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An Efficient Variant of the Restarted Shifted GMRES Method for Solving Shifted Linear Systems

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Abstract We investigate the restart of the Restarted Shifted GMRES method for solving shifted linear systems. Recently the variant of the GMRES(m) method with the *unfixed update* has been proposed to improve the convergence of the GMRES(m) method for solving linear systems, and shown to have an efficient convergence property. In this paper, by applying the unfixed update to the Restarted Shifted GMRES method, we propose a variant of the Restarted Shifted GMRES method. We show a potentiality for efficient convergence within the variant by some numerical results.

Keywords shifted linear systems; the Restarted Shifted GMRES method; restart techniques.

MR(2010) Subject Classification 65F10

1. Introduction

We consider solving large and sparse shifted linear systems of the form:

$$(A+\sigma_i I)\boldsymbol{x}(\sigma_i)=\boldsymbol{b}, \quad i=1,2,\ldots,t, \tag{1}$$

where $A\in\mathbb{R}^{n\times n}$, $\boldsymbol{x}(\sigma_i),\boldsymbol{b}\in\mathbb{R}^n$ and $\sigma_i\in\mathbb{R}$. The coefficient matrices $A(\sigma_i):=A+\sigma_i I$ are assumed to be nonsymmetric and nonsingular for all σ_i. Such shifted linear systems (1) arise from higher-order implicit methods for solving time-dependent partial differential equations, control theory, lattice gauge computations in quantum chromodynamics and so on.

One of the simplest ideas for solving the shifted linear systems (1) is to apply some Krylov subspace method with a powerful preconditioner to each linear system one by one. If the powerful preconditioner is constructed, then the shifted linear systems (1) can be efficiently solved. In this regard, however, the efficient preconditioners depend heavily on σ_i, therefore how to construct the powerful preconditioner is critical in this approach for the preconditioning techniques specialized in the shifted linear systems [1].

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As another approach, the shifted Krylov subspace methods have been recently proposed and actively studied to solve the shifted linear systems (1) at once. The shifted Krylov subspace methods are based on the shift-invariance property of the Krylov subspaces: if the initial vectors are collinear, then the Krylov subspaces corresponding to the matrix $A(\sigma_i)$ are equal for any σ_i; the details will be shown in Section 2. The shift-invariance property makes it possible to reuse the basis of the Krylov subspace whose construction can be one of the most time-consuming parts of the Krylov subspace methods. Thus the shifted Krylov subspace methods have attracted much attention for large and sparse shifted linear systems, typically in the case that the number of shift t is large.

The general ideas of the shifted Krylov subspace methods were firstly introduced by Freund in [2] as an extension of the CG method [3]. Since then, several authors have well studied on the efficient algorithms for large shifted linear systems (1) such as the shifted QMR method [4], the shifted Bi-CGSTAB(l) method [5] and the shifted GMRES method [6].

The shifted GMRES method, which is a natural extension of the GMRES method [7], finds the minimum residual solutions for each system based on the Arnoldi procedure and the minimum residual condition. As well as the GMRES method, the long-term recurrence based on the Arnoldi procedure causes difficulties in terms of computational cost and storage requirements, therefore it is naturally expected to apply so-called the *restart* to the shifted GMRES method. Unfortunately, it is known that the residual vectors obtained from the shifted GMRES method are not collinear in general, so that the shifted GMRES method cannot be efficiently restarted.

To overcome this difficulty, the Restarted Shifted GMRES method was proposed in 1998 by Frommer and Glässner [8] which imposes the collinearity condition on the residuals. The collinearity condition makes it possible to apply the restart for the shifted linear systems.

We investigate the restart of the Restarted Shifted GMRES method. Recently the variant of the GMRES(m) method with the unfixed update has been proposed to improve the convergence of the GMRES(m) method for solving linear systems, and shown to have an efficient convergence property [9]. In this paper, by applying the unfixed update to the Restarted Shifted GMRES method, we propose a variant of the Restarted Shifted GMRES method with the unfixed update. Then, we show a potentiality for efficient convergence within the variant by some numerical results.

This paper is organized as follows. In Section 2, we briefly describe the basic definitions of the shifted Krylov subspace methods and introduce the algorithm of the Restarted Shifted GMRES method. In Section 3, we briefly introduce the unfixed update for the GMRES(m) method, then we propose a variant of the Restarted Shifted GMRES method with the unfixed update. In Section 4, we test the performance of the variant of the Restarted Shifted GMRES method from some numerical experiments. For the end of this paper, we make some conclusions in Section 5.

Throughout this paper, I denotes the identity matrix, $\mathbf{0}$ denotes the zero vector and $(\boldsymbol{x}, \boldsymbol{y})$ for vectors $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^n$ denotes the inner product: $(\boldsymbol{x}, \boldsymbol{y}) = \sum_{i=1}^{n} x_i y_i = \boldsymbol{y}^{\mathrm{T}} \boldsymbol{x}$.

2. The Restarted Shifted GMRES method

In Section 2.1, we describe the basic definitions of the shifted Krylov subspace methods for solving shifted linear systems (1). In Sections 2.2 and 2.3, we introduce the algorithms of the shifted GMRES method and the Restarted Shifted GMRES method, respectively, especially focused on the restart part.

2.1. Basic definitions of shifted Krylov subspace methods

Let $A \in \mathbb{R}^{n\times n}$ and the vectors $\boldsymbol{v}, \boldsymbol{w} \in \mathbb{R}^n$ be collinear: $\boldsymbol{v} = c\boldsymbol{w}$, $c \in \mathbb{R}$. Then the Krylov subspaces

$$\mathscr{K}_k(A, \boldsymbol{v}) := \mathrm{span}\{\boldsymbol{v}, A\boldsymbol{v}, A^2\boldsymbol{v}, \ldots, A^{k-1}\boldsymbol{v}\}$$

satisfy

$$\mathscr{K}_k(A + \sigma_i I, \boldsymbol{v}) = \mathscr{K}_k(A + \sigma_j I, \boldsymbol{w}) \tag{2}$$

for any $\sigma_i, \sigma_j \in \mathbb{R}$. This is called the shift-invariance property of the Krylov subspaces.

Based on the shift-invariance property (2), the shifted Krylov subspace methods construct the Krylov basis vectors for just one of the systems (1) termed the seed system. Then the constructed basis can be used also for solving the rest systems called the add systems (additional systems).

