A flexible and adaptive Simpler GMRES with deflated restarting for shifted linear systems

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Abstract: In this paper, two efficient iterative algorithms based on the simpler GMRES method are proposed for solving shifted linear systems. To make full use of the shifted structure, the proposed algorithms utilizing the deflated restarting strategy and flexible preconditioning can significantly reduce the number of matrix-vector products and the elapsed CPU time. Numerical experiments are reported to illustrate the performance and effectiveness of the proposed algorithms.

Keywords: Shifted linear system, Adaptive Simpler GMRES, Flexible preconditioning, Deflated restarting.

AMS classifications: 65F15, 65F10, 65Y20.

1 Introduction

In this study, we are interested in efficiently simultaneous solutions of the following large shifted linear systems

$$(A + \alpha_jI)x(\alpha_j) = b, \quad j = 1, \cdots, s.$$  \hfill (1.1)

In general, $A \in \mathbb{C}^{n \times n}$ is non-singular and non-Hermitian, $\alpha_j \in \mathbb{C}$ is the shift such that $A + \alpha_jI$ is also non-singular, and $\alpha_j$ varies in a wide range, the right-hand side $b \in \mathbb{C}^n$ is fixed. Usually we take $\alpha_1 = 0$ as default, otherwise, Eq. (1.1) can be reset after a shift $\alpha_1$. The first linear system is called the seed system, others are the add systems. Such problem occurs in many scientific and engineering applications, such as structural dynamics \cite{1,2}, quantum chromodynamics \cite{3}, web search ranking \cite{4}, control theory \cite{5,6} and so on. Therefore, there is a strong need for establishing efficient solutions of Eq. (1.1).

Many traditional methods (such as direct and iterative linear systems solvers) for the above problem are to solve $(A + \alpha_jI)x(\alpha_j) = b$ for each $\alpha_j$, this trick can be quite expensive and prohibited when $s$ and $n$ are large. Fortunately, owing to the shift-invariance property of Krylov subspaces, the Krylov subspace methods can solve Eq. (1.1) simultaneously \cite{7}. That is, the Krylov subspace holds that

$$\mathcal{K}_m(A, b) = \mathcal{K}_m(A + \alpha_jI, b), \quad \forall \alpha_j \in \mathbb{C}.$$

Hence, all approximate solutions for (1.1) can be sought in a single space generated by the matrix $A$ with the vector $b$.

The GMRES algorithm \cite{8} is such a famous Krylov subspace method that it calculates the basis for $\mathcal{K}_k(A, b)$ by once Arnoldi process with the initial guess $x_0 = 0$, hence the shifted system (1.1)
can be solved cheaply if GMRES is performed for it simultaneously [5]. However, since the residuals
\( r_m(\alpha_j) = b - (A + \alpha_j I)x_m(\alpha_j) \) are not colinear, so that \( \mathcal{K}_m(A, r_m) \neq \mathcal{K}_m(A + \alpha_j I, r_m(\alpha_j)) \) with \( m \) being the restarting frequency. As a remedy, Frommer and Glässner have forced the residual vectors to be
colinear [9], then restarts can again solve Eq. (1.1) cheaply. There are many variants based on GMRES for
solving shifted linear systems. For instance, Gu, Zhang and Li proposed a variant of the restarted GMRES
augmented with some approximate eigenvectors for the shifted system (1.1), refer to [10] for details. Later,
Gu improved the restarted GMRES by augmenting the Krylov subspace with harmonic Ritz vectors
for Eq. (1.1) [11]. By deflating eigenvalues for matrices that have a few small eigenvalues, Darnell,
Morgan and Wilcox [12] presented an improved GMRES method with deflated restarting to accelerate
the convergence. Gu, Zhou and Lin from another aspect of enhancing the convergence speed, proposed
a flexible preconditioned Arnoldi method that needs to exactly solve a linear system with the coefficient
matrix \( A + \sigma_k I \) at the \( k \)-th iteration, where \( \sigma_k \) is the precondition reference value that draws near \( \alpha_j \). They also showed that their proposed method is greatly faster than the traditional preconditioning
strategies [13]. Saibaba, Bakhos and Kitanidis have further extended the flexible preconditioning idea
for solving generalized shifted linear systems arising from oscillatory hydraulic tomography [14]. Sun,
Huang and Jing et al. [15, 16] promoted the block version of GMRES method with deflated restarting
for solving linear systems with multiple shifts and multiple right-hand sides. For other related methods,
refer oneself to some studies in [17–26] and references therein.

As a cheaper implementation of GMRES, the Simpler GMRES algorithm (SGMRES) is another
famous Krylov subspace method [27]. It runs the Arnoldi process begin with \( Ar_0 \) instead of \( r_0 \), where
\( r_0 = b - Ax_0 \). At each iteration, it only requires to solve an upper-triangular least-squares problem rather
than an upper Hessenberg least-squares problem of GMRES, thus the SGMRES solver often spends
less computational cost. Recently, Jing, Yuan and Huang applied the SGMRES and its stable variant:
adaptive SGMRES (Ad-SGMRES) to solve the shifted system (1.1) [28]. For dealing with the non-
colinearity of \( r_m \) and \( r_m(\alpha_j) \), Jing, Yuan and Huang provided a remedy by forcing \( r_m(\alpha_j) \perp \mathcal{K}_m(A, r_0) \).
Besides to this advanced point, at each iteration step, from the non-converged systems, they took the
linear system with the maximum residual norm as the seed system of the restart iteration.

However, in each cycle of the restarted methods, the convergence will slow down, since the dimension
of the Krylov subspace is limited [13, 29–32]. Especially for the problem with \( A + \alpha_j I \) having small
eigenvalues (in modulas). The main reason is that at each cycle, the Krylov subspace does not contain
good approximations of the eigenvectors corresponding to such small eigenvalues. These make the thick-
restarting and preconditioning techniques beneficial for solving Eq. (1.1). Unfortunately, as far as
we know, unlike the shifted GMRES, there are not so many improved strategies applied to accelerate
SGMRES for solving shifted linear systems (1.1). Thus, in this paper, we will first apply the flexible
preconditioning technique [34] to the Ad-SGMRES for solving shifted linear systems (1.1), then consider
restarting the new algorithm with the deflated restarting strategy introduced in [30, 31]. The flexible
preconditioning technique we used in this paper is the inexact preconditioning [33] instead of exact which
used in [13]. The details will be located in Section 2.

