# Global GMRES with Deflated Restarting for Families of Shifted Linear Systems 

Jing Meng, Peiyong Zhu, Houbiao Li

Abstract-Many problems in science and engineering field require the solution of shifted linear systems with multiple right hand sides and multiple shifts. To solve such systems efficiently, the implicitly restarted global GMRES algorithm is extended in this paper. However, the shift invariant property could no longer hold over the augmented global Krylov subspace due to adding the harmonic Ritz matrices. To remedy this situation, we enforce the collinearity condition on the shifted system and propose shift implicitly restarted global GMRES. The new method not only improves the convergence but also has a potential to simultaneously compute approximate solution for the shifted systems using only as many matrix vector multiplications as the solution of the seed system requires. In addition, some numerical experiments also confirm the effectiveness of our method.

Keywords-Shifted linear systems, global Krylov subspace, GLGMRESIR, GLGMRESIRsh, harmonic Ritz matrix, harmonic Ritz vector.

## I. Introduction

W$E$ consider the solution of a sequence of families of linear systems:

$$
\begin{equation*}
\left(A-\sigma_{i} I\right) x_{i}^{j}=b^{j} \tag{1}
\end{equation*}
$$

with $j=1, \ldots, p$ and $i=1, \ldots, s$. Here $A \in \mathbb{C}^{n \times n}$ is a nonsingular matrix and all the $b^{j} \in \mathbb{C}^{n}$ are available simultaneously. Then (1) can be written as

$$
\begin{equation*}
\left(A-\sigma_{i} I\right) X_{i}=B \tag{2}
\end{equation*}
$$

where $B=\left[b^{1}, b^{2}, \ldots, b^{p}\right]$ and $X_{i}=\left[x_{i}^{1}, x_{i}^{2}, \ldots, x_{i}^{p}\right]$ are $N \times$ $p$ rectangular matrices. We call the numbers $\left\{\sigma_{i}\right\}_{i=1}^{s} \in \mathbb{C}$ shifts.

Systems with multiple right hand sides and multiple shifts arise in many scientific and engineering applications. For example, control theory [4], time dependent differential equations [16] and lattice quantum chromodynamics (lattice QCD) [1].

For simplicity of discussion, we frequently will focus on one family of linear systems with only one shift and drop the index $i$, yielding two systems of the form

$$
\begin{gather*}
A X=B  \tag{3}\\
(A-\sigma I) X_{\sigma}=B \tag{4}
\end{gather*}
$$

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The first equation is referred as the seed systems while the second one is termed as the shifted systems. All of them are the systems with multiple right hand sides.

A number of recent articles have established the benefits of using the shift invariance when solving shift linear systems with a single right hand $(p=1)$. Methods that are based on the nonsymmetric Lanczos process have been straightforwardly derived (1), such as CG [17], QMR, TFQMR [6], BiCGstab [7] and a recently proposed method IDR [15]. Restarted Krylov methods are not as straightforward. After a restart, all residual vectors formed at the end of a cycle of the Krylov method need to be parallel to each other. For FOM method, thid happens automatically [14]. However, this collinearity does not occur for restarted GMRES [8]. To handle this situation, Frommer and Glässner enforced the residuals to be collinear and proposed shifted GMRES [8]. This is an efficient method for solving families of shifted linear systems $(p=1)$, but it inherits the properties of stagnation and unpredictable convergence exhibited by restarted GMRES, see, e.g. [13], [5]. Deflated version of restarted GMRES can improve this. One of these approaches is related to Morgan's GMRESDR [12], and in [3], this method has been extended to simultaneously solve a family of shift systems with a single right hand side.

Recently, Lin combine restarted global GMRES method with deflation technology and proposed the implicitly global GMRES (GLGMRESIR) approach [11] for solving the seed systems. It has been observed that significant improvements in convergence rates can be achieved from global Krylov subspace methods by adding these harmonic Ritz matrices. Therefore, we consider an extension of GLGMRESIR to solve shifted linear systems with multiple right hand sides and multiple shifts in this section. Thus, we will have an efficient method which not only improves the convergence but also has a potential to simultaneously compute approximate solution for the shifted systems as the expense of only $p$ matrix vector multiplications per iteration.

The structure of the paper is as follows. In the next section, we recall some properties of global Krylov subspace. In Section $I I I$, we describe the implicitly global GMRES method aimed at accelerating convergence. We introduce our new method to address shifted linear systems in Section $I V$. The effectiveness of the proposed method is also demonstrated in Section $V$. Finally, some conclusions are summarized in Section VI.

