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E. Agullo*, L. Giraud*, Y.-F. Jing[†]

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Abstract: We consider the solution of large linear systems with multiple right-hand sides using a block GMRES approach. We introduce a new algorithm that effectively handles the situation of almost rank deficient block generated by the block Arnoldi procedure and that enables the recycling of spectral information at restart. The first feature is inherited from an algorithm introduced by Robbé and Sadkane [M. Robbé and M. Sadkane. Exact and inexact breakdowns in the block GMRES method. *Linear Algebra and its Applications*, 419: 265-285, 2006.], while the second one is obtained by extending the deflated restarting strategy proposed by Morgan [R. B. Morgan. Restarted block GMRES with deflation of eigenvalues. *Applied Numerical Mathematics*, 54(2): 222-236, 2005.]. Through numerical experiments, we show that the new algorithm combines efficiently the attractive numerical features of its two parents that it outperforms.

Key-words: Block GMRES, multiple right-hand sides, numerical rank deficiency, subspace augmentation, harmonic Ritz values

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GMRES par bloc avec inexact breakdowns et deflation au restart

Résumé : Nous considérons la résolution de systèmes linéaires avec second-membres multiples par une approche GMRES par bloc. Nous introduisons un nouvel algorithme qui gère efficacement d'une part la situation de perte de rang numérique dans les blocs générés par la méthode d'Arnoldi d'autre part le recyclage d'information spectrale au redémarrage via une technique d'augmentation d'espace. La première propriété est héritée de l'algorithme introduit par Robbé and Sadkane [M. Robbé and M. Sadkane. Exact and inexact breakdowns in the block GMRES method. *Linear Algebra and its Applications*, 419: 265-285, 2006.], et la seconde est obtenue en étendant la stratégie de redémarrage proposée par Morgan [R. B. Morgan. Restarted block GMRES with deflation of eigenvalues. *Applied Numerical Mathematics*, 54(2): 222-236, 2005.]. Via des expérimentations numériques, nous montrons que ce nouvel algorithme combine efficacement les deux propriétés de ces deux parents dont il améliore les performances.

Mots-clés : bloc GMRES, second-membres multiples, perte de rang numérique, augmentation de sous-espace, valeurs de Ritz harmoniques

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1 Introduction

We consider the solution of the linear system with p right-hand sides given simultaneously

$$AX = B, \tag{1}$$

where, $A \in \mathbb{C}^{n \times n}$ is a square nonsingular matrix of large dimension n , $B = [b^{(1)}, b^{(2)}, \dots, b^{(p)}] \in \mathbb{C}^{n \times p}$ are the given right-hand sides of full rank with $p \ll n$, and $X \in \mathbb{C}^{n \times p}$ are the solutions to be computed. Many large scientific and industrial applications, such as in radar cross section calculation in electromagnetism, wave scattering and wave propagation in acoustics, various source locations in seismic and parametric studies in general, require the solution of a sequence of linear systems with several right-hand sides given simultaneously. In that framework, block Krylov approaches appear as good candidates for the solution as the Krylov subspaces associated with each right-hand side are shared to enlarge the search space. They are attractive not only because of this numerical feature (larger search subspace), but also from a computational view point as they enable the use of BLAS3 like implementation. Their block-structures exhibit nice properties with respect to data locality and re-usability that comply with the memory constraint of modern multicore architectures. For a recent survey on block Krylov subspace methods, we refer to [18].

One difficulty when considering block Krylov methods is the situation when for a prescribed accuracy some right-hand sides converge much faster than others or when a linear combination of right-hand sides converges. In order to ensure the robustness of the numerical scheme and reduce the computational effort, a deflation strategy should be implemented to manage the space expansion [13]. In a block Arnoldi context, an exact convergence translates into a rank deficiency of the block of vectors to be used to expand the space and consequently leads to a breakdown (which contrary to the non-block counterpart is not a happy breakdown). To address convergence at a targeted numerical threshold, Robbé and Sadkane [33] introduced the idea of the inexact breakdowns. Instead of discarding some directions for the next space expansion, technique that might slow down the convergence [22], they keep the related information of subspaces spanned by these vectors and possibly reintroduce them later. They derive an algorithm that still exhibits a block Arnoldi-like recursion and they propose two criteria (W -criterion and R -criterion) to detect the inexact breakdowns to carry out BGMRES. They show that the R -criterion is more advisable to use than the W -criterion because it can efficiently detect inexact breakdowns when BGMRES is restarted and this criterion can be closely related to the backward error used to define the stopping criterion.. Therefore, only the R -criterion is considered in this paper; the corresponding BGMRES using this R -criterion to detect Inexact Breakdowns is referred to as IB-BGMRES.

It is well known that convergence of Krylov subspace methods for systems of linear equations depends to a large degree on the distribution of eigenvalues. Different numerical techniques have been proposed in the GMRES context to alleviate the effect of part of the spectrum either through preconditioning updates [15] or via information recycling at restart [14, 19]. In many approaches, some estimate of the invariant subspace is searched in the Krylov subspace and reused in the next restart either by augmenting the space [6, 26, 34], by deflating over the subspace [27] or by ensuring some orthogonality properties with respect to that space [31]. One of the most recent work in this field based on a deflation approach is GMRES-DR [27] extended to block-GMRES (referred to as BGMRES-DR) in [28]. This proposed BGMRES-DR is shown to perform much better than standard block-GMRES (referred to as BGMRES) [36, 42].

In this paper we study and design a block variant that combines effectively the key features of IB-BGMRES and BGMRES-DR. Numerical experiments demonstrate that this approach substantially keeps the efficiency of BGMRES-DR by augmenting the space with directions associ-

ated with some approximations of selected eigenvalues while it allows a decrease of the computational cost thanks to the detection and proper management of partial convergences. For other variants of BGMRES, we refer to the rich literature, for instance [1, 2, 5, 7, 8, 17, 20, 23, 24, 32, 34, 38, 37].

The remainder of this paper is organized as follows. In Section 2, the block Arnoldi process [18, 33, 35, 40] and some insights of IB-BGMRES are firstly reviewed. Some fundamental properties, similar to those of BGMRES-DR, are established in Section 3.1.1 for the harmonic residual vectors as well as their relationships with the residual vectors of the linear systems. In Section 3.1.2 we derive the new restarting procedure that enables to start with a subspace containing the selected spectral information and the linear system residuals. At restart, the new Arnoldi recursion for the new starting subspace is computed at low computational cost without involving any additional matrix-vector product with A . We show in Section 3.1.4, how the inexact breakdowns affect the right-hand sides of the least-squares problems and how they can be incrementally computed (contrarily to classical implementations where these right-hand sides are just expanded with zero entries to account for the increase of the Krylov space). The new block variant – IB-BGMRES-DR is presented in Section 3.2. In Section 3.3, we discuss the stopping criterion and its consequences on quality of the computed solutions by IB-BGMRES-DR in a backward error framework. Numerical experiments on a set of typical test problems are reported in Section 4 and concluding remarks are discussed in Section 5.

The symbol $\|\cdot\|_q$ denotes the Euclidean norm when $q = 2$ and the Frobenius norm when $q = F$. The superscript “ H ” denotes the transpose conjugate of a vector or matrix. For convenience of algorithm illustration and presentation, some MATLAB notation is used. A subscript “ k ” for a scalar or a matrix is used to indicate that the scalar or the matrix is obtained at iteration k . A matrix $C \in \mathbb{C}^{k \times \ell}$ consisting of k rows and ℓ columns sometimes is denoted as $C_{k \times \ell}$ explicitly. The identity and null matrices of dimension k are denoted respectively by I_k and 0_k or just I and 0 when the order is evident from the context. If $C \in \mathbb{C}^{k \times \ell}$, the singular values of C are denoted by $\sigma_1(C) \geq \dots \geq \sigma_{\min(k, \ell)}(C)$ in descent order.

2 Background: Block Arnoldi and inexact breakdowns

Denote by X_0 the initial block guesses, and by $R_0 = B - AX_0$ the corresponding nonsingular initial block residuals. Block GMRES builds the Krylov space $\mathcal{K}_j(A, R_0) = \text{span}(R_0, AR_0, \dots, A^{j-1}R_0)$ and searches for approximated solutions that minimize the 2-norms of the residuals associated with the individual right-hand sides. When one solution or a linear combination of the solutions has converged to the target accuracy, the block-Arnoldi procedure implemented to build an orthonormal basis of $\mathcal{K}_j(A, R_0)$ needs to be modified to account for this partial convergence. This partial convergence is characterized by a numerical rank deficiency in the new p directions one attempts to introduce for enlarging the Krylov space. In [33], the authors present an elegant numerical variant that enables the detection of what is referred to as inexact breakdowns. In that approach the directions that have a low contribution to the residual block are discarded from the set of vectors used to expand the space at the next iteration. In this section, we try to give an insight and the main equalities required to derive the IB-BGMRES-DR algorithm. We refer the reader to the original paper [33] for a detailed and complete description. For the sake of simplicity of exposure and easy cross-reading, we adopt most of the notations from [33].

Let $R_0 = V_1 \Lambda_1$ be the reduced QR -factorization of R_0 , where $V_1 \in \mathbb{C}^{n \times p}$ is matrix with orthonormal columns and $\Lambda_1 \in \mathbb{C}^{p \times p}$ is an upper triangular full rank matrix. Then an orthonormal basis of block Krylov subspace

$$\mathcal{K}_j(A, V_1) = \text{span}(V_1, AV_1, \dots, A^{j-1}V_1),$$

can be constructed using a block Arnoldi process described in Algorithm 1.

Algorithm 1 *Block Arnoldi with blockwise modified Gram-Schmidt orthogonalization*

```

1: Choose a unitary matrix  $V_1$  of size  $n \times p$ 
2: for  $j = 1, 2, \dots, m$  do
3:   Compute  $W_j = AV_j$ 
4:   for  $i = 1, 2, \dots, j$  do
5:      $H_{i,j} = V_i^H W_j$ 
6:      $W_j = W_j - V_i H_{i,j}$ 
7:   end for
8:    $W_j = V_{j+1} H_{j+1,j}$  (reduced  $QR$ -factorization)
9: end for

```

Because when an inexact breakdown occurs, not all the space spanned by W_j is considered to build V_{j+1} in order to expand the space (Step 8 of the Algorithm 1), where a subscript j is added to denote its block number of columns. Let $p_1 = p$ and denote by p_{j+1} the column rank of the block orthonormal basis vector V_{j+1} . Then $V_{j+1} \in \mathbb{C}^{n \times p_{j+1}}$, $W_j \in \mathbb{C}^{n \times p_j}$ and $H_{j+1,j} \in \mathbb{C}^{p_{j+1} \times p_j}$. As a consequence the dimension of the search space $\mathcal{K}_j(A, V_1)$ considered at the j^{th} iteration is no longer necessarily equal to $j \times p$ but is equal to $n_j = \sum_{i=1}^j p_i$; that is, the sum of the column ranks of V_i 's ($i = 1, \dots, j$). $\mathcal{V}_j = [V_1, \dots, V_j] \in \mathbb{C}^{n \times n_j}$ ($\mathcal{V}_{j+1} = [\mathcal{V}_j, V_{j+1}]$) denotes the orthonormal basis of $\mathcal{K}_j(A, V_1)$ (respectively $\mathcal{K}_{j+1}(A, V_1)$). Associated with these bases we define $\mathcal{H}_j = \begin{bmatrix} \mathcal{H}_j \\ 0 \dots 0 \end{bmatrix} \in \mathbb{C}^{n_{j+1} \times n_j}$ the block upper Hessenberg matrix, where $\mathcal{H}_j = (H_{i,\ell})_{1 \leq i, \ell \leq j} \in \mathbb{C}^{n_j \times n_j}$.

