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BLOCK GMRES METHOD WITH INEXACT BREAKDOWNS AND DEFLATED RESTARTING*

E. AGULLO†, L. GIRAUD†, AND Y.-F. JING‡

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 [*Linear Algebra Appl.*, 419 (2006), pp. 265–285], while the second one is obtained by extending the deflated restarting strategy proposed by Morgan [*Appl. Numer. Math.*, 54 (2005), pp. 222–236]. Through numerical experiments, we show that the new algorithm combines efficiently the attractive numerical features of its two parents and outperforms them.

Key words. block GMRES, deflated restarting, block inexact rank deficiency

AMS subject classifications. 65F10, 65N22, 15A06

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1. Introduction.

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

$$AX = B, \tag{1.1}$$

where $A \in \mathbb{C}^{n\times n}$ is a square nonsingular matrix of large dimension n, $B = [b^{(1)}, b^{(2)}, \ldots, b^{(p)}] \in \mathbb{C}^{n\times p}$ 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, and 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 reusability that comply with the memory constraint of modern multicore architectures. For a recent survey on block Krylov subspace methods, we refer to [20].

One difficulty when considering block Krylov methods is the situation when for a presribed 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

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†INRIA, Bordeaux INP, CNRS (LaBRI UMR5800), Université de Bordeaux, Toulouse F-31057, France (emmanuel.agullo@inria.fr, luc.giraud@inria.fr).

‡Corresponding author. School of Mathematical Sciences/Institute of Computational Science, University of Electronic Science and Technology of China, Chengdu, Sichuan, 611731, People's Republic of China (yanfeijing@uestc.edu.cn, 00jyfvictory@163.com). The research of this author was supported by the Inria fund, NSFC (61170311, 11201055), the Chinese Universities Specialized Research Fund for the Doctoral Program (20120185120026), the State Scholarship Fund from the China Scholarship Council, and the Fundamental Research Funds for the Central Universities.

the numerical scheme and reduce the computational effort, a deflation strategy should be implemented to manage the space expansion [15, 20]. 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 nonblock counterpart is not a happy breakdown). To address convergence at a targeted numerical threshold, Robbé and Sadkane [36] introduced the idea of inexact breakdowns. Instead of discarding some directions for the next space expansion, a technique that might slow down the convergence [24], 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 block GMRES. They show that the R-criterion is more advisable to use than the W-criterion because it can efficiently detect inexact breakdowns when block GMRES 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 block GMRES 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 [17] or via information recycling at restart [16, 21]. In many approaches, some estimate of the invariant subspace is searched in the Krylov subspace and reused in the next restart by augmenting the space [7, 28, 37], by deflating over the subspace [29], or by ensuring some orthogonality properties with respect to that space [34]. One of the most recent works in this field based on a deflation approach is GMRES-DR [29] extended to block GMRES (referred to as BGMRES-DR) in [30]. This proposed BGMRES-DR is shown to perform much better than standard block GMRES [39, 45].

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 associated 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 block GMRES, we refer to the rich literature, for instance, [2, 3, 6, 8, 9, 19, 22, 25, 26, 35, 37, 41, 40].

The remainder of this paper is organized as follows. In section 2, the block Arnoldi process [20, 36, 38, 43] and some insights of IB-BGMRES are first 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 us 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 the 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 $\sigma_1(C) \geq \cdots \geq \sigma_{min(k,\ell)}(C)$ 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 $\mathscr{K}_j(A, R_0) = \text{span}(R_0, A R_0, \ldots, A^{j-1}R_0)$ 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 $\mathscr{K}_j(A, R_0)$ 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 [36], 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 [36] for a detailed and complete description. For simplicity of exposition and easy cross-reading, we adopt most of the notation from [36].

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 a 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

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

can be constructed using a block Arnoldi process described in Algorithm 1. From now on, let W_j denote the matrix obtained at the end of the i-loop of Algorithm 1, that is, the candidate directions to enlarge the search space at next block iteration (to be orthogonalized by a reduced QR-factorization on line 8).

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 Algorithm 1), 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 $\mathscr{K}_j(A, V_1)$ considered at the jth 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 $V_i's$ $(i = 1, \ldots, j)$. $\mathscr{V}_j = [V_1, \ldots, V_j] \in \mathbb{C}^{n\times n_j}$ $(\mathscr{V}_{j+1} = [\mathscr{V}_j, \quad V_{j+1}])$ denotes the orthonormal basis of $\mathscr{K}_j(A, V_1)$ (respectively, $\mathscr{K}_{j+1}(A, V_1)$). Associated with these bases we define $\underline{\mathscr{H}}_j = [{}_{0\ldots0}\ {}^{\mathscr{H}_j}_{H_{j+1,j}}] \in \mathbb{C}^{n_{j+1}\times n_j}$ the block upper Hessenberg matrix, where $\mathscr{H}_j = (H_{i,\ell})_{1\leq i,\ell\leq j} \in \mathbb{C}^{n_j\times n_j}$.

ALGORITHM 1. BLOCK ARNOLDI WITH BLOCKWISE MODIFIED GRAM–SCHMIDT ORTHOGONALIZATION.

```
Choose a unitary matrix V_1 of size n × p
for j = 1, 2, ..., m do
    Compute W_j = A V_j
    for i = 1, 2, ..., j do
        H_{i,j} = V_i^H W_j
        W_j = W_j − V_i H_{i,j}
    end for
    W_j = V_{j+1} H_{j+1,j} (reduced QR-factorization)
end for
```

When no inexact breakdown has occurred $p_{j+1} = p_j = \cdots = p_1 = p$, the range of W_j has always been used to enlarge the search space. Consequently, one obtains the standard block Arnoldi relation [38] from Algorithm 1,

$$A\mathscr{V}_j = \mathscr{V}_j\mathscr{H}_j + [0_{n\times n_{j-1}}, \quad W_j] = \mathscr{V}_{j+1}\underline{\mathscr{H}}_j. \tag{2.1}$$

The traditional block minimum residual norm approaches, such as block GMRES [39, 45], build approximations to the solutions X at iteration j of the form

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

where Y_j solves the least-squares problem

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

because $\mathscr{V}_{j+1}$ forms an orthonormal basis and $\Lambda_j = \left[\begin{smallmatrix}\Lambda_1\\ 0\end{smallmatrix}\right] \in \mathbb{C}^{n_{j+1}\times p}$.

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 [36] proposed to split,

$$W_j = V_{j+1}H_{j+1,j} + Q_j, \tag{2.2}$$

so that the columns of Q_j and V_{j+1} are orthogonal to each other and only V_{j+1} is used to enlarge $\mathscr{V}_j$ to form $\mathscr{V}_{j+1}$. Nonzero columns of $V_{j+1}H_{j+1,j}$ are matched by zero columns of Q_j and vice versa. We can then extend (2.1) into

$$A\mathscr{V}_j = \mathscr{V}_j\mathscr{H}_j + [\mathcal{Q}_{j-1}, \quad W_j], \tag{2.3}$$

where $\mathcal{Q}_{j-1} = [Q_1, \ldots, Q_{j-1}] \in \mathbb{C}^{n\times n_{j-1}}$ accounts for all the abandoned directions. The matrix $\mathcal{Q}_{j-1}$ is rank deficient and reduces to zero matrix of $\mathbb{C}^{n\times n_{j-1}}$ when no inexact breakdown has occurred; in that case (2.3) reduces to (2.1).

