Error Indicators for Fully Automatic Extraction of Heat-Transfer Macromodels for MEMS

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Short title
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Abstract

In this paper, we present three heuristic error indicators for the iterative model order reduction of electro-thermal MEMS models via the Arnoldi algorithm. Such error indicators help a designer to choose an optimal order of the reduced model, required to achieve a desired accuracy, and hence allow a completely automatic extraction of heat-transfer macromodels for MEMS. We first suggest a convergence criterion between two successive reduced models of order r and $r + 1$. We further propose to use a solution of the Lyapunov equations for reduced-order systems in each iteration, and alternatively to employ sequential model order reduction, which is based on consecutively applying Arnoldi and control-theory methods.

key words: *error estimates, model order reduction, Arnoldi process, heat-transfer macromodel*

1. Introduction

Numerous MEMS devices, such as thermal actuators [1], thermal flow sensors [2], microhotplate gas sensors [3], [4] or tunable optical filters [5], [6], are based on thermal effects. The heating changes optical properties in optical filters, reduces activation energies to allow metal oxides to detect gases, causes mechanical stress and thus movement in actuators. The heat transfer through the moving fluid allows us to measure the flow rate in heat-flow sensors. For such devices, thermal modeling and simulation play an important role during design flow, for computation of power assumption, or prediction of the temperature distribution for the given electrical input. Furthermore, the perfor-

mance of most applications is improved by employing feedback loops for precise control and hence, system-level modeling is required as well. Spatial discretisation methods allow us to make accurate but high dimensional (10^5 equations is routine) thermal models, whose computation in turn requires high computational costs. Hence, it is prohibitive to use these models during system-level simulation. Instead, compact and accurate heat transfer models are required. Thus, the here proposed tools for automatic creation of compact thermal models greatly support design and development of a large number of MEMS sensors and actuators.

In recent years, the application of Krylov-subspace methods for extracting heat-transfer macromodels of microelectronics and MEMS devices have gained great popularity among engineers [7], [8], [9], [10]. They are based on Padé or Padé-type [13] approximations of the transfer function via either the Lanzcos [14] or Arnoldi [15], [16] algorithm. The main advantage of these methods versus commonly used lumped-element [11] or modal approaches [12] is that they can be made fully automatic, i. e., without a designer's pre-knowledge about the extraction of RC-ladder networks or dominant modes of the observed system.

In order to apply Krylov-subspace based model order reduction (MOR), 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.

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. 1.

Unfortunately, an effective error estimate for Krylov-subspace methods is still an open research question. To our knowledge, only local (single-frequency) error estimates have been suggested so far [21], [22], [23]. Recent suggestions for the Arnoldi reduction algorithm can be found in [24] and [25]. For engineering applications, an error estimate should be implemented in the design flow in such a way as to fit in the iterative framework of Krylov-based MOR.

In this paper we propose three "heuristic" approaches for estimating the error of the reduced-order model computed via the Arnoldi algorithm. Since we can not yet prove rigorous error bounds, we refer to our results as error indicators. The idea is either to compute the relative error between the successive reduced order models (similar as in [23]) or alternatively, to compute the Hankel singular values of the reduced model in each iteration of the Arnoldi algorithm. The third approach is based on sequential strategies [17], [18]. The proposed strategies can be used by MEMS designers to automatically create heat-transfer macromodels using the Arnoldi algorithm.

We want to stress that an insufficiently accurate original model cannot be improved by model order reduction. Hence, the original model resulting from a spatial discretisation of the thermal domain, has to be validated. The problem of building an accurate FE device model lies out of the scope of this paper. In the following, we make an assumption that a validated FE model is already available, and we discuss how to efficiently obtain a compact model from it.

This paper is organized as follows: Section 2 contains MOR results for two electro-thermal MEMS case studies. In section 3 the convergence of the relative error between two successive reduced order models is presented. Section 4 describes the convergence of the Hankel singular values of the reduced models, and how this observation can be used to approximate a global error bound available for control-theory methods. Section 5 contains the results of sequential MOR, when first applying a partial Arnoldi reduction and then subsequently either a balanced truncation approximation, or a singular perturbation approximation, or a hankel norm approximation. Finally, section 6 concludes the paper with a discussion and some practical recommendations.

