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Model Order Reduction for Dynamic electro-Thermal simulation of Microsystems

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Abstract

In this paper we present a methodology for applying mathematical model order reduction (MOR) to electro-thermal MEMS models. We have applied MOR to successfully create dynamic compact thermal models (DCTM) of several novel MEMS devices. It is currently possible to use software tool mor4ANSYS to automatically create reduced order thermal models, directly from ANSYS models with more than 100,000 degrees of freedom. Model order reduction is automatic and based on the Pade approximation of the transfer function via the Arnoldi algorithm. Reduced models are easily convertible into hardware description language form, and can be directly used for system-level simulation. We have tested them using SABER simulator.

1 Introduction

The modeling of electro-thermal processes, e. g., Joule heating, becomes increasingly important during microsystems development. 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's self-heating and the thermal interaction with tightly placed neighboring devices cannot be neglected because excessive temperatures may cause the malfunction or even destruction of the device. Whereas Joule heating in microelectronics is a "parasitic" effect, some other devices like microsensors and microactuators use it (directly or indirectly) as a functioning principle.

In both cases, the engineer's task is to predict the temperature distribution for the given electrical input and the impact of the 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 simulation the temperature field is computed on a discrete grid whose size, easily exceeds 100,000 degrees of freedom (DOF), i. e. ordinary differential equations. Even though modern computers are able to handle this size of engineering problems, the system-level simulation would become prohibitive if the full models were directly used. Hence, an efficient computational technique is needed. An alternative to "classical compact modeling", which is based on parametrization of equivalent thermal networks is mathematical model order reduction, which is formal, robust and can be made fully automated. It is based on the formal conversion of the physical model, that is, governing partial differential equation (PDE) to a low-dimensional ordinary differential equation (ODE) system. The intermediate level is a device level, which is a high dimensional ODE system (see Fig. 1). The first conversion of the physical to the device model is done via the finite element (FE) discretisation. The goal of this work was to enable and automatize a second step, that is a conversion from the device to the system level simulation.

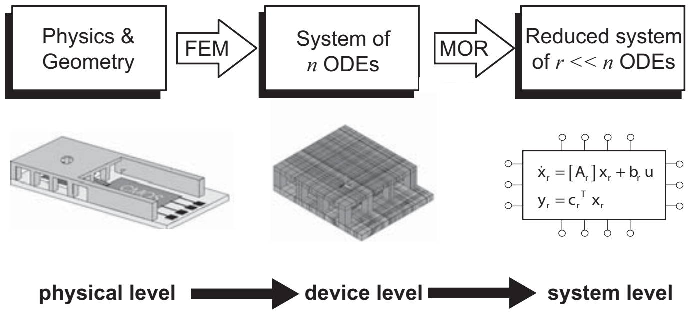

Fig. 1 Motivation for model order reduction.

2 Applications

Three novel MEMS devices (Fig. 2) are used as case studies for MOR. The pyrotechnical microthruster is based on the integration of solid fuel with a silicon micromachined structure. The thermally tunable optical filter is a Fabry-Perot interferometer fabricated as a free-standing membrane. The microhotplate gas sensor is supported by glass pillars emanating from a glass cap above the silicon wafer, which assures robust design and thermal isolation of the membrane from the surrounding wafer. The heat transfer within each hotplate is described through the following equations:

$$\nabla \bullet (\kappa \nabla T) + Q - \rho c \frac{\partial T}{\partial t} = 0 \, , \; Q = \boldsymbol{j}^2 R \tag{1}$$

where $\kappa(r)$ is the thermal conductivity in W/mK at the position r, $C_p(r)$ is the specific heat capacity (a material property that indicates the amount of energy a body stores for each degree increase in temperature, on a per unit mass basis) in J/kgK, $\rho(r)$ is the mass density in kg/m^3, $T(r, t)$ is the temperature distribution and $Q(r, t)$ is the heat generation rate per unit volume in W/m^3. Assuming that the heat generation is uniformly distributed within the heater, and that the system matrices are temperature independent around the working point, the finite element based spatial discretization of (1) leads to a large linear ODE system of the form:

$$\begin{aligned} C \cdot \dot{T} + K \cdot T &= F \cdot I^2(t) R(T) \\ y &= E^T \cdot T \end{aligned} \tag{2}$$

where C and K are the global heat capacity and heat conductivity matrices, F is the load vector (matrix) and E is the output vector. (2) contains 1,071, 1,668 and 73,955 equations for the microthruster, optical filter and gas sensor device respectively.

