbf{M}_\sigma^{\frac{1}{2}}\tilde{\mathbf{S}}^\top\Phi\Phi^\top\tilde{\mathbf{S}}\mathbf{M}_\sigma^{\frac{1}{2}}\mathbf{1}_i\right)\mathbf{1}_i, \tag{4}$$

with $\mathbf{P}$ a projection matrix that enables to compute the heat source at the grid nodes [4], [5], $\mathbf{1}_i$ the $i$-th basis column vector, and the sum carried out over all grid primary edges [1], [2], [6]. We partition $\Phi$ and $\mathbf{T}$ into $\{\Phi_\mathrm{d}, \mathbf{T}_\mathrm{d}\}$ and $\{\Phi_\mathrm{b}, \mathbf{T}_\mathrm{b}\}$, that is the degrees of *freedom* and *boundary* potentials and temperatures. After some mathematical manipulations, we arrive at

$$\tilde{\mathbf{S}}_\mathrm{d}\mathbf{M}_\sigma\tilde{\mathbf{S}}_\mathrm{d}^\top\Phi_\mathrm{d} = -\tilde{\mathbf{S}}_\mathrm{d}\mathbf{M}_\sigma\tilde{\mathbf{S}}_\mathrm{b}^\top\Phi_\mathrm{b}, \tag{5}$$

$$\begin{aligned}\mathbf{M}_{\mathrm{c;d}}\frac{\partial}{\partial t}\mathbf{T}_\mathrm{d} = &-\tilde{\mathbf{S}}_\mathrm{d}\mathbf{M}_\kappa\tilde{\mathbf{S}}_\mathrm{d}^\top\mathbf{T}_\mathrm{d} - \tilde{\mathbf{S}}_\mathrm{d}\mathbf{M}_\kappa\tilde{\mathbf{S}}_\mathrm{b}^\top\mathbf{T}_\mathrm{b}\\ &+ \Phi_\mathrm{d}^\top\mathbf{H}_\mathrm{dd}\Phi_\mathrm{d} + \Phi_\mathrm{d}^\top\mathbf{H}_\mathrm{db}\Phi_\mathrm{b},\end{aligned} \tag{6}$$

where $\mathbf{H}_\mathrm{dd}$ and $\mathbf{H}_\mathrm{db}$ are *heat* tensors[1]. The system (5)–(6) is an index-1 DAE that can be readily solved by the implicit Euler method [6]. However, we obtain the solution by means of a decoupling fractional step approach endowed with an error correction scheme. The later permits to retain the temporal

[1]Three-dimensional arrays of depth equal to the length of $\mathbf{T}_\mathrm{d}$, and where the subscripts $_\mathrm{dd}$ and $_\mathrm{db}$ denote the number of rows and columns, respectively.

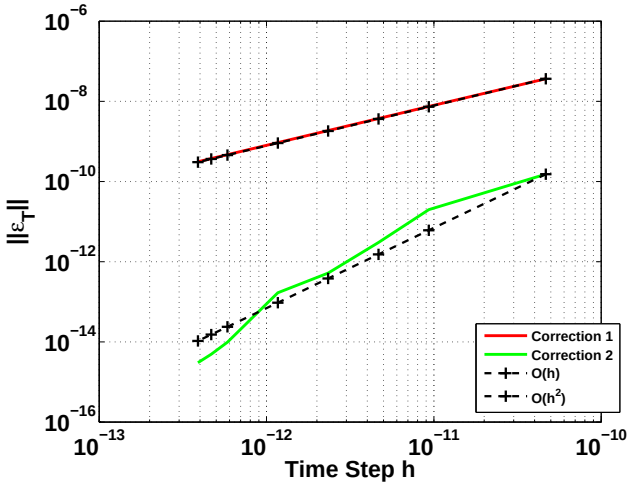


Fig. 2. Correction error $\|\mathbf{e_T}\|$ *versus* the time step $h$.

convergence order while avoiding the burden of the monolithic solution.

