Analysis of the structure of the Krylov subspace in various preconditioned CGS algorithms

Shoji Itoh* and Masaaki Sugihara†

Abstract

An improved preconditioned CGS (PCGS) algorithm has recently been proposed, and it performs much better than the conventional PCGS algorithm. In this paper, the improved PCGS algorithm is verified as a coordinator to the left-preconditioned system; this is done by comparing, analyzing, and executing numerical examinations of various PCGS algorithms, including the most recently proposed one. We show that the direction of the preconditioned system for the CGS method is determined by the operations of $\alpha_k$ and $\beta_k$ in the PCGS algorithm. By comparing the logical structures of these algorithms, we show that the direction can be switched by the construction and setting of the initial shadow residual vector.

1 Introduction

The conjugate gradient squared (CGS) method [13] is one of various methods used to solve systems of linear equations

$$Ax = b,$$

where the coefficient matrix $A$ of size $n \times n$ is usually nonsymmetric, $x$ is the solution vector, and $b$ is the right-hand side (RHS) vector.

The CGS method is a bi-Lanczos method that belongs to the class of Krylov subspace methods. Bi-Lanczos-type methods are derived from the biconjugate gradient (BiCG) method [4, 10], which assumes the existence of a dual system $A^T x^\# = b^\#$ (we will refer to this as the “shadow system”). Bi-Lanczos-type algorithms have the advantage of requiring less memory than Arnoldi-type algorithms, which is another class of Krylov subspace methods. Furthermore, a variety of bi-Lanczos-type algorithms, such as the biconjugate gradient stabilized (BiCGStab) [15] and the generalized product-type method based on the BiCG (GPBiCG) [16], have been constructed by adopting the idea behind the derivation of the CGS. Various iterative methods, including bi-Lanczos-type algorithms, are often used following a preconditioning operation that is used to improve the properties of the linear equations. Such algorithms are called preconditioned algorithms; for example, the preconditioned CGS (PCGS). Therefore, it is very important to study the properties of the PCGS so that its performance can be improved.

Generally, the degree $k$ of the Krylov subspace generated by $A$ and $r_0$ is displayed as $K_k(A, r_0) = \text{span}\{r_0, A r_0, A^2 r_0, \ldots, A^{k-1} r_0\}$, where $r_0$ is the initial residual vector $r_0 = b - A x_0$, where $x_0$ is the initial guess at the solution. The Krylov subspace $K_k(A, r_0)$ generated by the $k$-th iteration forms the structure of $x_k \in x_0 + K_k(A, r_0)$, where $x_k$ is the approximate solution vector (or simply the “solution vector”). However, for a given preconditioned Krylov subspace method, there are various different algorithms that can be used for the preconditioning conversion. In such cases, the structure of the approximate solution formed by the Krylov subspace is often different for different algorithms, and the performance of these various algorithms can also differ substantially [8].

An improved PCGS algorithm has been proposed [8]. Reference [8] illustrates that this improved algorithm has many advantages over the conventional PCGS algorithms [1, 12, 15]. In this paper, a variety of PCGS algorithms are discussed. We begin by considering two typical PCGS algorithms, and we analyze the structure of the solution vector for each Krylov subspace. We then perform the
same analysis for two improved PCGS algorithms, one of which was mentioned above [8] and the other is presented in the present paper.

In this paper, when we refer to a \textit{preconditioned algorithm}, we mean one that uses a preconditioning operator \( M \) or a preconditioning matrix, and by \textit{preconditioned system}, we mean one that has been converted by some operator(s) based on \( M \). These terms never indicate the \textit{algorithm for the preconditioning operation itself}, such as incomplete LU decomposition or by using the approximate inverse. For example, under a preconditioned system, the original linear system \((1.1)\) becomes

\[
\tilde{A}\tilde{x} = \tilde{b},
\]

\[
\tilde{A} = M_L^{-1}AM_R^{-1}, \quad \tilde{x} = M_Rx, \quad \tilde{b} = M_L^{-1}b,
\]

with the preconditioner \( M = M_LM_R \) (\( M \approx A \)). In this paper, the matrix and the vector under the preconditioned system are denoted by the tilde (\( \tilde{\cdot} \)). However, the conversions in \((1.2)\) and \((1.3)\) are not implemented directly; rather, we construct the preconditioned algorithm that is equivalent to solving \((1.2)\).

This paper is organized as follows. Section 2 provides various preconditioned CGS algorithms; in particular, we consider right- and left-preconditioned systems for CGS algorithms. The improved PCGS algorithms are shown to be coordinative to the left-preconditioned system. Section 3 discusses properties of the various PCGS algorithms discussed in section 2, and we illustrate the effect of switching the direction of the preconditioned system for the CGS algorithm in section 3. Finally, our conclusions are presented in section 4.

### 2 Analyses of various PCGS algorithms

In this section, four kinds of PCGS algorithms are analyzed. These PCGS algorithms can be derived as follows.

\textbf{Algorithm 1. CGS method under preconditioned system:}

\( x_0 \) is the initial guess, \( \tilde{r}_0 = \tilde{b} - \tilde{A}x_0 \), set \( \beta_{PCGS}^0 = 0 \),

\( \left( \tilde{r}_0^\text{\#}, \tilde{r}_0 \right) \neq 0 \), e.g., \( \tilde{r}_0^\text{\#} = \tilde{r}_0 \),

For \( k = 0, 1, 2, \cdots \), until convergence, Do:

\[
\tilde{u}_k = \tilde{r}_k + \beta_{k-1}^\text{PCGS} \tilde{q}_{k-1},
\]

\[
\tilde{p}_k = \tilde{u}_k + \beta_{k-1}^\text{PCGS} (\tilde{q}_{k-1} + \beta_{k-1}^\text{PCGS} \tilde{p}_{k-1}),
\]

\[
\alpha_k^\text{PCGS} = \left( \tilde{r}_0^\text{\#}, \tilde{r}_k \right) / \left( \tilde{r}_0^\text{\#}, \tilde{A}\tilde{p}_k \right),
\]

\[
\tilde{q}_k = \tilde{u}_k - \alpha_k^\text{PCGS} \tilde{A}\tilde{p}_k,
\]

\[
\tilde{x}_{k+1} = \tilde{x}_k + \alpha_k^\text{PCGS} (\tilde{u}_k + \tilde{q}_k),
\]

\[
\tilde{r}_{k+1} = \tilde{r}_k - \alpha_k^\text{PCGS} \tilde{A}(\tilde{u}_k + \tilde{q}_k),
\]

\[
\beta_{k}^\text{PCGS} = \left( \tilde{r}_0^\text{\#}, \tilde{r}_{k+1} \right) / \left( \tilde{r}_0^\text{\#}, \tilde{r}_k \right),
\]

End Do

Any preconditioned algorithm can be derived by substituting the matrix with the preconditioner for the matrix with the tilde and the vectors with the preconditioner for the vectors with the tilde. Obviously, Algorithm 1 without the preconditioning conversion is the same as the CGS method. If \( \tilde{A} \) is a symmetric positive definite matrix and \( \tilde{r}_0^\text{\#} = \tilde{r}_0 \), then Algorithm 1 is mathematically equivalent to the conjugate gradient (CG) method [6] under a preconditioned system.
The case of (1.3) is called two-sided preconditioning, the case in which \( M_L = M \) and \( M_R = I \) is called left preconditioning, and the case in which \( M_L = I \) and \( M_R = M \) is called right preconditioning, where \( I \) denotes the identity matrix. We now formally define these [4].