In order to characterize a minimum norm solution in the space spanned by $\mathscr{V}_j$ using (2.3) we need to form an orthonormal basis of the space spanned by $[\mathscr{V}_j, \mathcal{Q}_{j-1}, W_j]$. This is performed by first orthogonalizing $\mathcal{Q}_{j-1}$ against $\mathscr{V}_j$, that is, $\widetilde{\mathcal{Q}}_{j-1} = (I - \mathscr{V}_j\mathscr{V}_j^H)\mathcal{Q}_{j-1}$. Because $\mathcal{Q}_{j-1}$ is low rank, so is $\widetilde{\mathcal{Q}}_{j-1}$, which can be written

$$\widetilde{\mathcal{Q}}_{j-1} = P_{j-1}G_{j-1} \text{ with } \begin{cases} P_{j-1} \in \mathbb{C}^{n\times\widetilde{q}_{j-1}} \text{ has orthonormal columns with } \mathscr{V}_j^H P_{j-1} = 0, \\ G_{j-1} \in \mathbb{C}^{\widetilde{q}_{j-1}\times n_{j-1}} \text{ is of full rank.} \end{cases} \tag{2.4}$$

Next W_j, which is already orthogonal to $\mathscr{V}_j$, 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 $\widetilde{W}_j D_j$ the reduced QR-factorization of $W_j - P_{j-1}C_j$. Eventually, the columns of the matrix $[\mathscr{V}_j, P_{j-1}, \widetilde{W}_j]$ form an orthonormal basis of the space spanned by $[\mathscr{V}_j, \mathcal{Q}_{j-1}, W_j]$.

With this new basis (2.3) is written

(2.5)
$$A\mathscr{V}_j = \mathscr{V}_j \mathscr{L}_j + \left[P_{j-1}G_{j-1}, \left[P_{j-1}, \widetilde{W}_j\right] \begin{bmatrix} C_j \\ D_j \end{bmatrix}\right] = \left[\mathscr{V}_j, P_{j-1}, \widetilde{W}_j\right] \begin{bmatrix} \mathscr{L}_j & \\ G_{j-1} & \begin{matrix} C_j \\ D_j \end{matrix} \\ 0 & \end{bmatrix},$$

where

$$\mathscr{L}_j = \begin{bmatrix} H_{1,1} & \cdots & \cdots & \cdots & H_{1,j} \\ H_{2,1} & \ddots & & & \vdots \\ V_3^H Q_1 & \ddots & \ddots & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ V_j^H Q_1 & \cdots & V_j^H Q_{j-2} & H_{j,j-1} & H_{j,j} \end{bmatrix} \in \mathbb{C}^{n_j \times n_j}$$

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 (2.5) becomes

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

with

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

so that (2.3) is written in a more compact form as

$$A\mathscr{V}_j = \left[\mathscr{V}_j, [P_{j-1}, \widetilde{W}_j]\right] \mathscr{F}_j. \tag{2.6}$$

Robbé and Sadkane [36] introduced the so-called R-criterion to extract from $[P_{j-1}, \widetilde{W}_j]$ the subspace to be used to build V_{j+1} as follows. Based on the SVD of the coordinate vector of the residual $\Lambda_j - \mathscr{F}_j Y_j = \mathbb{U}_1 \Sigma_1 \mathbb{V}_1^H + \mathbb{U}_2 \Sigma_2 \mathbb{V}_2^H$, where Σ_1 contains the singular values larger than a prescribed threshold $\epsilon^{(R)}$, they decompose $\mathbb{U}_1 = \left(\begin{smallmatrix} \mathbb{U}_1^{(1)} \\ \mathbb{U}_1^{(2)} \end{smallmatrix}\right)$ in accordance with $[\mathscr{V}_j, [P_{j-1}, \widetilde{W}_j]]$ and consider $[\mathbb{W}_1, \mathbb{W}_2]$ unitary so that $\text{Range}(\mathbb{W}_1) = \text{Range}(\mathbb{U}_1^{(2)})$. The new set of vectors selected to expand the search space

$$V_{j+1} = \left[P_{j-1}, \widetilde{W}_j\right] \mathbb{W}_1 \tag{2.7}$$

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 [36] for a complete description, only stating that via this decomposition the main terms that appear in (2.5) can be computed incrementally from one iteration to the next as follows:

- Based on the recurrence

$$\mathscr{L}_j = \begin{bmatrix} & H_{1,j} \\ \underline{\mathscr{L}}_{j-1} & \vdots \\ & H_{j,j} \end{bmatrix},$$

where $\underline{\mathscr{L}}_{j-1} = \begin{bmatrix} \mathscr{L}_{j-1} \\ V_j^H \mathcal{Q}_{j-2} \; H_{j,j-1} \end{bmatrix}$, the last block row of $\underline{\mathscr{L}}_j$ at the next iteration $(j+1)$ is given by $\underline{\mathscr{L}}_{j+1,:} = \mathbb{W}_1^H \begin{bmatrix} G_{j-1} & C_j \\ 0 & D_j \end{bmatrix}$. The last block column of $\mathscr{L}_{j+1}$ 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

$$A\mathscr{V}_j = \mathscr{V}_{j+1}\underline{\mathscr{L}}_j + \widetilde{\mathcal{Q}}_j. \tag{2.8}$$

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

$$P_j = \left[P_{j-1}, \widetilde{W}_j\right] \mathbb{W}_2, \tag{2.9}$$

and 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 (2.6)? 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 one 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 [18, 27, 31, 33, 42] 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 3.1 (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,

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

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

Lemma 3.2 presents the harmonic Ritz formulation used in the block GMRES variant with inexact breakdowns and deflated restarting.

LEMMA 3.2. *Let $\mathcal{U} = \mathrm{span}(\mathcal{V}_m)$, where $\mathcal{V}_m$ is the orthonormal basis built by IB-BGMRES at the end of a cycle. The harmonic Ritz pairs $(\widetilde{\theta}_i, \widetilde{g}_i)$ associated with $\mathcal{V}_m$ satisfy the following property:*

$$\mathscr{F}_m^H \left(\mathscr{F}_m \widetilde{g}_i - \widetilde{\theta}_i \begin{bmatrix} \widetilde{g}_i \\ 0_p \end{bmatrix} \right) = 0 \ (i = 1, \ldots, n_m), \tag{3.1}$$

where $\mathscr{F}_m$ is defined by (2.6), $\widetilde{g}_i \in \mathbb{C}^{n_m}$, and $\mathcal{V}_m \widetilde{g}_i$ $(i = 1, \ldots, n_m)$ are the harmonic Ritz vectors associated with the corresponding harmonic Ritz values $\widetilde{\theta}_i$ $(i = 1, \ldots, n_m)$.

Proof. Assume that we have performed a first cycle of block Arnoldi with inexact breakdowns (see Algorithm 3). By the Petrov–Galerkin condition defined in Definition 3.1, the harmonic Ritz pairs satisfy

$$(A\mathcal{V}_m)^H (A\mathcal{V}_m \widetilde{g}_i - \widetilde{\theta}_i \mathcal{V}_m \widetilde{g}_i) = 0 \quad (i = 1, \ldots, n_m). \tag{3.2}$$

Substituting (2.6) with $j = m$ into (3.2), we get

$$\mathscr{F}_m^H \left[\mathcal{V}_m, [P_{m-1}, \widetilde{W}_m] \right]^H \left(\left[\mathcal{V}_m, [P_{m-1}, \widetilde{W}_m] \right] \mathscr{F}_m \widetilde{g}_i - \widetilde{\theta}_i \mathcal{V}_m \widetilde{g}_i \right) = 0 \ (i = 1, \ldots, n_m),$$

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

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

$$\left(\mathscr{L}_m^H \mathscr{L}_m + \mathbb{H}_m^H \mathbb{H}_m \right) \widetilde{g}_i = \widetilde{\theta}_i \mathscr{L}_m^H \widetilde{g}_i, \ i = 1, \ldots, n_m. \tag{3.3}$$

Therefore, we compute the k targeted eigenpairs $(\widetilde{\theta}_i, \widetilde{g}_i)$ of the matrix $\mathscr{L}_m + \mathscr{L}_m^{-H} \mathbb{H}_m^H \mathbb{H}_m$ (see step 3 of Algorithm 2). In practice, it might be more stable to solve the generalized eigenvalue problem in (3.3) if $\mathscr{L}_m$ is nearly singular.

