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# A Structured Quasi-Arnoldi procedure for model order reduction of second-order systems

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ABSTRACT

Existing Krylov subspace-based structure-preserving model order reduction methods for the second-order systems proceed in two stages. The first stage is to generate a basis matrix of the underlying Krylov subspace. The second stage is to employ an explicit subspace projection to obtain a reduced-order model with a moment-matching property. An open problem is how to avoid explicit projection so that it will be efficient for truly large scale systems. In addition, it is also desired that a structure-preserving reduced system of order $n$ matches maximum $2n$ moments.

In this paper we propose a new procedure to compute a so-called Structured Quasi-Arnoldi (SQA) decomposition. Once the SQA decomposition is computed, a structure-preserving reduced-order model can be defined immediately from the decomposition without the explicit subspace projection. Furthermore, the reduced model of order $n$ matches maximum $2n$ moments. Numerical examples demonstrate that the transpose-free SQA-based reduced model is compatible with the two-sided structure-preserving explicit projection methods and is more accurate than the one-sided structure-preserving explicit projection methods due to the higher number of matched moments.



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## 1. Introduction

A continuous time-invariant single-input single-output second-order system of state dimension $N$ is described by

$$\Sigma_N \ : \ \begin{cases} \mathbf{M}\ddot{\mathbf{x}}(t) + \mathbf{D}\dot{\mathbf{x}}(t) + \mathbf{K}\mathbf{x}(t) = \mathbf{r}u(t), \\ y(t) = \mathbf{w}^\top \dot{\mathbf{x}}(t) + \mathbf{v}^\top \mathbf{x}(t), \end{cases} \tag{1.1}$$

with initial conditions $\mathbf{x}(0) = \mathbf{x}_0$ and $\dot{\mathbf{x}}(0) = \dot{\mathbf{x}}_0$. Here coefficient matrices $\mathbf{M}$, $\mathbf{D}$ and $\mathbf{K} \in \mathbb{R}^{N\times N}$ represent the underlying physical systems, such as mass, damping and stiffness in structural dynamics. The vector $\mathbf{x}(t) \in \mathbb{R}^N$ is the state variables, and $\dot{\mathbf{x}}(t)$ represents differentiation with respect to time $t$. Scalar functions $u(t)$ and $y(t)$ are the input force and output measurement, respectively. The vector $\mathbf{r} \in \mathbb{R}^N$ is the input distribution, and vectors $\mathbf{w}, \mathbf{v} \in \mathbb{R}^N$ are the output measurements.

The second-order systems of the form (1.1) arise from a wide variety of applications, such as structural mechanical systems, circuit simulation, microelectronic mechanical systems and computational electromagnetics [5,1,25,11,26,20,16]. In practice, it is often that the state-space dimension $N$ is too large to allow efficient solutions of control or simulation tasks. Therefore, it is desirable to obtain a reduced-order system of much smaller state dimension, which approximates the original model with sufficient accuracy and meanwhile retains essential properties as well. A structure-preserving model order reduction method is to construct a reduced second-order system of the same form

$$\Sigma_n \ : \ \begin{cases} \mathbf{M}_n\ddot{\boldsymbol{\xi}}(t) + \mathbf{D}_n\dot{\boldsymbol{\xi}}(t) + \mathbf{K}_n\boldsymbol{\xi}(t) = \mathbf{r}_n u(t), \\ \eta(t) = \mathbf{w}_n^\top \dot{\boldsymbol{\xi}}(t) + \mathbf{v}_n^\top \boldsymbol{\xi}(t), \end{cases} \tag{1.2}$$

where the state vector $\boldsymbol{\xi}(t)$ is of dimension $n$, which is typically $n \ll N$, the coefficient matrices $\mathbf{M}_n, \mathbf{D}_n, \mathbf{K}_n \in \mathbb{R}^{n\times n}$ and the vectors $\mathbf{r}_n, \mathbf{w}_n, \mathbf{v}_n \in \mathbb{R}^n$. The output function $\eta(t)$ is a sufficient approximation of the original output function $y(t)$.

In recent years, there has been a lot of progress in structure-preserving model order reduction methods for the structured systems, see for examples [21,9,7,3,19,4,6,17]. In particular, a class of methods for the second-order systems is to first generate an orthonormal basis $\mathbf{V}_n$ of a so-called second-order Krylov subspace, and then explicitly project the original system to the subspace to obtain a reduced-order system, namely the coefficient matrices of reduced system is defined by $(\mathbf{M}_n, \mathbf{D}_n, \mathbf{K}_n) = \mathbf{V}_n^\top(\mathbf{M}, \mathbf{D}, \mathbf{K})\mathbf{V}_n$ via explicit matrix–matrix multiplications. The first such kind of methods is proposed in [24]. Recent studies are reported in [3,13] under the names of Second-Order ARnoldi (SOAR) method and Quadratic Arnoldi (Q-Arnoldi) method. The reduced model of order $n$ generated via these one-sided projection methods matches only $n$ moments. To increase the number of matched moments, both left and right second-order Krylov subspaces can be used to lead a Two-Sided Second-Order Arnoldi (TS-SOAR) method [19]. In the TS-SOAR method, one first generates left and right basis matrices $\mathbf{W}_n$ and $\mathbf{V}_n$, respectively, and then constructs the reduced model by a two-sided explicit projection $(\mathbf{M}_n, \mathbf{D}_n, \mathbf{K}_n) = \mathbf{W}_n^\top(\mathbf{M}, \mathbf{D}, \mathbf{K})\mathbf{V}_n$ to match $2n$ moments. We note that for computing the left Krylov subspace, the operations of the transpose matrix–vector products must be available. Another class of methods is to first generate an orthonormal basis of the Krylov subspace corresponding to the equivalent linear system of $\Sigma_N$, and then use some suitable partitioning of the basis matrix to perform explicit subspace projection to obtain a structure-preserving reduced-order model [9,10].

All these methods proceed in two stages. The second stage is to perform explicit subspace projection, i.e., matrix–matrix multiplications, using the projection basis matrices generated from the first stage. It could be prohibitively expensive in the memory and floating point arithmetic costs for truly large scale systems. In this paper we propose a procedure to compute a Structured Quasi-Arnoldi (SQA) decomposition. Once the SQA decomposition is computed, a structure-preserving reduced-order model can be defined immediately from the decomposition without the need of explicit subspace projection. In terms of the moment-matching property, the transpose-free SQA model is equivalent to the TS-SOAR method such that the reduced model of order $n$ matches maximum $2n$ moments. Numerical examples demonstrate the SQA-based reduced model is compatible with the TS-SOAR and benefits in accuracy due to the higher number of moments that are matched than the one-sided SOAR method. We should also note that there are other methods that also avoid explicit projection, such as the data-driven model order reduction approach proposed in [12].

The rest of this paper is organized as follows. In Section 2, we review the definitions of transfer function and moment of the second-order system $\Sigma_N$ and describe the goals of structure-preserving model order reduction. In Section 3, we introduce the SQA decomposition and derive a procedure to compute the SQA decomposition. In Section 4, we define the reduced-order model $\Sigma_n$ via the SQA decomposition. Numerical examples and concluding remarks are in Sections 5 and 6, respectively.

Throughout this paper, we follow the conventional notations commonly used in matrix computations. We use boldface capital letters to denote the matrices, boldface lower case letters for vectors, $\mathbf{0}$ for zero vector or matrix, $\mathbf{I}_k$ for the $k \times k$ identity matrix, $\mathbf{e}_j$ for the $j$th column of $\mathbf{I}_k$. $\mathbf{X}^\top$ is the transpose of matrix $\mathbf{X}$. $\|\cdot\|_p$ is the matrix or vector $p$-norm. $\mathbf{v}(i:j)$ denotes the subvector of the vector $\mathbf{v}$ that contains the $i$th to the $j$th entries of $\mathbf{v}$. $\mathbf{G}(i:j, k:\ell)$ denotes the submatrix of the matrix $\mathbf{G}$ that consists of the intersection of the rows $i$ to $j$ and the columns $k$ to $\ell$. The notation $\mathcal{K}_n(\mathbf{A};\mathbf{b})$ stands for the $n$th Krylov subspace introduced by $\mathbf{A}$ and $\mathbf{b}$, i.e., $\mathcal{K}_n(\mathbf{A};\mathbf{b}) = \text{span}\{\mathbf{b}, \mathbf{Ab}, \mathbf{A}^2\mathbf{b}, \ldots, \mathbf{A}^{n-1}\mathbf{b}\}$.

