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Introduction

This text addresses the application of a modern mathematical approach, referred to as model order reduction (MOR), for efficient simulation of electro-thermal microsystems. It is written for engineers that use high-dimensional finite element models (alternatively, spatial discretization can be used as well) during device simulation. It describes the automatic generation of accurate dynamic compact thermal models directly from finite element models. Such compact models are convertible into hardware description language form and can be directly used in system-level simulation or employed for extremely effective design optimization of electro-thermal microsystems.

In general, the design of microsystem devices often depends on large-scale transient simulation of coupled physical domains, such as thermal, mechanical, electrical, etc. This requires the solution of very large systems of ordinary differential equations (ODEs), resulting from the spatial discretization of a computational domain. However, instead of a common "brute force" approach to integrate a large system of ODEs, one can use modern mathematical methods to drastically reduce the problem dimension, and thereby achieve dramatic speedup of the calculation time. Hence, nowadays it is possible to simulate models that only several years ago were too large (due to lack of time, computer memory or computer speed). Indeed, it has been shown that for many MEMS devices, such as accelerometers, gyroscopes and many different electro-thermal devices, the number of ODEs obtained from finite element modeling can be reduced by several orders of magnitude almost without sacrificing precision.

This book describes a complete MOR methodology and software environment at the engineering level. It is equipped with a large number of practical examples, to show readers how to considerably speed up simulation in a concrete problem. Although the model order reduction approach can be applied to different physical domains, in this book we focus on electro-thermal MEMS.

1.1 MEMS, Compact Modeling and Model Order Reduction

The development of increasingly complex microstructures (in the following we will call all microsystems MEMS[1], even if functionality other than micro-electromechanical is employed) demands sophisticated simulation techniques for design, control and optimization [1, 2]. Often, system-level simulation, which includes several single devices placed on a chip together with their driving circuitry, is indispensable. Although no universal simulation strategy currently exists to cover all MEMS design situations [3], reduction of the problem size drastically reduces the computational work. This book is an overview on how to automatically produce reduced models for system-level simulation of MEMS, using modern mathematical approaches.

Traditionally size reduction is performed via compact modeling, which was developed in electrical engineering long before MEMS. The goal of compact modeling is to create a small size equivalent network of resistors, capacitors, inductors, etc. which accurately describes the dynamics of the device and can be directly inserted into SPICE-like simulators. Naturally, MEMS engineers try to use the same methodology. Mathematically speaking, compact modeling starts by choosing the topology of a small-dimensional equivalent circuit (see Figure 1.1). During the second step, parameters within this network (resistivities and capacitances) are found by fitting model parameters to measured or simulated curves. This approach requires the designer to choose the correct network topology intuitively, i.e. without strict guidelines, and then to perform a model parametrization. It should be noted that although the second step requires time-consuming data fitting, the first step usually takes even more time in practice as it is based on intuition.

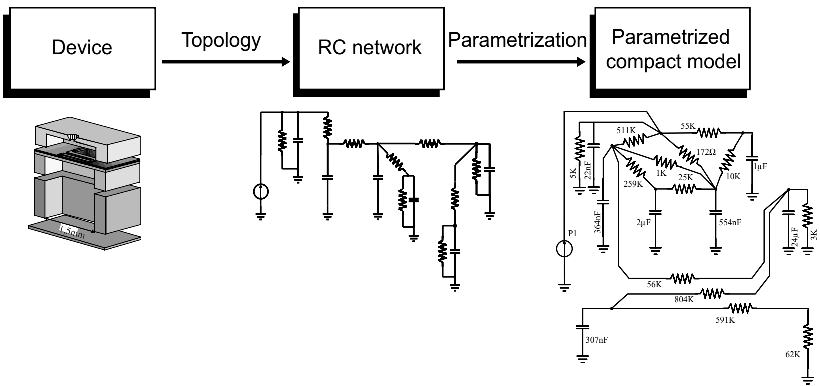

Fig. 1.1. Compact modeling flow of the example thermal MEMS model. RC network pictures courtesy of M. Salleras (UB, Spain).

[1]MEMS traditionally stands for micro-electromechanical systems.