2. Model Order Reduction of Electro-Thermal MEMS

2.1 Dynamics of Thermal Systems

The instationary heat conduction equation takes the form:

$$\rho C_p \frac{\partial T}{\partial t} - \nabla \bullet (\kappa \nabla T) = Q \tag{1}$$

where κ is the thermal conductivity, C_p is the specific heat capacity, ρ is the mass density, T is the temperature distribution and Q is the heat generation rate. In the following a linearity assumption will be made, which implies that all relevant material properties are considered to be temperature independent. This assumption is common for dynamic compact thermal models [26]. Under the assumption that Q is uniformly distributed within the heating area, the finite element based spatial discretization converts (1) into a large linear ODE system of the form:

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

where $C, K \in R^{nxn}$ are the global heat capacity and heat conductivity matrices, $\boldsymbol{T}(t), \boldsymbol{F}, E \in R^n$ are the temperature (state), the load and the output vectors and n is

the dimension of the system. For simplicity, we will assume a Single-Input-Single-Output setup in the following, as well as zero initial temperature distribution and Dirichlet boundary conditions $T_\Gamma = 0$ (at the bottom Γ of the chip). Please note that in general the heat generation rate, which originates mostly from Joule heating, is a function of temperature $Q(t, T)$, due to the temperature dependence of the lumped heater's resistivity.

2.2 Model Order Reduction by Arnoldi

The Arnoldi algorithm transforms equation system (2) into a similar system:

$$\begin{aligned} C_r\dot{z} + K_r z &= \boldsymbol{F}_r Q(t) \\ y_r &= E_r^T \cdot z \end{aligned} \tag{3}$$

with much smaller dimension $r \ll n$. A generalized coordinate z can be seen as a projection of the n-dimensional temperature vector onto an r-dimensional subspace, subject to some error ε:

$$\boldsymbol{T} = V \cdot z + \varepsilon, \quad z \in R^r, \quad r \ll n \tag{4}$$

and $y_r = E_r^T \cdot z$ is that linear combination of the reduced states which corresponds to the required output y in equation (2). The matrix V in (4) is composed from r n-dimensional vectors that form a basis for the reduced subspace. When the subspace is found, equation (2) is projected onto it by applying (4) and then multiplying (2) from the left side by V^T. This projection process produces a reduced order system (3) as follows:

$$C_r = V^T C V;\ K_r = V^T K V;\ \boldsymbol{F}_r = V^T \boldsymbol{F};\ E_r = V^T E \tag{5}$$

For large linear systems, a transformation matrix V can be effectively computed from an orthogonal basis for the Krylov subspace of dimension r:

$$K_r\{A, \boldsymbol{b}\} = span\{\boldsymbol{b}, A\boldsymbol{b}, \ldots, A^{r-1}\boldsymbol{b}\} \tag{6}$$

with $A = -K^{-1}C$, $\boldsymbol{b} = -K^{-1}\boldsymbol{F}$. It can be shown [15] that the transfer functions of the

systems (2) and (3) defined as $G(s) = E^T(sC + K)^{-1}F$ and $G_r(s) = E_r{}^T(sC_r + K_r)^{-1}F_r$, when developed into Taylor expansions around s_0:

$$\begin{aligned} G(s) &= \sum_{i=0}^{\infty} m_i(s-s_0)^i \quad with \quad m_i = E^T(-K^{-1}C)^i K^{-1}F \\ G_r(s) &= \sum_{i=0}^{\infty} m_{r_i}(s-s_0)^i \; with \; m_{r_i} = E_r{}^T(-K_r{}^{-1}C_r)^i K_r{}^{-1}F_r \end{aligned} \tag{7}$$

where m_i and m_{r_i} are called the i-*th* moments, match in the first r moments:

$$m_i = m_{r_i}, i = 0, \ldots, r-1 \tag{8}$$

Furthermore, the passivity and stability of the original system are preserved in the reduced system [27].

The transformation matrix V is a direct output of the Arnoldi algorithm, whereas K, C and the target reduced order r are its inputs. The Arnoldi vectors, which form a basis for (6), are computed iteratively. This requires a new matrix-vector product in each iteration, namely:

$$\begin{aligned} v_1 &= \boldsymbol{b} = -K^{-1}\boldsymbol{F} \\ v_2 &= A\boldsymbol{b} = K^{-1}C \cdot K^{-1}\boldsymbol{F} \\ v_3 &= A \cdot A\boldsymbol{b} = -K^{-1}C \cdot K^{-1}C \cdot K^{-1}\boldsymbol{F} \end{aligned} \tag{9}$$

etc. An important computational aspect here is that, if a direct solver is available, there is no need to invert the matrix K and compute $v_{new} = K^{-1}C \cdot v_{previous}$ for different $v_{previous}$ over again. Instead, an LU or Cholesky decomposition of K can be made once, and then, in each iteration, a fast back substitution is performed. In this way, model order reduction by Arnoldi can be performed approximately at the cost of a stationary system solution.

