Error-amplification analysis of subiteration-preconditioned GMRES for fluid-structure interaction

C. Michler, E.H. van Brummelen and R. de Borst
Delft University of Technology, Faculty of Aerospace Engineering,
P.O. Box 5058, NL-2600 GB Delft, The Netherlands

ABSTRACT
The customary subiteration method for solving fluid-structure-interaction problems exhibits several deficiencies, viz., only conditional stability, potential convergence difficulties due to nonnormality-induced divergence, and the inability to reuse information from previously solved similar problems. To overcome these deficiencies, a novel solution method is considered, in which subiteration is used as a preconditioner to GMRES. This paper treats the linear-algebra aspects of the subiteration method, and of the subiteration-preconditioned GMRES method, on the basis of properties of the error-amplification matrix for the aggregated fluid-structure system. An analysis of the error-amplification matrix of subiteration establishes that subiteration condenses errors into a low-dimensional subspace which can be associated with the interface degrees-of-freedom. Therefore, the GMRES acceleration of subiteration can be confined to the interface degrees-of-freedom. The error-amplification analysis provides a clear explanation of the relation between the $local$ GMRES acceleration (i.e., on the interface degrees-of-freedom), and the $global$ error-amplification properties (i.e., for the aggregated system). Moreover, we show that the subiteration iterates span a Krylov space corresponding to a preconditioned aggregated system. We then address the implications of the nonnormality of the subiteration preconditioner for the convergence of GMRES. The subiteration-preconditioned GMRES method enables the optional reuse of Krylov vectors in subsequent invocations of GMRES, which can substantially enhance the efficiency of the method. To assess the potential and the limitations of the reuse option, we analyse the error-amplification matrix of the GMRES method with reuse. Furthermore, we establish that the GMRES acceleration on the interface degrees-of-freedom generates an approximation to the Schur complement for the aggregated system. The GMRES acceleration and the reuse of Krylov vectors are then assessed in terms of the approximation properties for the Schur complement, and in terms of the properties of the corresponding error-amplification matrices. Numerical experiments on a model fluid-structure-interaction problem illustrate the developed theory. In particular, we analyse the convergence of the respective methods in terms of spectral radii, matrix norms and sharp convergence upper bounds.

Keywords and Phrases: fluid-structure interaction, subiteration, GMRES, preconditioning, reuse of Krylov vectors, error-amplification analysis, convergence bounds.

1. Introduction

Fluid-structure interactions are of great relevance in many engineering disciplines such as aerospace engineering [1, 2], civil engineering [3, 4] and bio-mechanics [5]. The numerical solution of fluid-structure-interaction problems commonly employs *subiteration*, i.e., fluid and structure equations are solved alternately subject to complementary partitions of the interface conditions; see, e.g., Refs. [6, 7, 8]. This process essentially constitutes a block Gauss-Seidel method. Although subiteration is a good solver for many problems, it converges only slowly or even diverges for problems with large computational time steps or large fluid-to-structure mass ratios. Subiteration is only conditionally stable, but even despite formal stability, transient divergence can precede asymptotic convergence. These convergence difficulties can be attributed to the nonnormality of the subiteration operator; see Ref. [9]. Such non-monotonous convergence behaviour can even lead to failure of the solution method despite formal stability. Moreover, subiteration is generally employed in a sequential time-integration process and, hence, it solves a sequence of similar problems. However, the method cannot exploit

this property by reusing generated information, for instance, for preconditioning purposes. Therefore, subiteration is to be considered inefficient.

In Ref. [10], we proposed to overcome the deficiencies of subiteration by combining it with GMRES acceleration [11]. As the latter can be confined to the interface degrees-of-freedom, we refer to the method also as *Interface-GMRES*. Restriction of the GMRES acceleration to the interface renders storage requirements for the Krylov space and computational cost of the least-squares problem low in contrast to approaches which apply GMRES to the aggregated equations [12, 13], or to the Schur complement associated with the structure [14]. In Ref. [10], we established the Interface-GMRES method in a continuum setting of a generic fluid-structure-interaction problem, which implies that the method is generic, and that its performance is asymptotically independent of the discretization of the underlying problem. Moreover, the proposed method enables optional reuse of Krylov vectors in subsequent invocations of GMRES, which can considerably enhance the efficiency of the method. The proposed method is easily implemented in existing codes which use subiteration as a solver, as it fully maintains the software modularity of segregated approaches; see, e.g., Ref. [15].

The present paper treats the linear-algebra aspects of the Interface-GMRES method on the basis of properties of the error-amplification matrix for the aggregated system. The linear-algebra setting enables a clear explanation of the relation between the *local* GMRES acceleration (i.e., on the interface degrees-of-freedom), and the *global* error-amplification properties (i.e., for the aggregated system). Moreover, the error-amplification matrix of the GMRES method with reuse serves to assess the potential of and the limitations on the reuse option.

To establish the error-amplification matrix, we consider a system of nonlinear-algebraic equations in conformity with discretizations of fluid-structure-interaction problems. We then investigate the iterative solution of a corresponding linear system by means of standard subiteration, and by means of the novel combined subiteration/GMRES method. By virtue of the linear-algebra setting, it is possible to derive precise expressions for the error-amplification properties of subiteration separately, and of subiteration combined with GMRES, with and without the reuse option. On the basis of the error-amplification matrix of subiteration, we can show that subiteration condenses errors into a low-dimensional subspace which can be associated with the interface degrees-of-freedom, and that the GMRES acceleration can be confined to the interface. Moreover, the nonnormality of the subiteration operator, and its implications for the combined subiteration/GMRES method, can be traced immediately to properties of the error-amplification matrix. Next, we show that the subiteration iterates span a Krylov space corresponding to a preconditioned aggregated system. The properties of the subiteration-preconditioned GMRES method are then considered and, in particular, the relation between GMRES convergence and nonnormality of the subiteration preconditioner is addressed. Furthermore, we establish that the GMRES acceleration on the interface degrees-of-freedom generates an approximation to the Schur complement for the aggregated system. The GMRES acceleration and the reuse of Krylov vectors in subsequent invocations of GMRES are then assessed in terms of the approximation properties for the Schur complement, and in terms of the properties of the corresponding error-amplification matrices.

The theory is illustrated by numerical experiments on a model fluid-structure-interaction problem with a van-der-Pol oscillator. As this model problem exhibits qualitative changes in its solution behaviour in time, it is particularly suitable to investigate the effect of the reuse of Krylov vectors on the error-amplification properties of the subiteration-preconditioned GMRES method. Moreover, we provide worst-case convergence bounds for the methods in terms of matrix norms.

The contents of this paper are organized as follows: Section 2 establishes the linear-algebra setting of the problem. Section 3 derives the error-amplification matrix of the subiteration method, and elaborates on the preconditioning perspective and on the nonnormality of subiteration. Section 4 analyses the error-amplification properties of the subiteration-preconditioned GMRES method with and without reuse in terms of the Schur-complement approximation and in terms of the error-amplification matrices. Section 5 provides numerical experiments and results. Section 6 contains concluding remarks.

2. Algebraic problem statement

In this section, we introduce the system of algebraic equations that emanates from a discretization of a generic fluid-structure-interaction problem; for a description of the latter we refer to Ref. [10]. We consider the system of linear-algebraic equations that arises from the application of Newton's method. This linear-algebraic system forms the basis of the error-amplification analysis for an inexact Newton method in Section 2.2. The subiteration method and the subiteration-preconditioned GMRES method can be construed as special instances of such an inexact Newton method.

2.1 The system of linear-algebraic fluid-structure-interaction equations

The system of fluid-structure-interaction equations comprises the initial-boundary-value problems of the fluid and the structure, complemented by kinematic and dynamic conditions at the fluid-structure interface. We consider the generic space-time variational formulation of such fluid-structure-interaction problems as presented in Ref. [10] and refer for a particular instance, viz., the piston problem, to Ref. [16]. The space-time finite-element discretization of this generic variational statement yields a system of aggregated algebraic equations for the fluid-structure system, which we condense into the abstract form

$$\boldsymbol{R}(\mathbf{q}) = \mathbf{0}, \tag{1a}$$

and, more specifically,

$$R_1(q_1, q_5) = 0, \tag{1b}$$
$$R_2(q_1, q_2) = 0, \tag{1c}$$
$$R_3(q_1, q_2, q_3) = 0, \tag{1d}$$
$$R_4(q_3, q_4) = 0, \tag{1e}$$
$$R_5(q_4, q_5) = 0. \tag{1f}$$

We denote aggregated quantities by bold symbols. In particular, in (1), $\boldsymbol{R} := [R_1, R_2, R_3, R_4, R_5]^T$ and $\mathbf{q} := [q_1, q_2, q_3, q_4, q_5]^T$ denote the residual operators and variables associated with kinematic interface condition, fluid equations, dynamic interface condition, structure equation and the restriction of the structure variables to the interface, respectively. Note that the fluid and structure variables, q_2 and q_4, are connected by the kinematic and dynamic interface conditions, R_1 and R_3, via the fluid-interface displacement and the interface traction exerted on the structure, q_1 and q_3, respectively. For transparency of the ensuing presentation, we have introduced an additional equation, Eq. (1f), given by

$$R_5(q_4, q_5) := T(q_4) - q_5 = 0, \tag{2}$$

where T represents the trace operator, which defines the structural displacement at the interface, q_5, in terms of the structural variables, q_4.

Given an initial estimate $\mathbf{q}^0$, the application of Newton's method to the nonlinear system (1) gives rise to a sequence of linear problems

$$\mathbf{A}(\mathbf{q}^{n+1} - \mathbf{q}^n) = -\boldsymbol{R}(\mathbf{q}^n), \tag{3a}$$

for $n = 0, 1, 2, \ldots$, which bear the particular form

$$\begin{pmatrix} A_{11} & 0 & 0 & 0 & A_{15} \\ A_{21} & A_{22} & 0 & 0 & 0 \\ A_{31} & A_{32} & A_{33} & 0 & 0 \\ 0 & 0 & A_{43} & A_{44} & 0 \\ 0 & 0 & 0 & A_{54} & A_{55} \end{pmatrix} \begin{bmatrix} q_1^{n+1} - q_1^n \\ q_2^{n+1} - q_2^n \\ q_3^{n+1} - q_3^n \\ q_4^{n+1} - q_4^n \\ q_5^{n+1} - q_5^n \end{bmatrix} = - \begin{bmatrix} R_1(\mathbf{q}^n) \\ R_2(\mathbf{q}^n) \\ R_3(\mathbf{q}^n) \\ R_4(\mathbf{q}^n) \\ R_5(\mathbf{q}^n) \end{bmatrix}. \tag{3b}$$

In (3b), A_{ij} denotes the Jacobian matrix corresponding to the residual-operator derivative $\partial R_i/\partial q_j$ and $R_i(\mathbf{q}^n)$ the residuals at the current linearization state $\mathbf{q}^n$. We remark that, in conformity with Eq. (2), $A_{55} = -I$ with I the identity matrix. If the initial estimate $\mathbf{q}^0$ is sufficiently close to the actual solution $\bar{\mathbf{q}}$ of Eq. (1a), then $\mathbf{q}^n$ converges to $\bar{\mathbf{q}}$ as $n \to \infty$.

The consideration of Newton's method is useful mainly for conceptual reasons, as it provides the framework for the ensuing error-amplification analysis in Section 2.2. For the solution of fluid-structure interaction problems, however, the application of Newton's method is actually prohibitive: The inherent interdependence between fluid and structure solutions induced by the interface conditions renders the matrix $\mathbf{A}$ in (3) inseparable. This interconnection requires, in principle, a simultaneous solution of fluid and structure equations and, hence, causes the loss of software modularity; cf. Ref. [15]. Moreover, the disparate properties and scales inherent in the fluid and structure problems generally render the matrix $\mathbf{A}$ severely ill-conditioned. Finally, Eq. (3b) necessitates the evaluation of so-called *shape derivatives*, i.e., the derivative of the fluid equations with respect to a perturbation in the interface position, represented by the entry A_{21}. The difficulty in the evaluation of A_{21} pertains to the fact that a perturbation in the interface position in principle generates a perturbation throughout the entire fluid domain and, hence, A_{21} acts as a non-local operator. Although there exist approaches to facilitate the evaluation of the shape derivatives, such as the *method of spines* [13], their applicability is typically restricted.