The rest of this paper is organized as follows. In Section 2, we first give a brief description of the
adaptive Simpler GMRES method (Ad-SGMRES), then present two variants of Ad-SGMRES for shifted
linear system (1.1). Numerical examples in Section 3 will illustrate the effectiveness of the proposed
algorithms. In Section 4, the paper closes with some conclusions.
2 A flexible and adaptive Simpler GMRES algorithm with deflated restarting for shifted linear systems

In this section, applying the flexible preconditioning technique [14,34], we first derive a flexible adaptive Simpler GMRES algorithm (FAd-SGMRES-Sh) for solving shifted linear systems (1.1) simultaneously. Then based on it, we thick-restart the new algorithm by using the deflated restarting strategy [30,31,45]. Hence, a flexible and adaptive Simpler GMRES algorithm with deflated restarting (FAd-SGMRES-DR-Sh) will be achieved for solving Eq. (1.1).

Before giving the new algorithms, we will first briefly review the adaptive Simpler GMRES method. By introducing a threshold parameter $\nu \in [0,1]$, Jiránek and Rozložník proposed the adaptive Simpler GMRES (Ad-SGMRES) [35], which is more stable than the Simpler GMRES, for solving the linear system $Ax = b$. The following algorithm is just the practical implementation of Ad-SGMRES.

Algorithm 1. The adaptive Simpler GMRES (Ad-SGMRES)

1. Given the initial guess $x_0$, a tolerance $\text{tol}$, a threshold parameter $\nu \in [0,1]$, let $m$ the maximal dimension of the solving subspace, $r_0 = b - Ax_0$;
2. For $k = 1, \cdots, m$, do
   
   (1) $z_k = \begin{cases} r_0/\|r_0\|_2, & \text{if } k = 1, \\ r_{k-1}/\|r_{k-1}\|_2, & \text{if } k > 1, \text{ and } \|r_{k-1}\|_2 \leq \nu \|r_{k-2}\|_2, \\ v_{k-1}, & \text{otherwise}. \end{cases}$
   
   (2) $v_k = Az_k$,
   
   (3) for $i = 1, \cdots, k - 1$
      
      $u_{ik} = v_i^H v_k, \; v_k = v_k - u_{ik}v_i$.
   
   $\text{end}$
   
   (4) $u_{kk} = \|v_k\|_2, \; v_k = v_k/\|v_k\|_2$.
   
   (5) $\xi_k = v_k^H r_{k-1}, \; r_k = r_{k-1} - v_k \xi_k, \; \text{if } \|r_k\|_2 \leq \text{tol}, \text{ then go to Step 3}.$

$\text{end}$

3. Let $k$ be the final iteration number of Step 2, solve: $y_k = U_k^{-1}[\xi_1, \cdots, \xi_k]^H$. Set $x_k = x_0 + Z_k y_k$.

In Algorithm 1, the definitions of $U_k$ and $V_k$ can be found in the next section.

2.1 Flexible preconditioning

Suppose $r_0 = b - Ax_0 \neq 0$, where $x_0$ is the initial guess. At $k$-th iteration of Ad-SGMRES (stated in Algorithm 1) for solving the seed system $Ax = b$, we have

\[ AZ_k = V_k U_k, \]

where $Z_k = [z_1, \cdots, z_k] \in \mathbb{C}^{n \times k}$ is the basis of $\mathcal{K}(A, r_0)$, $V_k = [v_1, \cdots, v_k] \in \mathbb{C}^{n \times k}$ is the orthogonal basis of $A\mathcal{K}(A, r_0)$, $U_k = [u_{ij}] \in \mathbb{C}^{k \times k}$, $i, j = 1, \cdots, k$ is upper triangular, so $U_k$ is non-singular because the coefficient matrix $A$ is non-singular.

In [13], Gu, Zhou and Lin proposed a flexible preconditioning strategy for GMRES that it is needed to exactly solve a linear system with the coefficient matrix $A + \sigma_k I$ at the $k$-th iteration, and it will cost a lot of time especially for large size problems. In this section, we will use the inexact flexible preconditioning [33,34,36] instead of exact. It is known that the traditional right preconditioning is
applied to solve a modified system such as \( AM^{-1}(Mx) = b \), where \( AM^{-1} \) is well conditioned. The inexact flexible preconditioning is actually a modification to the right preconditioning, i.e., \( M_k \) replaces \( M \), so that inexact solver can be used. Based on such ideas, at each \( k \)-th iteration, we set \( w_k = M_k^{-1}z_k \), where \( M_k \) is a variable preconditioner. Denote \( W_k = [w_1, \ldots, w_k] \), obviously, the columns of \( W_k \) may not span a Krylov subspace. For the absence of misunderstanding, we still use notions \( V_k \) and \( U_k \).

The relation (2.1) can be rewritten in the following matrix equation:

\[
AW_k = V_k U_k. \tag{2.2}
\]

For seed system, we seek the approximate solution \( x_k = x_0 + W_k y_k \) in the affine subspace \( x_0 + \text{span}\{W_k\} \), \( y_k \in \mathbb{C}^k \) is a vector to be determined. Meanwhile, we seek the approximate solution \( x_k(\alpha_j) = x_0(\alpha_j) + W_k y_k(\alpha_j) \) in the affine subspace \( x_0(\alpha_j) + \text{span}\{W_k\} \) for add systems, where \( y_k(\alpha_j) \in \mathbb{C}^k \) is a vector to be determined. For the add systems, we have

\[
(A + \alpha_j I)W_k = AW_k + \alpha_j W_k
= V_k U_k + \alpha_j W_k.
\]

Since for \( W_k \) cannot be expressed by \( V_k \), therefore, similar as in SGMRES [27], there exists no \( U_k(\alpha_j) \) for the add systems to keep a similar relation to (2.2). Hence, it is impossible to force the residual vectors \( r_k(\alpha_j) \) to be colinear to \( r_k \).