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## II. Preliminaries

## A. Notations

Throughout this paper, $\|\cdot\|_{F}$ denotes the Frobenius norm, ${ }^{T}$ is referred to as the transpose conjugate operation of matrix, the identity matrix of order $k$ is designated as $I_{k}$ or $I$ and $\mathbf{0}_{i \times j}$ is defined as the zero rectangular matrix with $i$ rows and $j$ columns. $\mathcal{R}(\cdot)$ and tol denote the range of the matrix and the convergence threshold, respectively. For two rectangular matrices $X$ and $Y$, we define $<X, Y>_{F}=\operatorname{tr}\left(X^{T} Y\right)$, where $\operatorname{tr}(\cdot)$ denotes the trace of the square matrix $X^{T} Y$. If $X$ is an $n \times p$ matrix, the $x=\operatorname{vec}(X)$ is the $n s$ vector obtained by stacking the $p$ columns of the matrix $X$. The notations of MATLAB style are also used, for example, $U(1: i, 1: j)$ denotes the submatrix of the first $i$ rows and the first $j$ columns of $U, U(:, j)$ refers to its jth column and $U(i, j)$ corresponds to the $U_{i, j}$ entry of the matrix $U$.

## B. Global Krylov Subspace

Let $X_{0} \in \mathbb{C}^{n \times p}$ be the initial guess and $R_{0}=B-A X_{0}$. Global Krylov subspace generated by A from $R_{0}$ is defined as follows

$$
\mathcal{K}_{m}\left(A, R_{0}\right):=\operatorname{span}\left\{R_{0}, A R_{0}, A^{2} R_{0}, \ldots, A^{m-1} R_{0}\right\}
$$

Note that the definition of 'global span' means a linear combination of the $N \times p$ matrices, i.e., $\left\{\sum_{i=0}^{m-1} \gamma_{i} A^{i} R_{0}\right\}$, for some scalars $\gamma_{i}^{\prime} s \in \mathbb{C}$. We observe that the global Krylov subspace generated by $A$ and $R_{0}$ is invariant under any shift, i.e.,

$$
\mathcal{K}_{m}\left(A, R_{0}\right)=\mathcal{K}_{m}\left((A-\sigma I), R_{0}\right)
$$

as long as the starting rectangular matrices are collinear.
Thus, any $Z \in \mathcal{K}_{m}\left(A, R_{0}\right)$ can be expressed as $Z=$ $\Phi_{m-1}(A) R_{0}$ with $\Phi_{m-1}$ a polynomial of degree $\leq m-1$ or, equivalently, $Z=\Phi_{m-1}^{\sigma}(A-\sigma I) R_{0}$, where

$$
\Phi_{m-1}^{\sigma}(t)=\Phi_{m-1}(t+\sigma)
$$

Similar to the Krylov subspace, some properties of the global Krylov space were introduced in [10].

## III. Implicitly global GMRES method

## A. Global Arnoldi Process

We firstly review global Arnoldi Process that constructs an Frobenius orthonormal (Forthonormal) basis of the global Krylov subspace $\mathcal{K}_{m}\left(A, R_{0}\right)$, as described in [10].

The global Arnoldi algorithm constructs an Forthonormal basis $V_{1}, V_{2}, \ldots V_{m}$ satisfying

$$
\begin{align*}
& \operatorname{tr}\left(V_{i}^{T} V_{j}\right)=0, \text { for } i \neq j, i, j=1,2, \ldots, m \\
& \operatorname{tr}\left(V_{i}^{T} V_{i}\right)=1, \text { for } i=1,2, \ldots, m \tag{5}
\end{align*}
$$

Then we have a global Arnoldi relation

$$
\begin{gather*}
A \mathcal{V}_{m}=\mathcal{V}_{m+1}\left(H_{m} \otimes I_{p}\right)+h_{m+1, m}\left[0_{n \times p}, \ldots, 0_{n \times p}, V_{m+1}\right] \\
A \mathcal{V}_{m}=\mathcal{V}_{m+1}\left(\bar{H}_{m} \otimes I_{p}\right) \tag{6}
\end{gather*}
$$

```
Algorithm 1 Global Arnoldi Process [10]
    \(\beta=\|V\|_{F}, V_{1}=V / \beta ;\)
    for \(j=1, \ldots, m\), do
        \(U=A V_{j} ;\)
        for \(i=1,2, \ldots j\), do
            \(h_{i, j}=<U, V_{i}>_{F}\);
            \(U=U-V_{i} h_{i, j} ;\)
        end for
        \(H_{j+1, j}=\|U\|_{F}\)
        \(V_{j+1}=U / h_{j+1, j} ;\)
    end for
```

where $\mathcal{V}_{m+1}$ denotes the $n \times(m+1) p$ rectangular matrix: $\mathcal{V}_{m+1}=\left[V_{1}, V_{2}, \ldots V_{m+1}\right], \bar{H}_{m}$ denote the $(m+1) \times m$ upper Hessenberg matrix:

$$
\begin{aligned}
\bar{H}_{m} & =\left[\begin{array}{cccc}
h_{1,1} & h_{1,2} & \ldots & h_{1, m} \\
h_{2,1} & h_{2,2} & \ldots & h_{2, m} \\
0 & h_{3,2} & \ldots & h_{3, m} \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \ldots & h_{m+1, m}
\end{array}\right] \\
& =\left[\begin{array}{c}
H_{m} \\
h_{m+1, m} e_{m}^{H}
\end{array}\right] \in \mathbb{C}^{(m+1) \times m},
\end{aligned}
$$

with $e_{m}=[0, \ldots, 0,1]^{T}$ is the $m$ th vector of the canonical basis of $\mathbb{R}^{m}$.
Since $h_{i, j}=<U, V_{i}>_{F}=\operatorname{tr}\left(V_{i}^{T} U\right)=\operatorname{vec}\left(V_{i}\right)^{T} \operatorname{vec}(U)$, $h_{j+1, j}=\|U\|_{F}=\|\operatorname{vec}(U)\|_{2}$, the global Arnoldi process over the matrix $A$ with starting rectangle matrix $V$ is equivalent with the classical Arnoldi process over the matrix $\left(I_{p} \otimes A\right)$ with starting vector $\operatorname{vec}(V)$. Then we have the following relation:

$$
\begin{align*}
\left(I_{p}\right. & \otimes A)\left[\operatorname{vec}\left(V_{1}\right), \operatorname{vec}\left(V_{2}\right), \ldots, \operatorname{vec}\left(V_{m}\right)\right] \\
& =\left[\operatorname{vec}\left(V_{1}\right), \operatorname{vec}\left(V_{2}\right), \ldots, \operatorname{vec}\left(V_{m}\right)\right] H_{m} \\
& +h_{m+1, m} \operatorname{vec}\left(V_{m+1}\right) e_{m}^{T}  \tag{7}\\
& =\left[\operatorname{vec}\left(V_{1}\right), \operatorname{vec}\left(V_{2}\right), \ldots, \operatorname{vec}\left(V_{m}\right), \operatorname{vec}\left(V_{m+1}\right)\right] \bar{H}_{m}
\end{align*}
$$

## B. Implicitly Restarted Global GMRES

Let us assume that a global Arnoldi relation of type $A \mathcal{V}_{m}=$ $\mathcal{V}_{m+1}\left(\bar{H}_{m} \otimes I_{s}\right)$ holds. In the GLGMRESIR method, harmonic Ritz matrices corresponding to the small eigenvalues $\theta_{i}^{\prime} s$ are kept in the restarting scheme. We denote these harmonic Ritz matrices $Y_{k}=\mathcal{V}_{m}\left(g_{k} \otimes I_{p}\right)$, where the $k$ vectors $g_{i}$ 's corresponding to the smallest eigenvalues are obtained as solutions of the following generalized eigenvalue problem

$$
\begin{equation*}
<A \mathcal{V}_{m}, A \mathcal{V}_{m}\left(g_{i} \otimes I_{p}\right)-\mathcal{V}_{m}\left(\theta_{i} g_{i} \otimes I_{p}\right)>_{F}=0 \tag{8}
\end{equation*}
$$

Using (6), this becomes

$$
\begin{equation*}
\left(H_{m}+h_{m+1, m}^{2} H_{m}^{-T} e_{m} e_{m}^{-T}\right) g_{i}=\theta_{i} g_{i}, \quad 1 \leq i \leq k \tag{9}
\end{equation*}
$$

Let $R_{0}$ be the initial residual for the linear equations at the start of the new cycle. Together with harmonic Ritz matrices, these matrices $\left(\left[Y_{1}, \ldots, Y_{k}, R_{0}\right]\right)$ are used to construct a new

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Forthogonal basis of dimension $k+1$. It allows us to compute new matrices $\mathcal{V}_{k+1}^{\text {new }}$ and $H_{k}^{\text {new }}$ such that

$$
\begin{aligned}
A \mathcal{V}_{k}^{\text {new }} & =\mathcal{V}_{k+1}^{\text {new }}\left(H_{k}^{\text {new }} \otimes I_{p}\right), \\
<\mathcal{V}_{k}^{\text {new }}, \mathcal{V}_{k}^{\text {new }}>_{F} & =I_{k+1},
\end{aligned}
$$