**Definition 1** For the system and solution
\[
\begin{align*}
\tilde{A}x &= \tilde{b}, \\
A &= M_L^{-1}AM_R^{-1}, \quad \tilde{x} = M_Rx, \quad \tilde{b} = M_L^{-1}b,
\end{align*}
\]
we define the direction of a preconditioned system of linear equations as follows:

- The two-sided preconditioned system: Equation (1.3');
- The right-preconditioned system: \( M_L = I \) and \( M_R = M \) in (1.3');
- The left-preconditioned system: \( M_L = M \) and \( M_R = I \) in (1.3'),

where \( M \) is the preconditioner \( M = M_LM_R \) (\( M \approx A \)), and \( I \) is the identity matrix.

Other vectors in the solving method are not preconditioned. The initial guess is given as \( x_0 \), and \( \tilde{x}_0 = M_Rx_0 \).

The two-sided preconditioned system may be impracticable, but it is of theoretical interest.

The preconditioned system is different from the preconditioning conversion. There are various ways of performing a preconditioning conversion, but the direction of the preconditioned system is uniquely defined. (For example, see the preconditioning conversions (2.2) and (2.5) in Algorithm 2, Section 2.1.1.

Both the CGS and the PCGS extend the two-dimensional subspace in each iteration [2, 5], therefore, the Krylov subspace \( \mathcal{K}_{2k}(\tilde{A}, \tilde{r}_0) \) generated by the \( k \)-th iteration forms the structure of
\[
(2.1) \quad \tilde{x}_k \in \tilde{x}_0 + \mathcal{K}_{2k}(\tilde{A}, \tilde{r}_0).
\]

### 2.1 Two typical PCGS algorithms

In this subsection, we present two well-known and typical PCGS algorithms. One is a right-preconditioned system, although this is not always recognized, and the other is a left-preconditioned system. For both of these algorithms, we examine the structure of their Krylov subspace and the solution vector.

#### 2.1.1 Conventional right-preconditioned PCGS

This PCGS algorithm has been described in many manuscripts and numerical libraries, for example, see [1, 12, 15]. It is usually derived by the following preconditioning conversion [4].

\[
\begin{align*}
\tilde{A} &= M_L^{-1}AM_R^{-1}, \quad \tilde{x}_k = M_Rx_k, \quad \tilde{b} = M_L^{-1}b, \\
\tilde{r}_k &= M_L^{-1}r_k, \quad \tilde{r}_0 = M_L^{-1}r_0, \quad \tilde{p}_k = M_L^{-1}p_k, \quad \tilde{q}_k = M_L^{-1}q_k.
\end{align*}
\]

Finally, Algorithm 2 is derived.

**Algorithm 2.** Conventional PCGS algorithm:

- \( x_0 \) is the initial guess, \( r_0 = b - Ax_0 \), set \( \beta_{-1} = 0 \),
- \( (\tilde{r}_0, \tilde{r}_0) = (r_0^2, r_0) \neq 0 \), e.g., \( r_0^2 = r_0 \),
- For \( k = 0, 1, 2, \ldots \), until convergence, Do:

\[
\begin{align*}
u_k &= r_k + \beta_{k-1}q_{k-1} \\
p_k &= u_k + \beta_{k-1}(q_{k-1} + \beta_{k-1}p_{k-1})
\end{align*}
\]

---

1 Here, we have offered a general definition. However, for preconditioned bi-Lanczos-type algorithms, additional restrictions are necessary [2].

2 In this case, the initial shadow residual vector (ISR V) \( \tilde{r}_0^2 \) is converted to \( M_L^2r_0^2 \), but there is no problem with displaying \( M_L^2r_0^2 \) in the notation of the algorithm. However, its internal structure is \( r_0^{♯} = M^{-T}r_0^{♯} \). The notation \( r_0^{♯} \) will be discussed in section 3. The same applies to (2.4).
\[
\begin{align*}
\alpha_k &= \frac{(r_0^k, r_k)}{(r_0^k, AM^{-1} p_k)}, \\
q_k &= u_k - \alpha_k AM^{-1} p_k, \\
x_{k+1} &= x_k + \alpha_k M^{-1} (u_k + q_k), \\
r_{k+1} &= r_k - \alpha_k AM^{-1} (u_k + q_k), \\
\beta_k &= \frac{(r_0^k, r_{k+1})}{(r_0^k, r_k)},
\end{align*}
\]

(2.3)

End Do

The stopping criterion is

\[
\frac{\|r_{k+1}\|}{\|b\|} \leq \varepsilon.
\]

(2.4)

The results of this algorithm can also be derived by the following conversion:

\[
\begin{align*}
\tilde{A} &= AM^{-1}, \quad \tilde{x}_k = Mx_k, \quad \tilde{b} = b, \\
\tilde{r}_k &= r_k, \quad \tilde{r}_0^k = r_0^k, \quad \tilde{p}_k = p_k, \quad \tilde{u}_k = u_k, \quad \tilde{q}_k = q_k.
\end{align*}
\]

This is the same as using \(M_L = I\) and \(M_R = M\) in \(2.2\). Furthermore, this is the same as converting only \(\tilde{A}, \tilde{x}_k,\) and \(\tilde{b}\), that is, the right-preconditioned system.

2.1.2 Left-preconditioned CGS

The following conversion can be used to derive another PCGS algorithm:

\[
\begin{align*}
\tilde{A} &= M^{-1} A, \quad \tilde{x}_k = x_k, \quad \tilde{b} = M^{-1} b, \\
\tilde{r}_k &= r_k, \quad \tilde{r}_0^k = r_0^k, \quad \tilde{p}_k = p_k, \quad \tilde{u}_k = u_k, \quad \tilde{q}_k = q_k.
\end{align*}
\]

This is the same as applying \(M_L = M\) and \(M_R = I\) to \(\tilde{A}, \tilde{x}_k,\) and \(\tilde{b}\), that is, the left-preconditioned system.

