A modified adaptive-order rational Arnoldi method for model order reduction

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A Greedy-type expansion point selection for moment-matching methods in model order reduction mainly depends on the computation of a sequence of reduced order models. Typically, the adaptive-order rational Arnoldi (AORA) method resembles an efficient way for the computation of a Galerkin projection corresponding to a set of expansion points. We will provide an extension of the AORA method, in order to reuse the orthonormal basis from previous calls of the AORA method.

1 Introduction

We will discuss the application of moment-matching methods for model order reduction of linear dynamical systems

$$\mathcal{E}\dot{x}(t) \quad = \quad \mathcal{A}x(t) \quad + \quad \mathcal{B}u(t), \quad y(t) \quad = \quad \mathcal{C}x(t), \tag{1}$$

where $\mathcal{E}, \mathcal{A} \in \mathbb{R}^{N\times N}$, $\mathcal{B} \in \mathbb{R}^{N\times m}$ and $\mathcal{C} \in \mathbb{R}^{p\times N}$. Moreover, we denote the state variable via $x(t) \in \mathbb{R}^N$, while $u(t) \in \mathbb{R}^m$ and $y(t) \in \mathbb{R}^p$ refer to the input and output variable of the descriptor system. The transfer function of the dynamical system is given as $\mathcal{H}(s) = \mathcal{C}(s\mathcal{E} - \mathcal{A})^{-1}\mathcal{B}$. In general, the rational idea behind model order reduction results from the application of a Galerkin projection $\Pi = V_n V_n^{\mathrm{T}}$ to (1), in order to provide a reduced order quadruplet $(\tilde{\mathcal{E}}, \tilde{\mathcal{A}}, \tilde{\mathcal{B}}, \tilde{\mathcal{C}})$ of significant smaller dimension $n \ll N$. For moment-matching methods, the columns of the orthonormal matrix $V_n \in \mathbb{C}^{N\times n}$ span the input Krylov subspace $\mathcal{K}_n(-(s_0\mathcal{E} - \mathcal{A})^{-1}\mathcal{E}, (s_0\mathcal{E} - \mathcal{A})^{-1}\mathcal{B})$ with $s_0 \in \mathbb{C}$, in order to preserve the input-output behaviour of the dynamical system in the reduced order model [1]. Since the accuracy of the reduced order model remains limited for a single expansion point, we usually investigate an adequate set of expansion points $\{s_1, \ldots, s_p\} \subset \mathbb{C}$. The missing a-priori error estimation for moment-matching methods poses the problem of the reliable choice of a set of expansion points. Nevertheless, the accuracy of the reduced order model might be obtained from a heuristic error estimation introduced by Grimme et al. [5].

2 Adaptive-order rational Arnoldi method

In general, the Greedy-type expansion point selection for moment-matching methods follows from the computation of a sequence of reduced order models $\tilde{\mathcal{H}}_1(s), \ldots, \tilde{\mathcal{H}}_k(s)$ including different sets of expansion points $\mathcal{S}_l = \mathcal{S}_{l-1} \cup \{s_l\}$, $s_l \in \mathbb{C}$, for all $l > 1$, see [3]. If we assume that the dimension of the reduced order model has been chosen a-priori, each reduced order model $\tilde{\mathcal{H}}_i(s)$ $(i = 1, \ldots, k)$ follows from a rational Arnoldi-type method [7]. Thereby, the span of the orthonormal matrix $V_n \in \mathbb{C}^{N\times n}$ fulfills

$$\operatorname{span}(V_n) = \bigoplus_{l=1}^{i} \mathcal{K}_{j_l}(-(s_l\mathcal{E} - \mathcal{A})^{-1}\mathcal{E}, (s_l\mathcal{E} - \mathcal{A})^{-1}\mathcal{B}), \tag{2}$$

where $n = j_1 + \cdots + j_i$, see [4].

An efficient way for the adaptive computation of each dimension $j_l \geq 0$ $(l = 1, \ldots, i)$ remains from the adaptive-order rational Arnoldi (AORA) method [6]. Let $Y^{(j)}(s_l) \equiv \mathcal{C}X^{(j)}(s_l)$ denote the output moment of the linear dynamical system (1), where $X^{(j)}(s_l) = [-(s_l\mathcal{E} - \mathcal{A})^{-1}\mathcal{E}]^j(s_l\mathcal{E} - \mathcal{A})^{-1}\mathcal{B}$ refers to the state moment. If $\tilde{Y}^{(j)}(s_l) = \tilde{\mathcal{C}}\tilde{X}^{(j)}(s_l)$ determines the output moment of the reduced order model, the AORA method increases the Krylov subspace of the expansion point $s_{\max} = \arg\max_{s\in\mathcal{S}_l} |Y^{(j)}(s) - \tilde{Y}^{(j)}(s)|$ with an additional vector in each iteration step. We remark that the computation of the expansion point $s_{\max} \in \mathbb{C}$ from the transfer function error follows as a by-product of the rational Arnoldi method. Moreover, the modified Gram-Schmidt procedure already ensures the computation of an orthonormal basis $V_n \in \mathbb{C}^{N\times n}$.