For the seed system \( Ax = b \), since the orthogonal condition is \( r_k \perp \text{span}\{AW_k\} \), i.e., \( r_k \perp \text{span}\{V_k\} \), then using (2.2), we get

\[
0 = V_k^H (b - Ax_k)
= V_k^H (r_0 - AW_k y_k)
= V_k^H r_0 - U_k y_k,
\]

and

\[
 r_k = b - Ax_k
= r_0 - V_k U_k y_k
= r_0 - V_k V_k^H r_0
= r_{k-1} - v_k \xi_k,
\]

where \( \xi_k = v_k^H r_0 = v_k^H r_{k-1} \). Thus (2.3) can be rewritten as

\[
 [\xi_1, \ldots, \xi_k]^H = U_k y_k. \tag{2.5}
\]

Similar to the strategy in [28], for the add systems, we require the residual vector \( r_k(\alpha_j) = b - (A + \alpha_j I)x_k(\alpha_j) \) being orthogonal to \( \text{span}\{AW_k\} \), together with (2.2), we have

\[
0 = V_k^H [b - (A + \alpha_j I)x_k(\alpha_j)]
= V_k^H (r_0(\alpha_j) - (AW_k + \alpha_j W_k)y_k(\alpha_j))
= V_k^H r_0(\alpha_j) - (U_k + \alpha_j V_k^H W_k)y_k(\alpha_j).
\]

Thus, after solving (2.5) and (2.6) to obtain \( y_k \) and \( y_k(\alpha_j) \), the approximate solution of (1.1) is immediately accessed, and then

\[
r_k(\alpha_j) = r_0(\alpha_j) - (AW_k + \alpha_j W_k)y_k(\alpha_j) = r_0(\alpha_j) - (V_k U_k + \alpha_j W_k)y_k(\alpha_j). \tag{2.7}
\]
With the same seed system selection strategy in [28, 37], we summarize our flexible and adaptive Simpler GMRES for solving shifted linear systems (FAd-SGMRES-Sh) in Algorithm 2. If the \( \alpha_1 \) in seed system is not zero, we can reset

\[
A \doteq A - \alpha_1 I,
\]
\[
\alpha_j \doteq \alpha_j - \alpha_1,
\]

thus we take \( \alpha_1 = 0 \) as default.

**Algorithm 2. A flexible and adaptive Simpler GMRES for shifted linear systems (FAd-SGMRES-Sh)**

1. **Start:** Given the initial guess \( x_0(\alpha_j) \), a tolerance \( \text{tol} \), a threshold parameter \( \nu \in [0, 1] \), let \( m \) the maximal dimension of the solving subspace, \( r_0(\alpha_j) = b - Ax_0(\alpha_j) \);
2. Select seed system: At the first iteration (after the second iteration), for all systems (for non-converged systems), find \( ss \in \{1, \cdots, s\} \), where \( s \) is adjusted by the number of non-converged systems, such that

\[
\|r_0(\alpha_{ss})\|_2 = \max_{1 \leq j \leq s} \|r_0(\alpha_j)\|_2.
\]

Re-order \( r_0(\alpha_1), \cdots, r_0(\alpha_s) \), so that the residual of the seed system is placed in the first place. Thus, after re-ordering, \( ss = 1 \);
3. **Iterate:** For \( k = 1, \cdots, m \), do

\begin{enumerate}
\item \( z_k = \begin{cases} 
   r_0/\|r_0\|_2, & \text{if } k = 1, \\
   r_{k-1}/\|r_{k-1}\|_2, & \text{if } k > 1, \text{ and } \|r_{k-1}\|_2 \leq \nu \|r_{k-2}\|_2, \\
   v_{k-1}, & \text{otherwise}.
\end{cases} \)
\item \( w_k = M_k^{-1} z_k \),
\item \( v_k = Aw_k \),
\item For \( i = 1, \cdots, k - 1 \)
   \[
u_{ik} = w_i^H v_k, \quad v_k = v_k - u_{ik} v_i.
   \]
\item \( u_{kk} = \|v_k\|_2, \quad v_k = v_k / u_{kk} \).
\item \( \xi_k = v_i^H r_{k-1}, \quad r_k = r_{k-1} - v_k \xi_k, \text{ if } \|r_k\|_2 \leq \text{tol} \), then go to **Step 4**.
\end{enumerate}

4. Let \( k \) be the final iteration number of **Step 3**.

For seed system, solve (2.5);

For add systems, \( j = 2, \cdots, s \), solve (2.6), and update \( r_k(\alpha_j) \) using (2.7);

5. Set \( x_k(\alpha_j) = x_0(\alpha_j) + W_k y_k(\alpha_j), \quad j = 1, \cdots, s \). For the non-converged systems, reset \( r_0(\alpha_j) = r_k(\alpha_j) \), \( x_0(\alpha_j) = x_k(\alpha_j), \quad j = 1, \cdots, s \), go to **step 2**.

Some remarks of the implementation details for FAd-SGMRES-Sh are as follows.

**Remark 1.** In **Step 3**, \( M_k \) is the flexible preconditioner in the \( k \)-th step. To get the effect of preconditioning, \( M_k \) is usually selected to be the matrix near \( A \). In our algorithm, we choose to solve \( Aw_k = z_k \) inexact for the process \( w_k = M_k^{-1} z_k \). There are many choices of inexact solvers, such as ILU [38], IHSS [39], IGMRES [38], ISOR [38], IQR [40], and so on. In numerical examples section, we select IGMRES with 10 iterations as the preconditioner.
Remark 2. In Step 4, for add systems, the matrix $U_k + \alpha_j V_k^H W_k$ is generally not upper triangular. Because we usually choose a small value $m \ll n$, such as 20, thus for the solving step $V_k^H r_0(\alpha_j) = (U_k + \alpha_j V_k^H W_k) y_k(\alpha_j)$, the MATLAB code “\" can be directly used to get $y_k(\alpha_j)$. In addition, from (2.7), we can see the update of the residual vectors will also cost some time. Consequently, for solving add systems, similar to SGMRES [28], FAd-SGMRES-Sh may not faster than GMRES [17]. But fortunately, for seed system, due to without solving an upper Hessenberg least-square problem, and with inexact preconditioning, FAd-SGMRES-Sh is much faster than SGMRES, GMRES and FGMRES [13], especially for large-scale problems. Numerical experiments will illustrate the effect later.

### 2.2 Thick-restarting

Actually, some inexact preconditioned systems may still encounter the issues with small eigenvalues, thus it is necessary to consider to restart Algorithm 2 with the deflated restarting strategy [41,42,45]. Our aim is to improve the convergence of FAd-SGMRES-Sh by using the spectral information of the preconditioned seed system at restart. There are two keys involved. The first is how to compute the spectral information at each restart. The second is how to apply these information with a low computation cost at restart.