Further advantages of the Arnoldi algorithm are that, due to the fact that the nonlinear

input term $Q(t, T)$ doesn't explicitly partake in the model order reduction algorithm, it is possible to transfer it directly to the reduced system [28]. Furthermore, in [9] we have shown that, for linear dynamic thermal models (in the sense of temperature-independent system matrices), the Single-Input-Single-Output setup for the Arnoldi algorithm is sufficient to approximate not only a single output response but also the transient thermal response at all the finite element nodes of the original large-scale model. Hence, for thermal problems (8) is valid also if E is an identity matrix of dimension n.

In the present work, we assume that for majority of thermal MEMS devices, the preservation of steady-state within a reduced model is more important than the high frequency behavior. Hence, $f = 0Hz$ has been considered as an expansion point for the Arnoldi algorithm. Nevertheless, our results can be applied to any expansion point that a designer may freely choose according to the specific device requirements.

2.3 MEMS Case Studies

As a firs study we consider a tunable optical filter based on a Fabry-Perot interferometer [5]. An optical resonator is formed by using two dielectric Bragg reflectors as mirrors and a solid-state material within the optical path between them. The optical length of this resonator determines the transmitted wavelength, while the remaining spectrum is reflected. Wavelength tuning is achieved through thermal modulation of the membrane's temperature. As the refractive index of the resonator material varies with temperature, its optical thickness changes correspondingly. This causes the transmitted wavelength to shift. Tuning the filter wavelength is achieved without physically changing the separation of the mirrors. The filter is fabricated as a free-standing membrane, as shown in Fig. 2. This thermally isolates the membrane from the substrate and guarantees a homogenous temperature distribution at the center of the membrane. Such a filter

is essential for the monitoring and reconfiguration of optical communication networks and can also be used for spectroscopic applications.

As a stable temperature is most important for reliable operation of the filter, control and feedback circuitry are integrated as well. Hence, system-level simulation becomes necessary, and requires a compact thermal model. For evaluation purposes we have used a two-dimensional model, which, after the FE based spatial discretization of the governing heat transfer equation, results in a linear system of 1668 ODEs. The Arnoldi process was applied to this model to generate several reduced models with different orders. For each reduced model a transfer function $G_r(s)$ over a relevant range of frequencies from 1rad/s to $10^9 rad/s$ was computed. The magnitude of the frequency responses of the full-scale model and three reduced order models are shown in Fig. 3. We can observe a good match in the frequency domain around the expansion point s_0, which we have chosen to be zero. Fig. 4 shows a step response of the full-scale filter model and vanishing step response errors of the reduced order models. The simulation time for the transient solution of a full-scale model in ANSYS with 30 time-steps was $150s$, the time for model reduction to order 50 was $0.75s$ and the time integration of the reduced system in Mathematica lasted for $1s$.

Our second case study is a microhotplate gas sensor that uses a metal oxide as the sensing material and features low power operation. The fabrication approach enables the integration of various sensing areas in an array configuration [3]. The gas-dependant change in electrical conductivity relies upon diffusion of oxygen from an ambient gas (e. g. air) into the sensitive layer at room temperature. In the presence of a reducing or oxidizing gas, which is able to react with the absorbed oxygen at temperatures between $200°C$ and $400°C$, the oxygen surface concentration and so the electrical conductivity of metal oxide is altered. This device requires a homogeneous temperature distribution

over its gas sensitive regions, a good thermal decoupling between the hotplate and the silicon rim and a good mechanical stability at high temperatures. This is achieved through supporting the silicon micromachined platform by glass pillars emanating from a glass cap above the silicon wafer as shown in Fig. 5.

