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A Weighted Block GMRES method for solving linear systems with multiple right-hand sides

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Abstract

We investigate the Block GMRES method for solving large and sparse linear systems with multiple right-hand sides. For solving linear systems with a single right-hand side, the Weighted GMRES method based on the weighted minimal residual condition has been proposed as an improvement of the GMRES method. In this paper, by applying the idea of the Weighted GMRES method to the Block GMRES method, we propose a Weighted Block GMRES method. The numerical experiments indicate that the Weighted Block GMRES(m) method has higher performance for efficient convergence than the Block GMRES(m) method.

Keywords large linear systems with multiple right-hand sides, the Block GMRES method, the weighted minimal residual condition

Research Activity Group Algorithms for Matrix / Eigenvalue Problems and their Applications

1. Introduction

In this paper, we consider solving large and sparse linear systems with multiple right-hand sides of the form:

$$AX = B, \quad A \in \mathbb{C}^{n\times n}, \quad X, B \in \mathbb{C}^{n\times l}, \tag{1}$$

where the coefficient matrix A is assumed to be non-Hermitian and nonsingular. Such linear systems (1) often arise from the lattice quantum chromodynamics (lattice QCD) calculations, eigensolvers based on the contour integration and so on.

For solving such linear systems (1), two kinds of Krylov subspace based methods: the Global Krylov subspace methods [1, 2]; and the Block Krylov subspace methods [3, 4], have been well studied as extensions of the standard Krylov subspace methods.

In this paper, we investigate one of the most basic Block Krylov subspace methods: the Block GMRES method which is an extension of the GMRES method [5]. For solving linear systems with a single right-hand side, the Weighted GMRES method [6] based on the weighted minimal residual condition has been proposed as an improvement of the GMRES method. In order to improve the convergence property of the Block GMRES method, we apply the weighted minimal residual condition to the linear systems with multiple right-hand sides (1) and propose a Weighted Block GMRES method based on the weighted minimal residual condition.

This paper is organized as follows. In Section 2, we briefly describe the Weighted GMRES method for solving linear systems. In Section 3, we introduce the Block GMRES method and propose a Weighted Block GMRES method. The performance of the Weighted Block GMRES(m) method is evaluated by some numerical experiments in Section 4. Our conclusions are summarized in Section 5.

2. The Weighted GMRES method for solving linear systems

The Krylov subspace methods are the most commonly used methods for solving large and sparse linear systems:

$$A\boldsymbol{x} = \boldsymbol{b}, \quad A \in \mathbb{C}^{n\times n}, \quad \boldsymbol{x}, \boldsymbol{b} \in \mathbb{C}^{n}. \tag{2}$$

Let $\boldsymbol{x}_0$ be an initial guess, and $\boldsymbol{r}_0 := \boldsymbol{b} - A\boldsymbol{x}_0$ be the corresponding initial residual. Then the Krylov subspace methods construct the sequence of the approximate solution $\boldsymbol{x}_k$ and the corresponding residual $\boldsymbol{r}_k := \boldsymbol{b} - A\boldsymbol{x}_k$:

$$\boldsymbol{x}_k = \boldsymbol{x}_0 + V_k\boldsymbol{y}_k, \quad \boldsymbol{r}_k = \boldsymbol{r}_0 - AV_k\boldsymbol{y}_k, \quad \boldsymbol{y}_k \in \mathbb{C}^k,$$

where the columns of the matrix $V_k \in \mathbb{C}^{n\times k}$ are the basis vectors of the Krylov subspace $\mathcal{K}_k(A, \boldsymbol{r}_0) := \mathrm{span}\{\boldsymbol{r}_0, A\boldsymbol{r}_0, \ldots, A^{k-1}\boldsymbol{r}_0\}$.

In what follows, we introduce basic ideas of the GMRES method in Section 2.1 and the Weighted GMRES method in Section 2.2, respectively.