Let σ_{seed} be the shift parameter for the seed system. We also let the initial guesses $\boldsymbol{x}_0(\sigma_i)$ be set such that the initial residuals $\boldsymbol{r}_0(\sigma_i) := \boldsymbol{b} - A(\sigma_i)\boldsymbol{x}_0(\sigma_i)$ are collinear[1]:

$$\boldsymbol{r}_0(\sigma_i) = \gamma_0(\sigma_i)\boldsymbol{r}_0(\sigma_{\mathrm{seed}}), \quad \gamma_0(\sigma_i) \in \mathbb{R}.$$

Then, from the shift-invariance property (2), the approximate solutions $\boldsymbol{x}_k(\sigma_i)$ for all i are extracted from affine spaces spanned by the initial guesses $\boldsymbol{x}_0(\sigma_i)$ and the same Krylov subspace as follows:

$$\boldsymbol{x}_k(\sigma_i) = \boldsymbol{x}_0(\sigma_i) + V_k\boldsymbol{s}_k(\sigma_i), \quad \boldsymbol{r}_k(\sigma_i) = \boldsymbol{r}_0(\sigma_i) - A(\sigma_i)V_k\boldsymbol{s}_k(\sigma_i),$$

where V_k is an $n \times k$ matrix whose columns are the basis vectors of the Krylov subspace $\mathscr{K}_k(A(\sigma_{\mathrm{seed}}), \boldsymbol{r}_0(\sigma_{\mathrm{seed}}))$, and $\boldsymbol{s}_k(\sigma_i) \in \mathbb{R}^k$.

Because of this reusability of the basis V_k, the shifted Krylov subspace methods can solve the shifted linear systems (1) at once without matrix-vector multiplications for the add systems. As extensions of the standard Krylov subspace methods, several shifted Krylov subspace methods have been proposed and well studied [4–6, 8]. For the details, we refer to [10] and references therein.

In what follows, we assume that the shift parameter for the seed system is zero, $\sigma_{\mathrm{seed}} = 0$. Note that this assumption does not lose the generality, because if $\sigma_{\mathrm{seed}} \neq 0$, then we can rewrite (1) by $A := A - \sigma_{\mathrm{seed}}I$ and $\sigma_i := \sigma_i - \sigma_{\mathrm{seed}}$.

2.2. The shifted GMRES method

As a natural extension of the GMRES method to the shifted linear systems (1), the vectors $\boldsymbol{s}_k(\sigma_i)$ of the shifted GMRES method can be determined by the minimal residual condition as follows:

$$\boldsymbol{s}_k(\sigma_i) = \arg\min_{\boldsymbol{s}\in\mathbb{R}^k} \|\gamma_0(\sigma_i)\beta\boldsymbol{e}_1 - \widetilde{H}_k(\sigma_i)\boldsymbol{s}\|_2, \quad i = 1, 2, \ldots, t,$$

[1] This is easily achievable by e.g. $\boldsymbol{x}_0(\sigma_i) = \boldsymbol{0}$ for all i. In this case $\boldsymbol{r}_0(\sigma_i) = \boldsymbol{b}$ and $\gamma_0(\sigma_i) = 1$ for all i.

where $\widetilde{H}_k(\sigma_i) \in \mathbb{R}^{(k+1)\times k}$ is the upper Hessenberg matrix obtained from the matrix formula of the Arnoldi procedure, i.e.,

$$A(\sigma_i)V_k = V_{k+1}\widetilde{H}_k(\sigma_i), \quad \widetilde{H}_k(\sigma_i) := \widetilde{H}_k(\sigma_{\mathrm{seed}}) + \sigma_i \begin{bmatrix} I \\ \mathbf{0}^{\mathrm{T}} \end{bmatrix} \in \mathbb{R}^{(k+1)\times k}, \tag{3}$$

and $\beta = \|\boldsymbol{r}_0(\sigma_{\mathrm{seed}})\|_2$, $\boldsymbol{e}_1 = [1, 0, \ldots, 0]^{\mathrm{T}} \in \mathbb{R}^{k+1}$.

The shifted GMRES method can find the minimum residual solutions based on the minimum residual condition for all linear systems in (1) with no matrix-vector multiplications for the add systems. However, as noted in Section 1, the shifted GMRES method has difficulties due to the long-term recurrence based on the Arnoldi procedure as well as the GMRES method. Therefore the restart is required to apply to the shifted GMRES method.

Unfortunately, it is known that the residual vectors $\boldsymbol{r}_k(\sigma_i)$ obtained from the minimum residual condition are not collinear in general. Thus after restart, the shift-invariance property (2) cannot be used for solving shifted linear systems[2].

2.3. The Restarted Shifted GMRES method

As described in Section 2.2, the shifted GMRES method has the difficulty for the restart. To remedy this difficulty, Frommer and Glässner proposed in 1998 the Restarted Shifted GMRES method [8].

The basic idea of the Restarted Shifted GMRES method is to impose the collinearity condition:

$$\boldsymbol{r}_m(\sigma_i) = \gamma_m(\sigma_i)\boldsymbol{r}_m, \quad \gamma_m(\sigma_i) \in \mathbb{R}, \tag{4}$$

instead of the minimum residual condition for the add systems, where $\boldsymbol{r}_m := \boldsymbol{r}_m(\sigma_{\mathrm{seed}})$ is the residual vector of the seed system and m is the restart frequency. We note that, for the seed system, the Restarted Shifted GMRES method imposes the minimum residual condition on the residual vector like the shifted GMRES method.

For the seed system, the vector $\boldsymbol{s}_m := \boldsymbol{s}_m(\sigma_{\mathrm{seed}})$ is computed by solving the minimization problem:

$$\boldsymbol{s}_m = \arg\min_{\boldsymbol{s}\in\mathbb{R}^m} \|\beta\boldsymbol{e}_1 - \widetilde{H}_m\boldsymbol{s}\|_2,$$

where $\widetilde{H}_m := \widetilde{H}_m(\sigma_{\mathrm{seed}})$. The residual vector $\boldsymbol{r}_m$ can be written as

$$\boldsymbol{r}_m = V_{m+1}\boldsymbol{u}_{m+1}, \quad \boldsymbol{u}_{m+1} := \beta\boldsymbol{e}_1 - \widetilde{H}_m\boldsymbol{s}_m \in \mathbb{R}^{m+1}.$$

Thus, from the collinearity condition (4) for the add systems, we have

[2] Since the residual vectors obtained from the Ritz-Galerkin condition are collinear, the Ritz-Galerkin based methods can be naturally restarted. From this observation, Simoncini proposed in 2003 the Restarted Shifted FOM method [11] as a natural extension of the FOM(m) method. Since then, improvement techniques of the Restarted Shifted FOM method have been well studied; see [12, 13].

