A New Block Krylov Subspace Method for Computing High Accuracy Solutions

Hiroto TADANO[1)], Tetsuya SAKURAI[1)], and Yoshinobu KURAMASHI[2)]
1) Department of Computer Science, University of Tsukuba, 1-1-1 Tennodai, Tsukuba, Ibaraki 305-8573, Japan
2) Graduate School of Pure and Applied Sciences, University of Tsukuba, 1-1-1 Tennodai, Tsukuba, Ibaraki 305-8571, Japan
E-mail: {tadano, sakurai}@cs.tsukuba.ac.jp, kuramasi@het.ph.tsukuba.ac.jp

Abstract

In this paper, the influence of errors which arise in matrix multiplications on the accuracy of approximate solutions generated by the Block BiCGSTAB method is analyzed. In order to generate high accuracy solutions, a new Block Krylov subspace method is also proposed. Some numerical experiments illustrate that high accuracy solutions can be obtained by using the proposed method compared with the Block BiCGSTAB method.

Keywords: Block Krylov subspace methods, Block BiCGSTAB, linear systems with multiple right hand sides, high accuracy solutions

1 Introduction

Linear systems with multiple right hand sides

$$AX = B, \tag{1}$$

where $A \in \mathbb{C}^{n\times n}$, $X, B \in \mathbb{C}^{n\times L}$, appear in many scientific applications such as lattice quantum chromodynamics (lattice QCD) calculation of physical quantities [1], an eigensolver using contour integration [6]. To solve these linear systems, some Block Krylov subspace methods (e.g. Block BiCG [5], Block BiCGSTAB [3], Block QMR [2]) have been proposed.

Block Krylov subspace methods can compute approximate solutions of linear systems with multiple right hand sides efficiently compared with Krylov subspace methods for single right hand side [2]. However, the difference between the residual generated by the recursion of the Block BiCGSTAB method and the true residual may arise. In this paper, this difference which arises in the Block BiCGSTAB method is analyzed. Then, a new Block Krylov subspace method for computing high accuracy approximate solutions of (1) is also proposed.

This paper is organized as follows. In Section 2, a matrix-valued polynomial and an operation are defined. The Block BiCGSTAB method is briefly described in Section 3. In Section 4, the influence of errors which arise in matrix multiplications on the accuracy of approximate solutions of the Block BiCGSTAB method. In Section 5, a new Block Krylov subspace method is proposed for computing high accuracy approximate solutions. Then the true residual of the proposed method is also evaluated. In Section 6, the true residual norm of the Block BiCGSTAB method and the proposed method is verified by numerical experiments. The paper is concluded in Section 7.

2 Matrix-valued polynomial

Let $\mathcal{M}_k(z)$ be a matrix-valued polynomial of degree k defined by

$$\mathcal{M}_k(z) \equiv \sum_{j=0}^{k} z^j M_j,$$

where $M_j \in \mathbb{C}^{L\times L}$ and $z \in \mathbb{C}$. The operation $\circ$ is used in this paper for the multiplication

$$\mathcal{M}_k(A) \circ V \equiv \sum_{j=0}^{k} A^j V M_j,$$

where $V \in \mathbb{C}^{n\times L}$. This operation satisfies the following properties [3].

Proposition 2.1. *Let $\mathcal{M}(z)$ and $\mathcal{N}(z)$ be matrix-valued polynomials of degree k and let V and ξ be an $n \times L$ matrix and an $L \times L$ matrix, respectively. Then, the following properties are satisfied.*
(1) $(\mathcal{M}(A) \circ V)\xi = (\mathcal{M}\xi)(A) \circ V$,
(2) $(\mathcal{M} + \mathcal{N})(A) \circ V = \mathcal{M}(A) \circ V + \mathcal{N}(A) \circ V$.

