

Model reduction of constrained mechanical systems in M-M.E.S.S. [★]

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Abstract: We discuss balanced truncation model reduction of constrained mechanical systems. The incorporation of the algebraic constraints leads to linear differential-algebraic control systems of index 2 or 3. Then for the square-root method in balanced truncation, the solution of projected Lyapunov equations is required. In this paper we discuss how to avoid the explicit construction of the projectors and the formulation of a projection-avoiding balanced truncation method which is suitable for efficient numerical computations. We have implemented this method in the MATLAB package M-M.E.S.S. and present some numerical results for illustration.

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1. INTRODUCTION

In this paper we consider the class of second-order differential-algebraic systems of the form

$$\begin{aligned} M\ddot{\xi}(t) &= K\xi(t) + D\dot{\xi}(t) + G_3^T\mu_3(t) + G_2^T\mu_2(t) + B_\xi u(t), \\ 0 &= G_3\xi(t) + G_2\dot{\xi}(t), \\ y(t) &= C_1\xi(t) + C_2\dot{\xi}(t), \end{aligned} \tag{1}$$

for the displacements $\xi(t) \in \mathbb{R}^{n_\xi}$ (i.e., $\dot{\xi}(t)$ and $\ddot{\xi}(t)$ represent the velocities and accelerations of the masses). Here, $M, K, D \in \mathbb{R}^{n_\xi \times n_\xi}$ are the possibly large and sparse, symmetric positive definite (spd) mass, stiffness, and damping matrices. Algebraic constraints are given by the full row-rank constraint matrices $G_3 \in \mathbb{R}^{n_\mu \times n_\xi}$, $G_2 \in \mathbb{R}^{n_\mu \times n_\xi}$ and corresponding Lagrange multipliers $\mu_2, \mu_3 \in \mathbb{R}^{n_\mu}$ with $n_\mu < n_\xi$. Furthermore, $B_\xi \in \mathbb{R}^{n_\xi \times m}$ is the input matrix corresponding to the input vector $u(t) \in \mathbb{R}^m$, and $C_1, C_2 \in \mathbb{R}^{q \times n_\xi}$ are the output matrices associated to the output vector $y(t) \in \mathbb{R}^q$.

Systems of this structure arise in a large variety of applications, in particular in the modeling of constrained vibrational systems as depicted in Eich-Soellner and Führer (1998); Mehrmann and Stykel (2005). Similar problems arise for electrical networks (see, e.g., Rianza (2008); Reis (2010)).

We focus on two most important special cases, namely:

- i) The constraints act only on the velocity level, i.e., $G_3 = 0$ and G_2 has full row-rank. By setting $\xi_1(t) :=$

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$\xi(t), \xi_2(t) := \dot{\xi}(t), \mu(t) := \mu_2(t)$, and linearizing, we obtain

$$\begin{aligned} \underbrace{\begin{bmatrix} I_{n_\xi} & 0 & 0 \\ 0 & M & 0 \\ 0 & 0 & 0 \end{bmatrix}}_{=: \mathcal{E}} \underbrace{\begin{bmatrix} \xi_1(t) \\ \xi_2(t) \\ \dot{\mu}(t) \end{bmatrix}}_{=: \dot{x}(t)} &= \underbrace{\begin{bmatrix} 0 & I_{n_\xi} & 0 \\ K & D & G_2^T \\ 0 & G_2 & 0 \end{bmatrix}}_{=: \mathcal{A}_2} \underbrace{\begin{bmatrix} \xi_1(t) \\ \xi_2(t) \\ \mu(t) \end{bmatrix}}_{=: x(t)} + \underbrace{\begin{bmatrix} 0 \\ B_\xi \\ 0 \end{bmatrix}}_{=: \mathcal{B}} u(t), \\ y(t) &= \underbrace{\begin{bmatrix} C_1 & C_2 & 0 \end{bmatrix}}_{=: \mathcal{C}} \underbrace{\begin{bmatrix} \xi_1(t) \\ \xi_2(t) \\ \mu(t) \end{bmatrix}}_{=: x(t)}, \end{aligned} \tag{2}$$

which is a *first-order differential-algebraic system of index 2*.