Algorithm 3. Left-preconditioned CGS algorithm (Left-PCGS):

\[
\begin{align*}
&x_0 \text{ is the initial guess, } r_0^+ = M^{-1} (b - Ax_0), \text{ set } \beta_{-1} = 0, \\
&\left(\tilde{r}_0^k, \tilde{r}_0\right) = \left(r_0^k, r_0^+\right) \neq 0, \text{ e.g., } r_0^k = r_0^+ \\
&\text{For } k = 0, 1, 2, \cdots, \text{ until convergence, Do:} \\
&\quad u_k^+ = r_k^+ + \beta_{k-1} q_{k-1}^+, \\
&\quad p_k^+ = u_k^+ + \beta_{k-1} (q_{k-1}^+ + \beta_{k-1} p_{k-1}^+), \\
&\quad \alpha_k = \frac{(r_0^k, r_k^+)}{(r_0^k, M^{-1} A p_k^+)}, \\
&\quad q_k^+ = u_k^+ - \alpha_k M^{-1} A p_k^+, \\
&\quad x_{k+1} = x_k + \alpha_k (u_k^+ + q_k^+), \\
&\quad r_{k+1}^+ = r_k^+ - \alpha_k M^{-1} A (u_k^+ + q_k^+), \\
&\quad \beta_k = \frac{(r_0^k, r_{k+1}^+)}{(r_0^k, r_k^+)}. \\
&\text{End Do}
\end{align*}
\]

In this paper, \(r_k^+\) denotes the residual vector under the left-preconditioned system, its internal structure is \(r_k^+ \equiv M^{-1} r_k\), and this is the definition of \(r_k^+\). Note that \(p_k^+, u_k^+,\) and \(q_k^+\) achieve

\[\footnote{The notation \(r_k^+\) will be discussed in sections \(2.3\), \(2.4\) and \(3\) but there is no problem with displaying \(r_k^+\) in the notation of the algorithm. Note that this is also true for \(p_k^+, u_k^+,\) and \(q_k^+\).} \]
the same purpose. Here, $r_k^+ \in \text{Algorithm 3}$ provides different information to the residual vector $r_k = b - Ax_k$, and here, the stopping criterion is

$$\frac{\|r_{k+1}\|}{\|M^{-1}b\|} \leq \varepsilon.$$  

Note that this also different from (2.4), and this is an example of incomplete judging, because $r_{k+1}^+$ never provides important information about $b - Ax_k$.

This algorithm can also be derived by the following conversion:

$$\begin{align*}
\hat{A} &= M_L^{-1}AM_R^{-1}, \quad \hat{x}_k = M_Rx_k, \quad \hat{b} = M_L^{-1}b, \\
\hat{r}_k &= M_Rr_k^+, \quad \hat{r}_0^+ = M_R^{-1}r_0^+, \quad \hat{p}_k = M_Rp_k^+, \quad \hat{u}_k = M_Ru_k^+, \quad \hat{q}_k = M_Rq_k^+.
\end{align*}$$

If $M_L = M$ and $M_R = I$ are substituted into (2.8), then (2.6) is obtained.

### 2.1.3 Comparison between two typical PCGS algorithms

Here, we compare the conventional PCGS (Algorithm 2) with the left-PCGS (Algorithm 3); we will focus on the structures of their Krylov subspaces and the solution vectors.

The conventional PCGS (Algorithm 2) is the right-preconditioned system that is, $(AM^{-1})(Mx) = b$, and $r_k = b - (AM^{-1})(Mx_k)$. The relation between the Krylov subspace and the solution vector is

$$Mx_k \in Mx_0 + K_{2k}^R (AM^{-1}, r_0).$$

This means that the Krylov subspace $K_{2k}^R (AM^{-1}, r_0)$ generates the solution vector as $Mx_k$, not $x_k$ directly, but $x_k$ is calculated with corrections, as in (2.3) in Algorithm 2.

The left-PCGS (Algorithm 3) is $M^{-1}Ax = M^{-1}b$, $r_k^+ = M^{-1}(b - Ax_k)$. The relation between its Krylov subspace and the solution vector is

$$x_k \in x_0 + K_{2k}^L (M^{-1}A, r_0^+).$$

Therefore, the Krylov subspace $K_{2k}^L (M^{-1}A, r_0^+)$ generates the solution vector directly as $x_k$ (Algorithm 3).

These are summarized in Table 1.

It is important to note that the structures are different for the two Krylov subspaces, $K_{2k}^R (AM^{-1}, r_0)$ for the conventional PCGS (the right system) and $K_{2k}^L (M^{-1}A, r_0^+)$ of the left-PCGS, because their scalar parameters $\alpha_k$ and $\beta_k$ are not equivalent [8, 9]. We summarize this here; for details, see [9]. The recurrences of the BiCG under the preconditioned system are

$$\begin{align*}
R_0(\hat{\lambda}) &= 1, \quad P_0(\hat{\lambda}) = 1, \\
R_k(\hat{\lambda}) &= R_{k-1}(\hat{\lambda}) - \alpha_{k-1}^{PBiCG} \hat{\lambda} P_{k-1}(\hat{\lambda}), \\
P_k(\hat{\lambda}) &= R_k(\hat{\lambda}) + \beta_{k-1}^{PBiCG} P_{k-1}(\hat{\lambda}).
\end{align*}$$

Here, $R_k(\hat{\lambda})$ is the degree $k$ of the residual polynomial, and $P_k(\hat{\lambda})$ is the degree $k$ of the probing direction polynomial, that is, $\hat{r}_k = R_k(\hat{A})\hat{r}_0$ and $\hat{p}_k = P_k(\hat{A})\hat{r}_0$. For example, in the left-PCGS, (2.11) is shown as $R_k^L(\hat{\lambda}) = R_{k-1}^L(\hat{\lambda}) - \alpha_{k-1}^L \hat{\lambda} P_{k-1}^L(\hat{\lambda})$, so $\hat{r}_k \in K_{k+1}^L (\hat{A}, \hat{r}_0)$.

### 2.2 Improved preconditioned CGS algorithms

An improved PCGS algorithm has been proposed [8]. This algorithm retains some mathematical properties that are associated with the CGS derivation from the BiCG method under a non-preconditioned system. The improved PCGS algorithm from [8] will be referred to as “Improved1.” Another improved PCGS algorithm will be presented, and it will be referred to as “Improved2.” We note that Improved2 is mathematically equivalent to Improved1. The stopping criterion for both algorithms is (2.24).
2.2.1 The Improved1 PCGS algorithm (Improved1) [8]

Improved1 can be derived from the following conversion:

\[
\tilde{A} = M_L^{-1} A M_R^{-1}, \quad \tilde{x}_k = M_R x_k, \quad \tilde{b} = M_L^{-1} b,
\]

\[
\tilde{r}_k = M_L^{-1} r_k, \quad \tilde{r}_0^s = M_R^{-T} r_0^s, \quad \tilde{p}_k = M_R p_k^+, \quad \tilde{u}_k = M_R u_k^+, \quad \tilde{q}_k = M_R q_k^+. 
\]

Algorithm 4. Improved PCGS algorithm (Improved1):

1. \( x_0 \) is the initial guess, \( r_0 = b - A x_0 \), set \( \beta_{-1} = 0 \), \( \tilde{r}_0^s, \tilde{r}_0 \) = \( \tilde{r}_0^s, M^{-1} r_0 \) \( \neq 0 \), e.g., \( r_0^s = M^{-1} r_0 \).