3 The Block BiCGSTAB method

The $(k+1)$-th residual $R_{k+1} \in \mathbb{C}^{n\times L}$ of the Block BiCGSTAB method is defined by

$$R_{k+1} = B - AX_{k+1} \equiv (\mathcal{Q}_{k+1}\mathcal{R}_{k+1})(A) \circ R_0, \tag{2}$$

where $R_0 = B - AX_0$ is an initial residual. The matrix-valued polynomial $\mathcal{R}_{k+1}(z)$ of degree $(k+1)$ which appears in (2) can be computed by the following recursions

$$\begin{aligned}
\mathcal{R}_0(z) &= \mathcal{P}_0(z) = I_L,\\
\mathcal{R}_{k+1}(z) &= \mathcal{R}_k(z) - z\mathcal{P}_k(z)\alpha_k,\\
\mathcal{P}_{k+1}(z) &= \mathcal{R}_{k+1}(z) + \mathcal{P}_k(z)\beta_k,
\end{aligned}$$

where $\mathcal{P}_{k+1}(z)$ is an auxiliary matrix-valued polynomial of degree $(k+1)$, I_L is an $L \times L$ identity matrix, α_k and β_k are $L \times L$ complex matrices. The polynomial $\mathcal{Q}_{k+1}(z)$ of degree $(k+1)$ can be computed by

$$\begin{aligned}
\mathcal{Q}_0(z) &= 1,\\
\mathcal{Q}_{k+1}(z) &= (1 - \zeta_k z)\mathcal{Q}_k(z),
\end{aligned}$$

where $\zeta_k \in \mathbb{C}$. The residual R_{k+1} can be computed by the following recursions,

$$\begin{aligned}
R_{k+1} &= T_k - \zeta_k A T_k, &(3)\\
P_{k+1} &= R_{k+1} + (P_k - \zeta_k A P_k)\beta_k,\\
T_k &= R_k - A P_k \alpha_k, &(4)
\end{aligned}$$

$X_0 \in \mathbb{C}^{n \times L}$ is an initial guess,
Compute $R_0 = B - AX_0$,
Set $P_0 = R_0$,
Choose $\tilde{R}_0 \in \mathbb{C}^{n \times L}$,
For $k = 0, 1, \ldots,$ **until** $\|R_k\|_{\mathrm{F}} \le \varepsilon \|B\|_{\mathrm{F}}$ **do:**

$V_k = AP_k$,
Solve $(\tilde{R}_0^{\mathrm{H}} V_k)\alpha_k = \tilde{R}_0^{\mathrm{H}} R_k$ for α_k,
$T_k = R_k - V_k \alpha_k$,
$Z_k = AT_k$,
$\zeta_k = \mathrm{Tr}\left[Z_k^{\mathrm{H}} T_k\right] / \mathrm{Tr}\left[Z_k^{\mathrm{H}} Z_k\right]$,
$X_{k+1} = X_k + P_k \alpha_k + \zeta_k T_k$,
$R_{k+1} = T_k - \zeta_k Z_k$,
Solve $(\tilde{R}_0^{\mathrm{H}} V_k)\beta_k = -\tilde{R}_0^{\mathrm{H}} Z_k$ for β_k,
$P_{k+1} = R_{k+1} + (P_k - \zeta_k V_k)\beta_k$,

End

Figure 1: Algorithm of the Block BiCGSTAB method.

where matrices P_{k+1} and T_k are defined by $P_{k+1} \equiv (\mathcal{Q}_{k+1}\mathcal{P}_{k+1})(A) \circ R_0$ and $T_k \equiv (\mathcal{Q}_k \mathcal{R}_{k+1})(A) \circ R_0$, respectively. From Eqs. (2), (3), and (4), recursion for the approximate solution X_{k+1} can be obtained by

$$X_{k+1} = X_k + P_k \alpha_k + \zeta_k T_k. \tag{5}$$

The $L \times L$ matrices α_k and β_k are determined so that bi-orthogonal conditions:

$$\tilde{R}_0^{\mathrm{H}} A^j (\mathcal{R}_k(A) \circ R_0) = O_L, \; j = 0, 1, \ldots, k-1, \tag{6}$$

