COMPUTER-AIDED ENGINEERING OF ELECTRO-THERMAL MST DEVICES: MOVING FROM DEVICE TO SYSTEM SIMULATION

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Abstract

A general *overview* of electro-thermal simulation is presented with emphasis on how to *generate* compact thermal models. The current status of the mathematical theory for approximating large-scale linear dynamic systems is described. We discuss how this theory can assist engineers to obtain reliable compact thermal models in a completely *automatic* fashion. A *case study* of a microthruster is reported in order to demonstrate the feasibility of the ideas. Unsolved mathematical *challenges* pertaining to the topic are listed.

Introduction

The success of engineering practise is often strongly tied with new advances in mathematics, because progress in mathematical theory can, e.g., help to simulate a particular device with a higher level of detail within a shorter time and hence decrease the product development period significantly. In the present paper, we describe a recurring situation with electro-thermal simulations, which, in our view, can be greatly improved by employing mathematical results from the theory of approximation of large-scale linear dynamic systems.

Electro-thermal simulation has become an essential part of many instances of microsystem engineering. In general, it requires the solution of a coupled system of partial differential equations (PDEs) within a device-level simulation. This can be done in principle, but for real devices and systems it requires a considerable amount of computational time. Usually the focus of the simulation is to develop an electrically and thermally optimized electrical circuit, so that this system of ODEs has be solved repeatedly with different electrical input functions during a system-level simulation. Using compact thermal models would greatly increase efficiency, but generating the models still remains a challenge.

A closer look at the mathematical electro-thermal problem has revealed that, under some reasonable approximations, the thermal part of an electro-thermal simulation can be modeled by a linear dynamic system. Now, the approximation of large-scale linear dynamic systems is a rapidly developing area of modern applied mathematics. A detailed study of these methods has allowed us to suggest a rigid mathematical framework with which to automatically generate compact thermal models, which we will detail here. A block diagram of the basic idea is shown in Figure 1.

A microthruster device arranged in an array will be considered as a case study. The device is somewhat unusual for the electro-thermal community, as a primary design goal for the device is to reach a critical high temperature rather than to escape it. However, the underlying mathematical model is exactly the same as the usual case, as is the need to avoid thermal cross-talk between adjacent devices.

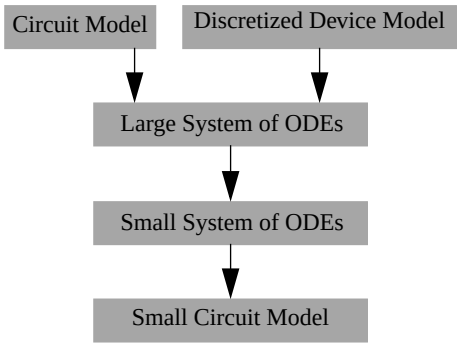

Figure 1. Model Order Reduction Steps.

At the end of the paper, we list some mathematical and numerical challenges, the solution of which is necessary for the further development of efficient electro-thermal simulators.

Electro-thermal Simulation in MEMS

Microsystem technology (MST) allows engineers to combine electrical circuitry and other microdevices for “ambient intelligence” applications. Many of these microdevices are powered by electrical current, so that they can sense their environment and, depending on circumstances, even produce some action. An important part of the design process is to take into consideration inevitable electro-thermal effects, which very often play a parasitic role through Joule heating. There are also a number of thermo-electric effects [1] that may be useful but they are outside of the scope of our paper.

Electro-thermal simulation therefore has become an essential design task in microsystem technology [2, 3]. A search at IEEE Xplore for the last six years reveals that, in this area, the IEEE journals and conferences annually publish about 20 publications, see Figure 2. The area of application is very broad: it ranges over power transistors, thick-film circuits, prediction of electrostatic discharge, hotplate sensors, oxide-confined vertical-cavity lasers, infrared sensors, flow meters, electro-thermal actuators, and so on.