Prior to fabrication, a thermal simulation is performed to determine the heating efficiency and temperature homogeneity of the gas sensor. As the device is connected to circuitry for heating power control and sensing resistor readout, a system-level simulation is needed here as well. Hence, a compact thermal model must be generated. The FE based spatial discretization of the governing heat transfer equation in ANSYS results in a linear system of 73955 ODEs. We have applied the Arnoldi process to this model and have generated several reduced models of different orders. For each reduced model a transfer function over a relevant range of frequencies from 0.01Hz to 10Hz was also computed for the purpose of evaluation. The magnitude of the frequency responses of the full-scale model and three reduced order models are shown in Fig. 6. Again, we can observe a good match of all models in the low-frequency domain. Fig. 7 shows a step response of the full-scale sensor model and vanishing step response errors of the reduced order models. The simulation time for the transient solution of the full-scale model in ANSYS with 30 time-steps was $6840s$, the time for model reduction to order 50 was $228s$ and the time integration of the reduced system in Mathematica lasted for $1s$.

As expected, both presented thermal models show low-pass filter characteristics (see Fig. 3 and Fig. 6). Hence, the connection between the rise-time and the cutoff frequency can be approximated through the ideal low-pass filter equation:

$$\tau = \frac{1}{2 \cdot f_g} \tag{10}$$

As a conclusion to this section, we can state that model reduction appears to work excellently for heat transfer in 2D and 3D. This is consistent with the observations of other groups [7] [8]. The main practical question that remains is, how to automatically choose the reduced order r. We additionally require that the error estimate should fit within the iterative framework of the Arnoldi algorithm.

3. Convergence of Relative error

Probably the simplest approach to estimate the model error in either the time- or frequency-domain is to compute the difference between two "neighbored" reduced models with order r and $r + 1$. Let us define a relative frequency-response error as:

$$E_r(s) = \frac{|G(s) - G_r(s)|}{|G(s)|} \tag{11}$$

where $G(s)$ and $G_r(s)$ are the transfer functions of the original model (2) and of the reduced order model (3), respectively. Let us further define a relative frequency-response error between two successive reduced models as:

$$\hat{E}_r(s) = \frac{|G_r(s) - G_{r+1}(s)|}{|G_r(s)|} \tag{12}$$

We have observed that, for both test cases from section 2.3,

$$E_r(s) \approx \hat{E}_r(s) \tag{13}$$

for a wide range of frequencies around the expansion point $s_0 = 0$. Fig. 8 through Fig. 10 compare the true error $E_r(s)$ (dashed line) to the estimate $\hat{E}_r(s)$ (dotted line) for different frequencies, for the optical filter model. We can see that both curves match well. We further observe convergence behavior when a treshold reduced system is reached. This means that, for the optical filter model for e. g., $\omega = 10 rad/s$, it is not possible to approximate the system better by using more than 6 Arnoldi vectors. This convergence occurs because the machine's numerical precision has been reached. The

minimal errors of the approximation for given machine precision, for the optical filter model are $\hat{E}_6$, $\hat{E}_{16}$ and $\hat{E}_{80}$ for the frequencies of 10, 10^3 and 10^4 rad/s (see Fig. 8 through Fig. 10). The system order necessary to reach convergence increases towards higher frequencies, as may be expected.

Similar results can be observed for the gas sensor model. Fig. 11 and Fig. 12 compare the true error $E_r(s)$ (dashed line) to the estimate $\hat{E}_r(s)$ (dotted line) for two different frequencies, for the gas sensor model.

It is important to note that, for very high frequencies (far away from the expansion point $s_0 = 0$) the observed convergence behavior may be replaced by fluctuations. Some results showing this phenomena can be found in [29]. In such a case, another expansion point has to be chosen.

This error indicator can be applied in the time-domain as well. Let us define a quadratic relative step-response error as:

$$\varepsilon(r) = \frac{1}{N} \cdot \sqrt{\sum_{t_i = 0}^{N \cdot \Delta t} \left(\frac{y(t_i) - y_r(t_i)}{y(t_i)} \right)^2} \tag{14}$$

where $y(t_i)$ and $y_r(t_i)$ are the system outputs of the full and order r reduced systems in N equidistant time-points spaced Δt apart. Let us further define a quadratic relative step-response error between two successive reduced order models as:

$$\hat{\varepsilon}(r) = \frac{1}{N} \cdot \sqrt{\sum_{t_i = 0}^{N \cdot \Delta t} \left(\frac{y_r(t_i) - y_{r+1}(t_i)}{y_r(t_i)} \right)^2} \tag{15}$$

Again, for the electrothermal MEMS models from section 2.3 it can be shown that:

$$\varepsilon(r) \approx \hat{\varepsilon}(r) \tag{16}$$

Please note that (14) and (15) are not functions of time, but rather of the system order,

and that they require a time integration of system outputs for a chosen output variable. Hence, they are slightly more expensive to compute than the frequency-response errors (11) and (12) and are susceptible to error accumulation. Fig. 13 and Fig. 14 show the time domain indicators for the optical filter and gas sensor devices. Integration time intervals for error indicators were chosen based on the rise time of the devices (Fig. 4 and Fig. 7).