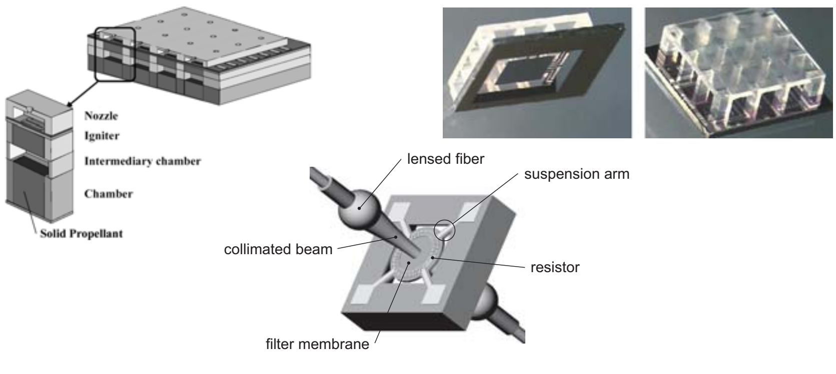

Fig. 2 MEMS case studies: microthruster (top left), gas sensor (top right), optical filter (bottom).

3 Model Order Reduction

As above number of equations is too high for system simulation, MOR is performed and a new, reduced system of equations (of the same form (2)) is used to generate a system-level model. Software tool mor4ANSYS [1] uses Arnoldi reduction algorithm, which can be viewed as a projection, from the full space to the reduced Krylov-subspace:

$$K_r\{A, b\} = span\{b, A^2 b, \ldots, A^{r-1} b\} \tag{3}$$

with $A = -K^{-1}C$ and $b = -K^{-1}F$. This projection is based on the transformation of the state vector T to the vector of generalized coordinates z, subjected to some small error ε:

$$T = V \cdot z + \varepsilon \tag{4}$$

and subsequent left side multiplication of (2) with the V^T. The transformation matrix $V \in R^{nxr}$, where $r \ll n$ are the dimensions of the reduced and the full system, respectively, is a direct output of Arnoldi algorithm. The property of the Krylov-subspace (3) is such that the transfer function of (2) is approximated through the first r coefficients of its Taylor series around an arbitrary chosen frequency. For our case studies the expansion frequency was set to zero in order to preserve the steady-state. The fact that neither input term $I^2(t)R(T)$ nor the output matrix E take part in order reduction, brings along two important properties of Arnoldi algorithm, which make it stands out from other MOR methods: the approximation of the full output, described in [2] and the reduction of weakly nonlinear systems (those with the temperature dependant input power), described in [3]. The comparison between the Arnoldi algorithm and the commercially available reduced order modeling via Guyan can be found in [4].

Using mor4ANSYS we have reduced a gas sensor model with 73.955 ODEs to 10 ODEs and implemented the reduced model in MAST. Fig. 3-4 show the schematic structure of the implemented HDL model for gas sensor and numerical simulation results of the full-scale model integrated in ANSYS, the reduced order model integrated in Mathematica and the MAST model integrated in SABER.

4 Error Estimation

In order to apply Arnoldi-based model order reduction, the MEMS designer has to provide a discretized model (e. g. a finite element (FE) model) of the device and to specify which frequency band should be well approximated by the compact model. This is done by choosing one or more expansion points in the frequency domain. The next important step is to specify the desired order of the target reduced system. A key question is: which order of the reduced system do we need to select in order to achieve a desired accuracy. A reduced model is an approximation of the original large-scale model. Hence, the difference between the two can be characterized by some error norm. In order to automate the MOR process completely, one should be able to estimate this error as a function of the reduced model's dimension. The automatic procedure from device-level to system-level modeling is schematically shown in Fig. 5.