2. For \( k = 0,1,2, \ldots \), until convergence, Do:

   \[
   u_k^+ = M^{-1} r_k + \beta_{k-1} q_{k-1}^+,
   \]

   \[
   p_k^+ = u_k^+ + \beta_{k-1} (q_{k-1}^+ + \beta_{k-1} p_{k-1}^+),
   \]

   \[
   \alpha_k = \begin{pmatrix} r_0^s, M^{-1} r_k \end{pmatrix},
   \]

   \[
   q_k^+ = u_k^+ - \alpha_k M^{-1} p_k^+,
   \]

   \[
   x_{k+1} = x_k + \alpha_k (u_k^+ + q_k^+),
   \]

   \[
   r_{k+1} = r_k - \alpha_k A (u_k^+ + q_k^+),
   \]

   \[
   \beta_k = \begin{pmatrix} r_0^s, M^{-1} r_{k+1} \end{pmatrix}. 
   \]

3. End Do

2.2.2 Improved2 PCGS algorithm (Improved2)

Improved2 can be derived from the following conversion:

\[
\hat{A} = M_L^{-1} A M_R^{-1}, \quad \hat{x}_k = M_R x_k, \quad \hat{b} = M_L^{-1} b,
\]

\[
\hat{r}_k = M_L^{-1} r_k, \quad \hat{r}_0^s = M_R^{-T} r_0^s, \quad \hat{p}_k = M_L^{-1} p_k, \quad \hat{u}_k = M_L^{-1} u_k, \quad \hat{q}_k = M_L^{-1} q_k. 
\]

Note that this conversion is different than (2.13) for \( \tilde{p}_k, \tilde{u}_k, \) and \( \tilde{q}_k \).

Algorithm 5. Another improved PCGS algorithm (Improved2):

1. \( x_0 \) is the initial guess, \( r_0 = b - A x_0 \), set \( \beta_{-1} = 0 \), \( \tilde{r}_0^s, \tilde{r}_0 \) = \( \tilde{r}_0^s, M^{-1} r_0 \) \( \neq 0 \), e.g., \( r_0^s = M^{-1} r_0 \).

2. For \( k = 0,1,2, \ldots \), until convergence, Do:

   \[
   u_k = r_k + \beta_{k-1} q_{k-1},
   \]

   \[
   p_k = u_k + \beta_{k-1} (q_{k-1} + \beta_{k-1} p_{k-1}),
   \]

   \[
   \alpha_k = \begin{pmatrix} M^{-T} r_0^s, r_k \end{pmatrix},
   \]

   \[
   q_k = M_L^{-1} q_k. 
   \]
\[ q_k = u_k - \alpha_k A M^{-1} p_k, \]
\[ x_{k+1} = x_k + \alpha_k M^{-1} (u_k + q_k), \]
\[ r_{k+1} = r_k - \alpha_k A M^{-1} (u_k + q_k), \]
\[ \beta_k = \frac{(M^{-T}r_0^+, r_{k+1})}{(M^{-T}r_0^+, r_k)}. \]

End Do

2.3 Analysis of the four kinds of PCGS algorithms

We will now analyze the four PCGS algorithms presented above.

We split the residual vector of the left-PCGS (Algorithm 3) \( r_k^+ \) into

\[ r_k^+ \mapsto M^{-1} r_k, \quad (k = 0, 1, 2, \ldots) \]

and give the necessary deformations; then the left-PCGS (Algorithm 3) is reduced to Improved1 (Algorithm 4). Alternatively, we can derive Algorithm 3 from Algorithm 4 by substituting \( M^{-1} r_k \) for \( r_k^+ \), that is, \( r_k^+ \equiv M^{-1} r_k \). By this means, we can explain the relationships between the four kinds of PCGS algorithms, as shown in Figure 1.

![Diagram](image)

Figure 1: Relations between the four different PCGS algorithms. \( \mapsto \) : Splitting left vector to right members (preconditioner and vector), \( \equiv \) : Substituting left vector for right members.

In addition, if we apply (2.15) to (2.10) for the structure of Krylov subspace of Algorithm 3 then

\[ \mathcal{K}_{2k}^L (M^{-1} A, r_0^+) \mapsto \mathcal{K}_{2k}^L (M^{-1} A, M^{-1} r_0) = M^{-1} \mathcal{K}_{2k}^L (AM^{-1}, r_0). \]

The structure of the solution vector for the Krylov subspace is then

\[ x_k \in x_0 + \mathcal{K}_{2k}^L (M^{-1} A, r_0^+) \mapsto x_k \in x_0 + M^{-1} \mathcal{K}_{2k}^L (AM^{-1}, r_0). \]

Therefore, the system of Improved1 (Algorithm 4) is coordinative to that of the left-PCGS (Algorithm 3), and Improved2 (Algorithm 5) is equivalent to Improved1 (Algorithm 4). Both algorithms have important advantages over the left-PCGS, because their residual vector is \( r_k \), and their stopping criterion is (2.4), not \( \| r_{k+1}^+ \| / \| M^{-1} b \| \).

Table 2 shows the structure of the residual vector and the structure of the solution vector for the Krylov subspace for each of the four PCGS algorithms.

In this summary, we see that the structures of the Krylov subspaces differ: \( \mathcal{K}_{2k}^R (AM^{-1}, r_0) \) of the conventional PCGS (the right-preconditioned system) is different from \( \mathcal{K}_{2k}^L (AM^{-1}, r_0) \) of both
improved PCGS (coordinative to the left-preconditioned systems), because the scalar parameters $\alpha_k$ and $\beta_k$ are not equivalent [8, 9].

Furthermore, there is superficially the same recurrence relation for the solution vector for both the conventional PCGS (Algorithm 2) and Improved2 (Algorithm 5): $x_{k+1} = x_k + \alpha_k M^{-1} (u_k + q_k)$. However, each recurrence relation belongs to a different system, because the components of the conventional PCGS are $\alpha_R^k$, $u_R^k$, and $q_R^k$, and those of Improved2 are $\alpha_L^k$, $u_L^k$, and $q_L^k$.

The structure of the residual vector of Improved1 (Algorithm 4) and Improved2 (Algorithm 5) is illustrated as $M^{-1} r_k = M^{-1} (b - (A M^{-1})(M x_k))$ in Table 2, because they are both from the left-PCGS and the structure of their Krylov subspace is $M^{-1} K_{2k} (A M^{-1}, r_0)$.

### 3 Congruence of preconditioning conversion, and direction of preconditioned system for the CGS

In a previous section, we defined the general direction of a preconditioned CGS system (see Definition 1). However, the direction of a preconditioned system is different from the direction of a preconditioning conversion. We will show that the direction of a preconditioned system is switched by the construction of the ISRV.

#### 3.1 Congruence of preconditioning conversion for PCGS

Here, we consider the congruence of a preconditioning conversion for PCGS in the following proposition.

**Proposition 1 (Congruency)** There is congruence to a PCGS algorithm in the direction of the preconditioning conversion.

**Proof** We have already shown instances of this. For example, Algorithm 2 can be derived by the two-sided conversion (2.2), and if $M_L = I$, $M_R = M$, and the conversion (2.2) is reduced to (2.9), then Algorithm 2 is derived. If $M_L = M$ and $M_R = I$, then Algorithm 2 can be derived. The other preconditioned algorithms (Algorithms 3, 4, and 5) and their corresponding preconditioning conversions are also the same.