where $\mathcal{V}_{k}^{\text {new }}$ is the Forthogonal basis of $\left[Y_{1}, \ldots, Y_{k}, R_{0}\right]$ and $H_{k}^{\text {new }}$ is a $(k+1) \times k$ rectangular matrix. Then we run $m-$ $k-1$ steps of the global Arnoldi process with starting matrices $\mathcal{V}_{k+1}^{\text {new }}(:, k p+1:(k+1) p)$ to eventually build $\mathcal{V}_{m+1}$ and $\bar{H}_{m}$. At the end of each cycle of GLGMRESDR, a global Arnldi relation is generated,

$$
\begin{aligned}
A \mathcal{V}_{m} & =\mathcal{V}_{m+1}\left(\bar{H}_{m} \otimes I_{s}\right), \\
<\mathcal{V}_{m+1}, \mathcal{V}_{m+1}>_{F} & =I_{m+1},
\end{aligned}
$$

where $V_{i}=\mathcal{V}_{k+1}^{\text {new }}(:,(i-1) p+1: i p), 1 \leq i \leq k+1$ and $\bar{H}_{m}$ now is an upper Hessenberg matrix, except for a full leading $k+1$ by $k+1$ portion. Remarkably, $\mathcal{V}_{m}$ is the Forthonormal basis of a global Krylov subspace of dimension $m$,
$\mathcal{S}=\operatorname{span}\left\{Y_{1}, Y_{2}, \ldots, Y_{k}, R_{0}, A R_{0}, A^{2} R_{0}, \ldots, A^{m-k-1} R_{0}\right\}$.
An approximate solution $X_{m} \in \mathbb{C}^{n \times p}$ is then found by minimizing the residual norm $\left\|R_{0}-A \mathcal{V}_{m} Y\right\|$ over the space $X_{0}+\mathcal{S}$. Details of the GLGMRESIR method are given in Algorithm 2.

```
Algorithm 2 GLGMRESIR [11]
Input: \(A \in \mathbb{C}^{n \times n}\) nonsingular, \(B \in \mathbb{C}^{n \times p} . X_{0}=\mathbf{0}_{n \times p}\), tol
Output: \(\quad X_{m} \in \mathbb{C}^{n \times p}\) with \(X_{m} \approx A^{-1} B\).
    : Choose an initial guess matrix \(X_{0}\) and compute the
    residual matrix \(R_{0}=B-A X_{0} . \beta_{0}=\left\|R_{0}\right\|_{F}, V_{1}=\)
    \(R_{0} / \beta_{0}\). Generate \(\mathcal{V}_{m+1}\) and \(\bar{H}_{m}\) with the global Arnoldi
    process. Set \(c=\left[\beta^{T}, 0, \ldots, 0\right]^{T}\).
    Solve min \(\left\|c-\bar{H}_{m} y\right\|_{2}\) for \(Y_{m}\). Set \(X_{m}=X_{0}+\)
    \(\mathcal{V}_{m}\left(y_{m} \otimes I_{p}\right), R_{m}=B-A X_{m}\). Check residual norms
    for convergence, and process if not satisfied.
    Compute the \(k\) smallest eigenpairs \(\left(\theta_{j}, g_{j}\right)\) of \(\left(H_{m}+\right.\)
    \(\left.h_{m+1, m}^{2} H_{m}^{-T} e_{m} e_{m}^{-T}\right)\).
    4: Orthonormalize the vectors \(g_{i}^{\prime} \mathrm{s}\) by the first separating into
    real and imaginary parts if complex, to form the columns
    of \(G_{k} \in \mathbb{R}^{m \times k}\). (It may be necessary to adjust \(k\) to include
    both the real and imaginary part of complex eigenvectors.)
    Extend with zero entries the vectors \(p_{1}, \ldots, p_{k}\) to length
    \(m+1\), then orthonormalize the columns of \(z=c-\bar{H}_{m} y_{m}\)
    against the columns of \(\left[\begin{array}{c}G_{k} \\ 0\end{array}\right]\) to form \(g_{k+1}\). Set \(G_{k+1}=\)
    \(\left[\begin{array}{cc}G_{k} & \\ 0 & g_{k+1}\end{array}\right]\)
    Set \(\mathcal{V}_{k+p}^{\text {new }}=\mathcal{V}_{m+1}\left(G_{k+1} \otimes I_{p}\right), H_{k}^{\text {new }}=G_{k+1}^{T} \bar{H}_{m} G_{k}\).
    Apply the global Arnoldi algorithm to extend \(H_{k}^{\text {new }}\) and
    \(V_{k+p}^{\text {new }}\) to \(\bar{H}_{m}\) and \(\mathcal{V}_{m+1}\).
    7: Let \(c_{i}=<V_{i}, R_{m}>_{F}, i=1, \ldots, m+1\) and \(X_{0}=X_{m}\).
        Go to step 2 .
```