2.2 Error-amplification analysis of inexact Newton methods

In order to bypass the aforementioned disadvantages of Newton's method, one generally reverts to alternative solution methods such as subiteration. For the error-amplification analysis of these methods, it is convenient to construe them, on linear approximation, as particular instances of an *inexact* Newton method. At variance with Eq. (3a), such inexact Newton methods determine an approximation $\tilde{\mathbf{q}}^{n+1}$ from the solution of

$$\tilde{\mathbf{A}}(\tilde{\mathbf{q}}^{n+1} - \mathbf{q}^n) = -\boldsymbol{R}(\mathbf{q}^n), \tag{4}$$

where $\tilde{\mathbf{A}}$ denotes an approximate Jacobian that is 'in some sense' similar to $\mathbf{A}$, but easier to invert. The error induced by this approximation can be assessed as follows. The exact Newton method solves Eq. (3a) and, hence, on linear approximation, eliminates the error in a single step. Thus, on linear approximation, $\mathbf{q}^{n+1}$ corresponds to the solution $\bar{\mathbf{q}}$ of (1a), and Eq. (3a) translates into

$$-\mathbf{A}\boldsymbol{\epsilon}^n = -\boldsymbol{R}(\mathbf{q}^n), \tag{5}$$

where $\boldsymbol{\epsilon}^n := \mathbf{q}^n - \bar{\mathbf{q}}$ denotes the error in the approximation $\mathbf{q}^n$. Likewise, we denote by $\boldsymbol{\epsilon}^{n+1} := \tilde{\mathbf{q}}^{n+1} - \bar{\mathbf{q}}$. Substituting Eq. (5) into Eq. (4) and adding suitable partitions of zero, we obtain

$$\tilde{\mathbf{A}}(\boldsymbol{\epsilon}^{n+1} - \boldsymbol{\epsilon}^n) = -\mathbf{A}\boldsymbol{\epsilon}^n, \tag{6}$$

which yields the error-amplification relation

$$\boldsymbol{\epsilon}^{n+1} = \mathbf{E}\boldsymbol{\epsilon}^n \tag{7a}$$

with

$$\mathbf{E} := \mathbf{I} - \tilde{\mathbf{A}}^{-1}\mathbf{A} \tag{7b}$$

the error-amplification matrix of the inexact Newton method with approximate Jacobian $\tilde{\mathbf{A}}$. The inexact Newton method is formally convergent, if the spectral radius of the error-amplification matrix is smaller than unity, i.e., $\mathrm{spr}(\mathbf{E}) < 1$. With the setting $\tilde{\mathbf{A}} = \mathbf{A}$, we recover the exact Newton method, which yields $\mathbf{E} = \mathbf{0}$. We elaborate in Sections 3 and 4 that the customary subiteration method and the novel subiteration-preconditioned GMRES method with and without reuse can be associated with specific choices of $\tilde{\mathbf{A}}$. This enables a comparison of their respective error-amplification properties from a unified viewpoint.

3. Error-amplification analysis of the subiteration method

This section presents a detailed analysis of the error-amplification properties of the subiteration method. To this end, we recall the basic subiteration algorithm in Section 3.1. In Section 3.2, we establish the error-amplification matrix, and we derive the precise form of its entries, which enables us to relate the error-amplification behaviour to specific entries. We show that the error-amplification matrix is rank-deficient, which provides the theoretical basis for the restriction of the GMRES acceleration to the interface degrees-of-freedom. Moreover, we consider the norm, spectral radius, and the nonnormality of the error-amplification matrix in Section 3.3. Nonnormality has important implications for the convergence of the subiteration method, and for the GMRES convergence bounds discussed in Section 4.5. Finally, in Section 3.4, we elaborate on the preconditioning perspective of subiteration, which provides the motivation of using it as a preconditioner to GMRES.

3.1 The subiteration method

The subiteration method is defined by the following iterative procedure: Provided with an initial approximation of the structure displacement at the interface, $q_5^0(t)$, for $n = 1, 2, \ldots$

(S1) Solve the kinematic condition: find q_1^n such that $R_1(q_1^n, q_5^{n-1}) = 0$

(S2) Solve the fluid equations: find q_2^n such that $R_2(q_1^n, q_2^n) = 0$

(S3) Solve the dynamic condition: find q_3^n such that $R_3(q_1^n, q_2^n, q_3^n) = 0$

(S4) Solve the structure equations: find q_4^n such that $R_4(q_3^n, q_4^n) = 0$

(S5) Determine the structure displacement at the interface: find q_5^n such that $R_5(q_4^n, q_5^n) = 0$

We remark that in an actual computation, the subiteration process solves the nonlinear equations. However, for our analysis we shall apply it to the linearized equations.

Note that the subiteration procedure obviates the simultaneous treatment of the fluid and the structure and, thus, enables software modularity. For applications of the subiteration method to fluid-structure-interaction problems see, e.g., Refs. [6, 7, 8]. We remark that the customary *partitioned* and *staggered* time-integration methods for fluid-structure-interaction problems (see, e.g., Refs. [15, 17, 18, 19]) are essentially identical to the above subiteration method; however, they do not repeat the iterative process.

For convenience of the ensuing presentation, let us introduce the notation $z := q_5$. To facilitate the subsequent analysis of the subiteration method separately, and of the combined subiteration/GMRES method, we construe the subiteration process as a mapping from one structure interface displacement to the next, i.e.,

$$C : z^n \mapsto z^{n+1} = Cz^n, \tag{8}$$

where C denotes the operator induced by the subiteration process as defined by (S1)–(S5); see Refs. [9, 10] for further elaboration. Accordingly, the subiteration process can be characterized by recursion of the nonlinear operator C on the interface displacement z. Thus, subiteration can be conceived as a fixed-point iteration. The fixed point

$$\bar{z} : \bar{z} = C\bar{z} \tag{9}$$

corresponds to the solution of (1). The nonlinear fixed-point problem (9) can be reformulated as

$$R_{\mathrm{Sub}}\bar{z} = 0 \tag{10}$$

with $R_{\mathrm{Sub}} := C - I$ the residual operator defined in conformity with (9) and I the identity. Clearly, $\bar{z}$ being a solution of Eq. (10) is equivalent to $\bar{z}$ being a fixed point of Eq. (9). The residual of an iterate is

$$r^n := R_{\mathrm{Sub}} z^n = (C - I)z^n = Cz^n - z^n = z^{n+1} - z^n. \tag{11}$$

Note that, upon providing the subiteration process with the solution $\bar{q}_5 = \bar{z}$, the steps (S1)–(S5) yield the solution $\bar{\mathbf{q}} = (\bar{q}_1, \bar{q}_2, \bar{q}_3, \bar{q}_4, \bar{q}_5)$ of the aggregated nonlinear equations (1) in a single iteration, provided that the equations in each step are solved exactly.

3.2 Error-amplification analysis

This section analyses the error-amplification properties of the subiteration method. To this end, we recall from Section 3.1 that the subiteration method solves the nonlinear equations. For the error-amplification analysis we consider the linearization of these equations in conformity with Eq. (3). The subiteration algorithm then translates into the solution of the following equations:

$$\begin{pmatrix} A_{11} & 0 & 0 & 0 & 0 \\ A_{21} & A_{22} & 0 & 0 & 0 \\ A_{31} & A_{32} & A_{33} & 0 & 0 \\ 0 & 0 & A_{43} & A_{44} & 0 \\ 0 & 0 & 0 & A_{54} & A_{55} \end{pmatrix} \begin{bmatrix} \tilde{q}_1^{n+1} - q_1^n \\ \tilde{q}_2^{n+1} - q_2^n \\ \tilde{q}_3^{n+1} - q_3^n \\ \tilde{q}_4^{n+1} - q_4^n \\ \tilde{q}_5^{n+1} - q_5^n \end{bmatrix} = - \begin{bmatrix} R_1(\mathbf{q}^n) \\ R_2(\mathbf{q}^n) \\ R_3(\mathbf{q}^n) \\ R_4(\mathbf{q}^n) \\ R_5(\mathbf{q}^n) \end{bmatrix}, \tag{12a}$$

which can be condensed into the form

$$\tilde{\mathbf{A}}_{\mathrm{Sub}}(\tilde{\mathbf{q}}^{n+1} - \mathbf{q}^n) = -\boldsymbol{R}(\mathbf{q}^n). \tag{12b}$$

From Eq. (12) it is apparent that we can associate a Jacobian matrix $\tilde{\mathbf{A}}_{\mathrm{Sub}}$ with the subiteration process, that corresponds to the lower-triangular part of $\mathbf{A}$, i.e., it is identical to matrix $\mathbf{A}$ in Eq. (3), but with the A_{15} block set to zero. Because $\tilde{\mathbf{A}}_{\mathrm{Sub}}$ is lower block-triangular, the subproblems involving the inversion of the Jacobian $\tilde{\mathbf{A}}_{\mathrm{Sub}}$ can be solved conveniently by forward substitution. Hence, the subiteration process essentially corresponds to a block Gauss-Seidel method.

Having identified the approximate Jacobian matrix $\tilde{\mathbf{A}}_{\mathrm{Sub}}$ induced by the subiteration process, we determine the corresponding error-amplification matrix according to Eq. (7) as $\mathbf{E}_{\mathrm{Sub}} := \mathbf{I} - \tilde{\mathbf{A}}_{\mathrm{Sub}}^{-1}\mathbf{A} = \tilde{\mathbf{A}}_{\mathrm{Sub}}^{-1}(\tilde{\mathbf{A}}_{\mathrm{Sub}} - \mathbf{A})$ such that the error-amplification relation (7) translates into

$$\begin{bmatrix} \epsilon_1^{n+1} \\ \epsilon_2^{n+1} \\ \epsilon_3^{n+1} \\ \epsilon_4^{n+1} \\ \epsilon_5^{n+1} \end{bmatrix} = \begin{pmatrix} 0 & 0 & 0 & 0 & E_{15} \\ 0 & 0 & 0 & 0 & E_{25} \\ 0 & 0 & 0 & 0 & E_{35} \\ 0 & 0 & 0 & 0 & E_{45} \\ 0 & 0 & 0 & 0 & E_{55} \end{pmatrix} \begin{bmatrix} \epsilon_1^n \\ \epsilon_2^n \\ \epsilon_3^n \\ \epsilon_4^n \\ \epsilon_5^n \end{bmatrix}, \tag{13a}$$

where the entries are defined as

$$E_{15} = -A_{11}^{-1}A_{15}, \tag{13b}$$
$$E_{25} = A_{22}^{-1}A_{21}A_{11}^{-1}A_{15}, \tag{13c}$$
$$E_{35} = -A_{33}^{-1}(A_{32}A_{22}^{-1}A_{21} - A_{31})A_{11}^{-1}A_{15}, \tag{13d}$$
$$E_{45} = A_{44}^{-1}A_{43}A_{33}^{-1}(A_{32}A_{22}^{-1}A_{21} - A_{31})A_{11}^{-1}A_{15}, \tag{13e}$$
$$E_{55} = -A_{55}^{-1}A_{54}A_{44}^{-1}A_{43}A_{33}^{-1}(A_{32}A_{22}^{-1}A_{21} - A_{31})A_{11}^{-1}A_{15}. \tag{13f}$$

Eq. (13) conveys that the subiteration error-amplification matrix is highly rank-deficient and, more specifically, its rank is equal to the minimum rank of the contributing block matrices in E_{55}.

It is important to note that in general the dimensions of the block matrices A_{11}, A_{33} and A_{55} associated with the interface variables are negligible compared to the dimensions of the fluid and structure block matrices, A_{22} and A_{44}, respectively, because the former refer to interface functions. Hence, the rank of the error-amplification matrix will generally be determined by the dimension of a block matrix associated with the interface. This rank-deficiency has important consequences. In particular, it implies that the error components $\epsilon_1^n, \ldots, \epsilon_4^n$ are mapped onto zero and, hence, do not contribute to $\boldsymbol{\epsilon}^{n+1}$. The only error component that propagates from $\boldsymbol{\epsilon}^n$ to $\boldsymbol{\epsilon}^{n+1}$ is ϵ_5^n. More precisely, ϵ_5^n contributes to all components in $\boldsymbol{\epsilon}^{n+1}$ due to the particular structure of the error-amplification matrix in (13). Thus, if the subiteration process is provided with the exact structure displacement $\bar{q}_5 = \bar{z}$, and, accordingly, $\epsilon_5 = 0$, then the method yields the solution to the aggregated equations in a

single iteration. Moreover, from Eqs. (7) and (13), it is possible to derive a bound on the aggregated error, $\boldsymbol{\epsilon}$, in terms of the error in the structure interface displacement, ϵ_5, as follows

$$\|\boldsymbol{\epsilon}^{n+1}\| \leq \gamma \|E_{55}^n\| \|\epsilon_5^0\|, \qquad \gamma \in \mathbb{R}_+ \,, \tag{14}$$

with γ a constant depending on $\|\mathbf{E}_{\mathrm{Sub}}\|$, but independent of n. If the spectral radius $\mathrm{spr}(E_{55}) < 1$, then $\boldsymbol{\epsilon}^n \to 0$ and, hence, $\mathbf{q}^n \to \bar{\mathbf{q}}$ as $n \to \infty$. Moreover, from Eq. (14) it is apparent that the precise convergence behaviour of subiteration is determined by the properties of E_{55}; see Section 3.3 for further elaboration.