Although this property has been repeatedly discussed in the literature, it should be considered when evaluating the direction of a preconditioned system.

#### 3.2 Direction of a preconditioned system and that of the PCGS

The direction of a preconditioned system is different from the direction of a preconditioning conversion.

**Proposition 2** The direction of a preconditioned system is determined by the operations of $\alpha_k$ and $\beta_k$ in each PCGS algorithm. These intrinsic operations are based on biorthogonality and biconjugacy.

**Proof**. The operations of biorthogonality and biconjugacy in each PCGS algorithm and the structure of the solution vector for each Krylov subspace are shown below. The underlined inner products are the actual operators for each PCGS.
Only the conventional PCGS (Algorithm 2) algorithm has the ISRV in the form $r_0^+$; in all other algorithms, it is $r_0^\ast$. The ISRV $r_0^\ast$ never splits as $M^{-T}r_0^\ast$ in this algorithm, and the preconditioned coefficient matrix for the biconjugacy is fixed as $AM^{-1}$, that is, the right-preconditioned system.

- **Conventional (Algorithm 2)**:
  \[
  r_0^\ast = r_0, \\
  \left(\tilde{r}_0^\ast, \tilde{r}_k\right) = \left(M_L^TR_0^\ast, M_L^{-1}r_k\right) = \left(r_0^\ast, r_k\right), \\
  \left(\tilde{r}_0^\ast, \tilde{A}p_k\right) = \left(M_L^TR_0^\ast, (M_L^{-1}AM_R^{-1})(M_L^{-1}p_k)\right) = \left(r_0^\ast, (AM^{-1})p_k\right).
  \]
  \[
  Mx_k \in Mx_0 + k_{2k}^L(AM^{-1}, r_0).\]

- **Left-PCGS (Algorithm 3)**:
  \[
  r_0^\ast = r_0^+, \\
  \left(\tilde{r}_0^\ast, \tilde{r}_k\right) = \left(r_0^+, r_k^+\right), \\
  \left(\tilde{r}_0^\ast, \tilde{A}p_k\right) = \left(r_0^+, (M^{-1}A)p_k^+\right), \\
  x_k \in x_0 + k_{2k}^L(AM^{-1}, r_0^+).\]

- **Improved1 (Algorithm 4)**:
  \[
  r_0^\ast = M^{-1}r_0, \\
  \left(\tilde{r}_0^\ast, \tilde{r}_k\right) = \left(M_R^{-T}r_0^\ast, M_L^{-1}r_k\right) = \left(r_0^\ast, M^{-1}r_k\right), \\
  \left(\tilde{r}_0^\ast, \tilde{A}p_k\right) = \left(M_R^{-T}r_0^\ast, (M_L^{-1}AM_R^{-1})(M_L^{-1}p_k)\right) = \left(r_0^\ast, (M^{-1}A)p_k^+\right), \\
  x_k \in x_0 + M^{-1}k_{2k}^L(AM^{-1}, r_0).\]

- **Improved2 (Algorithm 5)**:
  \[
  r_0^\ast = M^{-1}r_0, \\
  \left(\tilde{r}_0^\ast, \tilde{r}_k\right) = \left(M_R^{-T}r_0^\ast, M_L^{-1}r_k\right) = \left(M^{-T}r_0^\ast, r_k\right) = \left(r_0^\ast, M^{-1}r_k\right), \\
  \left(\tilde{r}_0^\ast, \tilde{A}p_k\right) = \left(M_R^{-T}r_0^\ast, (M_L^{-1}AM_R^{-1})(M_L^{-1}p_k)\right) = \left(M^{-T}r_0^\ast, (M^{-1}A)(M^{-1}p_k)\right), \\
  x_k \in x_0 + M^{-1}k_{2k}^L(AM^{-1}, r_0).\]

We present the following proposition and corollary.

**Proposition 3** On the structure of biorthogonality $(\tilde{r}_0^\ast, \tilde{r}_k)$ in the iterated part of each PCGS algorithm, there exists a single preconditioning operator between $r_k$ (basic form of the residual vector) and $r_0^\ast$ (basic form of the ISRV) such that $M^{-1}$ operates on $r_k$ or $M^{-T}$ operates on $r_0^\ast$.

**Proof.** We split $r_0^\ast \mapsto M^{-T}r_0^\ast$ and $r_k^+ \mapsto M^{-1}r_k$ in Algorithms 2 to 5 and obtain
\[
\left(\tilde{r}_0^\ast, \tilde{r}_k\right) = \left(r_0^\ast, r_k\right) \mapsto \left(M^{-T}r_0^\ast, r_k\right), \\
\left(\tilde{r}_0^\ast, \tilde{r}_k\right) = \left(r_0^\ast, r_k^+\right) \mapsto \left(r_0^\ast, M^{-1}r_k\right), \\
\left(\tilde{r}_0^\ast, \tilde{r}_k\right) = \left(r_0^\ast, M^{-1}r_k\right), \\
\left(\tilde{r}_0^\ast, \tilde{r}_k\right) = \left(M^{-T}r_0^\ast, r_k\right) = \left(r_0^\ast, M^{-1}r_k\right).\]
The underlined inner products are the actual operators for each PCGS.

In addition, for the two-sided conversion, we obtain

\[
\left( \tilde{r}_0^0, \tilde{r}_k \right) = \left( M_R^{T} \tilde{r}_0^0, M_L^{-1} r_k \right) = \left( M^{-T} r_0^0, r_k \right) = \left( r_0^0, M^{-1} r_k \right). \quad \Box
\]

**Corollary 1** On the structure of biconjugacy \((\tilde{r}_0^0, \tilde{A}\tilde{p}_k)\) in the iterated part of each PCGS algorithm, there exists a single preconditioning operator between \(A\) (coefficient matrix) and \(r_0^0\) (basic form of the ISRV), such that \(M^{-1}\) operates on \(A\) or \(M^{-T}\) operates on \(r_0^0\). Furthermore, there exists a single preconditioning operator between \(A\) and \(p_k\) (basic form of probing direction vector).

From Propositions 2 and 3 and Corollary 1, the intrinsic operations on the biorthogonality and the biconjugacy for the four PCGS algorithms have the same matrix and vector structures, even though the superficial descriptions of these algorithms are different.

### 3.3 ISRV switches the direction of the preconditioned system for the CGS

Although the mathematical properties of the conventional PCGS (Algorithm 2) and Improved2 (Algorithm 5) are quite different, the structures of these algorithms are very similar. This can be seen by replacing \(M^{-T} r_0^0\) with \(r_0^0\) in Algorithm 5 and in the initial part, we have

\[
(3.1) \quad \left( \tilde{r}_0^0, \tilde{r}_0 \right) = \left( M_R^{T} r_0^0, M_L^{-1} r_0 \right) = \left( M^{-T} r_0^0, r_0 \right)
\]

\[
= \left( r_0^0, r_0 \right) \neq 0, \quad \text{e.g., } r_0^0 = r_0;
\]

then Algorithm 5 becomes Algorithm 2.

**Theorem 1** The direction of a preconditioned system for the CGS method is switched by construction and setting of the ISRV.