The lumped representation of an electrical circuit is a well-established area in electrical engineering, in which a

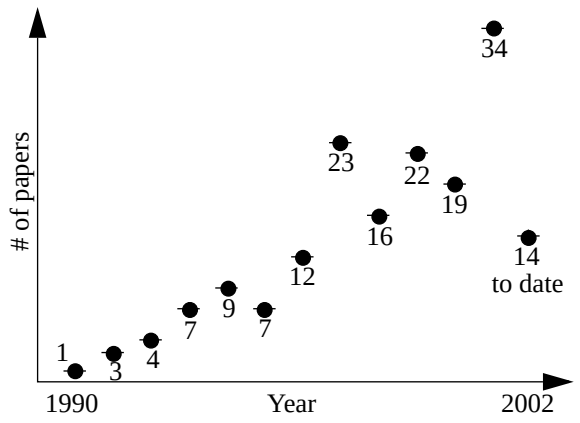

Figure 2. Number of IEEE electro-thermal papers.

system of ordinary differential equations (ODEs) is directly created for a given circuit. There are a number of tools (e.g. SPICE) with which electrical engineers have successfully developed circuitry for many years. However, the addition of a thermal model to such a system-level simulation happens not to be straightforward.

The main question for an electro-thermal simulation is: *how to convert the heat transfer partial differential equation (PDE) [4] to a system of ODEs in order to include it in a system-level circuit simulation*? Unfortunately, the straightforward solution by means of a semidiscretization of the governing PDEs leads to a high dimensional system of ODEs, which, due to its size, is not feasible to add to the system level circuit model.

The conventional approach is first to develop a compact thermal model that describes the temperature behavior at prescribed spacial positions. A typical way to proceed here, and which can be found in available software, is to make several device-level simulations and then to try to fit these results to some low-order lumped model based on the idea of thermal impedance. Yet, as the functional form of appropriate low-order models is not known a priory, this process may take up a lot of time of highly-qualified personnel, because the success highly depends on a person's intuition. *Hence it is quite essential to automate the procedure of generating compact thermal models completely.* We will now consider a way to do so.

Mathematical Problem Analysis

Heat transfer in a solid material is expressed by a partial differential equation as follows

$$\nabla \bullet (\kappa \nabla T) + Q - \rho C_p \frac{\partial T}{\partial t} = 0, \qquad (1)$$

where κ is the thermal conductivity (assumed to be isotropic), C_p is the specific heat capacity, ρ is the mass density, Q is the heat generation rate per unit volume (this term is non-zero within the heat source region only) and T is the unknown temperature distribution that is to be determined over the device domain Ω with boundary Γ. This equation holds at each point within the solid material.

The coupling of Eq (1) with an electrical circuit is made through the heat generation rate that, for the case of dissipative Joule heating, is given by

$$Q = \frac{\boldsymbol{j}^2}{\sigma}. \qquad (2)$$

where $\boldsymbol{j}$ is the electrical current density vector and σ is the conductivity at a given point. In the general case, in order to find the electrical current density distribution within the heat source region, one has to solve a Poisson equation. As a result, the combined task becomes computationally demanding as it is necessary to solve both the Poisson and heat transfer equation.

A considerable simplification can be made under the assumption of homogeneous heat generation rate within the heat source, in other words, by introducing lumped electrical resistors in which heat generation occurs. In some devices, for example hotplate sensors, heat generation resistor elements are already lumped by design. In others, like transistors, the applicability of such an assumption requires special considerations.

The homogeneous heat generation hypothesis decouples electrical and thermal parts because now the heat generation rate can be computed as follows

$$Q = I^2 R / V, \qquad (3)$$

where I is the total current passing through the lumped resistor, R its total resistance and V is its volume. After this step, one can make a semidiscretization of Eq (1) in space (e.g. by the FEM, see Figure 3) and obtain a system

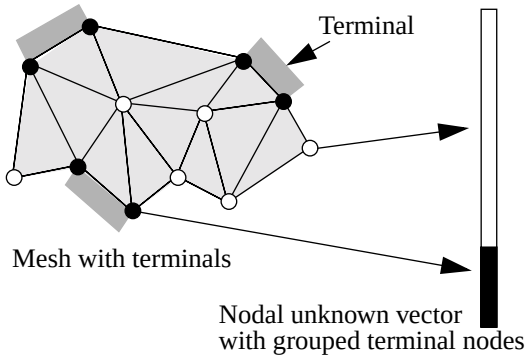

Figure 3. Spatial semidiscretization and nodal unknown grouping.

of ordinary differential equations

$$\frac{d\boldsymbol{T}}{dt} = A \cdot \boldsymbol{T} + \boldsymbol{b}u \qquad (4)$$

where $\boldsymbol{T}$ is a vector of unknown temperatures at the nodes introduced during the discretization, A is the system matrix, $\boldsymbol{b}$ is a load vector and $u = I^2 R$ is a scalar input function. Eq (4) allows us now to make simple black box connections between the thermal and electric parts and to merge the systems of ODE for the electrical circuit and heat transfer in a natural way (see Figures 4 and 5)