- ii) The constraints act only on the position level, i.e., $G_2 = 0$ and G_3 has full row-rank. By setting $\xi_1(t) := \xi(t), \xi_2(t) := \dot{\xi}(t), \mu(t) := \mu_3(t)$, and linearizing (1), we obtain

$$\begin{aligned} \underbrace{\begin{bmatrix} I_{n_\xi} & 0 & 0 \\ 0 & M & 0 \\ 0 & 0 & 0 \end{bmatrix}}_{=: \mathcal{E}} \underbrace{\begin{bmatrix} \xi_1(t) \\ \xi_2(t) \\ \dot{\mu}(t) \end{bmatrix}}_{=: \dot{x}(t)} &= \underbrace{\begin{bmatrix} 0 & I_{n_\xi} & 0 \\ K & D & G_3^T \\ G_3 & 0 & 0 \end{bmatrix}}_{=: \mathcal{A}_3} \underbrace{\begin{bmatrix} \xi_1(t) \\ \xi_2(t) \\ \mu(t) \end{bmatrix}}_{=: x(t)} + \underbrace{\begin{bmatrix} 0 \\ B_\xi \\ 0 \end{bmatrix}}_{=: \mathcal{B}} u(t), \\ y(t) &= \underbrace{\begin{bmatrix} C_1 & C_2 & 0 \end{bmatrix}}_{=: \mathcal{C}} \underbrace{\begin{bmatrix} \xi_1(t) \\ \xi_2(t) \\ \mu(t) \end{bmatrix}}_{=: x(t)}, \end{aligned} \tag{3}$$

which is a *first-order differential-algebraic system of index 3*.

The two most frequently applied modern MOR methods are balanced truncation (see Moore (1981); Tombs and Postlethwaite (1987)) and rational interpolation of the transfer function by the iterative rational Krylov algorithm

(IRKA) from Gugercin et al. (2008). Both approaches have also been extended to general descriptor systems in Stykel (2004); Gugercin et al. (2013). In this case one has to apply certain projections to the model in order to decouple the differential from the algebraic equations. However, the computation and application of the projectors can be very demanding in terms of computational complexity, as well as memory requirements and also rises some robustness issues if the number of constraints, i.e., the number of rows in G_2 or G_3 become large.

In case of structured systems of the form (2) there exists an easier approach. It is possible to explicitly construct the projector onto the differential part of the system from the given problem data. In this way the algebraic equations can be eliminated following Heinkenschloss et al. (2008); Gugercin et al. (2013). Then, exploiting certain technical properties of the projector, one can directly apply the methods for ODE systems to the projected system. This procedure has, however, only been studied for structured first-order systems of index two. Note that both approaches are essentially projecting to the same subspace. They only differ in the topology underlying the projection. The classical Stykel-type spectral projection is orthogonal in the state-space equipped with the standard Euclidean inner product. The projection derived from the problem structure is oblique in this setting, but orthogonal in the inner product induced by the mass matrix. In the context of the linearized Navier-Stokes equations discussed in Heinkenschloss et al. (2008), the projection is in fact the discretized version of the well known Leray projection to the divergence-free velocity functions.

Until now there only exist first investigations for both the second-order index-2 or index-3 systems as in (1). This paper is mainly devoted to closing the gap in the open software and also to the generation of a unifying framework for these kind of systems. Here, we will focus on balanced truncation model reduction using the software infrastructure in M-M.E.S.S., but in principle our results can also be directly applied to obtain a generalized version of IRKA following the lines of Gugercin et al. (2013), see also Ahmad and Benner (2014).

The paper is structured as follows. In Section 2 we will repeat some preliminaries, in particular we briefly review balanced truncation model reduction and the low-rank ADI method to solve the arising large-scale Lyapunov equations. Furthermore, we will introduce the general projection technique to reduce structured differential-algebraic systems to ODE systems. In Section 3 we will describe details about carrying out this projection with the focus on resolving certain numerical difficulties. Finally, we present computational results in Section 4 and summarize the paper in Section 5.

2. PRELIMINARIES

In this section we briefly review some fundamental concepts and results including balanced truncation, the low-rank alternating directions implicit (ADI) iteration for the solution of the arising Lyapunov equations, and projection techniques for descriptor systems that will be used throughout this paper.

2.1 Balanced Truncation and Low-Rank ADI

Among all other techniques of model order reduction, the method of balanced truncation is particularly attractive due to the availability of an a priori error bound, and the guaranteed stability of the reduced order model (see, e.g., Antoulas (2005) and references therein). The low-rank ADI method for the solution of large-scale Lyapunov equations is a desirable solver since it does only rely on basic linear algebra manipulations and in contrast to projection based methods does not pose additional requirements on the system properties. We will discuss these two in the current section.

