The Improved BiCG Method for Large and Sparse Linear Systems on Parallel Distributed Memory Architectures *

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Abstract

For the solutions of large and sparse linear systems of equations with unsymmetric coefficient matrices, we propose an improved version of the BiConjugate Gradient method (IBiCG) method based on [5, 6] by using the Lanczos process as a major component combining elements of numerical stability and parallel algorithm design. For Lanczos process, stability is obtained by a coupled two-term procedure that generates Lanczos vectors scaled to unit length. The algorithm is derived such that all inner products, matrix-vector multiplications and vector updates of a single iteration step are independent and communication time required for inner product can be overlapped efficiently with computation time of vector updates. Therefore, the cost of global communication on parallel distributed memory computers can be significantly reduced. The resulting IBiCG algorithm maintains the favorable properties of the Lanczos process while not increasing computational costs. Data distribution suitable for both irregularly and regularly structured matrices based on the analysis of the non-zero matrix elements is presented. Communication scheme is supported by overlapping execution of computation and communication to reduce waiting times. The efficiency of this method is demonstrated by numerical experimental results carried out on a massively parallel distributed memory system.

1 Introduction

Solving linear systems, which arise very frequently in scientific and engineering computing, is one of the fundamental task of numerical computing. Examples include finite difference or finite element approximations to partial differential equations, as intermediate steps in computing the solution of nonlinear problems or as subproblems in linear and nonlinear programming.

If we deal with small size linear systems, the standard approach is to use direct methods, such as LU decomposition which obtains the solution through a factorization of the coefficient matrix. In contrast with direct methods, iterative methods use successive approximations to obtain more accurate solutions to the linear systems at subsequent steps. Generally speaking, iterative methods are computationally more attractive than the direct methods particularly for large and sparse systems [11].

The family of Krylov subspace methods [10, 14] is a powerful iterative type method involving the coefficient matrix only in the form of matrix-by-vector products for the solution of large and sparse linear systems with unsymmetric positive definite coefficient matrices. These methods basically consist of the generation of a suitable basis of a vector space called Krylov subspace and the choice of the actual iterate within that space. In this paper, one of the Krylov subspace methods, namely, the BiConjugate Gradient algorithm [10, 14], is considered mainly for large and sparse linear systems with unsymmetric coefficient matrices.

There are three basic time-consuming computational kernels of Krylov subspace methods, namely: inner products, vector updates, matrix-vector multiplications on massively parallel computers. For many scientific and engineering problems especially when matrix operations are well-structured, these operations are suitable to be implemented on vector and shared memory parallel computers [9]. But for parallel distributed memory machines, we have to cope with it differently because the matrices and vectors are distributed over the processors, so that even when the matrix operations can be implemented efficiently by parallel operations, we still can not avoid the global communication,

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i.e. accumulation of data from all to one processor, required for inner product computations. Vector updates are perfectly parallelizable and, for large sparse matrices, matrix-vector multiplications can be implemented with communication between only nearby processors. The bottleneck is usually due to inner products enforcing global communication. There are some discussions and improvements on the communication problem on distributed memory systems in [7, 8, 16]. These global communication costs become relatively more and more important when the number of parallel processors is increased and thus they have the potential to affect the scalability of the algorithm in a negative way [7, 8].

A new modified version of the BiConjugate Gradient (MBiCG) method recently by Bücker et al. [5, 6]. The algorithm is derived that both generated sequences of Lanczos vectors are scalable and is reorganized without changing the numerical stability so that all inner products and matrix-vector multiplications of a single iteration step are independent. There is only a single global synchronization point per iteration. Therefore, the cost of global communication on parallel distributed memory computers can be reduced. Based on their similar ideas, we propose a new improved two-term recurrences Lanczos process without look-ahead as the underlying process for the new Improved BiConjugate Gradient (IBiCG) method. The algorithm is reorganized without changing the numerical stability so that all inner products, matrix-vector multiplications and vector updates of a single iteration step are independent, and subsequently communication time required for inner product can be overlapped efficiently with computation time of vector updates. Therefore, the cost of global communication on parallel distributed memory computers can be significantly reduced. The resulting IBiCG algorithm maintains the favorable properties of the Lanczos process while not increasing computational costs. The efficient parallel implementation details, in particularly, data distribution and communication scheme, will be addressed as well. The efficiency of this method is demonstrated by numerical experimental results carried out on a massively parallel distributed memory computer, the Parsytec system.