Algorithm 1 One restart cycle of the Restarted Shifted GMRES method [8]

Compute $\boldsymbol{r}_0 = \boldsymbol{b} - A\boldsymbol{x}_0$ and set $\beta = \|\boldsymbol{r}_0\|_2, \boldsymbol{v}_1 = \boldsymbol{r}_0/\beta$
for $j = 1, 2, \ldots, m$, **do**
  Compute $\boldsymbol{w}_j = A\boldsymbol{v}_j$
  for $i = 1, 2, \ldots, j$, **do**
    $h_{i,j} = (\boldsymbol{w}_j, \boldsymbol{v}_i)$
    $\boldsymbol{w}_j = \boldsymbol{w}_j - h_{i,j}\boldsymbol{v}_i$
  end for
  $h_{j+1,j} = \|\boldsymbol{w}_j\|_2$
  $\boldsymbol{v}_{j+1} = \boldsymbol{w}_j/h_{j+1,j}$
end for
Define the $(m+1) \times m$ Hessenberg matrix $\widetilde{H}_m = \{h_{i,j}\}_{1\le i\le m+1, 1\le j\le m}$
Compute $\boldsymbol{s}_m = \arg\min_{\boldsymbol{s}\in\mathbb{R}^m} \|\beta\boldsymbol{e}_1 - \widetilde{H}_m\boldsymbol{s}\|_2$ and set $\boldsymbol{u}_{m+1} = \beta\boldsymbol{e}_1 - \widetilde{H}_m\boldsymbol{s}_m$
for $i = 1, 2, \ldots, t$, **do**
  Solve $\left[\widetilde{H}_m(\sigma_i) \,\middle|\, \boldsymbol{u}_{m+1}\right] \begin{bmatrix} \boldsymbol{s}_m(\sigma_i) \\ \gamma_m(\sigma_i) \end{bmatrix} = \gamma_0(\sigma_i)\beta\boldsymbol{e}_1$
  $\boldsymbol{x}_m(\sigma_i) = \boldsymbol{x}_0(\sigma_i) + V_m\boldsymbol{s}_m(\sigma_i)$
end for

$$
\begin{aligned}
& & \boldsymbol{r}_m(\sigma_i) &= \gamma_m(\sigma_i)\boldsymbol{r}_m \\
&\Leftrightarrow & \boldsymbol{b} - A(\sigma_i)\{\boldsymbol{x}_0(\sigma_i) + V_m\boldsymbol{s}_m(\sigma_i)\} &= \gamma_m(\sigma_i)V_{m+1}\boldsymbol{u}_{m+1} \\
&\Leftrightarrow & \boldsymbol{r}_0(\sigma_i) - A(\sigma_i)V_m\boldsymbol{s}_m(\sigma_i) &= V_{m+1}\boldsymbol{u}_{m+1}\gamma_m(\sigma_i) \\
&\Leftrightarrow & \gamma_0(\sigma_i)\boldsymbol{r}_0 - V_{m+1}\widetilde{H}(\sigma_i)\boldsymbol{s}_m(\sigma_i) &= V_{m+1}\boldsymbol{u}_{m+1}\gamma_m(\sigma_i) \\
&\Leftrightarrow & V_{m+1}\{\widetilde{H}(\sigma_i)\boldsymbol{s}_m(\sigma_i) + \boldsymbol{u}_{m+1}\gamma_m(\sigma_i)\} &= \gamma_0(\sigma_i)\boldsymbol{r}_0 \\
&\Leftrightarrow & \widetilde{H}(\sigma_i)\boldsymbol{s}_m(\sigma_i) + \boldsymbol{u}_{m+1}\gamma_m(\sigma_i) &= \gamma_0(\sigma_i)\beta\boldsymbol{e}_1,
\end{aligned}
$$

using the matrix formula of the Arnoldi procedure (3); see [8].

From the above relation, $\boldsymbol{s}_m(\sigma_i)$ and $\gamma_m(\sigma_i)$ can be written as the solution of the $(m+1) \times (m+1)$ linear systems, i.e.,

$$
\left[\widetilde{H}_m(\sigma_i) \,\middle|\, \boldsymbol{u}_{m+1}\right] \begin{bmatrix} \boldsymbol{s}_m(\sigma_i) \\ \gamma_m(\sigma_i) \end{bmatrix} = \gamma_0(\sigma_i)\beta\boldsymbol{e}_1, \tag{5}
$$

for $i = 1, 2, \ldots, t$. The linear systems (5) are solved efficiently by using the Givens-rotation, because the coefficient matrices are upper Hessenberg matrices.

Note that each system (5) has a unique solution if and only if $P_m(-\sigma_i) \neq 0$, where $P_m(\lambda)$ is the residual polynomial of m iterations of the GMRES method for the seed system [8, Lemma 2.4].

The algorithm of one restart cycle (m iterations) of the Restarted Shifted GMRES method with the initial guesses $\boldsymbol{x}_0(\sigma_i)$ such that $\boldsymbol{r}_0(\sigma_i) = \gamma_0(\sigma_i)\boldsymbol{r}_0$ is given in Algorithm 1. Then the restarted version of Algorithm 1, the Restarted Shifted GMRES method, can be shown in Algorithm 2 by the simplified description.

If the coefficient matrix A is positive definite: $(A\boldsymbol{x}, \boldsymbol{x}) > 0, \forall\boldsymbol{x} \neq \boldsymbol{0}$, and $\sigma_i > 0$ for all i, then

Algorithm 2 The Restarted Shifted GMRES method [8]

1: Choose the restart frequency m and the initial guesses $\boldsymbol{x}_0^{(1)}(\sigma_i)$ such that $\boldsymbol{r}_0^{(1)}(\sigma_i) = \gamma_0^{(1)}(\sigma_i)\boldsymbol{r}_0^{(1)}$, e.g., $\boldsymbol{x}_0^{(1)}(\sigma_i) = \mathbf{0}$ for all i
2: **for** $l = 1, 2, \ldots,$ until convergence **do**
3: Run m iterations of Algorithm 1 with the initial guesses $\boldsymbol{x}_0^{(l)}(\sigma_i)$ and $\gamma_0^{(l)}(\sigma_i)$, and get the approximate solutions $\boldsymbol{x}_m^{(l)}(\sigma_i)$ and $\gamma_m^{(l)}(\sigma_i)$
4: Update $\underline{\boldsymbol{x}_0^{(l+1)}(\sigma_i) := \boldsymbol{x}_m^{(l)}(\sigma_i)}$ and $\gamma_0^{(l+1)}(\sigma_i) := \gamma_m^{(l)}(\sigma_i)$ for all i
5: **end for**

Algorithm 3 The GMRES(m) method [7]

1: Choose the restart frequency m and the initial guess $\boldsymbol{x}_0^{(1)}$
2: **for** $l = 1, 2, \ldots,$ until convergence **do**
3: Solve (approximately) $A\boldsymbol{x} = \boldsymbol{b}$ by m iterations of the GMRES method with the initial guess $\boldsymbol{x}_0^{(l)}$, and get the approximate solution $\boldsymbol{x}_m^{(l)}$
4: Update the initial guess $\underline{\boldsymbol{x}_0^{(l+1)} := \boldsymbol{x}_m^{(l)}}$
5: **end for**

the Restarted Shifted GMRES method (Algorithm 2) converges for the seed and the add systems for every restart frequency m, because in this case Eq. (5) has a unique solution [8, Theorem 3.3]. Moreover if the smallest σ_i is chosen as the seed, and the initial guesses $\boldsymbol{x}_0(\sigma_i)$ of the 1st restart cycle are set at $\boldsymbol{x}_0(\sigma_i) = \mathbf{0}$, then the add systems converge more rapidly than the seed system [8, Theorem 3.3]. Therefore in this case, we do not need to use the shift switching technique[3].