## 2. Second-order systems and MOR

Let us begin with an equivalent first-order form of the second-order system $\Sigma_N$ defined in (1.1):

$$\begin{cases} \mathbf{C}\,\dot{\mathbf{q}}(t) + \mathbf{G}\,\mathbf{q}(t) = \mathbf{b}\,u(t), \\ y(t) = \mathbf{l}^\top \mathbf{q}(t), \end{cases} \tag{2.1}$$

where

$$\mathbf{C} = \begin{bmatrix} \mathbf{D} & \mathbf{M} \\ -\mathbf{I} & \mathbf{0} \end{bmatrix}, \quad \mathbf{G} = \begin{bmatrix} \mathbf{K} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{bmatrix}, \quad \mathbf{q}(t) = \begin{bmatrix} \mathbf{x}(t) \\ \dot{\mathbf{x}}(t) \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} \mathbf{r} \\ \mathbf{0} \end{bmatrix}, \quad \mathbf{l} = \begin{bmatrix} \mathbf{v} \\ \mathbf{w} \end{bmatrix}.$$

Assuming that $\mathbf{K}$ is nonsingular, then the first-order form (2.1) can be written as

$$\begin{cases} \mathbf{A}\dot{\mathbf{q}}(t) + \mathbf{q}(t) = \mathbf{b}_0 u(t) \\ y(t) = \mathbf{l}^\top \mathbf{q}(t), \end{cases} \tag{2.2}$$

where $\mathbf{A} = \mathbf{G}^{-1}\mathbf{C}$ and $\mathbf{b}_0 = \mathbf{G}^{-1}\mathbf{b}$. The transfer function of the second-order system (1.1), or equivalently the first-order forms (2.1) and (2.2), is given by

$$\begin{aligned} h(s) &= (s\mathbf{w}^\top + \mathbf{v}^\top)(s^2\mathbf{M} + s\mathbf{D} + \mathbf{K})^{-1}\mathbf{r} \\ &= \mathbf{l}^\top(s\mathbf{C} + \mathbf{G})^{-1}\mathbf{b} \\ &= \mathbf{l}^\top(\mathbf{I} + s\mathbf{A})^{-1}\mathbf{b}_0, \end{aligned}$$

where it is assumed that we have homogeneous initial conditions $\mathbf{x}(0) = \mathbf{0}$, $\dot{\mathbf{x}}(0) = \mathbf{0}$ and $u(0) = 0$. The power series expansion of $h(s)$ at $s = 0$ is given by

$$h(s) = \sum_{i=0}^{\infty} m_i s^i,$$

where $m_i = (-1)^i \mathbf{l}^\top \mathbf{A}^i \mathbf{b}_0$ are referred to as the *moments* of the system $\Sigma_N$.

A popular model order reduction technique is to use subspace projection. Roughly speaking, the subspace projection approach is to first compute a basis matrix $\mathbf{X}_{2n}$ of a projection subspace $\mathcal{K}$. Then by approximating the state vector $\mathbf{q}(t)$ by $\mathbf{X}_{2n}\mathbf{z}(t)$:

$$\mathbf{q}(t) \approx \mathbf{X}_{2n}\mathbf{z}(t) \quad \text{for some } \mathbf{z}(t) \in \mathbb{R}^{2n},$$

it yields the following over-determined linear system

$$\begin{cases} \mathbf{A}\mathbf{X}_{2n}\dot{\mathbf{z}}(t) + \mathbf{X}_{2n}\mathbf{z}(t) = \mathbf{b}_0 u(t) \\ \eta(t) = \mathbf{l}^\top \mathbf{X}_{2n}\mathbf{z}(t). \end{cases} \tag{2.3}$$

After multiplying the first equation of (2.3) from the left by $\mathbf{Y}_{2n}^\top$, where $\mathbf{Y}_{2n} \in \mathbb{R}^{2N\times 2n}$ of full column rank, we obtain a reduced-order system

$$\begin{cases} \mathbf{Y}_{2n}^\top\mathbf{A}\mathbf{X}_{2n}\dot{\mathbf{z}}(t) + \mathbf{Y}_{2n}^\top\mathbf{X}_{2n}\mathbf{z}(t) = \mathbf{Y}_{2n}^\top\mathbf{b}_0 u(t) \\ \eta(t) = \mathbf{l}^\top \mathbf{X}_{2n}\mathbf{z}(t). \end{cases} \tag{2.4}$$

The goal of a structure-preserving reduced-order method is to choose proper right and left projectors $\mathbf{X}_{2n}$ and $\mathbf{Y}_{2n}$ such that the reduced model (2.4) can be recast in the second-order form $\Sigma_n$ (1.2). One way to achieve this goal is to preserve the $2 \times 2$ block structure of $\mathbf{A}$ in the two-sided projection $\mathbf{Y}_{2n}^\top\mathbf{A}\mathbf{X}_{2n}$. Specifically, we want to choose $\mathbf{X}_{2n}$ and $\mathbf{Y}_{2n}$ satisfying the following properties:

$$\mathbf{Y}_{2n}^\top\mathbf{X}_{2n} = \mathbf{I}_{2n}, \quad \mathbf{Y}_{2n}^\top\mathbf{A}\mathbf{X}_{2n} = \begin{bmatrix} \mathbf{R}_n & \mathbf{S}_n \\ \mathbf{T}_n & \mathbf{0} \end{bmatrix}, \quad \mathbf{Y}_{2n}^\top\mathbf{b}_0 = \begin{bmatrix} \mathbf{r}_n \\ \mathbf{0} \end{bmatrix}, \quad \mathbf{X}_{2n}^\top\mathbf{l} = \begin{bmatrix} \widehat{\mathbf{v}}_n \\ \widehat{\mathbf{w}}_n \end{bmatrix}.$$

Consequently, by the congruence transformation

$$\begin{bmatrix} \mathbf{I}_n & \mathbf{0} \\ \mathbf{0} & -\mathbf{T}_n^{-1} \end{bmatrix} \begin{bmatrix} \mathbf{R}_n & \mathbf{S}_n \\ \mathbf{T}_n & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{I}_n & \mathbf{0} \\ \mathbf{0} & -\mathbf{T}_n \end{bmatrix} = \begin{bmatrix} \mathbf{R}_n & -\mathbf{S}_n\mathbf{T}_n \\ -\mathbf{I}_n & \mathbf{0} \end{bmatrix},$$

the reduced first-order model (2.4) can immediately be rewritten as an equivalent second-order model (1.2) with the coefficient matrices $\mathbf{M}_n = -\mathbf{S}_n\mathbf{T}_n$, $\mathbf{D}_n = \mathbf{R}_n$, and $\mathbf{K}_n = \mathbf{I}_n$. The input vector is $\mathbf{r}_n$ and output vectors are $\mathbf{v}_n = \widehat{\mathbf{v}}_n$ and $\mathbf{w}_n = -\mathbf{T}_n\widehat{\mathbf{w}}_n$.

An additional objective of a proper choice of $\mathbf{X}_{2n}$ and $\mathbf{Y}_{2n}$ is to match as many leading moments as possible, i.e., for as large $q$ as possible, it satisfies

$$m_i = m_i^{(n)} \quad \text{for} \quad i = 0, 1, \ldots, q-1, \tag{2.5}$$

where $m_i^{(n)} = (-1)^i\mathbf{l}^\top\mathbf{X}_{2n}(\mathbf{Y}_{2n}^\top\mathbf{A}\mathbf{X}_{2n})^i\mathbf{Y}_{2n}^\top\mathbf{b}_0$ are the moments of the reduced-system (2.4). The identity (2.5) implies that the reduced system $\Sigma_n$ is an order of $q$ approximation of the original system $\Sigma_N$, namely $h(s) = h_n(s) + O(s^q)$.

## 3. Structured Quasi-Arnoldi decomposition and procedure

Let us define a Structured Quasi-Arnoldi (SQA) decomposition of the following form:

$$\mathbf{A}\mathbf{X}_{2n} = \mathbf{X}_{2n} \begin{bmatrix} \mathbf{R}_n & \mathbf{S}_n \\ \mathbf{T}_n & \mathbf{0} \end{bmatrix} + s_{n+1,n}\mathbf{x}_{2n+1}\mathbf{e}_{2n}^\top, \tag{3.1}$$

where $\mathbf{X}_{2n}$ is an $N \times 2n$ matrix, $\mathbf{x}_{2n+1}$ is a column vector of length $N$, $\mathbf{R}_n$ and $\mathbf{T}_n$ are $n \times n$ upper triangular matrices and $\mathbf{S}_n$ is an $n \times n$ upper Hessenberg matrix. First, we note that the SQA decomposition (3.1) can be compactly expressed as

$$\mathbf{A}\mathbf{X}_{2n} = \mathbf{X}_{2n+1}\widehat{\mathbf{H}}_{2n}, \tag{3.2}$$

where

$$\mathbf{X}_{2n+1} = \begin{bmatrix} \mathbf{X}_{2n} & \mathbf{x}_{2n+1} \end{bmatrix} \quad \text{and} \quad \widehat{\mathbf{H}}_{2n} = \begin{bmatrix} \mathbf{R}_n & \mathbf{S}_n \\ \mathbf{T}_n & \mathbf{0} \\ \mathbf{0} & s_{n+1,n}\mathbf{e}_n^\top \end{bmatrix}.$$

In the following theorem, we show that the subspace spanned by $\mathbf{X}_{2n+1}$ is indeed the Krylov subspace $\mathcal{K}_{2n+1}(\mathbf{A}; \mathbf{x}_1)$, where $\mathbf{x}_1$ is the first column of $\mathbf{X}_{2n+1}$.