In fact, we use the harmonic Ritz value information of the seed system $Ax = b$ at each restart. That is required, after one cycle, the harmonic Ritz pair $(\lambda_i, g_i \equiv W_m g_i)$ of $A$ in $\text{span}\{W_m\}$ and orthogonal to $\text{span}\{A W_m\}$ satisfying [43]:

$$AW_m g_i - \lambda_i W_m g_i \perp \text{span}\{A W_m\} \Leftrightarrow (V_m U_m)^H (AW_m g_i - \lambda_i W_m g_i) = 0.$$  

From (2.2), and $U_m$ non-singular, the above equation is equivalent to

$$U_m g_i = \lambda_i V_m^H W_m g_i.$$  

Consequently, the harmonic Ritz pairs can be calculated at each iteration of FAd-SGMRES-Sh. Let $(\lambda_i, g_i), i = 1, \ldots, e (e \leq m)$ are the eigenpairs of the reduced generalized eigenvalues problem (2.8). Let $G_e = [g_1, \ldots, g_e]$, suppose that $P_e L_e = G_e$ is the QR decomposition of $G_e$, where matrix $P_e = [p_1, \ldots, p_e] \in \mathbb{C}^{k \times e}$ is orthogonal. Postmultiplying (2.2) by $P_e$ yields

$$AW_m P_e = V_m U_m P_e.$$  

Let $U_m P_e = \hat{P} e U_e^{new}$ be the QR decomposition, then from (2.9) we have

$$AW_m P_e = V_m \hat{P} e U_e^{new}.$$  

Define $W_e^{new} = W_m P_e$ and $V_e^{new} = V_m \hat{P} e$, then we obtain

$$AW_e^{new} = V_e^{new} U_e^{new},$$  

where $V_e^{new} \in \mathbb{C}^{n \times e}$ is orthogonal, $U_e^{new} \in \mathbb{C}^{e \times e}$ is upper triangular. Let $W_e = W_e^{new}$, $V_e = V_e^{new}$ and $U_e = U_e^{new}$. To establish the equation (2.2) for the current cycle, the flexible and adaptive Simpler GMRES with deflated restarting executes the remaining $(m - e)$ steps with $w_i = M_i^{-1} z_i (e + 1 \leq i \leq m)$ where $M_i$ is the flexible preconditioner and

$$z_i = \begin{cases} r_e / \| r_e \|_2, & \text{if } i = e + 1, \\ r_{i-1} / \| r_{i-1} \|_2, & \text{if } i > e + 1 \text{ and } \| r_{i-1} \|_2 \leq \nu \| r_{i-2} \|_2, \\ v_{i-1}, & \text{otherwise.} \end{cases}$$
After each cycle of the new algorithm, we restart the algorithm by setting $x_0^{new}(\alpha_j) = x_m(\alpha_j)$ and $r_0^{new}(\alpha_j) = r_m(\alpha_j)$. We use the symbols such as $x_m^{new}(\alpha_j)$, $r_m^{new}(\alpha_j)$, $W_m^{new}$, $V_m^{new}$ and $U_m^{new}$ for current cycle to distinguish the ones from the last cycle.

For the seed system, after one cycle of FAd-SGMRES-Sh, from (2.4), we have

$$r_0^{new} = r_m = r_0 - V_m^H r_0,$$

and

$$r_e^{new} = r_0^{new} - V_e^{new}(V_e^{new})^H r_0^{new}.$$ 

Note that

$$(V_e^{new})^H r_0^{new} = \hat{\beta}^H V_m^H (r_0 - V_m V_m^H r_0) = 0.$$ 

Thus

$$r_e^{new} = r_0^{new}, \quad \xi_i^{new} = (v_i^{new})^H r_0^{new} = 0, \quad i = 1, \ldots, e,$$

then from (2.3) and (2.4), we need to solve

$$U_m^{new} y_m^{new} = [0, \ldots, 0, \xi_{e+1}^{new}, \ldots, \xi_m^{new}]^T,$$ 

where $\xi_i^{new} = (u_i^{new})^H r_0^{new} = (u_i^{new})^H r_{i-1}^{new}, i = e + 1, \ldots, m$, and update

$$r_i^{new} = r_{i-1}^{new} - v_i^{new} \xi_i^{new}.$$ 

For add systems, from (2.6) we can get

$$(V_m^{new})^H r_0^{new}(\alpha_j)^{new} = \hat{\beta}^H V_m^H r_m(\alpha_j) = 0,$$

thus,

$$(V_m^{new})^H r_0(\alpha_j)^{new} = [0, \ldots, 0, \xi_{e+1}(\alpha_j)^{new}, \ldots, \xi_m(\alpha_j)^{new}]^T,$$

where $\xi_i(\alpha_j)^{new} = (u_i^{new})^H r_0(\alpha_j)^{new}, i = e + 1, \ldots, m$. Consequently, from (2.6), we need to solve

$$[0, \ldots, 0, \xi_{e+1}(\alpha_j)^{new}, \ldots, \xi_m(\alpha_j)^{new}]^T = (U_k^{new} + \alpha_j(\alpha_j)^{new}) V_k^{new} y_k(\alpha_j)^{new},$$

and we still exploit (2.7) to update the residual vector. Now it is ready to present the main algorithm of this paper.

**Algorithm 3.** A flexible and adaptive Simpler GMRES with deflated restarting for shifted linear systems (FAd-SGMRES-DR-Sh)

1. **Start:** Given the initial guess $x_0(\alpha_j)$, an integer $e$, a tolerance tol, a threshold parameter $\nu \in [0, 1]$, let $m$ the maximal dimension of the solving subspace, $r_0(\alpha_j) = b - x_0(\alpha_j)$;
2. **Select seed system:** At the first iteration (after the second iteration), for all systems (for non-converged systems), find $ss \in \{1, \ldots, s\}$, where $s$ is adjusted by the number of non-converged systems, such that

$$\|r_0(\alpha_{ss})\|_2 = \max_{1 \leq s \leq s} \|r_0(\alpha_j)\|_2.$$ 

Re-order $r_0(\alpha_1), \ldots, r_0(\alpha_s)$, so that the residual of the seed system is placed in the first place. Thus, after re-ordering, $ss = 1$;
3. **Apply one cycle of FAd-SGMRES-Sh to the seed system $Ax = b$, generate $W_m, V_m, U_m, x_m,$ and $r_m$;**
4. Compute the eigenvalues and eigenvectors of the generalized eigenvalue problem (2.8) by using the QZ algorithm. Let $g_1, \cdots, g_e$ be the eigenvectors corresponding to the $e$ smallest eigenvalues of (2.8). Set $G_e = [g_1, \cdots, g_e]$, and compute the QR decompositions of $G_e$ and $U_m P_e$: $G_e = P_e L_e$, $U_m P_e = \tilde{P}_e U_e^{\text{new}}$. Let $W_e^{\text{new}} = W_m P_e$ and $V_e^{\text{new}} = V_m \tilde{P}_e$.