In Lemma 3.3, we detail a useful relation as a basis for Proposition 3.4 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 3.3. *Assume that $\mathscr{L}_m$ is of full rank after performing a first cycle of Algorithm 3; then the column vectors $(\mathscr{F}_m \widetilde{g}_i - \widetilde{\theta}_i \left[\begin{smallmatrix} \widetilde{g}_i \\ 0 \end{smallmatrix} \right]) \in \mathbb{C}^{n_m+p}$ $(i = 1, \ldots, n_m)$ are all contained in the subspace spanned by the least-squares residuals $R_{LS_m} = (\Lambda_m - \mathscr{F}_m Y_m) \in \mathbb{C}^{(n_m+p)\times p}$, i.e., $\exists \alpha_i \in \mathbb{C}^p$ so that*

$$\mathscr{F}_m\widetilde{g}_i - \widetilde{\theta}_i \begin{bmatrix} \widetilde{g}_i \\ 0 \end{bmatrix} = R_{LS_m}\alpha_i. \tag{3.4}$$

Proof. From the preceding lemma, we have that $(\mathscr{F}_m\widetilde{g}_i - \widetilde{\theta}_i[\begin{smallmatrix}\widetilde{g}_i\\0\end{smallmatrix}]) \in \mathrm{Null}(\mathscr{F}_m^H)$, $(i = 1, \ldots, n_m)$. Furthermore, we have $n_m + p = \dim(\mathrm{Range}(\mathscr{F}_m^H)) + \dim(\mathrm{Null}(\mathscr{F}_m^H))$. Because $\mathscr{L}_m$ is assumed of full rank, we have $\dim(\mathrm{Null}(\mathscr{F}_m^H)) = p$.

On the other hand, $Y_m = \mathrm{argmin}_{Y\in\mathbb{C}^{n_m\times p}} \|\Lambda_m - \mathscr{F}_m Y\|_F$, and then $\mathscr{F}_m Y_m$ are the orthogonal projections of Λ_m on $\mathrm{Range}(\mathscr{F}_m)$ and $(\Lambda_m - \mathscr{F}_m Y_m) \perp \mathrm{Range}(\mathscr{F}_m)$. That is, $(\Lambda_m - \mathscr{F}_m Y_m) \in \mathrm{Null}(\mathscr{F}_m^H)$ thanks to $\mathrm{Range}(\mathscr{F}_m)^\perp = \mathrm{Null}(\mathscr{F}_m^H)$, which together with $\mathrm{rank}(\Lambda_m - \mathscr{F}_m Y_m) = p$ indicates that $\mathrm{span}(\Lambda_m - \mathscr{F}_m Y_m) = \mathrm{Null}(\mathscr{F}_m^H)$. Then consequently $(\mathscr{F}_m\widetilde{g}_i - \widetilde{\theta}_i[\begin{smallmatrix}\widetilde{g}_i\\0\end{smallmatrix}]) \in \mathrm{span}(\Lambda_m - \mathscr{F}_m Y_m)$ $(i = 1, \ldots, n_m)$, yielding (3.4). ∎

Using Lemma 3.3 and (2.6) 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 [30, Lemma 2] when inexact breakdowns occur and are handled.

PROPOSITION 3.4. *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 $[\mathscr{V}_m, [P_{m-1}, \widetilde{W}_m]]$ and the relation $A\mathscr{V}_m = [\mathscr{V}_m, [P_{m-1}, \widetilde{W}_m]]\mathscr{F}_m$ from (2.6). The harmonic residual vectors $R_{\mathrm{har}}^{(i)} = A\mathscr{V}_m\widetilde{g}_i - \widetilde{\theta}_i\mathscr{V}_m\widetilde{g}_i$ $(i = 1, \ldots, n_m)$ and the residual vectors $R_m = B - AX_m$ from the minimum residual solutions of the linear equation problem respectively satisfy

$$R_{\mathrm{har}}^{(i)} = A\mathscr{V}_m\widetilde{g}_i - \widetilde{\theta}_i\mathscr{V}_m\widetilde{g}_i = \left[\mathscr{V}_m, [P_{m-1}, \widetilde{W}_m]\right]\left(\mathscr{F}_m\widetilde{g}_i - \widetilde{\theta}_i\begin{bmatrix}\widetilde{g}_i\\0\end{bmatrix}\right)(i = 1, \ldots, n_m),$$

$$R_m = B - AX_m = R_0 - A\mathscr{V}_m Y_m = V_1\Lambda_1 - A\mathscr{V}_m Y_m = \left[\mathscr{V}_m, [P_{m-1}, \widetilde{W}_m]\right] R_{LS_m}.$$

Because $[\mathscr{V}_m, [P_{m-1}, \widetilde{W}_m]]$ is an orthonormal basis, Lemma 3.3 shows that R_{har} and R_m are in the same p-dimensional space, which concludes the proof. ∎

3.1.2. Block GMRES with inexact breakdowns relations at restart. Next, we will show that the block-Arnoldi-like recurrence formulae (2.6) and (2.8) 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 $\mathscr{V}_m\widetilde{G}$ the k targeted harmonic Ritz vectors, where $\widetilde{G} = [\widetilde{g}_1, \ldots, \widetilde{g}_k] \in \mathbb{C}^{n_m\times k}$. First add zero rows of size p to $\widetilde{G}$ and then append R_{LS_m} to form a new matrix denoted as $\underline{G} = [\begin{smallmatrix}\widetilde{G} & R_{LS_m}\\ 0_{p\times k} & \end{smallmatrix}]$ 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

$$Q_{\underline{G}} = \begin{bmatrix} \Gamma_1 & \Gamma_2 \\ 0_{p\times k} & \end{bmatrix} \in \mathbb{C}^{(n_m+p)\times(k+p)}, \tag{3.5}$$

$$R_{\underline{G}} = \begin{bmatrix} \Theta_1 & \Theta_2 \\ 0_{p\times k} & \end{bmatrix} \in \mathbb{C}^{(k+p)\times(k+p)}, \tag{3.6}$$

with $\Gamma_1 = Q_{\underline{G}}(1:n_m, 1:k)$, $\Gamma_2 = Q_{\underline{G}}(:, k+1:k+p)$, $\Theta_1 = R_{\underline{G}}(1:k, 1:k)$, and $\Theta_2 = R_{\underline{G}}(:, k+1:k+p)$, and

$$\widetilde{G} = \Gamma_1 \Theta_1, \tag{3.7}$$

$$R_{LS_m} = Q_{\underline{G}} \Theta_2. \tag{3.8}$$

Proposition 3.5 shows that the block-Arnoldi-like recurrence formulae of IB-BGMRES [36] can be recovered without involving any matrix-vector product with A when restarting with some harmonic information.