**Proof.** Proposition 2 shows that the direction of a preconditioned system for the CGS algorithm is determined by the structures of the biorthogonality and the biconjugacy. Here, we show that their structures are switched by the ISRV. The underlined inner products are the actual operators for each PCGS.

- **ISRV1**: \( r_0^0 = M^{-1} r_0 \) (Based on left conversion)

\[
(3.2) \quad \left( \tilde{r}_0^0, \tilde{r}_0 \right) = \left( M_R^{T} r_0^0, M_L^{-1} r_0 \right) = \left( r_0^0, M^{-1} r_0 \right) \neq 0,
\]

\[
eq (r_0, r_0), \quad \text{e.g., } r_0^0 = M^{-1} r_0.
\]

- **ISRV2**: \( r_0^0 = M^T r_0 \) (Based on right conversion)

\[
(3.3) \quad \left( \tilde{r}_0^0, \tilde{r}_0 \right) = \left( M_R^{T} r_0^0, M_L^{-1} r_0 \right) = \left( M^{-T} r_0^0, r_0 \right) \neq 0,
\]

\[
eq (r_0^0, r_0), \quad \text{e.g., } M^{-T} r_0^0 = r_0 \rightarrow r_0^0 = M^T r_0.
\]

If we apply ISRV2 to Algorithm 5 then Algorithm 5 is equivalent to Algorithm 2 with \(r_0^0 = r_0\):

\[
\left( \tilde{r}_0^0, \tilde{r}_k \right) = \left( M^{-T} r_0^0, r_k \right) = (r_0, r_k),
\]

\[
\tilde{r}_0^0, \tilde{A}\tilde{p}_k = \left( M^{-T} r_0^0, A(M^{-1} p_k) \right) = (r_0, (AM^{-1}) p_k).
\]

Alternatively, if we apply \(r_0^0 = M^{-T} M^{-1} r_0\) (we will call this ISRV9) to Algorithm 2 then Algorithm 2 is equivalent to Algorithm 5 with ISRV1:

\[
\left( \tilde{r}_0^0, \tilde{r}_k \right) = \left( r_0^0, r_k \right) = (M^{-T}(M^{-1} r_0), r_k),
\]

\[
\tilde{r}_0^0, \tilde{A}\tilde{p}_k = \left( r_0^0, (AM^{-1}) p_k \right) = (M^{-T}(M^{-1} r_0), (AM^{-1}) p_k). \quad \Box
\]

If we change Improved2 (Algorithm 5) to Improved1 (Algorithm 1), then we will obtain the same results.

In the next section, Theorem 1 is verified numerically.
4 Numerical experiments

Convergence of the four PCGS algorithms of section 2 is confirmed in section 4.1 by evaluating three cases. Furthermore, in section 4.2, the ability of the ISRV to switch the direction of the preconditioned system (as discussed in section 3.3) and Theorem 1 are verified.

4.1 Comparison of the four PCGS algorithms

The test problems were generated by building real nonsymmetric matrices corresponding to linear systems taken from the University of Florida Sparse Matrix Collection [3] and the Matrix Market [11]. The RHS vector $b$ of (1.1) was generated by setting all elements of the exact solution vector $x^{\text{exact}}$ to 1.0 and substituting this into (1.1). The solution algorithm was implemented using the sequential mode of the Lis numerical computation library (version 1.1.2 [14]) in double precision, with the compiler options registered in the Lis "Makefile." Furthermore, we set the initial solution to $x_0 = 0$. The maximum number of iterations was set to 1000.

The numerical experiments were executed on a DELL Precision T7400 (Intel Xeon E5420, 2.5 GHz CPU, 16 GB RAM) running the Cent OS (kernel 2.6.18) and the Intel icc 10.1, ifort 10.1 compiler.

In all tests, ILU(0) was adopted as a preconditioning operation with each PCGS algorithm; here, the value “zero” means the fill-in level. The ISRVs were set as $r_0^\delta = r_0$ in the conventional PCGS (Algorithm 2), $r_0^\# = r_0^\dagger$ in the left-PCGS (Algorithm 3), and $r_0^{\delta} = M^{-1}r_0$ in Improved1 and Improved2 (Algorithms 4 and 5, respectively).

We considered the following three cases:

(a) Evaluating the algorithm relative residual (see Figure 2, 5, and Table 3);
(b) Evaluating the true relative residual (see Figure 3, 6, and Table 4);
(c) Evaluating the true relative error (see Figure 4, 7, and Table 5).

We adopted the following stopping criteria: For case (a), we adopted the 2-norm of (2.4) for Algorithms 2, 4, and 5, and we adopted the 2-norm of (2.7) for Algorithm 3. For case (b), we adopted $\| b - Ax_k \|_2 / \| b \|_2 \leq \varepsilon$ for all algorithms. For case (c), we adopted $\| x_k - x^{\text{exact}} \|_2 / \| x^{\text{exact}} \|_2 \leq \varepsilon$ for all algorithms. We set $\varepsilon = 10^{-12}$ for all cases.
Table 3: (a) Numerical evaluation using the relative residual of each algorithm. N is the problem size, and NNZ is the number of nonzero elements. The three numbers in each row for the column for each method are as follows: the leftmost number is the true relative residual $\log_{10}$ 2-norm, the number in parentheses is the number of iterations required to reach convergence, and the lower number is the true relative error $\log_{10}$ 2-norm.

| Matrix | N   | NNZ | Conventional (Algorithm 2) | Left-PCGS (Algorithm 3) | Improved1 (Algorithm 4) | Improved2 (Algorithm 5) |
|--------|-----|-----|-----------------------------|--------------------------|-------------------------|-------------------------|
| add32  | 4960| 19848| -12.17 (35)                  | -12.17                   | -12.04 (35)             | -12.04 (35)             |
|        |     |     |                             | -13.06 (37)              | -12.04 (35)             | -12.04 (35)             |
|        |     |     |                             | -12.96                   | -11.96                   | -11.96                   |
| bfwa782| 782 | 7514| -9.36 (93)                   | -12.37 (83)              | -12.82 (78)             | -12.17 (84)             |
|        |     |     |                             | -12.09                   | -12.48                   | -12.22                   |
|        |     |     | Breakdown                   | -11.83 (15)              | -12.44 (16)             | -12.44 (16)             |
|        |     |     |                             | -12.10                   | -12.53                   | -12.53                   |
|        |     |     | Breakdown                   | -12.17 (38)              | -12.20 (34)             | -12.21 (33)             |
|        |     |     |                             | -10.64                   | -8.05                    | -8.00                    |
|        |     |     | Breakdown                   | -12.11 (35)              | -9.77                    | -9.77                    |
|        |     |     | Breakdown                   | -12.11 (35)              | -9.77                    | -9.77                    |
|        |     |     | Breakdown                   | -12.11 (35)              | -9.77                    | -9.77                    |

Table 4: (b) Numerical evaluation using the true relative residual of each algorithm.