### C. Error Correction Scheme

We introduce a staggered grid pair in time, i.e., $\mathbf{t} = [t_1, t_2, \ldots, t_n]$ with time step $h_i$. The dual grid is shifted by half of a time step. Then, we proceed to decouple $\Phi_\mathrm{d}$ and $\mathbf{T}_\mathrm{d}$ over a time step $h_i$, viz.

$$\frac{\partial}{\partial t}\Phi_\mathrm{d} \equiv 0 \Rightarrow \tilde{\Phi}_\mathrm{d}^{(n+\frac{1}{2})} = \tilde{\Phi}_\mathrm{d}^{(n)}, \qquad t_n \leq t < t_n + \frac{h_i}{2}, \tag{7}$$

$$\frac{\partial}{\partial t}\mathbf{T}_\mathrm{d} \equiv 0 \Rightarrow \tilde{\mathbf{T}}_\mathrm{d}^{(n+1)} = \tilde{\mathbf{T}}_\mathrm{d}^{(n+\frac{1}{2})}, \, t_n + \frac{h_i}{2} \leq t < t_n + h_i, \tag{8}$$

where $\tilde{}$ denotes approximations. The resulting system is solved by means of the implicit Euler method thus generating a first estimation of $\{\Phi_\mathrm{d}, \mathbf{T}_\mathrm{d}\}$, viz.

$$\begin{aligned}\mathbf{M}_{\mathrm{c;d}} \frac{\tilde{\mathbf{T}}_\mathrm{d}^{(n+\frac{1}{2})} - \tilde{\mathbf{T}}_\mathrm{d}^{(n)}}{h_i/2} = &- \tilde{\mathbf{S}}_\mathrm{d}\tilde{\mathbf{M}}_\kappa\tilde{\mathbf{S}}_\mathrm{d}^\top\tilde{\mathbf{T}}_\mathrm{d}^{(n+\frac{1}{2})} - \tilde{\mathbf{S}}_\mathrm{d}\tilde{\mathbf{M}}_\kappa\tilde{\mathbf{S}}_\mathrm{b}^\top\mathbf{T}_\mathrm{b} \\ &+ \tilde{\Phi}_\mathrm{d}^{\top(n)}\tilde{\mathbf{H}}_\mathrm{dd}\tilde{\Phi}_\mathrm{d}^{(n)} + \tilde{\Phi}_\mathrm{d}^{\top(n)}\tilde{\mathbf{H}}_\mathrm{db}\Phi_\mathrm{b},\end{aligned} \tag{9}$$

$$\tilde{\mathbf{S}}_\mathrm{d}\tilde{\mathbf{M}}_\sigma^{(n+\frac{1}{2})}\tilde{\mathbf{S}}_\mathrm{d}^\top\tilde{\Phi}_\mathrm{d} = - \tilde{\mathbf{S}}_\mathrm{d}\tilde{\mathbf{M}}_\sigma^{(n+\frac{1}{2})}\tilde{\mathbf{S}}_\mathrm{b}^\top\Phi_\mathrm{b}. \tag{10}$$

Subsequently, we define the errors $\mathbf{e}_\Phi = \Phi - \tilde{\Phi}$ and $\mathbf{e_T} = \mathbf{T} - \tilde{\mathbf{T}}$. These errors consist of two contributions; one coming from the time discretisation and the other coming from the decoupling. Both error contributions are $\mathcal{O}(h_i)$. We reduce these errors by solving the associated error equation in a recursive fashion, viz.