Let $\overline{\mathcal{V}}_{m}=\left[\operatorname{vec}\left(V_{1}\right), \operatorname{vec}\left(V_{2}\right), \ldots, \operatorname{vec}\left(V_{m}\right)\right]$. Note that (8) is equivalent with

$$
\begin{equation*}
\left(I_{p} \otimes A\right) \overline{\mathcal{V}}_{m} \perp\left[\left(I_{p} \otimes A\right) \overline{\mathcal{V}}_{m} g_{i}-\theta_{i} \overline{\mathcal{V}}_{m} g_{i}\right] . \tag{10}
\end{equation*}
$$

The residual vector $\operatorname{vec}\left(R_{m}\right)$ is orthogonal to the subspace spanned by the columns of $\left(I_{p} \otimes A\right) \overline{\mathcal{V}}_{m}$. From (9), we observe that harmonic residual vectors $\operatorname{vec}\left(\tilde{R}_{j}\right)=\left(I_{p} \otimes\right.$ $A) \operatorname{vec}\left(Y_{j}\right)-\theta_{j} \operatorname{vec}\left(Y_{j}\right)$ is also is orthogonal to the subspace $\mathcal{R}\left(\left(I_{p} \otimes A\right) \overline{\mathcal{V}}_{m}\right)$. The harmonic residual vectors and the residual vector $\operatorname{vec}\left(R_{m}\right)$ all reside in the Krylov subspace of dimension $m+1$ and are orthogonal to the same subspace of dimension $m$, so they must be multiples of each other, i.e., $\operatorname{vec}\left(\tilde{R}_{j}\right)=\zeta_{j} \operatorname{vec}\left(R_{m}\right), j=1, \ldots, k$. Then we have

$$
\tilde{R}_{j}=A Y_{j}-\theta_{j} Y_{j}=\zeta_{j} R_{m}, j=1, \ldots, k
$$

## IV. GLGMRESIR FOR SHIFTED LINEAR SYSTEMS

As mentioned above, GLGMRESIR generates the matrix subspace of dimension $m$, i.e., $\mathcal{S}$. Any vector $X_{k} \in X_{0}+\mathcal{S}$ can be represented as

$$
\begin{equation*}
X_{m}=X_{0}+P_{m-k-1}(A) R_{0}+\sum_{i=1}^{k} \alpha_{i} Y_{i} \tag{11}
\end{equation*}
$$

where $P_{m-k-1}$ is a polynomial of degree $\leq m-k-1$ with $P_{m-k-1}(0)=1$. Then, the corresponding residual $R_{m}=B-$ $A X_{m}$ satisfies

$$
\begin{aligned}
R_{m} & =R_{0}-A P_{m-k-1}(A) R_{0}-\sum_{i=1}^{k} \alpha_{i} A Y_{i} \\
& =\Phi_{m-k}(A) R_{0}-\sum_{i=1}^{k} \alpha_{i} A Y_{i}
\end{aligned}
$$

where $\Phi_{m-k}(t)=1-t P_{m-k-1}(t)$ is a polynomial of degree $\leq m-k$ with $\Phi_{m-k}(0)=1$.
For the shifted systems, we have

$$
\begin{aligned}
& X_{m}^{\sigma}=X_{0}^{\sigma}+P_{m-k-1}^{\sigma}(A-\sigma I) R_{0}^{\sigma}+\sum_{i=1}^{k} \alpha_{i}^{\sigma} Y_{i}, \\
R_{m}^{\sigma}= & R_{0}^{\sigma}-(A-\sigma I) P_{m-k-1}^{\sigma}(A-\sigma I) R_{0}^{\sigma}-\sum_{i=1}^{k} \alpha_{i}^{\sigma}(A-\sigma I) Y_{i} \\
= & \Phi_{m-k}^{\sigma}(A-\sigma I) R_{0}^{\sigma}-\sum_{i=1}^{k} \alpha_{i}^{\sigma}(A-\sigma I) Y_{i}
\end{aligned}
$$

where $\Phi_{m-k}(t)=1-t P_{m-k-1}(t)$ is a polynomial of degree $\leq m-k$ with $\Phi_{m-k}(0)=1$.