2.1 *The GMRES method*

The GMRES method is one of the most successful Krylov subspace methods for solving non-Hermitian linear systems (2). It constructs the orthonormal basis $V_k, V_k^{\mathrm{H}}V_k = I$ by the Arnoldi procedure and computes the approximate solution by the minimal residual condition:

$$\min \|\boldsymbol{r}_k\|_2 \Leftrightarrow \min_{\boldsymbol{y}\in\mathbb{C}^k} \|\boldsymbol{r}_0 - AV_k\boldsymbol{y}\|_2. \tag{3}$$

From the matrix formula of the Arnoldi procedure $AV_k = V_{k+1}\underline{H}_k$ and the minimal residual condition (3), the vector $\boldsymbol{y}_k$ is computed by

$$\boldsymbol{y}_k = \arg\min_{\boldsymbol{y}\in\mathbb{C}^k} \|\beta\boldsymbol{e}_1 - \underline{H}_k\boldsymbol{y}\|_2,$$

where $\beta = \|\boldsymbol{r}_0\|_2, \boldsymbol{e}_1 = [1, 0, \ldots, 0]^{\mathrm{T}} \in \mathbb{R}^{k+1}$, and $\underline{H}_k$ is

Algorithm 1 The GMRES(m) method [5]

1: Set an initial guess $\boldsymbol{x}_0$ and the restart frequency m
2: Compute $\boldsymbol{r}_0 := \boldsymbol{b} - A\boldsymbol{x}_0$
3: Compute $\beta := \|\boldsymbol{r}_0\|_2, \boldsymbol{v}_1 := \boldsymbol{r}_0/\beta$
4: **for** $j = 1, 2, \ldots, m$ **do:**
5:   Compute $\boldsymbol{w}_j = A\boldsymbol{v}_j$
6:   **for** $i = 1, 2, \ldots, j$ **do:**
7:     $h_{i,j} = \boldsymbol{v}_i^{\mathrm{H}}\boldsymbol{w}_j$
8:     $\boldsymbol{w}_j = \boldsymbol{w}_j - h_{i,j}\boldsymbol{v}_j$
9:   **end for**
10:   $h_{j+1,j} = \|\boldsymbol{w}_j\|_2$
11:   $\boldsymbol{v}_{j+1} = \boldsymbol{w}_j/h_{j+1,j}$
12: **end for**
13: Set $V_m = [\boldsymbol{v}_1, \boldsymbol{v}_2, \ldots, \boldsymbol{v}_m], \underline{H}_m = \{h_{i,j}\}_{1\leq i\leq m+1, 1\leq j\leq m}$
14: Compute $\boldsymbol{y}_m = \arg\min_{\boldsymbol{y}\in\mathbb{C}^m} \|\beta\boldsymbol{e}_1 - \underline{H}_m\boldsymbol{y}\|_2$
15: Compute $\boldsymbol{x}_m = \boldsymbol{x}_0 + V_m\boldsymbol{y}_m$, **if** satisfied **then** stop
16: Update $\boldsymbol{x}_0 = \boldsymbol{x}_m$, and go to 2

a $(k+1)\times k$ upper Hessenberg matrix.

The algorithm of the restarted version of the GMRES method: the GMRES(m) method, can be shown in Algorithm 1, where m is the restart frequency.

2.2 The Weighted GMRES method

In order to accelerate the convergence of the GMRES method, the Weighted GMRES method has been proposed by Essai in 1998 [6].

The D-inner product $(\boldsymbol{u}, \boldsymbol{v})_D := \boldsymbol{u}^{\mathrm{H}}D\boldsymbol{v}$ and the corresponding D-norm $\|\boldsymbol{u}\|_D := \sqrt{\boldsymbol{u}^{\mathrm{H}}D\boldsymbol{u}}$ have been introduced in the paper [6], where D is a diagonal matrix whose diagonal entries are all positive. The D-norm $\|\boldsymbol{u}\|_D$ satisfies the following relation:

$$V^{\mathrm{H}}DV = I \Rightarrow \|V\boldsymbol{u}\|_D = \|\boldsymbol{u}\|_2. \tag{4}$$

Then, by using the D-orthonormal basis $\widetilde{V}_k, \widetilde{V}_k^{\mathrm{H}}D\widetilde{V}_k = I$ of the Krylov subspace, the Weighted GMRES method adopts the weighted minimal residual condition:

$$\min \|\boldsymbol{r}_k\|_D \Leftrightarrow \min_{\boldsymbol{y}\in\mathbb{C}^k} \|\boldsymbol{r}_0 - A\widetilde{V}_k\boldsymbol{y}\|_D, \tag{5}$$

instead of the minimal residual condition (3) of the GMRES method.