3. A variant of the Restarted Shifted GMRES method

In this section, we briefly introduce the unfixed update for the GMRES(m) method proposed in [9], then we propose a variant of the Restarted Shifted GMRES method with the unfixed update [4].

3.1. The variant of the GMRES(m) method with the unfixed update for solving linear systems

In this section, we focus on the GMRES(m) method for solving linear systems, especially we investigate the restart itself. Then we briefly introduce the unfixed update for the GMRES(m) method proposed in [9].

The restart of the GMRES(m) method is composed of the following three major parts:

Part 1 Choose the restart frequency m and the initial guess $\boldsymbol{x}_0^{(1)}$ of the 1st restart cycle.

Part 2 Solve (approximately) $A\boldsymbol{x} = \boldsymbol{b}$ by m iterations of the GMRES method with the initial guess $\boldsymbol{x}_0^{(l)}$, and get the approximate solution $\boldsymbol{x}_m^{(l)}$.

Part 3 Update the initial guess of the next restart cycle, i.e., $\boldsymbol{x}_0^{(l+1)} := \boldsymbol{x}_m^{(l)}$.

Based on these three major parts, the algorithm of the GMRES(m) method can be simplified as shown in Algorithm 3.

[3] In general, the seed system may converge faster than the add systems. In this case, for efficient computation, we need to change the seed into one of the rest systems, this technique is called the seed switching technique [14].
[4] It is expected that a variant of the Restarted Shifted FOM method can also be proposed as an improvement of Restarted Shifted FOM [11] in essentially the same way.

Algorithm 4 The variant of the GMRES(m) method with the unfixed update [9]

1: Choose the restart frequency m and the initial guess $\boldsymbol{x}_0^{(1)}$
2: **for** $l = 1, 2, \dots,$ until convergence **do**
3: Solve (approximately) $A\boldsymbol{x} = \boldsymbol{b}$ by m iterations of the GMRES method with the initial guess $\boldsymbol{x}_0^{(l)}$, and get the approximate solution $\boldsymbol{x}_m^{(l)}$
4: Set the vector $\boldsymbol{y}^{(l+1)} \in \mathbb{R}^n$ based on a certain strategy
5: Update the initial guess $\underline{\boldsymbol{x}_0^{(l+1)} := \boldsymbol{x}_m^{(l)} + \boldsymbol{y}^{(l+1)}}$
6: **end for**

The restart remedies the difficulties of the GMRES method due to the long-term recurrence of the Arnoldi procedure; however, the restart generally slows the convergence of the GMRES method. Therefore, several improvement techniques have been recently proposed for Part 1 and Part 2; see [9,10] and references therein.

On the other hand, Part 3 has been regarded only as the connection in terms of convergence. Thus, in the algorithm of the GMRES(m) method, also with some improvement techniques, the initial guess of each restart cycle is updated such that

$$\boldsymbol{x}_0^{(l+1)} := \boldsymbol{x}_m^{(l)}, \tag{6}$$

which is the same as original paper [7].

Instead of this fixed update (6), the unfixed update

$$\boldsymbol{x}_0^{(l+1)} := \boldsymbol{x}_m^{(l)} + \boldsymbol{y}^{(l+1)} \tag{7}$$

has been introduced in [9], where $\boldsymbol{y}^{(l+1)} \in \mathbb{R}^n$ is determined by a certain strategy. Then the algorithm of the efficient variant of GMRES(m) method with the unfixed update (7) have been introduced as shown in Algorithm 4. Note that the variant of GMRES(m) method with the unfixed update can be regarded as a natural extension of the GMRES(m) method in terms of the error equations and the iterative refinement scheme [9].

Here, in general, an arbitrary vector $\boldsymbol{y}^{(l+1)}$ cannot guarantee good convergence. Thus, we require a suitable strategy to define $\boldsymbol{y}^{(l+1)}$ for efficient convergence compared with the traditional GMRES(m) method. In [9], one example of such strategy has been provided, i.e.,

$$\boldsymbol{y}^{(l+1)} = \begin{cases} \boldsymbol{0}, & l = 1, \\ \mu^{(l)} \Delta \boldsymbol{x}^{(l)}, & l \geq 2, \end{cases} \tag{8}$$

where $\Delta \boldsymbol{x}^{(l)} := \boldsymbol{x}_m^{(l)} - \boldsymbol{x}_0^{(l-1)}$ and $\mu^{(l)} = \arg\min_{\mu \in \mathbb{R}} \|\boldsymbol{r}_m^{(l)} - \mu A \Delta \boldsymbol{x}^{(l)}\|_2$. From some numerical experiments, the variant of the GMRES(m) method with this strategy (8) has been shown to have more efficient convergence property than the GMRES(m) method [9].

The computational cost for computing the vector $\boldsymbol{y}^{(l+1)}$ based on (8) is one matrix-vector multiplication and some AXPY[5] and inner products. We also note that this strategy (8) guarantees the monotonic decrease in the residual 2-norm as well as the GMRES(m) method, i.e.,

$$\|\boldsymbol{r}_m^{(l+1)}\|_2 \leq \|\boldsymbol{r}_0^{(l+1)}\|_2 = \|\boldsymbol{r}_m^{(l)} - A\boldsymbol{y}^{(l+1)}\|_2 \leq \|\boldsymbol{r}_m^{(l)}\|_2.$$

3.2. A variant of Restarted Shifted GMRES with the unfixed update for solving shifted linear systems

[5] Addition of scaled vectors.

In this section, we propose a variant of the Restarted Shifted GMRES method with the unfixed update described in Section 3.1.

As shown in Algorithm 2, the initial guesses $\boldsymbol{x}_0^{(l+1)}(\sigma_i)$ of each restart cycle are updated by the fixed update, i.e.,

$$\boldsymbol{x}_0^{(l+1)}(\sigma_i) := \boldsymbol{x}_m^{(l)}(\sigma_i), \quad i = 1, 2, \dots, t,$$

like the GMRES(m) method; see Eq. (6). We note that this is not only for the traditional algorithm in [8], but also for its improvement techniques [15, 16]. Here we can also consider the unfixed update:

$$\boldsymbol{x}_0^{(l+1)}(\sigma_i) := \boldsymbol{x}_m^{(l)}(\sigma_i) + \boldsymbol{y}^{(l+1)}(\sigma_i), \quad i = 1, 2, \dots, t, \tag{9}$$

instead of the fixed update under the same idea as introduced in [9].