$$\tilde{R}_0^{\mathrm{H}} A^{j+1} (\mathcal{P}_k(A) \circ R_0) = O_L, \; j = 0, 1, \ldots, k-1, \tag{7}$$

are satisfied. Here, $\tilde{R}_0$ is an $n \times L$ nonzero matrix, O_L is an $L \times L$ zero matrix, and $\| \cdot \|_{\mathrm{F}}$ denotes the Frobenius norm of a matrix. The scalar parameter ζ_k is determined so that $\|R_{k+1}\|_{\mathrm{F}}$ is minimized. Fig. 1 shows the algorithm of the Block BiCGSTAB method. Here, $\mathrm{Tr}[\,\cdot\,]$ denotes the trace of a matrix, and $\varepsilon > 0$ is a sufficiently small value for the stopping criterion.

4 Evaluation of the true residual of the Block BiCGSTAB method

In this section, it is assumed that computation errors arise in the multiplications with $\alpha_0, \alpha_1, \ldots, \alpha_k$ which appear in the Block BiCGSTAB method. The influence of these errors on the true residual of the Block BiCGSTAB method is considered. A matrix enclosed by a symbol $\langle \cdot \rangle$ denotes the perturbed matrix. Throughout this section, it is assumed that no calculation errors arise except for multiplications with $\alpha_0, \alpha_1, \ldots, \alpha_k$.

The perturbed matrices $\langle P_j\alpha_j\rangle$ and $\langle (AP_j)\alpha_j\rangle$ are required for the computation of X_{j+1} and R_{j+1}, respectively. These matrices can be written as follows:

$$\langle P_j\alpha_j\rangle = P_j\alpha_j + F_j, \tag{8}$$
$$\langle (AP_j)\alpha_j\rangle = AP_j\alpha_j + G_j, \tag{9}$$

where F_j and G_j denote error matrices.

From Eqs. (5) and (8), X_{k+1} is written as

$$\begin{aligned} X_{k+1} &= X_k + \langle P_k\alpha_k\rangle + \zeta_k T_k \\ &= X_k + P_k\alpha_k + \zeta_k T_k + F_k \\ &= X_0 + \sum_{j=0}^{k} (P_j\alpha_j + \zeta_j T_j) + \sum_{j=0}^{k} F_j. \end{aligned} \tag{10}$$

By using the Eq. (9), the residual R_{k+1} generated by the recursion (3) is also written as

$$\begin{aligned} R_{k+1} &= R_k - \langle (AP_k)\alpha_k\rangle - \zeta_k AT_k \\ &= R_k - AP_k\alpha_k - \zeta_k AT_k - G_k \\ &= R_0 - \sum_{j=0}^{k} (AP_j\alpha_j + \zeta_j AT_j) - \sum_{j=0}^{k} G_j. \end{aligned} \tag{11}$$

By using Eqs. (10) and (11), the true residual $B - AX_{k+1}$ of the Block BiCGSTAB method is given by

$$\begin{aligned} B - AX_{k+1} &= R_0 - \sum_{j=0}^{k} (AP_j\alpha_j + \zeta_j AT_j) - \sum_{j=0}^{k} AF_j \\ &= R_{k+1} + \sum_{j=0}^{k} E_j, \end{aligned} \tag{12}$$

where the matrix E_j is defined by $E_j \equiv G_j - AF_j$. From Eqs. (8) and (9), the matrix E_j can be represented by

$$E_j = \langle (AP_j)\alpha_j\rangle - A\langle P_j\alpha_j\rangle.$$

The error matrices $E_0, E_1, \ldots, E_k$ appear in (12) when the computation errors occur in the multiplications with $\alpha_0, \alpha_1, \ldots, \alpha_k$. The Eq. (12) implies that the true residual $B - AX_{k+1}$ of the Block BiCGSTAB method approaches to $\sum_{j=0}^{k} E_j$ when the residual norm $\|R_{k+1}\|_{\mathrm{F}}$ is sufficiently small.