PROPOSITION 3.5. *At each restart of block GMRES with inexact breakdowns and deflated restarting, the initial block-Arnoldi-like recurrence formulae* (2.6) *and* (2.8) *still hold in exact arithmetic as*

$$A\mathscr{V}_1^{new} = \left[\mathscr{V}_1^{new}, [P_0, \widetilde{W}_1]^{new}\right] \mathscr{F}_1^{new}, \tag{3.9}$$

$$A\mathscr{V}_1^{new} = \mathscr{V}_2^{new} \underline{\mathscr{L}}_1^{new} + \widetilde{\mathcal{Q}}_1^{new} \tag{3.10}$$

with

$$\begin{aligned}
\left[\mathscr{V}_1^{new}, [P_0, \widetilde{W}_1]^{new}\right] &= \left[\mathscr{V}_m, [P_{m-1}, \widetilde{W}_m]\right] Q_{\underline{G}},\\
R_0 &= \left[\mathscr{V}_1^{new}, [P_0, \widetilde{W}_1]^{new}\right] \Lambda_1^{new} \text{ with } \Lambda_1^{new} = \Theta_2,\\
\mathscr{L}_1^{new} &= \Gamma_1^H \mathscr{L}_m \Gamma_1, \quad \mathbb{H}_1^{new} = \Gamma_2^H \mathscr{F}_m \Gamma_1, \quad \mathscr{F}_1^{new} = \begin{bmatrix} \mathscr{L}_1^{new} \\ \mathbb{H}_1^{new} \end{bmatrix},\\
V_2^{new} &= [P_0, \widetilde{W}_1]^{new} \mathbb{W}_1^{new}, \; P_1^{new} = [P_0, \widetilde{W}_1]^{new} \mathbb{W}_2^{new},\\
\mathscr{L}_{2,:}^{new} &= \mathbb{W}_1^{newH} \mathbb{H}_1^{new}, \; G_1^{new} = \mathbb{W}_2^{newH} \mathbb{H}_1^{new},\\
\mathscr{V}_2^{new} &= [\mathscr{V}_1^{new}, V_2^{new}], \; \underline{\mathscr{L}}_1^{new} = \begin{bmatrix} \mathscr{L}_1^{new} \\ \mathscr{L}_{2,:}^{new} \end{bmatrix}, \; \widetilde{\mathcal{Q}}_1^{new} = P_1^{new} G_1^{new},
\end{aligned}$$

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

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

with

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

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

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

Proof.

• Show that (3.9) holds. From (3.4) of Lemma 3.3, we have, $\forall i \in 1, \ldots, k$, $\exists \alpha_i \in \mathbb{C}^p$,

$$\mathscr{F}_m \widetilde{g}_i - \widetilde{\theta}_i \begin{bmatrix} \widetilde{g}_i \\ 0 \end{bmatrix} = R_{LS_m} \alpha_i. \tag{3.11}$$

Multiplying both sides of (3.11) with $[\mathscr{V}_m, [P_{m-1}, \widetilde{W}_m]]$ gives

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

Using (2.6), we can write the above equation as

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

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

$$A\mathscr{V}_m \widetilde{G} = \left[\mathscr{V}_m, [P_{m-1}, \widetilde{W}_m]\right] \underline{G} \begin{pmatrix} \operatorname{diag}(\widetilde{\theta}_1, \ldots, \widetilde{\theta}_k) \\ \alpha_1, \ldots, \alpha_k \end{pmatrix}.$$

Using the reduced QR-factorization of $\underline{G}$ and the structure of $\widetilde{G}$ as shown in (3.7), we have

$$A\mathscr{V}_m \Gamma_1 \Theta_1 = \left[\mathscr{V}_m, [P_{m-1}, \widetilde{W}_m]\right] Q_{\underline{G}} R_{\underline{G}} \begin{pmatrix} \operatorname{diag}(\widetilde{\theta}_1, \ldots, \widetilde{\theta}_k) \\ \alpha_1, \ldots, \alpha_k \end{pmatrix},$$

which, by multiplication of Θ^{-1} from the right-hand side and with partition of $Q_{\underline{G}}$ in (3.5), is

$$A\mathscr{V}_m \Gamma_1 = \left[\mathscr{V}_m \Gamma_1, \left[\mathscr{V}_m, [P_{m-1}, \widetilde{W}_m]\right] \Gamma_2\right] R_{\underline{G}} \begin{pmatrix} \operatorname{diag}(\widetilde{\theta}_1, \ldots, \widetilde{\theta}_k) \\ \alpha_1, \ldots, \alpha_k \end{pmatrix} \Theta^{-1}. \tag{3.12}$$

On the other hand, (3.11) can be rewritten in a matrix reformulation as

$$\mathscr{F}_m \widetilde{G} - \begin{pmatrix} \widetilde{G} \\ 0 \end{pmatrix} \operatorname{diag}(\widetilde{\theta}_1, \ldots, \widetilde{\theta}_k) = R_{LS_m} [\alpha_1, \ldots, \alpha_k],$$

which proceeds similarly to the above manipulations as

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

Based on the structure of $\mathscr{F}_m$ in (2.6) and the partition of $Q_{\underline{G}}$ in (3.5), we make

$$\begin{pmatrix} \Gamma_1^H \mathscr{L}_m \Gamma_1 \\ \Gamma_2^H \mathscr{F}_m \Gamma_1 \end{pmatrix} = R_{\underline{G}} \begin{pmatrix} \mathrm{diag}(\widetilde{\theta}_1, \ldots, \widetilde{\theta}_k) \\ \alpha_1, \ldots, \alpha_k \end{pmatrix} \Theta_1^{-1}. \tag{3.13}$$

If we denote

$$\begin{aligned} [P_0, \widetilde{W}_1]^{\mathrm{new}} &= \left[\mathscr{V}_m, [P_{m-1}, \widetilde{W}_m]\right] \Gamma_2, \quad \mathscr{V}_1^{\mathrm{new}} = \mathscr{V}_m \Gamma_1, \\ \mathscr{L}_1^{\mathrm{new}} &= \Gamma_1^H \mathscr{L}_m \Gamma_1, \\ \mathbb{H}_1^{\mathrm{new}} &= \Gamma_2^H \mathscr{F}_m \Gamma_1, \quad \mathscr{F}_1^{\mathrm{new}} = \begin{bmatrix} \mathscr{L}_1^{\mathrm{new}} \\ \mathbb{H}_1^{\mathrm{new}} \end{bmatrix}, \end{aligned}$$

and substitute (3.13) into (3.12), then (3.9) is obtained.

- Show $R_0 = [\mathscr{V}_1^{\mathrm{new}}, [P_0, \widetilde{W}_1]^{\mathrm{new}}]\Lambda_1^{\mathrm{new}}$. At restart we have

$$\begin{aligned} R_0 &= R_m \\ &= \left[\mathscr{V}_m, [P_{m-1}, \widetilde{W}_m]\right] R_{LS_m} \\ &= \left[\mathscr{V}_m, [P_{m-1}, \widetilde{W}_m]\right] Q_{\underline{G}} \Theta_2 \\ &= \left[\mathscr{V}_1^{\mathrm{new}}, [P_0, \widetilde{W}_1]^{\mathrm{new}}\right] \Lambda_1^{\mathrm{new}}. \end{aligned}$$

- Show that equality (3.10) holds. Because $[\mathbb{W}_1^{\mathrm{new}}, \mathbb{W}_2^{\mathrm{new}}]$ is unitary, we have

$$[P_0, \widetilde{W}_1]^{\mathrm{new}} = [P_0, \widetilde{W}_1]^{\mathrm{new}} \left[\mathbb{W}_1^{\mathrm{new}} \mathbb{W}_1^{\mathrm{new}\,H} + \mathbb{W}_2 \mathbb{W}_2^{\mathrm{new}\,H}\right],$$

