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A New Shifted Block GMRES Method with Inexact Breakdowns for Solving Multi-Shifted and Multiple Right-Hand Sides Linear Systems

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Abstract

We consider the efficient solution of linear systems with multiple shifts and multiple right-hand sides given simultaneously that arise frequently in large-scale scientific and engineering simulations. We introduce a new shifted block GMRES method that can solve the whole sequence of linear systems simultaneously, it handles effectively the situation of inexact breakdowns in the inner block Arnoldi procedure for improved robustness, and recycles spectral information at restart to achieve faster convergence. Numerical experiments are reported on a suite of sparse matrix problems and in realistic quantum chromodynamics application to show the potential of the new proposed method to solve general multi-shifted and multiple right-hand sides linear systems fast and efficiently.

Keywords Shifted block Krylov subspace methods · Deflated restarting · Inexact breakdowns · Preconditioning techniques

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1 Introduction

We consider the iterative solution of sequences of shifted linear systems with L shifts and p different right-hand sides given at once of the form

$$(A - \sigma_i I)X_i = B, \quad i = 1, 2, \dots, L, \quad (1)$$

where the scalars $\{\sigma_i\}_{i=1}^L \subset \mathbb{C}$ are the shifts, $A - \sigma_i I \in \mathbb{C}^{n \times n}$ are large square non-singular matrices of dimension n , and we denote by I the identity matrix of order n , by $B = [b^{(1)}, b^{(2)}, \dots, b^{(p)}]$ the $n \times p$ matrix of right-hand sides $b^{(j)}$, $j = 1, \dots, p$ and by $X_i \in \mathbb{C}^{n \times p}$ the unknown solution matrix corresponding to the shift σ_i . In the following, we assume that B is a full rank matrix; we refer to $(A - \sigma_1 I)X_1 = B$ as the base block system and to $(A - \sigma_i I)X_i = B$, for $i = 2, \dots, L$, as the shifted block systems. Multi-shifted linear systems with multiple right-hand sides of the form (1) arise in the solution of many large-scale scientific and engineering applications. In quenched quantum chromodynamics (QCD) using Wilson and Clover fermions, with application to quark propagator calculations, the right-hand sides represent different noise vectors and the shifts correspond to different quark masses that are used in an extrapolation process [17,23]. Other relevant examples of applications include hydraulic tomography [37], seismic problems [4] and PageRank computation [22]. Sparse direct methods based on variants of Gaussian elimination would require at best $L \cdot \mathcal{O}(n + \tau)$ operations to factorize the whole sequence of shifted matrices appearing in (1), where τ is the number of nonzeros of A , and they need to access all the entries of the coefficient matrix. A computationally attractive alternative to direct solvers is to use shifted variants of iterative methods that exploit the shift-invariance property of block Krylov subspaces,

$$\mathbb{K}_m(A - \sigma_i I, R_0) = \mathbb{K}_m(A - \sigma_1 I, R_0), \quad i = 2, \dots, L, \quad (2)$$

where we denote by

$$\mathbb{K}_m(A, R_0) = \text{span} \{R_0, AR_0, \dots, A^{m-1}R_0\} \quad (3)$$

the block Krylov subspace of dimension m generated by A and by the initial block residuals $R_0 = B - AX_0$ corresponding to the initial block guess X_0 . Because of (2), the same Krylov basis generated for the base block system can be used to approximate the solution of the additional shifted block systems simultaneously by performing matrix-free operations [41,42]. This approach is clearly more efficient than applying shifted Krylov subspace methods to the sequence of linear systems with multiple shifts [4,11,14,15,24,25,37], or block Krylov subspace methods to each single shifted linear system with multiple right-hand sides separately [1,5,6,13,16,21,28].

Recently, Sun et al. have introduced a new shifted block generalized minimum residual method with a deflated restarting strategy (denoted as BGMRES-DR-Sh) for the simultaneous solution of sequence (1), that attempts to overcome some of the typical convergence problems of shifted Krylov solvers by augmenting the search subspace with directions associated with the approximate smallest eigenvalues of A [41]. Although the distribution of the eigenvalues alone may not play any role in the convergence of iterative Krylov solvers for non-Hermitian systems [19], it has been observed that for many problems and applications a tightly clustered spectrum around a single point away from the origin is generally very beneficial, whereas widely spread eigenvalues and the presence of clusters close to zero are often disadvantageous. Krylov methods build a polynomial expansion of the coefficient matrix that must be equal to one at zero and has to approximate zero on the set of eigenvalues. Clearly, a low-degree

polynomial with value 1 at the origin cannot be small at such many points [18]; therefore, “removing” the smallest eigenvalues can greatly improve the convergence [2,8–10,29–32].

The first cycle of the BGMRES-DR-Sh method applied to the base block system is the standard BGMRES method [21]. Let $R_0 = V_1 R$ be the QR-decomposition of the initial block residuals R_0 , where $V_1 \in \mathbb{C}^{n \times p}$ is a matrix with orthonormal columns and $R \in \mathbb{C}^{p \times p}$ is an upper triangular full-rank matrix. BGMRES uses the block Arnoldi procedure based on the Modified Block Gram–Schmidt process described in Algorithm 1 to compute an orthonormal basis $\mathcal{V}_m$ for the space (3). After m steps of the block Arnoldi procedure, the following decomposition is computed

$$A\mathcal{V}_m = \mathcal{V}_m \mathcal{H}_m + [0_{n \times (m-1)p} \ W_m] = \mathcal{V}_{m+1} \tilde{\mathcal{H}}_m, \quad (4)$$

where $W_m = V_{m+1} H_{m+1,m}$ and $\tilde{\mathcal{H}}_m = \begin{bmatrix} \mathcal{H}_m \\ 0 \dots 0, H_{m+1,m} \end{bmatrix}$ is the block upper Hessenberg matrix with $\mathcal{H}_m = (H_{i,j})_{1 \leq i,j \leq m} \in \mathbb{C}^{mp \times mp}$. Due to the block shift-invariance property (2), the following shifted block Arnoldi-like relation, analogous to (4), can be established for shifted linear systems

$$(A - \sigma_i I)\mathcal{V}_m = \mathcal{V}_{m+1} \tilde{\mathcal{H}}_m^i, \quad (5)$$

with

$$\tilde{\mathcal{H}}_m^i = \tilde{\mathcal{H}}_m - \sigma_i \begin{bmatrix} I_{mp \times mp} \\ 0_{p \times mp} \end{bmatrix}.$$

The BGMRES approximate solution of the base block system is written as $X_m^1 = X_0^1 + \mathcal{V}_m Y_m^1$, where X_0^1 is the initial approximation and Y_m^1 minimizes the block residual norm onto $\mathbb{K}_m((A - \sigma_1 I), R_0^1)$. By using Eq. (5), the base block residual R_m^1 at the end of the first cycle is written as

$$\begin{aligned} R_m^1 &= R_0^1 - (A - \sigma_1 I)\mathcal{V}_m Y_m^1, \\ &= \mathcal{V}_{m+1}(ER - \tilde{\mathcal{H}}_m^1 Y_m^1), \end{aligned}$$

where $R_0^1 = \mathcal{V}_{m+1} ER$ and E is the $(m+1)p \times p$ matrix with upper $p \times p$ principal block equal to the identity matrix. As $\mathcal{V}_{m+1}$ is orthonormal, Y_m^1 is the solution to the following minimization problem

$$Y_m^1 = \underset{Y^1}{\operatorname{argmin}} \|ER - \tilde{\mathcal{H}}_m^1 Y^1\|_F. \quad (6)$$

At this stage, if the residual norm satisfies the convergence criterion, the algorithm stops; otherwise, the Krylov subspace is enlarged with new directions for the next search.

Algorithm 1 Block Arnoldi with 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-decomposition)
 - 9: **end for**
 - 10: Define $\mathcal{V}_{m+1} = [V_1, V_2, \dots, V_{m+1}]$, $\tilde{\mathcal{H}}_m = (H_{k,l})_{1 \leq k \leq m+1, 1 \leq l \leq m}$
-

In the BGMRES-DR-Sh method, after every cycle of m steps approximate eigenvectors corresponding to the small eigenvalues in magnitude of the coefficient matrix are computed and are added to the subspace (3). The spectral information recycled at restart is the so-called harmonic Ritz vectors defined as follows:

Definition 1 (Harmonic Ritz pair [33]). 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 called a harmonic Ritz pair of B with respect to $\mathcal{U}$ if and only if

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

or, equivalently, using the canonical scalar product, if and only if

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

The vector y is called the harmonic Ritz vector associated with the harmonic Ritz value λ . At the end of the cycle, the k desired harmonic Ritz vectors are computed and new matrices $\mathcal{V}_{k+p}^{new} \in \mathbb{C}^{n \times (k+p)}$ and $(\tilde{\mathcal{H}}_k^1)^{new} \in \mathbb{C}^{(k+p) \times k}$ are formed such that

$$(A - \sigma_1 I) \mathcal{V}_k^{new} = \mathcal{V}_{k+p}^{new} (\tilde{\mathcal{H}}_k^1)^{new},$$

where the columns of the $n \times k$ matrix $\mathcal{V}_k^{new}$ span the subspace of the harmonic Ritz vectors. The block Arnoldi process eventually builds matrices $\mathcal{V}_{m+1}$ and $\tilde{\mathcal{H}}_m^1$ to generate a relation similar to (5). We have shown in [41] that the shifted block Arnoldi-like relation still holds when the deflated restarting procedure is used, similar to the recycled GMRES methods in the single right-hand side case [38] and in the multiple right-hand sides case [34]. Finally, the minimization problem (6) can be solved for Y_m^1 to form the approximate solution of the base block system.