When no inexact breakdown has occurred $p_{j+1} = p_j = \dots = p_1 = p$, the range of W_j has always been used to enlarge the search space. Consequently, one obtains the standard block Arnoldi relation [35] from Algorithm 1

$$A\mathcal{V}_j = \mathcal{V}_j \mathcal{H}_j + [0_{n \times n_{j-1}}, W_j] = \mathcal{V}_{j+1} \mathcal{H}_j. \quad (2)$$

The block minimum residual norm approaches, such as BGMRES [36, 42] build approximations to the solutions X at iteration j of the form

$$X_j = X_0 + \mathcal{V}_j Y_j,$$

where Y_j solves the least-squares problem

$$\|B - AX_j\|_F = \min_{Y \in \mathbb{C}^{n_j \times p}} \|\mathcal{V}_{j+1} (\Lambda_j - \mathcal{H}_j Y)\|_F = \min_{Y \in \mathbb{C}^{n_j \times p}} \|\Lambda_j - \mathcal{H}_j Y\|_F$$

because \mathcal{V}_{j+1} forms an orthonormal basis and $\Lambda_j = \begin{bmatrix} \Lambda_1 \\ 0 \end{bmatrix} \in \mathbb{C}^{n_{j+1} \times p}$.

To account for a numerical deficiency in the residual block $R_j = B - AX_j$ in a way that is described later, Robbé and Sadkane [33] proposed to split

$$W_j = V_{j+1} H_{j+1,j} + Q_j. \quad (3)$$

so that Q_j and V_{j+1} are orthogonal and only V_{j+1} is used to enlarge \mathcal{V}_j to form \mathcal{V}_{j+1} . We can then extend Equation (2) into

$$A\mathcal{V}_j = \mathcal{V}_j \mathcal{H}_j + [Q_{j-1}, W_j], \quad (4)$$

where $Q_{j-1} = [Q_1, \dots, Q_{j-1}] \in \mathbb{C}^{n \times n_{j-1}}$ accounts for all the abandoned directions. The matrix Q_{j-1} is rank deficient, that reduces to zero matrix of $\mathbb{C}^{n \times n_{j-1}}$ when no inexact breakdown has occurred; in that case Equation (4) reduces to Equation (2).

In order to characterize a minimum norm solution in the space spanned by \mathcal{V}_j using Equation (4) we need to form an orthonormal basis of the space spanned by $[\mathcal{V}_j, \mathcal{Q}_{j-1}, W_j]$. This is performed by first orthogonalizing \mathcal{Q}_{j-1} against \mathcal{V}_j , that is $\tilde{\mathcal{Q}}_{j-1} = (I - \mathcal{V}_j \mathcal{V}_j^H) \mathcal{Q}_{j-1}$. Because \mathcal{Q}_{j-1} is low rank so is $\tilde{\mathcal{Q}}_{j-1}$ that can be written

$$\tilde{\mathcal{Q}}_{j-1} = P_{j-1} G_{j-1} \text{ with } \begin{cases} P_{j-1} \in \mathbb{C}^{n \times \tilde{q}_{j-1}} \text{ has orthonormal columns with } \mathcal{V}_j^H P_{j-1} = 0, \\ G_{j-1} \in \mathbb{C}^{\tilde{q}_{j-1} \times n_{j-1}} \text{ is of full rank.} \end{cases} \quad (5)$$

Next W_j , that is already orthogonal to \mathcal{V}_j , is made to be orthogonal to P_{j-1} with $W_j - P_{j-1} C_j$ where $C_j = P_{j-1}^H W_j$; then one computes $\tilde{W}_j D_j$ the reduced QR factorization of $W_j - P_{j-1} C_j$. Eventually, the columns of the matrix $[\mathcal{V}_j, P_{j-1}, \tilde{W}_j]$ form an orthonormal basis of the space spanned by $[\mathcal{V}_j, \mathcal{Q}_{j-1}, W_j]$.

With this new basis Equation (4) writes

$$A \mathcal{V}_j = \mathcal{V}_j \mathcal{L}_j + \begin{bmatrix} P_{j-1} G_{j-1}, [P_{j-1}, \tilde{W}_j] \end{bmatrix} \begin{bmatrix} C_j \\ D_j \end{bmatrix} = [\mathcal{V}_j, P_{j-1}, \tilde{W}_j] \begin{bmatrix} \mathcal{L}_j & & \\ G_{j-1} & C_j & \\ 0 & D_j & \end{bmatrix} \quad (6)$$

where $\mathcal{L}_j = \begin{bmatrix} H_{1,1} & \cdots & \cdots & \cdots & H_{1,j} \\ H_{2,1} & \ddots & & & \vdots \\ V_3^H Q_1 & \ddots & \ddots & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ V_j^H Q_1 & \cdots & V_j^H Q_{j-2} & H_{j,j-1} & H_{j,j} \end{bmatrix} \in \mathbb{C}^{n_j \times n_j}$ is no longer upper Hessenberg as soon as one inexact breakdown occurs, i.e., $\exists \ell Q_\ell \neq 0$.

The least-squares problem to be solved to compute the minimum norm solution associated with the generalized Arnoldi Equation (6) becomes

$$Y_j = \underset{Y \in \mathbb{C}^{n_j \times p}}{\operatorname{argmin}} \| \Lambda_j - \mathcal{F}_j Y \|_F,$$

with

$$\mathcal{F}_j = \begin{bmatrix} \mathcal{L}_j & & \\ G_{j-1} & C_j & \\ 0 & D_j & \end{bmatrix} \quad \text{and} \quad \Lambda_j = \begin{bmatrix} \Lambda_1 \\ 0 \\ 0 \end{bmatrix},$$

so that Equation (4) writes in a more compact form as

$$A \mathcal{V}_j = [\mathcal{V}_j, [P_{j-1}, \tilde{W}_j]] \mathcal{F}_j. \quad (7)$$

Robbé and Sadkane [33], introduced the so-called R-criterion to extract from the $[P_{j-1}, \tilde{W}_j]$ the subspace to be used to build V_{j+1} as follows. Based on the SVD of the projected residual $\Lambda_j - \mathcal{F}_j Y_j = \mathbb{U}_1 \Sigma_1 \mathbb{V}_1^H + \mathbb{U}_2 \Sigma_2 \mathbb{V}_2^H$ where Σ_1 contains the singular values larger than a prescribed threshold $\epsilon^{(R)}$, they decompose $\mathbb{U}_1 = \begin{pmatrix} \mathbb{U}_1^{(1)} \\ \mathbb{U}_1^{(2)} \end{pmatrix}$ in accordance with $[\mathcal{V}_j, [P_{j-1}, \tilde{W}_j]]$, and consider $[\mathbb{W}_1, \mathbb{W}_2]$ unitary so that $\operatorname{Range}(\mathbb{W}_1) = \operatorname{Range}(\mathbb{U}_1^{(2)})$. The new set of vectors selected to expand the search space

$$V_{j+1} = [P_{j-1}, \tilde{W}_j] \mathbb{W}_1 \quad (8)$$

is the one that contributes the most to the residual. Through this mechanism, directions that have been abandoned at a given iteration can be reintroduced, if the residual block has a large component along them. Furthermore, this selection strategy ensures that all the solutions have

converged when p inexact breakdowns have been detected; we refer to Section 3.3 for the discussion on how $\epsilon^{(R)}$ should be defined to ensure a convergence of all the solutions to a prescribed backward error.

We do not give the details of the calculation and refer to [33] for a complete description, but only state that via this decomposition the main terms that appear in Equation (6) can be computed incrementally from one iteration to the next as follows:

- based on the following recurrence $\mathcal{L}_j = \begin{bmatrix} \mathcal{L}_{j-1} & H_{1,j} \\ & \vdots \\ & H_{j,j} \end{bmatrix}$ where $\mathcal{L}_{j-1} = \begin{bmatrix} \mathcal{L}_{j-1} & \\ V_j^H \mathcal{Q}_{j-2} & H_{j,j-1} \end{bmatrix}$

the last block row of \mathcal{L}_j at next iteration $(j+1)$ is given by $\mathcal{L}_{j+1,:} = \mathbb{W}_1^H \begin{bmatrix} G_{j-1} & C_j \\ 0 & D_j \end{bmatrix}$.

The last block column of \mathcal{L}_{j+1} results from the block Arnoldi orthogonalization. Those matrices play a central role in IB-BGMRES since they define the procedure to enlarge the space and follow the equation below:

$$A\mathcal{V}_j = \mathcal{V}_{j+1}\mathcal{L}_j + \tilde{\mathcal{Q}}_j. \quad (9)$$

- the new compressed form of the abandoned directions $\tilde{\mathcal{Q}}_j$ is given by the new orthonormal set of vectors

$$P_j = [P_{j-1}, \tilde{W}_j] \mathbb{W}_2, \quad (10)$$

the complementary part of V_{j+1} and their components in the space spanned by P_j are

$$G_j = \mathbb{W}_2^H \begin{bmatrix} G_{j-1} & C_j \\ 0 & D_j \end{bmatrix}.$$

3 Block GMRES with inexact breakdowns and deflated restarting

In this section we present the new block algorithm that effectively handles the inexact breakdowns and that enables the recycling of spectral information at restart. These features are obtained by extending to IB-BGMRES the augmentation strategy of BGMRES-DR.

3.1 Analysis of a cycle

We discuss now the two main points related to the extension of BGMRES-DR in an inexact breakdown setting: what is the harmonic Ritz information recovered at restart and is it still possible to restart at low computational cost a block Arnoldi-like recurrence formula similar to Equation (7)? Both issues will be addressed in the next section.

3.1.1 Harmonic Ritz vectors and residuals

In order to describe how a restarting strategy enabling to recycle spectral information can be implemented in combination with the block GMRES with inexact breakdown, we first need to establish some key properties. In particular, we first characterize the subspace to be considered in order to define the harmonic Ritz vectors [16, 25, 29, 30, 39] that will be recycled at restart. These properties enable us to ensure that both the residuals of the linear systems and the harmonic Ritz vectors to be recycled can be represented in a same subspace at restart, while maintaining a block Arnoldi-like relation at low computational cost.

Definition 1. *Harmonic Ritz pair.* Consider a subspace \mathcal{U} of \mathbb{C}^n . Given a matrix $B \in \mathbb{C}^{n \times n}$, $\lambda \in \mathbb{C}$ and $y \in \mathcal{U}$, (λ, y) is a harmonic Ritz pair of B with respect to \mathcal{U} if and only if

$$By - \lambda y \perp B\mathcal{U}$$

or equivalently, for the canonical scalar product,

$$\forall w \in \text{Range}(B\mathcal{U}) \quad w^H (By - \lambda y) = 0.$$

The vector y is a harmonic Ritz vector associated with the harmonic Ritz value λ .

Lemma 1 presents the harmonic Ritz formulation used in the block GMRES variant with inexact breakdowns and deflated restarting.

Lemma 1. Let $\mathcal{U} = \text{span}(\mathcal{V}_m)$, where \mathcal{V}_m is the orthonormal basis built by IB-BGMRES at the end of a cycle. The harmonic Ritz pairs (θ_i, \tilde{g}_i) associated with \mathcal{V}_m satisfy the following property

$$\mathcal{F}_m^H \left(\mathcal{F}_m \tilde{g}_i - \tilde{\theta}_i \begin{bmatrix} \tilde{g}_i \\ 0_p \end{bmatrix} \right) = 0, \quad (i = 1, \dots, n_m), \quad (11)$$

where \mathcal{F}_m is defined by Equation (7), $\tilde{g}_i \in \mathbb{C}^{n_m}$, and $\mathcal{V}_m \tilde{g}_i$ ($i = 1, \dots, n_m$) are the harmonic Ritz vectors associated with the corresponding harmonic Ritz values θ_i ($i = 1, \dots, n_m$).