We can assign a particular meaning to the block matrix E_{55} in Eq. (13), which specifies the error amplification in the structure interface displacement, viz.,

$$\epsilon_5^{n+1} = E_{55} \epsilon_5^n . \tag{15a}$$

To this end, we linearize Eq.(8) around the solution $\bar{z} = \bar{q}_5$, subtract the fixed-point equation and obtain

$$\epsilon_5^{n+1} = C' \epsilon_5^n . \tag{15b}$$

From Eqs. (15a) and (15b), we can identify the block matrix E_{55} as the discrete representation of the subiteration-operator derivative C'.

Another observation that can be made from Eq. (13) is that the block matrices associated with the fluid and the structure, A_{22} and A_{44}, respectively, contribute to E_{55} only through projections onto the interface; see Eq. (13f). This indicates that the interior complexity of fluid and structure models yields only an indirect effect on the convergence of the subiteration method.

3.3 Nonnormality of subiteration

In this section, we briefly elaborate on the nonnormality of the subiteration operator, as such nonnormality has severe implications for the convergence behaviour of the subiteration method; see Ref. [9] for details. Moreover, nonnormality has implications also for the GMRES convergence bounds; see Section 4.5.

On linear approximation, convergence of the subiteration process requires that the spectral radius of the subiteration-operator derivative C' is strictly less than one, i.e., $\mathrm{spr}(C') < 1$ or, equivalently, $\mathrm{spr}(E_{55}) < 1$ in conformity with Eq. (15). Note, however, that the spectral radius only determines the asymptotic convergence behaviour of the method. The transient convergence behaviour is determined by the norm $\|C'\|$ or, equivalently, by $\|E_{55}\|$. Due to nonnormality of the subiteration-operator derivative C', the spectral radius and norm can be disparate and, in particular, $\mathrm{spr}(E_{55})$ can be much smaller than $\|E_{55}\|$. This disparity can give rise to non-monotonous convergence of the method, i.e., transient divergence can precede asymptotic convergence; see Ref. [20, ch. 2] for examples and, more specifically, Ref. [9]. To elucidate the above elaboration, we note that the error in the n-th iterate can be bounded in conformity with Eq. (15) as

$$(\mathrm{spr}(E_{55}))^n \leq \|\epsilon_5^n\| / \|\epsilon_5^0\| \leq \|E_{55}^n\| \leq \kappa(X) (\mathrm{spr}(E_{55}))^n , \tag{16}$$

where $\kappa(X) := \|X\| \|X^{-1}\|$ denotes the condition number of the matrix of eigenvectors, X, of E_{55}. For a normal matrix, the eigenvectors are orthonormal and, accordingly, $\kappa(X) = 1$, so that the upper and lower bounds in (16) coincide. For a nonnormal matrix, however, the eigenvectors are non-orthogonal and $\kappa(X)$ can be very large. In combination with the upper bound $\|E_{55}^n\| \leq \|E_{55}\|^n$, the bounds in (16) imply that if $\mathrm{spr}(E_{55}) < 1 < \|E_{55}\|$ and $\kappa(X)$ is large, then the initial error can be amplified by many orders of magnitude before it eventually decreases at an asymptotic rate determined by $\mathrm{spr}(E_{55})$. The transient error growth can cause failure of the iterative method despite formal stability. In order to control nonnormality-induced divergence, the computational time step can be reduced; see Ref. [9]. However, this generally renders the method inefficient.

3.4 Subiteration preconditioning

For the ensuing presentation of the combined subiteration/GMRES method in Section 4, it is elucidating to construe subiteration as a preconditioner for GMRES, following the concepts of Ref. [21].

The subiteration iterates computed according to the recursion (12) span a Krylov space corresponding to a left-preconditioned aggregated system:

$$\mathbf{q}^{n+1} - \mathbf{q}^n \in \mathrm{span}\{\tilde{\mathbf{A}}^{-1}\mathbf{r}^0, (\tilde{\mathbf{A}}^{-1}\mathbf{A})\tilde{\mathbf{A}}^{-1}\mathbf{r}^0, \ldots, (\tilde{\mathbf{A}}^{-1}\mathbf{A})^n\tilde{\mathbf{A}}^{-1}\mathbf{r}^0\} = \boldsymbol{\mathcal{K}}^{n+1}(\tilde{\mathbf{A}}^{-1}\mathbf{A}, \tilde{\mathbf{A}}^{-1}\mathbf{r}^0), \quad n = 0, 1, \ldots, \tag{17}$$

where for ease of notation we have dropped the subscript in $\tilde{\mathbf{A}}_{\mathrm{Sub}}$ and the tilde in $\tilde{\mathbf{q}}^{n+1}$, and denoted the Krylov space of dimension $n+1$ by $\boldsymbol{\mathcal{K}}^{n+1}$. Moreover, in Eq. (17), we have implied that, on linear approximation, the residual of the linear problem (3)

$$\mathbf{r}^n := \mathbf{A}\mathbf{q}^n - \mathbf{A}\mathbf{q}^{n-1} + \mathbf{R}(\mathbf{q}^{n-1}), \quad n = 1, 2, \ldots \tag{18}$$

is identical to the residual of the nonlinear problem (1), i.e., $\mathbf{r}^n = \mathbf{R}(\mathbf{q}^n)$. With this identity and provided with $\mathbf{r}^0 = \mathbf{R}(\mathbf{q}^0)$, the residual of the linear problem can be defined recursively as

$$\mathbf{r}^n := \mathbf{A}\mathbf{q}^n - \mathbf{A}\mathbf{q}^{n-1} + \mathbf{r}^{n-1}, \quad n = 1, 2, \ldots, \tag{19}$$

and Eq. (12) can be rewritten as

$$\mathbf{q}^{n+1} - \mathbf{q}^n = -\tilde{\mathbf{A}}^{-1}\mathbf{r}^n, \quad n = 0, 1, \ldots. \tag{20}$$

The proof of Eq. (17) follows straightforwardly by induction. Clearly, the assertion holds for $n = 0$:

$$\mathbf{q}^1 - \mathbf{q}^0 = -\tilde{\mathbf{A}}^{-1}\mathbf{r}^0 \in \mathrm{span}\{\tilde{\mathbf{A}}^{-1}\mathbf{r}^0\} \tag{21}$$

in conformity with Eq. (20). The induction makes use of the premise

$$\mathbf{q}^n - \mathbf{q}^{n-1} \in \mathrm{span}\{\tilde{\mathbf{A}}^{-1}\mathbf{r}^0, \ldots, (\tilde{\mathbf{A}}^{-1}\mathbf{A})^{n-1}\tilde{\mathbf{A}}^{-1}\mathbf{r}^0\}. \tag{22}$$

Starting from the left-hand-side of Eq. (17) and invoking Eqs. (19), (20) and (22), it holds that

$$\begin{aligned}
\mathbf{q}^{n+1} - \mathbf{q}^n = -\tilde{\mathbf{A}}^{-1}\mathbf{r}^n &= -\tilde{\mathbf{A}}^{-1}(\mathbf{A}\mathbf{q}^n - \mathbf{A}\mathbf{q}^{n-1} + \mathbf{r}^{n-1}) = -\tilde{\mathbf{A}}^{-1}(\mathbf{A}[\mathbf{q}^{n-1} - \tilde{\mathbf{A}}^{-1}\mathbf{r}^{n-1}] - \mathbf{A}\mathbf{q}^{n-1} + \mathbf{r}^{n-1}) \\
&= -\tilde{\mathbf{A}}^{-1}\mathbf{r}^{n-1} + (\tilde{\mathbf{A}}^{-1}\mathbf{A})\tilde{\mathbf{A}}^{-1}\mathbf{r}^{n-1} \\
&\in \mathrm{span}\{\tilde{\mathbf{A}}^{-1}\mathbf{r}^0, \ldots, (\tilde{\mathbf{A}}^{-1}\mathbf{A})^{n-1}\tilde{\mathbf{A}}^{-1}\mathbf{r}^0\} + (\tilde{\mathbf{A}}^{-1}\mathbf{A})\mathrm{span}\{\tilde{\mathbf{A}}^{-1}\mathbf{r}^0, \ldots, (\tilde{\mathbf{A}}^{-1}\mathbf{A})^{n-1}\tilde{\mathbf{A}}^{-1}\mathbf{r}^0\} \\
&= \mathrm{span}\{\tilde{\mathbf{A}}^{-1}\mathbf{r}^0, \ldots, (\tilde{\mathbf{A}}^{-1}\mathbf{A})^{n-1}\tilde{\mathbf{A}}^{-1}\mathbf{r}^0, (\tilde{\mathbf{A}}^{-1}\mathbf{A})^n\tilde{\mathbf{A}}^{-1}\mathbf{r}^0\} \\
&= \boldsymbol{\mathcal{K}}^{n+1}(\tilde{\mathbf{A}}^{-1}\mathbf{A}, \tilde{\mathbf{A}}^{-1}\mathbf{r}^0).
\end{aligned} \tag{23}$$

This completes the proof of Eq. (17).

Our error-amplification analysis in Section 3.2 conveys that the eigenvalues of $\tilde{\mathbf{A}}^{-1}\mathbf{A}$ exhibit a much more favourable distribution than those of $\mathbf{A}$. In particular, Eq. (13) imparts that most eigenvalues of $\tilde{\mathbf{A}}^{-1}\mathbf{A}$ are 1. This makes subiteration a good preconditioner for the aggregated equations. Thus, instead of using subiteration as a solver, we will employ it as a preconditioner for GMRES; see Section 4.

The rank-deficiency of $\tilde{\mathbf{A}}^{-1}\mathbf{A}$ and, moreover, the fact that the error-amplification behaviour is essentially determined by the properties of E_{55} (see Eq. (14)), have important implications for the Krylov method. In particular, it follows that a Krylov method solves the linear system (3) in at most N steps, where $N := \mathrm{rank}(\tilde{\mathbf{A}}^{-1}\mathbf{A}) = \mathrm{rank}(E_{55})$. Moreover, on account of the rank-deficiency and the particular structure of $\tilde{\mathbf{A}}^{-1}\mathbf{A}$, the Krylov vectors need not contain all degrees-of-freedom, but only those associated with the interface degrees-of-freedom. This enables an efficient storage of the Krylov space and, moreover, renders the computational cost of the least-squares problem low in contrast to approaches which apply GMRES to the aggregated equations [12, 13], or to the Schur complement pertaining to the structure [14].

4. Error-amplification analysis of subiteration-preconditioned GMRES

In this section, we present a detailed error-amplification analysis of the combined subiteration/GMRES method. To this end, we introduce in Section 4.1 the GMRES method with subiteration preconditioning. Moreover, we establish the Schur complement associated with the interface displacement. The Schur complement plays a central role in our investigation in that it enables us to analyse the considered solution methods in terms of their approximation properties for the Schur complement. The subiteration-preconditioned GMRES method allows for optional reuse of Krylov vectors in subsequent invocations of GMRES. This reuse option is considered in Section 4.2. Next, we analyse the error-amplification properties of the subiteration-preconditioned GMRES method, first without the reuse option (Section 4.3), and subsequently with reuse (Section 4.4). Finally, in Section 4.5, we consider the convergence behaviour of subiteration-preconditioned GMRES, and we derive sharp upper bounds for the GMRES residual.

4.1 Subiteration-preconditioned GMRES

On account of the fact that the subiteration iterates span a Krylov space, and that subiteration exhibits favourable error-amplification properties, subiteration constitutes an apt preconditioner for GMRES. The combined subiteration/GMRES method comprises the following steps: firstly, one subiteration to condense the errors into a low-dimensional subspace and, moreover, to obtain a particular form of the Schur complement, and secondly, the application of GMRES to the Schur-complement equation, which yields the solution of the structure interface displacement. Finally, another subiteration is required to compute the remaining components of the solution vector.

