Parameter Preserving Model Reduction for MEMS System-level Simulation and Design

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Abstract. Model reduction is a very helpful tool to generate compact models for system-level simulation. Quite often however, system matrices depend on design parameters and the new goal is not only to reduce the original system but also to preserve system parameters in the symbolic form during model reduction. We introduce multivariate moment matching as a possible solution to this problem. We consider several examples from MEMS to demonstrate the feasibility of the approach: a device cooled by airflow, a microhotplate, a flow meter (anemometer) and a microelectrode. Finally, we discuss problems that should be overcome in order to use this technique in software for engineering design applications.

1. Introduction

The microelectronic industry enjoys tremendous productivity levels due to its high level of design automation (EDA). This is possible because the industry has agreed on how design should progress, and what the future priorities are in terms of necessary achievements. In microsystem and nanosystem development this has not yet happened [1][2][3], mainly because the industry is not yet mature enough, but especially because the microsystem design automation industry is in its infancy.

The key to success in design automation is an accurate compact model of the MEMS/NEMS device. Yet, it happens that conventional compact modeling does not work well for the MST area where the number of different devices is too big to hope that one can apply a simple empirical approach. Here a community working on a particular device just does not have researchers with enough experience and intuition to develop compact models. And when the compact model is finally developed, it well may be that the interested parties have already switched to another technology.

Model order reduction is a rapidly developing interdisciplinary area [4][5][6]. There is considerable progress in the application of modern model reduction to MST for the last five years and, in our opinion, model reduciton can be considered as Compact Modeling on Demand.

It so happens that a high-dimensional ordinary differential equation system, as generated from e.g. a semidiscretized finite element model, possesses an inherent mathematical property that allows us to drastically reduce its dimension without sacrificing the precision of solution. Mathematically speaking, this is due the rapid decay of the system Hankel singular values [4]. There is much evidence that this is the case for most discretized MEMS models and the savings in computational speed are dramatic.

Model reduction of a linear system of ODEs can be considered as almost a solved problem. In this case, model reduction gradually becomes a common practice among engineering groups. There are good chances that this feature will be available in commercial tools in a few years.

However, conventional model reduction fails to preserve parameters during model reduction process. This limits severely its applicability for the design flow and system-level simulation. In the present paper we consider how one can overcome this limit. We start by a short overview of available approaches from the literature. Then, we review our results scattered over several conference papers. We present three engineering MEMS applications that require us to preserve parameters in a compact model and review results on parametric model reduction for these devices. After that, we discuss how to choose moments to include into the reduced model automatically.

2. Overview of Parametric Model Reduction

Because of its semi-empirical nature, compact modeling allows us to include some parameters in the symbolic form. For example, compact transistor models include some geometry parameters [7]. This is possible to some

extent because compact modeling always includes a parameterization step when numerical values of unknown coefficients are found based on data fitting to experimental curves. Unfortunately, the process is hard to use in practice as it is inherently based on intuition.

A formal approach related to parametric model reduction is a reduced-basis method [8][9][10]. An idea is to obtain several solutions distributed in the parameter space and then to use them to estimate a solution for an arbitrary point in the parameter space. Yet, the method is limited to a stationary problem.

In our view, the best choice is the multivariate Pade-type approximation that is a natural generalization of the moment matching method in conventional model reduction [5][6]. It was first suggested in [11] for an electromagnetic problem and then employed for interconnect modeling in [12][13].

Let us consider the last approach in more detail. The discretization in space (for example, by the finite element method) leads to a system of ordinary differential equations as follows

$$\begin{aligned} E\frac{dx(t)}{dt} &= Ax(t) + Bu(t), \\ y(t) &= Cx(t) \end{aligned} \tag{1}$$

where $x(t)$ is the vector of unknowns. E and A are the system matrices, B is the input matrix, and C is the output matrix. The vector u comprises inputs functions. The output matrix specifies particular linear combinations of $x(t)$ that of interest to an engineer.