Proof. Assume that we have performed a first cycle of block Arnoldi with inexact breakdowns (see Algorithm 3). By Petrov-Galerkin condition defined in Definition 1, the harmonic Ritz pairs satisfy

$$(A\mathcal{V}_m)^H (A\mathcal{V}_m \tilde{g}_i - \tilde{\theta}_i \mathcal{V}_m \tilde{g}_i) = 0, \quad (i = 1, \dots, n_m). \quad (12)$$

Substituting (7) with $j = m$ into (12), we get

$$\mathcal{F}_m^H [\mathcal{V}_m, [P_{m-1}, \tilde{W}_m]]^H ([\mathcal{V}_m, [P_{m-1}, \tilde{W}_m]] \mathcal{F}_m \tilde{g}_i - \tilde{\theta}_i \mathcal{V}_m \tilde{g}_i) = 0, \quad (i = 1, \dots, n_m),$$

which gives the desired result because $[\mathcal{V}_m, [P_{m-1}, \tilde{W}_m]]$ has orthonormal columns. \square

Because $\mathcal{F}_m = \begin{bmatrix} \mathcal{L}_m \\ \mathbb{H}_m \end{bmatrix}$ with $\mathbb{H}_m = \begin{bmatrix} G_{m-1} & C_m \\ 0 & D_m \end{bmatrix} \in \mathbb{C}^{p \times n_m}$, it also reads

$$(\mathcal{L}_m^H \mathcal{L}_m + \mathbb{H}_m^H \mathbb{H}_m) \tilde{g}_i = \tilde{\theta}_i \mathcal{L}_m^H \tilde{g}_i, \quad i = 1, \dots, n_m. \quad (13)$$

Therefore, we compute the k targeted eigenpairs $(\tilde{\theta}_i, \tilde{g}_i)$ of the matrix $\mathcal{L}_m + \mathcal{L}_m^{-H} \mathbb{H}_m^H \mathbb{H}_m$ (see Step 3 of Algorithm 2). In practice, it might be more stable to solve the generalized eigenvalue problem in Equation (13) if \mathcal{L}_m is nearly singular.

In Lemma 2, we detail a useful relation as a basis for Proposition 1 showing that the residuals of the linear systems and the residuals of the harmonic Ritz vectors to be recycled can be represented in the same subspace at restart.

Lemma 2. Assume that \mathcal{L}_m is of full rank after performing a first cycle of Algorithm 3, then the column vectors $(\mathcal{F}_m \tilde{g}_i - \tilde{\theta}_i \begin{bmatrix} \tilde{g}_i \\ 0 \end{bmatrix}) \in \mathbb{C}^{n_m+p}$ ($i = 1, \dots, n_m$) are all contained in the subspace spanned by the least-squares residuals $R_{LS_m} = (\Lambda_m - \mathcal{F}_m Y_m) \in \mathbb{C}^{(n_m+p) \times p}$, i.e., $\exists \alpha_i \in \mathbb{C}^p$ so that

$$\mathcal{F}_m \tilde{g}_i - \tilde{\theta}_i \begin{bmatrix} \tilde{g}_i \\ 0 \end{bmatrix} = R_{LS_m} \alpha_i. \quad (14)$$

Proof. From the preceding lemma, we have that $(\mathcal{F}_m \tilde{g}_i - \tilde{\theta}_i \begin{bmatrix} \tilde{g}_i \\ 0 \end{bmatrix}) \in \text{Null}(\mathcal{F}_m^H)$, $(i = 1, \dots, n_m)$. Furthermore, we have $n_m + p = \dim(\text{Range}(\mathcal{F}_m^H)) + \dim(\text{Null}(\mathcal{F}_m^H))$. Because \mathcal{L}_m is assumed of full rank, we have $\dim(\text{Null}(\mathcal{F}_m^H)) = p$.

On the other hand, $Y_m = \arg\min_{Y \in \mathbb{C}^{n_m \times p}} \|\Lambda_m - \mathcal{F}_m Y\|_F$, then $\mathcal{F}_m Y_m$ are the orthogonal projections of Λ_m on $\text{Range}(\mathcal{F}_m)$ and $(\Lambda_m - \mathcal{F}_m Y_m) \perp \text{Range}(\mathcal{F}_m)$. That is $(\Lambda_m - \mathcal{F}_m Y_m) \in \text{Null}(\mathcal{F}_m^H)$ thanks to $\text{Range}(\mathcal{F}_m)^\perp = \text{Null}(\mathcal{F}_m^H)$, which together with $\text{rank}(\Lambda_m - \mathcal{F}_m Y_m) = p$ indicates that $\text{span}(\Lambda_m - \mathcal{F}_m Y_m) = \text{Null}(\mathcal{F}_m^H)$. Then consequently $(\mathcal{F}_m \tilde{g}_i - \tilde{\theta}_i \begin{bmatrix} \tilde{g}_i \\ 0 \end{bmatrix}) \in \text{span}(\Lambda_m - \mathcal{F}_m Y_m)$, $(i = 1, \dots, n_m)$, yielding Equation (14). \square

Using Lemma 2 and Equation (7) for $j = m$, we can characterize the relationship between harmonic residuals and linear systems residuals in the inexact breakdown framework. This result can be viewed as a generalization of [28, Lemma 2] when inexact breakdowns occur and are handled.

Proposition 1. *The harmonic residual vectors are all linear combinations of the residual vectors from the minimum residual solutions of the linear equation problem after performing a first cycle of Algorithm 3.*

Proof. After performing a first cycle of Algorithm 3, we have obtained the orthonormal matrix $[\mathcal{V}_m, [P_{m-1}, \tilde{W}_m]]$ and the relation $A\mathcal{V}_m = [\mathcal{V}_m, [P_{m-1}, \tilde{W}_m]] \mathcal{F}_m$ from Equation (7). The harmonic residual vectors $R_{\text{har}}^{(i)} = A\mathcal{V}_m \tilde{g}_i - \tilde{\theta}_i \mathcal{V}_m \tilde{g}_i$ ($i = 1, \dots, n_m$) and the residual vectors $R_m = B - AX_m$ from the minimum residual solutions of the linear equation problem respectively satisfy

$$\begin{aligned} R_{\text{har}}^{(i)} &= A\mathcal{V}_m \tilde{g}_i - \tilde{\theta}_i \mathcal{V}_m \tilde{g}_i = [\mathcal{V}_m, [P_{m-1}, \tilde{W}_m]] \left(\mathcal{F}_m \tilde{g}_i - \tilde{\theta}_i \begin{bmatrix} \tilde{g}_i \\ 0 \end{bmatrix} \right), \quad (i = 1, \dots, n_m), \\ R_m &= B - AX_m = R_0 - A\mathcal{V}_m Y_m = V_1 \Lambda_1 - A\mathcal{V}_m Y_m = [\mathcal{V}_m, [P_{m-1}, \tilde{W}_m]] R_{LS_m}. \end{aligned}$$

Because $[\mathcal{V}_m, [P_{m-1}, \tilde{W}_m]]$ is an orthonormal basis, Lemma 2 shows that R_{har} and R_m are in the same p -dimensional space which concludes the proof. \square

3.1.2 Block GMRES with inexact breakdowns relations at restart

Next, we will show that the block Arnoldi-like recurrence formulae (7) and (9) still hold after building initial block orthonormal basis vectors of the new search subspace at each restart combined with refined information associated with the prescribed number k of targeted harmonic Ritz vectors calculated at the end of the previous cycle at low computational cost.

Let us further denote by $\mathcal{V}_m \tilde{G}$ the k targeted harmonic Ritz vectors, where $\tilde{G} = [\tilde{g}_1, \dots, \tilde{g}_k] \in \mathbb{C}^{n_m \times k}$. First add zero rows of size p to \tilde{G} and then append R_{LS_m} to form a new matrix denoted as $\underline{G} = \begin{bmatrix} \tilde{G} & R_{LS_m} \\ 0_{p \times k} & \end{bmatrix}$ of dimension $(n_m + p) \times (k + p)$. We denote $\underline{G} = Q_{\underline{G}} R_{\underline{G}}$ the reduced QR-factorization of \underline{G} , where the reduced factors can be partitioned as follows

$$Q_{\underline{G}} = \begin{bmatrix} \Gamma_1 & \Gamma_2 \\ 0_{p \times k} & \end{bmatrix} \in \mathbb{C}^{(n_m+p) \times (k+p)}, \quad (15)$$

$$R_{\underline{G}} = \begin{bmatrix} \Theta_1 & \Theta_2 \\ 0_{p \times k} & \end{bmatrix} \in \mathbb{C}^{(k+p) \times (k+p)}, \quad (16)$$

with $\Gamma_1 = Q_G(1:n_m, 1:k)$, $\Gamma_2 = Q_G(:, k+1:k+p)$, $\Theta_1 = R_G(1:k, 1:k)$ and $\Theta_2 = R_G(:, k+1:k+p)$ and

$$\tilde{G} = \Gamma_1 \Theta_1, \quad (17)$$

$$R_{LS_m} = Q_G \Theta_2. \quad (18)$$

Proposition 2 shows that the block Arnoldi-like recurrence formulae of IB-BGMRES [33] can be recovered without involving any matrix-vector product with A when restarting with some harmonic information.

Proposition 2. *At each restart of block GMRES with inexact breakdowns and deflated restarting, the initial block Arnoldi-like recurrence formulae (7) and (9) still hold in exact arithmetic as*

$$A\mathcal{V}_1^{new} = [\mathcal{V}_1^{new}, [P_0, \tilde{W}_1]^{new}] \mathcal{F}_1^{new}, \quad (19)$$

$$A\mathcal{V}_1^{new} = \mathcal{V}_2^{new} \underline{\mathcal{L}}_1^{new} + \tilde{\mathcal{Q}}_1^{new}, \quad (20)$$

with

$$[\mathcal{V}_1^{new}, [P_0, \tilde{W}_1]^{new}] = [\mathcal{V}_m, [P_{m-1}, \tilde{W}_m]] Q_G,$$

$$R_0 = [\mathcal{V}_1^{new}, [P_0, \tilde{W}_1]^{new}] \Lambda_1^{new} \text{ with } \Lambda_1^{new} = \Theta_2,$$

$$\underline{\mathcal{L}}_1^{new} = \Gamma_1^H \mathcal{L}_m \Gamma_1, \quad \mathbb{H}_1^{new} = \Gamma_2^H \mathcal{F}_m \Gamma_1, \quad \mathcal{F}_1^{new} = \begin{bmatrix} \mathcal{L}_1^{new} \\ \mathbb{H}_1^{new} \end{bmatrix},$$

$$V_2^{new} = [P_0, \tilde{W}_1]^{new} \mathbb{W}_1^{new}, \quad P_1^{new} = [P_0, \tilde{W}_1]^{new} \mathbb{W}_2^{new}, \quad \mathcal{L}_{2,:}^{new} = \mathbb{W}_1^{newH} \mathbb{H}_1^{new}, \quad G_1^{new} = \mathbb{W}_2^{newH} \mathbb{H}_1^{new},$$

$$\mathcal{V}_2^{new} = [\mathcal{V}_1^{new}, V_2^{new}], \quad \underline{\mathcal{L}}_1^{new} = \begin{bmatrix} \mathcal{L}_1^{new} \\ \mathcal{L}_{2,:}^{new} \end{bmatrix}, \quad \tilde{\mathcal{Q}}_1^{new} = P_1^{new} G_1^{new},$$

where \mathbb{W}_1^{new} and \mathbb{W}_2^{new} satisfy

$$\text{Range}(\mathbb{W}_1^{new}) = \text{Range}(\mathbb{U}_1^{new(2)}) \text{ with } \mathbb{U}_1^{new} = \begin{bmatrix} \mathbb{U}_1^{new(1)} \\ \mathbb{U}_1^{new(2)} \end{bmatrix} \text{ and } [\mathbb{W}_1^{new}, \mathbb{W}_2^{new}] \text{ is unitary}$$

with

$$\Lambda_1^{new} - \mathcal{F}_1^{new} Y_1^{new} = \mathbb{U}_1^{new} \Sigma_1^{new} \mathbb{V}_1^{newH} + \mathbb{U}_2^{new} \Sigma_2^{new} \mathbb{V}_2^{newH}, \text{ where } \sigma_{\min}(\Sigma_1^{new}) \geq \epsilon^{(R)} > \sigma_{\max}(\Sigma_2^{new})$$

the SVD to detect inexact breakdown in the restarting block residual where

$$Y_1^{new} = \underset{Y \in \mathbb{C}^{n_1 \times p}}{\text{argmin}} \|\Lambda_1^{new} - \mathcal{F}_1^{new} Y\|_F.$$

Proof. • Show that Equation (19) holds:

From Equation (14) of Lemma 2, we have, $\forall i \in 1, \dots, k$, $\exists \alpha_i \in \mathbb{C}^p$,

$$\mathcal{F}_m \tilde{g}_i - \tilde{\theta}_i \begin{bmatrix} \tilde{g}_i \\ 0 \end{bmatrix} = R_{LS_m} \alpha_i. \quad (21)$$