From the matrix formula of the Weighted Arnoldi procedure $A\widetilde{V}_k = \widetilde{V}_{k+1}\underline{\widetilde{H}}_k$ and (4), the weighted minimal residual condition (5) can be rewritten as

$$\boldsymbol{y}_k = \arg\min_{\boldsymbol{y}\in\mathbb{C}^k} \|\widetilde{\beta}\boldsymbol{e}_1 - \underline{\widetilde{H}}_k\boldsymbol{y}\|_2,$$

where $\widetilde{\beta} = \|\boldsymbol{r}_0\|_D, \boldsymbol{e}_1 = [1, 0, \ldots, 0]^{\mathrm{T}} \in \mathbb{R}^{k+1}$.

For an efficient convergence, the weight matrix D can be dynamically set in each restart cycle. In the paper [6], the following definition was introduced:

$$D = \mathrm{diag}(\boldsymbol{d}), \quad d_i = \frac{\sqrt{n}}{\|\boldsymbol{r}_0\|_2}|(\boldsymbol{r}_0)_i|, \tag{6}$$

where D is normalized such that $\|D\|_{\mathrm{F}} = \|I\|_{\mathrm{F}} = \sqrt{n}$. The algorithm of the Weighted GMRES(m) method can be shown in Algorithm 2.

Note that the Weighted GMRES(m) method can also be regarded as the GMRES(m) method for solving $(D^{1/2}AD^{-1/2})(D^{1/2})\boldsymbol{x} = D^{1/2}\boldsymbol{b}$, where the diagonal matrix D is dynamically set in each restart cycle.

Algorithm 2 The Weighted GMRES(m) method [6]

1: Set an initial guess $\boldsymbol{x}_0$ and the restart frequency m
2: Compute $\boldsymbol{r}_0 := \boldsymbol{b} - A\boldsymbol{x}_0$
3: Set D, e.g., $D := \mathrm{diag}(\boldsymbol{d}), d_i = \sqrt{n}|(\boldsymbol{r}_0)_i|/\|\boldsymbol{r}_0\|_2$
4: Compute $\widetilde{\beta} := \|\boldsymbol{r}_0\|_D, \widetilde{\boldsymbol{v}}_1 := \boldsymbol{r}_0/\widetilde{\beta}$
5: **for** $j = 1, 2, \ldots, m$ **do:**
6:   Compute $\widetilde{\boldsymbol{w}}_j = A\widetilde{\boldsymbol{v}}_j$
7:   **for** $i = 1, 2, \ldots, j$ **do:**
8:     $\widetilde{h}_{i,j} = \widetilde{\boldsymbol{v}}_i^{\mathrm{H}}D\widetilde{\boldsymbol{w}}_j$
9:     $\widetilde{\boldsymbol{w}}_j = \widetilde{\boldsymbol{w}}_j - \widetilde{h}_{i,j}\widetilde{\boldsymbol{v}}_j$
10:   **end for**
11:   $\widetilde{h}_{j+1,j} = \|\widetilde{\boldsymbol{w}}_j\|_D$
12:   $\widetilde{\boldsymbol{v}}_{j+1} = \widetilde{\boldsymbol{w}}_j/\widetilde{h}_{j+1,j}$
13: **end for**
14: Set $\widetilde{V}_m = [\widetilde{\boldsymbol{v}}_1, \widetilde{\boldsymbol{v}}_2, \ldots, \widetilde{\boldsymbol{v}}_m], \underline{\widetilde{H}}_m = \{\widetilde{h}_{i,j}\}_{1\leq i\leq m+1, 1\leq j\leq m}$
15: Compute $\boldsymbol{y}_m = \arg\min_{\boldsymbol{y}\in\mathbb{C}^m} \|\widetilde{\beta}\boldsymbol{e}_1 - \underline{\widetilde{H}}_m\boldsymbol{y}\|_2$
16: Compute $\boldsymbol{x}_m = \boldsymbol{x}_0 + \widetilde{V}_m\boldsymbol{y}_m$, **if** satisfied **then** stop
17: Update $\boldsymbol{x}_0 = \boldsymbol{x}_m$, and go to 2