## A. Collinear Residuals

Following the similar steps as in [9], we provide a simple analysis which justifies the residual $R_{m}^{\sigma}$ is unique if the approximate collinearity condition exist.
Suppose that the initial residuals for the base and shifted systems are collinear, $R_{0}^{\sigma}=\beta_{0} R_{0}, \beta_{0} \in \mathbb{C}$. We enforce the condition that the residual $R_{m}^{\sigma}$ is parallel to the minimized residual $R_{m}$, i.e.,

$$
R_{m}^{\sigma}=\beta_{m} R_{m}, \beta_{m} \in \mathbb{C}
$$

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which amounts to

$$
\begin{aligned}
\beta_{0} \Phi_{m-k}^{\sigma}(A-\sigma I) R_{0}^{\sigma} & -\sum_{i=1}^{k} \alpha_{i}^{\sigma}(A-\sigma I) Y_{i} \\
& =\beta_{s} \Phi_{m-k}(A) R_{0}-\sum_{i=1}^{k} \alpha_{i} A Y_{i}
\end{aligned}
$$

Combining the conditions $A Y_{i}-\theta_{i} Y_{i}=\tilde{R}_{i},(A-\sigma I) Y_{i}=$ $\left(\theta_{i}-\sigma\right) Y_{i}+\tilde{R}_{i}$ and $\tilde{R}_{i}=\zeta_{i} R_{m}$ yield

$$
\begin{aligned}
\beta_{0} \Phi_{m-k}^{\sigma}(A-\sigma I) R_{0} & -\sum_{i=1}^{k}\left(\alpha_{i}^{\sigma} \zeta_{i}\right. \\
& \left.-\beta_{s} \alpha_{i} \zeta_{i}\right) R_{0}-\beta_{s} \Phi_{m-k}(A) R_{0} \\
& =\sum_{i=1}^{k}\left(\alpha_{i}^{\sigma}\left(\theta_{i}-\sigma\right)-\beta_{s} \alpha_{i} \theta_{i}\right) Y_{i}
\end{aligned}
$$

Since the vectors $Y_{1}, \ldots, Y_{k}, R_{0}, A R_{0}, \ldots, A^{m-k-1} R_{0}$ are Forthogonal, it holds that

$$
\begin{gathered}
\beta_{0} \Phi_{m-k}^{\sigma}(t-\sigma)-\sum_{i=1}^{k}\left(\alpha_{i}^{\sigma} \zeta_{i}-\beta_{s} \alpha_{i} \zeta_{i}\right)-\beta_{s} \Phi_{m-k}(t)=0 \\
\alpha_{i}^{\sigma}\left(\theta_{i}-\sigma\right)-\beta_{s} \alpha_{i} \theta_{i}=0, i=1, \ldots, k
\end{gathered}
$$

Using the relation $\Phi_{m-k}^{\sigma}(0)=1$, we have

$$
\left(\begin{array}{cccc}
\Phi_{m-k}(\sigma)-\sum_{i=1}^{k} \alpha_{i} \zeta_{i} & \zeta_{1} & \cdots & \zeta_{k} \\
\alpha_{1} \zeta_{1} & \sigma-\theta_{1} & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
\alpha_{k} \zeta_{k} & 0 & \cdots & \sigma-\theta_{k}
\end{array}\right)\left(\begin{array}{c}
\beta_{s} \\
\alpha_{1}^{\sigma} \\
\vdots \\
\alpha_{k}^{\sigma}
\end{array}\right)
$$

$$
=\left(\begin{array}{c}
\beta_{0}  \tag{12}\\
0 \\
\vdots \\
0
\end{array}\right) .
$$

Observe that when $\theta_{j} \neq \sigma, i=1, \ldots, k$ and $\Phi_{m-k}(\sigma) \neq$ $\sum_{i=1}^{k} \alpha_{i} \zeta_{i} \sigma /\left(\sigma-\theta_{i}\right)$, the above system has a unique solution. It is shown that the colinearity condition cannot be satisfied, but if it can, the residual $R_{m}^{\sigma}$ is unique.

In practice, the corresponding polynomials $\Phi_{m-k}$ are not calculated. We now work out how the shifted systems can be practically computed when the GLGMRESIR iteration is performed on the seed systems.

Our basic assumption is that $R_{0}^{\sigma}=\beta_{0} R_{0}$. As mentioned above, at the end of each cycle of GLGMRESIR, a global Arnoldi relation is generated

$$
A \mathcal{V}_{m}=\mathcal{V}_{m+1}\left(\bar{H}_{m} \otimes I_{p}\right),
$$

with a shifted Arnoldi relation

$$
(A-\sigma I) \mathcal{V}_{m}=\mathcal{V}_{m+1}\left(\left(\bar{H}_{m}-\sigma I_{m}\right) \otimes I_{p}\right),
$$

We enforce the condition that the residual for the shifted system is parallel to the minimized residual of the base system, i.e.,

$$
\begin{equation*}
R_{m}^{\sigma}=\beta_{m} R_{m} . \tag{13}
\end{equation*}
$$