A Short Introduction to Balanced Truncation for Generalized State Space Systems In Antoulas (2005) four general approaches for computing the balancing and truncating transformations are described, among which we will focus on the square root method. For a linear time-invariant dynamical system

$$\begin{aligned} E\dot{x}(t) &= Ax(t) + Bu(t), \\ y(t) &= Cx(t), \end{aligned} \quad (4)$$

with $E, A \in \mathbb{R}^{n \times n}$, $B \in \mathbb{R}^{n \times p}$ and $C \in \mathbb{R}^{m \times n}$, state $x(t) \in \mathbb{R}^n$, input $u(t) \in \mathbb{R}^p$, and output $y(t) \in \mathbb{R}^m$ at time $t \geq 0$, we want to repeat the basic procedure here. In this section we assume that E is nonsingular and we describe how to pull the structured DAEs back to this case in the later sections. Moreover, we assume the system to be asymptotically stable. The key idea in the square root method is to perform a simultaneous diagonalization of the two system Gramians, whose diagonal entries will then be the decreasingly ordered Hankel singular values (HSVs) of the system. Then the states corresponding to small HSVs are truncated, leading to a much smaller system. The well-known balanced truncation error bound is then simply formed by twice the sum of the truncated HSVs.

The two system Gramians are computed as the solutions of the controllability and observability Lyapunov equations

$$APE^T + EPA^T = -BB^T, \quad (5a)$$

$$A^TQE + E^TQA = -C^TC. \quad (5b)$$

Let $P = RR^T$ and $Q = SS^T$ be symmetric factorizations of these Gramians. In the case where n is large, E and A are sparse, and $m, p \ll n$, then S and R are usually of low rank and can be computed by a low-rank solver for the large-scale equations (5). Here, we will focus on the low-rank ADI, see Kürschner (2016) for the most recent formulation.

The avoidance of the explicit application of the projectors is the main problem that we discuss here. This can be solved by a careful initialization of the ADI algorithm. The main operation in ADI is the solution of shifted linear systems of equations, as in the rational Krylov subspace method (RKSM) for computing the Gramian factors, see Druskin et al. (2011). Therefore, everything we present here carries over to RKSM and model reduction via IRKA as well (see Gugercin et al. (2013); Ahmad and Benner (2014)).

To perform the balancing operation we compute the singular value decomposition

Algorithm 1: LR-ADI iteration for the Lyapunov equation (5a).

Input : $E, A \in \mathbb{R}^{n \times n}$, $B \in \mathbb{R}^{n \times m}$, proper shift parameters $\{\alpha_1, \dots, \alpha_{j_{\max}}\} \subset \mathbb{C}_{<0} := \{\alpha \in \mathbb{C} \mid \operatorname{Re}(\alpha) < 0\}$, and a tolerance $0 < \tau \ll 1$ for the normalized residual.
Output: $Z \in \mathbb{R}^{n \times m_{j_{\max}}}$ such that $P \approx ZZ^T$, where P solves (5a).
 Initialize $W_0 := B$, $Z_0 := [\]$, and $j := 1$.
while $\|W_{j-1}^T W_{j-1}\| \geq \tau \|B^T B\|$ **do**
 Solve $(A + \alpha_j E)V_j = W_{j-1}$ for V_j .
 if $\operatorname{Im}(\alpha_j) = 0$ **then**
 Set $W_j := W_{j-1} - 2 \operatorname{Re}(\alpha_j) E V_j$.
 Set $Z_j := [Z_{j-1} \quad \sqrt{-2\alpha_j} V_j]$.
 else
 Set $\gamma_j := 2\sqrt{-\operatorname{Re}(\alpha_j)}$, $\delta_j := \frac{\operatorname{Re}(\alpha_j)}{\operatorname{Im}(\alpha_j)}$, and
 $\varphi_j := \gamma_j \sqrt{(\delta_j^2 + 1)}$.
 Set $W_{j+1} := W_{j-1} + \gamma_j^2 E (\operatorname{Re}(V_j) + \delta_j \operatorname{Im}(V_j))$.
 Set $Z_{j+1} := [Z_{j-1} \quad \gamma_j (\operatorname{Re}(V_j) + \delta_j \operatorname{Im}(V_j)) \quad \varphi_j \operatorname{Im}(V_j)]$.
 Set $j := j + 1$.
 Set $j := j + 1$.

$$S^T E R = U \Sigma V = [U_1 \ U_2] \begin{bmatrix} \Sigma_1 & 0 \\ 0 & \Sigma_2 \end{bmatrix} \begin{bmatrix} V_1^T \\ V_2^T \end{bmatrix}, \quad (6)$$

where $\Sigma_1 = \operatorname{diag}(\sigma_1, \dots, \sigma_r)$ contains the HSVs we want to keep, whereas $\Sigma_2 = \operatorname{diag}(\sigma_{r+1}, \dots, \sigma_n)$ contains the HSVs we want to truncate. Using R, S, U_1, V_1 , and Σ_1 we can then construct the left and right projection matrices, that are balancing and truncating the system at the same time as

$$T_L = S U_1 \Sigma_1^{-\frac{1}{2}}, \quad T_R = R V_1 \Sigma_1^{-\frac{1}{2}}. \quad (7)$$