The difference from conventional model reduction is that the system matrix A contains some parameters to be preserved during model reduction. In the linear case, one can partition the original matrix as follows

$$A = A_0 + \sum\nolimits_i k_i A_i , \tag{2}$$

where k_i is the parameter to be preserved. The transfer function of (1) with the condition (2)

$$H(s) = C\{sE - (A_0 + \sum\nolimits_i k_i A_i)\}^{-1} B , \tag{3}$$

in addition to Laplace variable s contains the parameter k_i.

Model reduction is based on an assumption that there exists a low-dimensional subspace V that accurately enough captures the dynamics of the state vector $x(t)$:

$$x \approx Vz . \tag{4}$$

In the moment matching approach [5][6], the subspace V is found in such a way as to preserve moments of the transfer function (3) in respect to the Laplace variable s around some value s_0 chosen a priori. Yet, these moments depend on k_i and, as result, conventional subspace V does not work well in the case of Eq (2).

In order to make V not depend on k_i, the transfer function (3) can be treated as a function in many variables (s and k_i) and one can perform its multivariate expansion. The next step is to find V so that to match multivariate moments [11][12][13]. This way, V does not depend on parameters in Eqs (2) and (3).

Provided V is known, one obtain a low-dimensional model by projecting (1) and (2) on V as follows

$$\begin{aligned} V^T EV\frac{dx(t)}{dt} &= \{V^T A_0 V + \sum\nolimits_i k_i V^T A_i V\}z(t) + V^T Bu(t) . \\ y(t) &= CVz(t) \end{aligned} \tag{5}$$

Eq (5) preserves the original parameters k_i and as a result we call this approach as parametric model reduction.

3. MEMS Case Studies

We have chosen three important MST applications that require parametric model reduction expressed by Eq (1) and (2). They are described below.

A. Compact thermal models for electro-thermal simulation

In the development of integrated circuits and microsystems, thermal management is always essential [14][15]. There are several electro-thermal and thermo-electric coupling effects but probably the biggest concern is about the Joule heating, which generates heat during conduction of the electric current through a resistor. In an integrated circuit, one has to remove the generated heat to keep the board temperature within acceptable limits. In microsystems, the Joule heating is often employed to keep a designated part (hotplate) at a given elevated temperature. In any case, the right temperature regime is crucial for the correct system functioning and its reliability.

The finite element method allows us to make an accurate model to describe heat transfer but its high dimensionality prevents engineers to employ it during system-level simulation. Hence, an important practical question is how one can make accurate but low-dimensional thermal models.

The two European projects, DELHPI and PROFIT have addressed this need: to produce an accurate but a small thermal model of a chip [16][17][18]. The DELHPI project has identified a number of requirements for a compact thermal model, one of the most important being that the compact model must be boundary condition independent. This means that a chip producer does not know conditions under which the chip will be used and hence the chip compact thermal model must allow an engineer to research on how the change in the environment influences the chip temperature. The chip benchmarks representing boundary condition independent requirements have been described [18].

Recently, modern methods of model order reduction have been successfully applied to automatically generate a compact thermal model [19][20][21][22], however they do not meet the criterion of boundary condition independence.

It should be noted that the term "boundary condition independence" is a bit ambiguous as different engineering groups refer to different requirements. Eqs (1) and (2) fit the case when thermal engineers use convection boundary conditions to separate the thermal model from environment. This assumes that the normal heat flux $q_\perp$ is proportional to the temperature difference between the boundary T and the bulk temperature T_{bulk} of the neighboring bulk phase

$$q_\perp = k(T - T_{bulk}), \tag{6}$$

where k is the film coefficient that depends on the flow condition. As flow conditions may change at system level simulation, the film coefficient is to be preserved during model reduction.

The thermal model usually has different film coefficients for different surfaces. After the discretization in space of the heat transfer equation, we obtain Eq (1) and (2) where k_i is the film coefficient for the i-th boundary. Another important engineering requirement for this case is that the film coefficient can be changed in a huge range of values up to nine orders of magnitude [18].