However, in several circumstances, the approximation space required to satisfactorily approximate all shifted systems appears to be too large, and the method needs to be restarted, taking the current system residual as a new generating vector. In other words, all systems need to have collinear residuals for the restarted Krylov subspace methods, like shifted GMRES [15]. The natural analog to this property for shifted block Krylov subspace methods is that the block residuals need to have columns spanning the same subspace. In this paper, we adopt the same terminology used in [16] and denote blocks having this property as “cospatial”. Upon restarting after m steps, the block residuals R_m^1 and R_m^i , ($i = 2, \dots, L$) of the base block system and of the shifted block systems are no longer cospatial in general. In order to reinstate the shift-invariance property, the BGMRES-DR-Sh method forces the additional shifted block residuals to be cospatial at restart by imposing the condition

$$R_m^i = R_m^1 W_m^i, \quad i = 2, \dots, L, \quad (7)$$

where R_m^i , ($i = 2, \dots, L$) are the residuals of the additional shifted block systems and W_m^i are some $p \times p$ nonsingular matrices. Assuming that the initial shifted block residuals are cospatial, that is $R_0^i = R_0^1 W_0^i$, for $i = 2, \dots, L$ (note that this relation is satisfied by taking, e.g., $X_0^i = 0$), the additional shifted block residuals R_m^i can be obtained from Eq. (7) by writing

$$R_0^i - (A - \sigma_i I) \mathcal{V}_m Y_m^i = (R_0^1 - (A - \sigma_1 I) \mathcal{V}_m Y_m^1) W_m^i, \quad i = 2, 3, \dots, L, \quad (8)$$

or, equivalently, by using the Arnoldi relation

$$\left[\tilde{\mathcal{H}}_m^i \quad \hat{V} \right] \begin{bmatrix} Y_m^i \\ W_m^i \end{bmatrix} = E R W_0^i, \quad i = 2, 3, \dots, L. \quad (9)$$

In Eq. (9) we have set $R_{LS} = ER - \tilde{H}_m^1 Y_m^1$, $\widehat{W}_m^i = \widehat{R} W_m^i$ and $\widehat{V}$, $\widehat{R}$ are the QR factors of the reduced QR -decomposition of R_{LS} . The approximate solutions of the shifted block systems can be expressed as $X_m^i = X_0^1 + \mathcal{V}_m Y_m^i$, ($i = 2, \dots, L$), where Y_m^i , ($i = 2, \dots, L$) is the solution of Eq. (9). Several experiments reported in [41] on linear systems arising from different fields have shown that the deflated restarting strategy implemented in the BGMRES-DR-Sh method can be very effective to reduce the number of Krylov iterations.

Some special care, however, needs to be taken to handle the circumstance where a linear combination of the systems has converged or some of the right-hand sides converge much faster than others, that is when the matrix $(R_0^1, (A - \sigma_1 I) R_0^1, \dots, (A - \sigma_1 I)^{m-1} R_0^1)$ becomes nearly rank-deficient. This situation is referred to as inexact or partial breakdown [26, sect 2.6]. It is worth noting that, differently from a *lucky breakdown* that may occur for nonblock methods [36, p. 148], the block Arnoldi procedure breaks down due to the rank deficiency of the new block of vectors generated to expand the Krylov basis. An exact breakdown situation signals that some of the exact solutions are linearly dependent. By discarding the approximately linearly dependent directions from the Krylov basis, it is possible to reduce overall solutions costs and stabilize the convergence to some extent. The initial deflation strategy proposed in [21, section 12] detects approximate linear dependencies in the right-hand sides matrix B or in the initial block residual matrix R_0 before running the block Arnoldi procedure. If the Krylov method is restarted, the strategy can be applied again at the beginning of each cycle, after the computation of the block residual, to reduce effectively the Krylov space dimension [7,40]. The Arnoldi deflation strategy proposed in [21, section 13] detects the rank deficiency of the matrix W_j computed at step 8 of Algorithm 1 and reduces the Krylov space dimension accordingly. In [35], Robbé and Sadkane proposed to exclude the linearly dependent directions of the block Krylov basis from the matrix-vector products, but to reintroduce them in the next iterations to preserve the quality of the orthogonalization. Two different deflation criteria are introduced in [35], based on either the numerical rank of the generated block Krylov basis (the so-called W -criterion, which is implemented in the BGMRES-W method) or the numerical rank of the block residual (the so-called R -criterion implemented in the BGMRES-R method). The BGMRES-W method deflates whenever W_j is nearly rank-deficient, by discarding from the next space expansion those directions corresponding to the singular values of $H_{j+1,j}$ with magnitude below a threshold. The BGMRES-R method filters the singular values of the block residual matrix to remove the linear independent columns in the next block Arnoldi process and the deflated directions are used in the block Arnoldi algorithm for orthogonalization purposes only. Note that the R -criterion is advisable to use because it can detect efficiently the inexact breakdowns when BGMRES is restarted whereas W -criterion tends to deflate only at the end of the convergence history. Therefore, in our study we consider the R -criterion. We refer to the R -criterion-based variant of the BGMRES method as IB-BGMRES.

In this paper we present a Shifted, Augmented and Deflated (SAD) BGMRES method (named as SAD-BGMRES) developed upon the BGMRES-DR-Sh algorithm proposed in [41] that can solve the whole sequence of linear systems simultaneously, recycles spectral information at restart for faster convergence, and can detect effectively inexact breakdowns. Numerical experiments show that this approach can combine the favourable numerical properties of both the BGMRES-DR-Sh and IB-BGMRES methods. The remainder of the paper is organized as follows. In Sect. 2 we introduce the new block shifted GMRES method. Numerical experiments are illustrated in Sect. 3 to support the theoretical findings and to show the effectiveness of the new method against other state-of-the art solvers, with and without preconditioning. We conclude the paper in Sect. 4 with some final remarks.

Throughout this paper, 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 a matrix and the superscript i ($i = 1, \dots, L$) on X and R denotes quantities related to the i th shift. A superscript *new* for a matrix is used to indicate that the matrix is obtained according to the harmonic Ritz vectors. $I_k \in \mathbb{C}^{k \times k}$ is the identity matrix of dimension k , and $0_{i \times j} \in \mathbb{C}^{i \times j}$ is the zero rectangular matrix with i rows and j columns. In addition, MATLAB notation is used; for example, $R(i, j)$ denotes the (i, j) th entry of matrix R , and $R(1 : m, 1 : j)$ refers to the submatrix consisting of the first m rows and the first j columns of R .

2 Method and Algorithm

Similar to the BGMRES-DR-Sh method presented in Sect. 1, in SAD-BGMRES the solution of the base block system is separated from the solution of the shifted block systems. We describe these two stages of the computation in the coming sections.

2.1 Solution of the Base Block System

In the first cycle, we use the BGMRES method with inexact breakdowns [35]. At step j of the block Arnoldi method (Algorithm 1), we denote by $\mathcal{V}_j = [V_1, \dots, V_j] \in \mathbb{C}^{n \times n_j}$ the orthonormal basis of the block Krylov subspace (3) with dimension $n_j = \sum_{i=1}^j p_i$, while $V_{j+1} \in \mathbb{C}^{n \times p_{j+1}}$ is the Krylov block with linearly independent columns computed at line 8 by the reduced QR -decomposition

$$W_j = V_{j+1}H_{j+1,j},$$

where $W_j \in \mathbb{C}^{n \times p_j}$, $H_{j+1,j} \in \mathbb{C}^{p_{j+1} \times p_j}$, and $\text{rank}(W_j) = \text{rank}(H_{j+1,j}) = p_{j+1}$. When no breakdown occurs, that is $p_{j+1} = p_j = \dots = p_1 = p$, the matrix-matrix product carried out at line 3 represent the most costly part of Algorithm 1. We aim at reducing this cost in the occurrence of inexact breakdowns, that is when the matrix $\{R_0, AR_0, \dots, A^{j-1}R_0\}$ is *almost* rank-deficient.