3. A Weighted Block GMRES method for solving linear systems with multiple right-hand sides

One of the simplest ideas for solving the linear systems with multiple right-hand sides (1) is to apply some (preconditioned) Krylov subspace method to the linear system with each right-hand side individually. In this approach, the Krylov subspaces are constructed and used only for each right-hand side. As another approach, the Block Krylov subspace methods have been proposed and actively studied for solving the linear systems (1) simultaneously.

The basic idea of the Block Krylov subspace methods is to reuse each Krylov subspace for all right-hand sides. Let X_0 be an initial guess, and $R_0 = [\boldsymbol{r}_0^{(1)}, \boldsymbol{r}_0^{(2)}, \ldots, \boldsymbol{r}_0^{(l)}] := B - AX_0$ be the corresponding initial residual. Then the Block Krylov subspace methods construct the approximate solution X_k and the corresponding residual $R_k := B - AX_k$ as follows:

$$X_k = X_0 + V_k^{\square}Y_k, \quad R_k = R_0 - AV_k^{\square}Y_k, \quad Y_k \in \mathbb{C}^{(k\times l)\times l},$$

where the columns of $V_k^{\square} \in \mathbb{C}^{n\times(k\times l)}$ are the basis of the sum of the Krylov subspaces, i.e.,

$$\mathcal{K}_k^{\square}(A, R_0) := \mathcal{K}_k(A, \boldsymbol{r}_0^{(1)}) + \mathcal{K}_k(A, \boldsymbol{r}_0^{(2)}) + \cdots + \mathcal{K}_k(A, \boldsymbol{r}_0^{(l)}).$$

By reusing the Krylov subspace, the Block Krylov subspace methods often show more efficient convergence property than the traditional Krylov subspace methods. For the details, see, e.g., [7, 8] and references therein.

Here we note that the Global Krylov subspace methods use the Krylov subspaces $\mathcal{K}_k(A, \boldsymbol{r}_0^{(i)})$ independently for constructing the approximate solutions, whereas the Block Krylov subspace methods use the sum of the Krylov subspaces $\mathcal{K}_k^{\square}(A, R_0)$, see, e.g., [1, 2].

In what follows, we introduce basic ideas of the Block GMRES method in Section 3.1 and propose a Weighted Block GMRES method in Section 3.2.

Algorithm 3 The Block GMRES(m) method [4]

1: Set an initial guess X_0 and the restart frequency m
2: Compute $R_0 := B - AX_0$
3: Compute QR decomposition $R_0 = V_1 \beta^{\square}$
4: **for** $j = 1, 2, \ldots, m$ **do:**
5: Compute $W_j = AV_j$
6: **for** $i = 1, 2, \ldots, j$ **do:**
7: $H_{i,j} = V_i^{\mathrm{H}} W_j$
8: $W_j = W_j - V_j H_{i,j}$
9: **end for**
10: Compute QR decomposition $W_j = V_{j+1} H_{j+1,j}$
11: **end for**
12: Set $V_m^{\square} = [V_1, V_2, \ldots, V_m], \underline{H}_m^{\square} = \{H_{i,j}\}_{1 \le i \le m+1, 1 \le j \le m}$
13: Compute $Y_m = \arg\min_{Y \in \mathbb{C}^{(m \times l) \times l}} \|E_1 \beta^{\square} - \underline{H}_m^{\square} Y\|_{\mathrm{F}}$
14: Compute $X_m = X_0 + V_m^{\square} Y_m$, **if** satisfied **then** stop
15: Update $X_0 = X_m$, and go to 2

3.1 *The Block GMRES method*

The Block GMRES method is a natural extension of the GMRES method for solving linear systems with multiple right-hand sides (1). It constructs the orthonormal basis $V_k^{\square}, V_k^{\square \mathrm{H}} V_k^{\square} = I$ by the Block Arnoldi procedure and computes the approximate solution by the minimal residual condition:

$$\min \|R_k\|_{\mathrm{F}} \Leftrightarrow \min_{Y \in \mathbb{C}^{(k \times l) \times l}} \|R_0 - AV_k^{\square} Y\|_{\mathrm{F}}. \tag{7}$$