**Theorem 3.1.** *Suppose that $\mathbf{X}_{2n+1}$ satisfies the decomposition (3.2), diagonal elements $t_{11}, \ldots, t_{nn}$ of $\mathbf{T}_n$ and the sub-diagonal elements $s_{21}, \ldots, s_{n,n-1}$ of $\mathbf{S}_n$ together with $s_{n+1,n}$ are nonzero, then span$\{\mathbf{X}_{2n}\} = \mathcal{K}_{2n}(\mathbf{A}; \mathbf{x}_1)$ and span$\{\mathbf{X}_{2n+1}\} = \mathcal{K}_{2n+1}(\mathbf{A}; \mathbf{x}_1)$.*

**Proof.** Let us denote the permutations $\mathbf{\Pi}_{2n} \in \mathbb{R}^{2n\times 2n}$ and $\mathbf{\Pi}_{2n+1} \in \mathbb{R}^{(2n+1)\times(2n+1)}$ by

$$\mathbf{\Pi}_{2n} = [\,\mathbf{e}_1, \mathbf{e}_{n+1}, \mathbf{e}_2, \mathbf{e}_{n+2}, \ldots, \mathbf{e}_n, \mathbf{e}_{2n}\,] \quad \text{and} \quad \mathbf{\Pi}_{2n+1} = \begin{bmatrix} \mathbf{\Pi}_{2n} & \mathbf{0} \\ 0 & 1 \end{bmatrix}. \tag{3.3}$$

Note that $\mathbf{\Pi}_{2n}$ is the result of perfectly shuffling the $2n$ column vectors of the identity matrix $\mathbf{I}_{2n}$ [8]. Then by multiplying the structured Arnoldi decomposition (3.2) from the right by $\mathbf{\Pi}_{2n}$, we obtain

$$\mathbf{A}\mathbf{X}_{2n}\mathbf{\Pi}_{2n} = \mathbf{X}_{2n+1}\mathbf{\Pi}_{2n+1}\widetilde{\mathbf{H}}_{2n}, \tag{3.4}$$

where $\widetilde{\mathbf{H}}_{2n} = \mathbf{\Pi}_{2n+1}^\top \widehat{\mathbf{H}}_{2n}\mathbf{\Pi}_{2n}$. Note that $\mathbf{\Pi}_{2n+1}\mathbf{\Pi}_{2n+1}^\top = \mathbf{I}_{2n+1}$.

It is easy to verify that the matrix $\widetilde{\mathbf{H}}_{2n}$ is an upper Hessenberg matrix with sub-diagonal elements $t_{11}, s_{21}, t_{22}, s_{32}, \ldots, t_{nn}, s_{n+1,n}$. Hence the decomposition (3.4) is a Krylov-type decomposition [23]. Furthermore, note that $\widetilde{\mathbf{H}}_{2n}$ is an unreduced upper Hessenberg matrix. Since the first column of $\mathbf{X}_{2n}\mathbf{\Pi}_{2n}$ is $\mathbf{x}_1$ and the sub-diagonal elements of $\widetilde{\mathbf{H}}_{2n}$ are nonzero, by [2, Lemma 2.2], we conclude that the columns of $\mathbf{X}_{2n}$ and $\mathbf{X}_{2n+1}$ span Krylov subspaces $\mathcal{K}_{2n}(\mathbf{A}; \mathbf{x}_1)$ and $\mathcal{K}_{2n+1}(\mathbf{A}; \mathbf{x}_1)$, respectively. □

For ease of reference, let us denote the first $n$ columns of $\mathbf{X}_{2n}$ as $\mathbf{Q}_n$, the trailing $n$ columns as $\mathbf{P}_n$ and $\mathbf{x}_{2n+1} = \mathbf{q}_{n+1}$, i.e., $[\,\mathbf{X}_{2n} \mid \mathbf{x}_{2n+1}\,] = [\,\mathbf{Q}_n\ \mathbf{P}_n \mid \mathbf{q}_{n+1}\,]$. Then the decomposition (3.1) can be written as

$$\mathbf{A}\begin{bmatrix} \mathbf{Q}_n & \mathbf{P}_n \end{bmatrix} = \begin{bmatrix} \mathbf{Q}_n & \mathbf{P}_n \end{bmatrix}\begin{bmatrix} \mathbf{R}_n & \mathbf{S}_n \\ \mathbf{T}_n & \mathbf{0} \end{bmatrix} + s_{n+1,n}\mathbf{q}_{n+1}\mathbf{e}_{2n}^\top. \tag{3.5}$$

There are a number of ways to impose the orthogonality among the vectors of $\mathbf{Q}_{n+1} = [\,\mathbf{Q}_n\, \mathbf{q}_{n+1}\,]$ and $\mathbf{P}_n$. Here we impose that $\mathbf{Q}_{n+1}$ and $\mathbf{P}_n$ satisfy the following three conditions:

$$\text{(a)}\, \mathbf{Q}_{n+1}^\top \mathbf{Q}_{n+1} = \mathbf{I}_{n+1}, \quad \text{(b)}\, \mathbf{P}_n^\top \mathbf{P}_n = \mathbf{I}_n, \quad \text{(c)}\, \mathbf{p}_i^\top \mathbf{q}_j = 0 \quad \text{for} \quad i \geqslant j. \tag{3.6}$$

Note that condition (c) of (3.6) is equivalent to $\mathbf{P}_n^\top \mathbf{Q}_n$ being strictly upper triangular.

The motivation of imposing orthogonality conditions (3.6) is illustrated as follows. In the Krylov decomposition (3.4), the upper Hessenberg matrix $\widetilde{\mathbf{H}}_{2n}$ has less nonzeros than the upper Hessenberg matrix in the standard Arnoldi decomposition of order $2n$. Consequently we will not expect to have an orthogonal matrix $\mathbf{X}_{2n}\mathbf{\Pi}_{2n} = [\,\mathbf{Q}_n\, \mathbf{P}_n\,]\mathbf{\Pi}_{2n} = [\,\mathbf{q}_1, \mathbf{p}_1, \ldots, \mathbf{q}_n, \mathbf{p}_n\,]$. Instead we first impose the orthogonality conditions in the $\mathbf{q}_i's$ vectors and the $\mathbf{p}_i's$ vectors, respectively, i.e., conditions (a) and (b) of (3.6). Subsequently, we explore the orthogonal relation between $\mathbf{q}_i's$ and $\mathbf{p}_i's$ vectors in condition (c) of (3.6). The geometric interpretation of the conditions (b) and (c) of (3.6) is that $\mathbf{p}_j$ is perpendicular to the subspace spanned by its preceding vectors, i.e., span$\{\mathbf{q}_1, \mathbf{p}_1, \mathbf{q}_2, \mathbf{p}_2, \ldots, \mathbf{q}_j\}$. Thus if the columns of $[\,\mathbf{Q}_j\, \mathbf{P}_{j-1}\,]$ are linearly independent, then the columns of $[\,\mathbf{Q}_j\, \mathbf{P}_j\,]$ are linearly independent as well.

We now derive a procedure to compute the SQA decomposition (3.5) with the orthogonality conditions (3.6). We essentially apply a partial Gram–Schmidt procedure in an alternating fashion. Let us begin with computing $\mathbf{p}_1$ and $\mathbf{q}_2$. By equating the first column of (3.5), we have

$$\mathbf{A}\mathbf{q}_1 = \mathbf{q}_1 r_{11} + \mathbf{p}_1 t_{11},$$

where $r_{11}$, $t_{11}$ and $\mathbf{p}_1$ are to be determined. Let $\mathbf{f} = \mathbf{A}\mathbf{q}_1 - \mathbf{q}_1 r_{11}$. Then it is easy to see that if $r_{11} = \mathbf{q}_1^\top \mathbf{A}\mathbf{q}_1$, $\mathbf{f}$ is a projection of $\mathbf{A}\mathbf{q}_1$ onto the orthogonal complement of span$\{\mathbf{q}_1\}$. If $t_{11} = \|\mathbf{f}\|_2 \neq 0$, then $\mathbf{p}_1 = \mathbf{f}/t_{11}$. If $t_{11} = 0$, then the procedure terminates, and is referred to as the *case-A breakdown*. In this case, the subspace span$\{\mathbf{q}_1\} = \mathcal{K}_1(\mathbf{A}; \mathbf{q}_1)$ is an invariant subspace of $\mathbf{A}$.

To compute the vector $\mathbf{q}_2$, by equating the $n+1$ columns of (3.5), we have

$$\mathbf{A}\mathbf{p}_1 = \mathbf{q}_1 s_{11} + \mathbf{q}_2 s_{21},$$

where $s_{11}$, $s_{21}$ and $\mathbf{q}_2$ are to be determined. Let $\mathbf{g} = \mathbf{A}\mathbf{p}_1 - \mathbf{q}_1 s_{11}$. Then if $s_{11} = \mathbf{q}_1^\top \mathbf{A}\mathbf{p}_1$, the vector $\mathbf{g} = (\mathbf{I} - \mathbf{q}_1\mathbf{q}_1^\top)\mathbf{A}\mathbf{p}_1$ is a projection of $\mathbf{A}\mathbf{p}_1$ onto span$\{\mathbf{q}_1\}^\perp$. If $s_{21} = \|\mathbf{g}\|_2 \neq 0$, then $\mathbf{q}_2 = \mathbf{g}/s_{21}$ and $\mathbf{Q}_2^\top \mathbf{Q}_2 = \mathbf{I}_2$. If $s_{21} = 0$, then the procedure terminates. This is referred to as the *case-B breakdown*. In this case, we have $\mathbf{A}\mathbf{p}_1 = \mathbf{q}_1 s_{11}$, which yields that $\mathbf{A}^2\mathbf{q}_1 \in$ span$\{\mathbf{q}_1, \mathbf{p}_1\}$ and the subspace span$\{\mathbf{q}_1, \ \mathbf{p}_1\} = \mathcal{K}_2(\mathbf{A}; \mathbf{q}_1)$ is an invariant subspace.