So

$$
\begin{align*}
B-(A-\sigma I)\left(X_{0}^{\sigma}+\mathcal{V}_{m}\left(y_{m}^{\sigma} \otimes I_{p}\right)\right) & =\beta_{m} \mathcal{V}_{m+1}\left(z \otimes I_{p}\right) \\
\beta_{0} R_{0}^{\sigma}-\mathcal{V}_{m+1}\left(\left(\bar{H}_{m}-\sigma I_{m}\right) y_{m}^{\sigma} \otimes I_{p}\right) & =\mathcal{V}_{m+1}\left(\beta_{m} z \otimes I_{p}\right) \\
\mathcal{V}_{m+1}\left(\left(\beta_{0} c-\left(\bar{H}_{m}-\sigma I_{m}\right) y_{m}^{\sigma}\right) \otimes I_{p}\right) & =\mathcal{V}_{m+1}\left(\beta_{m} z \otimes I_{p}\right) \tag{14}
\end{align*}
$$

By straightforward computations, it is shown that if $z=$ $c-\bar{H}_{m} y_{m}$ then for (13) to hold, we must have

$$
\left(\bar{H}_{m}-\sigma I_{m}\right) y_{m}^{\sigma}+z \beta_{m}=\beta_{0} c
$$

Thus, we can compute both $y_{m}^{\sigma}$ and $\beta_{m}$ by solving the augmented linear system,

$$
\left[\begin{array}{ll}
\bar{H}_{m}-\sigma I_{m}, & z
\end{array}\right]\left[\begin{array}{c}
y_{m}^{\sigma}  \tag{15}\\
\beta_{m}
\end{array}\right]=\beta_{0} c
$$

Note that we only compute the minimum residual solution using a Petrov Galerkin condition for the base systems. We enforce collinearity of the residuals to compute the approximation for the shifted systems. It is shown that a solution to (13) is exist if and only is the residual polynomial satisfies $\theta_{j} \neq \sigma, i=1, \ldots, l$ and $\Phi_{m-k}(\sigma) \neq$ $\sum_{i=0}^{k} \alpha_{i} \zeta_{j} \sigma /\left(\sigma-\theta_{j}\right)$, otherwise, the system is singular. We can compute the QR factorization of $\left[\bar{H}_{m}-\sigma I_{m}, z\right]=Q R$ to detect numerical singularity by examining the last diagonal entry of $R$. In the case that the solution does not exist, we simply perform one more iteration and check condition again.
To make this idea more concrete, we present outline of the shifted GLGMRESIR (GLGMRESIRsh) for solving the systems (1) in Algorithm 3.

Algorithm 3 GLGMRESIRsh algorithm.
1: At the beginning of a cycle of GLGMRESIRSh, assume the current problem is $\left(A-\sigma_{i} I\right)\left(X_{i}-X_{0, i}\right)=\beta_{i} R_{0}$, with $\beta_{1}=1$, and where $X_{0, i}$ is the current approximate solution to the $i$ th shifted system.
2: Apply GLGMRESIR to $A$ and generate equation $A \mathcal{V}_{m}=$ $\mathcal{V}_{m+1}\left(\bar{H}_{m} \otimes I_{p}\right)$.
3: For the base system, solve the minimum residual reduced problem min $\left\|c-\bar{H}_{m} y\right\|$ for $y_{1}$, where $c_{i}=<V_{i}{ }^{T} R_{m}>_{F}$ , $i=1, \ldots, m+1$. The new approximate solution is $X_{1}=$ $X_{0,1}+\mathcal{V}_{m}\left(y_{1} \otimes I_{p}\right)$; The new residual vector is $R_{1}=$ $R_{0,1}-A \mathcal{V}_{m} y_{1}=R_{0,1}-\mathcal{V}_{m+1}\left(\bar{H}_{m} y_{1} \otimes I_{p}\right)$
4: For the other shifted systems $i, \ldots, s$, form $z=c-\bar{H}_{m} y_{1}$. Apply a QR factorization : $\left[\bar{H}_{m}-\sigma I_{m}, z\right]=Q R$. Solve $R y_{i}=\beta_{i} Q^{T} c-\beta_{i}^{\text {new }} Q^{T} z$, using the last row to solve for $\beta_{i}^{\text {new }}$ and the first $m$ rows for $y_{i}$.
5: The new approximate solution of the $i$ th system is $X_{i}=$ $X_{i, 1}+\mathcal{V}_{m}\left(y_{i} \otimes I_{p}\right)$, and the new residual is $R_{i}=\beta_{i}^{\text {new }} R_{1}$
6: Test the residual norms for convergence. If not satisfied, for $i=2, \ldots, s$, set $\beta_{i}=\beta_{i}^{\text {new }}$ and for $i=1, \ldots, s$, set $X_{0, i}=X_{i}$ and $R_{0, i}=R_{i}$. Then go back to Step 1 .