Notice that, for the Restarted Shifted GMRES method to solve shifted linear systems (1), the vectors $\boldsymbol{y}^{(l+1)}(\sigma_i)$ of the unfixed update (9) are required to set such that the initial residual vectors $\boldsymbol{r}_0^{(l+1)}(\sigma_i) = \boldsymbol{r}_m^{(l)}(\sigma_i) - A(\sigma_i)\boldsymbol{y}^{(l+1)}(\sigma_i)$ of the $(l+1)$th restart cycle satisfy the collinearity condition:

$$\boldsymbol{r}_0^{(l+1)}(\sigma_i) = \gamma_0^{(l+1)}(\sigma_i)\boldsymbol{r}_0^{(l+1)}, \quad \gamma_0^{(l+1)} \in \mathbb{R}. \tag{10}$$

The algorithm of a variant of the Restarted Shifted GMRES method with the unfixed update (9) is shown in Algorithm 5.

Algorithm 5 A variant of the Restarted Shifted GMRES method with the unfixed update

1: Choose the restart frequency m and the initial guesses $\boldsymbol{x}_0^{(1)}(\sigma_i)$ such that $\boldsymbol{r}_0^{(1)}(\sigma_i) = \gamma_0^{(1)}(\sigma_i)\boldsymbol{r}_0^{(1)}$, e.g., $\boldsymbol{x}_0^{(1)}(\sigma_i) = \boldsymbol{0}$ for all i
2: **for** $l = 1, 2, \dots,$ until convergence **do**
3: Run m iterations of Algorithm 1 with the initial guesses $\boldsymbol{x}_0^{(l)}(\sigma_i)$ and $\gamma_0^{(l)}(\sigma_i)$, and get the approximate solutions $\boldsymbol{x}_m^{(l)}(\sigma_i)$ and $\gamma_m^{(l)}(\sigma_i)$
4: Set the vectors $\boldsymbol{y}^{(l+1)}(\sigma_i) \in \mathbb{R}^n$ such that the residual vectors $\boldsymbol{r}_0^{(l+1)}(\sigma_i) = \boldsymbol{r}_m^{(l)}(\sigma_i) - A(\sigma_i)\boldsymbol{y}^{(l+1)}(\sigma_i)$ are collinear: $\boldsymbol{r}_0^{(l+1)}(\sigma_i) = \gamma_0^{(l+1)}\boldsymbol{r}_0^{(l+1)}$
5: Update $\underline{\boldsymbol{x}_0^{(l+1)}(\sigma_i) := \boldsymbol{x}_m^{(l)}(\sigma_i) + \boldsymbol{y}^{(l+1)}(\sigma_i)}$ for all i
6: **end for**

3.3. An example of how to define $\boldsymbol{y}^{(l+1)}(\sigma_i)$ for efficient convergence

As well as the variant of the GMRES(m) method, an arbitrary vector $\boldsymbol{y}^{(l+1)}(\sigma_i)$ cannot guarantee good convergence, then we require a suitable strategy to define $\boldsymbol{y}^{(l+1)}(\sigma_i)$ for efficient convergence compared with the traditional Restarted Shifted GMRES method. In this section, we provide an example of how to define $\boldsymbol{y}^{(l+1)}(\sigma_i)$ for efficient convergence based on the strategy (8) introduced in [9].

Now we let $\Delta\boldsymbol{x}^{(l)}(\sigma_i)$ and $\Delta\boldsymbol{r}^{(l)}(\sigma_i)$ be

$$\Delta\boldsymbol{x}^{(l)}(\sigma_i) := \boldsymbol{x}_m^{(l)}(\sigma_i) - \boldsymbol{x}_0^{(l-1)}(\sigma_i), \quad \Delta\boldsymbol{r}^{(l)}(\sigma_i) := \boldsymbol{r}_m^{(l)}(\sigma_i) - \boldsymbol{r}_0^{(l-1)}(\sigma_i),$$

respectively, then we consider setting the vectors $\boldsymbol{y}^{(l+1)}(\sigma_i)$ as follows:

$$\boldsymbol{y}^{(l+1)}(\sigma_i) = \mu^{(l)}(\sigma_i)\Delta\boldsymbol{x}^{(l)}(\sigma_i), \quad \mu^{(l)}(\sigma_i) \in \mathbb{R}. \tag{11}$$

From the relation $\Delta \boldsymbol{r}^{(l)}(\sigma_i) = -A(\sigma_i)\Delta \boldsymbol{x}^{(l)}(\sigma_i)$, the initial approximate solutions and corresponding residuals for the $(l+1)$th restart cycle can be shown by

$$\begin{cases} \boldsymbol{x}_0^{(l+1)}(\sigma_i) = \boldsymbol{x}_m^{(l)}(\sigma_i) + \mu^{(l)}(\sigma_i)\Delta \boldsymbol{x}^{(l)}(\sigma_i), \\ \boldsymbol{r}_0^{(l+1)}(\sigma_i) = \boldsymbol{r}_m^{(l)}(\sigma_i) + \mu^{(l)}(\sigma_i)\Delta \boldsymbol{r}^{(l)}(\sigma_i). \end{cases} \tag{12}$$

Here from the strategy (11) and the collinearity condition (10), we now have the following proposition.

Proposition 1 *Let the vectors $\boldsymbol{r}, \widehat{\boldsymbol{r}} \in \mathbb{R}^n$ and $\boldsymbol{r}^{\mathrm{old}}, \widehat{\boldsymbol{r}}^{\mathrm{old}} \in \mathbb{R}^n$ be the collinear respectively: $\widehat{\boldsymbol{r}} = \gamma \boldsymbol{r}, \widehat{\boldsymbol{r}}^{\mathrm{old}} = \gamma^{\mathrm{old}} \boldsymbol{r}^{\mathrm{old}}$, where $\gamma, \gamma^{\mathrm{old}} \in \mathbb{R}$, and we assume that $\boldsymbol{r}$ is not parallel to $\boldsymbol{r}^{\mathrm{old}}$. We also let the vectors $\boldsymbol{r}^{\mathrm{new}}, \widehat{\boldsymbol{r}}^{\mathrm{new}}$ be defined by*

$$\boldsymbol{r}^{\mathrm{new}} = \boldsymbol{r} + \mu(\boldsymbol{r} - \boldsymbol{r}^{\mathrm{old}}), \quad \widehat{\boldsymbol{r}}^{\mathrm{new}} = \widehat{\boldsymbol{r}} + \widehat{\mu}(\widehat{\boldsymbol{r}} - \widehat{\boldsymbol{r}}^{\mathrm{old}}),$$

where $\mu, \widehat{\mu} \in \mathbb{R}$.