B. Electrochemical scanning microscopy

Electrochemical scanning microscopy [23] involves the measurement of the current through an ultramicroelectrode when it is moved in electrolyte in the vicinity of a substrate. It allows us to study homogeneous and heterogeneous reactions, for high resolution imaging of chemical reactivity and topography of various interfaces [24], especially for biological systems [25]. In addition it can also be used for nano-patterning [26].

An experimental design of SECM eliminates many nonlinear effects such as convection [27]. A final mathematical model is a combination of linear multi-species diffusion equation with the Butler-Volmer equation to describe the reaction at the electrode. The latter is expressed as linear mixed boundary conditions

$$\nabla c_{i,\perp} = k(U) = be^{az_iU}, \tag{7}$$

where $\nabla c_{i,\perp}$ is the normal flux of the i-th species, z_i is the species charge, U is the applied voltage and a and b are some constants.

A typical run includes cyclic voltammogram when current is measured as a function of the applied voltage U. After the discretization, the voltage enters the system matrices and this leads to similar requirements as in the previous section: the reduced model must preserve the voltage in the symbolic form.

C. Flow meter (Anemometer)

A common way to measure the flow rate by means of MST technology is a combination of a heater with thermocouples positioned from both sides of the heater [28][29]. The flow influences the temperature distribution and, thus, the thermocouple signals can be converted to flow rate. An engineering requirement in this case is a compact flow meter model that allows us to use flow velocity as a parameter.

The complete model is quite involved as it is necessary to solve Navier-Stokes equations coupled with the heat transfer through the surrounding. Yet, it can be simplified in the case of a given velocity profile with an assumption that a flow meter does not influence significantly the flow profile. In this case, a mathematical model is a linear convection-diffusion heat transfer [30]. The system matrix depends linearly on the flow velocity v as follows

$$A = A_0 + vA_1, \tag{8}$$

4. Results

In this section, we review our results obtained by the multivariate Pade-type approximation for the models from the previous section. More information can be found in the original papers.

We have modified a microthruster benchmark in order to make it similar to a chip model with different film coefficients [31] (see Fig. 1). The model is a generic example of a device with a single heat source when the generated heat dissipates through the device to the surroundings. The exchange between surrounding and the device is modeled by convection boundary conditions. From this viewpoint, it is quite similar to a chip model used as a benchmark in [18].

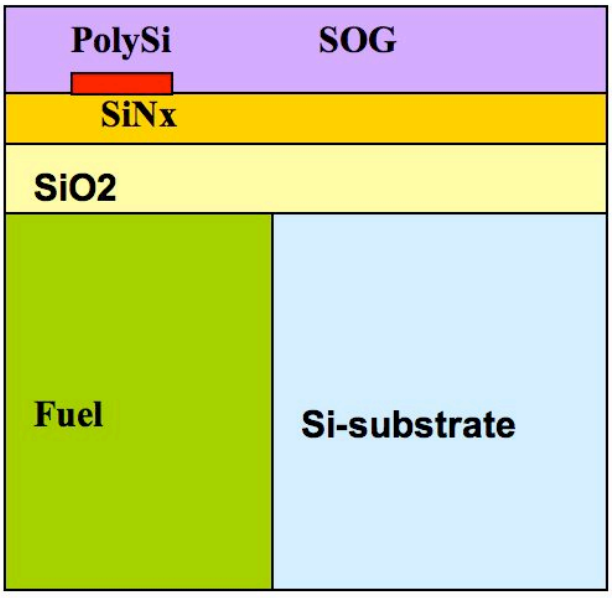

Fig. 1. A 2D-axisymmetrical model of the microthruster unit (not scaled). The axis of symmetry is on the left side. A heater is shown by the red block.

Result for parametric model reduction, when the same film coefficient is assumed for all surfaces, are described in Ref [32][33] and shown in Fig. 2. The dimension of the original model is 4725. We have made two reduced models with a dimension 33 and 49 respectively. Fig. 2 shows a relative error between transient simulation of the full scale and reduced models as a function of the film coefficient. Note the logarithmic scale for the film coefficient. The approximation error is within 1% for a very wide parameter range. Such an agreement is very good for engineering applications [18].