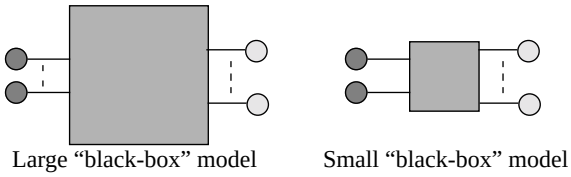

Figure 4. Model and reduced model with terminals.

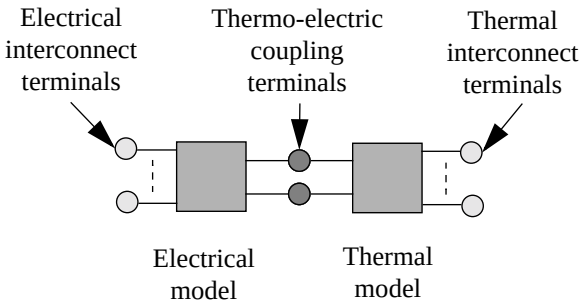

Figure 5. Electrothermal block diagram.

The main problem with Eq (4) is still the high dimensionality of the vector $\boldsymbol{T}$, which can easily reach hundreds of thousands for three-dimensional geometries discretized by e.g. the finite element method (FEM). This in turn leads to the high dimension of system matrices and finally to the huge computational cost to solve the system’s response. A solution to this problem is model reduction, and will be considered in the next section. However, before we do this, let us remind ourselves that engineers are frequently not interested in the solution of Eq (4) over the entire computational domain, that is, to know the temperatures at all nodes. Instead, they often only require a few of their combinations, that is, a few thermal outputs $\boldsymbol{y}$ expressed by an output matrix C

$$\boldsymbol{y} = C \cdot \boldsymbol{T} \tag{5}$$

Approximation of Large-scale Linear Dynamic Systems

The *goal* of model order reduction is to find a low-order system that reasonably well approximates the large scale dynamic system (4) and (5), that is, for the same inputs and outputs to reduce the dimension of the state vector $\boldsymbol{T}$ [5, 6], see Figure 6. For a linear dynamic system, there are many important results which we summarize below.

The most advanced results here are established by control theory, which allows us to make the strong statement that model reduction of a linear dynamic system is solved *in principle*. This means that there are methods (for example the truncated balanced approximation, the singular perturbation approximation, and the Hankel-norm approximation) with guaranteed error bounds for the difference between the transfer function of the original high-dimensional and reduced low-dimensional systems. This means that model reduction based on these methods can be made *fully automatic*. A user merely has to set an error bound, and then the algorithm will find the smallest possible dimension of the reduced system which satisfies that bound. Alternatively, a user specifies the required dimension of the reduced system and then the algorithm estimates the error bound for the reduced system. Unfortunately, the computational complexity of this algorithms is of order $O(N^3)$, with N the order of the system of ODEs. Hence, if the system order doubles, the time required to solve a new problem will increase about eight fold. In other words, even though this theory is valid for all linear dynamic systems, practically we can use it for “small” systems only.

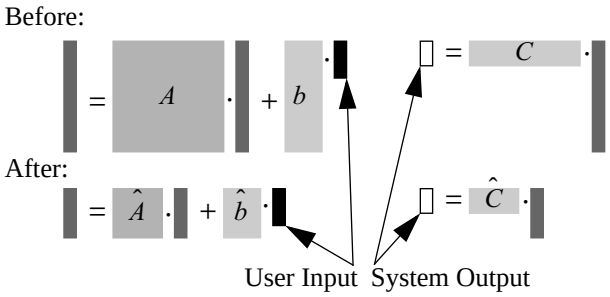

Figure 6. ODE system model order reduction details.

Most of the practical work in model reduction of large linear dynamic systems has been tied to Padé approximants (so-called moment matching) of the transfer function via Krylov subspaces by means of either the Arnoldi or the Lanczos process. In the literature, there are some spectacular examples where, using this technique, the dimension of a system of ordinary differential equations was reduced by *several orders of magnitude*, almost without sacrificing precision. The disadvantage is that Padé approximants do not have a global error estimate, and hence it is necessary to select the order of the reduced system manually.