**Remark 3.1.** We note that even if $s_{21} \neq 0$, the basis matrix $\mathbf{X}_3 = [\,\mathbf{q}_1, \mathbf{p}_1, \mathbf{q}_2\,]$ could still be rank deficient. For instance, the columns of $\mathbf{X}_3 = [\,\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_2\,]$ generated by

$$\mathbf{A} = \begin{bmatrix} 1 & 0 \\ 1 & 1 \end{bmatrix} \quad \text{and} \quad \mathbf{q}_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

are linearly dependent. This will cause a breakdown when we proceed to compute $\mathbf{p}_2$. It will be referred to as the *case-C breakdown*.

In general, let us assume we have computed the SQA decomposition (3.5) of order $j-1$ for $j \geqslant 2$. To compute the decomposition (3.5) of order $j$, let us first consider the $j$th column of (3.5):

$$\mathbf{A}\mathbf{q}_j = \mathbf{q}_1 r_{1j} + \cdots + \mathbf{q}_j r_{jj} + \mathbf{p}_1 t_{1j} + \cdots + \mathbf{p}_j t_{jj},$$

where $r_{1j}, \ldots, r_{jj}, t_{1j}, \ldots, t_{jj}$ and $\mathbf{p}_j$ are to be determined. Since the first column $\mathbf{q}_1$ of $\mathbf{X}_{2j-1} = [\,\mathbf{Q}_{j-1}\ \mathbf{P}_{j-1}\ \mathbf{q}_j\,]$ is orthogonal to the rest of the columns of $\mathbf{X}_{2j-1}$, we have $r_{1j} = \mathbf{q}_1^\top \mathbf{A}\mathbf{q}_j$. Let

$$\mathbf{f} = \widehat{\mathbf{f}} - \mathbf{X}_{2j-1}(:, 2:2j-1)\mathbf{d}_*,$$

where $\widehat{\mathbf{f}} = \mathbf{A}\mathbf{q}_j - \mathbf{q}_1 r_{1j}$, $\mathbf{d}_* = [\,\check{\mathbf{r}}_j^\top,\ \tilde{\mathbf{t}}_j^\top,\ r_{jj}\,]^\top$, $\check{\mathbf{r}}_j^\top = [\,r_{2j}, \ldots, r_{j-1,j}\,]$ and $\tilde{\mathbf{t}}_j^\top = [\,t_{1j}, \ldots, t_{j-1,j}\,]$. Then we need to determine the vector $\mathbf{d}_*$ such that $\mathbf{f}$ is a projection of $\mathbf{A}\mathbf{q}_j$ onto the orthogonal complement of span$\{\mathbf{X}_{2j-1}\}$. There are two possible cases, namely, $\mathbf{X}_{2j-1}(:, 2:2j-1)$ is of full column rank or rank deficient. If $\mathbf{X}_{2j-1}(:, 2:2j-1)$ is of full rank, then

$$\mathbf{d}_* = \mathbf{X}_{2j-1}^\dagger(:, 2:2j-1)\widehat{\mathbf{f}}, \tag{3.7}$$

where $\mathbf{X}^\dagger$ is the pseudoinverse of $\mathbf{X}$; $\mathbf{X}^\dagger = (\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top$, see for example [22, p. 252]. Subsequently, if $t_{jj} = \|\mathbf{f}\|_2 \neq 0$, then we have $\mathbf{p}_j = \mathbf{f}/t_{jj}$. If $t_{jj} = 0$, then we have the case-A breakdown, and have computed the decomposition

$$\mathbf{A}\mathbf{X}_{2j-1} = \mathbf{X}_{2j-1} \begin{bmatrix} \mathbf{R}_j & \widehat{\mathbf{S}}_j \\ \widehat{\mathbf{T}}_j & \mathbf{0} \end{bmatrix}, \tag{3.8}$$

where $\mathbf{R}_j$ is $j \times j$ upper triangular, $\widehat{\mathbf{S}}_j$ is $j \times (j-1)$ upper triangular and $\widehat{\mathbf{T}}_j$ is $(j-1) \times j$ upper triangular. Since $\mathbf{A}\mathbf{q}_j \in \text{span}\{\mathbf{X}_{2j-1}\}$, the subspace $\text{span}\{\mathbf{X}_{2j-1}\} = \mathcal{K}_{2j-1}(\mathbf{A}; \mathbf{q}_1)$ is an invariant subspace of $\mathbf{A}$.

If $\mathbf{X}_{2j-1}(:, 2:2j-1)$ is rank deficient, the SQA procedure terminates. This is referred to as the *case-C breakdown*. In this case, $\mathbf{X}_{2j-1}$ must also be rank deficient due to the fact that $\mathbf{q}_1 = \mathbf{X}_{2j-1}\mathbf{e}_1$ is known to be orthogonal to $\mathbf{X}_{2j-1}(:, 2:2j-1)$. Since $\mathbf{X}_{2j-1}$ is rank deficient, $\mathbf{A}\mathbf{q}_j \in \text{span}\{\mathbf{X}_{2j-1}\} = \text{span}\{\mathbf{X}_{2j-2}\}$. Therefore the subspace $\text{span}\{\mathbf{X}_{2j-2}\} = \mathcal{K}_{2j-2}(\mathbf{A}; \mathbf{q}_1)$ is an invariant subspace. The matrix $\mathbf{X}_{2j-1}$ and the vector $\mathbf{q}_j$ satisfy the following decomposition:

$$\mathbf{A}\mathbf{X}_{2j-2} = \mathbf{X}_{2j-2} \begin{bmatrix} \mathbf{R}_{j-1} & \mathbf{S}_{j-1} \\ \mathbf{T}_{j-1} & \mathbf{0} \end{bmatrix} + s_{j,j-1}\mathbf{q}_j\mathbf{e}_{2j-2}^{\top}. \tag{3.9}$$

Now let us turn to the second part of computing the SQA decomposition (3.5) of order $j$, namely compute the $j$th column of $\mathbf{S}_n$ and the vector $\mathbf{q}_{j+1}$ in (3.5). By equating the $2j$th column of (3.5), we have

$$\mathbf{A}\mathbf{p}_j = \mathbf{q}_1 s_{1j} + \cdots + \mathbf{q}_j s_{jj} + \mathbf{q}_{j+1} s_{j+1,j} = \mathbf{Q}_j\mathbf{s}_j + \mathbf{q}_{j+1} s_{j+1,j},$$

where $\mathbf{s}_j = [\, s_{1j}, \ \ldots, \ s_{jj} \,]^{\top}$ and $\mathbf{q}_{j+1}$ are to be determined. Let $\mathbf{g} = \mathbf{A}\mathbf{p}_j - \mathbf{Q}_j\mathbf{s}_j$, then if $\mathbf{s}_j = \mathbf{Q}_j^{\top}\mathbf{A}\mathbf{p}_j$, $\mathbf{g}$ is a projection of $\mathbf{A}\mathbf{p}_j$ onto the orthogonal complement of $\text{span}\{\mathbf{Q}_j\}$. If $s_{j+1,j} = \|\mathbf{g}\|_2 \neq 0$, then $\mathbf{q}_{j+1} = \mathbf{g}/s_{j+1,j}$. If $s_{j+1,j} = 0$, then we have the case-B breakdown and have computed the decomposition

$$\mathbf{A}\mathbf{X}_{2j} = \mathbf{X}_{2j} \begin{bmatrix} \mathbf{R}_j & \mathbf{S}_j \\ \mathbf{T}_j & \mathbf{0} \end{bmatrix}, \tag{3.10}$$

since $\mathbf{A}\mathbf{p}_j \in \text{span}\{\mathbf{Q}_j\}$ and the subspace $\text{span}\{\mathbf{X}_{2j}\} = \mathcal{K}_{2j}(\mathbf{A}; \mathbf{q}_1)$ is an invariant subspace.

This completes the derivation of the procedure to compute the SQA decomposition (3.5). Before presenting a pseudocode for the complete algorithm, two remarks are in order.

**Remark 3.2.** The main computational cost of the procedure is to compute the vector $\mathbf{d}_*$ defined in (3.7) and determine whether the basis matrix $\mathbf{X}_{2j-1}(:, 2:2j-1)$ is of full column rank. Note that the vector $\mathbf{d}_*$ is the solution of the least squares (LS) problem:

$$\mathbf{d}_* = \text{argmin}_{\mathbf{d}} \left\| \widehat{\mathbf{f}} - \mathbf{X}_{2j-1}(:, 2:2j-1)\mathbf{d} \right\|_2. \tag{3.11}$$

A stable method described in [22, p. 297] to solve the problem (3.11) is to first compute the following QR factorization of an augmented LS matrix:

$$\begin{bmatrix} \mathbf{X}_{2j-1}(:, 2:2j-1) & \widehat{\mathbf{f}} \end{bmatrix} = \begin{bmatrix} \mathbf{Q} & \mathbf{q} \end{bmatrix} \begin{bmatrix} \mathbf{R} & \mathbf{r} \\ \mathbf{0} & \rho \end{bmatrix}. \tag{3.12}$$

If $\mathbf{R}$ is nonsingular, then $\mathbf{X}_{2j-1}(:, 2:2j-1)$ is full rank, and the solution vector $\mathbf{d}_*$ is obtained by solving the upper triangular system

$$\mathbf{R}\mathbf{d}_* = \mathbf{r}. \tag{3.13}$$

If $\mathbf{R}$ is singular, then $\mathbf{X}_{2j-1}(:, 2:2j-1)$ is rank deficient. This is the case-C breakdown.