and substituting this into (3.9) gives

$$\begin{aligned} A\mathscr{V}_1^{\mathrm{new}} &= \left[\mathscr{V}_1^{\mathrm{new}}, [P_0, \widetilde{W}_1]^{\mathrm{new}} \left(\mathbb{W}_1^{\mathrm{new}} \mathbb{W}_1^{\mathrm{new}\,H} + \mathbb{W}_2^{\mathrm{new}} \mathbb{W}_2^{\mathrm{new}\,H}\right)\right] \begin{bmatrix} \mathscr{L}_1^{\mathrm{new}} \\ \mathbb{H}_1^{\mathrm{new}} \end{bmatrix} \\ &= \mathscr{V}_1^{\mathrm{new}} \mathscr{L}_1^{\mathrm{new}} + [P_0, \widetilde{W}_1]^{\mathrm{new}} \left(\mathbb{W}_1^{\mathrm{new}} \mathbb{W}_1^{\mathrm{new}\,H} + \mathbb{W}_2^{\mathrm{new}} \mathbb{W}_2^{\mathrm{new}\,H}\right) \mathbb{H}_1^{\mathrm{new}} \\ &= \mathscr{V}_1^{\mathrm{new}} \mathscr{L}_1^{\mathrm{new}} + [P_0, \widetilde{W}_1]^{\mathrm{new}} \mathbb{W}_1^{\mathrm{new}} \mathbb{W}_1^{\mathrm{new}\,H} \mathbb{H}_1^{\mathrm{new}} + [P_0, \widetilde{W}_1]^{\mathrm{new}} \mathbb{W}_2^{\mathrm{new}} \mathbb{W}_2^{\mathrm{new}\,H} \mathbb{H}_1^{\mathrm{new}} \\ &= \mathscr{V}_1^{\mathrm{new}} \mathscr{L}_1^{\mathrm{new}} + V_2^{\mathrm{new}} \mathscr{L}_{2,:}^{\mathrm{new}} + P_1^{\mathrm{new}} G_1^{\mathrm{new}} \\ &= [\mathscr{V}_1^{\mathrm{new}}, \quad V_2^{\mathrm{new}}] \begin{bmatrix} \mathscr{L}_1^{\mathrm{new}} \\ \mathscr{L}_{2,:}^{\mathrm{new}} \end{bmatrix} + P_1^{\mathrm{new}} G_1^{\mathrm{new}}, \end{aligned}$$

which shows (3.10). ∎

It is noticed that the matrix $[P_0, \widetilde{W}_1]^{\mathrm{new}}$ is treated as an integrated matrix during the computation in Proposition 3.5 and it is not necessary to tell the explicit forms of P_0^{new} and $\widetilde{W}_1^{\mathrm{new}}$. As a matter of fact, continuing Algorithm 3 for $j = 2, \ldots, m$ with the initialization proposed in Proposition 3.5 as shown in steps 4 and 5 of Algorithm 2, i.e., setting $\mathscr{V}_2 = \mathscr{V}_2^{\mathrm{new}}$, $\underline{\mathscr{L}}_1 = \underline{\mathscr{L}}_1^{\mathrm{new}}$, $P_1 = P_1^{\mathrm{new}}$, $G_1 = G_1^{\mathrm{new}}$, we can consequently see that the block-Arnoldi-like recurrence formulae of IB-BGMRES still hold for 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 steps (4)–(7) of BGMRES-DR in [30] under the inexact-breakdown circumstances. Note 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 $[P_0, \widetilde{W}_1]^{\text{new}}$ and $\mathscr{V}_1^{\text{new}}$. 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 3.5 to easily see that the initial block-Arnoldi-like recurrence formulae (3.9) and (3.10) stay 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 nonzero 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

$$R_0 = \left[\mathscr{V}_1, [P_0, \widetilde{W}_1]\right] \Lambda_1. \tag{3.14}$$

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 $[P_0, \widetilde{W}_1]$, those directions are not kept as is in the search space. As the method progresses, the directions of $[P_0, \widetilde{W}_1]$ will contribute to the construction of V_j or P_{j-1} to expand the search space. Proposition 3.6 indicates how the least-squares right-hand sides can be incrementally and cheaply computed at each iteration of the block algorithm.

PROPOSITION 3.6. *At each iteration (see step* 5 *of Algorithm* 2*), the new least-squares problem reads*

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

with the right-hand sides being

$$\Lambda_{j+1} = \begin{bmatrix} I_{p_1} \\ 0_{(n_{j+1}+p-p_1)\times p_1} \end{bmatrix} \Phi_{j+1} \Lambda_1, \tag{3.15}$$

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*

$$\Phi_{j+1} = \begin{bmatrix} \Phi_j(1:n_j,:) \\ [\mathbb{W}_1, \mathbb{W}_2]^H \begin{bmatrix} \Phi_j(n_j+1:n_j+p-p_j,:) \\ 0_{p_j \times p} \end{bmatrix} \\ 0_{p_{j+1}\times p} \end{bmatrix}, \tag{3.16}$$

where $[\mathbb{W}_1, \mathbb{W}_2]$ *are respectively defined in* (2.7) *and* (2.9) *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

$$
\begin{aligned}
\Lambda_{j+1} &= \left[\mathscr{V}_{j+1}, \left[P_j, \widetilde{W}_{j+1}\right]\right]^H R_0, \\
&= \left[\mathscr{V}_j, V_{j+1}, \left[P_j, \widetilde{W}_{j+1}\right]\right]^H R_0, \\
&= \left[\mathscr{V}_j, \left[P_{j-1}, \widetilde{W}_j\right]\mathbb{W}_1, \left[P_{j-1}, \widetilde{W}_j\right]\mathbb{W}_2, \widetilde{W}_{j+1}\right]^H R_0 \text{ using (2.7) and (2.9)}, \\
&= \left[\mathscr{V}_j, \left[P_{j-1}, \widetilde{W}_j\right][\mathbb{W}_1, \mathbb{W}_2], \widetilde{W}_{j+1}\right]^H R_0, \\
&= \left[\mathscr{V}_j, \left[P_{j-1}, \widetilde{W}_j\right][\mathbb{W}_1, \mathbb{W}_2], \widetilde{W}_{j+1}\right]^H \left[\mathscr{V}_1, [P_0, \widetilde{W}_1]\right]\Lambda_1, \\
&= \begin{bmatrix} \mathscr{V}_j^H\mathscr{V}_1 & \mathscr{V}_j^H[P_0, \widetilde{W}_1] \\ [V_{j+1}, P_j]^H\mathscr{V}_1 & [\mathbb{W}_1, \mathbb{W}_2]^H[P_{j-1}, \widetilde{W}_j]^H[P_0, \widetilde{W}_1] \\ \widetilde{W}_{j+1}^H\mathscr{V}_1 & \widetilde{W}_{j+1}^H[P_0, \widetilde{W}_1] \end{bmatrix}\Lambda_1 \\
&= \begin{bmatrix} \begin{bmatrix} I_{p_1} \\ 0_{(n_j-p_1)\times p_1} \end{bmatrix} & \Phi_j(1:n_j, :) \\ 0_{p\times p_1} & [\mathbb{W}_1, \mathbb{W}_2]^H \begin{bmatrix} \Phi_j(n_j+1:n_j+p-p_j, :) \\ 0_{p_j\times p} \end{bmatrix} \\ 0_{p_{j+1}\times p_1} & 0_{p_{j+1}\times p} \end{bmatrix}\Lambda_1.
\end{aligned}
$$

The last equality results mainly from the facts that $\text{Range}([P_0, \widetilde{W}_1]) \subset \text{Range}([\mathscr{V}_j, P_{j-1}, \widetilde{W}_j])$ $(j = 1, \ldots, m)$, $\widetilde{W}_{j+1} \perp \text{Range}([P_0, \widetilde{W}_1])$ $(j = 1, \ldots, m-1)$, and that the basis $[\mathscr{V}_j, P_{j-1}, \widetilde{W}_j]$ $(j = 1, \ldots, m)$ is orthonormal. ∎

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.

We do not derive a computational complexity comparison between BGMRES-DR and IB-BGMRES-DR as it is identical to the one presented in [36, p. 280] for BGMRES versus IB-BGMRES. We only mention that this analysis indicates that the IB variants tend to require fewer floating point operations than their classical counterparts, as will be illustrated by experiments in section 4.

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 3.7. *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*

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

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 $B = [b^{(1)}, b^{(2)}, \ldots, b^{(p)}]$. 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, $X_0 = [x_0^{(1)}, x_0^{(2)}, \ldots, x_0^{(p)}]$ the initial guesses. Let $r_0^{(i)} = b^{(i)} - Ax_0^{(i)},\ i = 1, \ldots, p$. Denote $R_0 = [r_0^{(1)}, r_0^{(2)}, \ldots, r_0^{(p)}]$ the initial nonsingular block residuals. The recast problems are $A(x^{(i)} - x_0^{(i)}) = r_0^{(i)},\ i = 1, \ldots, p$.