2.1.1 Detecting Inexact Breakdowns

When an inexact breakdown occurs at the j th iteration, not all the Krylov directions spanned by W_j should be used to build the new block basis V_{j+1} and to expand the Krylov subspace at step 8 of Algorithm 1. The modified block Arnoldi algorithm proposed by Robbé and Sadkane in [35] relies on the numerical rank of the block residuals to select the linear independent columns of V_{j+1} to use in the next iteration (BGMRES-R). Let us assume that at step j an inexact breakdown has been detected according to the R -criterion. Then the reduced QR -decomposition at line 8 of Algorithm 1 is modified as

$$W_j = V_{j+1}H_{j+1,j} + Q_j, \quad (10)$$

where Q_j is a perturbation matrix that takes into account the numerical rank in the QR -decomposition, and $\text{range}(Q_j) \perp \text{range}(V_{j+1})$. Note that in (10), the size of matrix V_{j+1} is still $n \times p_{j+1}$ whereas the rank of W_j can be different from p_{j+1} , and $H_{j+1,j}$ can be rank-deficient, with $\text{rank}(W_j) = \text{rank}(Q_j) + p_{j+1} \leq p_1$. By using (4) and (10), we obtain

the following relation at the j th step of Algorithm 1

$$AV_j = \mathcal{V}_j \begin{bmatrix} H_{1,j} \\ \vdots \\ H_{j,j} \end{bmatrix} + V_{j+1} H_{j+1,j} + Q_j,$$

and the standard block Arnoldi relation (4) writes as

$$AV_j = \mathcal{V}_j \mathcal{H}_j + [Q_{j-1} \ W_j], \quad (11)$$

where the matrix $Q_{j-1} = [Q_1, \dots, Q_{j-1}]$ contains all the discarded directions. The discarded columns of V_{j+1} are excluded from the matrix-matrix computation at line 3 in the next step of Algorithm 1, but they are kept for orthogonalization purposes. If no inexact breakdown occurs, Q_j reduces to the zero matrix like in the standard block Arnoldi process; in that case (11) reduces to (4). The following theorem shows that an Arnoldi-like relation can be derived from (11) when the Q'_j s are used in the block Arnoldi process. In order to compute the minimum norm solution, we need to form an orthonormal basis of the space spanned by $[V_j, Q_{j-1}, W_j]$.

Theorem 1 *The block Arnoldi with inexact deflation admits the relation*

$$\begin{aligned} A\mathcal{V}_j &= \mathcal{V}_j \mathcal{L}_j + \begin{bmatrix} P_{j-1} G_{j-1}, [P_{j-1}, \tilde{W}_j] \begin{bmatrix} C_j \\ D_j \end{bmatrix} \end{bmatrix}, \\ &= [\mathcal{V}_j, [P_{j-1}, \tilde{W}_j]] \mathcal{F}_j, \end{aligned}$$

where $\mathcal{F}_j = \begin{bmatrix} \mathcal{L}_j \\ \mathbb{H}_j \end{bmatrix}$, $\mathcal{L}_j = \begin{bmatrix} H_{1,1} & \cdots & \cdots & \cdots & H_{1,j} \\ H_{2,1} & \ddots & & & \\ V_3^H Q_1 & \ddots & \ddots & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ V_j^H Q_1 & \ddots & V_j^H Q_{j-2} & H_{j,j-1} & H_{j,j} \end{bmatrix} \in \mathbb{C}^{n_j \times n_j}$, and $\mathbb{H}_j = \begin{bmatrix} G_{j-1} & C_j \\ 0 & D_j \end{bmatrix}$.

(12)

In (12), matrices P_{j-1} and $\tilde{W}_j$ are orthogonal.

Proof In order to obtain the orthonormal basis of the space spanned by $[V_j, Q_{j-1}, W_j]$, we need Q_{j-1} orthogonal to V_j and W_j orthogonal to Q_{j-1} where W_j is already orthogonal to V_j . We orthogonalize Q_{j-1} against V_j yielding $\tilde{Q}_{j-1} = (I - V_j V_j^H) Q_{j-1}$. Then we compute the reduced QR -factorization of $\tilde{Q}_{j-1}$, that is, $\tilde{Q}_{j-1} = P_{j-1} G_{j-1}$. Note that P_{j-1} is the needed orthogonal matrix. Similarly, the other orthogonal matrix $\tilde{W}_j$ can be obtained as $\tilde{W}_j D_j = (I - P_{j-1} P_{j-1}^H) W_j$. Here we denote $C_j = P_{j-1}^H W_j$. Finally, the columns of the matrix $[\mathcal{V}_j, [P_{j-1}, \tilde{W}_j]]$ form an orthonormal basis of the space spanned by $[V_j, Q_{j-1}, W_j]$. That is, Eq. (11) can be rewritten as Eq. (12). $\square$

Corollary 1 *For shifted systems, the shifted Arnoldi-like relation holds*

$$(A - \sigma_i I) \mathcal{V}_j = [\mathcal{V}_j, [P_{j-1}, \tilde{W}_j]] \mathcal{F}_j^i, \quad i = 1, \dots, L, \text{ with } \mathcal{F}_j^i = \begin{bmatrix} \mathcal{L}_j^i \\ \mathbb{H}_j \end{bmatrix} \text{ and } \mathcal{L}_j^i = \mathcal{L}_j - \sigma_i I. \quad (13)$$

Proof By subtracting $\sigma_i V_j$ from both sides of Eq. (12), it is straightforward to obtain the analogous shifted Arnoldi-like relation (13). $\square$

Therefore, the approximate solutions at iteration j of the base block system has the form

$$X_j^1 = X_0^1 + \mathcal{V}_j Y_j^1, \quad (14)$$

where Y_j^1 minimizes the base block residual

$$\begin{aligned} R_j^1 &= R_0^1 - (A - \sigma_1 I) \mathcal{V}_j Y_j^1, \\ &= [\mathcal{V}_j, [P_{j-1}, \tilde{W}_j]] (\Lambda_j - \mathcal{F}_j^1 Y_j^1), \\ &= [\mathcal{V}_j, [P_{j-1}, \tilde{W}_j]] R_{LS}, \end{aligned} \quad (15)$$

with $R_0^1 = [\mathcal{V}_j, [P_{j-1}, \tilde{W}_j]] \Lambda_j$, $\Lambda_j = \begin{bmatrix} \Lambda_1 \\ 0 \\ 0 \end{bmatrix}$. In (15), we denoted the base block quasi-residual as $R_{LS} = \Lambda_j - \mathcal{F}_j^1 Y_j^1$. Then, Y_j^1 can be computed by solving the least-squares problem

$$Y_j^1 = \operatorname{argmin}_{Y^1 \in \mathbb{C}^{n_j \times p}} \left\| \Lambda_j - \mathcal{F}_j^1 Y^1 \right\|_F.$$

2.1.2 Implementation of the R -Criterion

Similar to [35], in the SAD-BGMRES method the R -criterion is used to detect an approximate linear dependence in the base block residual vectors and select only the linear independent columns of the matrix V_{j+1} for the next block Arnoldi iteration. Since the columns of $[\mathcal{V}_j, [P_{j-1}, \tilde{W}_j]]$ are orthonormal, we compute the singular value decomposition of the base block quasi-residual

$$\begin{aligned} R_{LS} &= U \Sigma V^H, \\ &= U_1 \Sigma_1 V_1^H + U_2 \Sigma_2 V_2^H, \end{aligned}$$

where Σ_1 contains the singular values larger than a prescribed threshold $\epsilon^{(R)}$, that is,

$$\sigma(\Sigma_1) \geq \epsilon^{(R)} \geq \sigma(\Sigma_2),$$

and write

$$\begin{aligned} R_j^1 &= [\mathcal{V}_j, [P_{j-1}, \tilde{W}_j]] U \Sigma V^H, \\ &= [\mathcal{V}_j, [P_{j-1}, \tilde{W}_j]] U_1 \Sigma_1 V_1^H + [\mathcal{V}_j, [P_{j-1}, \tilde{W}_j]] U_2 \Sigma_2 V_2^H. \end{aligned} \quad (16)$$

Small singular values below a threshold would signal the near rank-deficient of the base residuals. The splitting (16) suggests to decompose the orthogonal projection subspace of R_j^1 onto $\mathcal{V}_j$ as

$$\operatorname{range}((I - \mathcal{V}_j \mathcal{V}_j^H) R_j^1) = \operatorname{range}(V_{j+1}) \oplus \operatorname{range}(P_j), \quad (17)$$

with $\operatorname{range}(V_{j+1}) = \operatorname{range}((I - \mathcal{V}_j \mathcal{V}_j^H) R_j^1 \mathbb{V}_1)$ and $\operatorname{range}(P_j) = \operatorname{range}((I - \mathcal{V}_j \mathcal{V}_j^H) R_j^1 \mathbb{V}_2)$. That is, the new Krylov basis columns V_{j+1} are the effective directions of the largest singular values and the columns of P_j are the deflated directions corresponding to the smallest singular values.