Based on our numerical results, we propose three heuristic error indicators for the iterative model order reduction of electro-thermal MEMS models via the Arnoldi algorithm. We first suggest a convergence criterion between two successive reduced models of order r and $r + 1$. We further propose to approximate a global error bound provided by the exact control-theory methods and alternatively to employ sequential model order reduction, which is based on consecutively applying Arnoldi and control-theory methods. Fig. 6 shows the convergence of relative error for the microthruster model

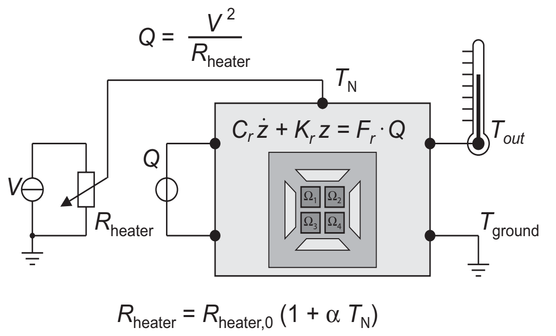

Fig. 3 HDL model structure containing back coupled teperature dependant heater

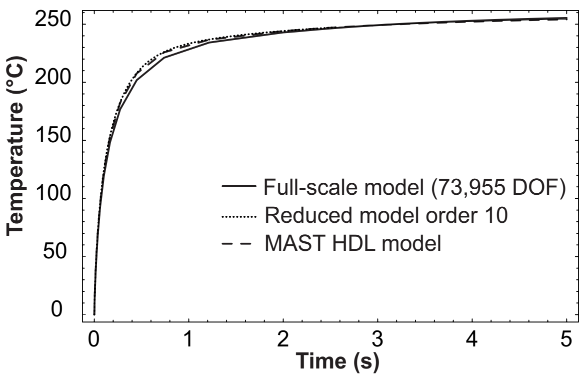

Fig. 4 Solution of the full-scale system (73. 955 DOF) and of the reduced order 10 system in a central hotplate node of

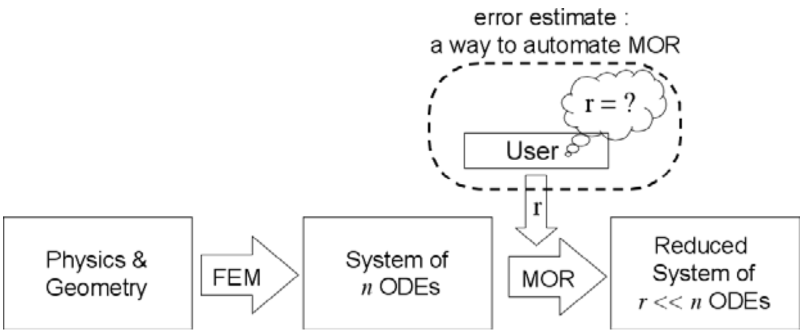

Fig. 5 Compact model extraction. Eliminating the need for user iteration makes the process fully automatic.

for two different frequencies. The system order necessary to reach the convergence increases towards higher frequencies, as may be expected for the expansion around zero. It should be noted that for the frequencies far away from the expansion point the oscillations may occur. Our observation is that the error indicator approximates the true error with high accuracy.

At the present stage, the convergence of relative error and sequential MOR can be recommended for practical use. They are both straightforward to implement, as shown in [5].

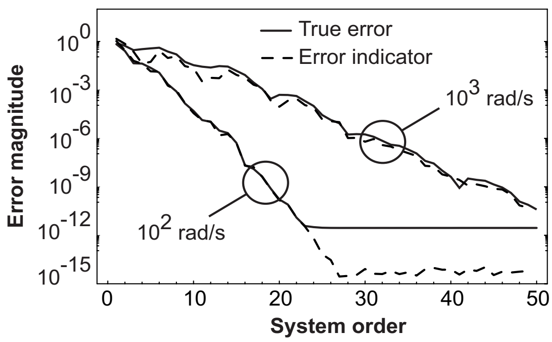

Fig. 6 Convergence of relative error between the two successive reduced models for the microthruster.