The Schur complement associated with the interface constitutes a key element in the analysis of the subiteration-preconditioned GMRES method. Therefore, let us first introduce the notion of the Schur complement associated with the structure interface displacement q_5 and the linear-algebraic system (3b). To this end, we translate the system (3b) into Schur form

$$\begin{pmatrix} A_{11} & 0 & 0 & 0 & A_{15} \\ A_{21} & A_{22} & 0 & 0 & 0 \\ A_{31} & A_{32} & A_{33} & 0 & 0 \\ 0 & 0 & A_{43} & A_{44} & 0 \\ 0 & 0 & 0 & 0 & S \end{pmatrix} \begin{bmatrix} q_1^{n+1} - q_1^n \\ q_2^{n+1} - q_2^n \\ q_3^{n+1} - q_3^n \\ q_4^{n+1} - q_4^n \\ q_5^{n+1} - q_5^n \end{bmatrix} = - \begin{bmatrix} R_1(\mathbf{q}^n) \\ R_2(\mathbf{q}^n) \\ R_3(\mathbf{q}^n) \\ R_4(\mathbf{q}^n) \\ R_S(\mathbf{q}^n) \end{bmatrix} \tag{24a}$$

with the Schur-complement matrix S and the corresponding right-hand-side vector $R_S(\mathbf{q}^n)$ defined respectively as

$$S := -A_{55}^{-1} A_{54} A_{44}^{-1} A_{43} A_{33}^{-1} (A_{32} A_{22}^{-1} A_{21} - A_{31}) A_{11}^{-1} A_{15} - I \tag{24b}$$

and

$$\begin{aligned} R_S(\mathbf{q}^n) := A_{55}^{-1} \big(-R_5(\mathbf{q}^n) + A_{54} A_{44}^{-1} \big(R_4(\mathbf{q}^n) + A_{43} A_{33}^{-1} \left(-R_3(\mathbf{q}^n) \right. \\ \left. + A_{32} A_{22}^{-1} \left(R_2(\mathbf{q}^n) - A_{21} A_{11}^{-1} R_1(\mathbf{q}^n) \right) + A_{31} A_{11}^{-1} R_1(\mathbf{q}^n) \right) \big) \big) . \end{aligned} \tag{24c}$$

Note that the fifth equation in (24a) decouples. This equation constitutes the Schur-complement equation, viz.,

$$S(q_5^{n+1} - q_5^n) = -R_S(\mathbf{q}^n). \tag{25}$$

The expression of the right-hand-side vector $R_S(\mathbf{q}^n)$ in (24c) can be significantly simplified when provided with residuals $R_1(\mathbf{q}^n), \ldots, R_5(\mathbf{q}^n)$ based on a $\mathbf{q}^n$ that has been generated by subiteration. To substantiate this assertion, we recall from Section 3.1 that, provided with an initial approximation of the structure interface displacement q_5^{n-1}, the subiteration steps (S1)–(S5) can be conceived as a sequence of mappings, viz., $q_5^{n-1} \mapsto q_1^n \mapsto q_2^n \mapsto q_3^n \mapsto q_4^n \mapsto q_5^n$. For convenience, and without loss of generality, let us shift the indices according to $q_5^n \mapsto q_1^n \mapsto q_2^n \mapsto q_3^n \mapsto q_4^n \mapsto \hat{q}_5^{n+1}$. The 'hat' symbol serves to indicate that $\hat{q}_5^{n+1}$ constitutes only an intermediate value which will be replaced by the

subsequent invocation of GMRES. Note that, in conformity with the mapping above and Eq. (1), the residuals $R_1(\mathbf{q}^n), \ldots, R_4(\mathbf{q}^n)$ are identically zero, and $R_5(\mathbf{q}^n) = R_{\mathrm{Sub}}(q_5^n) = \hat{q}_5^{n+1} - q_5^n$ in accordance with Eqs. (2) and (11). In summary, one subiteration generates a vector $\mathbf{q}^n = [q_1^n, q_2^n, q_3^n, q_4^n, q_5^n]$ such that the corresponding residual vector is $\boldsymbol{R}(\mathbf{q}^n) = [0, 0, 0, 0, \hat{q}_5^{n+1} - q_5^n]$. Provided with the residual vector $\boldsymbol{R}(\mathbf{q}^n)$ and noting that $A_{55} = -I$, Eq. (24c) simplifies considerably. Using the notation $z := q_5$ introduced in Section 3.1, the Schur-complement equation (25) can then be written as

$$S(z^{n+1} - z^n) = -(\hat{z}^{n+1} - z^n)\,. \tag{26a}$$

With the definition (13f), the expression for the Schur complement (24b) can be specified as

$$S = E_{55} - I. \tag{26b}$$

Recall from Section 3.2 that the matrix E_{55} constitutes the discrete representation of the subiteration-operator derivative C'. Hence, Eq. (26a) can be identified as a Newton iteration for the fixed-point residual equation (10), viz.,

$$R'_{\mathrm{Sub}}(z^{n+1} - z^n) = -R_{\mathrm{Sub}}(z^n), \tag{27}$$

and $S = R'_{\mathrm{Sub}}$. Note that one subiteration is required to provide the residual $R_{\mathrm{Sub}}(z^n)$ that forms the right-hand-side of the Schur-complement equation (26a).

The Schur-complement matrix S in (26a) is generally not known explicitly. However, if a Krylov method is used to solve the linear system (26a), then S is only required in the form of matrix-vector products, which can be approximated by finite differences. To this end, we note that on linear approximation

$$S(z_j^{n+1} - z^n) = r_j^{n+1} - r^n, \tag{28}$$

where j indicates the counter for the GMRES iterations. In Eq. (28), the action of the Schur-complement matrix S on the increment vector $(z_j^{n+1} - z^n)$ yields the corresponding residual sensitivity $(r_j^{n+1} - r^n)$. For a Krylov method that makes use of the finite-difference approximation (28), we thus require a space of *search directions* in the form of updates around the current linearization state z^n, and the corresponding space of *residual sensitivities* in the form of increments around r^n. We then seek an approximation to the solution of Eq. (26a) from the search space $\mathcal{K}^m$, according to

$$(z^{n+1} - z^n) \in \mathcal{K}^m := \mathrm{span}\{z_j^{n+1} - z^n\}_{j=1}^{j=m}, \tag{29}$$

where the z_j^{n+1} are generated by successive subiterations. For a formal proof that $\mathcal{K}^m$ constitutes a Krylov space we refer to Ref. [10]. Denoting the vectors of search directions by $u_j = z_j^{n+1} - z^n$ with $j = 1, \ldots, m$, we collect them in a matrix $U_m := [u_1, \ldots, u_m]$. Moreover, we require the space of residual sensitivities, $\mathcal{R}^m$, that corresponds to the space of search vectors, viz.,

$$(r^{n+1} - r^n) \in \mathcal{R}^m := \mathrm{span}\{r_j^{n+1} - r^n\}_{j=1}^{j=m}. \tag{30}$$

Denoting the residual-sensitivity vectors by $v_j = r_j^{n+1} - r^n$ with $j = 1, \ldots, m$, we collect them in a matrix $V_m := [v_1, \ldots, v_m]$. In conformity with Eq. (28), V is the image of U under S, i.e.,

$$SU = V. \tag{31}$$

We remark that the generation of the search and residual-sensitivity space implicitly builds an approximation to the Schur-complement matrix. If the spaces U and V are complete and have full rank, then S can be obtained from Eq. (31) by $S = VU^{-1}$.

Provided with the linearization state z^n and the corresponding residual r^n, the generation of one pair of search direction and corresponding residual sensitivity, $(u_j, v_j) = (z_j^{n+1} - z^n, r_j^{n+1} - r^n)$, is at the expense of one subiteration. The subiteration is required for the evaluation of the residual

$r_j^{n+1} := R_{\mathrm{Sub}}(z_j^{n+1}) = z_{j+1}^{n+1} - z_j^{n+1}$. At the same time, it also generates a new search direction $u_{j+1} = z_{j+1}^{n+1} - z^n$. In practice, though, the search direction must be orthogonalized with respect to the previously generated search directions to avoid ill-conditioning of the search space.

To construct an approximation to the solution of the linear problem (26a), we make the following ansatz

$$z^{n+1} - z^n = \sum_{j=1}^{j=m} \alpha_j u_j \tag{32}$$

with coefficients α_j that are determined from the requirement that the update (32) minimizes the residual of the Schur-complement equation (26a), viz.,

$$\bar{\boldsymbol{\alpha}} = \arg\min_{\boldsymbol{\alpha}} \| r^n + S \sum_{j=1}^{j=m} \alpha_j u_j \| = \arg\min_{\boldsymbol{\alpha}} \| r^n + \sum_{j=1}^{j=m} \alpha_j v_j \| \tag{33}$$

in conformity with the finite-difference approximation (28). Hence, the considered Krylov method is a minimal-residual method. As the spaces $\mathcal{K}^m$ and $\mathcal{R}^m$ are generally not complete, Eq. (33) is solved in a least-squares sense (see, e.g., Ref. [22, ch. 5.3]), i.e., the coefficients $\bar{\boldsymbol{\alpha}}$ are obtained from the solution of the normal equation

$$V^T V \bar{\boldsymbol{\alpha}} = -V^T r^n. \tag{34}$$

The computational cost involved in solving Eq. (34) is small in comparison to that of a subiteration, because the least-squares problem (33) is confined to the interface degrees-of-freedom. With coefficients $\bar{\boldsymbol{\alpha}}$ determined from the solution of Eq. (34), the norm of the residual of the Schur-complement equation (26a) is given by

$$\xi_m := \| r^n + \sum_{j=1}^{j=m} \bar{\alpha}_j v_j \|. \tag{35}$$

If the residual norm ξ_m in (35) satisfies a given tolerance, the coefficients $\bar{\boldsymbol{\alpha}}$ are used to determine the corresponding approximate solution z^{n+1} from Eq. (32). Note that in the actual nonlinear process, the residual norm given by Eq. (35) constitutes an estimate for the norm of the nonlinear residual; cf. Ref. [10].

Having established the equations solved by subiteration and GMRES, we can now establish the aggregated system that is solved by the combined subiteration/GMRES method. To this end, we recall that the subiteration process acting on the aggregated system (12) and the GMRES method acting on the Schur-complement equation (26a) correspond to the mappings $q_5^n \mapsto \tilde{q}_1^{n+1} \mapsto \ldots \mapsto \tilde{q}_4^{n+1} \mapsto \hat{q}_5^{n+1}$ and $\hat{q}_5^{n+1} \mapsto q_5^{n+1}$, respectively. The combined subiteration/GMRES method then corresponds to the combined mapping $q_5^n \mapsto q_5^{n+1}$. Upon combining the Schur-complement equation (26a) with the system (12a) associated with subiteration, we obtain

$$\begin{pmatrix} A_{11} & 0 & 0 & 0 & 0 \\ A_{21} & A_{22} & 0 & 0 & 0 \\ A_{31} & A_{32} & A_{33} & 0 & 0 \\ 0 & 0 & A_{43} & A_{44} & 0 \\ 0 & 0 & 0 & A_{54} & -A_{55}S \end{pmatrix} \begin{bmatrix} \tilde{q}_1^{n+1} - q_1^n \\ \tilde{q}_2^{n+1} - q_2^n \\ \tilde{q}_3^{n+1} - q_3^n \\ \tilde{q}_4^{n+1} - q_4^n \\ q_5^{n+1} - q_5^n \end{bmatrix} = - \begin{bmatrix} R_1(\mathbf{q}^n) \\ R_2(\mathbf{q}^n) \\ R_3(\mathbf{q}^n) \\ R_4(\mathbf{q}^n) \\ \hat{q}_5^{n+1} - q_5^n \end{bmatrix}. \tag{36}$$

Clearly, the system (36) retains the lower block-triangular structure induced by the subiteration method. As subiteration discards the A_{15} entry in (3b), two iterations are required to compute the aggregated solution vector: Upon solution of Eq. (36) only the component q_5^{n+1}, obtained from the Schur-complement equation, corresponds to the solution of (3b). To determine the remaining components of the solution vector, one additional subiteration needs to be carried out; see also Section 3.1.

As we already mentioned in the beginning of this section with respect to the combined subiteration/GMRES method, prior to an invocation of GMRES, a subiteration needs to be carried out,

which serves two purposes. Firstly, it condenses all error components into a low-dimensional subspace associated with the interface; cf. Section 3.2. Secondly, the subiteration process provides the right-hand-side residual for the Schur-complement equation.

So far we have exclusively considered the solution of the linear-algebraic system (3). However, in practice, the system of equations (1) is nonlinear. The application of Newton's method to the nonlinear system gives rise to a sequence of linear systems. We solve these linear systems by subiteration-preconditioned GMRES. Hence, we can alternatively classify the considered solution technique as a *Newton-Krylov method* [23], in which subiteration acts as a preconditioner.

Having established the subiteration-preconditioned GMRES method, let us briefly address some algorithmic aspects of the method; for details see Ref. [10]. For computational efficiency, it is customary to set the convergence tolerance of the linear problem (3) relative to the norm of the actual residual of the nonlinear problem (1). Moreover, it is important to endow the method with Gram-Schmidt orthonormalization and underrelaxation. The former improves the robustness, the latter facilitates the subiteration process and allows the combination of GMRES with subiteration even if subiteration is formally unstable.