**Remark 3.3.** There is an efficient solver for the LS problem (3.11) by updating the QR factorization (3.12) from steps $j$ to $j+1$. It is based on the relation

$$\widetilde{\mathbf{X}}_{2j-1} = \begin{bmatrix} \widetilde{\mathbf{X}}_{2j-3} & \mathbf{p}_{j-1} & \mathbf{q}_j \end{bmatrix}, \tag{3.14}$$

where $\widetilde{\mathbf{X}}_{2j-1} = \mathbf{X}_{2j-1}\mathbf{\Pi}_{2j-1}$ and $\widetilde{\mathbf{X}}_{2j-3} = \mathbf{X}_{2j-3}\mathbf{\Pi}_{2j-3}$. Permutations $\mathbf{\Pi}_{2j-1}$ and $\mathbf{\Pi}_{2j-3}$ are defined by $\mathbf{\Pi}_{2j-1} = \begin{bmatrix} \mathbf{\Pi}_{2j-2} & \mathbf{0} \\ 0 & 1 \end{bmatrix}$ and $\mathbf{\Pi}_{2j-3} = \begin{bmatrix} \mathbf{\Pi}_{2j-4} & \mathbf{0} \\ 0 & 1 \end{bmatrix}$ with the perfect shuffles $\mathbf{\Pi}_{2j-2}$ and $\mathbf{\Pi}_{2j-4}$ defined in (3.3). By the identity (3.14), we know that the $Q$-factor of the QR factorization of $\widetilde{\mathbf{X}}_{2j-3}(:, 2:2j-3)$ is the first $2j-4$ columns of the $Q$-factor of the QR factorization of $\widetilde{\mathbf{X}}_{2j-1}(:, 2:2j-1)$. Note that the first columns of $\widetilde{\mathbf{X}}_{2j-1}$ and $\widetilde{\mathbf{X}}_{2j-3}$ are the same. Hence we can rewrite the LS problem (3.11) as

$$\mathbf{d}_* = \operatorname{argmin}_{\mathbf{h}} \left\| \widehat{\mathbf{f}} - \widetilde{\mathbf{X}}_{2j-1}(:, 2:2j-1)\widetilde{\mathbf{\Pi}}_{2j-2}^{\top}\mathbf{h} \right\|_2, \tag{3.15}$$

where $\widetilde{\mathbf{\Pi}}_{2j-2} = [\, \mathbf{e}_{j-1},\ \mathbf{e}_1, \mathbf{e}_j,\ \mathbf{e}_2, \ldots, \mathbf{e}_{2j-3}, \mathbf{e}_{2j-2} \,]$. To solve the LS problem (3.15), we first compute a QR factorization of the augmented LS matrix

$$\left[\widetilde{\mathbf{X}}_{2j-1}(:, 2:2j-1)\ \widehat{\mathbf{f}}\right] = \left[\mathbf{Q}\ \ \mathbf{q}\right]\begin{bmatrix} \mathbf{R} & \mathbf{r} \\ \mathbf{0} & \rho \end{bmatrix} \tag{3.16}$$

and then solve the triangular linear system

$$\mathbf{R}\widetilde{\mathbf{\Pi}}_{2j-2}^{\top}\mathbf{d}_* = \mathbf{r} \tag{3.17}$$

for $\mathbf{d}_*$ by back substitution and permutation. An advantage of calculating the vector $\mathbf{d}_*$ through (3.16) and (3.17) instead of (3.12) and (3.13) is that we can obtain the QR factorization (3.16) from updating the QR factorization of $\widetilde{\mathbf{X}}_{2j-3}(:, 2{:}2j{-}3)$. An efficient QR updating algorithm can be found in [22, p. 338].

The following pseudocode summarizes the procedure to compute the SQA decomposition (3.5) with the orthogonality conditions (3.6).

**SQA algorithm**

$\widetilde{\mathbf{X}}(:, 1) = \mathbf{b}/\|\mathbf{b}\|_2$,
**for** $j = 1, 2, \ldots, n$ **do**
  $\mathbf{f} = \mathbf{A}\widetilde{\mathbf{X}}(:, 2j-1)$
  $r_{1j} = \widetilde{\mathbf{X}}(:, 1)^{\top}\mathbf{f}$
  $\mathbf{f} := \mathbf{f} - \widetilde{\mathbf{X}}(:, 1)r_{1j}$
  **if** $j \geqslant 2$ **then**
    update the QR factorization $\left[\widetilde{\mathbf{X}}(:, 2:2j-1)\ \mathbf{f}\right] = \left[\mathbf{Q}\ \ \mathbf{q}\right]\begin{bmatrix} \mathbf{R} & \mathbf{r} \\ \mathbf{0} & \rho \end{bmatrix}$
    if $\mathbf{R}$ is singular, stop (case-C breakdown)
    solve $\mathbf{R}\widetilde{\mathbf{\Pi}}_{2j-2}^{\top}\mathbf{d} = \mathbf{r}$ for $\mathbf{d}$, where $\widetilde{\mathbf{\Pi}}_{2j-2} = [\, \mathbf{e}_{j-1},\ \mathbf{e}_1, \mathbf{e}_j,\ \mathbf{e}_2, \ldots, \mathbf{e}_{2j-3}, \mathbf{e}_{2j-2} \,]$.
    $\mathbf{f} := \mathbf{f} - \widetilde{\mathbf{X}}(:, 2:2j-1)\widetilde{\mathbf{\Pi}}_{2j-2}^{\top}\mathbf{d}$
  **end if**
  $t_{jj} = \|\mathbf{f}\|_2$. If $t_{jj} = 0$, stop (case-A breakdown)
  $\widetilde{\mathbf{X}}(:, 2j) = \mathbf{f}/t_{jj}$
  $\mathbf{g} = \mathbf{A}\widetilde{\mathbf{X}}(:, 2j)$
  **for** $i = 1, 2, \ldots, j$ **do**
    $s_{ij} = \widetilde{\mathbf{X}}(:, 2j-1)^{\top}\mathbf{g}$
    $\mathbf{g} := \mathbf{g} - \widetilde{\mathbf{X}}(:, 2j-1)s_{ij}$
  **end for**
  $s_{j+1,j} = \|\mathbf{g}\|_2$. If $s_{j+1,j} = 0$, stop (case-B breakdown)
  $\widetilde{\mathbf{X}}(:, 2j+1) = \mathbf{g}/s_{j+1,j}$
**end for**

By the discussion in Remark 3.3, the QR factorization at line 7 of the algorithm is computed via updating the QR factorization of $\widetilde{\mathbf{X}}_{2j-3}(:, 2:2j-3)$ with appending of the three column vectors $\mathbf{p}_{j-1}$, $\mathbf{q}_j$ and $\mathbf{f}$. To numerically detect the breakdowns, we need to provide a tolerance $\epsilon$ in lines 8, 12 and 19.

## 4. Model reduction based on the SQA procedure

In this section, we construct a reduced second-order system $\Sigma_n$ (1.2) via the SQA decomposition (3.1) computed by the SQA algorithm with

$$\mathbf{A} = \mathbf{G}^{-1}\mathbf{C} = \begin{bmatrix} \mathbf{K}^{-1}\mathbf{D} & \mathbf{K}^{-1}\mathbf{M} \\ -\mathbf{I} & \mathbf{0} \end{bmatrix} \quad \text{and} \quad \mathbf{b}_0 = \mathbf{G}^{-1}\mathbf{b} = \begin{bmatrix} \mathbf{K}^{-1}\mathbf{r} \\ \mathbf{0} \end{bmatrix}.$$

Let us first consider the situation where there is no breakdown. In this case, $\mathbf{X}_{2n+1}$ is of full rank. Define

$$\mathbf{Y}_{2n} = (\mathbf{X}_{2n+1}^{\dagger})^{\top} \begin{bmatrix} \mathbf{I}_{2n} \\ \mathbf{0} \end{bmatrix}.$$

Then it can be verified that $\mathbf{Y}_{2n}$ and $\mathbf{X}_{2n}$ are biorthogonal $\mathbf{Y}_{2n}^{\top}\mathbf{X}_{2n} = \mathbf{I}_{2n}$ and $\mathbf{Y}_{2n}^{\top}\mathbf{q}_{n+1} = \mathbf{0}$. Consequently by the decomposition (3.1), we have

$$\mathbf{Y}_{2n}^{\top}\mathbf{A}\mathbf{X}_{2n} = \begin{bmatrix} \mathbf{R}_n & \mathbf{S}_n \\ \mathbf{T}_n & \mathbf{0} \end{bmatrix}.$$

Furthermore, since $\mathbf{b}_0 = \gamma \mathbf{x}_1$ with $\gamma = \|\mathbf{K}^{-1}\mathbf{r}\|_2$, we have

$$\mathbf{Y}_{2n}^{\top}\mathbf{b}_0 = \mathbf{Y}_{2n}^{\top}(\gamma \mathbf{x}_1) = \gamma \mathbf{Y}_{2n}^{\top}\mathbf{X}_{2n}\mathbf{e}_1 = \gamma \mathbf{e}_1.$$

Finally, for $\mathbf{X}_{2n} = [\,\mathbf{Q}_n\ \mathbf{P}_n\,]$, the matrix–vector multiplication $\mathbf{X}_{2n}^{\top}\mathbf{l}$ has the natural partition

$$\mathbf{X}_{2n}^{\top}\mathbf{l} = \begin{bmatrix} \mathbf{Q}_n^{\top}\mathbf{l} \\ \mathbf{P}_n^{\top}\mathbf{l} \end{bmatrix}.$$

Following the projection framework presented in Section 2, we immediately have the following reduced second-order system of order $n$:

$$\Sigma_n \ : \ \begin{cases} \mathbf{M}_n\ddot{\boldsymbol{\xi}}(t) + \mathbf{D}_n\dot{\boldsymbol{\xi}}(t) + \mathbf{K}_n\boldsymbol{\xi}(t) = \mathbf{r}_n u(t), \\ \eta(t) = \mathbf{w}_n^{\top}\dot{\boldsymbol{\xi}}(t) + \mathbf{v}_n^{\top}\boldsymbol{\xi}(t), \end{cases} \tag{4.1}$$

where the system matrices are $\mathbf{M}_n = -\mathbf{S}_n\mathbf{T}_n$, $\mathbf{D}_n = \mathbf{R}_n$ and $\mathbf{K}_n = \mathbf{I}_n$. The input and output vectors are $\mathbf{r}_n = \gamma\mathbf{e}_1$, $\mathbf{v}_n = \mathbf{Q}_n^{\top}\mathbf{l}$ and $\mathbf{w}_n = -\mathbf{T}_n^{\top}\mathbf{P}_n^{\top}\mathbf{l}$.