2: *Find approximate solutions for the first cycle.* Implement the first cycle of Algorithm 3. Form the new approximate solutions $X_m = X_0 + \mathscr{V}_m Y_m$. Compute the residual vectors $R_m = B - AX_m = [\mathscr{V}_m, [P_{m-1}, \widetilde{W}_m]](\Lambda_m - \mathscr{F}_m Y_m)$. 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 $(\widetilde{\theta}_i, \widetilde{g}_i)$ $(i = 1, \ldots, k)$ of the matrix $\mathscr{L}_m + \mathscr{L}_m^{-H} \mathbb{H}_m^H \mathbb{H}_m$. (The $\widetilde{\theta}_i$ $(i = 1, \ldots, k)$ are harmonic Ritz values.) Then store the $\widetilde{g}_i$ $(i = 1, \ldots, k)$ into the matrix G. For real matrices, it is necessary to separate $\widetilde{g}_i$ $(i = 1, \ldots, k)$ 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* $j = 2, \ldots, m$. 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.

6: *Form the approximate solutions.* Form the new approximate solutions $X_m = X_0 + \mathscr{V}_m Y_m$. Compute the residual vectors $R_m = B - AX_m = [\mathscr{V}_m, [P_{m-1}, \widetilde{W}_m]](\Lambda_m - \mathscr{F}_m Y_m)$.

7: Check convergence, and restart if convergence is not achieved, i.e., go to 3.

Assuming p inexact breakdowns have occurred at iterations s of IB-BGMRES (also IB-BGMRES-DR) solving for $B = [b^{(1)}, b^{(2)}, \ldots, b^{(p)}]$, according to [36, equation (47)], we have

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

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

(3.17)
$$\eta_{b^{(i)}}(x_s^{(i)}) = \frac{||b^{(i)} - Ax_s^{(i)}||_2}{||b^{(i)}||_2} \leq \frac{||B - AX_s||_2}{||b^{(i)}||_2} \leq \frac{||B - AX_s||_2}{\min\limits_{i=1,\ldots,p} \left\|b^{(i)}\right\|_2} \leq \frac{\epsilon^{(R)}}{\min\limits_{i=1,\ldots,p} \left\|b^{(i)}\right\|_2}$$

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

$$\epsilon^{(R)} = \varepsilon \times \min_{i=1,\ldots,p} \left\|b^{(i)}\right\|_2 \tag{3.18}$$

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 [30] and IB-BGMRES [36] in terms of number of matrix-vector products (referred to as *mvps*) 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 [30], the sixth matrix is used in [36], and the last two are used in [23]. For a 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 $0.1, 1, 2, 3, \ldots, 999$. Matrix 2 has diagonal entries $1, 2, 3, \ldots, 1000$, matrix 3 has diagonal entries $11, 12, 13, \ldots, 1010$, while matrix 4 has diagonal entries $10.1, 10.2, 10.3, \ldots, 19.9, 20, 21, 22, \ldots, 919, 920$. 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 [11]. 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 [10]. For those experiments, the k smallest harmonic Ritz values are chosen 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 $B = [b^{(1)}, b^{(2)}, \ldots, b^{(p)}] \in \mathbb{C}^{n\times p}$ 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 $\eta_{b^{(i)}} < \varepsilon$ $(i = 1, \ldots, p)$, 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* = 10,000 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 sides of Figures 1 and 2, we display the upper bounds on the backward errors for IB-BGMRES and IB-BGMRES-DR given by (3.17) and the largest backward error. It can be seen that the upper bound is quite sharp and deserves to be considered in designing 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,

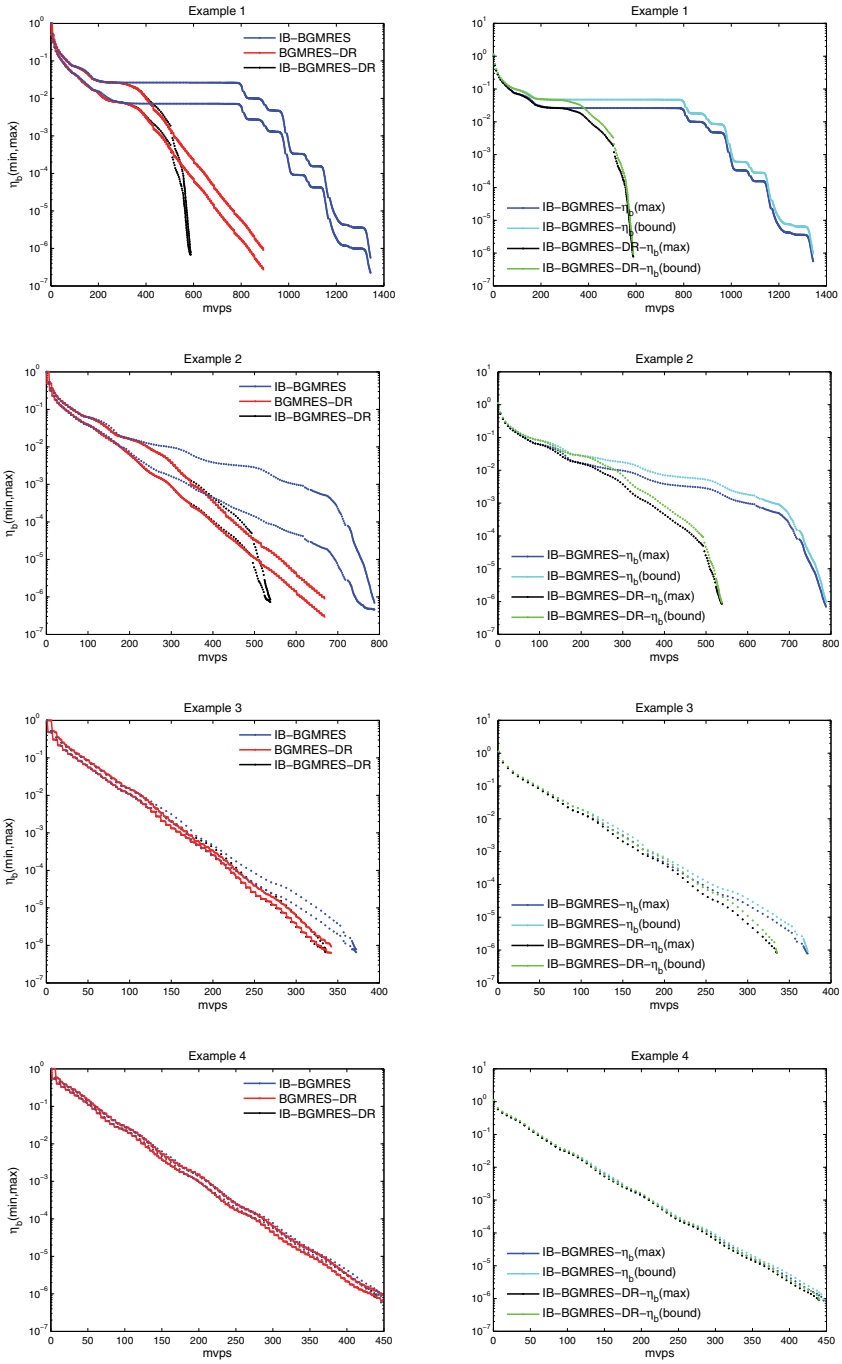

FIG. 1. *Convergence histories for the first four examples. Left: convergence histories of the largest/smallest* $\eta_{b^{(i)}}$ *at each mvps. Right: upper bounds of* $\eta_{b^{(i)}}$ *and* $max(\eta_{b^{(i)}})$ *at each mvps.*