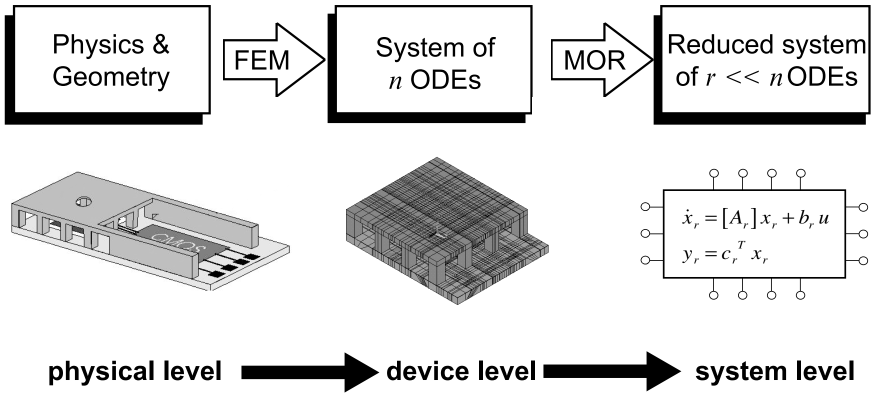

Fig. 1.2. Model order reduction: a switch from device to system level simulation.

An alternative to compact modeling is mathematical model order reduction (also called the approximation of large-scale dynamic systems [4]). Figure 1.2 shows the MOR flow. The simulation of a single device starts with the governing partial differential equations (PDEs). One example is a heat transfer PDE, Eq. 2.5, which takes a central place in this book. The next step is the discretization in space of the original PDE, using, for example, the finite element method (FEM), which integrates the PDE over a number of small nonoverlapping subsets of the complete domain. This results in a system of ordinary differential equations, whose dimension is proportional to the number of introduced nodes. The finer the spatial discretization required, the more nodes are produced. Due to the complex nature of MEMS, its discrete models are usually large (100,000 equations are the engineering standard nowadays). The second step is mathematical model order reduction, which is based on the transformation of a high-dimensional system of ODEs to a low-dimensional one, done by projection. This conversion is formal, robust and can be fully automated. If necessary, the reduced system can also be represented as an equivalent electrical circuit and inserted into a system-level simulator. Hence, mathematical model order reduction can be considered as "compact modeling on demand" [5].

In Table 1.1 the most important properties of compact modeling and mathematical model order reduction are contrasted. Compact modeling requires the designer to intuitively choose the topology of a small-sized equivalent network, which is not a trivial task. It further requires either simulation of the original large-scale system or the use of experimental data. These are then used for the parametrization (via data fitting) of the compact model. No mathematical properties of the original system matrices, or their connection to the matrices of the reduced ODE system are taken into account. Model order reduction, on the other hand, does not require simulation of the original system. Instead, it reduces the original large-scale system matrices using the concept of mathematical projection (explained in detail in Chapter 3). Hence, the reduced system is obtained completely formally and without relying on intuition.

Table 1.1. Compact modeling vs. model order reduction (MOR)

Method properties	Compact modeling	MOR
reduced model topology	obtained by intuition	formally obtained
simulation of the original model	necessary	not necessary
parameter extraction	necessary	not necessary
experimental results	can be used	cannot be used
system matrices of the original model	not used	used

In this book, we focus on MOR, because for linear systems and systems with nonlinear input functions[2] it is much more effective than compact modeling. Presently, the development of model order reduction is strongly driven by diverse MEMS engineering applications [6, 7] that would benefit significantly if the dimension reduction could be done in a completely automatic fashion. In general, one can say that the development of efficient MOR methods for automatically creating accurate low-order dynamic models is about to become a major subject of MEMS simulation and modeling research.

1.2 MEMS and Electro-thermal Simulation

Modeling of electro-thermal processes, e.g. Joule heating, becomes increasingly important during microsystems development [8]. For example, with the decreasing size and growing complexity of micro electronic systems, the power dissipation of integrated circuits has become a critical concern. The thermal influence upon the device caused by each transistor self-heating and the thermal interaction with tightly placed neighboring devices cannot be neglected because excessive temperatures change transistor characteristics and may cause malfunction or even destruction of the device. Whereas Joule heating in microelectronics is a "parasitic" effect, many MEMS devices, such as microsensors and microactuators, use it (directly or indirectly) as a functioning principle. For example, microhotplate-based devices can use Joule heating to achieve the operating temperature. Micromechanical devices with electro-thermal actuation can use Joule heating for electro-thermal expansion. Microfluidic devices employ Joule heating to expel microdroplets out of microfabricated reservoirs, etc. In all design situations above, the engineer's task is to predict the temperature distribution for the given electrical input and the impact of temperature on the device electronics in turn, i.e. to run an electro-thermal simulation. To go a step further, in each sequence of joint electro-thermal simulations the temperature field is computed on a discrete grid whose size, as already mentioned, easily exceeds 100 000 degrees of freedom, i.e. ordinary differential equations.