5 Coupling of Reduced Models

As MEMS are often composed of identical devices that are interconnected, array structures for example, it is desirable, especially with a large number of subsystems, to reduce each subsystem on its own and then to couple them back together. Hence, we seek a kind of compact thermal multiport representation which allows thermal fluxes to cross the boundaries and enables straightforward coupling to the next thermal multiport. The main problem thereby is that the thermal flow is not lumped by nature as, for example, the electrical flow is along metallic wire interconnects. The ratio of electrical conductivity of metals and that of insulators is of the order of 10^8. Hence, the electrical current flow takes place almost solely in metal paths. This is not the case with heat flow because the ratio of thermal conductivities in microtechnology is only of the order of 10^2. Therefore, it is unclear how to lump the thermal fluxes at shared surfaces between two finite element (FE) models in order to form the thermal ports (Fig. 7) which would serve to couple together several compact models.

Presently it is possible to use two methods for model order reduction of thermal MEMS arrays, Block Arnoldi and Guyan-based substructuring (available in ANSYS). The application of the block Arnoldi algorithm (classical Arnoldi which is suitable for multiple-input-multiple-output systems) is straightforward. It reduces the entire array model and results in a much smaller reduced model sizes than by using substructuring. Its main disadvantage is that it is not well scalable to a large number of devices within an array. Substructuring decouples the array model and physically preserves the shared nodes. This allows easy back-coupling of the reduced models, but results in unnecessary large array model sizes. Both methods are described in [6]. Fig. 9 compares the step response of the substructured microhotplate test array with the step responses of the full-scale model and of the block Arnoldi reduced model.

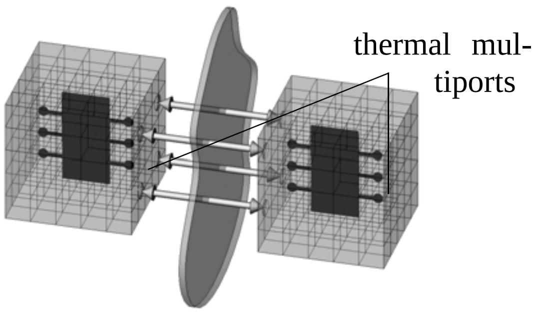

Fig. 7 Continuous thermal flux through the shared interface of two FE models. The goal is to model the "FE cubes" as thermal multiports i. e. to lump a flux.

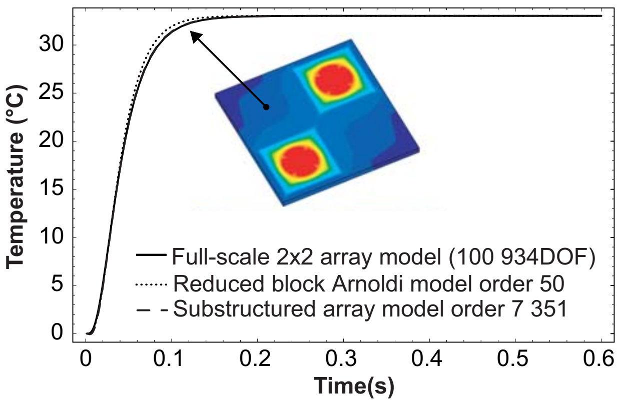

Fig. 8 Solution of the full scale system (73. 955 DOF) and of the reduced order 10 system in a central hotplate node of gas sensor device.

In [7] we have also described a general technique of coupling two reduced thermal models gained by projection (e. g. when the Arnoldi algorithm is used). In such case the coupling is done via surface fluxes.

5 Summary

We have developed a methodology and a software tool for applying mathematical model order reduction to the automatic generation of dynamic compact thermal models for MEMS. We have shown that with Arnoldi it is possible to reduce linear thermal ODE systems of around 100,000 equations to orders between 20 and 50 with only a minimal loss of accuracy. This increases computational efficiency by more than 10 times in the case of a microhotplate gas sensor and in general reduces computational time to the time comparable with a single stationary solution of the original system.

Further advantages of Arnoldi-based reduction are the approximation of the complete output and the reduction of models with temperature dependent heating power. Its main disadvantage was the fact that no error estimate between the original and the reduced models exists. We have suggested three heuristic strategies for error estimation. At the present stage, the convergence of relative error and sequential model order reduction can be recommended for practical use. They are both straightforward to implement.
We have researched the possibilities for model order reduction of MEMS array structures. Presently, we are able to apply Block Arnoldi and Guyan-based substructuring. Block Arnoldi can be recommended in cases of a moderate number of devices within an array. However, when the number of interconnected devices grows, both methods need alternatives.

6 References

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