The numerical error to integrate in time the original high-dimensional system is much higher than for the case of harmonic simulation. This can be seen in Fig. 14 where the results of the two different transient integrations, with 50 and 200 timesteps, are compared with the same reduced system. The difference between these two curves allows us to estimate the numerical error which is due to the time integration alone. So for example, the integration in ANSYS6.1 with 50 time steps already causes an error of about 1%. With 200 time steps an improvement of about 8% (difference between both true errors computed as in (14)) can be detected. Eventually, the true error and error estimate fit together.

The presented strategy, schematically summarized in Fig. 15, is similar to [21] with the advantage that it is computationally cheaper, and that it does perform an oscillations and convergence check. Concerning the choice of the frequency range of interest, for electro-thermal models, their low-pass filter characteristics (Fig. 3 and Fig. 6) can be used to connect the rise-time and the cutoff frequency according to equation (10), and hence to estimate a suitable frequency range.

4. Convergence of the Hankel singular Values

The second approach proposed is based on the computation of the Hankel singular values (HSV) of the reduced system. The Hankel singular values of a linear dynamic sys-

tem (2) of order n can be computed by solving two Lyapunov equations:

$$\begin{aligned} AP + PA^T &= -\boldsymbol{b}\boldsymbol{b}^T \\ A^T Q + QA &= -\boldsymbol{c}\boldsymbol{c}^T \end{aligned} \tag{17}$$

with $A = -C^{-1}K$, $\boldsymbol{b} = C^{-1}\boldsymbol{F}$, for the controlability grammian P and the observability grammian Q. The Hankel singular values are defined as:

$$\sigma_i = \sqrt{\lambda_i(P \cdot Q)}, i = 1, \ldots, n \tag{18}$$

Well established model order reduction methods from control theory offer a global error bound for an approximant of order r, based on the sum of the tail of the ordered set of Hankel singular values $\Sigma = \{\sigma_1, \sigma_2, \ldots, \sigma_n\}$, $\sigma_{i+1} \geq \sigma_i$ beginning with entry $r+1$:

$$\left\| G(s) - G_r(s) \right\|_\infty \leq 2(\sigma_{r+1} + \ldots + \sigma_n) \tag{19}$$

$G(s)$ is the transfer function of the original state-space model (2) and $G_r(s)$ is the transfer function of it's reduced order-r model, obtained by using projectors originating from the solutions to (17).

Since the computational complexity of (17) scales with $O(n^3)$, it is impractical to compute the HSV for large-scale systems. Luckily we could show that, for our test cases, the frequency-response error of Arnoldi reduction can be approximated by (19), by only computing the HSV $\hat{\sigma}_{ij}$ of the reduced system in each Arnoldi iteration. In this way, after i iterations we have a matrix-like structure:

$$H_i = \begin{bmatrix} \hat{\sigma}_{11} & 0 & \ldots & 0 \\ \hat{\sigma}_{21} & \hat{\sigma}_{22} & \ldots & 0 \\ & \ldots & & \\ \hat{\sigma}_{i1} & \hat{\sigma}_{12} & \ldots & \hat{\sigma}_{ii} \end{bmatrix} \tag{20}$$

where $\hat{\sigma}_{ij}$ is the j-th HSV of the i-th order reduced model. We have observed that, for the presented electro-thermal MEMS models after a number of Arnoldi iterations, the

largest $\hat{\sigma}_{ij}$ of the reduced order models converge towards the HSV of the original model. Fig. 16 shows that for the large scale gas sensor model, the reduced system of order 50 already reproduces the original 8 largest HSV. Furthermore, in each iteration, one new value is added towards the end of the set, while the beginning values further converge slowly. This means that after a number of iterations we can consider the largest original HSV of each model (those which do not change further when increasing the reduced system order) as known and use (19) to approximate the frequency response error. To demonstrate this, let us set an error bound of 10% for the transfer function of optical filter model and query the order of the reduced system needed to fulfill this error:

$$\left|G(s) - G_r(s)\right| \le 0.1,\ r\ =\ ? \tag{21}$$

Fig. 17 shows that, already after the second iteration, the first two Hankel singular Values of optical filter seems to have converged, which means that the difference between two consecutive values is negligible. Hence, we can consider them both as known. Observing the matrix H_6 we further see that the third reduced HSV $\hat{\sigma}_{i3}$ converges towards $\sigma_3 = 0.04$ i. e., has an order of magnitude of 10^{-2}.