**Remark 4.1.** System matrices $\mathbf{M}_n$, $\mathbf{D}_n$ and $\mathbf{K}_n$ of the reduced-order systems $\Sigma_n$ are obtained from $\mathbf{R}_n$, $\mathbf{S}_n$ and $\mathbf{T}_n$ of the SQA procedure directly. To form the output vectors $\mathbf{v}_n$ and $\mathbf{w}_n$, we need to compute the matrix–vector products $\mathbf{Q}_n^{\top}\mathbf{l}$ and $\mathbf{P}_n^{\top}\mathbf{l}$. These operations can be embedded in the SQA algorithm. Therefore, there is no need to return the basis matrices $\mathbf{Q}_n$ and $\mathbf{P}_n$ from the SQA algorithm and compute the matrix–vector explicitly to obtain the reduced-order model.

When the SQA procedure terminates at the $j$th step for $j < n$, there are three possibilities as discussed in Section 3. First, for the case-A breakdown, we have the decomposition (3.8). In this case, we can use the SQA decomposition of order $2j-2$

$$\mathbf{A}\mathbf{X}_{2j-2} = \mathbf{X}_{2j-2}\begin{bmatrix}\mathbf{R}_{j-1} & \mathbf{S}_{j-1}\\ \mathbf{T}_{j-1} & \mathbf{0}\end{bmatrix} + s_{j,j-1}\mathbf{q}_j\mathbf{e}_{2j-2}^\top$$

to define a reduced-order model. Specifically, define

$$\mathbf{Y}_{2j-2} = (\mathbf{X}_{2j-1}^\dagger)^\top\begin{bmatrix}\mathbf{I}_{2j-2}\\ \mathbf{0}\end{bmatrix}.$$

Then it can be verified that $\mathbf{Y}_{2j-2}$ and $\mathbf{X}_{2j-2}$ are biorthogonal, $\mathbf{Y}_{2j-2}^\top\mathbf{X}_{2j-2} = \mathbf{I}_{2j-2}$, and $\mathbf{Y}_{2j-2}^\top\mathbf{q}_j = \mathbf{0}$, and

$$\mathbf{Y}_{2j-2}^\top\mathbf{A}\mathbf{X}_{2j-2} = \begin{bmatrix}\mathbf{R}_{j-1} & \mathbf{S}_{j-1}\\ \mathbf{T}_{j-1} & \mathbf{0}\end{bmatrix}.$$

Furthermore, we have $\mathbf{Y}_{2j-2}^\top\mathbf{b}_0 = \gamma\mathbf{e}_1$ where $\gamma = \|\mathbf{K}^{-1}\mathbf{r}\|_2$, and $\mathbf{X}_{2j-2}^\top\mathbf{l} = \begin{bmatrix}\mathbf{Q}_{j-1}^\top\mathbf{l}\\ \mathbf{P}_{j-1}^\top\mathbf{l}\end{bmatrix}$. Consequently, we have a reduced second-order system of order $j-1$:

$$\Sigma_{j-1}\ :\ \begin{cases}\mathbf{M}_{j-1}\ddot{\boldsymbol{\xi}}(t) + \mathbf{D}_{j-1}\dot{\boldsymbol{\xi}}(t) + \mathbf{K}_{j-1}\boldsymbol{\xi}(t) = \mathbf{r}_n u(t),\\ \eta(t) = \mathbf{w}_{j-1}^\top\dot{\boldsymbol{\xi}}(t) + \mathbf{v}_{j-1}^\top\boldsymbol{\xi}(t),\end{cases} \tag{4.2}$$

where the system matrices are $\mathbf{M}_{j-1} = -\mathbf{S}_{j-1}\mathbf{T}_{j-1}$, $\mathbf{D}_{j-1} = \mathbf{R}_{j-1}$ and $\mathbf{K}_{j-1} = \mathbf{I}_{j-1}$. The input and output vectors are $\mathbf{r}_{j-1} = \gamma\mathbf{e}_1$, $\mathbf{v}_{j-1} = \mathbf{Q}_{j-1}^\top\mathbf{l}$ and $\mathbf{w}_{j-1} = -\mathbf{T}_{j-1}^\top\mathbf{P}_{j-1}^\top\mathbf{l}$.

Second, for the case-B breakdown, we have the decomposition (3.10) and span$\{\mathbf{X}_{2j}\}$ is an invariant subspace of $\mathbf{A}$. Define

$$\mathbf{Y}_{2j} = (\mathbf{X}_{2j}^\dagger)^\top.$$

Then we have

$$\mathbf{Y}_{2j}^\top\mathbf{A}\mathbf{X}_{2j} = \begin{bmatrix}\mathbf{R}_j & \mathbf{S}_j\\ \mathbf{T}_j & \mathbf{0}\end{bmatrix},$$

and $\mathbf{Y}_{2j}^\top\mathbf{b}_0 = \gamma\mathbf{e}_1$ where $\gamma = \|\mathbf{K}^{-1}\mathbf{r}\|_2$, and $\mathbf{X}_{2j}^\top\mathbf{l} = \begin{bmatrix}\mathbf{Q}_j^\top\mathbf{l}\\ \mathbf{P}_j^\top\mathbf{l}\end{bmatrix}$. Consequently, we have a reduced second-order system $\Sigma_j$ of order $j$ defined as (4.2) with the system matrices $\mathbf{M}_j = -\mathbf{S}_j\mathbf{T}_j$, $\mathbf{D}_j = \mathbf{R}_j$ and $\mathbf{K}_j = \mathbf{I}_j$. The input and output vectors are $\mathbf{r}_j = \gamma\mathbf{e}_1$, $\mathbf{v}_j = \mathbf{Q}_j^\top\mathbf{l}$ and $\mathbf{w}_j = -\mathbf{T}_j^\top\mathbf{P}_j^\top\mathbf{l}$.

Finally, for the case-C breakdown, we have the decomposition (3.9) and the subspace span$\{\mathbf{X}_{2j-2}\} = \mathcal{K}_{2j-2}(\mathbf{A};\mathbf{q}_1)$ is an invariant subspace. Since $\mathbf{q}_j \in \mathcal{K}_{2j-2}(\mathbf{A};\mathbf{q}_1)$, we can compute the vectors $\boldsymbol{\upsilon}, \boldsymbol{\varphi} \in \mathbb{R}^{j-1}$ such that

$$\mathbf{s}_{j,j-1}\mathbf{q}_j = \mathbf{X}_{2j-2}\begin{bmatrix}\boldsymbol{\upsilon}\\ \boldsymbol{\varphi}\end{bmatrix}. \tag{4.3}$$

Substituting the Eq. (4.3) into (3.9), we have

$$\mathbf{A}\mathbf{X}_{2j-2} = \mathbf{X}_{2j-2}\begin{bmatrix} \mathbf{R}_{j-1} & \widetilde{\mathbf{S}}_{j-1} \\ \mathbf{T}_{j-1} & \varphi\mathbf{e}_{j-1}^{\top} \end{bmatrix}, \tag{4.4}$$

where $\widetilde{\mathbf{S}}_{j-1} = \mathbf{S}_{j-1} + \boldsymbol{\upsilon}\mathbf{e}_{j-1}^{\top}$. Furthermore, let

$$\mathbf{F} = \begin{bmatrix} \mathbf{I}_{j-1} & -\mathbf{F}_{12} \\ \mathbf{0} & \mathbf{I}_{j-1} \end{bmatrix},$$

where $\mathbf{F}_{12} = \mathbf{T}_{j-1}^{-1}\varphi\mathbf{e}_{j-1}^{\top}$. Then we have

$$\mathbf{F}^{-1}\begin{bmatrix} \mathbf{R}_{j-1} & \widetilde{\mathbf{S}}_{j-1} \\ \mathbf{T}_{j-1} & \varphi\mathbf{e}_{j-1}^{\top} \end{bmatrix}\mathbf{F} = \begin{bmatrix} \widehat{\mathbf{R}}_{j-1} & \widehat{\mathbf{S}}_{j-1} \\ \mathbf{T}_{j-1} & \mathbf{0} \end{bmatrix}, \tag{4.5}$$

where $\widehat{\mathbf{R}}_{j-1} = \mathbf{R}_{j-1} + \mathbf{F}_{12}\mathbf{T}_{j-1}$ and $\widehat{\mathbf{S}}_{j-1} = \widetilde{\mathbf{S}}_{j-1} - \mathbf{R}_{j-1}\mathbf{F}_{12}$. Combining (4.4) and (4.5), it yields the decomposition

$$\mathbf{A}\mathbf{X}_{2j-2}\mathbf{F} = \mathbf{X}_{2j-2}\mathbf{F}\begin{bmatrix} \widehat{\mathbf{R}}_{j-1} & \widehat{\mathbf{S}}_{j-1} \\ \mathbf{T}_{j-1} & \mathbf{0} \end{bmatrix}.$$