The desired reduced order model

$$\begin{aligned} \widehat{E} \dot{\widehat{x}}(t) &= \widehat{A} \widehat{x}(t) + \widehat{B} u(t), \\ \widehat{y}(t) &= \widehat{C} \widehat{x}(t), \end{aligned} \quad (8)$$

is computed as $\widehat{E} = T_L^T E T_R = I_r$, $\widehat{A} = T_L^T A T_R$, $\widehat{B} = T_L^T B$ and $\widehat{C} = C T_R$ and we get the error bound

$$\|y - \widehat{y}\|_{\mathcal{L}_2(\mathbb{R}_{\geq 0}, \mathbb{R}^p)} \leq \left(2 \sum_{i=r+1}^n \sigma_i \right) \|u\|_{\mathcal{L}_2(\mathbb{R}_{\geq 0}, \mathbb{R}^m)}$$

for inputs $u \in \mathcal{L}_2(\mathbb{R}_{\geq 0}, \mathbb{R}^m)$ and $\mathbb{R}_{\geq 0} := [0, \infty)$.

Low-Rank Alternating Directions Implicit Iteration Low-rank ADI can be understood as a clever low-rank formulation of a relaxation based fixed point iteration for the Lyapunov operator. For the sake of simplicity we will simply use the most recent formulation as a recipe in Algorithm 1. A detailed derivation and a discussion of the state-of-the-art of the shift parameter problem is available in Kürschner (2016). Note that Algorithm 1 expects the shifts to be proper, i.e., they are either real or come in pairs of two consecutive complex conjugate shifts in the ordered set $\{\alpha_1, \dots, \alpha_{j_{\max}}\}$.

2.2 *Balanced Truncation for Stokes-like Systems*

We follow the projection idea of Heinkenschloss et al. (2008) for systems of the form

$$\begin{bmatrix} E & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \dot{v}(t) \\ \dot{p}(t) \end{bmatrix} = \begin{bmatrix} A & H^T \\ G & 0 \end{bmatrix} \begin{bmatrix} v(t) \\ p(t) \end{bmatrix} + \begin{bmatrix} B_v \\ 0 \end{bmatrix} u(t), \quad (9)$$

$$y(t) = C_v v(t) + C_p p(t).$$

Here $v(t) \in \mathbb{R}^{n_v}$ and $p(t) \in \mathbb{R}^{n_p}$ for each $t \geq 0$. We assume that $E \in \mathbb{R}^{n_v \times n_v}$ is spd, $A \in \mathbb{R}^{n_v \times n_v}$, $G, H \in \mathbb{R}^{n_p \times n_v}$, $B_v \in \mathbb{R}^{n_v \times m}$, $C_v \in \mathbb{R}^{q \times n_v}$, and $C_p \in \mathbb{R}^{q \times n_p}$. As in Heinkenschloss et al. (2008), for now, we assume that $G = H$. The extension to the case $G \neq H$ is covered by Gugercin et al. (2013).

From (9) we obtain $Gv(t) = 0$ implying $G\dot{v}(t) = 0$ and thus,

$$0 = GE^{-1}Av(t) + GE^{-1}G^T p(t) + GE^{-1}B_v u(t).$$

This yields

$$\begin{aligned} p(t) &= -(GE^{-1}G^T)^{-1} GE^{-1}Av(t) \\ &\quad - (GE^{-1}G^T)^{-1} GE^{-1}B_v u(t). \end{aligned}$$

Defining the matrices

$$\begin{aligned} \Pi &:= I_{n_v} - G^T (GE^{-1}G^T)^{-1} GE^{-1}, \\ C &:= C_v - C_p (GE^{-1}G^T)^{-1} GE^{-1}A, \\ D &:= -C_p (GE^{-1}G^T)^{-1} GE^{-1}B_v, \end{aligned} \quad (10)$$

and inserting $p(t)$ into (9), we obtain

$$\begin{aligned} E\dot{v}(t) &= \Pi Av(t) + \Pi B_v u(t), \\ y(t) &= Cv(t) + Du(t). \end{aligned} \quad (11)$$

In the following we will frequently use the following result.