Then, $\boldsymbol{r}^{\mathrm{new}}$ and $\widehat{\boldsymbol{r}}^{\mathrm{new}}$ satisfy the collinearity condition:

$$\widehat{\boldsymbol{r}}^{\mathrm{new}} = \gamma^{\mathrm{new}} \boldsymbol{r}^{\mathrm{new}}, \quad \gamma^{\mathrm{new}} \in \mathbb{R}, \tag{13}$$

if and only if the parameters $\widehat{\mu}, \gamma^{\mathrm{new}}$ are obtained by the solution of the linear system:

$$\begin{bmatrix} 1+\mu & -\gamma \\ \mu & -\gamma^{\mathrm{old}} \end{bmatrix} \begin{bmatrix} \gamma^{\mathrm{new}} \\ \widehat{\mu} \end{bmatrix} = \begin{bmatrix} \gamma \\ 0 \end{bmatrix}.$$

Proof From the required collinearity condition (13), we have

$$\begin{aligned} & \widehat{\boldsymbol{r}}^{\mathrm{new}} = \gamma^{\mathrm{new}} \boldsymbol{r}^{\mathrm{new}} \\ \Leftrightarrow \quad & \gamma(1+\widehat{\mu})\boldsymbol{r} - \gamma^{\mathrm{old}}\widehat{\mu}\boldsymbol{r}^{\mathrm{old}} = \gamma^{\mathrm{new}}\{(1+\mu)\boldsymbol{r} - \mu \boldsymbol{r}^{\mathrm{old}}\} \\ \Leftrightarrow \quad & \begin{cases} \gamma(1+\widehat{\mu}) & = \gamma^{\mathrm{new}}(1+\mu) \\ \gamma^{\mathrm{old}}\widehat{\mu} & = \gamma^{\mathrm{new}}\mu \end{cases} \\ \Leftrightarrow \quad & \begin{bmatrix} 1+\mu & -\gamma \\ \mu & -\gamma^{\mathrm{old}} \end{bmatrix} \begin{bmatrix} \gamma^{\mathrm{new}} \\ \widehat{\mu} \end{bmatrix} = \begin{bmatrix} \gamma \\ 0 \end{bmatrix}. \end{aligned}$$

Therefore the proposition is proved.

Proposition 1 means that the residual vectors $\boldsymbol{r}_0^{(l+1)}(\sigma_i)$ obtained from Eq. (12) based on the solutions of the linear systems

$$\begin{bmatrix} 1+\mu^{(l)} & -\gamma_m^{(l)}(\sigma_i) \\ \mu^{(l)} & -\gamma_0^{(l-1)}(\sigma_i) \end{bmatrix} \begin{bmatrix} \gamma_0^{(l+1)}(\sigma_i) \\ \mu^{(l)}(\sigma_i) \end{bmatrix} = \begin{bmatrix} \gamma_m^{(l)}(\sigma_i) \\ 0 \end{bmatrix} \tag{14}$$

satisfy the collinearity condition (10), where $\mu^{(l)} := \mu^{(l)}(\sigma_{\mathrm{seed}})$.

If $\mu^{(l)}$ are set at 0 for all restart cycle l, then the algorithm is mathematically equivalent to the Restarted Shifted GMRES method, because in this case $\mu^{(l)}(\sigma_i)$ obtained by Eq. (14) are also 0. In this paper, we set $\mu^{(l)}$ as follows:

$$\mu^{(l)} := \mu^{(l)}(\sigma_{\mathrm{seed}}) = \arg\min_{\mu \in \mathbb{R}} \|\boldsymbol{r}_m^{(l)}(\sigma_{\mathrm{seed}}) - \mu A(\sigma_{\mathrm{seed}})\Delta \boldsymbol{x}^{(l)}(\sigma_{\mathrm{seed}})\|_2$$

as well as [9].

Notice that the linear systems (14) have no solutions if the coefficient matrix of (14) is singular and the right-hand side of (14) does not belong to the range space of the coefficient matrix of (14). This corresponds to the case that $\boldsymbol{r}_0^{(l+1)}$ is parallel to $\Delta\boldsymbol{r}^{(l)}(\sigma_i)$.

For the seed systems, the variant of the Restarted Shifted GMRES method is mathematically equivalent to the variant of the GMRES(m) method proposed in [9]. Therefore, if we focus only on the seed system, the residual 2-norm of the variant of the Restarted Shifted GMRES method monotonically decreases. However, we note that monotonical decrease of the residual 2-norm of the add systems is not guaranteed as well as the Restarted Shifted GMRES method.

4. Numerical experiments and results

In this section, we test the performance of the Restarted Shifted GMRES method and the variant of the Restarted Shifted GMRES method with (11) for solving shifted linear systems (1). The performance of these methods is evaluated by the test problems from The University of Florida Sparse Matrix Collection [17] with five shift parameters which are set at $\sigma_i = 0.0, 1.0 \times 10^{-4}, \ldots, 4.0 \times 10^{-4}$.

Matrix name	n	Nnz	$Ave.Nnz$	Application area
CAVITY05	1182	32747	27.70	Computational fluid dynamics
CAVITY16	4562	138187	30.29	Computational fluid dynamics
COUPLED	11341	98523	8.69	Circuit simulation
EPB1	14734	95053	6.45	Thermal problem
FEM_3D_THERMAL2	147900	3489300	23.59	Thermal problem
MEMPLUS	17758	126150	7.10	Electronic circuit design
NS3DA	20414	1679599	82.28	Computational fluid dynamics
POISSON3DB	85623	2374949	27.74	Computational fluid dynamics
RAEFSKY1	3242	294276	90.77	Computational fluid dynamics
RAEFSKY2	3242	294276	90.77	Computational fluid dynamics
RAJAT03	7602	32653	4.30	Circuit simulation
RDB5000	5000	29600	5.92	Computational fluid dynamics
XENON1	48600	1181120	24.30	Materials problem
XENON2	157464	3866688	24.56	Materials problem

Table 1 Characteristics of the coefficient matrices of the test problems for the Restarted Shifted GMRES method and the variant of the Restarted Shifted GMRES method.

The characteristics of the coefficient matrices of the test problems are shown in Table 1, where n, Nnz and $Ave.Nnz$ denote the number of dimension, the number of nonzero elements and the average nonzero elements per row or column respectively.

We set $\boldsymbol{b} = [1, 1, \ldots, 1]^{\mathrm{T}}$ as the right-hand side, $\boldsymbol{x}_0^{(1)}(\sigma_i) = [0, 0, \ldots, 0]^{\mathrm{T}}$ for the initial guess of each systems. We also set $m = 30, 50$ as the restart frequency and stopping criterion was set as $\|\boldsymbol{r}_k(\sigma_i)\|_2 / \|\boldsymbol{b}\|_2 \leq 10^{-10}$ for all σ_i. The seed system is firstly set at $\sigma_1 = 0.0$, then the seed is switched every restart cycle to the latest system in terms of the residual 2-norm.

All the numerical experiments were carried out in double precision arithmetic on OS: CentOS 64bit, CPU: 1 core of Intel Xeon X5550 2.67GHz, Memory: 48GB, Compiler: GNU Fortran ver. 4.1.2, Compile option: -O3.

[Numerical results]

Firstly, we present the numerical results in Tables 2 and 3. We analyze the results in terms of two aspects: convergence rate of each system and total computation time.