Now define $\mathbf{Y}_{2j-2}$ as a pseudoinverse of $\mathbf{X}_{2j-2}\mathbf{F}$:

$$\mathbf{Y}_{2j-2} = \mathbf{X}_{2j-2}\mathbf{F}(\mathbf{F}^{\top}\mathbf{X}_{2j-2}^{\top}\mathbf{X}_{2j-2}\mathbf{F})^{-1}.$$

Then we have $\mathbf{Y}_{2j-2}^{\top}(\mathbf{X}_{2j-2}\mathbf{F}) = \mathbf{I}_{2j-2}$ and

$$\mathbf{Y}_{2j-2}^{\top}\mathbf{A}(\mathbf{X}_{2j-2}\mathbf{F}) = \begin{bmatrix} \widehat{\mathbf{R}}_{j-1} & \widehat{\mathbf{S}}_{j-1} \\ \mathbf{T}_{j-1} & \mathbf{0} \end{bmatrix}.$$

Since $\mathbf{X}_{2j-2}\mathbf{F}\mathbf{e}_1 = \mathbf{X}_{2j-2}\mathbf{e}_1 = \mathbf{b}_0/\gamma$ where $\gamma = \|\mathbf{K}^{-1}\mathbf{r}\|_2$, we have

$$\mathbf{Y}_{2j-2}^{\top}\mathbf{b}_0 = \gamma\mathbf{Y}_{2j-2}^{\top}\mathbf{X}_{2j-2}\mathbf{F}\mathbf{e}_1 = \gamma\mathbf{e}_1.$$

The matrix–vector multiplication $\mathbf{F}^{\top}\mathbf{X}_{2j-2}^{\top}\mathbf{l}$ has the partitioned form

$$\mathbf{F}^{\top}\mathbf{X}_{2j-2}\mathbf{l} = \begin{bmatrix} \mathbf{Q}_{j-1}^{\top}\mathbf{l} \\ -\mathbf{F}_{12}^{\top}\mathbf{Q}_{j-1}^{\top}\mathbf{l} + \mathbf{P}_j^{\top}\mathbf{l} \end{bmatrix} \equiv \begin{bmatrix} \mathbf{v}_{j-1} \\ \widehat{\mathbf{w}}_{j-1} \end{bmatrix}.$$

Consequently, we have a reduced second-order system $\Sigma_j$ of order $j$ defined as (4.2) with the system matrices $\mathbf{M}_{j-1} = -\widehat{\mathbf{S}}_{j-1}\mathbf{T}_{j-1}$, $\mathbf{D}_{j-1} = \widehat{\mathbf{R}}_{j-1}$ and $\mathbf{K}_{j-1} = \mathbf{I}_{j-1}$. The input and output vectors are $\mathbf{r}_{j-1} = \gamma\mathbf{e}_1$, $\mathbf{v}_{j-1} = \mathbf{Q}_{j-1}^{\top}\mathbf{l}$ and $\mathbf{w}_{j-1} = -\mathbf{T}_{j-1}^{\top}\widehat{\mathbf{w}}_{j-1}$.

In the rest of this section, we give the moment-matching property of the reduced second-order systems. First we have the following theorem for the case where there is no breakdown.

**Theorem 4.1.** *The first* $2n$ *moments of the original system* (1.1) *and the reduced second-order system* $\Sigma_n$ (4.1) *coincide, i.e.,*

$$m_i = (-1)^i \mathbf{l}^\top \mathbf{A}^i \mathbf{b}_0 = (-1)^i \mathbf{l}^\top \mathbf{X}_{2n} (\mathbf{Y}_{2n}^\top \mathbf{A} \mathbf{X}_{2n})^i \mathbf{Y}_{2n}^\top \mathbf{b}_0 = m_i^{(n)} \tag{4.6}$$

*for* $i = 0, 1, 2, \ldots, 2n-1$. *Hence* $h_n(s)$ *of* $\Sigma_n$ *is a Padé approximant of* $h(s)$:

$$h(s) = h_n(s) + O(s^{2n}).$$

**Proof.** By Theorem 3.1, it is known that $\mathbf{X}_{2n}$ is a basis of the Krylov subspace $\mathcal{K}_{2n}(\mathbf{A}; \mathbf{b}_0)$. Hence there exist vectors $\mathbf{v}_i \in \mathbb{R}^{2n}$ such that $\mathbf{A}^i \mathbf{b}_0 = \mathbf{X}_{2n} \mathbf{v}_i$ for $i = 0, 1, \ldots, 2n-1$. Together with $\mathbf{Y}_{2n}^\top \mathbf{X}_{2n} = \mathbf{I}_{2n}$, it yields that

$$\mathbf{X}_{2n} \mathbf{Y}_{2n}^\top \mathbf{A}^i \mathbf{b}_0 = \mathbf{X}_{2n} \mathbf{Y}_{2n}^\top \mathbf{X}_{2n} \mathbf{v}_i = \mathbf{X}_{2n} \mathbf{v}_i = \mathbf{A}^i \mathbf{b}_0, \quad \text{for} \;\; i = 0, 1, 2, \ldots, 2n-1. \tag{4.7}$$

Next, we show by induction that

$$\mathbf{X}_{2n} (\mathbf{Y}_{2n}^\top \mathbf{A} \mathbf{X}_{2n})^i \mathbf{Y}_{2n}^\top \mathbf{b}_0 = \mathbf{A}^i \mathbf{b}_0, \tag{4.8}$$

for $i = 0, 1, \ldots, 2n-1$. At the basis step $i = 0$, the identity (4.8) is the identity (4.7) for $i = 0$. When $i = 1$, using the identity (4.7) with $i = 0$ and $i = 1$, we have

$$\mathbf{X}_{2n} (\mathbf{Y}_{2n}^\top \mathbf{A} \mathbf{X}_{2n}) \mathbf{Y}_{2n}^\top \mathbf{b}_0 = \mathbf{X}_{2n} \mathbf{Y}_{2n}^\top \mathbf{A} (\mathbf{X}_{2n} \mathbf{Y}_{2n}^\top \mathbf{b}_0) = \mathbf{X}_{2n} \mathbf{Y}_{2n}^\top \mathbf{A} \mathbf{b}_0 = \mathbf{A} \mathbf{b}_0$$

At the inductive step, for $2 \leqslant i \leqslant 2n-1$,

$$\begin{aligned} \mathbf{X}_{2n} (\mathbf{Y}_{2n}^\top \mathbf{A} \mathbf{X}_{2n})^i \mathbf{Y}_{2n}^\top \mathbf{b}_0 &= \mathbf{X}_{2n} (\mathbf{Y}_{2n}^\top \mathbf{A} \mathbf{X}_{2n}) (\mathbf{Y}_{2n}^\top \mathbf{A} \mathbf{X}_{2n})^{i-1} \mathbf{Y}_{2n}^\top \mathbf{b}_0 \\ &= \mathbf{X}_{2n} \mathbf{Y}_{2n}^\top \mathbf{A} \left[ \mathbf{X}_{2n} (\mathbf{Y}_{2n}^\top \mathbf{A} \mathbf{X}_{2n})^{i-1} \mathbf{Y}_{2n}^\top \mathbf{b}_0 \right] \\ &= \mathbf{X}_{2n} \mathbf{Y}_{2n}^\top \mathbf{A} \mathbf{A}^{i-1} \mathbf{b}_0 \\ &= \mathbf{A}^i \mathbf{b}_0, \end{aligned}$$

where for the second equality we used the hypothesis of the induction, and for the fourth equality we use the identity (4.7). The moment-matching property (4.6) is followed immediately from the identity (4.8). □

Theorem 4.1 shows that the reduced system $\Sigma_n$ of dimension $n$ matches $2n$ moments of the original system $\Sigma_N$. In contrast, the order-$n$ reduced system generated by the SOAR method [3] or the SPRIM method [9] generally matches only $n$ moments.

When a breakdown occurs, the moment-matching properties of the original system $\Sigma_N$ and the reduced second-order system $\Sigma_{j-1}$ or $\Sigma_j$ are summarized in the following two theorems. First, by an analogous proof of Theorem 4.1, we have the following theorem for the case-A breakdown.

**Theorem 4.2.** *If SQA has the case-A breakdown at the* $j$*th step, then the first* $2j-2$ *moments of the original system* (1.1) *and the reduced second-order system* $\Sigma_{j-1}$ (4.2) *coincide.*

At the case-B and case-C breakdowns, we use invariant Krylov subspaces $\mathcal{K}_{2j}(\mathbf{A}; \mathbf{b}_0)$ and $\mathcal{K}_{2j-2}(\mathbf{A}; \mathbf{b}_0)$ to define reduced second-order systems. For these cases, we have the following theorem.