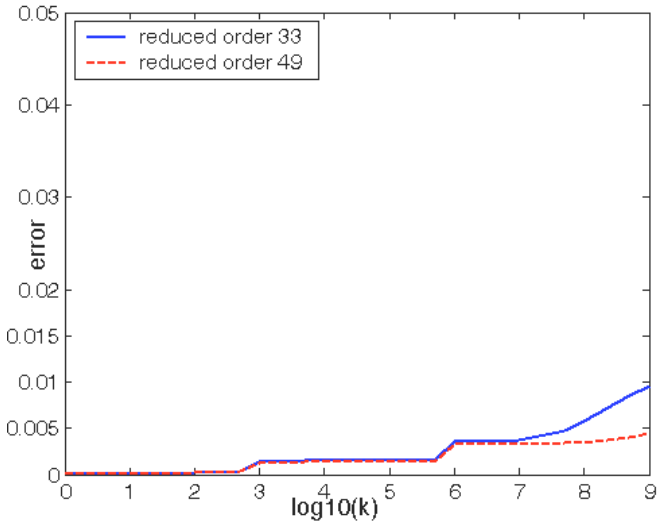

Fig. 2. The error of transient simulation for a reduced model as a function of the film coefficient. Note that the film coefficient changes by nine orders of magnitude.

A model for electrochemical simulation related to scanning electrochemical microscopy is described in [34] and schematically shown in Fig. 3. The computation domain under a 2D-axisymmetrical approximation includes the electrolyte under the electrode. We assume that the concentration does not depend on the rotation angle. A single chemical reaction takes place on the electrode:

$$Ox + e^- \underset{k_b}{\overset{k_f}{\Leftrightarrow}} Red \tag{9}$$

A feature of the electrochemistry model is nonzero initial conditions as the concentration of all species cannot be zero. Our way to deal with this is presented in [34].

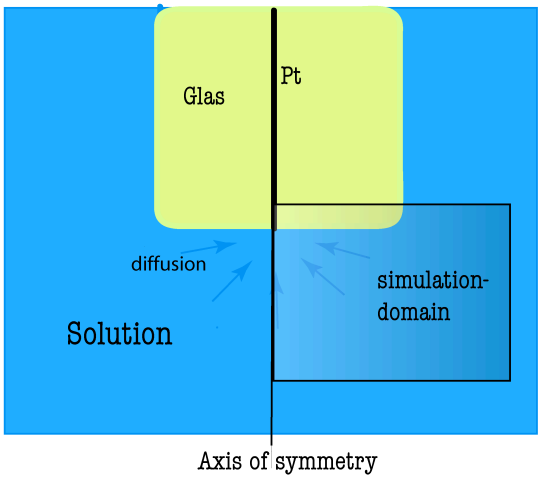

Fig. 3. The layout of electrochemistry simulation.

Parametric model reduction for simulation of voltammograms is presented in [35]. Fig. 4 shows simulation results for the original model of a dimension 16912 and a reduced model of a dimension 202. The figures display the current as a function of voltage (not in time) as this is the usual way to represent voltammograms. The solid line is the result computed by full simulation of the original large model, the dashed line is the result computed by the reduced model. It should be noted that the results of the reduced model are accurate for a wide range of the dynamic behavior when the voltage rate (du/dt) changes by three orders of magnitude (0.0005-0.5) [35].

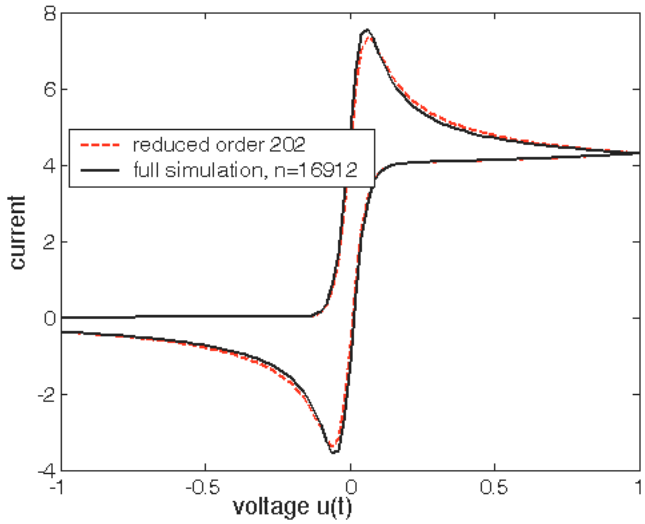

Fig. 4. Simulation results of the cyclic voltammogram when $du/dt = \pm 0.5$.