| Matrix | N   | NNZ | Conventional (Algorithm 2) | Left-PCGS (Algorithm 3) | Improved1 (Algorithm 4) | Improved2 (Algorithm 5) |
|--------|-----|-----|-----------------------------|--------------------------|-------------------------|-------------------------|
| add32  | 4960| 19848| -12.17 (35)                  | -12.17                   | -12.04 (35)             | -12.04 (35)             |
|        |     |     |                             | -12.17                   | -12.17                   | -12.17                   |
|        |     |     |                             | -13.06 (37)              | -12.04 (35)             | -12.04 (35)             |
|        |     |     |                             | -12.96                   | -12.04 (35)             | -12.04 (35)             |
|        |     |     |                             | -11.96                   | -11.96                   | -11.96                   |
| bfwa782| 782 | 7514| -9.36 (Stag.)               | -10.29                   | -12.37 (83)             | -12.17 (84)             |
|        |     |     |                             | -12.09                   | -12.48                   | -12.22                   |
|        |     |     | Breakdown                   | -11.83 (15)              | -12.44 (16)             | -12.44 (16)             |
|        |     |     |                             | -12.10                   | -12.53                   | -12.53                   |
|        |     |     | Breakdown                   | -12.17 (38)              | -12.20 (34)             | -12.21 (33)             |
|        |     |     |                             | -10.64                   | -8.05                    | -8.00                    |
|        |     |     | Breakdown                   | -12.11 (35)              | -9.77                    | -9.77                    |
|        |     |     | Breakdown                   | -12.11 (35)              | -9.77                    | -9.77                    |
|        |     |     | Breakdown                   | -12.11 (35)              | -9.77                    | -9.77                    |
|        |     |     | Breakdown                   | -12.11 (35)              | -9.77                    | -9.77                    |

12
Table 5: (c) Numerical evaluation using the true relative error of each algorithm.

| Matrix  | N   | NNZ  | Conventional (Algorithm 2) | Left-PCGS (Algorithm 3) | Improved1 (Algorithm 4) | Improved2 (Algorithm 5) |
|---------|-----|------|----------------------------|-------------------------|-------------------------|-------------------------|
| add32   | 4960| 19848| -12.17 (35)                | -12.00 (36)             | -12.00 (36)             | -12.00 (36)             |
| bfwa782 | 782 | 7514 | -10.36 (Stag.)             | -12.37 (83)             | -12.00 (77)             | -12.17 (84)             |
| jpwh_991| 991 | 6027 | Breakdown                  | -11.83 (15)             | -11.83 (15)             | -11.83 (15)             |
| olm5000 | 5000| 19996| -0.18 (Stag.)              | -12.79 (Stag.)          | -12.80 (49)             | -12.59 (52)             |
| poisson3Db | 85623 | 2374949 | -10.14 (111)            | -11.24 (111)           | -11.61 (117)          | -11.53 (116)          |
| sherman4| 1104| 3786 | -12.69 (34)                | -11.68 (32)             | -11.68 (32)             | -11.68 (32)             |
| wang4   | 26068| 177196| -12.48 (Stag.)           | -13.37 (68)            | -12.80 (66)           | -12.83 (66)           |
| watt_1  | 1856| 11360| -18.06 (41)                | -14.28 (40)             | -14.26 (40)             | -14.26 (40)             |

We will first focus on the results of the conventional PCGS (Algorithm 2), as shown in Tables 3 to 5. Breakdown occurs for *jpwh_991*, and stagnation occurs for *olm5000* at pitifully insufficient accuracy, although the other three algorithms (Algorithms 3 to 5) were able to solve them.

Next, it is very important to compare cases (a) and (b) (Tables 3 and 4) with case (c) (Table 5), in order to determine the crucial ways in which they differ. Because (a) and (b) can be evaluated without knowing the exact solution but (c) requires the exact solution, it is important to examine the results when the exact solution is known. Comparing the results for *bfwa782*, *poisson3Db*, and *watt_1* in cases (a) and (b) (Tables 3 and 4), the conventional PCGS (Algorithm 2) has results in which the true relative residual or true relative error (or both) are much less accurate than those obtained by the other algorithms, and only in the conventional PCGS does stagnation occur at insufficient accuracy. In particular, the conventional PCGS is the fastest to converge for *watt_1* in cases (a) and (b) (Tables 3 and 4), but this is undesirable, because when it converges too quickly, evaluating by the relative residual and by the true relative residual to satisfy the accuracy. On the other hand, evaluating by the true relative error in the case of (c) (Table 5), the conventional PCGS converges after almost the same number of iterations as do the other methods.

Next, in contrast, the results of the conventional PCGS with *wang4* gave the most accurate true relative error for cases (a) and (b) (Tables 3 and 4), but the conventional PCGS stagnated with *wang4*, and this resulted in the lowest accuracy for case (c) (Table 5).

From the graphs in Figures 2 to 7, we can see the following: in case (a), Improved1, Improved2, and the left-PCGS show different convergence behaviors, but in cases (b) and (c), they show similar behaviors. These results correspond to the analysis in section 2.3. Therefore, Algorithms 4 and 5 are coordinative to Algorithm 3 regarding the structure of the solution vector for the generated Krylov subspace, in spite of the difference between the residual vectors: \( r_k \) for the left-PCGS (Algorithm 3) and \( r_k^\dagger \) for Improved1 and Improved2 (Algorithms 4 and 5, respectively). The conventional PCGS had a convergence behavior that differs from those of all of the other algorithms for all cases (a) to (c).

These numerical results conform to the behavior expected from the discussion of the relation between the structure of solution vector and the Krylov subspace. We compared the numerical

---

5 The row marked *olm5000* in all tables contains the results after 1000 iterations; furthermore, *olm5000* by Algorithm 2 stagnated after 5000 iterations, due to the size of the matrix.

6 The results of *poisson3Db* with Improved2 in Table 4 and *olm5000* with the left-PCGS in Table 5 can be considered to be sufficiently accurate, because they were almost convergence with being close to \( 10^{-12} \). We note that \( \varepsilon = 10^{-12} \) is a stringent value for the tolerance for the true relative residual and the true relative error.
Figure 2: (a) Convergence histories of the algorithm relative residual 2-norm for each of the four algorithms (sherman4).

Figure 3: (b) Convergence histories of the true relative residual 2-norms (sherman4) for each of the four algorithms.

Figure 4: (c) Convergence histories of the true relative error 2-norm (sherman4) for each of the four algorithms.
Figure 5: (a) Convergence histories of the algorithm relative residual 2-norm (watt_1) for each of the four algorithms.

Figure 6: (b) Convergence histories of the true relative residual 2-norm (watt_1) for each of the four algorithms.

Figure 7: (c) Convergence histories of the true relative error 2-norm (watt_1) for each of the four algorithms.
results with the theoretical results of sections 2.1.3 and 2.3, and these are summarized as follows:

1. For case (a), the difference between the residual vector \( r_k^+ \) of the left-PCGS and \( r_k \) has been verified.