5 Derivation of a new Block Krylov subspace method

The matrices F_j and G_j give adverse effects to the true residual of Block BiCGSTAB. To negate the influence of these matrices, a condition $G_j = AF_j$ should be satisfied. In this section, a new Block Krylov subspace method is proposed to compute high accuracy solutions.

5.1 Construction of an algorithm

There are two ways of constructing the recursion for the residual $R_{k+1} = (\mathcal{Q}_{k+1}\mathcal{R}_{k+1})(A) \circ R_0$. In the Block BiCGSTAB method, firstly, the polynomial $\mathcal{Q}_{k+1}(z)$ is expanded. In this case, as shown in the Eq. (12), the true residual $B - AX_{k+1}$ is not equal to the residual R_{k+1} generated by the recursion. In the proposed method, firstly, the polynomial $\mathcal{R}_{k+1}$ is expanded for computing $\mathcal{Q}_{k+1}\mathcal{R}_{k+1}$. The recursion of this polynomial is given by

$$\mathcal{Q}_{k+1}\mathcal{R}_{k+1} = \mathcal{Q}_k\mathcal{R}_k - \zeta_k z\mathcal{Q}_k\mathcal{R}_k - z\mathcal{Q}_{k+1}\mathcal{P}_k\alpha_k.$$

The polynomials $\mathcal{Q}_{k+1}\mathcal{R}_k$ and $\mathcal{Q}_{k+1}\mathcal{P}_{k+1}$ are computed by the following recursions:

$$\begin{aligned} \mathcal{Q}_{k+1}\mathcal{P}_k &= \mathcal{Q}_k\mathcal{P}_k - \zeta_k z\mathcal{Q}_k\mathcal{P}_k, \\ \mathcal{Q}_{k+1}\mathcal{P}_{k+1} &= \mathcal{Q}_{k+1}\mathcal{R}_{k+1} + \mathcal{Q}_{k+1}\mathcal{P}_k\beta_k. \end{aligned}$$

From the above recursions, the residual R_{k+1} and auxiliary matrices can be computed by

$$\begin{aligned} R_{k+1} &= R_k - \zeta_k AR_k - AU_k, && (13) \\ P_{k+1} &= R_{k+1} + U_k\alpha_k^{-1}\beta_k, && (14) \\ S_k &= P_k - \zeta_k AP_k, \end{aligned}$$

where $S_k \equiv (\mathcal{Q}_{k+1}\mathcal{P}_k)(A) \circ R_0$ and $U_k \equiv S_k\alpha_k$. By Eqs. (2) and (13), the recursion for X_{k+1} can be obtained by

$$X_{k+1} = X_k + \zeta_k R_k + U_k. \tag{15}$$

Matrices α_k and β_k are determined so that bi-orthogonality conditions (6) and (7) are satisfied. From the Eq. (6), the matrix α_k can be computed by

$$\alpha_k = (\tilde{R}_0^{\mathrm{H}} AP_k)^{-1}\tilde{R}_0^{\mathrm{H}} R_k. \tag{16}$$

By the bi-orthogonality condition (7) and the relation

$$\tilde{R}_0^{\mathrm{H}} R_{k+1} = -\zeta_k\tilde{R}_0^{\mathrm{H}} AT_k,$$

the matrix β_k can be obtained by

$$\beta_k = (\tilde{R}_0^{\mathrm{H}} AP_k)^{-1}\tilde{R}_0^{\mathrm{H}} R_{k+1}/\zeta_k. \tag{17}$$

The matrix $\gamma_k \equiv \alpha_k^{-1}\beta_k$ is appeared in the Eq. (14). By using Eqs. (16) and (17), γ_k can be obtained by

$$\gamma_k = (\tilde{R}_0^{\mathrm{H}} R_k)^{-1}\tilde{R}_0^{\mathrm{H}} R_{k+1}/\zeta_k.$$