$$\begin{aligned}-\mathbf{r_T} \cong \mathbf{M}_{\mathrm{c;d}}\mathbf{e_T} &+ \int_0^t \tilde{\mathbf{S}}_\mathrm{d}\tilde{\mathbf{M}}_\kappa\tilde{\mathbf{S}}_\mathrm{d}^\top\mathbf{e_T} + \tilde{\mathbf{S}}_\mathrm{d}\mathbf{E}_\kappa\tilde{\mathbf{S}}_\mathrm{d}^\top\tilde{\mathbf{T}}_\mathrm{d}\,\mathrm{d}t \\ &+ \int_0^t \tilde{\mathbf{S}}_\mathrm{d}\mathbf{E}_\kappa\tilde{\mathbf{S}}_\mathrm{b}^\top\mathbf{T}_\mathrm{b}\,\mathrm{d}t - \int_0^t \tilde{\Phi}_\mathrm{d}^\top\mathbf{E}_\mathrm{dd}\tilde{\Phi}_\mathrm{d}\,\mathrm{d}t + \mathbf{e}_\Phi^\top\tilde{\mathbf{H}}_\mathrm{dd}\tilde{\Phi}_\mathrm{d}\,\mathrm{d}t \\ &- \int_0^t \tilde{\Phi}_\mathrm{d}^\top\tilde{\mathbf{H}}_\mathrm{dd}\mathbf{e}_\Phi\,\mathrm{d}t + \mathbf{e}_\Phi^\top\tilde{\mathbf{H}}_\mathrm{dd}\mathbf{e}_\Phi + \tilde{\Phi}_\mathrm{d}^\top\mathbf{E}_\mathrm{db}\Phi_\mathrm{b} + \mathbf{e}_\Phi^\top\tilde{\mathbf{H}}_\mathrm{db}\Phi_\mathrm{b}\,\mathrm{d}t,\end{aligned} \tag{11}$$

and

$$-\mathbf{r_\Phi} \cong -\tilde{\mathbf{S}}_\mathrm{d}\tilde{\mathbf{M}}_\sigma\tilde{\mathbf{S}}_\mathrm{d}^\top\mathbf{e}_\Phi - \tilde{\mathbf{S}}_\mathrm{d}\mathbf{E}_\sigma\tilde{\mathbf{S}}_\mathrm{d}^\top\tilde{\Phi}_\mathrm{d} - \tilde{\mathbf{S}}_\mathrm{d}\mathbf{E}_\sigma\tilde{\mathbf{S}}_\mathrm{b}^\top\Phi_\mathrm{b}, \tag{12}$$

where $\mathbf{r_T}$ and $\mathbf{r_\Phi}$ are residual functions, $\mathbf{E}_\kappa \equiv \mathbf{M}_\kappa - \tilde{\mathbf{M}}_\kappa$, $\mathbf{E}_\sigma \equiv \mathbf{M}_\sigma - \tilde{\mathbf{M}}_\sigma$, $\mathbf{E}_\mathrm{dd} \equiv \mathbf{H}_\mathrm{dd} - \tilde{\mathbf{H}}_\mathrm{dd}$, and $\mathbf{E}_\mathrm{db} \equiv \mathbf{H}_\mathrm{db} - \tilde{\mathbf{H}}_\mathrm{db}$ are function of $\mathbf{e_T}$.

## III. Numerical Example

The afore-described method has been applied to a electro-thermal problem from MAGWEL, modelled in their PTM-ET software, in which the temperature dependence of the material matrices $\mathbf{M}_\kappa$ and $\mathbf{M}_\sigma$, and heat tensors $\mathbf{H}_\mathrm{dd}$ and $\mathbf{H}_\mathrm{db}$, is given by polynomials $\Pi_{\kappa;\sigma}(\mathbf{T}, \mathbf{T}_\mathrm{o})$ with reference temperature $\mathbf{T}_\mathrm{o}$. We have solved for $\tilde{\Phi}_\mathrm{d}$ and $\tilde{\mathbf{T}}_\mathrm{d}$ using the implicit Euler method with iterative refinement. Figure 2 shows the correction error $\|\mathbf{e_T}\|$ after two recursions.

## IV. Conclusion

We have described an approach for the error correction of index-1 DAE describing electro-thermal systems. The method avoids the monolithic solution while retaining the time convergence order. Future research will investigate the combination of the iterative with a sub-problem-wise model order reduction technique.

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