When we started this research in 2001, MOR approaches were only used for electric circuit interconnects and structural mechanical problems. No efforts to apply MOR to electro-thermal MEMS models have been made so far. At the same

[2] Here we mean the dependence of the input function on state variables, such as the dependence of heater resistivity on temperature.

time, thermal problems, which after spatial discretization result in first-order ODE systems (see Eq. 2.14), are the “most convenient” case from the MOR point of view. Consequently, they provide the best examples to learn MOR and will be targeted in this book.

1.3 Thematic Outline

The purpose of this text is to guide MEMS engineers to apply MOR for efficient simulation of electro-thermal models or electro-thermal domains of coupled models. Along the way, the reader will develop a deeper understanding of

- electro-thermal modeling in general,
- how mathematical MOR works,
- how it can be applied to electro-thermal systems and to coupled systems which include thermal domains,
- how reduced order models can be used within system-level simulation or within a design optimization process.

We thus begin in Chapter 2 with an overview of dynamic electro-thermal simulation of microsystems. The solution of the heat transfer partial differential equation, Eq. 2.5, which is central to electro-thermal microsystem simulation, is discussed. Different levels of solution approaches are presented, starting from the most rigorous, when the heat transfer can only be modeled by a set of coupled partial differential equations, and finishing with the final level of approximation, which is compact thermal modeling.

In Chapter 3 we present the most important algorithms for MOR of linear first-order ODE systems. All MOR methods are based on the projection of a large-scale system to a low-dimensional subspace. Different projections characterize different methods. The central focus of this tutorial is the Arnoldi algorithm, which is based on the projection to a so-called Krylov subspace. We will also discuss the mathematically optimal control theory methods [9, 10], which already have a long tradition in MOR of linear systems of moderate size, and the commercially available Guyan algorithm [11], which up to now has been mostly used for mechanical engineering problems.

In Chapter 4 we describe the available software environment and give a practical guideline how to use it. The software tool *MOR for ANSYS* (pronounced “more for ANSYS) has been developed during the last five years at the laboratory in the simulation. Department of Microsystem Engineering, University of Freiburg (see [12]). It implements the Arnoldi algorithm to generate compact models directly from ANSYS models. Apart from electro-thermal models *MOR for ANSYS* can also be used for the reduction of second-order systems, i.e. for structural models. We also guide the reader in how to perform the substructuring in ANSYS, which is based on the Guyan algorithm (described in Chapter 3) and can be used for the MOR of electro-thermal models as well, although it originally targeted non-damped mechanical models. We further describe how to use the SLICOT library (see [13]), which implements the most important control theory methods and can be applied for MOR of arbitrary first-order ODE systems of moderate size.

In Chapter 5 we describe three novel MEMS devices used as case studies for MOR. These are a pyrotechnical microthruster, a thermally tunable optical filter and a microhotplate gas sensor. The formal switch from electro-thermal to "pure" thermal modeling, under the assumption of homogenous heat generation within the lumped resistor, is discussed as well. We further present the numerical results of model reduction for the three case studies and consider different important aspects of the Arnoldi algorithm, such as the approximation of the complete output and the reduction of systems with nonlinear input functions. Results of Arnoldi-based reduction are compared with the results of control theory methods and those of substructuring. The setup for the system-level simulation (using SABER) and the solution of the inverse thermal problem via MOR are presented in this chapter as well.

While Chapters 3 to 5 address the basic level of MOR that can be used in practice, Chapter 6 outlines advanced topics. These are the error estimate for MOR, MOR of interconnected MEMS systems, parametric MOR, MOR of nonlinear and second-order systems and methods based on low-rank Gramian approximation.

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