4.2 Reuse of Krylov vectors

As each Newton step involves the solution of a Schur-complement system by a Krylov method, the Newton-Krylov method lends itself naturally to reuse of Krylov vectors in subsequent Newton steps. Reuse of Krylov vectors only requires minor modifications. Essentially, it requires that the counter j in Eqs. (29)–(30) is not reset in each Newton step. The available search and residual-sensitivity spaces are then augmented instead of overwritten. Moreover, an additional residual estimate corresponding to the reduction of the updated nonlinear residual in the available space must be determined; see [10]. Depending on this initial residual estimate, the search and residual-sensitivity spaces are further augmented, or a Newton update is carried out. We remark that, once a single vector is reused, the search space does formally no longer constitute a Krylov space, which implies that the search directions do not necessarily constitute 'preferential' search directions. Nevertheless, typically much fewer Krylov vectors need to be added to the reused space than are generated for a reconstructed Krylov space, which can result in considerable computational savings. However, the viability and benefit of the reuse option is contingent on the similarity between the reused and the reconstructed space.

In addition to the reuse option within a single time step, reuse is also possible within subsequent time steps. In the latter case, the available search and residual-sensitivity spaces are carried over from one time interval to the next. There is, however, a difference between the two reuse options. Within a single time step, the nonlinear subiteration operator does not change, but only its linearization state does. In contrast, the subiteration operator does change between time steps on account of differences in initial conditions. As long as the operators in subsequent time steps are sufficiently similar, reuse will be beneficial. We will assess the potential and limitations of the reuse option based on an error-amplification analysis in Section 4.4.

Next, let us briefly discuss the effect of reuse on the Schur complement. We recall from Section 4.1 that search and residual-sensitivity space implicitly approximate the exact Schur-complement matrix S; cf. Eq. (31). Likewise, reusing the search and residual-sensitivity space implies an approximation $\tilde{S}$ to the exact S. With such an approximation $\tilde{S}$, the exact Schur-complement equation (26a) translates into

$$\tilde{S}(\tilde{q}_5^{n+1} - q_5^n) = -R(q_5^n), \tag{37}$$

which yields an approximation $\tilde{q}_5^{n+1}$ to q_5^{n+1}. The system solved by the subiteration-preconditioned GMRES method with reuse can still be cast in the form of Eq. (36), but with the Schur-complement matrix S replaced by $\tilde{S}$. The effect of reuse and augmentation of the spaces on the error-amplification behaviour can thus be investigated in terms of the approximation properties for the Schur complement.

To place the reuse option into context, we briefly consider two alternative approaches for reusing computational information, viz., so-called *search space injection* [24] and *nested preconditioning* [25].

In particular, we establish commonalities and differences between these approaches and our methodology of reusing Krylov vectors. We consider first the *search space injection* from Ref. [24]. A commonality with our approach consists in storing a search space and its image under the operator, which allows for straightforward reuse and augmentation of these spaces. An important difference to Ref. [24] is that in our problem the operator is not known explicitly, but its action on a vector has to be evaluated by subiteration. Moreover, in contrast to [24], we consider the reuse of Krylov vectors in subsequent invocations of GMRES for which the left-hand-side matrix as well as the right-hand-side vector have changed. Finally, at variance with [24], in our approach the Krylov space need only contain the interface degrees-of-freedom and, hence, storage is not an issue. Next, we consider *nested preconditioning* from Ref. [25]. Likewise, this approach solves the linear problems by a Krylov method. Upon solution of the linear system, the generated Krylov space is condensed into a preconditioning matrix. However, an incomplete Krylov space would translate into a rank-deficient preconditioning matrix. To ensure invertability of the preconditioner, some 'adhoc' terms are added to this matrix in [25]. The preconditioning matrix is then applied to the subsequent linear system, which is again solved by a Krylov method. Successive solution of the linear systems thus generates a sequence of preconditioners, which are applied in a 'nested' way to the subsequent linear problems. The disadvantages of this approach pertain to the 'adhoc' terms, which can interfere with the performance of subsequent preconditioners. Moreover, due to storage requirements, the number of preconditioners must be limited by restarts. These disadvantages can be avoided by methods in conformity with search space injection and reuse of Krylov vectors. Finally, we remark that Ref. [25] restricts reuse to subsequent Newton iterations, but does not consider reuse in subsequent time steps. However, it is in particular the reuse in subsequent time steps which can substantially reduce the computational cost in transient fluid-structure-interaction problems.

4.3 Error-amplification analysis

In this section, we derive the error-amplification matrix for the combined subiteration/GMRES method. In our analysis, the Schur complement from Section 4.1 plays a central role: the solution methods under consideration can all be conceived as instances of an inexact Newton method with a specific approximation to the Schur-complement matrix. Thus, an error-amplification analysis based on the Schur complement allows for a direct comparison of the subiteration process separately, the subiteration method with GMRES acceleration, and the subiteration method with GMRES acceleration and reuse, from a unified viewpoint.

As the subiteration-preconditioned GMRES method can be conceived as an instance of an inexact Newton method in conformity with Section 2.2, its error-amplification matrix is given in a general form by Eq. (7). The implied approximation $\tilde{\mathbf{A}}$ to the exact Jacobian $\mathbf{A}$ of the Newton process is given by Eq. (36). However, to analyse the general case with an approximation to the Schur complement, for instance due to reuse of Krylov vectors, we consider the Jacobian matrix from Eq. (36) with the Schur complement S replaced by a complete and full-rank approximation $\tilde{S}$. Substituting the expressions for $\mathbf{A}$ and $\tilde{\mathbf{A}}$ in Eq. (7) yields, after some straightforward manipulations, the error-amplification relation for the subiteration-preconditioned GMRES method:

$$\begin{bmatrix} \epsilon_1^{n+1} \\ \epsilon_2^{n+1} \\ \epsilon_3^{n+1} \\ \epsilon_4^{n+1} \\ \epsilon_5^{n+1} \end{bmatrix} = \begin{pmatrix} 0 & 0 & 0 & 0 & E_{15} \\ 0 & 0 & 0 & 0 & E_{25} \\ 0 & 0 & 0 & 0 & E_{35} \\ 0 & 0 & 0 & 0 & E_{45} \\ 0 & 0 & 0 & 0 & I - \tilde{S}^{-1}S \end{pmatrix} \begin{bmatrix} \epsilon_1^{n} \\ \epsilon_2^{n} \\ \epsilon_3^{n} \\ \epsilon_4^{n} \\ \epsilon_5^{n} \end{bmatrix}. \tag{38}$$

Eq. (38) expresses the error-amplification under a combined subiteration / GMRES step with an approximation $\tilde{S}$ to the Schur complement matrix S. In analogy to our observations in Section 3.2, we find that the error-amplification matrix in (38) is highly rank-deficient. In particular, the only non-zero eigenvalues are the ones of the lower block-diagonal matrix $I - \tilde{S}^{-1}S$, which expresses the mapping of one error in the structure interface displacement onto the next.

In fact, Eq. (38) is of a general form and encompasses the following three special cases: Firstly, upon setting $\tilde{S} = -I$, Eq. (38) reverts to Eq. (13a), and we recover the error-amplification matrix of the subiteration method. By virtue of the result from Section 4.1 that S constitutes the discrete approximation to $R'_{\mathrm{Sub}} := C' - I$, the identity $\tilde{S} = \tilde{S}_{\mathrm{Sub}} := -I$ conveys that $\tilde{S}_{\mathrm{Sub}}$ implies the most trivial approximation to R'_{Sub}. Secondly, upon setting $\tilde{S} = S$, the lower block-diagonal entry is zero, and we obtain the error-amplification matrix of subiteration combined with 'exact' GMRES, i.e., no approximations are made to search and residual-sensitivity space. This is not to be confused with the error-amplification matrix of the exact Newton method which is identically zero; cf. Section 2.2. In the case of subiteration combined with GMRES, the matrix in Eq. (38) is nilpotent of index 2, i.e., $E^n \equiv 0, n \geq 2$; see, e.g., [26, ch. 1]. This implies that, to eliminate all error components and, hence, to obtain the complete vector of solution components, two applications of Eq. (38) are required. This is in agreement with the elaboration in Section 4.1, according to which one step of subiteration-preconditioned GMRES eliminates the error in q_5, and a second step eliminates the error in the remaining components of the solution vector. Thirdly, Eq. (38) specifies the error-amplification matrix of subiteration combined with GMRES for the case that an approximation $\tilde{S}$ to the exact Schur-complement matrix S is used. Such an approximation can be obtained, for instance, by reusing the search and residual-sensitivity spaces generated for the solution of the linear system (26a) in a previous Newton or time step. The error-amplification behaviour for the combined subiteration/GMRES method with reuse will be discussed in more detail in Section 4.4.

The above elaboration assumes that the Schur-complement approximation $\tilde{S}$ is complete and has full rank and is thus invertible. In practice, the generation of a complete space V $(N \times N)$ with $N := \mathrm{rank}(\tilde{\mathbf{A}}^{-1}\mathbf{A}) = \mathrm{rank}(E_{55})$ is generally too expensive. However, it is usually also not required. An incomplete space $\tilde{V}$ $(N \times k)$ with $k < N$, however, implies rank-deficiency of the Schur-complement approximation $\tilde{S}$. In that case, $\tilde{S}$ can be determined as follows: With the solution $\bar{\boldsymbol{\alpha}}$ from the normal equation (34), we consider the Newton update $\tilde{z}^{n+1} = z^n + U\bar{\boldsymbol{\alpha}}$. With $r^n = S\epsilon_5^n$ and upon subtracting the solution $\bar{z}$, we can identify the Schur-complement approximation in analogy with Eq. (38) as

$$\tilde{S}^{-1} = (\tilde{U}(\tilde{V}^T\tilde{V})^{-1}\tilde{V}^T). \tag{39}$$

We remark, however, that incompleteness of $\tilde{U}$ and $\tilde{V}$ implies that $\tilde{S}$ has $N - k$ eigenvalues equal to zero and, hence, $I - \tilde{S}^{-1}S$ has $N - k$ eigenvalues equal to 1. This entails that the corresponding error components cannot be reduced in the available space. The precise error-amplification behaviour then depends specifically on the error in the initial approximation

4.4 Analysis of the reuse option

Reuse of Krylov spaces enhances the efficiency of the method at the expense of robustness. In this section, we discuss the limitations of the reuse option based on the effect of reuse on the error-amplification behaviour of GMRES. We restrict our considerations to the case that search and residual-sensitivity space are complete and have full rank. For rank-deficient spaces the elaboration in Section 4.3 applies likewise.

With reuse, the residual-sensitivity space $\tilde{V}$ is no longer equal to the image of the search space $\tilde{U}$ under the current Schur complement S, i.e., $\tilde{V} \neq S\tilde{U}$. This is due to the fact that $\tilde{V} := \tilde{S}\tilde{U}$ may have been generated with, possibly multiple, different Schur-complement matrices, here collectively denoted by $\tilde{S}$. The benefit and limitations of the reuse option therefore depend pivotally on the similarity between S and $\tilde{S}$. If the Schur complement changes significantly in subsequent Newton iterations and time steps, the disparity between S and $\tilde{S}$ can be substantial. Clearly, this is detrimental for the effectiveness of the reuse option. Reuse fails, if the spectral radius of the error-amplification matrix exceeds 1, i.e., if $\mathrm{spr}(I - \tilde{S}^{-1}S) > 1$, in conformity with Eq. (38). The reused space is then simply too inaccurate. In Section 5.4, we consider the properties of $I - \tilde{S}^{-1}S$ for a fluid-structure-interaction model problem.

For completeness let us briefly mention another 'failure mechanism' of the reuse option. If the reused space $\tilde{V}$ is rank-deficient, then certain error components cannot be eliminated in $\tilde{V}$. If these

error components are contained in the initial approximation, then the residual estimate stalls at some point, i.e., $\xi_m \nrightarrow 0$ for $m \to N$ with $N := \mathrm{rank}(\tilde{\mathbf{A}}^{-1}\mathbf{A}) = \mathrm{rank}(E_{55})$. In that case, the algorithm breaks down; cf. Ref. [10] for further elaboration.