5. Let $W_e = W_e^{\text{new}}$, $V_e = V_e^{\text{new}}$, $U_e = U_e^{\text{new}}$, and $x_0 = x_m$, $r_0 = r_m$, $r_e = r_0$;

6. Iterate: for $k = e + 1, \cdots, m$, do

\begin{align*}
(1) \quad & z_k = \begin{cases} 
  r_e / \|r_e\|_2, & \text{if } k = e + 1, \\
  r_{k-1} / \|r_{k-1}\|_2, & \text{if } k > e + 1, \text{ and } \|r_{k-1}\|_2 \leq \nu \|r_{k-2}\|_2, \\
  v_{k-1}, & \text{otherwise}.
\end{cases} \\
(2) \quad & w_k = M_k^{-1} z_k, \\
(3) \quad & v_k = A w_k, \\
(4) \quad & u_{ik} = v_i^T v_k, \quad v_k = v_k - u_{ik} v_k. \\
\end{align*}

7. Let $k$ be the final iteration number of Step 6.

For seed system, solve (2.10); For add systems, solve (2.6), and update $r_k(\alpha_j)$ using (2.7).

8. Set $x_k(\alpha_j) = x_0(\alpha_j) + W_k y_k(\alpha_j)$, $j = 1, \cdots, s$. For the non-converged systems, reset $r_0(\alpha_j) = r_k(\alpha_j)$, $x_0(\alpha_j) = x_k(\alpha_j)$, $j = 1, \cdots, s$, go to step 2.

In the end of this section, it is meaningful to evaluate the computational costs in a generic cycle of GMRES-Sh, Ad-SGMRES-Sh, FAd-SGMRES-Sh and FAd-SGMRES-DR-Sh, where the detail pseudo-codes of GMRES-Sh and Ad-SGMRES-Sh are be found in [28]. The comparisons are presented in Table 1 and Table 2. Here, we denote “mv” the number of matrix-vector products. “op$M_k$” denotes the number of the preconditioning process $M_k^{-1} z_k$ in one cycle, “vector updates” denotes the number of vectors that need to be updated in one cycle. We also write down the number of generalized eigenvalue problems by “G-p” in one cycle.

Table 1: Main computational costs per cycle for GMRES-Sh, Ad-SGMRES-Sh and FAd-SGMRES-Sh

|                  | GMRES-Sh | Ad-SGMRES-Sh | FAd-SGMRES-Sh |
|------------------|----------|--------------|---------------|
| mv               | $m$      | $m$          | $m$           |
| dot products     | $m (\sum_{k=1}^m (k-1) + 1)$ | $m (\sum_{k=1}^m (k-1) + 1 + s)$ | $m (\sum_{k=1}^m (k-1) + 1 + s)$ |
| saxpy            | $m (\sum_{k=1}^m (k-1) + 1) + m + s$ | $m (\sum_{k=1}^m (k-1) + 1 + 2s)$ | $m (\sum_{k=1}^m (k-1) + 1 + 2s)$ |
| op$M_k$          | $0$      | $0$          | $m$           |
| vector updates   | $m + s + 1$ | $2m + 2s$    | $2m + 2s$     |
| G-p              | $0$      | $0$          | $0$           |
Table 2: Main computational costs per cycle for the 1st cycle and the other cycle of FAd-SGMRES-DR-Sh

|                      | FAd-SGMRES-DR-Sh (1st cycle) | FAd-SGMRES-DR-Sh (other cycle) |
|----------------------|------------------------------|--------------------------------|
| mv                   | \( m \sum_{k=1}^{m} (k - 1) + 1 + s \) | \( (m - e)(\sum_{k=1}^{m} (k - 1) + 1 + s) \) |
| dot products         | \( m \sum_{k=1}^{m} (k - 1) + 1 + s \) | \( m \sum_{k=1}^{m} (k - 1) + 1 + 2s \) |
| saxpy                | \( m \sum_{k=1}^{m} (k - 1) + 1 + 2s \) | \( m \sum_{k=1}^{m} (k - 1) + 1 + 2s \) |
| operator \( \mathcal{M}_k \) | \( m \) | \( m - e \) |
| vector updates       | \( 2m + 2s \) | \( 2m + 2s \) |
| G-p                  | 1 | 1 |

3 Numerical results

In this section, numerical comparisons are made for GMRES-Sh [17], Ad-SGMRES-Sh [28], FGMRES-Sh [13], GMRD-SGMRSh [42], FAd-SGMRES-Sh and FAd-SGMRES-Dr-Sh according to the number of outer matrix-vector products (referred to as `mv`), and the elapsed CPU time in seconds (referred to as `cpu`). We set the stopping criterion as

\[
\frac{\|b - (A + \alpha_j I)x_k(\alpha_j)\|_2}{\|b\|_2} < 1 \times 10^{-6}, \quad j = 1, 2, \ldots, s.
\]

The bold values in the following tables indicate the fastest in the terms of `cpu`. The numerical results are obtained by using MATLAB R2014a (64bit) on a PC-Intel Core i5-6200U, CPU 2.4 GHz, 8 GB RAM with machine epsilon \( 10^{-16} \) in double precision floating point arithmetic.