Matrix	Method	Number of restart (N_{Restart})					Time[sec.]
		σ_1	σ_2	σ_3	σ_4	σ_5	t_{Total}
CAVITY05	RS-GMRES	574	163	99	82	69	2.15×10^0
	Variant	271	109	80	66	58	1.03×10^0
CAVITY16	RS-GMRES	†	708	246	174	142	†
	Variant	1797	160	106	91	78	2.72×10^1
COUPLED	RS-GMRES	†	†	†	†	†	†
	Variant	2735	2720	2681	2642	2629	7.86×10^1
EPB1	RS-GMRES	94	38	27	21	18	2.81×10^0
	Variant	67	31	22	18	16	2.01×10^0
FEM_3D_THERMAL2	RS-GMRES	36	25	20	17	15	2.03×10^1
	Variant	20	16	14	13	12	1.13×10^1
MEMPLUS	RS-GMRES	221	39	27	22	18	8.41×10^0
	Variant	77	26	19	15	14	2.97×10^0
NS3DA	RS-GMRES	78	75	73	70	68	1.71×10^1
	Variant	78	75	73	70	68	1.69×10^1
POISSON3DB	RS-GMRES	24	22	19	18	16	1.15×10^1
	Variant	19	16	15	14	13	9.01×10^0
RAEFSKY1	RS-GMRES	142	125	112	98	85	3.00×10^0
	Variant	86	70	61	54	49	1.81×10^0
RAEFSKY2	RS-GMRES	235	213	195	179	166	4.97×10^0
	Variant	195	177	163	151	141	4.17×10^0
RAJAT03	RS-GMRES	†	†	†	†	†	†
	Variant	400	304	257	240	234	6.03×10^0
RDB5000	RS-GMRES	31	31	31	31	31	3.25×10^{-1}
	Variant	34	34	34	34	34	3.60×10^{-1}
XENON1	RS-GMRES	384	384	384	384	384	7.46×10^1
	Variant	63	63	63	63	63	1.22×10^1
XENON2	RS-GMRES	523	523	523	523	523	3.24×10^2
	Variant	80	80	80	80	80	5.06×10^1

Table 2 Convergence results (N_{Restart}: number of restart cycles for each system and t_{Total}: total computation time) of the Restarted Shifted GMRES method and the variant of the Restarted Shifted GMRES method for the restart frequency $m = 30$.

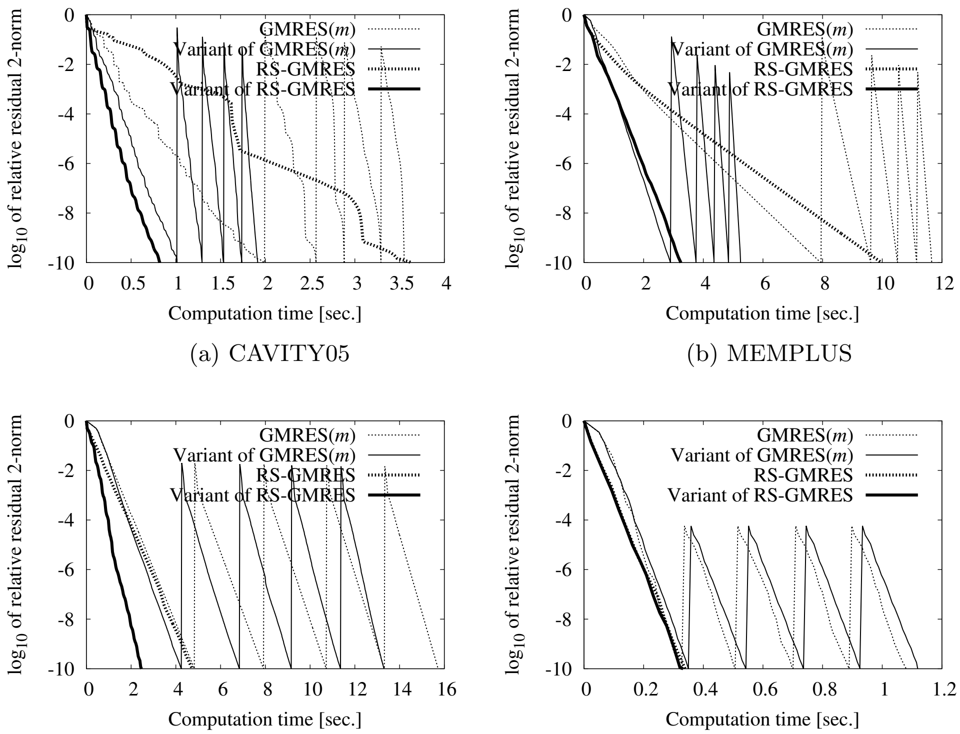
Matrix	Method	Number of restart (N_{Restart})					Time[sec.]
		σ_1	σ_2	σ_3	σ_4	σ_5	t_{Total}
CAVITY05	RS-GMRES	495	135	97	78	61	3.63×10^0
	Variant	111	45	36	33	28	8.19×10^{-1}
CAVITY16	RS-GMRES	†	100	69	54	44	†
	Variant	589	68	50	39	35	1.74×10^1
COUPLED	RS-GMRES	748	732	717	703	689	4.50×10^1
	Variant	543	538	532	528	525	3.22×10^1
EPB1	RS-GMRES	40	18	13	11	10	2.66×10^0
	Variant	36	17	13	11	10	2.39×10^0
FEM_3D_THERMAL2	RS-GMRES	16	12	10	9	8	1.78×10^1
	Variant	12	10	8	8	7	1.34×10^1
MEMPLUS	RS-GMRES	119	18	12	9	8	1.01×10^1
	Variant	38	13	10	8	7	3.25×10^0
NS3DA	RS-GMRES	47	45	44	42	41	1.77×10^1
	Variant	39	38	37	35	35	1.47×10^1
POISSON3DB	RS-GMRES	16	14	12	11	10	1.42×10^1
	Variant	11	10	9	9	8	9.80×10^0
RAEFSKY1	RS-GMRES	77	63	53	46	41	2.85×10^0
	Variant	47	39	34	31	28	1.74×10^0
RAEFSKY2	RS-GMRES	126	115	105	96	90	4.71×10^0
	Variant	66	61	57	54	51	2.46×10^0
RAJAT03	RS-GMRES	†	†	†	†	†	†
	Variant	165	113	96	81	78	5.41×10^0
RDB5000	RS-GMRES	15	15	15	15	15	3.43×10^{-1}
	Variant	14	14	14	14	15	3.42×10^{-1}
XENON1	RS-GMRES	141	141	141	141	141	5.33×10^1
	Variant	38	38	38	38	38	1.43×10^1
XENON2	RS-GMRES	190	190	190	190	190	2.35×10^2
	Variant	47	47	47	47	47	5.76×10^1

Table 3 Convergence results (N_{Restart}: number of restart cycles for each system and t_{Total}: total computation time) of the Restarted Shifted GMRES method and the variant of the Restarted Shifted GMRES method for the restart frequency $m = 50$.