4.5 GMRES convergence bounds

To elaborate the implications of the nonnormality of the subiteration operator for GMRES convergence, we recall from Section 3.3 that nonnormality of E_{55} is due to non-orthogonality of its eigenvectors. By virtue of the fact that E_{55} and the Schur complement $S = E_{55} - I$ have the same eigenvectors, S is also nonnormal. This has consequences for the solution of the Schur-complement equation (26a) by GMRES. Nonnormality typically implies a severe degradation in the sharpness of the usual GMRES convergence bounds, which renders such bounds unreliable; cf. Ref. [20, ch.3]. To substantiate this statement, let us recall from Ref. [20] the following sequence of GMRES convergence bounds:

$$\|r_k\| = \min_{p\in\mathcal{P}_k} \|p(S)r_0\| = \min_{p\in\mathcal{P}_k} \|Xp(\Lambda)X^{-1}r_0\| \leq \kappa(X) \min_{p\in\mathcal{P}_k} \|p(\Lambda)\|\|r_0\|, \tag{40a}$$

which implies

$$\|r_k\|/\|r_0\| \leq \kappa(X) \min_{p\in\mathcal{P}_k} \max_{\lambda\in\mathcal{L}} |p(\lambda)|, \tag{40b}$$

where $\|\cdot\|$ denotes the standard 2-norm, $\mathcal{P}_k$ is the set of k-th-order polynomials, defined by $\mathcal{P}_k(z) := 1 - \sum_{i=1}^{i=k} \alpha_k z^k$, $\mathcal{L}$ is the spectrum of S and $\Lambda := \mathrm{diag}(\lambda_1, \ldots, \lambda_n)$ is the diagonal matrix of eigenvalues of S, X is the matrix of right eigenvectors of S, and $\kappa(X) := \|X\|\|X^{-1}\|$ is the eigenvector-matrix condition number. Nonnormality of S implies that the eigenvectors of S are non-orthogonal. Hence, the corresponding eigenvector matrix X can be severely ill-conditioned, in which case $\kappa(X)$ can be very large. It is then not clear whether GMRES indeed converges slowly, or whether the bound is simply a large overestimate of the actual residual norm. This renders the bounds (40) virtually useless. For nonnormal matrices, a sharp convergence upper bound follows from

$$\|r_k\|/\|r_0\| \leq \max_{\|u\|=1} \min_{p\in\mathcal{P}_k} \|p(S)u\|. \tag{41}$$

This bound is sharp in the sense that there exists an r_0 for which the right-hand side value is actually attained. Eq. (41) delineates the worst-case convergence, independent of the specifics of the initial residual.

5. Numerical experiments

To illustrate the theoretical results from Sections 3 and 4, we conduct numerical experiments on a model fluid-structure-interaction problem. A concise setup of the model problem is provided in Section 5.1. Section 5.2 presents results for the subiteration method separately. In Section 5.3, we assess the convergence of the subiteration-preconditioned GMRES method and determine convergence upper bounds. In Section 5.4, we investigate the viability of reusing Krylov spaces by examining the properties of the corresponding error-amplification matrix.

5.1 Experimental setup

We conduct numerical experiments on a fluid-structure system consisting of the Euler equations of gas dynamics in one spatial dimension, in connection with a nonlinear structure, viz., the Van-der-Pol oscillator, at the interface. The Euler equations in conservative form are given by

$$\frac{\partial w}{\partial t} + \frac{\partial f}{\partial x} = 0, \quad t \in (0, T), \quad x \in (0, l + \alpha(t)) \tag{42a}$$

with $\alpha(t)$ the displacement of the fluid-structure interface and

$$w := \begin{pmatrix} \rho \\ \rho v \\ E \end{pmatrix}, \quad f(w) := \begin{pmatrix} w_2 \\ w_2^2/w_1 + p(w) \\ (p(w) + w_3)w_2/w_1 \end{pmatrix}, \quad p(w) := (\gamma - 1)\left(w_3 - \frac{w_2^2}{2w_1}\right) \tag{42b}$$

and γ a constant, typically, $\gamma = 1.4$. In Eq. (42b), ρ, v, E and p denote the density, velocity, total energy and pressure of the fluid, respectively.

Eq. (42) is subject to initial and boundary conditions $w_2(0,t) = 0$, $w_2(l+\alpha(t)) = w_1(l+\alpha(t))\dot{\alpha}(t)$ and $w(x,0) = w^0(x)$, where $w^0(x)$ denotes prescribed initial conditions. The initial conditions are determined from the linearized model problem in Ref. [16]. However, we remark that for the considered small initial deflections of the oscillator, the influence of the initial conditions is small.

The structure model consists of the Van-der-Pol oscillator, viz.,

$$M\ddot{z} + Kz + \mu\beta^{-2}(z^2 - \beta^2)\dot{z} = \pi - p^0 \tag{43}$$

with $z := z(t)$ the structure displacement from its equilibrium position and M, K, μ and β suitable constants. The right member of Eq. (43) is composed of the stress $\pi := \pi(t)$ exerted by the fluid on the structure through the interface and the constant external pressure p^0. The ordinary differential equation (43) is supplemented with the initial conditions $z(0) = z^0$ and $\dot{z}(0) = \dot{z}^0$. The fluid and the structure are connected by the dynamic interface condition $p(w(l+\alpha(t),t)) = \pi(t)$ and the kinematic interface condition $\alpha(t) = z(t)$.

With $\mu = 0$, Eq. (43) simplifies to the equation of a harmonic oscillator considered in Ref. [10]. The associated fluid-structure system admits periodic solutions; cf. the linearized-system analysis in Ref. [16]. In contrast, for $\mu > 0$, the fluid-structure system given by Eqs. (42)–(43) behaves distinctly different: For non-vanishing initial conditions, the amplitude of $z(t)$ in the Van-der-Pol equation increases to approximately 2β. As a consequence, the behaviour of the system at later times is in general distinctly different from its initial behaviour and, correspondingly, the subiteration operator changes. Therefore this model problem is particularly suitable to test the reuse of Krylov spaces under adverse conditions.

The fluid-structure system is discretized by means of space/time finite elements. The adopted discretization is essentially identical to that in Ref. [16]. For completeness, we briefly summarize its setup. The space/time fluid domain is covered with a tesselation of quadrilateral elements. The number of elements in spatial direction is denoted by $N^x_{\mathbb{W}}$, the number of elements in temporal direction per unit time by $N^t_{\mathbb{W}}$. The structure mesh consists of $N^t_{\mathbb{Z}}$ elements per unit time. The fluid equations are discretized by means of a discontinuous Galerkin method with the approximation space consisting of piecewise tensor products of polynomials of degree $P_{\mathbb{W}}$ (space, time). The approximation spaces admit discontinuities across element boundaries. The elements in the fluid are connected by the modified Osher scheme and weakly enforced initial conditions. The structure equation is discretized by means of a continuous Galerkin method. The approximation space of the structure consists of piecewise polynomials of degree $P_{\mathbb{Z}}$. The connection between the elements in the structure is provided by strongly enforced initial conditions through Lagrange multipliers. The interface approximation spaces associated with kinematic and dynamic conditions comprise $N_{\mathbb{A},\mathbb{P}} = N^t_{\mathbb{Z}}$ elements per unit time, and consist of piecewise polynomials of degree $P_{\mathbb{A}}$ and $P_{\mathbb{P}}$, respectively.

We consider the fluid-structure system for representative settings of the system parameters. The parameters are listed in Table 1. The discretization is sufficiently fine to ensure that the results are essentially mesh independent. The computational time step τ is chosen of the order of the period of the linearized system. We consider three representative settings of the parameter μ which determines the nonlinearity of the structure model. In particular, we choose $\mu = 2$, 0.5 and 0, corresponding to strong, medium and vanishing structural nonlinearity, respectively. We remark that the parameter μ moreover determines the initial-growth rate of the displacement, i.e., for larger μ the initial growth of $z(t)$ is more pronounced.

5.2 Convergence of subiteration

In this section, we consider the convergence of the standard subiteration method. To this end, we investigate the properties of the corresponding error-amplification matrix and, in particular, of the lower diagonal block matrix E_{55} which yields the only non-zero eigenvalues of the error-amplification matrix; cf. Section 3.2.

Table 1: System and discretization parameters ($*$ indicates a variable parameter).

z^0	$\dot{z}^0$	l	ρ^0	c^0	K	M	μ	β	τ	$P_{\mathbb{W}}$	$P_{\mathbb{A}}$	$P_{\mathbb{Z}}$	$P_{\mathbb{P}}$	$N^x_{\mathbb{W}}$	$N^t_{\mathbb{W}}$	$N^t_{\mathbb{Z}}$
10^{-4}	0	1	20	0.5	1	1	$*$	0.025	8	$(2,2)$	4	4	3	12	4	4

For reference, Fig. 1 plots the structure displacement versus time for $\mu = 0, 0.5, 2$. The figure illustrates the significant change in the solution behaviour of the system over time. For $\mu > 0$, the amplitude of the structure oscillation increases by a factor of 500, viz., from an initial deflection $z^0 = 10^{-4}$ to approximately $5 \cdot 10^{-2}$ when the oscillation has settled into a (quasi-)periodic regime. For the larger value of μ, the amplitude increases more rapidly on account of the stronger nonlinearity of Eq. (43) and, accordingly, the oscillation settles into its periodic regime faster. In contrast, for $\mu = 0$, the amplitude remains constant and equal to the initial deflection $z^0 = 10^{-4}$. For $\mu = 2$, a slight drift in the oscillation mean is visible in Fig. 1. Mesh refinement indicates that this drift is caused by discretization error and, moreover, that this discretization error does not significantly change the results presented in the sequel.

Fig. 2 plots the spectral radius of the error-amplification matrix of subiteration versus time, viz., $(E_{55})_j := S_j + I$ in accordance with (26b), with S_j the Schur-complement matrix pertaining to time step j. The Schur complement is computed as $S = VU^{-1}$ with, in particular,

$$V^T := \nu^{-1} \left\{ \begin{pmatrix} R_{\text{Sub}}\big(u_0 + \nu(u_1 - u_0)\big) \\ \vdots \\ R_{\text{Sub}}\big(u_0 + \nu(u_n - u_0)\big) \end{pmatrix} - \begin{pmatrix} R_{\text{Sub}}(u_0) \\ \vdots \\ R_{\text{Sub}}(u_0) \end{pmatrix} \right\}, \tag{44}$$

i.e., the image space V is determined by finite differencing of the nonlinear residual operator of the (local) subiteration process, R_{Sub}, as defined below (10). Throughout, we used $\nu = 10^{-8}$.

For $\mu = 2$, there is an initial growth in the spectral radius, before it decreases to an essentially constant value of approximately 2. This initial growth is apparently related to the strong initial growth of the solution; see Fig. 1. For $\mu = 0.5$, the initial growth of the spectral radius is absent, and the spectral radius decreases to approximately 3 in the periodic regime. In either case, however, the spectral radius is larger than one and, hence, the subiteration process diverges. For reference, we also computed the spectral radius for $\mu = 0$. This spectral radius is approximately 4. Clearly, for $\mu = 0$ the spectral radius remains essentially constant in time. For a detailed analysis of the convergence behaviour of subiteration for $\mu = 0$, we refer the reader to Refs. [9, 10].

5.3 GMRES convergence bounds

To assess the convergence of the subiteration-preconditioned GMRES method, we compute

$$\sigma_k := \sup_{u \in \mathbb{R}^n} J(u) \quad \text{with} \quad J(u) := \inf_{\alpha \in \mathbb{R}^k} J(u, \alpha), \quad J(u, \alpha) := \big\|u\big\|^{-1} \big\| \big(I - \sum_{i=1}^{i=k} \alpha_i S^i\big) u \big\| . \tag{45}$$

Let us note that the convergence behaviour of the GMRES method pertaining to a particular initial residual r_0 is given by

$$\|r_k\| = \min_{\alpha} \|(I - \sum_{i=1}^{i=k} \alpha_i S^i) r_0\|. \tag{46}$$

For an illustration of the convergence behaviour of the method for the piston problem ($\mu = 0$) in specific instances we refer to Ref. [10]. One easily infers that Eq. (45) provides an upper bound to the residual reduction, i.e., $\|r_k\|/\|r_0\| \leq \sigma_k$ for all $r_0 \in \mathbb{R}^n$. Moreover, the bound in (45) is sharp in the sense that there exists an initial residual for which the bound is actually attained, in contrast to the usual GMRES convergence bounds; see Section 4.5 and also Ref. [20].

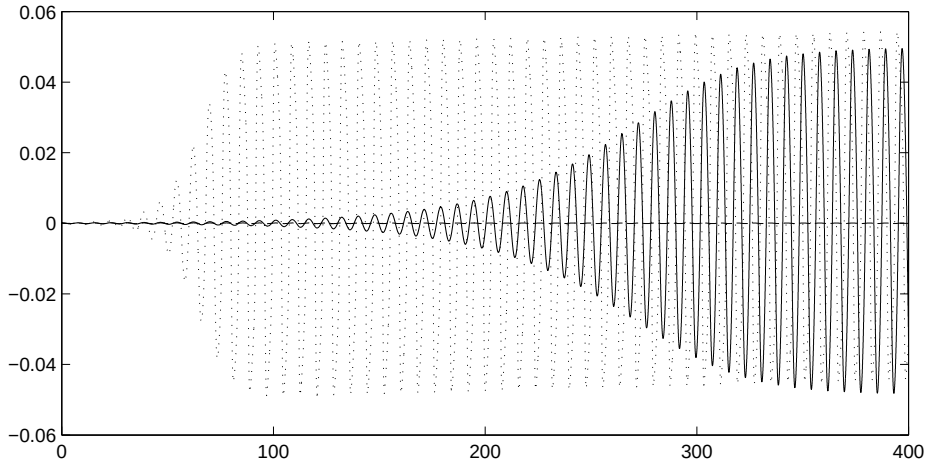

Figure 1: Structure displacement versus time for $\mu = 0.0\,(--)$, $\mu = 0.5\,(——)$ and $\mu = 2.0\,(\cdots)$.