Proposition 1. (Heinkenschloss et al. (2008)). The matrix Π is a projector onto $\operatorname{im} \Pi = \ker GE^{-1}$ along $\ker \Pi = \operatorname{im} G^T$ and it holds

$$\Pi E = E \Pi^T. \quad (12)$$

In particular, it can be shown that

$$Gv(t) = 0 \Leftrightarrow \Pi^T v(t) = v(t). \quad (13)$$

By using (12) and (13), (11) can be reformulated as

$$\begin{aligned} \Pi E \Pi^T \dot{v}(t) &= \Pi A \Pi^T v(t) + \Pi B_v u(t), \\ y(t) &= C \Pi^T v(t) + Du(t). \end{aligned} \quad (14)$$

In this formulation, the algebraic equations have been successfully eliminated. However, since in general Π is a singular matrix, the pencil $\lambda \Pi E \Pi^T - \Pi A \Pi^T$ is a singular pencil. This means, that besides differential equations, (14) also contains some redundant equations that are trivially fulfilled and will give no further information. To get rid of the redundant part, we use the factorization

$$\Pi = \Theta_l \Theta_r^T,$$

where $\Theta_l, \Theta_r \in \mathbb{R}^{n_v \times r}$, $\Theta_r^T \Theta_l = I_r$, and $r = \operatorname{rank}(\Pi)$. Then, the projected system (without redundant equations) is given by

$$\begin{aligned} \Theta_r^T E \Theta_r \dot{\tilde{v}}(t) &= \Theta_r^T A \Theta_r \tilde{v}(t) + \Theta_r^T B_v u(t), \\ y(t) &= C \Theta_r \tilde{v}(t) + Du(t), \end{aligned} \quad (15)$$

where $\tilde{v}(t) = \Theta_l^T v(t)$. Note, that both $\Theta_r^T E \Theta_r$ and $\Theta_r^T A \Theta_r$ are regular and (15) is in fact a system of ODEs just like (4). Thus, it can directly be treated with the methods from Section 2.1. In contrast to Heinkenschloss et al. (2008) where the ADI formulation for differential algebraic systems was used, we will formulate our results with Algorithm 1. This will require some further modifications as outlined below.

3. BALANCED TRUNCATION FOR CONSTRAINED MECHANICAL SYSTEMS

Employing similar ideas as presented in Section 2, we will show how one can derive the projections for mechanical systems (2) and (3), and later avoid their explicit use in the algorithm.

3.1 Derivation of Π for the Index-2 Case

The system (2) exactly resembles (9) by setting

$$\begin{aligned} E &:= \begin{bmatrix} I_{n_\xi} & 0 \\ 0 & M \end{bmatrix}, & A &:= \begin{bmatrix} 0 & I_{n_\xi} \\ K & D \end{bmatrix}, \\ G &:= [0 \ G_2], & H &:= G, \\ B_v &:= \begin{bmatrix} 0 \\ B_\xi \end{bmatrix}, & C_v &:= [C_1 \ C_2], & C_p &:= 0, \end{aligned}$$

and we are precisely in the framework of Section 2.2. Note that for the particular linearization treated here, the projector Π takes a special form, namely

$$\Pi = I_{2n_\xi} - G^T (GE^{-1}G^T)^{-1} GE^{-1} = \begin{bmatrix} I_{n_\xi} & 0 \\ 0 & \Pi_2 \end{bmatrix} \quad (16)$$

with

$$\Pi_2 := I_{n_\xi} - G_2^T (G_2 M^{-1} G_2^T)^{-1} G_2 M^{-1}.$$

Here, the projector Π_2 only acts on the velocities since they contain the only constraints of the system. Note also that Π_2 has exactly the same structure as Π formulated on the velocity level of the second-order system and thus immediately inherits the properties of Proposition 1.

For theoretical considerations this completes the story, but numerical implementations of the method require some additional thoughts. These open issues will be addressed in Section 3.3.

3.2 Derivation of Π for the Index-3 Case

The system (3) also resembles (9) by setting

$$\begin{aligned} E &:= \begin{bmatrix} I_{n_\xi} & 0 \\ 0 & M \end{bmatrix}, & A &:= \begin{bmatrix} 0 & I_{n_\xi} \\ K & D \end{bmatrix}, \\ G &:= [G_3 \ 0], & H &:= [0 \ G_3], \\ B_v &:= \begin{bmatrix} 0 \\ B_\xi \end{bmatrix}, & C_v &:= [C_1 \ C_2], & C_p &:= 0. \end{aligned} \quad (17)$$

Thus, using the two-sided projection approach by Gugercin et al. (2013), this case is similarly easy to treat as the above one. However, we can find a one-sided projection as follows. To this end, we follow the same steps as in Section 2.2.