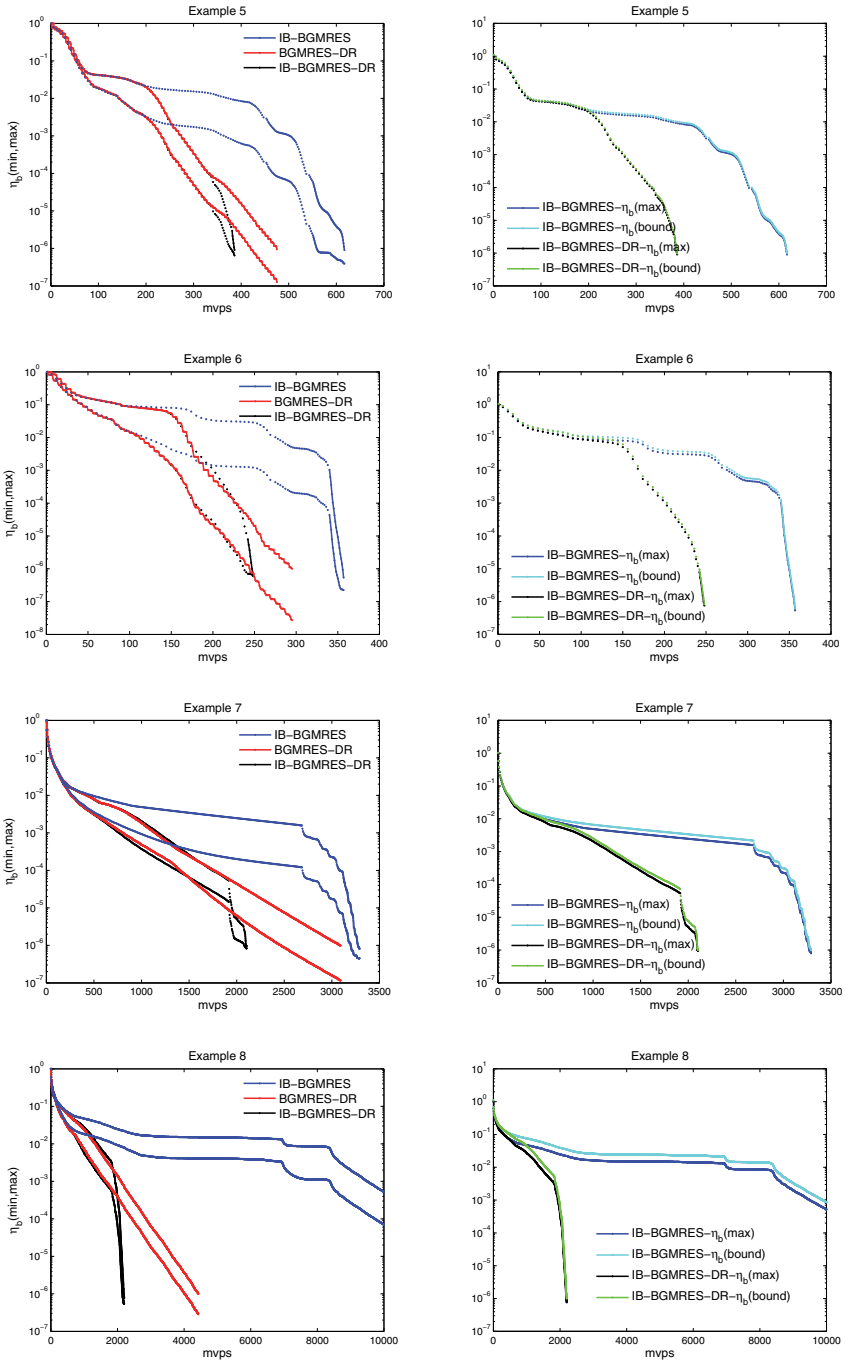

FIG. 2. *Convergence histories for the last four examples. Left: convergence histories of the largest/smallest* $\eta_{b^{(i)}}$ *at each mvps. Right: upper bounds of* $\eta_{b^{(i)}}$ *and* $max(\eta_{b^{(i)}})$ *at each mvps.*

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

Example	Method	*mvps*	$\eta_{b^{(i)}}$ $(i = 1, \ldots, p)$	
			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

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 performance of IB-BGMRES, BGMRES-DR, and IB-BGMRES-DR is 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. For all the examples, the IB-BGMRES-DR algorithm performs the best in terms of *mvps* which also translates in elapsed time decreases. Although not presented in this table, we mention that on our largest test problem, i.e., Example 7, we obtain a significant elapsed time reduction as IB-BGMRES-DR converges in 63.9 s, while BGMRES-DR requires 144.1 s. Furthermore, 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 fact of not taking into account the 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 simultaneously 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) [38]

TABLE 2
Number of mvps for regular GMRES, GMRES-DR, IB-BGMRES, BGMRES-DR, and IB-BGMRES-DR with $\varepsilon = 10^{-6}$.

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**

and GMRES-DR(m, k) [29] 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 terms of space dimension and stopping criterion, i.e., $\eta_{b^{(i)}} < \varepsilon$ $(i = 1, \ldots, p)$, or individual *mvps* exceeds *maxiter* ($p = 6,\ m = 90,\ k = 5, \varepsilon = 10^{-6},$ and *maxiter* = 10,000). 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, and 6; for Examples 3 and 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 in Example 7 while much less *mvps* than GMRES-DR in Example 8. Because of our experimental setting, the dimension of the Krylov search space for individual right-hand side is larger for the nonblock variants; that explains why GMRES-DR sometimes beats IB-BGMRES-DR.

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 this polynomial degree constant 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 behaviors are identical.

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

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

		Example							
p	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**

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

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

	Example			
p	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**

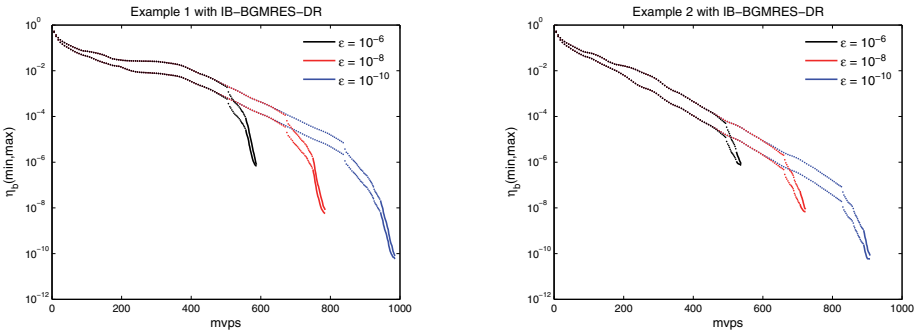

FIG. 3. *Convergence history of IB-GMRES-DR when the targeted accuracy is varied.*

p backward errors. Because the inexact breakdown threshold is related to ε by (3.18), 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 us to focus on what remains to be converged and then reduce the computational cost to achieve convergence.

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

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 mvps.

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

problems (see, e.g., [1, 4, 5, 12, 13, 14, 32] and related papers, e.g., [44]). In [4] 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 [4] can be extended in a straightfordward 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 [4] 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 *mvps* required by IB-BGMRES-DR. 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 also could be extended to other block 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 occured. Not addressed in [36], 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 [18].

Appendix 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 $\underline{\mathscr{L}}_0 = [\ ]$. Choose a targeted backward error ε and set the corresponding $\epsilon^{(R)}$.

3: **for** $j = 1, 2, \ldots, m$ **do**

4: Orthogonalize AV_j against previous block orthonormal basis $\mathscr{V}_j = [V_1, \ldots, V_j]$ as

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

5: Set $\mathscr{L}_j = \begin{bmatrix}\underline{\mathscr{L}}_{j-1}, & \mathscr{L}_{1,1:j}\end{bmatrix} \in \mathbb{C}^{n_j\times n_j}$.