Multiplying both sides of Equation (21) with $[\mathcal{V}_m, [P_{m-1}, \tilde{W}_m]]$ gives

$$[\mathcal{V}_m, [P_{m-1}, \tilde{W}_m]] \mathcal{F}_m \tilde{g}_i - [\mathcal{V}_m, [P_{m-1}, \tilde{W}_m]] \tilde{\theta}_i \begin{bmatrix} \tilde{g}_i \\ 0 \end{bmatrix} = [\mathcal{V}_m, [P_{m-1}, \tilde{W}_m]] R_{LS_m} \alpha_i.$$

Using (7), we can write the above equation as

$$A\mathcal{V}_m\tilde{g}_i = [\mathcal{V}_m, [P_{m-1}, \tilde{W}_m]] \left(\tilde{\theta}_i \begin{bmatrix} \tilde{g}_i \\ 0 \end{bmatrix} + R_{LS_m} \alpha_i \right),$$

which, according to the formulations of \tilde{G} and \underline{G} , can be reformulated in a matrix form as

$$A\mathcal{V}_m\tilde{G} = [\mathcal{V}_m, [P_{m-1}, \tilde{W}_m]] \underline{G} \begin{pmatrix} \text{diag}(\tilde{\theta}_1, \dots, \tilde{\theta}_k) \\ \alpha_1, \dots, \alpha_k \end{pmatrix}.$$

Using the reduced QR -factorization of \underline{G} and the structure of \tilde{G} as shown in Equation (17), we have

$$A\mathcal{V}_m\Gamma_1\Theta_1 = [\mathcal{V}_m, [P_{m-1}, \tilde{W}_m]] Q_{\underline{G}} R_{\underline{G}} \begin{pmatrix} \text{diag}(\tilde{\theta}_1, \dots, \tilde{\theta}_k) \\ \alpha_1, \dots, \alpha_k \end{pmatrix}.$$

Multiplying by Θ^{-1} from the right-hand side gives

$$A\mathcal{V}_m\Gamma_1 = [\mathcal{V}_m, [P_{m-1}, \tilde{W}_m]] Q_{\underline{G}} R_{\underline{G}} \begin{pmatrix} \text{diag}(\tilde{\theta}_1, \dots, \tilde{\theta}_k) \\ \alpha_1, \dots, \alpha_k \end{pmatrix} \Theta_1^{-1},$$

which, from the partition of $Q_{\underline{G}}$ in Equation (15), is

$$A\mathcal{V}_m\Gamma_1 = [\mathcal{V}_m\Gamma_1, [\mathcal{V}_m, [P_{m-1}, \tilde{W}_m]]\Gamma_2] R_{\underline{G}} \begin{pmatrix} \text{diag}(\tilde{\theta}_1, \dots, \tilde{\theta}_k) \\ \alpha_1, \dots, \alpha_k \end{pmatrix} \Theta^{-1}. \quad (22)$$

On the other hand, Equation (21) can be rewritten in a matrix reformulation as

$$\mathcal{F}_m\tilde{G} - \begin{pmatrix} \tilde{G} \\ 0 \end{pmatrix} \text{diag}(\tilde{\theta}_1, \dots, \tilde{\theta}_k) = R_{LS_m} [\alpha_1, \dots, \alpha_k],$$

which proceeds similarly to the above manipulations as

$$\begin{aligned} \mathcal{F}_m\tilde{G} &= \underline{G} \begin{pmatrix} \text{diag}(\tilde{\theta}_1, \dots, \tilde{\theta}_k) \\ \alpha_1, \dots, \alpha_k \end{pmatrix}, \\ \Rightarrow \mathcal{F}_m\Gamma_1\Theta_1 &= Q_{\underline{G}} R_{\underline{G}} \begin{pmatrix} \text{diag}(\tilde{\theta}_1, \dots, \tilde{\theta}_k) \\ \alpha_1, \dots, \alpha_k \end{pmatrix}, \\ \Rightarrow Q_{\underline{G}}^H \mathcal{F}_m\Gamma_1 &= R_{\underline{G}} \begin{pmatrix} \text{diag}(\tilde{\theta}_1, \dots, \tilde{\theta}_k) \\ \alpha_1, \dots, \alpha_k \end{pmatrix} \Theta^{-1}. \end{aligned}$$

Based on the structure of \mathcal{F}_m in Equation (7) and the partition of $Q_{\underline{G}}$ in Equation (15), we make

$$\begin{pmatrix} \Gamma_1^H \mathcal{L}_m \Gamma_1 \\ \Gamma_2^H \mathcal{F}_m \Gamma_1 \end{pmatrix} = R_{\underline{G}} \begin{pmatrix} \text{diag}(\tilde{\theta}_1, \dots, \tilde{\theta}_k) \\ \alpha_1, \dots, \alpha_k \end{pmatrix} \Theta_1^{-1}. \quad (23)$$

If we denote

$$\begin{aligned} [P_0, \tilde{W}_1]^{\text{new}} &= [\mathcal{V}_m, [P_{m-1}, \tilde{W}_m]] \Gamma_2, \quad \mathcal{V}_1^{\text{new}} = \mathcal{V}_m \Gamma_1, \\ \mathcal{L}_1^{\text{new}} &= \Gamma_1^H \mathcal{L}_m \Gamma_1, \\ \mathbb{H}_1^{\text{new}} &= \Gamma_2^H \mathcal{F}_m \Gamma_1, \quad \mathcal{F}_1^{\text{new}} = \begin{bmatrix} \mathcal{L}_1^{\text{new}} \\ \mathbb{H}_1^{\text{new}} \end{bmatrix} \end{aligned}$$

and substitute Equation (23) into Equation (22), Equation (19) is obtained.

- Show $R_0 = [\mathcal{V}_1^{\text{new}}, [P_0, \tilde{W}_1]^{\text{new}}] \Lambda_1^{\text{new}}$:

At restart we have

$$\begin{aligned} R_0 &= R_m \\ &= [\mathcal{V}_m, [P_{m-1}, \tilde{W}_m]] R_{LS_m} \\ &= [\mathcal{V}_m, [P_{m-1}, \tilde{W}_m]] Q_G \Theta_2 \\ &= [\mathcal{V}_1^{\text{new}}, [P_0, \tilde{W}_1]^{\text{new}}] \Lambda_1^{\text{new}}. \end{aligned}$$

- Show that Equality (20) holds:

Because $[\mathbb{W}_1^{\text{new}}, \mathbb{W}_2^{\text{new}}]$ is unitary, we have

$$[P_0, \tilde{W}_1]^{\text{new}} = [P_0, \tilde{W}_1]^{\text{new}} [\mathbb{W}_1^{\text{new}} \mathbb{W}_1^{\text{new}H} + \mathbb{W}_2 \mathbb{W}_2^{\text{new}H}],$$

substituting which into Equation (19) gives

$$\begin{aligned} A \mathcal{V}_1^{\text{new}} &= [\mathcal{V}_1^{\text{new}}, [P_0, \tilde{W}_1]^{\text{new}} (\mathbb{W}_1^{\text{new}} \mathbb{W}_1^{\text{new}H} + \mathbb{W}_2 \mathbb{W}_2^{\text{new}H})] \begin{bmatrix} \mathcal{L}_1^{\text{new}} \\ \mathbb{H}_1^{\text{new}} \end{bmatrix} \\ &= \mathcal{V}_1^{\text{new}} \mathcal{L}_1^{\text{new}} + [P_0, \tilde{W}_1]^{\text{new}} (\mathbb{W}_1^{\text{new}} \mathbb{W}_1^{\text{new}H} + \mathbb{W}_2 \mathbb{W}_2^{\text{new}H}) \mathbb{H}_1^{\text{new}} \\ &= \mathcal{V}_1^{\text{new}} \mathcal{L}_1^{\text{new}} + [P_0, \tilde{W}_1]^{\text{new}} \mathbb{W}_1^{\text{new}} \mathbb{W}_1^{\text{new}H} \mathbb{H}_1^{\text{new}} + [P_0, \tilde{W}_1]^{\text{new}} \mathbb{W}_2 \mathbb{W}_2^{\text{new}H} \mathbb{H}_1^{\text{new}} \\ &= \mathcal{V}_1^{\text{new}} \mathcal{L}_1^{\text{new}} + V_2^{\text{new}} \mathcal{L}_{2,:}^{\text{new}} + P_1^{\text{new}} G_1^{\text{new}} \\ &= [\mathcal{V}_1^{\text{new}}, V_2^{\text{new}}] \begin{bmatrix} \mathcal{L}_1^{\text{new}} \\ \mathcal{L}_{2,:}^{\text{new}} \end{bmatrix} + P_1^{\text{new}} G_1^{\text{new}}, \end{aligned}$$

which shows Equation (20). \square

It is noticed that the matrix $[P_0, \tilde{W}_1]^{\text{new}}$ is treated as an integrated matrix during the computation in Proposition 2 and it is not necessary to tell the explicit forms of P_0^{new} and \tilde{W}_1^{new} . As a matter of fact, continuing Algorithm 3 for $j = 2, \dots, m$ with the initialization proposed in Proposition 2 as shown in Steps 4 and 5 of Algorithm 2, i.e., setting $\mathcal{V}_2 = \mathcal{V}_2^{\text{new}}$, $\mathcal{L}_1 = \mathcal{L}_1^{\text{new}}$, $P_1 = P_1^{\text{new}}$, $G_1 = G_1^{\text{new}}$, we can consequently see that the block Arnoldi-like recurrence formulae of IB-BGMRES still hold for IB-BGMRES-DR. Then, an immediate corollary of Propositions 1 and 2 follows [28, Theorem 3] and reads:

Corollary 1. *The subspace for IB-BGMRES-DR is a block Krylov subspace, i.e., it is a combination of Krylov subspaces after a cycle of IB-BGMRES-DR.*

3.1.3 Algorithm for restarting with deflated targeted harmonic Ritz vectors

The glue procedure for adding the refined information of the targeted harmonic Ritz vectors at each restart of Algorithm 3 is summarized as in Algorithm 4. This glue procedure could be considered as counterparts of the implementations carried out at the Steps (4)-(7) of BGMRES-DR in [28] under the inexact-breakdown circumstances. It is remarked that in practical computation with finite precision arithmetic, it might be necessary to perform the reorthogonalization step as shown in Step 5 of Algorithm 4 to keep the orthogonality between $[P_0, \tilde{W}_1]^{\text{new}}$ and $\mathcal{V}_1^{\text{new}}$. As a consequence, the corresponding variables should be updated consequently as shown in Step 6 of Algorithm 4. One can follow the proof of Proposition 2 to easily see that the initial block Arnoldi-like recurrence formulae (19) and (20) keep the same.

3.1.4 Right-hand sides of the least-squares problem

For classical block-GMRES, the first residuals are in the initial search space so that the right-hand side of the least-squares problem has a special structure with non-zero entries only in its first leading block. When inexact breakdowns are handled, the right-hand side of the least-squares problem does not enjoy this property anymore and its calculation deserves some additional attention. At restart, instead of computing R_0 explicitly as $R_0 = B - AX_0$, we can express it alternatively as

$$R_0 = [\mathcal{V}_1, [P_0, \tilde{W}_1]] \Lambda_1. \quad (24)$$

The necessity and motivation to update the right-hand sides of the least-squares problem at each iteration is that R_0 has components in $[P_0, \tilde{W}_1]$, those directions are not kept as is in the search space. As the method progresses, the directions of $[P_0, \tilde{W}_1]$ will contribute to the construction of V_j or P_{j-1} to expand the search space. Proposition 3 indicates how the least-squares right-hand sides can be incrementally and cheaply computed at each iteration of the block algorithm.