From Eqs. (16) to (17), we orthogonalize R_j^1 against $\mathcal{V}_j$ to obtain V_{j+1} and decompose $\mathbb{U}_1 = \begin{bmatrix} \mathbb{U}_1^{(1)} \\ \mathbb{U}_1^{(2)} \end{bmatrix}$ in accordance with $[\mathcal{V}_j, [P_{j-1}, \tilde{W}_j]]$. We have

$$\begin{aligned} & (I - \mathcal{V}_j \mathcal{V}_j^H) [\mathcal{V}_j, [P_{j-1}, \tilde{W}_j]] \mathbb{U}_1, \\ &= [0, [P_{j-1}, \tilde{W}_j]] \begin{bmatrix} \mathbb{U}_1^{(1)} \\ \mathbb{U}_1^{(2)} \end{bmatrix}, \\ &= [P_{j-1}, \tilde{W}_j] \mathbb{U}_1^{(2)}. \end{aligned}$$

We refer to [35] for the details of the calculation and note that the main matrix that appear in (12) can be computed at moderate cost. Consider $\mathbb{W}_1$ and $\mathbb{W}_2$ such that $\text{range}(\mathbb{W}_1) = \text{range}(\mathbb{U}_1^{(2)})$, here $[\mathbb{W}_1 \ \mathbb{W}_2]$ is unitary and $\mathbb{W}_2$ is corresponding to $\mathbb{U}_1^{(2)}$. Then the V_{j+1} and P_j can be computed as

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

and

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

respectively. This process is summarized in Algorithm 4.

2.1.3 Computing the Harmonic Ritz Vectors

At the end of each cycle of the block Arnoldi process, in the SAD-BGMRES method we compute the approximate eigenvectors corresponding to the small eigenvalues in magnitude of the coefficient matrix, and we recycle this spectral information at restart as an attempt to improve the convergence at low memory and computational costs. The next lemma shows how the harmonic Ritz vectors can be obtained from the block Arnoldi process.

Lemma 1 *Let $\mathcal{U} = \text{span}\{\mathcal{V}_m\}$, where $\mathcal{V}_m$ is an orthogonal matrix built after m steps of the block Arnoldi process. The harmonic Ritz pairs $(\tilde{\theta}_i, \tilde{g}_i)$ associated with $\mathcal{V}_m$ satisfy the following property*

$$(\mathcal{F}_m^1)^H \left(\mathcal{F}_m^1 \tilde{g}_i - \tilde{\theta}_i \begin{bmatrix} \tilde{g}_i \\ 0_p \end{bmatrix} \right) = 0, \quad (18)$$

where $\mathcal{V}_m \tilde{g}_i$ are the harmonic Ritz vectors associated with the corresponding harmonic Ritz values $\tilde{\theta}_i$.

Proof It is known that the harmonic Ritz pairs of $A - \sigma_1 I$ in $\text{range}(\mathcal{V}_m)$ satisfies the following relation

$$(A - \sigma_1 I) \mathcal{V}_m - \tilde{\theta}_i \mathcal{V}_m \tilde{g}_i \perp \text{range}((A - \sigma_1 I) \mathcal{V}_m).$$

The proof then proceeds as in the proof of [1, Lemma 3.2]. $\square$

Using the expression of $\mathcal{F}_m^1$, Eq. (18) can be rewritten as

$$((\mathcal{L}_m^1)^H \mathcal{L}_m^1 + \mathbb{H}_m^H \mathbb{H}_m) \tilde{g}_i = \tilde{\theta}_i (\mathcal{L}_m^1)^H \tilde{g}_i,$$

which is used to compute the harmonic Ritz vectors over the SAD-BGMRES cycles. The next theorem shows the important result that the shifted block Arnoldi-like relation still holds at low computational cost when deflated restarting is applied.

Proposition 1 *At each restart of SAD-BGMRES method, the shifted block Arnoldi-like recurrence*

$$(A - \sigma_1 I) \mathcal{V}_k^{new} = [\mathcal{V}_k^{new}, [P_{k-1}, \tilde{W}_k]^{new}] (\mathcal{F}_k^1)^{new} \quad (19)$$

holds with

$$\begin{aligned} \mathcal{V}_k^{new} &= \mathcal{V}_m Q_k, \\ \mathcal{V}_{k+1}^{new} &= [\mathcal{V}_m, [P_{m-1}, \tilde{W}_m]] Q_{k+1}, \\ (\mathcal{F}_k^1)^{new} &= Q_{k+1}^H \mathcal{F}_m^1 Q_k. \end{aligned}$$

Proof The residuals of the harmonic Ritz vectors and the residuals of the base block linear system are in the same subspace at restart [1, Lemma 3.3], so that we can write

$$\mathcal{F}_m^1 \tilde{g}_i - \tilde{\theta}_i \begin{bmatrix} \tilde{g}_i \\ 0_p \end{bmatrix} = R_{LS} \alpha_i. \quad (20)$$

Multiplying both sides of (20) with $[\mathcal{V}_m, [P_{m-1}, \tilde{W}_m]]$ gives

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

Now, according to Lemma 1, the k targeted harmonic Ritz vectors are given by $\mathcal{V}_m \tilde{G}_k$, where $\tilde{G}_k = [\tilde{g}_1, \dots, \tilde{g}_k] \in \mathbb{C}^{n_m \times k}$. By adding zero rows of size p to $\tilde{G}_k$ and appending the quasi-residual R_{LS} to $\tilde{G}_k$, we define the new matrix denoted as $\tilde{G}_{k+1} = \begin{bmatrix} \tilde{G}_k \\ 0_{p \times k} \end{bmatrix}, R_{LS}$ of dimension $(n_{m+1}) \times (k+p)$. The reduced QR-decomposition of $\tilde{G}_{k+1} = Q_{k+1} R_{k+1}$ can be written as

$$\left[\begin{bmatrix} \tilde{G}_k \\ 0_{p \times k} \end{bmatrix}, R_{LS} \right] = \left[\begin{bmatrix} Q_k \\ 0_{p \times k} \end{bmatrix}, Q_2 \right] \left[\begin{bmatrix} R_k \\ 0_{p \times k} \end{bmatrix}, R_2 \right], \quad (21)$$

with

$$\tilde{G}_k = Q_k R_k. \quad (22)$$

We use Eqs. (13) and (22) to write

$$\begin{aligned} (A - \sigma_1 I) \mathcal{V}_m \tilde{G}_k &= [\mathcal{V}_m, [P_{m-1}, \tilde{W}_m]] \tilde{G}_{k+1} \begin{pmatrix} \text{diag}(\tilde{\theta}_1, \dots, \tilde{\theta}_k) \\ \alpha_1, \dots, \alpha_k \end{pmatrix}, \\ \Leftrightarrow (A - \sigma_1 I) \mathcal{V}_m Q_k &= [\mathcal{V}_m, [P_{m-1}, \tilde{W}_m]] Q_{k+1} R_{k+1} \begin{pmatrix} \text{diag}(\tilde{\theta}_1, \dots, \tilde{\theta}_k) \\ \alpha_1, \dots, \alpha_k \end{pmatrix} R_k^{-1}. \end{aligned} \quad (23)$$

From (13), since $Q_{k+1}^H Q_{k+1} = I$ we have

$$R_{k+1} \begin{pmatrix} \text{diag}(\tilde{\theta}_1, \dots, \tilde{\theta}_k) \\ \alpha_1, \dots, \alpha_k \end{pmatrix} R_k^{-1} = Q_{k+1}^H \mathcal{F}_m^1 Q_k. \quad (24)$$

We introduce two new matrices $\mathcal{V}_{k+1}^{new}$ and $(\mathcal{F}_k^1)^{new}$ defined as follows

$$\mathcal{V}_{k+1}^{new} = [\mathcal{V}_m, [P_{m-1}, \tilde{W}_m]] Q_{k+1}, \quad (\mathcal{F}_k^1)^{new} = Q_{k+1}^H \mathcal{F}_m^1 Q_k.$$

Based on the structure of Q_{k+1} in Eq. (21), we can write

$$\mathcal{V}_k^{new} = \mathcal{V}_m Q_k, \quad [P_{k-1}, \tilde{W}_k]^{new} = [\mathcal{V}_m, [P_{m-1}, \tilde{W}_m]] Q_2. \quad (25)$$

Finally, we set $\mathcal{V}_{k+1} = \mathcal{V}_{k+1}^{new}$, $\mathcal{F}_k^1 = (\mathcal{F}_k^1)^{new}$ and substitute (24) into (23) to obtain the shifted block Arnoldi-like relation. $\square$

At restart we define

$$\begin{aligned} R_0^1 &= R_m^1, \\ &= [\mathcal{V}_m, [P_{m-1}, \tilde{W}_m]] R_{LS}, \\ &= [\mathcal{V}_m, [P_{m-1}, \tilde{W}_m]] \left[\begin{bmatrix} Q_k \\ 0_{p \times k} \end{bmatrix}, Q_2 \right] R_2, \\ &= [\mathcal{V}_k^{new}, [P_{k-1}, \tilde{W}_k]^{new}] R_2. \end{aligned}$$

We set $\Lambda_k^{new} = R_2$, then we use the R -criterion to handle the inexact breakdowns. See steps 22–28 of Algorithm 3 for the complete details. After that, we carry out $\frac{n_m-k}{p}$ block Arnoldi steps with inexact breakdowns to get the shifted block Arnoldi-like relation, which is similar to (13). We seek an approximate solution $X_m^1 = X_0^1 + \mathcal{V}_m Y_m^1$ over the subspace $X_0^1 + \text{Range}(\mathcal{V}_m)$, where Y_m^1 is the solution of the following least-squares problem

$$Y_m^1 = \argmin_{Y^1} \|R_0^1 - (A - \sigma_1 I) \mathcal{V}_m Y^1\|_F = \argmin_{Y^1} \|\Lambda_m - \mathcal{F}_m^1 Y^1\|_F,$$

with $R_0^1 = [\mathcal{V}_m, [P_{m-1}, \tilde{W}_m]] \Lambda_m$.