Example 3.1 We consider the same matrices used in [28]. These matrices are from the University of Florida Sparse Matrix Collection and the Example 1 in [44]. Table 3 lists the matrices with their information. Here bidiag1 and bidiag2 are bidiagonal matrices with super-diagonal entries being all one. The diagonal elements of bidiag1 are \( 0, 1, 2, 3, \ldots, 999 \), and the ones of bidiag2 are \( 1, 2, 3, \ldots, 1000 \). All the initial vectors are zero in all examples. The right-hand side \( b \) is generated by the MATLAB code `randn(n,1)`, where \( n \) is the dimension of \( A \). The shift parameters are \( \alpha = 0, 0.4, 2 \). For FAd-SGMRES-Sh and FAd-SGMRES-Dr-Sh, the flexible preconditioner is chosen as running 10 steps of the un-restarted GMRES algorithm [8]. The same strategy is used in Example 3.2. For FGMRES-Sh, we use LU decomposition to exactly solve \( (A + \sigma_i I)w = v \) in the preconditioning process. Similar as in [13], we select the same \( \sigma_1 = 0.5 \) in the first \( m/2 \) steps, in the last \( m/2 \) steps for the same \( \sigma_2 = 1 \). Thus, the LU decomposition of \( A + \sigma_i I \) need to save for using in the first and last \( m/2 \) steps of each cycle. The same strategy is also used in Example 3.3.

In Table 4, we reported the `mv(cpu)` of each algorithm for listed matrices with size smaller than 1000, and the dimension of the approximate subspace in each cycle is set as \( m = 10, \mu = 0.9 \). For FAd-SGMRES-Dr-Sh, \( e \) is the number of harmonic eigenvectors retained from the previous cycle. We compare two cases, i.e., \( e = 3, 6 \). In Table 5, for comparison, we set \( m = 20 \) and \( e = 5, 10, 15 \), with \( \mu = 0.9 \), and the matrices size are all larger than 1000. In all tables, “†” stands for the algorithm fails to converge even after using 10000 outer matrix-vector products.

As seen from Table 4 and Table 5, for smaller matrices except for cdde1, FGMRES-Sh is the best solver among these algorithms, which is inseparable from the exact solution of \( (A + \sigma_k)w = v \) during the
Table 3: The test matrices used in Example 4.1

| Matrix ID | Matrix name | Size  | Nonzeros | Problem domain          |
|-----------|-------------|-------|----------|-------------------------|
| 1         | add20       | 2,395 | 13,151   | Circuit simulation      |
| 2         | bidiag1     | 1,000 | 1,999    | Academic                |
| 3         | bidiag2     | 1,000 | 1,999    | Academic                |
| 4         | cdde1       | 961   | 4,681    | Computational fluid dynamics |
| 5         | epb1        | 14,734| 95,053   | Thermal                 |
| 6         | sherman4    | 1,104 | 3,786    | Computational fluid dynamics |
| 7         | wang1       | 2,903 | 19,093   | Semiconductor device    |
| 8         | wang4       | 26,068| 177,196  | Semiconductor device    |
| 9         | young1c     | 841   | 4,089    | Acoustics               |
| 10        | young2c     | 841   | 4,089    | Acoustics               |

preconditioning process. But for the larger matrices, especially for wang4 whose size is 26068, the exact solving process of FGMRES-Sh obviously became a time-consuming obstacle, while FAd-SGMRES-DR-Sh performs best. It also can see for FAd-SGMRES-DR-Sh with different values \( e \), in some examples, e.g., epb1 in Table 5, even the number \( mv \) is smaller, but the elapsed CPU time is larger, this is because when using the harmonic Ritz value information, there needs to compute a generalized eigenvalue problem \( (2.8) \) and sort these eigenvalues, thus if the eigenvectors number \( e \) is larger, the elapsed CPU time for the previous procedure may be larger too. Thus, it is important to choose appropriate \( m \) and \( e \). For some matrices, such as bidiag2, cdde1, add20 and sherman4, we can see the number \( mv \) of FAd-SGMRES-DR-Sh is not much less than FAd-SGMRES-Sh, even equal to each other, this is because after preconditioning, the small eigenvalues problems of these matrices are well controlled, thus the effect of deflated restarting is not obvious, whereas the other matrices are still need the deflated restarting. Consequently, for large and difficult problems, FAd-SGMRES-DR-Sh still performs better than the other mentioned algorithms.

Example 3.2 In this example, we apply our algorithms to solve quantum chromodynamics (QCD) problems with multiple shifts, which is one of the most time-consuming supercomputer applications. \( D_i, 1 \leq i \leq 14 \) are denoted the complex matrices downloaded from Matrix Market\(^1\). These \( D_i \) are discretizations by the Dirac operator used in numerical simulation of quark behavior at different physical temperatures [3,21]. For each \( D_i \), we take \( A_i = (\frac{1}{k_c} + 10^{-3})I - D_i \) as the base matrix, where \( k_c \) is the critical value such that for \( \frac{1}{k_c} < \frac{1}{k} < \infty \), the matrix \( \frac{1}{k}I - D \) is real-positive. Table 6 lists the matrices \( D_i \) with their information. Moreover, the right-hand side \( b = \text{ones}(	ext{length}(A),1) \), and the initial guess in each example is zero vector. We take \([0.0001, 0.0002, \ldots, 0.0004, 0.001, 0.002, \ldots, 0.004, 0.01, 0.02, \ldots, 0.04]\) as the set of shifted values \( \alpha_j \). It is shown from Fig. 1 that the eigenvalues of base matrix \( A_1 \) are in the right-half of the complex plane, but partially surround the origin [12].

For seed matrices \( A_1 - A_7 \), we set \( m = 10, \mu = 0.9 \), and \( e = 3,6 \). Table 7 gives the results of the considered algorithms. Form Table 7, it can see that GMRES-DR-Sh does not converge for each matrix, and FGMRES-Sh costs too much time, whereas FAd-SGMRES-DR-Sh performs best, this implies that after adding inexact preconditioning and then deflating the small eigenvalues can accelerate the convergence. In Table 8, we compares the other algorithms besides FGMRES-Sh and GMRES-DR-Sh, and we set \( m = 20, \mu = 0.9, e = 5,10,15 \) for seed matrices \( A_8 - A_{14} \). As seen from Table 7 and Table

\(^1\)Refer to the website: [http://math.nist.gov/MatrixMarket/](http://math.nist.gov/MatrixMarket/).
Table 4: Convergence behaviors of the GMRES-Sh, Ad-SGMRES-Sh, FGMRES-Sh, FAd-SGMRES-Sh, GMRES-DR-Sh and FAd-SGMRES-DR-Sh with $\text{tol} = 10^{-6}$, $m = 10$ and $\mu = 0.9$.