From the constraint equation $G_3 \xi(t) = 0$ we directly obtain $G_3 \dot{\xi}(t) = 0$ and also $G_3 \ddot{\xi}(t) = 0$. Inserting these in (1) yields

$$\begin{aligned} 0 &= G_3 M^{-1} K \xi(t) + G_3 M^{-1} D \dot{\xi}(t) \\ &\quad + G_3 M^{-1} G_3^T \mu(t) + G_3 M^{-1} B_\xi u(t), \end{aligned}$$

and hence we can write the Lagrange multiplier as

$$\begin{aligned} \mu(t) &= - (G_3 M^{-1} G_3^T)^{-1} G_3 M^{-1} K \xi(t) \\ &\quad - (G_3 M^{-1} G_3^T)^{-1} G_3 M^{-1} D \dot{\xi}(t) \\ &\quad - (G_3 M^{-1} G_3^T)^{-1} G_3 M^{-1} B_\xi u(t). \end{aligned}$$

We define

$$\Pi_3 := I_{n_\xi} - G_3^T (G_3 M^{-1} G_3^T)^{-1} G_3 M^{-1},$$

and obtain

$$M \ddot{\xi}(t) = \Pi_3 D \dot{\xi}(t) + \Pi_3 K \xi(t) + \Pi_3 B_\xi u(t).$$

Obviously Π_3 is a projector and satisfies the equivalent properties of Proposition 1. Furthermore, by direct calculation it can be verified that

$$G_3 \xi(t) = 0 \Leftrightarrow \Pi_3^T \xi(t) = \xi(t),$$

$$\text{and } G_3 \dot{\xi}(t) = 0 \Leftrightarrow \Pi_3^T \dot{\xi}(t) = \dot{\xi}(t).$$

Therefore, similarly as for (14) we obtain

$$\begin{aligned} \Pi_3 M \Pi_3^T \ddot{\xi}(t) &= \Pi_3 D \Pi_3^T \dot{\xi}(t) + \Pi_3 K \Pi_3^T \xi(t) + \Pi_3 B_\xi u(t), \\ y(t) &= C_1 \Pi_3^T \xi(t) + C_2 \Pi_3^T \dot{\xi}(t). \end{aligned}$$

Again, this system contains redundant equations, which we eliminate using the factorization

$$\Pi_3 = \Psi_l \Psi_r^T,$$

where $\Psi_l, \Psi_r \in \mathbb{R}^{n_\xi \times r}$, $\Psi_r^T \Psi_l = I_r$, and $r = \text{rank}(\Pi_3)$. Then, the projected system (without redundant equations) is

$$\begin{aligned} \Psi_r^T M \Psi_r \ddot{\tilde{\xi}}(t) &= \Psi_r^T D \Psi_r \dot{\tilde{\xi}}(t) + \Psi_r^T K \Psi_r \tilde{\xi}(t) + \Psi_r^T B_\xi u(t), \\ y(t) &= C_1 \Psi_r \tilde{\xi}(t) + C_2 \Psi_r \dot{\tilde{\xi}}(t), \end{aligned}$$

where $\tilde{\xi}(t) = \Psi_l^T \xi(t)$ and therefore also $\dot{\tilde{\xi}}(t) = \Psi_l^T \dot{\xi}(t)$ and $\ddot{\tilde{\xi}}(t) = \Psi_l^T \ddot{\xi}(t)$.

Similarly to (16), the desired one-sided projector $\Pi \in \mathbb{R}^{2n_\xi \times 2n_\xi}$ for application in (3) attains the form

$$\Pi = \begin{bmatrix} \Pi_3 & 0 \\ 0 & \Pi_3 \end{bmatrix}.$$

3.3 Formulation of the Projection-Avoiding BT Algorithms

The main contribution in Heinkenschloss et al. (2008); Gugercin et al. (2013) is to show how the MOR can be carried out without explicitly forming the projected systems or the projection operators. In the formulation of the ADI in Algorithm 1 a few additional algorithmic subtleties arise that will be addressed in this section.