Proposition 3. *At each iteration (see Step 5 of Algorithm 2), the new least-squares problem reads*

$$Y_{j+1} = \underset{Y \in \mathbb{C}^{n_{j+1} \times p}}{\operatorname{argmin}} \| \Lambda_{j+1} - \mathcal{F}_{j+1} Y \|_F,$$

with the right-hand sides being

$$\Lambda_{j+1} = \begin{bmatrix} I_{p_1} & \\ 0_{(n_{j+1}+p-p_1) \times p_1} & \Phi_{j+1} \end{bmatrix} \Lambda_1, \quad (25)$$

where $\Lambda_1 \in \mathbb{C}^{(p_1+p) \times p}$ and $\Phi_{j+1} \in \mathbb{C}^{(n_{j+1}+p) \times p}$ can be iteratively updated as

$$\Phi_{j+1} = \begin{bmatrix} \Phi_j(1:n_j, :) \\ [\mathbb{W}_1, \mathbb{W}_2]^H \begin{bmatrix} \Phi_j(n_j+1:n_j+p-p_j, :) \\ 0_{p_j \times p} \end{bmatrix} \\ 0_{p_{j+1} \times p} \end{bmatrix}, \quad (26)$$

where, $[\mathbb{W}_1, \mathbb{W}_2]$ are respectively defined in Equations (8) and (10) at iteration j (see Step 7 of Algorithm 4 and Algorithm 3).

Proof. The right-hand side of the least-squares problem at iteration $(j+1)$ is defined by

$$\begin{aligned} \Lambda_{j+1} &= [\mathcal{V}_{j+1}, [P_j, \tilde{W}_{j+1}]]^H R_0, \\ &= [\mathcal{V}_j, V_{j+1}, [P_j, \tilde{W}_{j+1}]]^H R_0, \\ &= [\mathcal{V}_j, [P_{j-1}, \tilde{W}_j] \mathbb{W}_1, [P_{j-1}, \tilde{W}_j] \mathbb{W}_2, \tilde{W}_{j+1}]^H R_0, \text{ using Equations (8) and (10) }, \\ &= [\mathcal{V}_j, [P_{j-1}, \tilde{W}_j] [\mathbb{W}_1, \mathbb{W}_2], \tilde{W}_{j+1}]^H R_0, \\ &= [\mathcal{V}_j, [P_{j-1}, \tilde{W}_j] [\mathbb{W}_1, \mathbb{W}_2], \tilde{W}_{j+1}]^H [\mathcal{V}_1, [P_0, \tilde{W}_1]] \Lambda_1, \\ &= \begin{bmatrix} \mathcal{V}_j^H \mathcal{V}_1 & \mathcal{V}_j^H [P_0, \tilde{W}_1] \\ [V_{j+1}, P_j]^H \mathcal{V}_1 & [\mathbb{W}_1, \mathbb{W}_2]^H [P_{j-1}, \tilde{W}_j]^H [P_0, \tilde{W}_1] \\ \tilde{W}_{j+1}^H \mathcal{V}_1 & \tilde{W}_{j+1}^H [P_0, \tilde{W}_1] \end{bmatrix} \Lambda_1 \\ &= \begin{bmatrix} \begin{bmatrix} I_{p_1} \\ 0_{(n_j-p_1) \times p_1} \end{bmatrix} & \Phi_j(1:n_j, :) \\ 0_{p \times p_1} & [\mathbb{W}_1, \mathbb{W}_2]^H \begin{bmatrix} \Phi_j(n_j+1:n_j+p-p_j, :) \\ 0_{p_j \times p} \end{bmatrix} \\ 0_{p_{j+1} \times p_1} & 0_{p_{j+1} \times p} \end{bmatrix} \Lambda_1 \end{bmatrix} \end{aligned}$$

The last equality results mainly from the facts that $\text{Range}([P_0, \tilde{W}_1]) \subset \text{Range}([\mathcal{V}_j, P_{j-1}, \tilde{W}_j])$ ($j = 1, \dots, m$), $\tilde{W}_{j+1} \perp \text{Range}([P_0, \tilde{W}_1])$ ($j = 1, \dots, m-1$), and that the basis $[\mathcal{V}_j, P_{j-1}, \tilde{W}_j]$ ($j = 1, \dots, m$) are orthonormal. \square

3.2 The new block variant

With the properties and discussions stated in the previous three sections, we summarize and present the new block variant-IB-BGMRES-DR as in Algorithm 2. Notice that we take the same notation for IB-BGMRES-DR as that for IB-BGMRES for consistent algorithm presentation. However, it should be kept in mind that the quantities computed by IB-BGMRES-DR after the first cycle of Algorithm 2 are different from those by IB-BGMRES as shown in Algorithm 3.

Algorithm 2 *IB-BGMRES-DR: Block-GMRES-DR with R -criterion to detect inexact breakdowns.*

- 1: *Start.* Let the p linearly independent right-hand sides be $B = [b^{(1)}, b^{(2)}, \dots, b^{(p)}]$. Choose the maximal dimension of the underlying block approximation Krylov subspace in each cycle, k the desired number of approximate targeted eigenvectors, ε the targeted backward error, $X_0 = [x_0^{(1)}, x_0^{(2)}, \dots, x_0^{(p)}]$ the initial guesses. Let $r_0^{(i)} = b^{(i)} - Ax_0^{(i)}$, $i = 1, \dots, p$. Denote $R_0 = [r_0^{(1)}, r_0^{(2)}, \dots, r_0^{(p)}]$ the initial nonsingular block residuals. The recast problems are $A(x^{(i)} - x_0^{(i)}) = r_0^{(i)}$, $i = 1, \dots, p$.
 - 2: *Find approximate solutions for the first cycle.* Implement the first cycle of Algorithm 3. Form the new approximate solutions $X_m = X_0 + \mathcal{V}_m Y_m$. Compute the residual vectors $R_m = B - AX_m = [\mathcal{V}_m, [P_{m-1}, \tilde{W}_m]] (\Lambda_m - \mathcal{F}_m Y_m)$. Check convergence, and proceed if not satisfied.
 - 3: *Begin restart.* Let $X_0 = X_m$ and $R_0 = R_m$. Compute the k targeted eigenpairs $(\tilde{\theta}_i, \tilde{g}_i)$ ($i = 1, \dots, k$) of the matrix $\mathcal{L}_m + \mathcal{L}_m^{-H} \mathbb{H}_m^H \mathbb{H}_m$. (The $\tilde{\theta}_i$ ($i = 1, \dots, k$) are harmonic Ritz values.) Then store the \tilde{g}_i ($i = 1, \dots, k$) into the matrix G . For real matrices, it is necessary to separate \tilde{g}_i ($i = 1, \dots, k$) into real and imaginary parts if complex, in order to form an $n_m \times k$ matrix G . (It may be necessary to adjust k in order to make sure both parts of complex vectors are included.)
 - 4: *Implement Algorithm 4.* Fulfill the initialization of Algorithm 3 at each restart with refined information associated with the k targeted harmonic Ritz vectors G .
 - 5: *Implement Algorithm 3 for $j = 2, \dots, m$.* Complete the remaining iterations of a new cycle of Algorithm 3 after the initialization with Algorithm 4 and the update of the least-squares right-hand sides described in Proposition 3.
 - 6: *Form the approximate solutions.* Form the new approximate solutions $X_m = X_0 + \mathcal{V}_m Y_m$. Compute the residual vectors $R_m = B - AX_m = [\mathcal{V}_m, [P_{m-1}, \tilde{W}_m]] (\Lambda_m - \mathcal{F}_m Y_m)$.
 - 7: Check convergence, and restart if convergence is not achieved, i.e., go to 3.
-

3.3 Stopping criterion

We further discuss how the threshold parameter $\epsilon^{(R)}$ used to detect the inexact breakdowns should be related to the final targeted backward error of the individual linear systems. The normwise backward error associated with an approximate solution x with perturbation on one right-hand side b is defined as follows

Definition 2. *For the solution of a linear system, the normwise backward error associated with*

an approximate solution x with perturbation on one right-hand side b is defined by

$$\begin{aligned}\eta_b(x) &= \min_{\Delta b} \{ \tau > 0 : \|\Delta b\|_2 \leq \tau \|b\|_2 \text{ and } Ax = b + \Delta b \} \\ &= \frac{\|Ax - b\|_2}{\|b\|_2}.\end{aligned}$$

Assuming p inexact breakdowns have occurred at iterations s of IB-BGMRES (also IB-BGMRES-DR) solving for $B = [b^{(1)}, b^{(2)}, \dots, b^{(p)}]$, according to [33, Equation (47)], we have

$$\|B - AX_s\|_2 \leq \epsilon^{(R)}.$$

Then the normwise backward errors $\eta_{b^{(i)}} (i = 1, \dots, p)$ associated with each column of approximate solutions $X_s = [x_s^{(1)}, \dots, x_s^{(p)}]$ satisfy

$$\eta_{b^{(i)}}(x_s^{(i)}) = \frac{\|b^{(i)} - Ax_s^{(i)}\|_2}{\|b^{(i)}\|_2} \leq \frac{\|B - AX_s\|_2}{\|b^{(i)}\|_2} \leq \frac{\|B - AX_s\|_2}{\min_{i=1, \dots, p} \|b^{(i)}\|_2} \leq \frac{\epsilon^{(R)}}{\min_{i=1, \dots, p} \|b^{(i)}\|_2} \quad (27)$$

due to the property of matrix 2-norm. It follows that the choice

$$\epsilon^{(R)} = \varepsilon \times \min_{i=1, \dots, p} \|b^{(i)}\|_2 \quad (28)$$

ensures that all the linear systems have been solved to the target accuracy ε when p inexact breakdowns have been detected. We notice that this might induce some delay in the practical convergence check with wasted computational effort, but not much, as will be seen and discussed in the numerical experiments.

4 Numerical experiments

4.1 Test problems and experimental setting

In this section, we investigate the numerical features and convergence behaviors of IB-BGMRES-DR on a set of representative test problems. The performance obtained by IB-BGMRES-DR is evaluated in comparison with BGMRES-DR [28] and IB-BGMRES [33] in term of number of matrix-vector products (referred to as *mups*) that is often the most time consuming kernel in large calculations.

The test problems include eight matrices. For the sake of comparison with related works, the first five test matrices are taken as those of Example 1 in [28], the sixth matrix is used in [33], and the last two are used in [21]. From the point of view of convenient illustration, we briefly describe those examples. The first four matrices of size 1000 are bidiagonal with superdiagonal entries being all unity. Matrix 1 has diagonal entries $0.1, 1, 2, 3, \dots, 999$. Matrix 2 has diagonal entries $1, 2, 3, \dots, 1000$, matrix 3 has diagonal entries $11, 12, 13, \dots, 1010$, while matrix 4 has diagonal entries $10.1, 10.2, 10.3, \dots, 19.9, 20, 21, 22, \dots, 919, 920$. The fifth and sixth matrices are from oil reservoir simulation- SHERMAN4 of size 1104 and SHERMAN5 of size 3312 taken from the Harwell-Boeing collection of test matrices [10]. The last two matrices Dehghani/light_in_tissue of size 29282 and HB/young1c of size 841 as respectively arising from light transport in soft tissue and aero research, are borrowed from the University of Florida Sparse Matrix Collection [9]. For those experiments, the k smallest harmonic Ritz values are chosen as to select the harmonic vectors to be recycled in IB-BGMRES-DR and BGMRES-DR. The experiments have been carried out in double precision floating point arithmetic in MATLAB 7.0.4.

4.2 Some comparisons

All these tests are started with the initial block guess equal to $0 \in \mathbb{C}^{n \times p}$. The right-hand sides $B = [b^{(1)}, b^{(2)}, \dots, b^{(p)}] \in \mathbb{C}^{n \times p}$ have p linearly independent columns generated with normal distribution. For BGMRES-DR, the stopping criterion used here is that the p individual normwise backward error satisfies $\eta_{b^{(i)}} < \varepsilon$ ($i = 1, \dots, p$), or the number of matrix-vector multiplications exceeds the allowed maximal number (referred to as *maxiter*). For IB-BGMRES and IB-BGMRES-DR, the stopping criterion used here is that all p inexact breakdowns (monitored as described in Section 3.3) have occurred, or *mvps* exceeds *maxiter*. In those experiments we set the number of right-hand sides to $p = 6$, the maximum dimension of the search space is $m = 90$, the number of deflated harmonic Ritz vectors is $k = 5$, the targeted backward error is $\varepsilon = 10^{-6}$ and *maxiter* = 10000 for all tests. No preconditioning is used except for the sixth example, where a right ILU(0) preconditioner is implemented to ensure the convergence within a reasonable amount of iterations.