From the matrix formula of the Block Arnoldi procedure $AV_k^{\square} = V_{k+1}^{\square} \underline{H}_k^{\square}$ and the minimal residual condition (7), the matrix Y_k is computed by

$$Y_k = \arg \min_{Y \in \mathbb{C}^{(k \times l) \times l}} \|E_1 \beta^{\square} - \underline{H}_k^{\square} Y\|_{\mathrm{F}},$$

where $\beta^{\square} \in \mathbb{C}^{l \times l}$ is the upper triangular matrix computed by the QR decomposition of R_0: $R_0 = V_1 \beta^{\square}$, and $E_1 \in \mathbb{R}^{((k+1) \times l) \times l}$ is the first l columns of the identity matrix. Here we note that $\underline{H}_k^{\square}$ is the $[(k+1) \times l] \times (k \times l)$ upper banded Hessenberg matrix with bandwidth l.

The algorithm of the Block GMRES(m) method can be shown in Algorithm 3.

3.2 *Proposal for a Weighted Block GMRES method*

In order to improve the convergence property of the Block GMRES method, we propose a Weighted Block GMRES method based on a weighted minimal residual condition for the linear systems with multiple right-hand sides (1).

Firstly, we introduce a matrix D-norm as follows:

$$\|X\|_D := \sqrt{\mathrm{tr}(X^{\mathrm{H}} D X)},$$

as well as the Weighted GMRES method, where D is a diagonal matrix whose diagonal entries are all positive. This matrix D-norm satisfies the following relations:

$$\|X\|_D \ge 0, \quad \|X\|_D = 0 \text{ iff } X = O,$$

$$\|\alpha X\|_D = |\alpha| \|X\|_D, \quad \alpha \in \mathbb{C},$$

$$\|X + Y\|_D \le \|X\|_D + \|Y\|_D,$$

for any $X, Y \in \mathbb{C}^{n \times m}$, and

$$V^{\mathrm{H}} D V = I \Rightarrow \|VX\|_D = \|X\|_{\mathrm{F}}. \tag{8}$$

Algorithm 4 A Weighted Block GMRES(m) method

1: Set an initial guess X_0 and the restart frequency m
2: Compute $R_0 := B - AX_0$
3: Set D, e.g., (10).
4: Compute WQR decomposition $R_0 = \widetilde{V}_1 \widetilde{\beta}^{\square}$
5: **for** $j = 1, 2, \ldots, m$ **do:**
6: Compute $\widetilde{W}_j = A\widetilde{V}_j$
7: **for** $i = 1, 2, \ldots, j$ **do:**
8: $\widetilde{H}_{i,j} = \widetilde{V}_i^{\mathrm{H}} D \widetilde{W}_j$
9: $\widetilde{W}_j = \widetilde{W}_j - \widetilde{V}_j \widetilde{H}_{i,j}$
10: **end for**
11: Compute WQR decomposition $\widetilde{W}_j = \widetilde{V}_{j+1} \widetilde{H}_{j+1,j}$
12: **end for**
13: Set $\widetilde{V}_m^{\square} = [\widetilde{V}_1, \widetilde{V}_2, \ldots, \widetilde{V}_m], \underline{\widetilde{H}}_m^{\square} = \{\widetilde{H}_{i,j}\}_{1 \le i \le m+1, 1 \le j \le m}$
14: Compute $Y_m = \arg\min_{Y \in \mathbb{C}^{(m \times l) \times l}} \|E_1 \widetilde{\beta}^{\square} - \underline{\widetilde{H}}_m^{\square} Y\|_{\mathrm{F}}$
15: Compute $X_m = X_0 + \widetilde{V}_m^{\square} Y_m$, **if** satisfied **then** stop
16: Update $X_0 = X_m$, and go to 2