Initialization of Residual Factors In the formulation of the LR-ADI in Algorithm 1, we initialize the residual simply by assigning the right hand side factor $W_0 = B$. In the framework of Section 2.2 this becomes the projected right hand side factor $W_0 = \Pi B_v$. It is an easy task to check that in fact $\Theta = E^{-1} \Pi B_v$ solves the saddle point system

$$\begin{bmatrix} E & G^T \\ G & 0 \end{bmatrix} \begin{bmatrix} \Theta \\ \Lambda \end{bmatrix} = \begin{bmatrix} B_v \\ 0 \end{bmatrix}, \quad (18)$$

and thus the initial residual is $W_0 = E\Theta$ and can be computed without explicit usage of Π . After this initialization the update formula can be used without additional treatment since the updates are already projected by construction and thus all subsequent residual factors will automatically be invariant under projection with Π . This is obviously possible in the index-2 case introduced in Section 3.1. In Gugercin et al. (2013) one of the contributions is to show that the symmetry with respect to G in Heinkenschloss et al. (2008) is in fact not necessary. Thus, observing that the index-3 model in (3) is just the non-symmetric variant, we can do the same here.

ADI Shift Parameter Computation For fast convergence, Algorithm 1 relies on shift parameters that are often taken as a subset of eigenvalue approximations of the matrix pencil $\lambda E - A$. The matrix pencil $\lambda \begin{bmatrix} E & 0 \\ 0 & 0 \end{bmatrix} - \begin{bmatrix} A & G^T \\ G & 0 \end{bmatrix}$ in (9) has $2n_\mu$ infinite eigenvalues. Therefore, direct usage of Arnoldi’s method for the approximation of large magnitude eigenvalues is not possible. However, we can employ the strategy introduced in Cliffe et al. (1994) looking at the modified matrix pencil $\lambda \begin{bmatrix} E & \alpha G^T \\ \alpha G & 0 \end{bmatrix} - \begin{bmatrix} A & G^T \\ G & 0 \end{bmatrix}$ which moves all infinite eigenvalues to $\frac{1}{\alpha}$ ($\alpha \in \mathbb{R}$) and keeps the finite ones untouched. Although the original paper states the theorem (Cliffe et al., 1994, Theorem 3.1) only for the case $G = H$, the result also holds for G, H as in (17). This is due to the fact that by swapping the first two block columns in the matrices in (3) we obtain an equivalent matrix pencil, which provides exactly the same structure as in the index-2 case.

Now, first computing approximations to the small magnitude eigenvalues and choosing $\frac{1}{\alpha}$ close to them, enables the use of Arnoldi’s method with the modified pencil. Only, the matrix \mathcal{A}_2 in (2) is always singular and thus (Eich-Soellner and Führer, 1998, Theorem 2.7.3)¹ must be used to identify the nonzero finite spectra of the pencils $\lambda \mathcal{E} - \mathcal{A}_2$ and $\lambda \mathcal{E} - \mathcal{A}_3$ and, thus, always use \mathcal{A}_3 for the small magnitude eigenvalue computations. Note that $\mathcal{P}(\alpha) = \mathcal{A}_2 + \alpha \mathcal{E}$ is invertible for all $\alpha \neq 0$, although \mathcal{A}_2 is not, such that the linear systems in the actual algorithm are well-posed for all proper choices of α .

4. NUMERICAL RESULTS

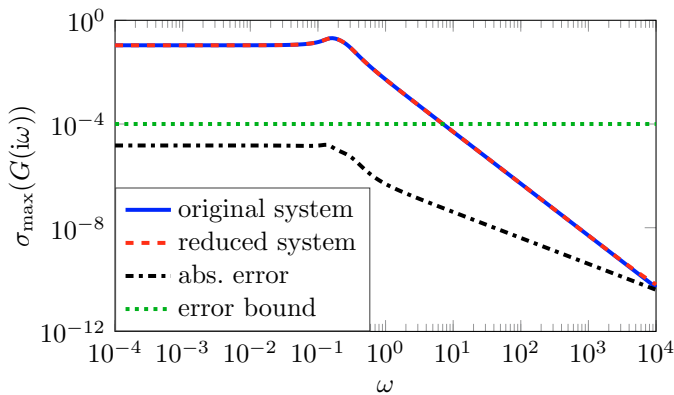


Fig. 1. Sigma plots of the original, reduced, and error systems for Stykel’s example.

In this section we present some computational results of our approach. We have tested it on three benchmark examples on a notebook with one Intel® Core™i7-3517U CPU running at 1.90GHz with 2 cores and 4GB of RAM. The experiments use Ubuntu 16.04.3 LTS, MATLAB® R2016b and M-M.E.S.S.-1.0.1. The experiments will be included as demonstration examples in the next M-M.E.S.S. release. We show the sigma plots of the transfer functions of the original system, the reduced one, and the error system evaluated at frequencies ω . In our plots, $\sigma_{\max}(\cdot)$ refers to the largest singular value of its matrix argument and G

¹ The theorem originates in Simeon et al. (1993) but we prefer the textbook reference.