On the right part of Figures 1 and 2, we display the upper bounds on the backward errors for IB-BGMRES and IB-BGMRES-DR given by Equation (27) and the largest backward error. It can be seen that the upper bound is quite sharp and deserves to be considered to design the stopping criterion especially when the norms of right-hand sides have similar magnitude. In the left part of these figures we display the convergence history of the three block methods reporting for each of them the smallest and largest backward errors among the p right-hand sides. For problems where slow convergence is caused by small eigenvalues as Examples 1, 2, 5, 6, 7 and 8, deflation of small eigenvalues makes IB-BGMRES-DR more attractive and efficient. It enables a significant reduction of *mvps* compared to IB-BGMRES and BGMRES-DR. For easier problems such as Examples 3 and 4, the performances of IB-BGMRES, BGMRES-DR and IB-BGMRES-DR are essentially similar. It can be observed that IB-BGMRES-DR essentially inherits the nice numerical features of its two ascendent methods namely IB-BGMRES and BGMRES-DR.

The *mvps* required and the attained accuracy in terms of the maximum and minimum of the p individual normwise backward errors associated with the initial right-hand sides B are reported in Table 1 where the symbol “-” indicates no convergence. It can be observed that the minimum components of the p individual normwise backward errors attained by BGMRES-DR are smaller than their counterparts obtained by IB-BGMRES and IB-BGMRES-DR in most cases. This illustrates that some computational resources are wasted due to the none detection of partial convergence, that is BGMRES-DR does continue to enlarge the space with constant dimension at each step and update all the approximated solutions including those that have converged. This is the main feature of the IB-BGMRES-DR and IB-BGMRES variants that ensure that all the solutions converge to the same accuracy.

In order to illustrate the benefit of using block variants in linear Krylov solvers, we present numerical experiments performed with regular single GMRES(m) [35] and GMRES-DR(m, k) [27] for solving in sequence the same set of right-hand sides. The *mvps* displayed are cumulated over the p solutions using the same experimental setting in term of space dimension and stopping criterion, i.e., $\eta_{b^{(i)}} < \varepsilon$ ($i = 1, \dots, p$), or individual *mvps* exceeds *maxiter* ($p = 6$, $m = 90$, $k = 5$, $\varepsilon = 10^{-6}$, and *maxiter* = 10000). The results are reported in Table 2, and they are most of the time significantly better for the block variants and only marginally worse on two examples (where it could be argued that the computer science benefit of BLAS-3 type operation can compensate the small numerical penalty). In particular, we can see that the block variants perform more efficiently than regular single vector counterparts for Examples 1, 2, 5, 6; for Examples 3, 4, all the solvers perform similarly. For Examples 7 and 8, BGMRES-DR is outperformed by its single vector counterpart GMRES-DR. In these latter two examples, IB-BGMRES-DR performs much better than BGMRES-DR, having almost the same *mvps* as GMRES-DR on Example 7 while

Example	Method	mvp s	$\eta_{b(i)} \ (i = 1, \dots, p)$	
			min	max
1	IB-BGMRES	1344	2.23e-7	5.64e-7
	BGMRES-DR	892	2.74e-7	9.13e-7
	IB-BGMRES-DR	588	6.86e-7	7.83e-7
2	IB-BGMRES	788	4.62e-7	6.98e-7
	BGMRES-DR	667	2.96e-7	9.04e-7
	IB-BGMRES-DR	538	7.31e-7	8.53e-7
3	IB-BGMRES	372	6.55e-7	7.85e-7
	BGMRES-DR	341	6.36e-7	9.34e-7
	IB-BGMRES-DR	335	6.59e-7	8.38e-7
4	IB-BGMRES	446	5.90e-7	8.78e-7
	BGMRES-DR	447	6.53e-7	9.18e-7
	IB-BGMRES-DR	440	8.18e-7	9.11e-7
5	IB-BGMRES	617	3.93e-7	9.03e-7
	BGMRES-DR	474	1.27e-7	9.48e-7
	IB-BGMRES-DR	386	6.50e-7	9.08e-7
6	IB-BGMRES	357	2.24e-7	5.36e-7
	BGMRES-DR	294	2.71e-8	9.97e-7
	IB-BGMRES-DR	248	6.01e-7	7.54e-7
7	IB-BGMRES	3291	4.51e-7	7.97e-7
	BGMRES-DR	3090	1.15e-7	9.85e-7
	IB-BGMRES-DR	2104	8.32e-7	9.55e-7
8	IB-BGMRES	-	7.01e-5	5.19e-4
	BGMRES-DR	4426	2.84e-7	9.90e-7
	IB-BGMRES-DR	2202	5.40e-7	7.63e-7

Table 1: Numerical behavior of IB-BGMRES, BGMRES-DR and IB-BGMRES-DR with $\varepsilon = 10^{-6}$.

much less *mvp*s than GMRES-DR on Example 8.

Example	GMRES	GMRES-DR	IB-BGMRES	BGMRES-DR	IB-BGMRES-DR
1	2536	1077	1344	892	588
2	1069	856	788	667	538
3	378	378	372	341	335
4	412	412	446	447	440
5	845	694	617	474	386
6	464	464	357	294	248
7	3154	2003	3291	3090	2104
8	10643	3110	-	4426	2202

Table 2: Number of *mvp*s for regular GMRES, GMRES-DR, IB-BGMRES, BGMRES-DR and IB-BGMRES-DR with $\varepsilon = 10^{-6}$.

4.3 Influence of the number of right-hand sides

In this section, we investigate the effect of the number of right-hand sides on the relative performance of the block solvers. In all the tables, we vary the number of right-hand sides $p = 6, 12, 18, 24$. First in Table 3 (Table 4) we consider $m = 90$ (respectively $m = 200$) for the maximal dimension of the search space. For the block GMRES variant, when p is increased the degree of the polynomial in A used to build the Krylov space decreases. For instance with $p = 24$, the degree is less than 4 which can explain why some block variants do not succeed to converge. When the value of n is increased to 200, the polynomial degree can be increased and the robustness of the block GMRES variant increases as well.

In order to further illustrate the effect of the polynomial degree on the block Krylov solver robustness we report in Table 5 numerical results where we attempt to keep constant this polynomial degree to 15 when the number of right-hand sides is varied. Consequently we set $m = 15 \times p$ and only select the largest test examples so that the maximum size of the search space remains a small fraction of the problem dimension. It can be observed that the numerical performance of all block GMRES improves. For $p = 24$, regular GMRES and GMRES-DR never perform restart so that their numerical behaviours are identical.

4.4 Inexact breakdowns versus targeted accuracy

In this section we illustrate the benefit of the tight coupling between the inexact breakdown detection and the targeted accuracy for the solution. In Figure 3, we display the convergence history of IB-BGMRES-DR for different values of ε for the largest and smallest of the p backward errors. Because the inexact breakdown threshold is related to ε by Equation (28), the inexact breakdown strategy will act earlier for larger values of ε . For instance it might be observed that the curves overlap until the first inexact breakdown is detected for $\varepsilon = 10^{-6}$, then the ones associated with $\varepsilon = 10^{-8}$ and 10^{-10} still overlap while the other one exhibits a faster decay to its target 10^{-8} . This characterizes the nice feature of the inexact breakdown mechanism that enables to focus on what remains to be converged and then reduce the computational cost to achieve convergence.

p	Example Method	1	2	3	4	5	6	7	8
6	GMRES	2536	1069	378	412	845	464	3154	-
	GMRES-DR	1077	856	378	412	694	464	2003	3110
	IB-BGMRES	1344	788	372	446	617	357	3291	-
	BGMRES-DR	892	667	341	447	474	294	3090	4426
	IB-BGMRES-DR	588	538	335	440	386	248	2104	2202
12	GMRES	4855	2132	753	825	1696	927	6343	-
	GMRES-DR	2141	1711	753	825	1404	927	4003	6225
	IB-BGMRES	2427	1556	790	1091	1182	713	7320	-
	BGMRES-DR	2324	1784	820	1139	1209	901	-	-
	IB-BGMRES-DR	1098	1074	694	1062	843	442	5823	4478
18	GMRES	7573	3235	1135	1238	2556	1393	9641	-
	GMRES-DR	3204	2553	1135	1238	2117	1393	6029	9332
	IB-BGMRES	3048	2322	1278	1902	1913	1116	-	-
	BGMRES-DR	5529	4207	1536	2587	2355	-	-	-
	IB-BGMRES-DR	1822	1687	1178	2058	1579	661	-	6794
24	GMRES	-	4332	1516	1648	3367	1859	-	-
	GMRES-DR	4277	3408	1516	1648	2824	1859	8015	-
	IB-BGMRES	4542	3244	1902	3589	2961	1589	-	-
	BGMRES-DR	-	6963	2375	4531	3741	-	-	-
	IB-BGMRES-DR	2402	2312	1648	3349	2473	846	-	8744

Table 3: Total number of *mvps* for different numbers of right-hand sides with $m = 90$.

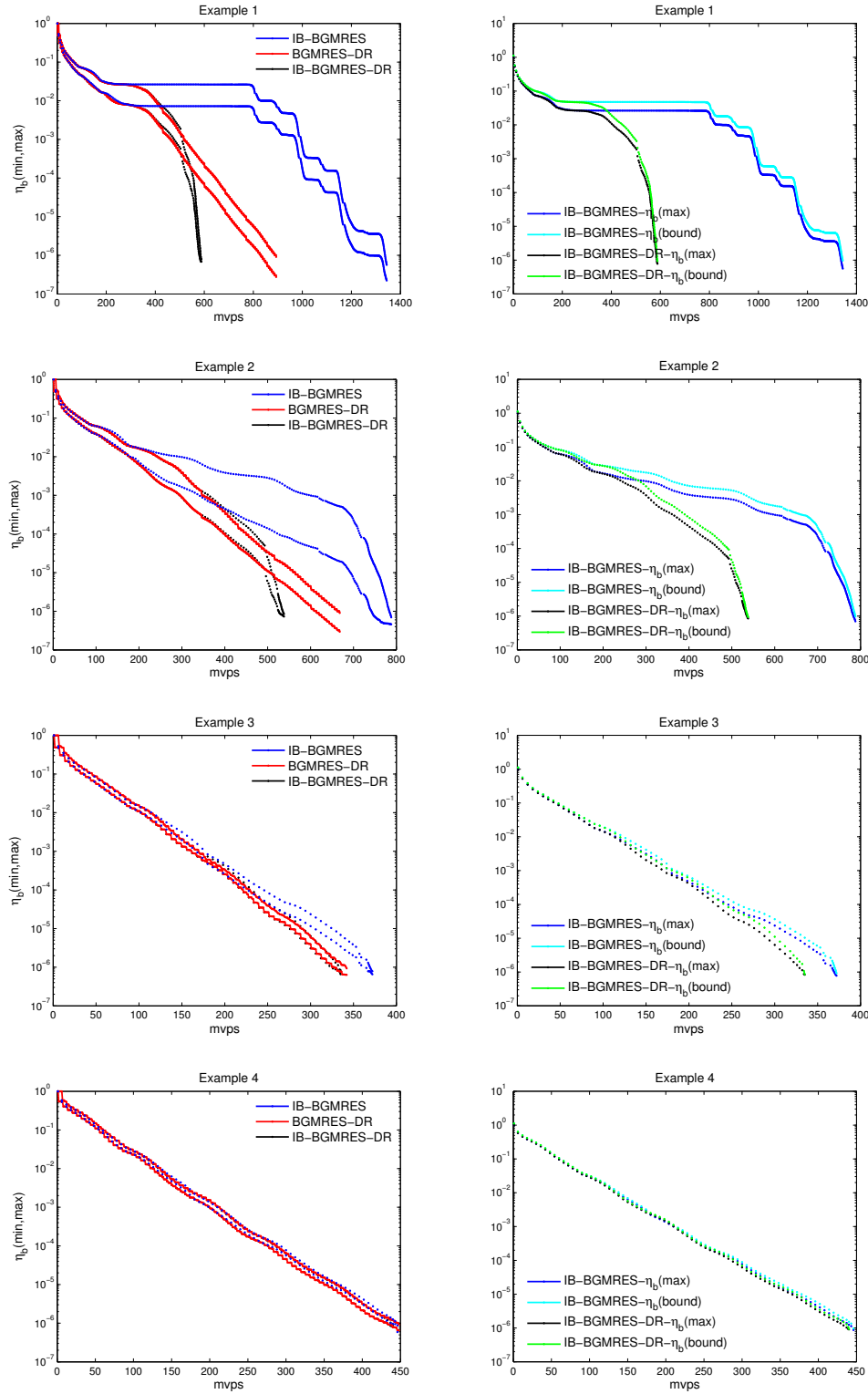


Figure 1: Convergence histories for the first four examples. Left: convergence histories of the largest/smallest $\eta_b(i)$ at each $mvps$. Right: upper bounds of $\eta_b(i)$ and $\max(\eta_b(i))$ at each $mvps$.