We consider the number of restart cycles (N_{Restart}) of both methods. In most cases, the variant of the Restarted Shifted GMRES method shows lower N_{Restart} than the Restarted Shifted GMRES method especially for the latest system. We can also see from the high convergence rate of the systems for all σ_i that the strategy (11) well played even for the add systems. Especially, for CAVITY16 ($m = 30, 50$), COUPLED ($m = 30$) and RAJAT03 ($m = 30, 50$), the Restarted Shifted GMRES method did not converge within 100000 iteration; on the other hand, the variant of the Restarted Shifted GMRES method converged to the solution satisfying the required accuracy.

We also consider the total computation time (t_{Total}). From the smaller N_{Restart}, we can see that the variant of the Restarted Shifted GMRES method converged within much smaller computation time except the case for RDB5000 ($m = 30$).

Next, we present in Figure 1 the relative residual 2-norm histories of the Restarted Shifted GMRES method and the variant of the Restarted Shifted GMRES method with $m = 30$ versus computation time for CAVITY05, MEMPLUS, RAEFSKY2 and RDB5000. In this figure, we also compare the GMRES(m) method [7] and the variant of the GMRES(m) method [9] for the linear systems described in Section 3.1. These methods are applied to each linear system of (1) one by one. In this regard, however, the obtained approximate solution of the previous shift parameter is used for the initial guess of the next system: $\boldsymbol{x}_0(\sigma_{i+1}) := \boldsymbol{x}_k(\sigma_i)$.



(a) CAVITY05 (b) MEMPLUS

(c) RAEFSKY2 (d) RDB5000

Figure 1 The relative residual 2-norm history versus computation time of the GMRES(m) method, the variant of the GMRES(m) method, the Restarted Shifted GMRES method and the variant of the Restarted Shifted GMRES method for CAVITY05, MEMPLUS, RAEFSKY2 and RDB5000.

The residual 2-norm histories of the GMRES(m) method and the variant of the GMRES(m) method have five peaks, which means that these methods were applied to each system sequentially. Here, since the obtained approximate solution is used for the next initial guess, this reduces the initial residual after second system, e.g., to $\approx 10^{-4}$ for RDB5000.

From Figure 1, we can see that the Restarted Shifted GMRES method and the variant of the Restarted Shifted GMRES method show monotonic decrease in the residual 2-norm. Then both shifted Krylov subspace methods can solve the test problems more efficiently than the

GMRES(m) method and the variant of the GMRES(m) method. Moreover, we can see that the strategy (11) well played, and then the variant of the Restarted Shifted GMRES method converged in much smaller computation time than the Restarted Shifted GMRES method except for RDB5000.

5. Conclusion

In this paper, we have investigated the restart of the Restarted Shifted GMRES method of Frommer and Glässner for solving large and sparse shifted linear systems. In order to improve the Restarted Shifted GMRES method, we have proposed the variant of the Restarted Shifted GMRES method with the unfixed update.

From our numerical experiments, we have learned that the strategy (11) well played not only for the seed system but also for the add systems, and then the variant of the Restarted Shifted GMRES method has a high potential for efficient convergence over the Restarted Shifted GMRES method, as well as the variant of the GMRES(m) method for linear systems proposed in [9].

In this paper, by some numerical experiments, we have tested the performance of the variant of the Restarted Shifted GMRES method. However, it remains our future work to apply it to real applications and evaluate its performance. Moreover, for further improvement, we also need to analyze the convergence behavior of the variant of the Restarted Shifted GMRES method, and design more suitable strategy to define the vectors $\boldsymbol{y}^{(l+1)}(\sigma_i)$.

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References

[1] M. BENZI, D. BERTACCINI. *Approximate inverse preconditioning for shifted linear systems.* BIT Numer. Math., 2003, **43**(2): 231–244.

[2] R. W. FREUND. *On conjugate gradient type methods and polynomial preconditioners for a class of complex non-Hermitian matrices.* Numer. Math., 1990, **57**(3): 285–312.

[3] M. R. HESTENES, E. STIEFEL. *Methods of conjugate gradients for solving linear systems.* J. Research Nat. Bur. Standards, 1952, **49**: 409–436.

[4] R. W. FREUND. *Solution of Shifted Linear Systems by Quasi-Minimal Residual Iterations.* de Gruyter, Berlin, 1993.

[5] A. FROMMER. *BiCGSTAB(l) for families of shifted linear systems.* Computing, 2003, **70**(2): 87–109.

[6] B. N. DATTA, Y. SAAD. *Arnoldi methods for large Sylvester-like observer matrix equations, and an associated algorithm for partial spectrum assignment.* Linear Algebra Appl., 1991, **154/156**: 225–244.

[7] Y. SAAD, M. H. SCHULTZ. *GMRES: a generalized minimal residual algorithm for solving nonsymmetric linear systems.* SIAM J. Sci. Statist. Comput., 1986, **7**(3): 856–869.

[8] A. FROMMER, U. GlÄSSNER. *Restarted GMRES for shifted linear systems.* SIAM J. Sci. Comput., 1998, **19**(1): 15–26.

[9] A. IMAKURA, T. SOGABE, Shaoliang ZHANG. *An efficient variant of the GMRES(m) method based on the error equations.* East Asian Journal on Appl. Math., 2012, **2**: 19–32.

[10] V. SIMONCINI, D. B. SZYLD. *Recent computational developments in Krylov subspace methods for linear systems.* Numer. Linear Algebra Appl., 2007, **14**(1): 1–59.

[11] V. SIMONCINI. *Restarted full orthogonalization method for shifted linear systems.* BIT, 2003, **43**(2): 459–466.

[12] Yanfei JING, Tingzhu HUANG. *Restarted weighted full orthogonalization method for shifted linear systems.* Comput. Math. Appl., 2009, **57**(9): 1583–1591.

[13] Zhanwen LI, Guiding GU. *Restarted FOM augmented with Ritz vectors for shifted linear systems*. Numer. Math. J. Chin. Univ. (Engl. Ser.), 2006, **15**(1): 40–49.

[14] T. SOGABE, T. HOSHI, Shaoliang ZHANG, et al. *A Numerical Method for Calculating the Green's Function Arising from Electronic Structure Theory*. Springer-Verlag, Berlin, 2007.

[15] D. DARNELL, R. B. MORGAN, W. WILCOX. *Deflated GMRES for systems with multiple shifts and multiple right-hand sides*. Linear Algebra Appl., 2008, **429**(10): 2415–2434.

[16] Guiding GU, Jianjun ZHANG, Zhanwen LI. *Restarted GMRES augmented with eigenvectors for shifted linear systems*. Int. J. Comput. Math., 2003, **80**(8): 1039–1049.

[17] T. A. DAVIS, Yifan HU. *The University of Florida sparse matrix collection*. ACM Trans. Math. Software, 2011, **38**(1): 1–25.