$$H_6 = \begin{bmatrix} 118.6 & 0 & 0 & 0 & 0 & 0 \\ 118 & 0.62 & 0 & 0 & 0 & 0 \\ 118 & 0.6 & 0.02 & 0 & 0 & 0 \\ 118 & 0.6 & 0.02 & 1.31 \cdot 10^{-5} & 0 & 0 \\ 118 & 0.58 & 0.04 & 2.4 \cdot 10^{-3} & 1.1 \cdot 10^{-4} & 0 \\ 118 & 0.58 & 0.04 & 1.5 \cdot 10^{-3} & 1.5 \cdot 10^{-4} & 3.8 \cdot 10^{-6} \end{bmatrix} \tag{22}$$

If we assume a worst case, that is, that $\sigma_4, \sigma_5, \ldots$ are of the same order of magnitude as σ_3 and apply the estimate (19) we get:

$$\left|G(s) - G_2(s)\right| \le 2 \cdot 1666 \cdot 10^{-2} \approx 33 \tag{23}$$

As we do assume a rapid decay of the HSV for our MEMS models [13], we need some

HSV decay estimate in order to correct the right side of (23). In [30] an inexpensive decay estimate for the eigenvalues $\lambda_i(P)$ of one grammian of the symmetric system has been proposed as:

$$\frac{\lambda_k(P)}{\lambda_1(P)} \leq \left(\prod_{j=0}^{k-1} \frac{\kappa(A)^{(2j+1)/(2k)} - 1}{\kappa(A)^{(2j+1)/(2k)} + 1} \right)^2 \tag{24}$$

It is based only on the knowledge of the condition number κ of A, which can be computed by iterative methods [31]. Since we have observed essentially the same quality of results for the decay estimate of HSV and $\lambda_i(P)$ for our case studies, we use formula (24) to estimate an upper bound for σ_i:

$$\frac{\tilde{\sigma}_i}{\sigma_1} \leq \left(\prod_{j=0}^{i-1} \frac{\kappa(A)^{(2j+1)/(2i)} - 1}{\kappa(A)^{(2j+1)/(2i)} + 1} \right)^2 \tag{25}$$

and so correct the right side of the inequality (23). In (25), $\tilde{\sigma}_i$ should be understood as an estimate of σ_i.

Let us mention here that another recently proposed HSV decay estimate [32] given by:

$$\frac{\lambda_k(P)}{\lambda_1(P)} = \frac{-1}{2 \cdot Re(\lambda_k)} \prod_{j=1}^{k-1} \left| \frac{\lambda_k - \lambda_j}{\lambda_k + \lambda_j} \right| \tag{26}$$

doesn't require symmetry of A, but depends on complete knowledge of the spectrum of the system matrix, and is not practical for large-scale systems.

The estimate (24) as well as a decay curve of the true Hankel singular values of the tunable optical filter are shown in Fig. 18. By adding up all the $\tilde{\sigma}_i$ estimates with order of magnitude smaller or equal to σ_3 we get:

$$\sum_{i=j}^{1668} \tilde{\sigma}_i \approx 0.085, \tilde{\sigma}_j \leq \sigma_3 \tag{27}$$

This sum already indicates that we could possibly fulfill our specified error bound with

only two iterations. Indeed for the original model it holds:

$$\left|G(s) - G_2(s)\right| \leq 2 \cdot (\sigma_3 + \ldots + \sigma_{1668}) \;=\; 0.049 \tag{28}$$

In the case of the large-scale model of a gas sensor it was not possible to compute true Hankel singular values, hence the estimate (25) was computed (Fig. 19 shows the first 1000 estimates). Let us follow the same logic as in the previous example. Once again, Fig. 16 shows that after less than 50 iterations, first eight Hankel singular values of the gas sensor model have converged. From the matrix H_{50} (not displayed) we find out that the ninth reduced HSV $\hat{\sigma}_{i9}$ converges towards $\sigma_9 \;=\; 0.02$, i. e., has an order of magnitude of 10^{-2}. A worst case gives:

$$\left|G(s) - G_8(s)\right| \leq 2 \cdot 73947 \cdot 10^{-2} \approx 147894 \tag{29}$$