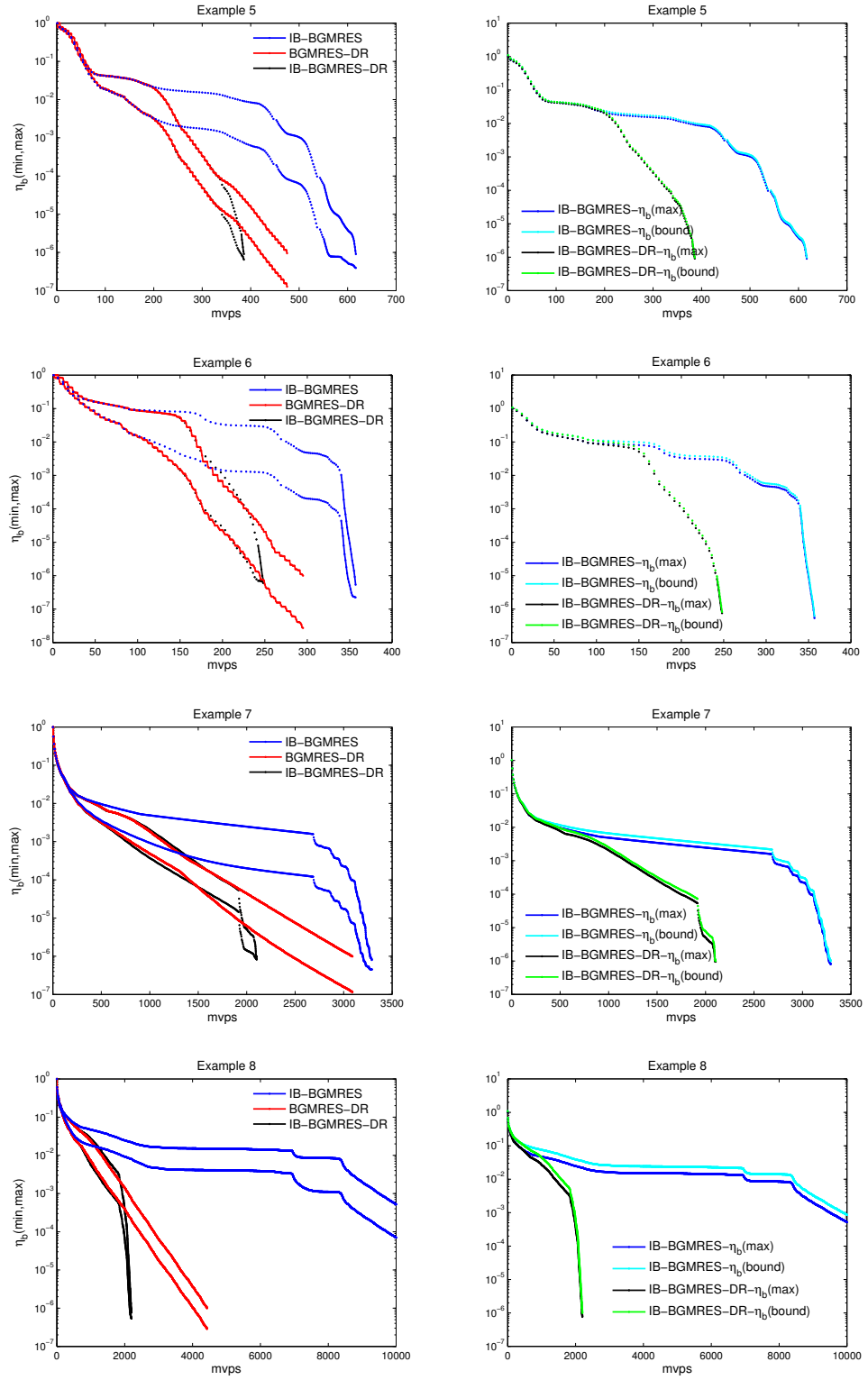


Figure 2: Convergence histories for the last four examples. Left: convergence histories of the largest/smallest $\eta_b(i)$ at each $mvps$. Right: upper bounds of $\eta_b(i)$ and $\max(\eta_b(i))$ at each $mvps$.

p	Example Method	1	2	3	4	5	6	7	8
6	GMRES	1062	849	378	412	660	464	2428	4012
	GMRES-DR	1062	849	378	412	660	464	1977	2211
	IB-BGMRES	759	596	327	410	367	184	2230	2738
	BGMRES-DR	677	582	328	417	371	225	2004	1645
	IB-BGMRES-DR	516	473	315	410	316	184	1524	1361
12	GMRES	2112	1698	753	825	1330	927	4829	8126
	GMRES-DR	2112	1698	753	825	1330	927	3951	4435
	IB-BGMRES	1183	1059	645	850	703	368	4481	4663
	BGMRES-DR	1219	981	627	853	699	393	5857	4474
	IB-BGMRES-DR	829	797	573	828	568	345	3342	2465
18	GMRES	3162	2533	1135	1238	2004	1393	7335	-
	GMRES-DR	3162	2533	1135	1238	2004	1393	5950	6650
	IB-BGMRES	1651	1469	947	1341	963	550	6944	8128
	BGMRES-DR	2667	1756	981	1453	1170	735	-	7580
	IB-BGMRES-DR	1189	1120	850	1316	855	475	6034	3527
24	GMRES	4220	3380	1516	1648	2671	1859	9670	-
	GMRES-DR	4220	3380	1516	1648	2671	1859	7907	8865
	IB-BGMRES	2170	1930	1217	1961	1386	731	-	-
	BGMRES-DR	3500	2856	1374	2103	1759	960	-	-
	IB-BGMRES-DR	1513	1500	1115	1905	1221	591	8731	4254

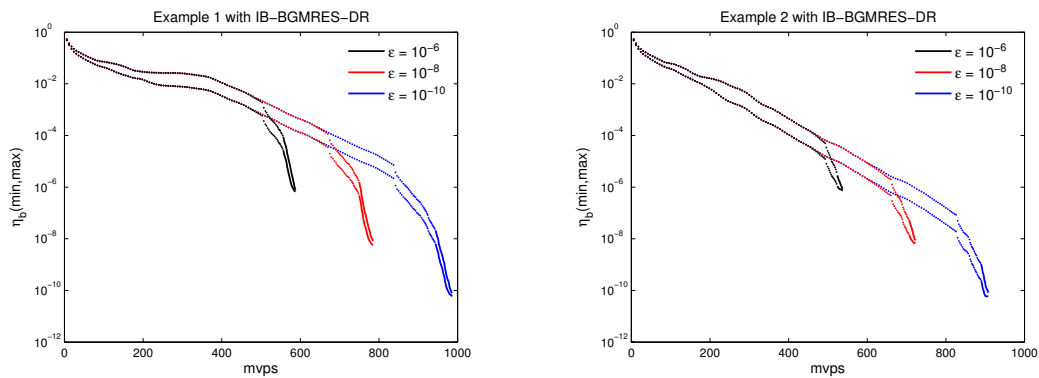
Table 4: Total number of $mvps$ for different numbers of right-hand sides with $m = 200$.

Figure 3: Convergence history of IB-GMRES-DR when the targeted accuracy is varied.

p	Example Method	5	6	7
6	GMRES	845	464	3154
	GMRES-DR	694	464	2003
	IB-BGMRES	617	357	3291
	BGMRES-DR	474	294	3090
	IB-BGMRES-DR	386	248	2104
12	GMRES	1330	927	4845
	GMRES-DR	1330	927	3946
	IB-BGMRES	673	406	4787
	BGMRES-DR	719	481	7567
	IB-BGMRES-DR	589	344	3576
18	GMRES	2004	1393	6270
	GMRES-DR	2004	1393	5963
	IB-BGMRES	831	454	5843
	BGMRES-DR	981	507	-
	IB-BGMRES-DR	744	427	4963
24	GMRES	2671	1859	7845
	GMRES-DR	2671	1859	7845
	IB-BGMRES	941	495	7149
	BGMRES-DR	1241	600	-
	IB-BGMRES-DR	852	437	6114

Table 5: Examples 5, 6 and 7: Comparison results of “iso-polynomial degree” experiments for different numbers of right-hand sides with $m = 15 \times p$.

4.5 Further improvement

The selection of the restart parameter for GMRES(m) depends mostly on the specific application context and on the affordable memory. Recently, it has been surprisingly noticed that small values of the restart parameter actually yield convergence in fewer iterations than larger values for some problems (see, e.g. [3, 4, 11, 12] and related papers, e.g. [41]). In [3] the authors proposed a simple strategy for varying the restart parameter of GMRES(m) with a negligible amount of overhead to accelerate convergence in terms of the time to solution by disrupting repetitive behaviors of the GMRES(m) residual vectors at the end of each restart cycle.

Corresponding to the selection of the restart parameter for GMRES(m), the selection of the maximal dimension n of the underlying block approximation Krylov subspace in each cycle of IB-BGMRES-DR is examined in this section. The strategy employed in [3] can be extended in a straightforward way to adjust n the maximal dimension of the block Krylov subspace in each cycle in IB-BGMRES-DR. Instead of using the residual norm as in [3] we use the bounds on the 2-norm of the residual block. The calculation of n is described in Algorithm 5 that involves a negligible extra computational effort.

As shown in Table 6, for small values of n , the adjusting strategy does help to further reduce mvp s required by IB-BGMRES-DR. While for larger ones, the strategy seems not to help much for some cases. However, from the point of view of the goal of restarting as a means of reducing computational and storage costs, this adjusting strategy could be recommended, especially when memory is a concern. It should be noted that this strategy could be also extended to other block

Example Method	1	2	3	4	5	6	7	8
IB-BGMRES-DR(30)	1043	917	508	728	709	304	5330	5064
α IB-BGMRES-DR(30,15)	671	581	364	476	476	270	1954	4691
IB-BGMRES-DR(60)	688	615	370	491	451	278	2705	2762
α IB-BGMRES-DR(60,15)	639	599	366	545	489	286	1691	2516
IB-BGMRES-DR(90)	588	538	335	440	386	248	2104	2202
α IB-BGMRES-DR(90,15)	603	545	335	440	387	248	1673	2359

Table 6: Comparison results for varying the maximal dimension of the underlying block approximation Krylov subspace in each cycle with $\varepsilon = 10^{-6}$ in terms of mvp s.

variants of GMRES(m), however this is out of the scope of this paper and we do not investigate it further.

5 Concluding remarks

In this paper we combine the numerical feature of BGMRES-DR and IB-BGMRES to develop a new block variant—IB-BGMRES-DR for systems of linear equations with multiple right-hand sides given simultaneously. We derive a restarting strategy that preserves the Arnoldi-like relation while ensuring that both the residuals and some spectral information are in the space at restart when inexact breakdown occurred. Not addressed in [33], we also show how the right-hand sides of the least-squares problems can be incrementally updated after the first restart of IB-BGMRES and IB-BGMRES-DR. Through extensive numerical experiments we illustrate that IB-BGMRES-DR inherits from the nice numerical features of its two ascendent methods. In particular, we indicate how the varying restart strategy of regular GMRES can be extended to this new block

variant. Finally, although not derived in this paper, a version of the proposed algorithm with flexible preconditioning can be developed using similar techniques as those presented in [16].