Recently, there have been considerable efforts to find computationally effective strategies in order to apply methods based on Hankel singular values to large-scale systems, the so-called SVD-Krylov methods based on low-rank Grammian approximants. However, they are currently under development and engineers will have to wait for the experience of mathematicians grows in this field.

Model Order Reduction for the Electro-Thermal Problem

The model order reduction methods described in the previous section are of of course of general importance. In our view, however, the thermal part of an electro-thermal simulation is an *almost ideal candidate* for these techniques, because:

- Compact thermal models are used repeatedly during system-level simulations;
- The nonlinearity in the thermal domain is small and thus it can be effectively treated by a linear dynamic model;
- The available numerical results support a view that the compression ratio of model order reduction for thermal problems is very high.

Let us elaborate these points. Model order reduction is done for a given device specification because it follows a semidiscretization step. For any change in the device specification, model order reduction must be repeated. This means that, if the solution of the PDEs is required only once, it is probably easier to obtain it by conventional means. For the case where a device is coupled to an electrical circuit, the device PDEs will be solved many times for different boundary conditions representing electrical inputs. In this case, model order reduction can greatly decrease the overall computational time.

There are several sources of nonlinearity that prevent us to employ the methods from the previous section. This is certainly the case when material properties in the heat transfer PDE depends on temperature. Because the temperature range in conventional devices is relatively small, this can often be treated by taking properties at an average temperature. After the homogenous heat generation approximation, the input functions may depend on temperature explicitly because the resistivity depends on temperature. This is another source of nonlinearity, because in the mathematical theories considered above an input function must depend on time only. However, from an engineering viewpoint we can close our eyes to this fact because, pragmatically speaking, the model order reduction algorithms do not depend on the input function. Thus, after model order reduction is done we can obtain the necessary temperature output from the reduced model in order to plug it back into the input function, see Figure 5.

Whether model order reduction is possible depends on the system matrix properties. One cannot exclude the possibility that, after the application of the formal mathematical methods, the result might be that for a given system and required precision the order of the reduced system is about the same as that of the original one. However, numerical results available so far indicate that the latter is not the case for the thermal domain, but rather, that the compression ratio can reach a very high value.

Microthruster: a case study

A new class of microthrusters is based on the integration of solid fuel with a silicon micromachined system [7, 8]. In addition to the space application, the device can be also used for gas generation or as a highly-energetic actuator. The goal of this project is to fabricate a working array of independently addressable solid propellant microthrusters on a single chip and to optimize its performance. The model for a microthruster array must include an involved electro-thermal simulation and must be able to perform a joint simulation of the array together with its driving circuitry.

In Ref. [9], model order reduction for a microthruster has been performed by three methods: truncated balanced approximation (BTA), Padé approximation via Arnoldi algorithms, and the Guyan method [10] as implemented in ANSYS [11]. The conclusions from the numerical results are as follows:

- For the same accuracy, the BTA method and Padé approximation allowed us to reduce the order of the original system by a factor of one hundred while the Guyan method achieved only a factor of five.
- For the same order of the reduced system, the BTA method produces more accurate results than the Padé approximation, just as the theory predicts.
- The application of the BTA method is limited to systems with an order of a few thousand.
- Even though the reduced model obtained by the Padé approximation is not optimal, the difference to the BTA approximation is not large, and hence it can be recommended for use with high dimensional systems.

Outlook: Directions for Further Research

We finish by a list of topics, which, in our view, requires work for further application to the area of electro-thermal simulation. Whenever it is possible, a reference is given to appropriate publications where authors already achieve some results to cope with the stated problem:

- The homogeneous heat generation hypothesis may not be appropriate in many cases. Here it is necessary to find a lumped representation of electric parts that contribute to the heat generation rate and assume that within each lumped element the heat generation rate is homogeneous.
- The input function, as was mentioned above, contains a nonlinear term. This requires more mathematical research to determine the limits of our approach.
- Model reduction is usually performed for a single device, and a very important question is, how to connect reduced thermal models to one another [12].
- The Padé approximation does not have a global error estimate. As a result, special efforts should be invested in determining how to choose an order for the reduced system [13].

- The current computational complexity of the control theory methods is $O(N^3)$. There is active research on how to reduce it to an acceptable level [14, 15, 16], for this remains the mathematically most robust method.

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