Assuming that p inexact breakdowns have occurred at iterations j of the SAD-BGMRES method, according to [35, Eq. (47)] we obtain the following inequality

$$\|R_j^1(:, i)\|_2 \leq \epsilon^{(R)}, \quad 1 \leq i \leq p. \quad (26)$$

Using relation (26), we have

$$\frac{\|R_j^1(:, i)\|_2}{\|B(:, i)\|_2} = \frac{\|R_j^1(:, i)\|_2}{\|b^{(i)}\|_2} \leq \frac{\epsilon^{(R)}}{\min_{i=1, \dots, p} \|b^{(i)}\|_2}.$$

From the above relation, we get the relation between the threshold parameter $\epsilon^{(R)}$ used to detect the inexact breakdowns and the stopping threshold tol as

$$\epsilon^{(R)} = tol \times \min_{i=1, \dots, p} \|b^{(i)}\|_2, \quad (27)$$

which we used in all our runs.

2.2 The Additional Shifted Block Systems

The additional shifted block systems can be solved inexpensively if we exploit the shifted block invariance property of the block Krylov subspace. However, this property may not be maintained if the SAD-BGMRES algorithm is restarted as the block residuals R_m^1 and R_m^i , ($i = 2, \dots, L$) of the base block system and of the shifted block systems are in general no longer cospatial. To overcome this problem, we force the additional shifted block residuals R_m^i , ($i = 2, \dots, L$) to be cospatial to R_m^1 similarly to the strategy used in [41], i.e., we impose that

$$R_m^i = R_m^1 N_m^i, \quad i = 2, \dots, L, \quad (28)$$

where N_m^i are some $p \times p$ nonsingular matrices. Here we assume that the initial shifted block residuals are cospatial, $R_0^i = R_0^1 N_0^i$, $i = 2, \dots, L$ (note that this relation is satisfied by taking $X_0^i = 0$). The approximate solutions of the additional shifted block systems can be formulated like Eq. (14),

$$X_m^i = X_0^i + \mathcal{V}_m Y_m^i, \quad i = 2, 3, \dots, L, \quad (29)$$

and the corresponding additional shifted block residuals written as

$$\begin{aligned} R_m^i &= R_0^i - (A - \sigma_i I) \mathcal{V}_m Y_m^i, \\ &= R_0^i - [\mathcal{V}_m, [P_{m-1}, \tilde{W}_m]] \mathcal{F}_m^i Y_m^i, \end{aligned} \quad (30)$$

where the last relation can be obtained from Eq.(13), i.e.,

$$(A - \sigma_i I) \mathcal{V}_m = [\mathcal{V}_m, [P_{m-1}, \tilde{W}_m]] \mathcal{F}_m^i, \quad i = 2, 3, \dots, L.$$

Requiring the cospatial relation (28), we use the Eqs. (15) and (30),

$$\begin{aligned} R_m^i &= R_m^1 N_m^i, \\ \Leftrightarrow R_0^i - [\mathcal{V}_m, [P_{m-1}, \tilde{W}_m]] \mathcal{F}_m^i Y_m^i &= [\mathcal{V}_m, [P_{m-1}, \tilde{W}_m]] R_{LS} N_m^i, \\ \Leftrightarrow R_0^1 N_0^i - [\mathcal{V}_m, [P_{m-1}, \tilde{W}_m]] \mathcal{F}_m^i Y_m^i &= [\mathcal{V}_m, [P_{m-1}, \tilde{W}_m]] R_{LS} N_m^i, \\ \Leftrightarrow [\mathcal{V}_m, [P_{m-1}, \tilde{W}_m]] (\mathcal{F}_m^i Y_m^i + R_{LS} N_m^i) &= R_0^1 N_0^i, \\ \Leftrightarrow [\mathcal{V}_m, [P_{m-1}, \tilde{W}_m]] (\mathcal{F}_m^i Y_m^i + R_{LS} N_m^i) &= [\mathcal{V}_m, [P_{m-1}, \tilde{W}_m]] \Lambda_m N_0^i. \end{aligned}$$

In terms of the unknowns Y_m^i and N_m^i , the last line can be written as the following linear systems

$$[\mathcal{F}_m^i \hat{V}] \begin{bmatrix} Y_m^i \\ \hat{R} N_m^i \end{bmatrix} = \Lambda_m N_0^i, \quad i = 2, 3, \dots, L,$$

with $R_{LS} = \hat{V} \hat{R}$ be the reduced QR -decomposition of R_{LS} . Finally, we can use these quantities to form the approximate solutions X_m^i of the additional shifted block linear systems [see Eq. (29)]. The complete pseudocode of the SAD-BGMRES method is sketched in Algorithm 2.

3 Numerical Experiments

We report on numerical experiments with the SAD-BGMRES method for solving sequences of shifted linear systems with multiple right-hand sides arising in different fields. In our experiments, the harmonic Ritz vectors were computed using the MATLAB built-in function *eigs* that calls the ARPACK package for eigenvalue problems [27]. We setup the $n \times p$ right-hand side matrix B with normally distributed values by calling the MATLAB built-in function *randn*. The iterative solution was always started from the initial guess $0 \in \mathbb{C}^{n \times p}$ and it was stopped when either the Euclidean norm of the columns of the block shifted residuals normalized by the corresponding right-hand side satisfies the stopping criterion

$$\frac{\|R_m^i(:, j)\|_2}{\|B(:, j)\|_2} \leq tol, \quad i = 1, \dots, L, \quad j = 1, \dots, p,$$

or when the number of iterations exceeded the positive integer parameter *maxiter*. The experiments were run under Windows 7 and MATLAB version R2015a, on a PC with an Inter(R) Core(TM) i5-4590 CPU @3.30 GHz and 8GB of memory. The timings reported in our experiments are expressed in seconds.

Algorithm 2 SAD-BGMRES method**Input:** $B, \{\sigma_i\}_{i=1}^L \subset \mathbb{C}, tol, maxiter, k$ **Output:** X_m^i

```

1: Choose an initial guess  $X_0^i \in \mathbb{C}^{n \times p}$  and set  $N_0^i = I$ .
2:  $R_0^i = B - (A - \sigma_i I)X_0^i$ .
3: for  $iter = 1, \dots, maxiter$  do
4:    $R_0^1 = V_1 \Lambda_1$  (reduced  $QR$ -decomposition)
5:   if  $iter = 1$  then
6:     Apply block Arnoldi using inexact breakdown (Algorithm 4) to  $A - \sigma_1 I$  and generate  $\mathcal{V}_m, P_{m-1}, \tilde{W}_m, \mathcal{F}_m^1$ 
7:   else
8:     Apply Algorithm 3 to recycle the harmonic Ritz information and generate  $\mathcal{V}_m, P_{m-1}, \tilde{W}_m, \mathcal{F}_m^1$ 
9:   end if
10:   $Y_m^1 = \underset{Y^1}{\operatorname{argmin}} \|\Lambda_m - \mathcal{F}_m^1 Y^1\|_F$ 
11:   $R_{LS} = \Lambda_m - \mathcal{F}_m^1 Y_m^1$ 
    % Solve the base system
12:   $X_m^1 = X_0^1 + \mathcal{V}_m Y_m^1$ 
13:   $R_m^1 = [\mathcal{V}_m, [P_{m-1}, \tilde{W}_m]] R_{LS}$ 
    % Solve the other shifted systems
14:  Solve  $[\mathcal{F}_m^i \hat{V}] \begin{bmatrix} Y_m^i \\ \hat{R} N_m^i \end{bmatrix} = \Lambda_m N_0^i, i = 2, 3, \dots, L$ 
15:   $X_m^i = X_0^i + \mathcal{V}_m Y_m^i$ 
16:   $R_m^i = R_m^1 N_m^i$ 
17:  Check convergence, and restart if convergence is not achieved
18:  Set  $X_0^1 = X_m^1$  and  $R_0^1 = R_m^1$ 
19: end for

```

Table 1 Set and characteristics of the test matrix problems used in our experiments

Example	Name	Size	Nonzeros	Problem kind
1	epb1	14,734	95,053	Thermal problem
2	poisson3Da	13,514	352,762	Computational fluid dynamics problem
3	poisson3Db	85,623	2,374,949	Computational fluid dynamics problem
4	FEM_3D_thermal2	147,900	3,489,300	Thermal problem
5	light_in_tissue	29,282	406,084	Electromagnetics problem
6	vfem	93,476	1,434,636	Electromagnetics problem

3.1 General Test Problems

Initially, we assessed the effectiveness of the inexact breakdown strategy by comparing the performance of the SAD-BGMRES method against the standard BGMRES-DR-Sh method introduced in [41] for solving a suite of selected linear systems from the University of Florida Sparse Matrix Collection [12] listed in Table 1. The two methods were compared in terms of number of matrix-vector products (*mvp*s), maximum true relative residuals norms (*trr*) and CPU solution time expressed in seconds (*cpu*). In our experiments, we used $p = 10$ right-hand sides, the set of shifts $\sigma_i = [-0.0001, -0.001, -0.01, -0.1, -1]$ and we deflated $k = 10$ harmonic Ritz vectors. We set the maximum dimension of the search space equal to $m = 90$, and $tol = 10^{-6}$ and we used $maxiter = 10000$ for the stopping criterion parameters.