This is also a natural extension of the Frobenius-norm, because of

$$\|X\|_I = \sqrt{\mathrm{tr}(X^{\mathrm{H}} X)} = \|X\|_{\mathrm{F}}.$$

Then, by using the D-orthonormal basis $\widetilde{V}_k^{\square}$ of $\mathcal{K}_k^{\square}(A, R_0)$, which satisfies $(\widetilde{V}_k^{\square})^{\mathrm{H}} D \widetilde{V}_k^{\square} = I$, the Weighted Block GMRES method adopts a weighted minimal residual condition for the linear systems with multiple right-hand sides (1), i.e.,

$$\min \|R_k\|_D \Leftrightarrow \min_{Y \in \mathbb{C}^{(k \times l) \times l}} \|R_0 - A\widetilde{V}_k^{\square} Y\|_D, \tag{9}$$

instead of the minimal residual condition (7) of the Block GMRES method. From the matrix formula of a Weighted Block Arnoldi procedure $A\widetilde{V}_k^{\square} = \widetilde{V}_{k+1}^{\square} \underline{\widetilde{H}}_k^{\square}$ and (8), the weighted minimal residual condition (9) can be rewritten as

$$Y_k = \arg \min_{Y \in \mathbb{C}^{(k \times l) \times l}} \|E_1 \widetilde{\beta}^{\square} - \underline{\widetilde{H}}_k^{\square} Y\|_{\mathrm{F}},$$

where $\widetilde{\beta}^{\square} \in \mathbb{C}^{l \times l}$ is the upper tridiagonal matrix computed by the Weight QR (WQR) decomposition of R_0: $R_0 = \widetilde{V}_1 \widetilde{\beta}^{\square}, \widetilde{V}_1^{\mathrm{H}} D \widetilde{V}_1 = I$, and $E_1 \in \mathbb{R}^{((k+1) \times l) \times l}$ is the first l columns of the identity matrix. Here we note that the Weighted Block GMRES method with $D = I$ is mathematically equivalent to the Block GMRES method. The algorithm of the Weighted Block GMRES(m) method, can be shown in Algorithm 4.

Note that the Weighted Block GMRES(m) method can also be regarded as the Block GMRES(m) method for solving $(D^{1/2} A D^{-1/2})(D^{1/2}) X = D^{1/2} B$, where the matrix D is dynamically set in each restart cycle.

4. Numerical experiments and results

In this section, we evaluate the performance of the Weighted Block GMRES(m) method, and compare it with the Block GMRES(m) method. Here we do not use any preconditioners, because the proposed method is independent of preconditioning techniques and we can similarly apply preconditioning techniques to both methods.

Table 1. Convergence results (Restart : number of restart cycle, t_{restart} : computation time per restart, t_{total} : total computation time, TRR : True Relative Residual) of the Block GMRES(m) method and the Weighted Block GMRES(m) method.

Method	Restart	Time [sec.] t_{restart}	Time [sec.] t_{total}	TRR
COUPLED				
Bl-GMRES	†	2.48E-01	8.26E+02	-5.05
W-Bl-GMRES	1526	2.48E-01	3.79E+02	-12.03
FEM_3D_THERMAL1				
Bl-GMRES	15	4.36E-01	6.54E+00	-12.44
W-Bl-GMRES	13	4.35E-01	5.66E+00	-12.71
MEMPLUS				
Bl-GMRES	393	3.96E-01	1.56E+02	-12.00
W-Bl-GMRES	161	3.99E-01	6.42E+01	-12.01
NS3DA				
Bl-GMRES	111	8.42E-01	9.35E+01	-12.08
W-Bl-GMRES	121	8.43E-01	1.02E+02	-12.07

4.1 Numerical experiments

For the test problems, we use the following matrices: COUPLED ($n = 11341$, $Nnz = 98523$) of the circuit simulation; FEM_3D_THERMAL1 ($n = 17880$, $Nnz = 430740$) of the thermal problem; MEMPLUS ($n = 17758$, $Nnz = 126150$) of the circuit simulation; NS3DA ($n = 20414$, $Nnz = 1679599$) of the fluid dynamics, which are obtained from [9].