2. For cases (b) and (c), we verified (2.16):
   \[
   x_k \in x_0 + K_{2k}^L (M^{-1}A, r_0^+) \rightarrow x_k \in x_0 + M^{-1}K_{2k}^L (AM^{-1}, r_0).
   \]

3. The differences between the conventional PCGS and the left-PCGS, Improved1, Improved2 have been confirmed through their convergence behaviors. That is, the relation of the solution vector and the Krylov subspace between the right system (the conventional PCGS) and the left-PCGS, the coordinative PCGSs to the left-PCGS (Improved1 and Improved2).

4.2 Behavior of the PCGS when it is switched by the ISRV

In this subsection, the experimental environment was same as that described in section 4.1, except that we used Matlab 7.8.0 (R2009a), and we gave different ISRVs to the conventional PCGS and Improved1.

We compared five different PCGS algorithms, including using a different ISRV. In the figures, we use the following labels. “Conventional” means the conventional PCGS (Algorithm 2), for which the ISRV is \( r_0^+ = r_0 \); this is a right-preconditioned system. “Impr1-ISRV1” means Improved1 (Algorithm 4) with ISRV1: \( r_0^+ = M^{-1}r_0 \). “Impr1-ISRV2” means Improved1 with ISRV2: \( r_0^+ = M^T r_0 \). “Left” means the left-PCGS (Algorithm 3), for which the ISRV is \( r_0^+ = r_0^+ \). “Conv-ISRV9” means the conventional PCGS with ISRV9: \( r_0^+ = M^{-T}M^{-1}r_0 \).

The convergence histories of “Conventional,” “Impr1-ISRV1,” and “Left” in both figures are the same as those of “Conventional,” “Improved1,” and “Left-PCGS,” respectively, in Figures 3 and 6.

In both figures, “Impr1-ISRV2” and “Conv-ISRV9” were added to verify Theorem1. The convergence history of “Impr1-ISRV2” is the same as that of “Conventional,” and those of “Impr1-ISRV1” and “Conv-ISRV9” are the same as that of “Left.”

We have numerically verified the discussion in section 3 in particular, we have verified Theorem1.

5 Conclusions

In this paper, an improved PCGS algorithm [8] has been analyzed by mathematically comparing four different PCGS algorithms, and we have focused on the structures of their Krylov subspace and the solution vector. From our analysis and numerical results, we have verified two improved PCGS algorithms. They are both coordinative to the left-preconditioned systems, although their residual vector maintains the basic form \( r_k^+ \), not \( r_k^+ \). For both algorithms, the structures of their Krylov subspace and the solution vector are \( x_k \in x_0 + M^{-1}K_{2k}^L (AM^{-1}, r_0) \). Further, the numerical results of the improved PCGS with the ILU(0) preconditioner show many advantages, such as effectiveness and consistency across several preconditioners, have also been shown; see [8].

We presented a general definition of the direction of a preconditioned system of linear equations. Furthermore, we have shown that the direction of a preconditioned system for CGS is switched by the construction and setting of the ISRV. This is because the direction of the preconditioning conversion is congruent. We have also shown that the direction of a preconditioned system for CGS is determined by the operations of \( \alpha_k \) and \( \beta_k \), and these intrinsic operations are based on biorthogonality and biconjugacy. However, the structures of these intrinsic operations are the same in all four of the PCGS algorithms. Therefore, we have focused on the ability of the ISRV to switch the direction of a preconditioned system, and such a mechanism may be unique to the bi-Lanczos-type algorithms that are based on the BiCG method.

As we analyzed the four PCGS algorithms, we paid particular attention to the vectors. We note that there exist preconditioned BiCG (PBiCG) algorithms that correspond to the preconditioning conversion of each of the PCGS algorithms. The polynomial structure of the PBiCG can be minutely analyzed by replacing the vectors of the PCGS. We have analyzed the four PBiCG algorithms in parallel [9], and each PBiCG corresponds to one of the four PCGS algorithms in this paper. In [9], using the ISRV to switch the direction of a preconditioned system was discussed in detail.
Figure 8: Convergence histories of the true relative residual 2-norm of the right- and left-preconditioned PCGS, for each of the five PCGS algorithms with ISRV switching (sherman4).

Figure 9: Convergence histories of true relative residual 2-norm of the right- and left-preconditioned PCGS, for each of the five PCGS algorithms with ISRV switching (watt_1).
References

[1] Barrett, R. et al., *Templates for the Solution of Linear Systems: Building Blocks for Iterative Methods*, SIAM, Philadelphia, PA, 1994.

[2] Bruaset, A. M., *A Survey of Preconditioned Iterative Methods*, Longman Scientific & Technical, Harlow, Essex, UK, 1995.

[3] Davis, T. A., *The University of Florida Sparse Matrix Collection*, http://www.cise.ufl.edu/research/sparse/matrices/

[4] Fletcher, R., *Conjugate gradient methods for indefinite systems*, in Numerical Analysis: Proceedings of the Dundee Conference on Numerical Analysis, 1975, G. Watson, ed., Lecture Notes in Math. 506, Springer, New York, 1976, pp. 73–89.

[5] Gutknecht, M. H., *On Lanczos-type methods for Wilson Fermions*, in Numerical Challenges in Lattice Quantum Chromodynamics, A. Frommer, T. Lippert, B. Medeke, and K. Schilling, eds., Lecture Notes in Computational Science and Engineering 15, Springer, Berlin, 2000, pp. 48–65.

[6] Hestenes, M. R. and Stiefel, E., *Methods of conjugate gradients for solving linear systems*, J. Res. Nat. Bur. Standards, 49 (1952), pp. 409–435.

[7] Itoh, S. and Sugihara, M., *Systematic performance evaluation of linear solvers using quality control techniques*, in Software Automatic Tuning From Concepts to State-of-the-Art Results, K. Naono, K. Teranishi, J. Cavazos, and R. Suda, eds., Springer, New York, 2010, pp. 135–152.

[8] Itoh, S. and Sugihara, M., *Formulation of a preconditioned algorithm for the conjugate gradient squared method in accordance with its logical structure*, Appl. Math., 6 (2015), pp. 1389–1406.

[9] Itoh, S. and Sugihara, M., *The structure of the polynomials in preconditioned BiCG algorithms and the switching direction of preconditioned systems*, arXiv, 2016.

[10] Lanczos, C., *Solution of systems of linear equations by minimized iterations*, J. Res. Nat. Bur. Standards, 49 (1952), pp. 33–53.

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

[12] Meurant, G., *Computer Solution of Large Linear Systems*, Elsevier, New York, 2005.

[13] Sonneveld, P., *CGS: A fast Lanczos-type solver for nonsymmetric linear systems*, SIAM J. Sci. Stat. Comput., 10 (1989), pp. 36–52.

[14] SSI project, *Lis: Library of iterative solvers for linear systems*, http://www.ssisc.org/lis/

[15] Van der Vorst, H. A., *Bi-CGSTAB: A fast and smoothly converging variant of Bi-CG for the solution of nonsymmetric linear systems*, SIAM J. Sci. Stat. Comput., 13 (1992), pp. 631–644.

[16] Zhang, S.-L., *GPBi-CG: Generalized product-type methods based on Bi-CG for solving nonsymmetric linear systems*, SIAM J. Sci. Comput., 18 (1997), pp. 537–551.