If the parameter ζ_k is determined so that $\|R_{k+1}\|_{\mathrm{F}}$ is minimized, then extra multiplications with A are required in the proposed method. To avoid the multiplications with A, the parameter ζ_k is computed by

$$\zeta_k = \mathrm{Tr}\left[(AR_k)^{\mathrm{H}} R_k\right] / \mathrm{Tr}\left[(AR_k)^{\mathrm{H}} AR_k\right].$$

In the proposed method, the three multiplications with A are required in each iteration. To reduce the number of multiplications with A, the matrix AP_{k+1} is computed by the following recursion

$$AP_{k+1} = AR_{k+1} + AU_k\gamma_k.$$

The proposed method can be summarized in Fig. 2.

$X_0 \in \mathbb{C}^{n\times L}$ is an initial guess,
Compute $R_0 = B - AX_0$,
Set $P_0 = R_0$ and $V_0 = W_0 = AR_0$,
Choose $\tilde{R}_0 \in \mathbb{C}^{n\times L}$,
For $k = 0, 1, \ldots,$ **until** $\|R_k\|_\mathrm{F} \le \varepsilon \|B\|_\mathrm{F}$ **do:**
Solve $(\tilde{R}_0^\mathrm{H} V_k)\alpha_k = \tilde{R}_0^\mathrm{H} R_k$ for α_k,
$\zeta_k = \mathrm{Tr}\left[W_k^\mathrm{H} R_k\right] / \mathrm{Tr}\left[W_k^\mathrm{H} W_k\right]$,
$S_k = P_k - \zeta_k V_k$,
$U_k = S_k \alpha_k$,
$Y_k = AU_k$,
$X_{k+1} = X_k + \zeta_k R_k + U_k$,
$R_{k+1} = R_k - \zeta_k W_k - Y_k$,
$W_{k+1} = AR_{k+1}$,
Solve $(\tilde{R}_0^\mathrm{H} R_k)\gamma_k = \tilde{R}_0^\mathrm{H} R_{k+1}/\zeta_k$ for γ_k,
$P_{k+1} = R_{k+1} + U_k\gamma_k$,
$V_{k+1} = W_{k+1} + Y_k\gamma_k$,
End

Figure 2: Algorithm of the proposed method.

5.2 Evaluation of the true residual

Similar to the previous section, assume that no calculation errors arise except for the multiplications with $\alpha_0, \alpha_1, \ldots, \alpha_k$. The multiplication with α_j is appeared in the computation of $U_j = S_j\alpha_j$. By using the symbol $\langle \quad \rangle$, the perturbed matrix $\langle S_j\alpha_j \rangle$ is represented by

$$\langle S_j\alpha_j \rangle = S_j\alpha_j + H_j, \tag{18}$$

where H_j is an error matrix. From Eqs. (15) and (18), the approximate solution X_{k+1} is written as

$$\begin{aligned} X_{k+1} &= X_k + \zeta_k R_k + \langle S_k\alpha_k \rangle \\ &= X_k + \zeta_k R_k + S_k\alpha_k + H_k \\ &= X_0 + \sum_{j=0}^{k} (\zeta_j R_j + S_j\alpha_j) + \sum_{j=0}^{k} H_j. \end{aligned} \tag{19}$$

By using Eqs. (13) and (19), R_{k+1} is represented by

$$\begin{aligned} R_{k+1} &= R_k - \zeta_k AR_k - A\langle S_k\alpha_k \rangle \\ &= R_k - \zeta_k AR_k - A[S_k\alpha_k + H_k] \\ &= R_0 - \sum_{j=0}^{k} (\zeta_j AR_j + AS_j\alpha_j) - \sum_{j=0}^{k} AH_j \end{aligned}$$

$$
\begin{aligned}
&= B - A\left[X_0 + \sum_{j=0}^{k}(\zeta_j R_j + S_j\alpha_j) + \sum_{j=0}^{k} H_j\right] \\
&= B - AX_{k+1}.
\end{aligned}
$$

By regarding the matrices H_j and AH_j as F_j and G_j, it is confirmed that the proposed method satisfies the condition $E_j = G_j - AF_j = O$.