| Method | $mv$ (cpu), $m = 10$, $\mu = 0.9$ |
|------------------|-----------------|-----------------|-----------------|-----------------|
|                | bidiag1 | bidiag2 | cdde1 | young1c | young2c |
| GMRES-Sh        | 4678(0.36) | 513(0.06) | †     | †     | †     |
| Ad-SGMRES-Sh    | 4678(0.34) | 513(0.06) | 9569(1.00) | †     | †     |
| FGMRES-Sh       | 7(0.02)    | 7(0.01)    | 118(0.07) | 12(0.13) | 11(0.12) |
| FAd-SGMRES-Sh   | 54(0.04)   | 35(0.03)   | 21(0.06) | 627(0.73) | 615(0.72) |
| GMRES-DR-Sh     | 351(0.81)  | 258(0.05)  | 174(0.10) | †     | †     |
| GMRES-DR-Sh $e = 3$ | 373(0.10)  | 240(0.06)  | 169(0.06) | †     | †     |
| GMRES-DR-Sh $e = 6$ | 39(0.02)   | 32(0.02)   | 19(0.06)  | 231(0.34) | 230(0.34) |
| FAd-SGMRES-DR-Sh $e = 3$ | 41(0.03)   | 32(0.02)   | 19(0.04)  | 193(0.25) | 178(0.24) |
| FAd-SGMRES-DR-Sh $e = 6$ | 41(0.03)   | 32(0.02)   | 19(0.04)  | 193(0.25) | 178(0.24) |

8. FAd-SGMRES-DR-Sh performs better than the other algorithms for most examples with deflating the small eigenvalues (in modulas). It is also known that the appropriate choice of $m$ and $e$ is important for FAd-SGMRES-DR-Sh, which will be subject to further investigations in the future.

Example 3.3 As we know, preconditioning is the critical point that effects the convergence of iteration methods directly [38]. However, different preconditioners will make different effects. In this example, some numerical results of FAd-SGMRES-Sh with different preconditioners are reported. We select ILU and IGMRES [38], and then denote the two algorithms by FAd-SGMRES-Sh(ILU) and FAd-SGMRES-Sh(IGMRES), respectively. At the same time, we also execute the flexible preconditioned GMRES with LU decomposition (FGMRES-Sh(LU)) [13] for comparison. All the matrices used in the

Fig. 1: The eigenvalues distribution of $A_1$. 
Table 5: Convergence behaviors of the GMRES-Sh, Ad-SGMRES-Sh, FGMRES-Sh, FAd-SGMRES-Sh, GMRES-DR-Sh and FAd-SGMRES-DR-Sh with $tol = 1e-6$, $m = 20$ and $\mu = 0.9$

| Method               | add20 (cpu) | ebp1 (cpu) | sherman4 (cpu) | wang1 (cpu) | wang2 (cpu) |
|----------------------|-------------|------------|----------------|-------------|-------------|
| GMRES-Sh             | 1231(0.32)  | 1300(1.17) | 548(0.17)      | 1049(0.33)  | †           |
| Ad-SGMRES-Sh         | 1231(0.27)  | 1310(1.70) | 548(0.10)      | 894(0.24)   | †           |
| FGMRES-Sh            | 635(11.39)  | 1099(9.74) | 14(0.07)       | 295(1.38)   | 3161(268.17) |
| FAd-SGMRES-Sh        | 55(0.10)    | 72(0.59)   | 23(0.05)       | 51(0.12)    | 148(2.30)   |
| GMRES-DR-Sh $e = 5$  | 629(0.27)   | 601(1.89)  | 134(0.09)      | 473(0.25)   | 1162(7.05)  |
| GMRES-DR-Sh $e = 10$ | †           | 591(2.30)  | 130(0.04)      | 496(0.23)   | †           |
| GMRES-DR-Sh $e = 15$ | †           | †          | 136(0.06)      | †           | †           |
| FAd-SGMRES-DR-Sh $e = 5$ | 56(0.11) | 63(0.58)   | 23(0.06)       | 44(0.11)    | 80(1.25)    |
| FAd-SGMRES-DR-Sh $e = 10$ | 55(0.08) | 63(0.59)   | 23(0.02)       | 44(0.07)    | 76(1.26)    |
| FAd-SGMRES-DR-Sh $e = 15$ | 56(0.09) | 63(0.70)   | 23(0.01)       | 44(0.08)    | 79(1.50)    |

above two examples are considered in our experiments, and record the typical results in Table 9. Here $\text{iter}$ denotes the iteration number of Arnoldi process.

As seen from Table 9, FGMRES-Sh(LU) and FAd-SGMRES-Sh(ILU) are almost the same performance for each matrices. Especially for smaller size matrices, they are both performing better than FAd-SGMRES-Sh(IGMRES). However, for large-scale matrices, FAd-SGMRES-Sh(IGMRES) will be the best solver. This is because the inner loop of FGMRES-Sh(LU) becomes time-consuming to exactly solve a linear system with the coefficient matrix $A + \sigma_i I$ using the LU decomposition, and the saving of the LU decomposition is another big cost. For FAd-SGMRES-Sh(ILU), although there is no storage about the LU decomposition, but in each cycle, there needs to calculate the incomplete LU decomposition of $A$ and solving two sparse triangular linear systems, these are still both flaws. While for FAd-SGMRES-Sh(IGMRES), 10 steps of the inexact GMRES will not cost too much time. Consequently, for smaller size matrices, it is better to use FGMRES-Sh(LU) and FAd-SGMRES-Sh(ILU) to solve shifted systems, and it is best to use FAd-SGMRES-Sh(IGMRES) for solving some large-scale shifted systems.

