A Posteriori Error Bounds for Krylov-based Fast Frequency Sweeps of Finite Element Systems

Y. Konkel, O. Farle, R. Dyczij-Edlinger Chair for Electromagnetic Theory, Saarland University, Saarbrücken, D-66123, Germany o.farle@lte.uni-saarland.de

Abstract—Projection-based model reduction is a well established methodology for computing fast frequency sweeps of finite element approximations to passive microwave structures. This contribution presents a novel provable error bound for momentmatching reduced-order models of lossless systems. It improves over existing methods by increasing the accuracy of the estimate and by reducing the numerical overhead. Numerical studies demonstrate the benefits of the suggested approach.

Index Terms—Reduced order systems, approximation error, finite element methods, microwave devices.

I. INTRODUCTION

Methods of model-order reduction (MOR) provide very efficient tools for computing fast frequency sweeps of linear timeinvariant systems. Most of them are subspace methods [1]-[4] that increase the dimension of their respective projection bases in an iterative process. To avoid the computational costs for constructing and solving an oversized reduced-order model (ROM), it is critical to stop the subspace iteration as soon as the ROM error meets a user-defined tolerance.

At present, the majority of the MOR methods utilizes heuristic stopping criteria. To the authors knowledge, computable and provable error bounds have only been reported in [3] and [4]. These estimates are based on a lower bound for the inf-sup constant, which is computed by the successive constraint method (SCM) [3]. Especially for resonant structures, the SCM is often more expensive than the whole process of generating the ROM, because eigenvalue problems of the dimension of the original system have to be solved. Furthermore, in the lossless case, the inf-sup constant corresponds to the distance from the working frequency to the nearest pole of the transfer function. Since the poles lie on the frequency axis, the distance may become arbitrarily small, which limits the usefulness of these methods in the lossless case.

We here propose a novel error estimator for lossless structures and MOR methods of Krylov type. Krylov subspace methods stand out for their efficiency, because they usually require only one single matrix factorization at a user-defined expansion point. The new error estimator is based on the fact that Krylov subspace methods quickly resolve the eigenvectors in the vicinity of the expansion point [5]. A spectral decomposition of the residual vector into converged and non-converged eigenvectors leads to the upper error bound. It is computable at very reasonable cost: Except for one additional matrix factorization for the whole frequency sweep, all quantities can be computed efficiently on the scale of the ROM. In its basic form, the error bound is only applicable to systems in immittance form, which may exhibit singularities. To overcome this shortcoming, the full paper will also include an asymptotical error estimator for scattering matrices. Our theoretical analysis does not include the effects of round-off errors.

Numerical examples demonstrate the efficiency and reliability of the suggested approach.

II. MODEL-ORDER REDUCTION

Finite element (FE) discretization of lossless microwave structures results in linear systems of the form

$$\left(\mathbf{S} - k_0^2 \mathbf{T}\right) \mathbf{x} = \mathbf{j} k_0 \eta_0 \mathbf{b}, \tag{1a}$$

$$z = \mathbf{b}^T \mathbf{x},\tag{1b}$$

where $\mathbf{S} \in \mathbb{C}^{N \times N}$ denotes the stiffness, $\mathbf{T} \in \mathbb{C}^{N \times N}$ the mass matrix, $\mathbf{b} \in \mathbb{R}^N$ the excitation vector, $\mathbf{x} \in \mathbb{C}^N$ the solution vector, and $k_0, \eta_0 \in \mathbb{R}$ the freespace wave number and characteristic impedance, respectively. For ease of presentation, we restrict ourselves in (1) to the single-input, single-ouput (SISO) case and transverse electromagnetic (TEM) modes as excitation. The extension to multiple-input, multiple-ouput (MIMO) systems is straightforward, and handling transverse electric (TE) or transverse magnetic (TM) modes as excitation just requires a post-processing scaling operation [2].

The expansion point $k_{0,exp}^2$ for the single-point MOR method is usually selected to be in the middle of the frequency band under investigation, \mathcal{B}_f . By introducing the shifted frequency parameter $\kappa = k_0^2 - k_{0,exp}^2$, we arrive at the system

$$(\mathbf{A} - \kappa \mathbf{T}) \mathbf{x} = \mathbf{b}, \tag{2a}$$

$$z = \mathbf{j}k_0\eta_0 \mathbf{b}^T \mathbf{x},\tag{2b}$$

where $\mathbf{A} = \mathbf{S} - k_{0,exp}^2 \mathbf{T}$ stands for the FE matrix at the expansion point. To achieve moment-matching, the projection matrix $\mathbf{Q} \in \mathbb{R}^{N \times n}$ has to span the Krylov subspace range(\mathbf{Q}) = $\mathcal{K}_n(\mathbf{A}^{-1}\mathbf{T}, \mathbf{A}^{-1}\mathbf{b})$ [1]. Note that the construction of the projection matrix just requires one single matrix factorization. Galerkin projection of (2) onto \mathbf{Q} leads to a ROM of the form

$$(\tilde{\mathbf{A}} - \kappa \tilde{\mathbf{T}}) \tilde{\mathbf{x}} = \tilde{\mathbf{b}},$$
 (3)

$$z = \mathbf{j}k_0\eta_0 \mathbf{\tilde{b}}^T \mathbf{\tilde{x}},\tag{4}$$

with

Â

$$\tilde{\mathbf{A}} = \mathbf{Q}^T \mathbf{A} \mathbf{Q}, \qquad \tilde{\mathbf{T}} = \mathbf{Q}^T \mathbf{T} \mathbf{Q}, \qquad \tilde{\mathbf{b}} = \mathbf{Q}^T \mathbf{b}.$$
 (5)

To ensure numerical robustness, the projection matrix \mathbf{Q} is computed by means of the Arnoldi algorithm [5].