6 Numerical experiments

Test matrices used in numerical experiments were PDE900, JPWH991, and CONF5.4-00L8X8-1000 [4]. The size and the number of nonzero elements of these matrices are shown in Table 1. The coefficient matrix of CONF5.4-00L8X8-1000 is constructed by $I_n - \kappa D$, where D is an $n \times n$ non-Hermitian matrix and κ is a real valued parameter. This parameter was set to 0.1782.

The initial solution X_0 was set to the zero matrix. The shadow residual $\tilde{R}_0$ was given by a random number generator. The right hand side B of (1) was given by $B = [\boldsymbol{e}_1, \boldsymbol{e}_2, \ldots, \boldsymbol{e}_L]$, where $\boldsymbol{e}_j$ is a j-th unit vector. The value ε for the stopping criterion was set to 1.0×10^{-14}.

All experiments were carried out in double precision arithmetic on CPU: Intel Core 2 Duo 2.4GHz, Memory: 4GBytes, Compiler: Intel Fortran ver. 10.1, Compile option: `-O3 -xT -openmp`. The multiplication with the coefficient matrix was parallelized by OpenMP.

The results of the Block BiCGSTAB method are shown in Table 2. In this Table, #Iter., Res, and True Res. denote the number of iterations, the relative residual norm $\|R_k\|_\mathrm{F}/\|B\|_\mathrm{F}$, and the true relative residual norm $\|B - AX_k\|_\mathrm{F}/\|B\|_\mathrm{F}$, respectively.

As shown in Table 2, the relative residual norms of the Block BiCGSTAB method were satisfied the convergence criterion. However, the true residual norms did not reach 10^{-14} when $L = 2, 4$.

The relation between the true relative residual norm and $\|\sum_{j=0}^{k} E_j\|_\mathrm{F}/\|B\|_\mathrm{F}$ for JPWH991 with $L = 4$ is shown in Fig. 3. The true relative residual norm became almost equal to the value $\|\sum_{j=0}^{k} E_j\|_\mathrm{F}/\|B\|_\mathrm{F}$. The Eq. (12) was verified through this numerical example.

The results of the proposed method are shown in Table 3. The true relative residual norms computed by the proposed method reached 10^{-14} except for JPWH991 with $L = 1$. By using the proposed method, high accuracy solutions can be obtained compared with the Block BiCGSTAB method.

Table 1: The size and the number of nonzero elements of test matrices. NNZ denotes the number of nonzero elements.

Matrix name	Size	NNZ
PDE900	900	4,380
JPWH991	991	6,027
CONF5.4-00L8X8-1000	49,152	1,916,928

Table 2: Results of the Block BiCGSTAB method.

PDE900				
L	#Iter.	Time/L [s]	Res.	True Res.
1	53	0.0096	4.8×10^{-15}	4.8×10^{-15}
2	46	0.0067	1.1×10^{-15}	2.0×10^{-13}
4	41	0.0031	4.8×10^{-15}	1.8×10^{-12}
JPWH991				
L	#Iter.	Time/L [s]	Res.	True Res.
1	56	0.0159	5.7×10^{-15}	1.2×10^{-14}
2	49	0.0083	8.3×10^{-15}	4.1×10^{-13}
4	43	0.0034	6.3×10^{-15}	5.9×10^{-12}
CONF5.4-00L8X8-1000				
L	#Iter.	Time/L [s]	Res.	True Res.
1	555	13.9408	8.9×10^{-15}	9.5×10^{-15}
2	452	7.5609	7.3×10^{-15}	2.5×10^{-13}
4	406	6.1544	8.7×10^{-15}	2.8×10^{-13}

Table 3: Results of the proposed method.