6: Orthogonalize W_j against P_{j-1} and carry out its reduced QR-factorization as

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

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

$$\min_{Y\in\mathbb{C}^{n_j\times p}} \|\Lambda_j - \mathscr{F}_j Y\|_F \ \text{ with}$$
$$\Lambda_j = \begin{pmatrix}\Lambda_1\\ 0\end{pmatrix} \in \mathbb{C}^{(n_j+p)\times p}, \mathscr{F}_j = \begin{pmatrix}\mathscr{L}_{\mathrm{j}}\\ \mathbb{H}_j\end{pmatrix} \in \mathbb{C}^{(n_j+p)\times n_j}, \text{ and}$$
$$\mathbb{H}_j = \begin{pmatrix}\mathrm{G_{j-1}} & \mathrm{C_j}\\ 0 & \mathrm{D_j}\end{pmatrix} \in \mathbb{C}^{p\times n_j}.$$

Carry out the singular value decomposition algorithm to detect inexact breakdowns in residuals

$$(\Lambda_j - \mathscr{F}_j Y_j) = \mathbb{U}_1\Sigma_1\mathbb{V}_1^H + \mathbb{U}_2\Sigma_2\mathbb{V}_2^H, \text{ where } \sigma_{\min}(\Sigma_1) \geq \epsilon^{(R)} > \sigma_{\max}(\Sigma_2).$$

Compute $\mathbb{W}_1$ and $\mathbb{W}_2$ such that
Range$(\mathbb{W}_1)$ = Range$(\mathbb{U}_1^{(2)})$ with $\mathbb{U}_1 = \begin{pmatrix}\mathbb{U}_1^{(1)}\\ \mathbb{U}_1^{(2)}\end{pmatrix}$ and $[\mathbb{W}_1, \quad \mathbb{W}_2]$ is unitary.
Compute orthonormal matrices V_{j+1} and P_j, the last block row matrix $\mathscr{L}_{j+1,:}$ of $\underline{\mathscr{L}}_j$, and G_j as

$$V_{j+1} = \begin{bmatrix}P_{j-1}, & \widetilde{W}_j\end{bmatrix}\mathbb{W}_1, \quad P_j = \begin{bmatrix}P_{j-1}, & \widetilde{W}_j\end{bmatrix}\mathbb{W}_2,$$
$$\mathscr{L}_{j+1,:} = \mathbb{W}_1^H\mathbb{H}_j, \qquad G_j = \mathbb{W}_2^H\mathbb{H}_j.$$

8: Set $\underline{\mathscr{L}}_j = \begin{pmatrix}\mathscr{L}_j\\ \mathscr{L}_{j+1,:}\end{pmatrix}$.

9: **end for**

Appendix B. Restarting procedure with deflation.

ALGORITHM 4. RESTARTING WITH DEFLATED TARGETED HARMONIC RITZ VECTORS.

1: Compute $R_{LS_m} = \Lambda_m - \mathscr{F}_m Y_m = [\mathscr{V}_m, [P_{m-1}, \widetilde{W}_m]]^H R_m \in \mathbb{C}^{(n_m+p)\times p}$ the least-squares residuals at the mth iteration of the first cycle of Algorithm 3. Denote by $\mathscr{V}_m \widetilde{G}$ the k targeted harmonic Ritz vectors, where $\widetilde{G} = [\widetilde{g}_1, \ldots, \widetilde{g}_k] \in \mathbb{C}^{n_m \times k}$.

2: Append R_{LS_m} to $\widetilde{G}$ by first adding zero rows of size p to $\widetilde{G}$ and then R_{LS_m} to form a new matrix denoted as $\underline{G} = \left[\begin{smallmatrix} \widetilde{G} & R_{LS_m} \\ 0 & \end{smallmatrix}\right]$ 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

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

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

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

6: Compute $\mathscr{L}_1 = \mathscr{L}_1^{\text{new}} + \widetilde{\mathbb{R}}(1 : k, :)\mathbb{H}_1^{\text{new}}$, $\mathbb{H}_1 = \widetilde{\mathbb{R}}(k+1 : k+p, :)\mathbb{H}_1^{\text{new}}$, $\Lambda_1 = \left[\begin{smallmatrix} I_k & \\ 0_{p\times k} & \widetilde{\mathbb{R}} \end{smallmatrix}\right]\Lambda_1^{\text{new}}$. Let $\mathscr{V}_1 = \mathscr{V}_1^{\text{new}}$ and $n_1 = k$. Set $\mathscr{F}_1 = \left(\begin{smallmatrix} \mathscr{L}_1 \\ \mathbb{H}_1 \end{smallmatrix}\right)$.

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

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

Carry out the singular value decomposition algorithm to detect inexact breakdown in first new block residuals

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

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

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

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

$$V_2 = [P_0, \widetilde{W}_1]\mathbb{W}_1, \; P_1 = [P_0, \widetilde{W}_1]\mathbb{W}_2, \; \mathscr{L}_{2,:} = \mathbb{W}_1^H \mathbb{H}_1, \; G_1 = \mathbb{W}_2^H \mathbb{H}_1.$$

8: Set $\underline{\mathscr{L}}_1 = \left(\begin{smallmatrix} \mathscr{L}_1 \\ \mathscr{L}_{2,:} \end{smallmatrix}\right)$.

Appendix C. Alpha variant of BGMRES with inexact breakdowns and deflated restarting.

ALGORITHM 5. αIB-BGMRES-DR $(n_{\text{MAX}}, n_{\text{MIN}})$: IB-BGMRES-DR WITH ADJUSTING NUMBER OF MATRIX-VECTOR PRODUCTS AT EACH RESTART.

Start. Let the p linearly independent right-hand sides be $B = [b^{(1)}, b^{(2)}, \ldots, b^{(p)}]$. 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 eigenvectors, ε the targeted backward error, $X_0 = [x_0^{(1)}, x_0^{(2)}, \ldots, x_0^{(p)}]$ the initial guesses. Let $r_0^{(i)} = b^{(i)} - Ax_0^{(i)}$, $i = 1, \ldots, p$. Denote $R_0 = [r_0^{(1)}, r_0^{(2)}, \ldots, r_0^{(p)}]$ the initial nonsingular block residuals. The recast problems are $A(x^{(i)} - x_0^{(i)}) = r_0^{(i)}$, $i = 1, \ldots, p$.
$cr = 1$; /* convergence rate */
$\max_{cr} = \cos(8)$; /* max conv. rate = cosine of 8 degrees ≈ 0.99 */
$\min_{cr} = \cos(80)$; /* min conv. rate = cosine of 80 degrees ≈ 0.175 */
$d = 3$; /* increment for adjusting */
$cycle = 1$; /* counter for restart cycles */
while (does not satisfy the stopping criterion) **do**
  /* calculate maximal dimension n of the underlying block approximation Krylov subspace in each cycle */
  if $cr > \max_{cr}$ or $cycle = 1$ **then**
    /* first cycle or near stagnation */
    $n_{\text{cycle}} = n_{\max}$
  else if $cr < \min_{cr}$ **then**
    /* converging well */
    $n_{\text{cycle}} = n_{\text{cycle-1}}$
  else
    /* adjust */
    if $n_{\text{cycle-1}} - d \geq n_{\min}$ **then**
      $n_{\text{cycle}} = n_{\text{cycle-1}} - d$
    else
      $n_{\text{cycle}} = n_{\max}$
    end if
  end if
  /* restart cycle */
  for $n_m \leq n_{\text{cycle}}$ **do**
    /* IB-BGMRES-DR block iterations */
    /* (break if stopping criterion is met) */
  end for
  $cycle = cycle + 1$
  /* calculate conv. rate (= cosine of the sequential angle) */
  $cr = \frac{||B - AX_{cycle}||_2}{||B - AX_{cycle-1}||_2}$
end while

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