Luckily, by adding up all the $\tilde{\sigma}_i$ estimates with order of magnitude smaller or equal to σ_9 we get:

$$\sum_{i\,=\,j}^{73955} \tilde{\sigma}_i \approx 0.2,\; \tilde{\sigma}_j \leq \sigma_9 \tag{30}$$

which indicates that the reduced model of order eight could have an approximate error given by:

$$\left|G(s) - G_8(s)\right| \leq 2 \cdot 0.2 \approx 0.4 \tag{31}$$

Let us mention that the sum in equation (30) must not necessarily be made over the complete model size, because already after $i \;=\; 1000$ has been reached, the order of magnitude of $\tilde{\sigma}_i$ is only 10^{-64}. Hence, the remaining terms can be neglected.

Note once more that $G_2(s)$ in (28) and $G_8(s)$ in (31) should be computed by e. g. balanced truncations and hence the method suggested here only indicates where to stop in an iterative model order reduction based on the Arnoldi process. The presented strategy is schematically summarized in Fig. 20.

The challenge in the above algorithm is to choose the right number of the largest HSV *m*, which must have converged if the error bound ε is to be fulfilled, as well as to specify a "convergence threshold". In the given example of the optical filter the convergence of the 2 largest HSV was enough to fulfill an error bound of $\varepsilon = 0.1$. If one however needs too many iterations to meet the order of magnitude of ε among the converged HSV, the solution of the Lyapunov equations may become too expensive, and hence the error bound ε must be increased. Presently there are no guidelines on how to coordinate these numbers.

5. Sequential Model Order Reduction

The idea in using sequential MOR is to first use the Arnoldi algorithm to reduce a large-scale ordinary differential equation system to some order r1, and then to switch to one of the mathematically superior control theory methods for further reduction from order r1 to chosen order r2. In this way we will at least have an exact error estimate between the reduced system of order r1 and that of order r2. The problem of choosing the proper r1 remains of course. Our suggestion is to choose r1 according to one of the stop criteria suggested in section 3 and 4. In fact, for the tested electro-thermal MEMS models r1 = 50 turns out to be a reasonable choice, as shown in Fig. 21 for the gas sensor model, when first using Arnoldi for the reduction from 73.955 to 200, 150, 100 and 50 respectively, and then singular perturbation approximation. Fig. 22 to Fig. 24 compare the results of sequential MOR for the gas sensor model with r1=50 and r2=5 using singular perturbation approximation (SPA), hankel norm approximation (HNA) and balanced truncation approximation (BTA) respectively, to the "pure" Arnoldi reductions with r=50 and r=5. We can observe that the target reduced order 5 can be reached with smaller error if using sequential MOR than by using the Arnoldi algorithm alone. Out of the three control theory methods only the SPA preserves the stationary state (Fig. 22).

HNA and BTA (Fig. 23 and Fig. 24) do not preserve the stationary state, but yield smaller errors within the transient phase than the SPA. HNA is considered by mathematicians [33] to be the optimal method in terms of additionally specifying the lower bound for the inequality (19). Nevertheless, the most popular method of the three is BTA, due to its shortest computational time.

To combine the error indicators from section 4 with sequential MOR, we should first compute the HSV in each Arnoldi iteration until some prescribed error ε_1 has been approximately fulfilled:

$$\left|G(s) - G_{r1}(s)\right| \leq \varepsilon_1 \tag{32}$$

and then use one of the three presented control theory methods to reduce the model further toward the target order r2 having:

$$\left|G_{r1}(s) - G_{r2}(s)\right| \leq \varepsilon_2 \tag{33}$$

Using a simple triangle rule $\|x - y\| \geq \|x\| - \|y\|$, the error between the target reduced system with order r2 and the full-scale system can be now expressed as:

$$|G(s)| - \left|G_{r2}(s)\right| \leq \varepsilon_1 + \varepsilon_2 \tag{34}$$

Please note that inequality (34) is only a guideline on how to approximately choose a reduced order model.

6. Conclusion

The computation of the modeling error involves a common trade-off, which is balancing computational efficiency against the accuracy of the result. We have described three strategies and as usual, each has its advantages and disadvantages (see Fig. 25). At the present stage, the convergence of relative error and sequential MOR can be recommended for practical use. They are both straightforward to implement.