III. Error estimation

The following error estimator is based on the assumption that the eigenvalues of a converged ROM coincide with the eigenvalues of the full model in the frequency range of interest. This assumption is justified by two facts: First, the shift-andinvert preconditioned Arnoldi method of Section II is known to first converge against the eigenvalues in the vicinity of the shift $k_{0,exp}^2$ [5]. Second, non-resolved eigenvalues give rise to noticeable errors in the transfer function, since the eigenvalues lie on the frequency axis. The error in the solution vector,

$$\mathbf{e} = \mathbf{x} - \mathbf{Q}\tilde{\mathbf{x}},\tag{6}$$

fulfills the residual equation

$$(\mathbf{A} - \kappa \mathbf{T})\mathbf{e} = \mathbf{r},\tag{7}$$

wherein **r** denotes the residual of (2a). Let (κ_i, \mathbf{v}_i) denote the eigenpair of the eigenvalue problem associated with (2a). Expanding the error **e** into eigenvectors \mathbf{v}_i of the original model, together with the Galerkin condition $\mathbf{Q}^T \mathbf{r} = \mathbf{0}$, leads to a representation of the error in system impedance e_z :

$$e_z = -\mathbf{j}k_0\eta_0 \mathbf{r}^T \mathbf{V} \operatorname{diag} \frac{1}{\kappa_i - \kappa} \mathbf{V}^T \mathbf{r}, \qquad (8)$$

with $\mathbf{V} = \begin{bmatrix} \mathbf{v}_1 & \dots & \mathbf{v}_N \end{bmatrix}$. Under the assumption that the eigenvectors of the original model are approximated well by the ROM in the frequency band \mathcal{B}_f , we can derive from (8) the error bound:

$$|e_{z}| \le k_{0}\eta_{0}\mathbf{r}^{T}\mathbf{V}\operatorname{diag}\frac{1}{|\kappa_{i}-\kappa|}\mathbf{V}^{T}\mathbf{r} \le \frac{k_{0}\eta_{0}}{\min_{\boldsymbol{\kappa}_{i}\notin\mathcal{B}}|\kappa_{i}-\kappa|}\mathbf{r}^{T}\mathbf{V}\mathbf{V}^{T}\mathbf{r}.$$
 (9)

Note that the term $\mathbf{r}^T \mathbf{V} \mathbf{V}^T \mathbf{r}$ can be evaluated efficiently on the level of the ROM, from quantities that are readily available in the Arnoldi iteration. Details will be given in the full paper.

IV. NUMERICAL EXAMPLE

Fig. 1 presents the structure of a bandpass filter. FE discretization results in a system of 213 472 degrees of freedom. We consider 201 equidistant evaluation points in the frequency band $\mathcal{B}_f = [0.58, 0.63]$ GHz and set the expansion point at f = 0.6 GHz. To quantify the overall error in the frequency band, we employ the error measure E_{∞} :

$$E_{\infty}(\mathbf{M}; \mathcal{B}_f) = \max_{i,j,n} \left| M_{ij}(f_n) \right|, \qquad (10)$$

where \mathbf{M} is a frequency-dependent error matrix. The estimated error is computed from (9), and the true one is given by

$$\mathbf{M} = \mathbf{Z}^{ROM} - \mathbf{Z}^{FE}.$$
 (11)

Fig. 2 presents a comparison between the true and the estimated error. The vertical line indicates the ROM dimension



Figure 1. Bandpass filter structure. All dimensions are in mm.



Figure 2. Comparison of true error and estimated error.

at which the eigenvalues in the frequency band are converged and the error estimate (9) becomes valid. As long as the true error is above the noise floor in the order of 10^{-8} , the proposed error estimate is an upper bound, as predicted by theory. The error estimator does not capture the noise floor correctly, because the Arnoldi algorithm underestimates roundoff errors in the residual. However, this represents no severe practical limitation, because underestimation only occurs when the ROM is already converged.

References

- P. Feldmann and R.W. Freund, "Efficient linear circuit analysis by Padé approximation via the Lanczos process," IEEE Trans. Comput. Aided Des. Integr. Circuits Syst., vol. 14, no. 5, pp. 639–649, 1995.
- [2] J. Rubio, J. Arroyo, and J. Zapata, "SFELP An efficient methodology for microwave circuit analysis," IEEE Trans. Microwave Theory Tech., vol. 49, no. 3, pp. 509–516, 2001.
- [3] Y. Chen, J.S. Hesthaven, Y. Maday and J. Rodríguez, "Certified reduced basis methods and output bounds for the harmonic Maxwell's equations," SIAM J. Sci. Comput., vol. 32, no. 2, pp. 970–996, 2010.
- [4] J. Pomplun and F. Schmidt, "Accelerated a posteriori error estimation for the reduced basis method with application to 3D electromagnetic scattering problems," SIAM J. Sci. Comput., vol. 32, no. 2, pp. 498– 520, 2010.
- [5] Y. Saad, "Numerical Methods for Large Eigenvalue Problems," SIAM, second edition, 2011.