An anemometer is a flow meter that consists of a heater and temperature sensors before and after the heater in the direction of the flow [36] (see Fig. 5). The flow influences the temperature field and thus leads to a temperature difference between the sensors. This temperature difference is measured and used to determine the fluid flow.

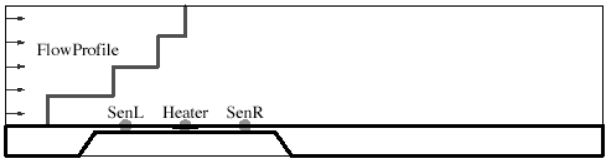

Fig. 5. Model of the anemometer. The flow enters from the left. A heater is surrounded by two thermosensors.

Parametric model reduction has been performed in [36]. Fig. 6 shows the temperature difference between sensors for steady state solutions with different velocities. The small graph within the figure shows the deviation between the reduced model of a dimension 102 and the original model of a dimension 29008. This deviation lies below 1% of the difference signal. The reduced model captures the dynamic behavior as well [36].

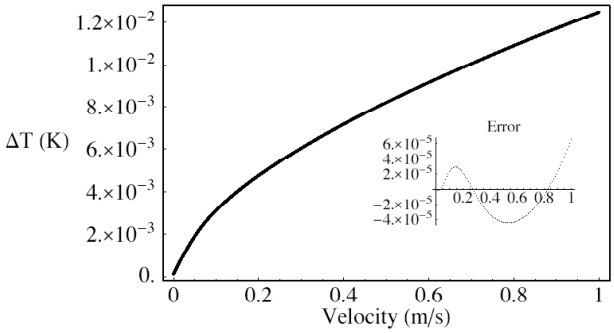

Fig. 6. Steady state solution for the temperature difference between the sensors for different flow velocities for the original and reduced models.

5. Discussion

We have presented three MEMS engineering problems that require parametric model reduction and reviewed our results obtained within the framework of multivariate Pade-type approximants. In all case studies we were able to reduce the model dimension considerably and at the same time to preserve the accuracy within engineering requirements. However, we should stress that the models considered were relatively simple, as they have contained only one or two parameters to be preserved. The generalization of the approach to engineering models with more parameters, unfortunately, may not be straightforward. Below we briefly list potential problems.

Methods in [12][13] use moments directly to construct the projection subspace and this may lead to the rapid accumulation of rounding errors. We have developed a Krylov-subspace based approach in [33] but its generalization to many parameters seems to be difficult.

A usual problem for moment matching methods is how to choose the number of moments to match. In the case of multivariate matching, the situation is much worse as there are many different types of derivatives. For example, in the case of a single parameter, we have derivatives of the transfer function in respect to the Laplace variable, derivatives in respect to a parameter, and then mixed derivatives. The more parameters are included in the transfer function, the more different derivative types we have. A straightforward approach to generate all the moments up to a given order does not scale well with the number of parameters [13]. For example, if we choose to preserve four film coefficients then a reduced model made from all first derivatives has the dimension of 6, a reduced model made from all second derivatives has the dimension of 21, and a reduced model from all third derivatives already has the dimension of 56 (see Appendix F in [13]). At the same time, we may need derivatives of higher order than three to describe accurately the transient behavior of the original model.

In order to treat the problem, we have suggested a heuristic procedure in Ref [37]. It is based on 1) neglecting the mixed moments; 2) employing the local error control to chose the right number of moments along the Laplace variable and each parameter. This has been applied for the first device to preserve three film coefficients independently and results of numerical experiments were promising. However, more research is needed to see to what extent this can be used in other applications.

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