## V. Numerical results

In this section, some numerical experiments will be described. The goal of these experiments is to examine the the effectiveness of GLGMRESIRsh (Algorithm 3).

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In all of our runs we use a $\mathbf{0}_{n \times p}$ initial guess and choose different values for $\sigma$. Here, $m$ and $k$ denote the number of iterations for each restart and the number of harmonic Ritz vectors, respectively. The parameters are taken as $m=30$, $k=15$ for all the experiments. The stopping criterion in all iterative methods is $\frac{\left\|R_{k}\right\|_{F}}{\left\|R_{0}\right\|_{F}} \leq 10^{-6}$.

All the numerical experiments were performed in MATLAB 2011b. The machine we have used is a PC Pentium(R), CPU $2.80 \mathrm{GHz}, 2.00 \mathrm{~GB}$ of RAM.

Example 1. Following [11], the first test matrix is a tridiagonal matrix with entries $0.01,0.02,0.03,0.04,0.05$, $6,7, \ldots, 1000$ on the main diagonal, subdiagonal entries all 1 and superdiagonal entries all -1 . The shifts are taken six different values $\{0,0.9 i, i, 0.6,-i,-1\}$. The right hand sides are chosen to be random vectors with $p=5$ or 10 .


Fig. 1. Convergence history of GLGMRESIRsh for tridiagonal problem. Left: $p=5$, Right: $p=10$.

The results in Fig. 1 highlight the interest of performing GLGMRESIRsh which could simultaneously solve all the linear systems at the expense of just the matrix vector multiplications for the seed systems.
Example 2. We test GLGMRESIRsh on the reaction diffusion Brusselator model matrices RDB1250 and RDB2048 from Matrix Market [2]. For the examples, we take six values for the shift, $\sigma=\left\{0, \frac{1}{2}+\frac{1}{5} i, \frac{1}{2}-\frac{1}{5} i, 2,1-\frac{1}{2} i, 1-\frac{1}{2} i\right\}$. As right hand sides we choose $\mathrm{B}=\operatorname{rand}(n, p)$ with $p=10$.


Fig. 2. Convergence history of GLGMRESIRsh for RDB1250 and RDB2048.

Fig. 2 depict the residual history of examples using the GLGMRESIRsh method. GLGMRESsh can simultaneously compute solutions for the seed and shifted systems without any additional matrix vector for iterates of the shifted systems. And the shifted systems enjoy a faster convergence.

## Example 3. Convection diffusion problem

The third example is the convection diffusion problem with Dirichlet boundary conditions in the unit square $[0,1]^{2}=$
$\Omega \bigcap \partial \Omega$, where $\Omega=(0,1)^{2}$,

$$
\left\{\begin{array}{l}
-\varepsilon \triangle u+c u_{x}+d u_{y}=g \quad \text { in } \quad \Omega \\
u=0 \quad \text { on } \quad \partial \Omega
\end{array}\right.
$$

This problem is discretized with a second order finite difference scheme for a vertex centered location of unknowns. We adopt $\frac{h}{\varepsilon} \max (|c|,|d|)=2$ to satisfy the Péclet condition, where $h=\frac{1}{N-1}$ is the mesh size and N is the number of points per direction. Here, $h=1 / 128(1 / 256), c=d=$ $256(512)$ and $\varepsilon=1$ are taken, then the problem size is $\left.129^{2}\left(257^{2}\right)=16641(66049)\right)$ and has $80137(324105)$ non zero entries, which is real, sparse and nonsymmetric. The right hand sides have normally distributed rand elements with $p=10$. The numerical behaviour of the GLGMRESIRsh approaches are plotted in Fig. 3.


Fig. 3. Convergence history of GLGMRESIRsh for convection diffusion problem. Left: $n=16641$, Right: $n=66049$.

The curves in Fig. 3 highlight interest of performing shift invariance with GLGMRESIR at each iteration. The curves for shifted systems enjoys a significant decrease in the number of matrix vector products than the one for seed system. In addition, GLGMRESIRsh simultaneously solve all shifted linear systems in only one global Krylov subspace, leading to large saving in storage and time. Thus, it is demonstrated that the potential effectiveness of our algorithm for the shift systems with multiple shifts and multiple right hand sides.

## VI. CONCLUSIONS

In this paper, we have derived the extension of GLGMRESIRsh for shifted linear systems with multiple shifts and multiple right hand sides (1). We use a strategy to make the residuals of the shift systems collinear. With this condition, our method not only enjoys the benefits of using deflation technique, but also can exploit the shift invariance, without computing additional matrix vector products for solving the shifted systems. Numerical examples also confirm the effectiveness of our method. Therefore, it is concluded that the GLGMRESIRsh is a competitive method for solving the linear systems with multiple right hand sides and multiple shifts.

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