Algorithm 3 SAD-BGMRES method: recycle the harmonic Ritz information

```

1:  $[\tilde{G}_k, \tilde{\Theta}_k] = \text{eigs}((\mathcal{L}_m^1)^H \mathcal{L}_m^1 + \mathbb{H}_m^H \mathbb{H}_m, (\mathcal{L}_m^1)^H, k)$ 
2:  $\tilde{G}_{k+1} = \left[ \begin{bmatrix} \tilde{G}_k \\ 0_{p \times k} \end{bmatrix}, R_{LS} \right] \in \mathbb{C}^{(n_{m+1} \times (k+p))}$ 
3:  $\tilde{G}_{k+1} = Q_{k+1} R_{k+1}$  (reduced  $QR$ -decomposition)
4:  $Q_k = Q_{k+1}(1:n_m, 1:k)$ ,  $R_2 = R_{k+1}(:, k+1:k+p)$ 
5:  $\mathcal{V}_k^{new} = \mathcal{V}_m Q_k$ 
6:  $PW \leftarrow [P_{k-1}, \tilde{W}_k]^{new} = [\mathcal{V}_m, [P_{m-1}, \tilde{W}_m]] Q_2$ 
7:  $V PW \leftarrow [\mathcal{V}_j^{new}, [P_{j-1}, \tilde{W}_j]^{new}]$ 
8:  $(\mathcal{F}_k^1)^{new} = Q_{k+1}^H \mathcal{F}_m^1 Q_k$ 
9:  $\Lambda_k^{new} = R_2$ 
10: for  $i = 1, \dots, p$  do
11:    $w = PW(:, i)$ 
12:   for  $j = 1, \dots, k$  do
13:      $\mathbb{R}(j, i) = V PW(:, j)^H w$ 
14:      $w = w - \mathbb{R}(j, i) V PW(:, j)$ 
15:   end for
16:    $\mathbb{R}(i+1, i) = \|w\|$ 
17:    $PW(:, i) = w / \mathbb{R}(i+1, i)$ 
18:    $k = k+1$ 
19: end for
20:  $\mathcal{F}_k^1 = \left[ \begin{bmatrix} I_k \\ 0_{p \times k} \end{bmatrix}, \mathbb{R} \right] (\mathcal{F}_k^1)^{new}, \Lambda_k = \left[ \begin{bmatrix} I_k \\ 0_{p \times k} \end{bmatrix}, \mathbb{R} \right] \Lambda_k^{new}$ 
21:  $Y_k^1 = \underset{Y^1 \in \mathbb{C}^{n_j \times p}}{\text{argmin}} \left\| \Lambda_k - \mathcal{F}_k^1 Y^1 \right\|$ 
    % Compute the SVD to detect inexact breakdowns in residuals
22:  $(\Lambda_k - \mathcal{F}_k^1 Y_k^1) = U_1 \Sigma_1 V_1^H + U_2 \Sigma_2 V_2^H$ , where  $\sigma_{\min}(\Sigma_1) \geq \epsilon^{(R)} > \sigma_{\max}(\Sigma_2)$ 
23: Compute  $\mathbb{W}_1$  and  $\mathbb{W}_2$  such that
    
$$\text{Range}(\mathbb{W}_1) = \text{Range}(U_1^{(2)}) \text{ with } U_1 = \begin{pmatrix} U_1^{(1)} \\ U_1^{(2)} \end{pmatrix} \text{ and } [\mathbb{W}_1, \mathbb{W}_2] \text{ is unitary.}$$

24:  $V_{k+1} = [P_{k-1}, \tilde{W}_k] \mathbb{W}_1$ 
25:  $P_k = [P_{k-1}, \tilde{W}_k] \mathbb{W}_2$ 
26:  $\mathcal{L}_{k+1,:} = \mathbb{W}_1^H \mathbb{H}_k$ 
27:  $G_k = \mathbb{W}_2^H \mathbb{H}_k$ 
28: Set  $\underline{\mathcal{L}}_k = \begin{pmatrix} \mathcal{L}_k \\ \mathcal{L}_{k+1,:} \end{pmatrix}$ 
29: Apply Algorithm 4 to form the rest of  $\mathcal{V}_{m+1}, P_{m-1}, \tilde{W}_m, \mathcal{F}_m^1$ 

```

We clearly see the stabilization effects of the inexact breakdown strategy on the convergence history of the SAD-BGMRES method in the plots displayed in the left sides of Figs. 1 and 2 for Examples 1–6, which report on the $\log_{10}$ of the maximum relative residual norms versus the number of matrix-vector products. For some of the plotted curves, the improvement versus the BGMRES-DR-Sh method is really notable, showing that the SAD-BGMRES method handled the inexact breakdown situation effectively when it occurred. For the sake of clarity we also display for each example a side-by-side convergence analysis between the SAD-BGMRES and BGMRES-DR-Sh methods at each time when the inexact breakdown occurred in the solution of the base system. The improvement of the inexact breakdown strategy is evident in the right plots of Figs. 1 and 2. In order to further illustrate the benefits of the inexact breakdown strategy, in Fig. 3 we display for each example the rank of the matrix V_{j+1} versus the number of *mvp*s over the iterations for the base block system. The inexact breakdown situation occurs anytime the rank of V_{j+1} is smaller than the number of right-

Algorithm 4 Block Arnoldi using R -criterion to detect inexact breakdowns [1]

```

1: Let  $P_0 = 0$ ,  $G_0 = 0$ ,  $\mathcal{L}_0 = [\ ]$ , and  $\epsilon^{(R)}$ 
2: for  $j = 1, 2, \dots, m$  do
3:    $\mathcal{L}_{1,1:j} = \mathcal{V}_j^H (AV_j)$ 
4:    $W_j = AV_j - \mathcal{V}_j \mathcal{L}_{1,1:j}$ 
5:   Set  $\mathcal{L}_j = [\mathcal{L}_{j-1}, \mathcal{L}_{1,1:j}] \in \mathbb{C}^{n_j \times n_j}$ 
6:    $C_j = P_{j-1}^H W_j$ 
7:    $\tilde{W}_j D_j = W_j - P_{j-1} C_j$  (reduced  $QR$ -decomposition)
8:   Set  $\mathbb{H}_j = \begin{pmatrix} G_{j-1} & C_j \\ 0 & D_j \end{pmatrix} \in \mathbb{C}^{p \times n_j}$ ,  $\mathcal{F}_j = \begin{pmatrix} \mathcal{L}_j \\ \mathbb{H}_j \end{pmatrix} \in \mathbb{C}^{(n_j+p) \times n_j}$ ,  $\Lambda_j = \begin{pmatrix} \Lambda_1 \\ 0 \end{pmatrix} \in \mathbb{C}^{(n_j+p) \times p}$ 
9:    $Y_j = \underset{Y \in \mathbb{C}^{n_j \times p}}{\operatorname{argmin}} \|\Lambda_j - \mathcal{F}_j Y\|_F$ 
   % Compute the SVD to detect inexact breakdowns in residuals
10:   $(\Lambda_j - \mathcal{F}_j Y_j) = \mathbb{U}_1 \Sigma_1 \mathbb{V}_1^H + \mathbb{U}_2 \Sigma_2 \mathbb{V}_2^H$ , where  $\sigma_{\min}(\Sigma_1) \geq \epsilon^{(R)} > \sigma_{\max}(\Sigma_2)$ 
11:  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  $[\mathbb{W}_1, \mathbb{W}_2]$  is unitary.
12:   $V_{j+1} = [P_{j-1}, \tilde{W}_j] \mathbb{W}_1$ 
13:   $P_j = [P_{j-1}, \tilde{W}_j] \mathbb{W}_2$ 
14:   $\mathcal{L}_{j+1,:} = \mathbb{W}_1^H \mathbb{H}_j$ 
15:   $G_j = \mathbb{W}_2^H \mathbb{H}_j$ 
16:  Set  $\mathcal{L}_j = \begin{pmatrix} \mathcal{L}_j \\ \mathcal{L}_{j+1,:} \end{pmatrix}$ 
17: end for

```

hand sides. Over the iterations, the approximate linear dependence of the base block residuals was detected according to the given deflation tolerance, and the block size was effectively reduced. The smaller the block size, the faster the convergence. The SAD-BGMRES method outperformed the BGMRES-DR-Sh method on all the problems in terms of both *mups* and *cpu* time, as it can be seen from Table 2. Note that the inexact breakdown strategy reduces not only reduce the *mups*, but also the number of iterations *Iters*.