3 Extension of rational Arnoldi-type methods

Of course, the drawback of the subsequent calls of the AORA method results from the fact, that the computation of the orthonormal basis $V_n^{(k)} \in \mathbb{C}^{N\times n}$ corresponding to the k–th call does not consider any previous orthonormal bases. Since we

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simply add a single expansion point $s_l \in \mathbb{C}$ during each call of the AORA method, the idea of the modified adaptive-order rational Arnoldi (mAORA) method is given as follows: At first, we call the AORA method subsequently with the expansion points $\{s_1\}, \{s_1, s_2\}, \ldots, \{s_1, \ldots, s_p\}$. Here, each call returns an orthonormal matrix $V_n^{(l)} \in \mathbb{C}^{N\times n}$ spanning the subspace (2) of dimension $n = j_{1,i} + \cdots + j_{l,i}$ $(i = 1, \ldots, p)$. Moreover, as long as $j_{i,l+1} \leq j_{i,l}$ $(i = 1, \ldots, l)$, we are able to reuse the orthonormal vectors from the previous call of the AORA method. Hence, we only have to explicitly solve a shifted linear system, whenever the new expansion point $s_{l+1} \in \mathbb{C}$ has been selected or the dimension $j_{i,l+1} > j_{i,l}$ exceeds the previous number of orthonormal vectors of the expansion point $s_i \in \mathbb{C}$ $(i = 1, \ldots, l)$.

We point out that the AORA and mAORA method coincide for at most two expansion points. More expansion points lead to a sufficient approximation of the AORA method avoiding the complete recomputation of the orthonormal basis $V_n^{(l)} \in \mathbb{C}^{N\times n}$ due to the reuse of previous orthonormal vectors from $V_n^{(l-1)} \in \mathbb{C}^{N\times n}$. In general, both methods lead to a comparable sequence $n = j_{1,i} + \cdots + j_{l,i}$ $(i = 1, \ldots, p)$ in each subsequent call.

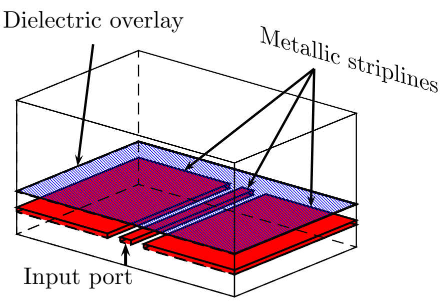
4 Numerical experiment

Finally, we will provide a numerical example for a Coplanar Waveguide[1] resulting from the time-harmonic, first-order Maxwell's equations

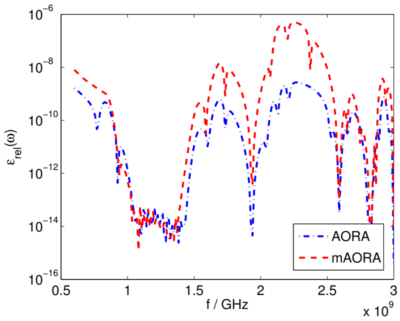
$$\imath\omega(\epsilon \boldsymbol{E}) = -\sigma \boldsymbol{E} + \nabla \times \boldsymbol{H}, \qquad \imath\omega(\mu \boldsymbol{H}) = \nabla \times \boldsymbol{E},$$

where $\boldsymbol{E}$ and $\boldsymbol{H}$ refer to the electric and magnetic field strength. The Coplanar Waveguide resembles a single-input, single-output dynamical system with the frequency range $[f_{\min}, f_{\max}] = [0.6, 3.0]$ GHz and $N = 32924$ degrees of freedom, cf. Figure 1(a). On the boundary of the computational domain, we have employed the PEC boundary condition $\boldsymbol{E} \times \boldsymbol{n} = 0$. However, the relative error $\epsilon_{rel}(\omega) = |\mathcal{H}(\imath\omega) - \tilde{\mathcal{H}}(\imath\omega)|/|\mathcal{H}(\imath\omega)|$, $\omega = 2\pi f$ and $f \in [f_{\min}, f_{\max}]$, in Figure 1(b) allows a comparison between the AORA and mAORA method for eight expansion points and the dimension $n = 25$. The expansion points have been determined adaptively on the basis of the rational Krylov residual, see [2].

In general, the numerical experiments indicate that the computational effort for the subsequent calls of the mAORA method reduces about a factor of three. This is due to saving a substantial amount of systems solves with large-scale and highly indefinite systems of the form $(s\mathcal{E} - \mathcal{A})x = f$, $s \in \mathbb{C}$.



(a) Coplanar Waveguide



(b) mAORA vs. AORA

Fig. 1: Adaptive-order rational Arnoldi method in computational electromagnetism.

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[1] The model problem has been developed within the MoreSim4Nano research project, see http://moresim4nano.org