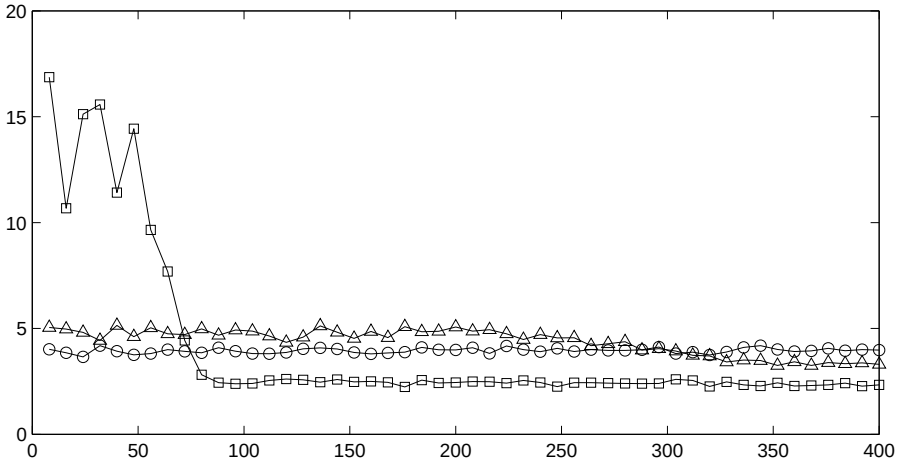

Figure 2: Spectral radius of the error-amplification matrix of subiteration, $\mathrm{spr}(E_{55})$, versus time for $\mu = 0.0\,(\circ)$, $\mu = 0.5\,(\triangle)$ and $\mu = 2\,(\square)$.

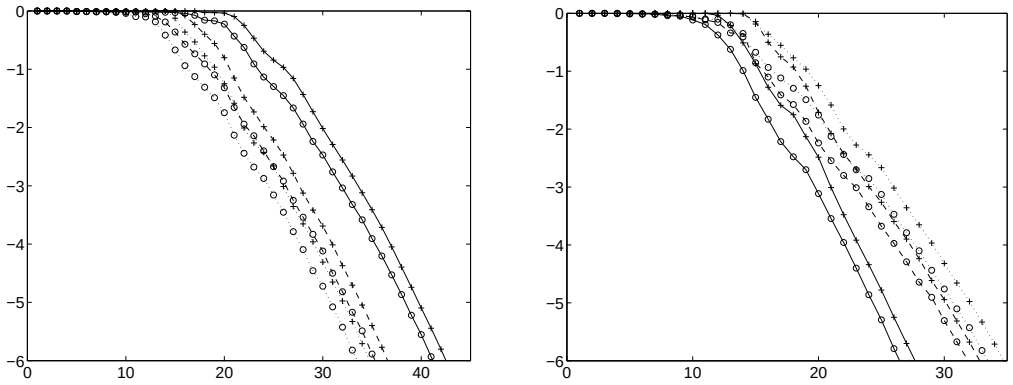

Figure 3: Convergence of the subiteration-preconditioned GMRES method: σ_k according to (45) (+) and the supremum of $J(u)$ over 10^6 random vectors u ($\circ$) versus k for $\mu = 0\,(\cdots), 0.5\,(--), 2\,(\text{——})$, in the initial time step (*left*) and the final time step (*right*). y-axis in $\log_{10}$-scale.

To determine the supremum over all u, we employ a steepest-ascent method (or *hill-climbing* algorithm), in combination with a line-search technique. Essentially, the steepest-ascent method determines the gradient J_u of $J(u)$ with respect to u, and updates u according to $u + \theta J_u$, with θ a small number determined by the line-search strategy. This process is repeated until $J_u = 0$ and, accordingly, u corresponds to a supremum of $J(u)$. As the functional $J(u)$ is nonconvex, the process is started from multiple initial guesses, and the maximum over all local extrema is determined, to ensure that the global supremum is computed.

Instead of computing the functional $J(u)$ according to its definition in (45), we first orthonormalize the Krylov space $[u, Su, S^2u, \ldots, S^ku]$ to avoid ill-conditioning. Although the orthonormalization changes the coefficients of the GMRES polynomial, it does not change σ_k. Such a change of basis can be straightforwardly incorporated in the functional, but the expression for the corresponding gradient is prohibitively complicated. Therefore, in the numerical procedure we apply the gradient for the non-orthonormalized functional. Consequently, the accuracy of the gradient deteriorates with increasing dimension of the Krylov space on account of the loss of digits, and the supremum is typically not attained. As a result, for large dimensions of the Krylov space, the steepest-ascent process yields a reasonably sharp lower estimate of the upper bound σ_k.

Fig. 3 displays the upper bound σ_k versus the dimension of the Krylov space k for $\mu = 0, 0.5, 2$ in the first time step (*left*), i.e., in the time interval $0 \le t \le \tau$, and in the final time step (*right*), viz., $(j-1)\tau \le t \le j\tau$ with $j = 50$. For reference and validation purposes, the figure also plots the supremum of the functional $J(u)$ over 10^6 random vectors u, versus the Krylov-space dimension k. Let us first note that the computed value of σ_k in all cases exceeds the supremum over the 10^6 random vectors. Hence, although the accuracy of the gradient deteriorates with increasing k and, accordingly, it cannot be ensured that the steepest-ascent algorithm converges to the supremum, it appears that the algorithm nonetheless yields a sharp estimate. Fig. 3 conveys that there is a lower bound to the dimension of the Krylov space in which a reduction of the residual can be ascertained. In particular, for dimensions k less than approximately 10 it holds that $\sigma_k \approx 1$. Furthermore, the figure shows that the convergence behaviour in the first time step deteriorates with increasing μ. Conjecturally, this can be attributed to the growth of the solution in the first time step. For $\mu = 0$, the convergence behaviour is essentially identical for all time steps. For $\mu = 0.5, 2$ the convergence behaviour in the final time step is better than in the initial time step. In contrast to the growth regime, it appears that in the periodic regime the convergence behaviour improves with increasing μ.

5.4 Error-amplification analysis of the reuse option

In this section, we investigate the viability of reuse of the Krylov space in subsequent invocations of GMRES. To this end, we consider the corresponding error-amplification matrix and, in particular, the lower diagonal block matrix $I - \tilde{S}^{-1}S$ which yields the only non-zero eigenvalues. We then examine its properties in terms of spectral radius, norm and pseudospectra.

We consider the reuse of the Krylov space generated in the first time step in the subsequent time steps. Fig. 4 plots the spectral radius of the error-amplification matrix versus time. The spectral radius expresses the quality of the Krylov space of the first time step as an approximation to the Krylov spaces of the subsequent time steps. In particular, if the spectral radius is large, then the first Krylov space constitutes a poor approximation and reuse is ineffective. In fact, if the spectral radius exceeds 1, then reuse leads to divergence of the method. The figure indicates that the quality of the reused space degrades in the growth regime of the solution, reflecting the change in the solution behaviour and the corresponding change in the subiteration operator. As the solution settles into its periodic regime, the spectral radius becomes essentially constant, modulo minor erratic variations. Moreover, Fig. 4 indicates that for large μ the deterioration of the approximation properties of the reused space is more severe. This can be attributed to the stronger nonlinearity of the structure associated with a larger value of μ. Even for $\mu = 2$, however, the spectral radius remains smaller than one and, hence, the reuse option is formally convergent. Conjecturally, the spectral radius of the error-amplification matrix with reuse can exceed one, thus causing the reuse option to fail. However, for the considered test case such failure appears to be rare, and we have not observed failure of the reuse option despite testing it under various extreme conditions.

Next, we consider error bounds for the GMRES method with reuse in conformity with

$$(\mathrm{spr}(I - \tilde{S}^{-1}S))^n \leq \|\epsilon_5^n\|/\|\epsilon_5^0\| \leq \|(I - \tilde{S}^{-1}S)^n\| \leq \kappa(X)(\mathrm{spr}(I - \tilde{S}^{-1}S))^n, \tag{47}$$

where ϵ_5^n denotes the error in the interface displacement after n iterations, and $\kappa(X) := \|X\|\|X^{-1}\|$ is the condition number of the matrix of eigenvectors, X, of $I - \tilde{S}^{-1}S$. To this end, we plot in Fig. 5 the norm of powers of the error-amplification matrix along with the bounds given by Eq. (47). The figure considers reuse of the Krylov space generated in the first time step in time step 50 for $\mu = 0$ (*left*), $\mu = 0.5$ (*center*) and $\mu = 2$ (*right*). In either case, the spectral radius is less than one, and the method with reuse is formally convergent. However, the condition numbers of the eigenvector matrices are very large, viz., $\kappa(X) = 3.1 \cdot 10^5$ for $\mu = 0$, $\kappa(X) = 6.9 \cdot 10^7$ for $\mu = 0.5$ and $\kappa(X) = 1.2 \cdot 10^8$ for $\mu = 2$. Moreover, the norm of the error-amplification matrix is smaller than one for $\mu = 0$, but it exceeds one for both $\mu = 0.5$ and $\mu = 2$. In combination with the upper bound $\|(I - \tilde{S}^{-1}S)^n\| \leq \|I - \tilde{S}^{-1}S\|^n$, the bounds in (47) then imply that for $\mu = 0$ convergence is monotonous, whereas for $\mu = 0.5, 2$ the initial error can be amplified by several orders of magnitude before it eventually decreases at an asymptotic rate determined by $\mathrm{spr}(I - \tilde{S}^{-1}S)$. For $\mu = 2$, the phase of transient divergence is much more pronounced, and the initial error can be amplified by more than five orders of magnitude before asymptotic convergence sets in. The transient divergence is indicative of the nonnormality of the GMRES method with reuse which is induced by the nonnormality of the underlying subiteration operator; cf. the discussion in Sections 3.3 and 4.5. We remark that the GMRES method without reuse converges monotonously; see Ref. [20] for the general theory, and Fig. 3 for an illustration.

Nonnormality also manifests itself in sensitivity of the spectrum to perturbations in the error-amplification matrix, e.g., due to discretization, linearization and round-off errors. To illustrate this effect, we plot in Fig. 6 the ε-pseudospectra[1] of the error-amplification matrices considered in Fig. 5. A perturbation of the error-amplification matrix according to $(I - \tilde{S}^{-1}S) + E'$ with $\|E'\| \leq \varepsilon$ can shift the eigenvalues anywhere within the corresponding ε-contour line; see [28]. For normal matrices the ε-pseudospectrum consists of all points in the complex plane at distance at most ε from the spectrum. For nonnormal matrices, however, the ε-pseudospectrum can be much larger. Although

[1] The pseudospectra plots in Fig. 6 were computed using the *EigTool* package by T.G. Wright, M. Embree and L.N. Trefethen; see [27] for further information.

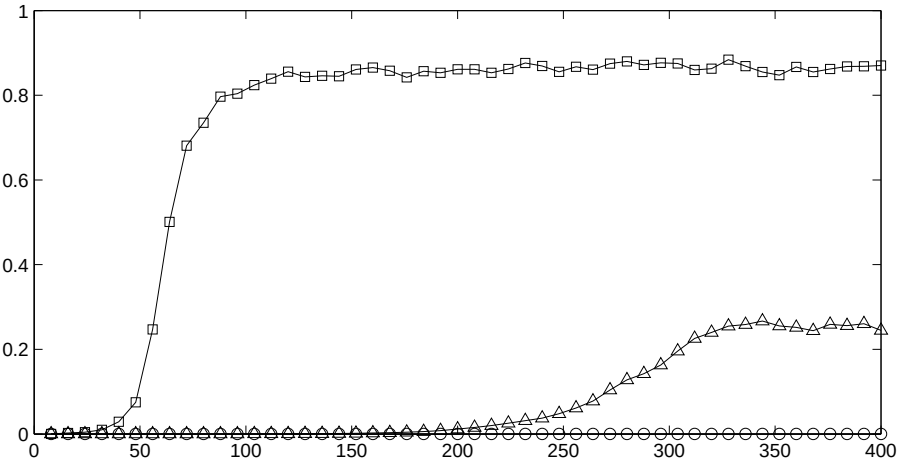

Figure 4: Reuse of the Krylov space generated in the first time step $0 \leq t \leq \tau$ in subsequent time steps $(j-1)\tau \leq t \leq j\tau$ with $1 \leq j \leq 50$: Spectral radius of the error-amplification matrix versus time for $\mu = 0.0\,(\circ)$, $\mu = 0.5\,(\triangle)$ and $\mu = 2\,(\square)$.