The extra computational time for the convergence of the relative error is very small,

provided it is estimated in the frequency domain. In this case, the strategy can be summarized in two main steps:

1. Choose an error required at the highest relevant (cutoff) frequency.

2. Solve a linear equation system for this frequency at each iteration.

This is the only method of the three where it is possible to detect (through the oscillations) whether the required frequency is too far from the expansion point or not.

The computational time for sequential model reduction is higher than for the convergence of the relative error, because first a maximum number of Arnoldi vectors (r_1) has to be estimated. Our tests show that for electro-thermal MEMS models $r_1 = 50$ might be enough. Now, the further reduction from r_1 to r_2 (which also has to be chosen) by BTA, SPA or HNA takes additional time. On the other hand, the order of the final reduced model might be lower than when it would be determined by the convergence of the relative error, for the same prescribed error bound. This is because the model of order r_2 includes information from r_1 Arnoldi vectors, although $r_1 > r_2$.

The convergence of the Hankel singular values requires the largest computational expense, because it is necessary to solve Lyapunov equations for the reduced model in each iteration. It also requires a decay estimate for the HSV. However, it is better suited for theoretical analysis than the other two methods. The advantages and disadvantages of each method are summarized in Fig. 25.

At this time we offer no theoretical justification for the proposed strategies. Whether they will function in general remains a question which requires further research with particularly more complex transfer functions than those of the low-pass filters. We have shown, however, that they currently offer sufficient accuracy for the presented engineering problems. Due to the simplicity of the implementation, the high computational effi-

ciency and a low susceptibility for numerical error accumulation, convergence of the relative error in the frequency domain takes priority, for automatic generation of electro-thermal compact models. Nevertheless, the convergence of the HSV as well as sequential MOR, and their application for error estimation, certainly deserve further research.

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Captions for figures

Fig. 1 Compact model extraction; Eliminating the need for user interaction makes the process fully automatic.

Fig. 2 Optical filter structure (by courtesy of D. Hohlfeld, IMTEK, Freiburg).

Fig. 3 Frequency response of optical filter.

Fig. 4 Step response (outer plot) and step response errors (inner plot) of optical filter. The errors for all three reduced models are less than 0.001% after 0.001s. The errors for all three reduced models are less than 0.001% after 0.001s.

Fig. 5 Gas sensor array structure (by courtesy of J. Wöllenstein, Fraunhofer IPM, Freiburg).

Fig. 6 Frequency response of gas sensor.

Fig. 7 Step response (outer plot) and step response errors (inner plot) of gas sensor.

Fig. 8 Error indicator for optical filter at $\omega = 10 rad/s$.

Fig. 9 Error indicator for optical filter at $\omega = 10^3 rad/s$.

Fig. 10 Error indicator for optical filter at $\omega = 10^5 rad/s$.

Fig. 11 Error indicator for gas sensor at $f = 0.01 Hz$.

Fig. 12 Error indicator for gas sensor at $f = 10 Hz$

Fig. 13 Time domain error indicator for optical filter computed for discrete times between 0s and 0.25s with $\Delta t = 0.01 s$.

Fig. 14 Time domain error indicator for gas sensor computed for discrete times between 0s and 5s.

Fig. 15 Error indicator algorithm based on convergence of relative errors.

Fig. 16 Largest 8 HSV of the Arnoldi reduced gas sensor models (order 1 to 50).

Fig. 17 Largest 8 HSV of the Arnoldi reduced optical filter models (order 1 to 20) normalized to the corresponding HSV of the original model.

Fig. 18 Decay estimate of HSV for tunable optical filter.

Fig. 19 Decay estimate of HSV for gas sensor.

Fig. 20 Error indicator algorithm based on computation of HSV of the reduced system.

Fig. 21 Sequential reduction of gas sensor using Arnoldi with r1=200, 150, 100 and 50 and SPA with r2=20.

Fig. 22 Sequential reduction of gas sensor using Arnoldi and SPA with r1=50 and r2=5.

Fig. 23 Sequential reduction of gas sensor using Arnoldi and HNA with r1=50 and r2=5.

Fig. 24 Sequential reduction of gas sensor using Arnoldi and BTA with r1=50 and r2=5.

Fig. 25 Advantages and disadvantages of proposed strategies.