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A Robbé, Sadkane Block Arnoldi with inexact breakdowns

Algorithm 3 *Block Arnoldi using R-criterion to detect inexact breakdowns*

- 1: Assuming $B \in \mathbb{C}^{n \times p}$ is of full rank, choose the initial block guesses X_0 , and compute the corresponding nonsingular initial block residuals $R_0 = B - AX_0$.
- 2: Form the initial unitary matrix V_1 from the initial block residuals $R_0 = V_1 \Lambda_1$ with reduced QR -factorization. Let $P_0 = 0, G_0 = 0$ and $\underline{\mathcal{L}}_0 = [\]$. Choose a targeted backward error ε and set the corresponding $\epsilon^{(R)}$.
- 3: **for** $j = 1, 2, \dots, m$ **do**
- 4: Orthogonalize AV_j against previous block orthonormal basis $\mathcal{V}_j = [V_1, \dots, V_j]$ as

$$\mathcal{L}_{1,1:j} = \mathcal{V}_j^H (AV_j), \quad W_j = AV_j - \mathcal{V}_j \mathcal{L}_{1,1:j}, \quad \text{where } \mathcal{L}_{1,1:j} \text{ is a block column matrix.}$$

- 5: Set $\underline{\mathcal{L}}_j = [\underline{\mathcal{L}}_{j-1}, \quad \mathcal{L}_{1,1:j}] \in \mathbb{C}^{n_j \times n_j}$.
- 6: Orthogonalize W_j against P_{j-1} and carry out its reduced QR -factorization as

$$C_j = P_{j-1}^H W_j, \quad \tilde{W}_j D_j = W_j - P_{j-1} C_j.$$

- 7: Compute Y_j the solution of the least-squares problem

$$\min_{Y \in \mathbb{C}^{n_j \times p}} \|\Lambda_j - \mathcal{F}_j Y\|_F \quad \text{with}$$

$$\Lambda_j = \begin{pmatrix} \Lambda_1 \\ 0 \end{pmatrix} \in \mathbb{C}^{(n_j+p) \times p}, \quad \mathcal{F}_j = \begin{pmatrix} \underline{\mathcal{L}}_j \\ \mathbb{H}_j \end{pmatrix} \in \mathbb{C}^{(n_j+p) \times n_j}, \quad \text{and } \mathbb{H}_j = \begin{pmatrix} G_{j-1} & C_j \\ 0 & D_j \end{pmatrix} \in \mathbb{C}^{p \times n_j}.$$

Carry out the Singular Value Decomposition algorithm to detect inexact breakdowns in residuals

$$(\Lambda_j - \mathcal{F}_j Y_j) = U_1 \Sigma_1 V_1^H + U_2 \Sigma_2 V_2^H, \quad \text{where } \sigma_{\min}(\Sigma_1) \geq \epsilon^{(R)} > \sigma_{\max}(\Sigma_2).$$

Compute \mathbb{W}_1 and \mathbb{W}_2 such that

$$\text{Range}(\mathbb{W}_1) = \text{Range}(U_1^{(2)}) \quad \text{with } U_1 = \begin{pmatrix} U_1^{(1)} \\ U_1^{(2)} \end{pmatrix} \quad \text{and } [\mathbb{W}_1, \quad \mathbb{W}_2] \text{ is unitary.}$$

Compute orthonormal matrices V_{j+1} and P_j , the last block row matrix $\mathcal{L}_{j+1,:}$ of $\underline{\mathcal{L}}_j$, and G_j as

$$V_{j+1} = [P_{j-1}, \quad \tilde{W}_j] \mathbb{W}_1, \quad P_j = [P_{j-1}, \quad \tilde{W}_j] \mathbb{W}_2, \\ \mathcal{L}_{j+1,:} = \mathbb{W}_1^H \mathbb{H}_j, \quad G_j = \mathbb{W}_2^H \mathbb{H}_j.$$

- 8: Set $\underline{\mathcal{L}}_j = \begin{pmatrix} \underline{\mathcal{L}}_j \\ \mathcal{L}_{j+1,:} \end{pmatrix}$.
 - 9: **end for**
-

B Restarting procedure with deflation

Algorithm 4 *Restarting with deflated targeted harmonic Ritz vectors*

Morgan [R. B. Morgan. Restarted block GMRES with deflation of eigenvalues. Applied Numerical Mathematics, 54(2): 222-236, 2005.].

- 1: Compute $R_{LS_m} = \Lambda_m - \mathcal{F}_m Y_m = [\mathcal{V}_m, [P_{m-1}, \tilde{W}_m]]^H R_m \in \mathbb{C}^{(n_m+p) \times p}$ the least-squares residuals at the m -th iteration of the first cycle of Algorithm 3. Denote by $\mathcal{V}_m \tilde{G}$ the k targeted harmonic Ritz vectors, where $\tilde{G} = [\tilde{g}_1, \dots, \tilde{g}_k] \in \mathbb{C}^{n_m \times k}$.
- 2: Append R_{LS_m} to \tilde{G} by first adding zero rows of size p to \tilde{G} and then R_{LS_m} to form a new matrix denoted as $\underline{G} = \begin{bmatrix} \tilde{G} & R_{LS_m} \\ 0 & \end{bmatrix}$ of dimension $(n_m + p) \times (k + p)$.
- 3: Form and store a unitary matrix $Q_{\underline{G}} \in \mathbb{C}^{(n_m+p) \times (k+p)}$ and the last p columns of an upper triangular matrix $R_{\underline{G}} \in \mathbb{C}^{(k+p) \times (k+p)}$ from the reduced QR -factorization of \underline{G} as $\underline{G} = Q_{\underline{G}} R_{\underline{G}}$. The matrix consisting of the last p columns of $R_{\underline{G}}$ is denoted as

$$\Lambda_1^{\text{new}} = R_{\underline{G}}(:, k+1 : k+p) \in \mathbb{C}^{(k+p) \times p}.$$

- 4: Compute

$$\begin{aligned} [P_0, \tilde{W}_1]^{\text{new}} &= [\mathcal{V}_m, [P_{m-1}, \tilde{W}_m]] Q_{\underline{G}}(:, k+1 : k+p), \quad \mathcal{V}_1^{\text{new}} = \mathcal{V}_m Q_{\underline{G}}(1 : n_m, 1 : k), \\ \mathcal{L}_1^{\text{new}} &= Q_{\underline{G}}(1 : n_m, 1 : k)^H \mathcal{L}_m Q_{\underline{G}}(1 : n_m, 1 : k), \\ \mathbb{H}_1^{\text{new}} &= Q_{\underline{G}}(:, k+1 : k+p)^H \mathcal{F}_m Q_{\underline{G}}(1 : n_m, 1 : k). \end{aligned}$$

- 5: Reorthogonalize $[P_0, \tilde{W}_1]^{\text{new}}$ against $\mathcal{V}_1^{\text{new}}$ such that

$$[\mathcal{V}_1^{\text{new}}, [P_0, \tilde{W}_1]^{\text{new}}] = [\mathcal{V}_1^{\text{new}}, [P_0, \tilde{W}_1]] \begin{bmatrix} I_k & \tilde{\mathbb{R}} \\ 0_{p \times k} & \end{bmatrix} \text{ with } \tilde{\mathbb{R}} \in \mathbb{C}^{(k+p) \times p}.$$

- 6: Compute $\mathcal{L}_1 = \mathcal{L}_1^{\text{new}} + \tilde{\mathbb{R}}(1 : k, :) \mathbb{H}_1^{\text{new}}$, $\mathbb{H}_1 = \tilde{\mathbb{R}}(k+1 : k+p, :) \mathbb{H}_1^{\text{new}}$, $\Lambda_1 = \begin{bmatrix} I_k & \\ 0_{p \times k} & \tilde{\mathbb{R}} \end{bmatrix} \Lambda_1^{\text{new}}$.

Let $\mathcal{V}_1 = \mathcal{V}_1^{\text{new}}$ and $n_1 = k$. Set $\mathcal{F}_1 = \begin{pmatrix} \mathcal{L}_1 \\ \mathbb{H}_1 \end{pmatrix}$.

- 7: Compute Y_1 the solution of the first new least-squares problem

$$\min_{Y \in \mathbb{C}^{n_1 \times p}} \|\Lambda_1 - \mathcal{F}_1 Y\|_F.$$

Carry out the Singular Value Decomposition algorithm to detect inexact breakdown in first new block residuals

$$(\Lambda_1 - \mathcal{F}_1 Y_1) = \mathbb{U}_1 \Sigma_1 \mathbb{V}_1^H + \mathbb{U}_2 \Sigma_2 \mathbb{V}_2^H, \text{ where } \sigma_{\min}(\Sigma_1) \geq \epsilon_j^{(R)} > \sigma_{\max}(\Sigma_2).$$

Compute \mathbb{W}_1 and \mathbb{W}_2 such that

$\text{Range}(\mathbb{W}_1) = \text{Range}(\mathbb{U}_1^{(2)})$ with $\mathbb{U}_1 = \begin{pmatrix} \mathbb{U}_1^{(1)} \\ \mathbb{U}_1^{(2)} \end{pmatrix}$ and $[\mathbb{W}_1, \mathbb{W}_2]$ is unitary.

Compute new orthonormal matrices V_2 and P_1 , the last block row matrix $\mathcal{L}_{2,:}$ of $\underline{\mathcal{L}}_1$, and G_1 as

$$V_2 = [P_0, \tilde{W}_1] \mathbb{W}_1, \quad P_1 = [P_0, \tilde{W}_1] \mathbb{W}_2, \quad \mathcal{L}_{2,:} = \mathbb{W}_1^H \mathbb{H}_1, \quad G_1 = \mathbb{W}_2^H \mathbb{H}_1.$$

- 8: Set $\underline{\mathcal{L}}_1 = \begin{pmatrix} \mathcal{L}_1 \\ \mathcal{L}_{2,:} \end{pmatrix}$.

C Alpha variant of BGMRES with inexact breakdowns and deflated restarting

Algorithm 5 α IB-BGMRES-DR (n_{\max}, n_{\min}): IB-BGMRES-DR with adjusting number of matrix-vector products at each restart.

```

1: Start. Let the  $p$  linearly independent right-hand sides be  $B = [b^{(1)}, b^{(2)}, \dots, b^{(p)}]$ . Choose
    $n_{\max}$  ( $n_{\min}$ ) the maximal (minimal) dimension of the underlying block approximation
   Krylov subspace in each cycle,  $k$  the desired number of approximate targeted eigenvec-
   tors,  $\varepsilon$  the targeted backward error,  $X_0 = [x_0^{(1)}, x_0^{(2)}, \dots, x_0^{(p)}]$  the initial guesses. Let
    $r_0^{(i)} = b^{(i)} - Ax_0^{(i)}$ ,  $i = 1, \dots, p$ . Denote  $R_0 = [r_0^{(1)}, r_0^{(2)}, \dots, r_0^{(p)}]$  the initial nonsingular block
   residuals. The recast problems are  $A(x^{(i)} - x_0^{(i)}) = r_0^{(i)}$ ,  $i = 1, \dots, p$ .
2:  $cr = 1$ ; /* convergence rate */
3:  $\max_{cr} = \cos(8)$ ; /* max conv. rate = cosine of 8 degrees  $\approx 0.99$  */
4:  $\min_{cr} = \cos(80)$ ; /* min conv. rate = cosine of 80 degrees  $\approx 0.175$  */
5:  $d = 3$ ; /* increment for adjusting */
6:  $cycle = 1$ ; /* counter for restart cycles */
7: while (does not satisfy the stopping criterion) do
8:   /* calculate maximal dimension  $n$  of the underlying block approximation Krylov subspace
      in each cycle */
9:   if  $cr > \max_{cr}$  or  $cycle = 1$  then
10:    /* first cycle or near stagnation */
11:     $n_{cycle} = n_{\max}$ 
12:   else if  $cr < \min_{cr}$  then
13:    /* converging well */
14:     $n_{cycle} = n_{cycle-1}$ 
15:   else
16:    /* adjust */
17:    if  $n_{cycle-1} - d \geq n_{\min}$  then
18:       $n_{cycle} = n_{cycle-1} - d$ 
19:    else
20:       $n_{cycle} = n_{\max}$ 
21:    end if
22:   end if
23:   /* restart cycle */
24:   for  $n_m \leq n_{cycle}$  do
25:    /* IB-BGMRES-DR block iterations */
26:    /* (break if stopping criterion is met) */
27:   end for
28:    $cycle = cycle + 1$ 
29:   /* calculate conv. rate (= cosine of the sequential angle) */
30:    $cr = \frac{\|B - AX_{cycle}\|_2}{\|B - AX_{cycle-1}\|_2}$ 
31: end while

```



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