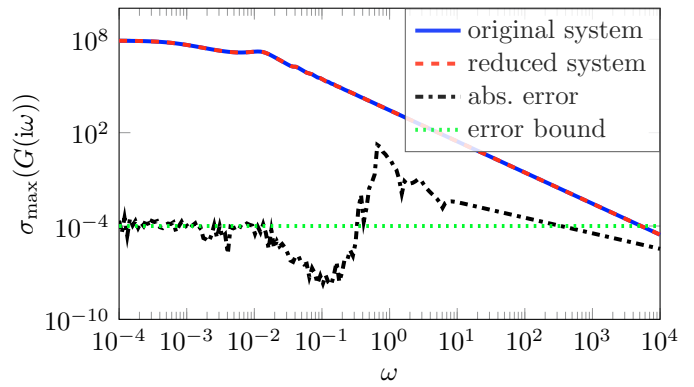


Fig. 2. Sigma plots of the original, reduced, and error systems for the constrained Truhar/Veselić example.

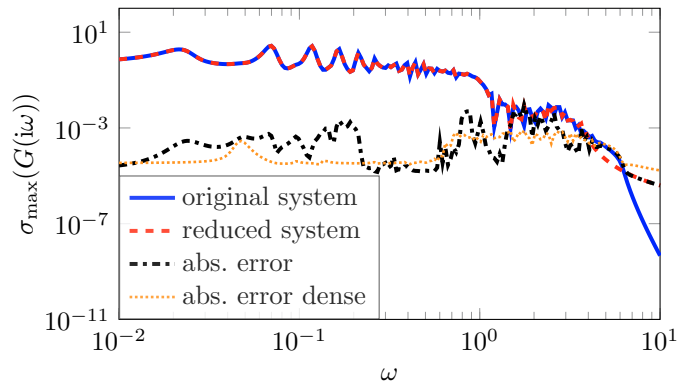


Fig. 3. Sigma plots of the original, reduced, and error systems for our modified Truhar/Veselić example.

denotes any of the transfer functions (Antoulas (2005)) under consideration.

First we consider the system from Mehrmann and Stykel (2005) whose linearization has as a state-space dimension of 12 001 and one input as well as one output. The Gramian factors computed by Algorithm 1 have 33 and 26 columns, respectively. The computation of the Gramian factors and the resulting reduced-order model of order 9 took 1.04 seconds. Figure 1 shows the sigma plots of the transfer functions of the original system and the reduced one, which match very well.

The second example is the triple chain oscillator taken from Truhar and Veselić (2009) with viscosities and internal damping set up as in Saak (2009). Here we consider a version with 1500 masses in each chain and a total system order of 9 008 due to 6 additional constraints. Our constraints rigidly couple the masses number 1 and 750, as well as 751 and 1500 in each chain. The input matrix B_ξ is the column of all ones just like the output matrix C_1 is the row of all ones. The matrix C_2 is chosen as the zero matrix. This simplifies the linearization and thus, the reduced order model (compare (10)). For this example the Gramian factors both have 301 columns, since the maximal iteration number is reached, i. e., the factors have not fully converged. Also the error bound inherits this inexactness, since it needs to be evaluated with respect to these approximate factors. Further, we prescribe a maximum of 250 for the order of the reduced order model, which is attained here. Therefore, the approximation can

not be expected to be as precise as in the previous example. The computation of the Gramian factors and the reduced model took 5.1 seconds and the still very convincing results can be found in Figure 2.

As the third example we choose an even more challenging version of the second example. In this case, the three chains contain only 151 masses. The remaining setup is as before, but now we only have three constraints coupling masses 1, 76, and 151 in a weighted sum in each chain. The three inputs go to the 5th mass in the first, the 81st mass in the second, and the 146th mass in the third chain, while the outputs are the displacements of the big coupling mass, the last mass in the second chain and 38th mass in the last chain. Together with the low internal damping, this example leads to very bad conditioning for the ADI procedure. The ADI iterations for both Gramian factors hardly converge at all. The normalized residual norms are $\mathcal{O}(10^{-1})$ after 300 iterations, each. However, the reduction results are even better than for the second example as Figure 3 clearly shows. For comparison, this figure also contains the absolute error for the dense reference computation (using `lyapcho1` in MATLAB) with explicit projection. Here, we fixed the reduced order to 300 for both approaches, rather than prescribing an error tolerance.

5. CONCLUSIONS

The results presented in this paper show the feasibility of the M-M.E.S.S. implementation of the implicit index reduction approach for balanced truncation model reduction of constrained mechanical systems.

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