In the experiments shown in Table 3 we increased the number of right-hand sides to $p = 12, 15$ and 18 , setting the maximum dimension of the search space m equal to $m = 90, 120$. Again, the SAD-BGMRES method outperformed the BGMRES-DR-Sh method in terms of *mups* and *cpu* time in all our runs, converging to the requested accuracy in cases where the BGMRES-DR-Sh method did not converge (this situation is represented in the table by the symbol “-”). The improvement was notable especially for small restart values and large right-hand sides number.

On Example 4, none of the methods converged to the requested accuracy using $p = 18$, $m = 120$. One possible explanation is that in this case the degree of the polynomial of A used to build the Krylov subspace is smaller than 7. Note that the polynomial degree decreases as the right-hand sides p increases. In fact, by increasing the maximum dimension of the search space to $m = 180$, the SAD-BGMRES method converged; however, the BGMRES-DR-Sh method still failed to converge. Obviously, preconditioning could be used to achieve convergence on difficult problems. Special preconditioners that maintain the shift-invariant property of the Krylov subspace need to be used, like e.g. polynomial [42], shift-and-invert [20,37] and multi-shifted preconditioners [3]. In our experiments we used a shift-and-invert preconditioner of the form $A_\tau = A - \tau I$:

$$(A - \sigma_i I)(A - \tau I)^{-1} \hat{X}_i = B, \quad i = 1, \dots, L,$$

Fig. 1 Convergence histories between the SAD-BGMRES and the BGMRES-DR-Sh methods for solving Examples 1–3. (Left: the different convergence curves correspond to different choice of the shift, right: convergence comparison between SAD-BGMRES and BGMRES-DR-Sh at each time when the inexact breakdown is occurred)

where $X_i = (A - \tau I)^{-1} \hat{X}_i$. The shift-invariance property for this preconditioner,

$$\mathbb{K}_m((A - \sigma_i I)(A - \tau I)^{-1}, B) = \mathbb{K}_m((A - \tau I)^{-1}, B),$$

follows from the identity $(A - \sigma_i I)(A - \tau I)^{-1} = I + (\tau - \sigma_i)(A - \tau I)^{-1}$. The implementation of the preconditioned SAD-BGMRES method is very similar to Algorithm 2, with the only difference that the block Arnoldi algorithm is run on the matrix $(A - \tau I)^{-1}$ starting from

Fig. 2 Convergence histories between the SAD-BGMRES and the BGMRES-DR-Sh methods for solving Examples 4–6. (Left: the different convergence curves correspond to different choice of the shift, right: convergence comparison between SAD-BGMRES and BGMRES-DR-Sh at each time when the inexact breakdown is occurred)

B. The effectiveness of this preconditioning strategy is shown in Table 4 on Example 4. The preconditioned SAD-BGMRES method converged favourably in terms of number of matrix-vector products and solution time, whereas it failed to converge without using a preconditioner in Table 3. Moreover, different preconditioners corresponding to different values of τ exhibited mixed performance, as illustrated in [20,37,40] for more details. In our implementation, we inverted the preconditioner matrix by using a sparse direct solver (the built-in MATLAB backslash ‘\’ operator).

Fig. 3 Effect of inexact breakdown strategy: the rank of V_{j+1} processed during the convergence of the SAD-BGMRES method for solving the base system in Examples 1–6

We analysed further the robustness of the SAD-BGMRES method by comparing the convergence of our solver against other popular Krylov algorithms for this problem class, namely the GMRES-DR-Sh [11], IB-BGMRES [35], IB-BGMRES-DR [1] and the recycled shifted block GMRES methods (rsbGMRES) [39]. In the experiments reported in Table 5 we set the number of right-hand sides to $p = 5$, since the rsbGMRES method requires this value to be equal to the number of shifts. We solved $p = 5$ multi-shifted linear systems separately by the GMRES-DR-Sh method, and $L = 5$ linear systems with multiple right-hand sides

Table 2 Performance comparison between the BGMRES-DR-Sh and SAD-BGMRES methods using a convergence tolerance $tol = 10^{-6}$ in the stopping criterion for solving general test problems

Example	Method	Iters	<i>Mvps</i>	<i>Trr</i> ($\times 10^{-7}$)	<i>Cpu</i>
1	BGMRES-DR-Sh	491	4901	9.9187 9.9153 9.6047 4.2500 7.2963	15.7966
	SAD-BGMRES	386	3303	8.9716 9.1456 9.6047 4.2500 7.2963	7.5463
2	BGMRES-DR-Sh	109	1081	9.6899 9.7957 9.6287 9.3944 3.5297	5.0595
	SAD-BGMRES	98	829	8.7851 9.8280 8.6855 9.3944 3.5297	2.9199
3	BGMRES-DR-Sh	313	3130	9.9654 9.8289 9.5669 7.5242 5.1765	74.6347
	SAD-BGMRES	231	2026	9.0564 9.5582 9.5661 7.5242 5.1765	44.2036
4	BGMRES-DR-Sh	686	6854	9.9725 9.6707 9.4991 8.3392 9.9730	323.2846
	SAD-BGMRES	579	5634	9.2840 9.6626 8.2865 8.3392 1.2376	167.7807
5	BGMRES-DR-Sh	640	6391	9.9201 9.7880 9.6858 9.6436 6.6052	87.6484
	SAD-BGMRES	423	3908	8.0562 9.7008 9.6813 9.6436 6.6052	47.6748
6	BGMRES-DR-Sh	157	1565	9.4637 9.6810 8.8717 7.1022 6.7966	61.7558
	SAD-BGMRES	153	1413	8.4281 7.3783 3.5241 1.8197 3.2435	57.2179

The best results are highlighted in bold

in sequence using the IB-BGMRES and IB-BGMRES-DR methods. For a fair comparison, we compared the number of matrix-vector products instead of the number of block matrix-vector products in the rsbGMRES code,¹ and we set the maximum dimension of the search space $m = 18$ in the GMRES-DR-Sh method. Observe that if the maximum dimension of the standard Krylov subspace method is equal to jp , then the maximum dimension for the corresponding block variant with p right-hand sides is j . As it can be seen in Table 5, shifted block solvers always outperformed shifted non-block solvers. Although the SAD-BGMRES method needed more *Mvps* than the rsbGMRES method for solving some of the problems, e.g. Examples 4 and 6, the total solution time was always significantly reduced.

3.2 Quantum Chromodynamics Application

Quantum chromodynamics (QCD) is generally accepted to be the fundamental physical theory of strong interactions among the quarks as constituents of matter [17]. Lattice gauge theory is a discretization of quantum chromodynamics based on the solution of the Dirac equation. Shifted linear systems of the form (1) arise naturally in lattice QCD for Wilson fermion matrices, where $A = I - \kappa D$ represents a periodic nearest-neighbour coupling on a four-dimensional Euclidean space-time lattice.

In our study we used two sets of QCD matrices available from the University of Florida Sparse Matrix Library [12] to compare the performance of the BGMRES-DR-Sh and SAD-BGMRES methods. The first is a collection of four $49, 152 \times 49, 152$ complex matrices and the other one is a collection of four 3072×3072 complex matrices, i.e., conf5_0- $8 \times 8-05$, conf5_0- $8 \times 8-15$, conf6_0- $8 \times 8-20$, conf6_0- $8 \times 8-80$, and conf5_0- $4 \times 4-14$, conf5_0- $4 \times 4-22$, conf6_0- $4 \times 4-20$, conf6_0- $4 \times 4-30$, respectively. For each matrix, say D , from the collection there exists a critical value κ_c with $\frac{1}{\kappa_c} < \frac{1}{\kappa} < \infty$ such that $A = I - \kappa D$ is real-positive. We defined $A = \left(\frac{1}{\kappa_c} + 10^{-3}\right) I - D$ as the base matrix. We considered $p = 6$ right-hand sides, $k = 10$ harmonic Ritz vectors, the shifts

¹ <https://zenodo.org/record/56157#.WtTbCvknbCA>.