PDE900				
L	#Iter.	Time/L [s]	Res.	True Res.
1	53	0.0107	3.2×10^{-15}	3.3×10^{-15}
2	46	0.0051	1.1×10^{-15}	1.4×10^{-15}
4	45	0.0031	5.5×10^{-15}	5.6×10^{-15}
JPWH991				
L	#Iter.	Time/L [s]	Res.	True Res.
1	52	0.0134	8.4×10^{-15}	1.3×10^{-14}
2	51	0.0082	3.7×10^{-15}	6.1×10^{-15}
4	44	0.0035	1.5×10^{-15}	2.3×10^{-15}
CONF5.4-00L8X8-1000				
L	#Iter.	Time/L [s]	Res.	True Res.
1	555	14.2714	7.4×10^{-15}	8.5×10^{-15}
2	456	8.1093	5.6×10^{-15}	6.7×10^{-15}
4	386	6.0348	7.4×10^{-15}	8.6×10^{-15}

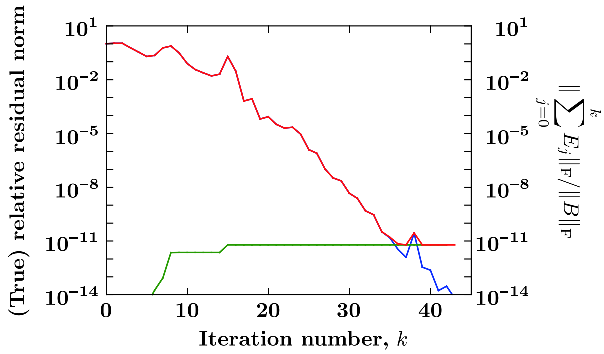

Figure 3: Relation between the true relative residual norm of Block BiCGSTAB and $\|\sum_{j=0}^{k} E_j\|_{\mathrm{F}}/\|B\|_{\mathrm{F}}$ (JPWH991, $L = 4$). — : true relative residual norm $\|B - AX_k\|_{\mathrm{F}}/\|B\|_{\mathrm{F}}$, — : relative residual norm $\|R_k\|_{\mathrm{F}}/\|B\|_{\mathrm{F}}$, — : $\|\sum_{j=0}^{k} E_j\|_{\mathrm{F}}/\|B\|_{\mathrm{F}}$.

7 Conclusions

In this paper, we have evaluated the true residual of the Block BiCGSTAB method when the computation errors arise in the multiplications with $\alpha_0, \alpha_1, \ldots, \alpha_k$. We have shown that the true residual of the Block BiCGSTAB method approaches to the sum of error matrices when the residual norm is sufficiently small. Then, we have proposed the new method for generating high accuracy approximate solutions. Through some numerical experiments, we have verified that the proposed method generates the high accuracy solutions compared with the Block BiCGSTAB method.

Acknowledgments

This work was supported by Grant-in-Aid for Young Scientists (Start-up) (No. 20800009).

References

[1] PACS-CS Collaboration, S. Aoki *et al.*, $2 + 1$ Flavor Lattice QCD toward the Physical Point, arXiv:0807.1661v1 [hep-lat].

[2] R. W. Freund, A Block QMR Algorithm for Non-Hermitian Linear Systems with Multiple Right-Hand Sides, Lin. Alg. Appl., Vol. 254, pp. 119–157, 1997.

[3] A. El Guennouni, K. Jbilou, and H. Sadok, A Block Version of BiCGSTAB for Linear Systems with Multiple Right-Hand Sides, Elec. Trans. Numer. Anal., Vol. 16, pp. 129–142, 2003.

[4] Matrix Market, `http://math.nist.gov/MatrixMarket/`

[5] D. P. O'Leary, The Block Conjugate Gradient Algorithm and Related Methods, Lin. Alg. Appl., Vol. 29, pp. 293–322, 1980.

[6] T. Sakurai, H. Tadano, T. Ikegami, and U. Nagashima, A Parallel Eigensolver Using Contour Integration for Generalized Eigenvalue Problems in Molecular Simulation, Tech. Rep. CS–TR–08–14, University of Tsukuba, 2008.