Fig. 6 indicates that as a result of nonnormality the spectrum of the error-amplification matrix is sensitive to perturbations, the presented results do not change significantly with mesh refinement or variations of the finite-differencing parameter ν involved in the evaluation of the image space according to Eq. (44).

6. Conclusions

We presented an error-amplification analysis of the subiteration-preconditioned GMRES method for fluid-structure-interaction problems. We considered the linear-algebra aspects of the subiteration method separately, and of the subiteration-preconditioned GMRES method, on the basis of properties of the error-amplification matrix for the aggregated fluid-structure system. We showed that the subiteration iterates span a Krylov space corresponding to a preconditioned aggregated system. The analysis of the error-amplification matrix of subiteration establishes that subiteration condenses errors into

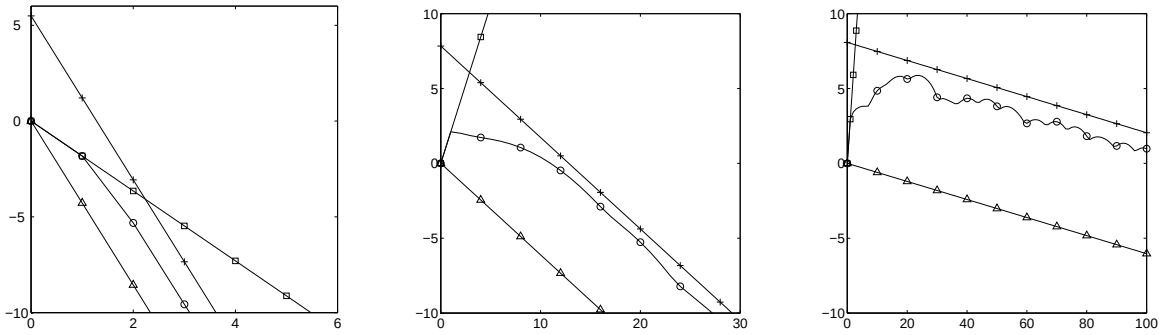

Figure 5: Reuse of the Krylov space generated in the first time step in time step 50 for $\mu = 0.0$ (*left*), $\mu = 0.5$ (*center*) and $\mu = 2$ (*right*): $\|(I - S_1^{-1}S_{50})^n\|\,(\circ)$, $\|I - S_1^{-1}S_{50}\|^n\,(\square)$, $(\mathrm{spr}(I - S_1^{-1}S_{50}))^n\,(\triangle)$ and $\kappa(X)(\mathrm{spr}(I - S_1^{-1}S_{50}))^n\,(+)$ versus n. y-axis in $\log_{10}$-scale.

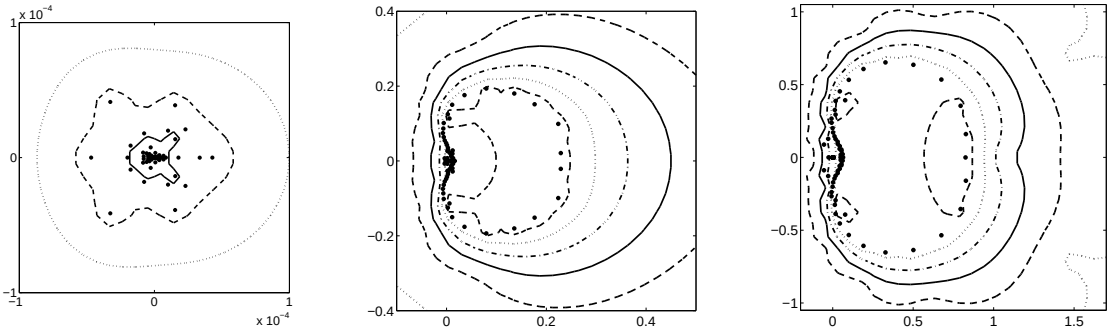

Figure 6: Spectra (•) and L_2 ε-pseudospectra of $(I - S_1^{-1}S_{50})$ in the complex plane for $\mu = 0.0$ (*left*), $\mu = 0.5$ (*center*) and $\mu = 2$ (*right*) and $\varepsilon = 10^{-9}$ (——), $\varepsilon = 10^{-8}$ (− −), $\varepsilon = 10^{-7}$ (···), $\varepsilon = 10^{-6}$ (−·), $\varepsilon = 10^{-5}$ (——), $\varepsilon = 10^{-4}$ (− −) and $\varepsilon = 10^{-3}$ (···).

a low-dimensional subspace which can be associated with the interface degrees-of-freedom. Therefore, the GMRES acceleration of subiteration can be confined to the interface degrees-of-freedom, which renders the storage requirements for the Krylov space and the computational cost of the least-squares problems low. The error-amplification analysis elucidates the connection between the *local* GMRES acceleration (i.e., on the interface degrees-of-freedom), and the *global* error-amplification properties (i.e., for the aggregated system).

An attractive feature of the subiteration-preconditioned GMRES method is that it enables the optional reuse of Krylov vectors in subsequent invocations of GMRES. This can substantially enhance the efficiency of the method, at the expense of robustness. We analysed the implications of reuse for the error-amplification behaviour. A pivotal element in the analysis is the observation that the GMRES acceleration on the interface degrees-of-freedom generates an approximation to the Schur complement for the aggregated system. The Schur complement allows for a concise expression of the error-amplification matrices, and enables the assessment of the GMRES acceleration and of the reuse of Krylov vectors in terms of the approximation properties for the Schur complement.

We illustrated the developed theory by numerical experiments on a model fluid-structure-interaction problem. In particular, we assessed convergence of the GMRES method with and without reuse in terms of spectral radius, norm and sharp convergence upper bounds. These bounds indicate that a minimum Krylov-space dimension is required to ensure a reduction of the residual. Moreover, the results show that significant changes in the solution due to nonlinearity can result in a degradation of the convergence behaviour.

Next, we investigated the viability of reusing Krylov vectors in subsequent invocations of GMRES. For the considered numerical experiments, the method with reuse is convergent, despite significant changes in the solution behaviour in time. Conjecturally, the spectral radius of the error-amplification matrix can exceed one, thus causing the reuse option to fail. However, such failure appears to be rare, and we have not observed it in the numerical investigations. This indicates that reuse constitutes a viable option, which renders it attractive for reducing the computational cost. However, the method with reuse appears to be affected by the nonnormality of the underlying subiteration operator. Thus, the method can exhibit transient divergence, whereas without reuse convergence is monotonous.

The presented error-amplification analysis of the subiteration-preconditioned GMRES methods is in principle generic. However, the specifics depend on the fluid-structure system under consideration.

Bibliography

[1] C. Farhat, P. Geuzaine, G. Brown, Application of a three-field nonlinear fluid-structure formulation to the prediction of the aeroelastic parameters of an F-16 fighter, Computers and Fluids 32 (2003) 3–29.

[2] C. Farhat, P. Geuzaine, C. Grandmont, The Discrete Geometric Conservation Law and the nonlinear stability of ALE schemes for the solution of flow problems on moving grids, Journal of Computational Physics 174 (2001) 669–694.

[3] I. Robertson, S. J. Sherwin, P. W. Bearman, Flutter instability prediction techniques for bridge deck sections, Int. J. Num. Methods Fluids 43 (2003) 1239–1256.

[4] B. Hübner, E. Walhorn, D. Dinkler, Numerical investigation to bridge aeroelasticity, in: Proceedings of the Fifth World Congress on Computational Mechanics (WCCM V) (H. A. Mang, F. G. Rammerstorfer and J. Eberhardsteiner, eds.), Vienna University of Technology, Austria, July 7-12 2002. Available at : `http://wccm.tuwien.ac.at/publications/Papers/fp81407.pdf`

[5] M. Heil, Stokes flow in an elastic tube - a large displacement fluid-structure interaction problem, Int. J. Num. Methods Fluids 28 (1998) 243–265.

[6] J.J. Alonso, A. Jameson, Fully-implicit time-marching aeroelastic solutions, AIAA 0056 (1994) 1–13.

[7] S.A. Morton, R.B. Melville, M.R. Visbal, Accuracy and coupling issues of aeroelastic Navier-Stokes solutions on deforming meshes, AIAA 1085 (1997) 252–262.

[8] P. LeTallec, J.Mouro, Fluid-structure interaction with large structural displacements, Comput. Methods Appl. Mech. Engrg. 190 (2001) 3039–3067.

[9] E.H. van Brummelen, R. de Borst, On the nonnormality of subiteration for a fluid-structure-interaction problem, SIAM J.-(2004). (Accepted for publication). Preprint available at : `http://www.em.lr.tudelft.nl/~brummelen/publications.html`

[10] E.H. van Brummelen, C. Michler, R. de Borst, Interface-GMRES(R) acceleration of subiteration for fluid-structure-interaction problems, Technical Report DACS-05-001, Delft University

of Technology, The Netherlands. Available at : http://www.em.lr.tudelft.nl/downloads/DACS-05-001.pdf

[11] Y. Saad, M.H. Schultz, GMRES: A generalized minimal residual algorithm for solving nonsymmetric linear systems, SIAM J. Sci. Comp. 7 (1986) 856–869.

[12] S.M. Rifai et.al., Multiphysics simulation of flow-induced vibrations and aeroelasticity on parallel computing platforms, Comput. Methods Appl. Mech. Engrg. 174 (1999) 393–417.

[13] M. Heil, An efficient solver for the fully-coupled solution of large-displacement fluid-structure interaction problems, Comput. Methods Appl. Mech. Engrg. 193 (2004) 1–23.

[14] H.G. Matthies, J. Steindorf, Partitioned strong coupling algorithms for fluid-structure interaction, Computers and Structures 81 (2003) 805–812.

[15] C.A. Felippa, K.C. Park, C. Farhat, Partitioned analysis of coupled mechanical systems, Comput. Methods Appl. Mech. Engrg., 190 (2001) 3247–3270.

[16] E.H. van Brummelen, S.J. Hulshoff, R. de Borst, Energy conservation under incompatibility for fluid-structure interaction problems, Comput. Methods Appl. Mech. Engrg. 192 (2003) 2727–2748.

[17] S. Piperno, C. Farhat, B. Larrouturou, Partitioned procedures for the transient solution of coupled aeroelastic problems - Part I : Model problem, theory and two-dimensional applications, Comput. Methods Appl. Mech. Engrg. 124 (1995) 79–112.

[18] S. Piperno, C. Farhat, Partitioned procedures for the transient solution of coupled aeroelastic problems - Part II : Energy transfer analysis and three-dimensional applications, Comput. Methods Appl. Mech. Engrg. 190 (2001) 3147–3170.

[19] S. Piperno, Explicit/implicit fluid/structure staggered procedures with a structural predictor and fluid subcycling for 2d inviscid aeroelastic simulations, Int. J. Num. Methods Fluids 25 (1997) 1207–1226.

[20] A. Greenbaum, Iterative Methods for Solving Linear Systems, volume 17 of Frontiers in Applied Mathematics, SIAM, Philadelphia, 1997.

[21] T. Washio, C.W. Oosterlee, Krylov subspace acceleration for nonlinear multigrid schemes, Electronic Transactions on Numerical Analysis 6 (1997) 271–290.

[22] G.H. Golub, C.F. van Loan, Matrix Computations, Johns Hopkins, 1996.

[23] P.N. Brown, Y. Saad, Hybrid Krylov methods for nonlinear systems of equations, SIAM J. Sci. Stat. Comput. 11 (1990) 450–481.

[24] M.E. Verbeek, Repairing near-singularity for dense EMC problems by adaptive basis techniques, Num. Lin. Alg. Appl. 7 (2000) 617–634.

[25] S. Deparis, Numerical analysis of axisymmetric flows and methods for fluid-structure interaction arising in blood flow simulation, PhD thesis, Ecole Polytechnique Fédérale de Lausanne, Switzerland, 2004.

[26] T. Kato, Perturbation Theory for Linear Operators, Number 132 in Grundlehren der Mathematischen Wissenschaft. Springer, Berlin, corr. pr. 2nd ed., 1984.

[27] T.G. Wright, Matlab Pseudospectra GUI. Oxford University Computing Laboratory. Available at : http://www.comlab.ox.ac.uk/pseudospectra/eigtool/.

[28] L.N. Trefethen, Pseudospectra of linear operators, SIAM Rev. 39 (1997) 383–406.