We set the number of linear systems $l = 4$ and the restart frequency $m = 30$. We also set B as a random matrix for the right-hand sides, $X_0 = O$ for the initial guess, and the stopping criterion was set as $\|R_k\|_{\mathrm{F}}/\|B\|_{\mathrm{F}} \leq 10^{-12}$. The weight matrix D of the Weighted Block GMRES(m) method was set as follows:

$$D = \mathrm{diag}(\boldsymbol{d}), \quad d_i = \frac{\sqrt{n}}{\|R_0\|_{\mathrm{F}}}\sqrt{\sum_{j=1}^{n}|(R_0)_{i,j}|^2}, \qquad (10)$$

where D was normalized such that $\|D\|_{\mathrm{F}} = \|I\|_{\mathrm{F}} = \sqrt{n}$. This is a natural extension of (6), because it is equivalent to (6) in the case of $l = 1$.

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

4.2 Numerical results

We present the numerical results in Table 1. In this table, a symbol † denotes that the method did not converge within 100000 iterations.

From Table 1, we can see that the Weighted Block GMRES(m) method shows almost the same or more efficient convergence property than the Block GMRES(m) method. Especially, for COUPLED, the Block GMRES(m) method did not converge within the 100000 iterations; on the other hand, the Weighted Block GMRES(m) method could obtain the approximate solution satisfies required accuracy $\|R_k\|_{\mathrm{F}}/\|B\|_{\mathrm{F}} \leq 10^{-12}$ with much smaller number of iterations.

In terms of the computation time per restart cycle (t_{restart}), we can also observe that the Block GMRES(m) method and the Weighted Block GMRES(m) method have almost the same t_{restart}. This derives from the fact that the incremental cost of the Weighted Block GMRES(m) method per restart cycle is only for computations with respect to the matrix D, which is relatively smaller than for the matrix operation with respect to A.

In terms of the total computation time (t_{total}), from the better convergence property and almost the same computation time per restart, the Weighted Block GMRES(m) method could solve the linear systems with multiple right-hand sides with the less computation time than the Block GMRES(m) method.

5. Conclusions

In this paper, in order to improve the convergence of the Block GMRES method, we have proposed the Weighted Block GMRES method based on the weighted minimal residual condition (9) for solving the linear systems with multiple right-hand sides (1). From our numerical experiments, we have learned that the Weighted Block GMRES(m) method is more robust than the Block GMRES(m) method.

For future work, we will compare the proposed method with other methods, e.g., the Weighted Global GMRES(m) method. We also need to investigate the specific definition of D for efficient convergence.

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References

[1] K. Jbilou, A. Messaoudi and H. Sadok, Global FOM and GMRES algorithms for matrix equations, Appl. Numer. Math., **31** (1999), 49–63.

[2] M. Heyouni and A. Essai, Matrix Krylov subspace methods for linear systems with multiple right-hand sides, Numer. Algorithms, **40** (2005), 137–156.

[3] A. El Guennouni, K. Jbilou and H. Sadok, A block version of BiCGSTAB for linear systems with multiple right-hand sides, Electron. Trans. Numer. Anal., **16** (2003), 129–142.

[4] B. Vital, Etude de quelques méthodes de résolution de problèmes linéaires de grande taille sur multiprocesseur, Ph. D. thesis, Univ. de Rennes I. Rennes, France, 1990.

[5] Y. Saad and M. H. Schultz, GMRES: A generalized minimal residual algorithm for solving nonsymmetric linear systems, SIAM J. Sci. Stat. Comput., **7** (1986), 856–869.

[6] A. Essai, Weighted FOM and GMRES for solving nonsymmetric linear systems, Numer. Algorithms, **18** (1998), 277–292.

[7] M. H. Gutknecht, Block Krylov space methods for linear systems with multiple right-hand sides: an introduction, in: Modern Mathematical Models, Methods and Algorithms for Real World Systems, A. H. Siddiqi et al. eds., pp. 420–447, Anamaya Publishers, New Delhi, India, 2007.

[8] H. Tadano and T. Sakurai, Numerical solvers for solving linear systems with multiple right-hand sides (in Japanese), OYOSURI, **21** (2011), 276–288.

[9] The University of Florida Sparse Matrix Collection, `http://www.cise.ufl.edu/research/sparse/matrices/`.