4 Conclusions

In the present paper, we established two iterative algorithms based on the Simpler GMRES for solving shifted linear systems simultaneously, namely FAd-SGMRES-Sh and FAd-SGMRES-DR-Sh. Moreover, these variants can be regarded as two improvements of Ad-SGMRES-Sh, which is recently proposed by Jing, Yuan and Huang in [28]. The resultant algorithms converge in less matrix-vector products than the other related solvers (GMRES-Sh, Ad-SGMRES-Sh, FAd-GMRES-Sh, and GMRES-DR-Sh), especially
Table 6: The matrices $D_i$ used in Example 4.2

| Matrix ID | Denotation       | Matrix name | Size   | Nonzeros | $k_c$   |
|-----------|------------------|-------------|--------|----------|---------|
| 1         | $D_1$            | CONF5.0-00L4X4-1000 | 3,072  | 119,808  | 0.20611 |
| 2         | $D_2$            | CONF5.0-00L4X4-1400 | 3,072  | 119,808  | 0.20328 |
| 3         | $D_3$            | CONF5.0-00L4X4-1800 | 3,072  | 119,808  | 0.20265 |
| 4         | $D_4$            | CONF5.0-00L4X4-2200 | 3,072  | 119,808  | 0.20235 |
| 5         | $D_5$            | CONF5.0-00L4X4-2600 | 3,072  | 119,808  | 0.21070 |
| 6         | $D_6$            | CONF6.0-00L4X4-2000 | 3,072  | 119,808  | 0.17968 |
| 7         | $D_7$            | CONF6.0-00L4X4-3000 | 3,072  | 119,808  | 0.16453 |
| 8         | $D_8$            | CONF5.4-00L8X8-0500 | 49,152 | 1,916,928 | 0.17865 |
| 9         | $D_9$            | CONF5.4-00L8X8-1000 | 49,152 | 1,916,928 | 0.17843 |
| 10        | $D_{10}$         | CONF5.4-00L8X8-1500 | 49,152 | 1,916,928 | 0.17689 |
| 11        | $D_{11}$         | CONF5.4-00L8X8-2000 | 49,152 | 1,916,928 | 0.17835 |
| 12        | $D_{12}$         | CONF6.0-00L8X8-2000 | 49,152 | 1,916,928 | 0.15717 |
| 13        | $D_{13}$         | CONF6.0-00L8X8-3000 | 49,152 | 1,916,928 | 0.15649 |
| 14        | $D_{14}$         | CONF6.0-00L8X8-8000 | 49,152 | 1,916,928 | 0.15623 |

Table 7: Convergence behaviors of the Ad-SGMRES-Sh, FAd-SGMRES-Sh and FAd-SGMRES-DR-Sh with $n = 3072$, $\text{tol} = 1e-6$, $m = 10$ and $\mu = 0.9$

| Method           | A1    | A2    | A3    | A4    | A5    | A6    | A7    |
|------------------|-------|-------|-------|-------|-------|-------|-------|
| GMRES-Sh         | 812(0.56) | 315(0.36) | 634(0.57) | 384(0.40) | 564(0.53) | 2357(1.78) | 176(0.26) |
| Ad-SGMRES-Sh     | 812(0.86) | 315(0.36) | 634(0.70) | 384(0.44) | 564(0.62) | 2357(2.53) | 176(0.22) |
| FGMRES-Sh        | 6(21.67)  | 6(32.21)  | 6(32.19)  | 6(21.60)  | 4(21.30)  | 4(21.56)  |       |
| FAd-SGMRES-Sh    | 105(0.71) | 60(0.46)  | 64(0.50)  | 63(0.46)  | 84(0.62)  | 70(0.49)  | 23(0.21) |
| GMRES-DR-Sh $e = 3$ |       |       |       |       |       |       |       |
| GMRES-DR-Sh $e = 6$ |       |       |       |       |       |       |       |
| FAd-SGMRES-DR-Sh $e = 3$ | 80(0.57) | 54(0.42) | 56(0.42) | 57(0.42) | 71(0.51) | 52(0.39) | 23(0.21) |
| FAd-SGMRES-DR-Sh $e = 6$ | 74(0.50) | 51(0.35) | 53(0.35) | 56(0.37) | 70(0.49) | 48(0.31) | 23(0.16) |

for large problems. Furthermore, although the cost per iteration of FAd-SGMRES-Sh and FAd-SGMRES-DR-Sh is higher, in our numerical experiences, the overall execution time is still lower. In addition, the FAd-SGMRES-DR-Sh performs better than FAd-SGMRES-Sh when the coefficient matrix of the seed system has many eigenvalues close to the origin as verified by numerical experiments. In conclusion, the proposed algorithms can be recommended as two efficient tools for solving shifted linear systems.

As an outlook for the future, the advanced development of preconditioning strategies (such as the polynomial preconditioning [6,26], the nested iterative technique [46] and other preconditioning strategies [22,47]) for solving shifted linear systems remains an meaningful topic of further research.
Table 8: Convergence behaviors of the Ad-SGMRES-Sh, FAd-SGMRES-Sh and FAd-SGMRES-DR-Sh with $n = 49152$, $tol = 1e-6$, $m = 20$ and $\mu = 0.9$.

| Matrix | Ad-SGMRES-Sh | FAd-SGMRES-Sh | FAd-SGMRES-DR-Sh |
|--------|--------------|---------------|------------------|
| $A_8$  | 872(18.71)   | 105(12.11)    | 95(11.27)        |
| $A_9$  | 584(12.90)   | 79(9.47)      | 77(9.10)         |
| $A_{10}$ | 471(10.34)   | 72(8.46)      | 71(8.50)         |
| $A_{11}$ | 431(9.61)    | 71(8.32)      | 72(8.66)         |
| $A_{12}$ | 659(15.11)   | 53(6.63)      | 50(6.06)         |
| $A_{13}$ | 1010(21.72)  | 54(6.27)      | 51(5.94)         |
| $A_{14}$ | 648(13.69)   | 54(6.13)      | 49(5.63)         |

Table 9: Convergence behaviors of the FGMRES-Sh(LU), FAd-SGMRES-Sh(ILU) and FAd-SGMRES-Sh(IGMRES) with $tol = 1e-6$, $m = 20$, $\mu = 0.9$, $\alpha = [0, 0.4, 2]$, and $\sigma_1 = 0.5$, $\sigma_2 = 1$.

| Matrix | FGMRES-Sh(LU) | FAd-SGMRES-Sh(ILU) | FAd-SGMRES-Sh(IGMRES) |
|--------|---------------|---------------------|------------------------|
| bidiag1 | 8(0.33)       | 3(0.06)             | 42(0.09)               |
| sherman4 | 14(0.07)     | 17(0.16)            | 24(0.10)               |
| wang4   | 1181(199.68)  | 1241(2433.90)       | 117(1.88)              |
| young1c | 11(0.15)      | 13(0.16)            | 299(0.41)              |
| young2c | 10(0.03)      | 13(0.11)            | 265(0.31)              |

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