**Theorem 4.3.** *When there is the case-B or case-C breakdown, the transfer function of the reduced second-order system* $\Sigma_j$ *or* $\Sigma_{j-1}$ *is identical to the transfer function of the original system* $\Sigma_N$ (1.1). *Hence, the case-B or case-C breakdown of the SQA procedure is regarded as a lucky breakdown.*

**Proof.** We can use an analogous argument for the proof of Theorem 4.1. The key difference here is that when the case-B breakdown occurs, $\mathbf{X}_{2j}$ is a basis of the invariant Krylov subspace $\mathcal{K}_{2j}(\mathbf{A};\mathbf{b}_0)$, there exist vectors $\mathbf{v}_i \in \mathbb{R}^{2j}$ such that $\mathbf{A}^i\mathbf{b}_0 = \mathbf{X}_{2j}\mathbf{v}_i$ for all $i \geqslant 0$. Thus together with the fact $\mathbf{Y}_{2j}^\top\mathbf{X}_{2j} = \mathbf{I}_{2j}$, it yields that $\mathbf{X}_{2j}\mathbf{Y}_{2j}^\top\mathbf{A}^i\mathbf{b}_0 = \mathbf{X}_{2j}\mathbf{Y}_{2j}^\top\mathbf{X}_{2j}\mathbf{v}_i = \mathbf{X}_{2j}\mathbf{v}_i = \mathbf{A}^i\mathbf{b}_0$ for all $i \geqslant 0$. For the case-C breakdown, we just need to note that since $\mathbf{F}$ is nonsingular, $\mathbf{X}_{2j-2}\mathbf{F}$ is also a basis of the invariant subspace $\mathcal{K}_{2j-2}(\mathbf{A};\mathbf{b}_0)$. □

## 5. Numerical examples

In this section, we present numerical examples to compare the accuracy of reduced-order models $\mathbf{\Sigma}_n$ of order $n$ generated by SQA, SOAR [3] and TS-SOAR [19]. In practice, often an approximation of the transfer function $h(s)$ of the original system $\Sigma_N$ around a selected expansion point $\sigma \neq 0$ is of interest. In this case, we can rewrite $h(s)$ in a shifted form

$$h(s) = \left((s-\sigma)\mathbf{w}^\top + \widetilde{\mathbf{v}}^\top\right)\left((s-\sigma)^2\mathbf{M} + (s-\sigma)\widetilde{\mathbf{D}} + \widetilde{\mathbf{K}}\right)^{-1}\mathbf{r},$$

where $\widetilde{\mathbf{v}} = \mathbf{v} + \sigma\mathbf{w}$, $\widetilde{\mathbf{D}} = 2\sigma\mathbf{M} + \mathbf{D}$ and $\widetilde{\mathbf{K}} = \sigma^2\mathbf{M} + \sigma\mathbf{D} + \mathbf{K}$, and then apply a model reduction method with the matrices $\mathbf{M}$, $\widetilde{\mathbf{D}}$ and $\widetilde{\mathbf{K}}$. All numerical experiments were run in MATLAB. The numerical tolerance $\epsilon$ for testing the breakdowns is set to be $10^{-15}$.

**Example 5.1.** We consider a proportionally damped second-order system (1.1), where $\mathbf{D} = \alpha\mathbf{M} + \beta\mathbf{K}$ and $\mathbf{w} = \mathbf{0}$. This is the butterfly gyroscope in the Oberwolfach benchmark collection [15,14]. It arises from simulating a vibrating micromechanical gyroscope. The full system has $N = 17{,}361$ degrees of freedom, 1 input and 12 outputs. For the experiments here the output vector $\mathbf{v}$ was taken to be the first column of the $17{,}361 \times 12$ selector output matrix. The damping matrix is assumed to be $\mathbf{D} = \beta\mathbf{K}$ where $\beta = 10^{-7}$. An expansion point $\sigma = 1.05 \times 10^5$ is used for approximating requested frequency range $10^4$–$10^6$ Hz. The Bode plot of $h(s)$ is shown in the left plot of Fig. 1.

We find that a reduced SQA system of order $n = 40$ is sufficient for the desired accuracy. The relative errors associated with SQA, SOAR and TS-SOAR are shown in the right plot of Fig. 1. The results demonstrate that SQA and TS-SOAR are compatible because they match the same number of moments. Both SQA and TS-SOAR models are more accurate than the SOAR model due to doubling the number of matched moments.

**Example 5.2.** This large example is from the frequency response analysis of a second-order system $\mathbf{\Sigma}_N$ arising from fluid–structure interaction at an acoustic level [18]. The state-space dimension of the original system $\mathbf{\Sigma}_N$ is $N = 89{,}120$. The nonsymmetric mass and stiffness matrices $\mathbf{M}$ and $\mathbf{K}$ come

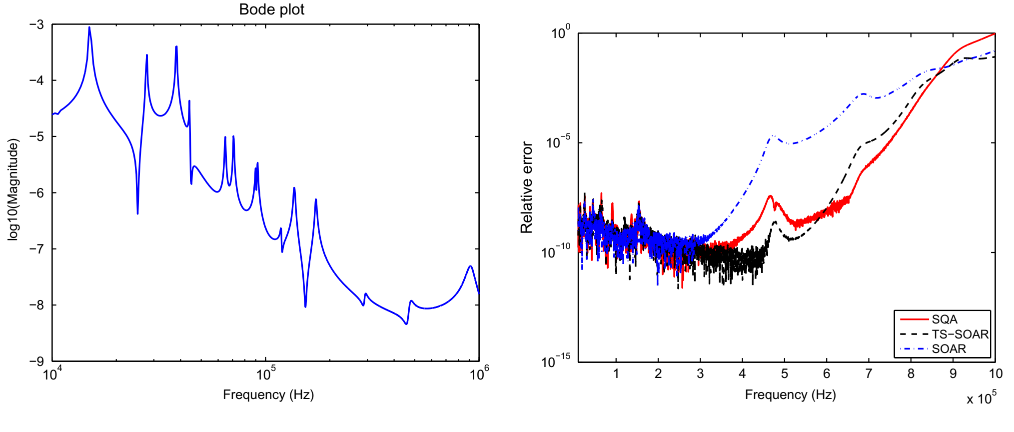


**Fig. 1.** Bode plot of the transfer function of Example 5.1, the relative errors of SQA, TS-SOAR and SOAR models at $n = 40$.

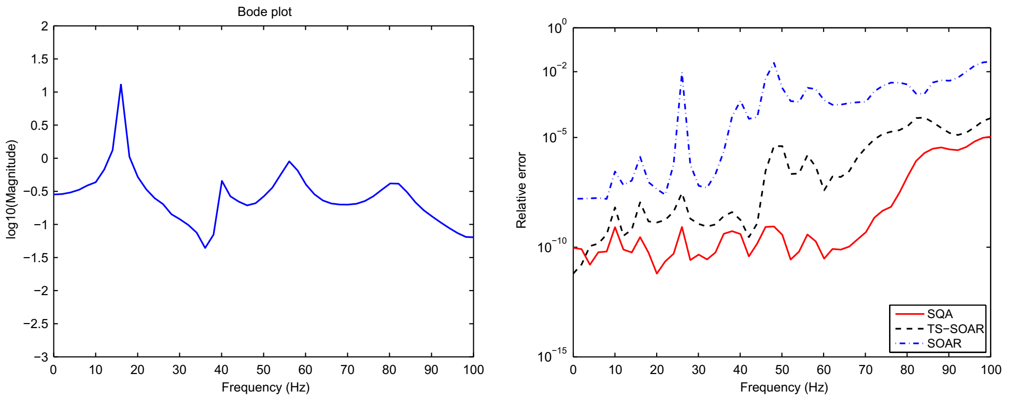


**Fig. 2**. Bode plot of the transfer function of Example 5.2, the relative errors of the SQA, TS-SOAR and SOAR models at $n = 100$.

from modeling fluid–structure coupling. The damping matrix $\mathbf{D}$ is symmetric. An expansion point $\sigma = 2\pi \times 50$ is used approximating requested frequency range 0–100 Hz. The shifted stiffness matrix $\widetilde{\mathbf{K}} = s_0^2\mathbf{M} + s_0\mathbf{D} + \mathbf{K}$ has 1-norm condition number $\mathcal{O}(10^{11})$. The Bode plot of $h(s)$ is shown in the left plot of Fig. 2.

We find that a reduced SQA model of order $n = 100$ is sufficient for the desired accuracy. The relative errors of SQA, TS-SOAR and SOAR models are shown in the right plot of Fig. 2. The results demonstrate that the SQA method constructs much better approximation than SOAR, and slightly more accurate than the TS-SOAR model although SQA and TS-SOAR models match the same number of moments.

## 6. Conclusions

We proposed a new SQA decomposition and the corresponding SQA procedure. The SQA decomposition can be used to define a structure-preserving model-order reduction of the second-order system $\Sigma_N$ (1.1) directly, without the explicit projection as in the existing structure-preserving model-order reduction methods. In terms of moment-matching property, it is equivalent to the TS-SOAR method. The proposed SQA method could significantly reduce the memory I/O and the extra floating-point arithmetic costs for very large systems on computer systems where the memory I/O costs have exceeded arithmetic costs by orders of magnitude. It is one of future work to provide quantitative performance measurement of the benefit. Other future work include efficiently detecting the numerical breakdowns, extension to the multiple expansion points and the development of the SQA method to preserve the symmetry of a symmetric second-order system.

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