Table 3 Number of matrix-vector products (*Mvps*) and solution time in seconds (*Cpu*) for the BGMRES-DR-Sh and SAD-BGMRES methods using a different number of right-hand sides and a different combinations of restarts for solving general test problems

$m = 90$		$p = 12$		$p = 15$		$p = 18$	
Example	Method	<i>Mvps</i>	<i>Cpu</i>	<i>Mvps</i>	<i>Cpu</i>	<i>Mvps</i>	<i>Cpu</i>
1	BGMRES-DR-Sh	6582	29.2151	8522	43.2141	—	—
	SAD-BGMRES	4501	11.0285	5695	14.6319	7058	18.2741
2	BGMRES-DR-Sh	1314	6.4061	1861	10.2433	2323	13.6924
	SAD-BGMRES	1039	3.1849	1356	4.0064	1728	5.5368
3	BGMRES-DR-Sh	3754	85.2554	5176	143.7784	7031	193.0596
	SAD-BGMRES	2613	50.7236	3662	80.7529	4298	94.3393
4	BGMRES-DR-Sh	—	—	—	—	—	—
	SAD-BGMRES	8306	220.9147	—	—	—	—
5	BGMRES-DR-Sh	8553	159.4412	—	—	—	—
	SAD-BGMRES	5400	58.6377	7826	87.8625	—	—
6	BGMRES-DR-Sh	2835	110.6439	4406	201.0116	6306	326.8536
	SAD-BGMRES	1834	67.1545	2690	105.5959	3851	154.7709
$m = 120$		$p = 12$		$p = 15$		$p = 18$	
Example	Method	<i>Mvps</i>	<i>Cpu</i>	<i>Mvps</i>	<i>Cpu</i>	<i>Mvps</i>	<i>Cpu</i>
1	BGMRES-DR-Sh	5070	28.5478	7381	43.4246	—	—
	SAD-BGMRES	3618	9.8557	4945	12.3239	6048	16.1242
2	BGMRES-DR-Sh	1126	6.8432	1536	9.7198	1920	13.3982
	SAD-BGMRES	919	2.7798	1169	3.4993	1422	4.4782
3	BGMRES-DR-Sh	3033	79.5724	4406	120.8334	5475	157.0843
	SAD-BGMRES	2209	44.4833	2956	59.1315	3722	74.7413
4	BGMRES-DR-Sh	7761	519.9304	—	—	—	—
	SAD-BGMRES	6040	166.2577	9047	254.3657	—	—
5	BGMRES-DR-Sh	5963	135.3786	8826	212.2614	—	—
	SAD-BGMRES	4014	46.5017	5880	65.2545	7565	86.4881
6	BGMRES-DR-Sh	1807	96.6953	2822	151.2565	4063	210.3583
	SAD-BGMRES	1461	56.5089	2098	80.2157	2808	108.5715

The best results are highlighted in bold

Table 4 Number of matrix-vector products (*Mvps*) and solution time in seconds (*Cpu*) for the SAD-BGMRES method using different preconditioners on Example 4

Example 4	$m = 90$				$m = 120$			
	$p = 15$		$p = 18$		$p = 15$		$p = 18$	
	<i>Mvps</i>	<i>Cpu</i>	<i>Mvps</i>	<i>Cpu</i>	<i>Mvps</i>	<i>Cpu</i>	<i>Mvps</i>	<i>Cpu</i>
$\tau = -0.0002$	192	594.3512	234	722.2651	192	591.7533	229	719.7767
$\tau = -0.002$	291	881.9244	350	1026.5642	288	822.6252	340	980.3509
$\tau = -0.02$	843	1734.8774	1107	2176.1557	760	1609.8043	968	1922.6312

The best results are highlighted in bold

Table 5 Number of *Mvps* and *Cpu* for GMRES-DR-Sh, IB-BGMRES, IB-BGMRES-DR, rsbGMRES, BGMRES-DR-Sh and SAD-BGMRES methods for solving general test problems

Method	Example 1		Example 2		Example 3	
	<i>Mvps</i>	<i>Cpu</i>	<i>Mvps</i>	<i>Cpu</i>	<i>Mvps</i>	<i>Cpu</i>
GMRES-DR-Sh	2440	8.6244	790	3.3173	1494	27.2411
IB-BGMRES	3206	6.3729	1470	4.4503	2509	55.9004
IB-BGMRES-DR	2387	6.1665	1176	3.4456	1944	40.1585
rsbGMRES	1730	26.7244	430	3.1887	910	100.4175
BGMRES-DR-Sh	1771	6.4928	501	2.7327	1076	22.1894
SAD-BGMRES	1467	3.9902	415	1.3312	864	18.8482
Method	Example 4		Example 5		Example 6	
	<i>Mvps</i>	<i>Cpu</i>	<i>Mvps</i>	<i>Cpu</i>	<i>Mvps</i>	<i>Cpu</i>
GMRES-DR-Sh	1932	76.7972	2020	32.3202	740	23.8921
IB-BGMRES	3305	108.8389	4629	58.6223	924	39.6715
IB-BGMRES-DR	2774	81.3387	3290	40.7117	814	31.1868
rsbGMRES	1170	207.7897	1905	202.6003	350	59.8205
BGMRES-DR-Sh	1803	84.4315	1776	29.4754	564	22.0863
SAD-BGMRES	1677	50.5453	1416	18.4266	558	20.0377

The best results are highlighted in bold

Table 6 Numerical behavior of BGMRES-DR-Sh and SAD-BGMRES with $tol = 10^{-6}$ for solving quantum chromodynamics application

Example	Method	<i>Mvps</i>	<i>Trr</i>	<i>Cpu</i>
Π_1	BGMRES-DR-Sh	2489	9.9331e-07 9.9754e-07 3.3935e-07	93.6452
	SAD-BGMRES	2022	8.8063e-07 9.8702e-07 3.3935e-07	60.2023
Π_2	BGMRES-DR-Sh	2151	9.7887e-07 9.7492e-07 3.3974e-07	72.7217
	SAD-BGMRES	1849	9.2417e-07 9.9093e-07 3.3974e-07	48.8799
Π_3	BGMRES-DR-Sh	1877	9.8258e-07 9.8029e-07 8.5653e-07	48.1522
	SAD-BGMRES	1375	8.9904e-07 9.5591e-07 8.5653e-07	36.2448
Π_4	BGMRES-DR-Sh	1769	9.6752e-07 9.8443e-07 8.6281e-07	45.4739
	SAD-BGMRES	1378	8.8008e-07 9.9086e-07 8.6281e-07	37.1091

The best results are highlighted in bold

were $\sigma = -[0.0001, 0.01, 10]$ in our runs, and we set the maximum number of iterations *maxiter* equal to 5000. Note that coefficient matrices with smaller shifts typically require more iterations to converge. The results are shown in Table 6. Again, overall the SAD-BGMRES method performs better than the BGMRES-DR-Sh method in terms of *mups* and *cpu* time.

In Table 7 we propose a performance comparison between the BGMRES-DR-Sh and SAD-BGMRES methods using a different number of right-hand sides and the following set of 15 shifts $[0.0001, 0.0002, 0.0003, 0.001, 0.002, 0.003, 0.01, 0.02, 0.03, 0.1, 0.2, 0.3, 1, 2, 3]$. The results show that the SAD-BGMRES method converges satisfactorily while the BGMRES-DR-Sh method does not converge especially when the number of right-hand sides is larger.

Table 7 Numerical behavior of BGMRES-DR-Sh and SAD-BGMRES methods with different number of right-hand sides for solving quantum chromodynamics application

Example	Method	$p = 6$		$p = 16$	
		<i>Mvps</i>	<i>Cpu</i>	<i>Mvps</i>	<i>Cpu</i>
Π_5	BGMRES-DR-Sh	1105	8.0663	–	–
	SAD-BGMRES	1005	3.4583	3084	10.2966
Π_6	BGMRES-DR-Sh	1052	7.4467	4907	50.6173
	SAD-BGMRES	972	3.3194	2736	8.8401
Π_7	BGMRES-DR-Sh	477	3.5053	1853	18.3657
	SAD-BGMRES	463	1.8551	1279	3.8312
Π_8	BGMRES-DR-Sh	518	3.8199	2027	19.7367
	SAD-BGMRES	480	1.8563	1427	4.1006

The best results are highlighted in bold

4 Conclusions

We have presented a new shifted block Krylov subspace method for solving large-scale multi-shifted linear systems with multiple right-hand sides arising in several science and engineering applications. The solver is remarkably robust as it can handle numerical problems due to the occurrence of inexact breakdowns in the block Arnoldi procedure. In addition, it recycles spectral information at restart for faster convergence. Finally, it solves the whole sequence of multi-shifted linear systems and multiple right-hand sides simultaneously exploiting the shift-invariance property of Krylov subspaces. Numerical experiments confirm the robustness and effectiveness of the new method that outperforms conventional block Krylov algorithms for solving general sparse linear systems arising from different fields. Especially when combined with preconditioning, the proposed iterative method can be suitable to use in different application areas, such as quantum chromodynamics, optimization and PageRank problems.

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