The rest of paper is organized as follows. In section 2, we will describe briefly the classical unsymmetric Lanczos algorithm. A sketch of a new improved variant, used as the underlying process for the Improved BiConjugate Gradient (IBiCG) method is described fully in section 3. In section 4, the parallel implementation details including data distribution and communication scheme are presented. Finally numerical experiments carried out on parallel distributed memory computers are reported and some comparisons between the new Improved BiConjugate Gradient (IBiCG) method and other approaches are given with regards to numerical accuracy, parallel performance and efficiency.

2 Lanczos Process Based Coupled Two-Term Recurrence

Although Lanczos used the similar technique as the coupled two-term recurrence in the early of 1950's, the majority of papers are dealing with the three-term recurrences process, until, recently, Freund et al. [13] reused this idea to improve numerical stability. They showed that, the latter variant of the Lanczos process, are numerically more stable. That is why we pursue further on this unsymmetric Lanczos process with two-recurrences as the underlying process of the BiCG method.

Recently, Bücker et al. [3, 4] propose a new parallel version of the quasi-minimal residual (QMR) method based on the coupled two-term recurrences Lanczos process without look-ahead strategy. The algorithm is derived that both generated sequences of Lanczos vectors are scaled to unit length and there is only one single global synchronization point per iteration. Based on their similar ideas, we will present a new improved coupled two-term recurrences Lanczos process without look-ahead technique.

Here we assume that the tridiagonal matrix T has an LU decomposition as

$$T = LU, \tag{1}$$

where the factors L and U are of lower and upper bidiagonal form, respectively. It is the bidiagonal structure of L and U that results in coupled two-term recurrences.

It has been pointed out by several authors [11, 12, 15, 17] that in practice we should scale both sequences of Lanczos vectors appropriately to unit length in order to avoid over- and underflow. This can only be achieved by giving up the bidiagonality $W^T V = I$ and setting $W^T V = D$ instead, where D is a diagonal matrix with diagonal entries $\delta_i \neq 0$ for $i = 1, 2, \cdots, n$.

The principal idea of the new approach suggested in [3, 4] is to start from scaling described above by using LU decomposition as well as introducing $P = VU^{-1}$ and $\tilde{Q} = WD^{-1}U^T$ which leads to

$$W^T V = D, \qquad V = PU, \tag{2}$$

and

$$\tilde{Q} = WD^{-1}U^T, \;\; AP = VL, \;\; A^T W = \tilde{Q}L^T D. \tag{3}$$

Assume that the matrices introduced by the above setting have column vectors according to

$$P = [p_1, p_2, \cdots, p_n] \quad \text{and} \quad \tilde{Q} = [\tilde{q}_1, \tilde{q}_2, \cdots, \tilde{q}_n].$$

Then, after some complicated derivations, we can get

$$\begin{aligned} p_n &= \frac{1}{\gamma_n}\tilde{v}_n - \mu_n p_{n-1}, \quad \tilde{v}_{n+1} = u_n - \frac{\tau_n}{\gamma_n}\tilde{v}_n, \\ u_n &= \frac{1}{\gamma_n}A\tilde{v}_n - \mu_n u_{n-1}, \quad \tilde{w}_{n+1} = q_n - \frac{\tau_n}{\xi_n}\tilde{w}_n, \\ q_n &= \frac{1}{\xi_n}A^T\tilde{w}_n - \frac{\gamma_n\mu_n}{\xi_n}q_{n-1}. \end{aligned}$$

and the corresponding coefficients are given as follows

$$\begin{aligned} \gamma_{n+1} &= (\tilde{v}_{n+1}, \tilde{v}_{n+1}), \quad \xi_{n+1} = (\tilde{w}_{n+1}, \tilde{w}_{n+1}), \\ \rho_{n+1} &= (\tilde{w}_{n+1}, \tilde{v}_{n+1}), \quad \varepsilon_{n+1} = (A^T\tilde{w}_{n+1}, \tilde{v}_{n+1}), \\ \mu_{n+1} &= \frac{\gamma_n\xi_n\rho_{n+1}}{\gamma_{n+1}\tau_n\rho_n}, \quad \tau_{n+1} = \frac{\varepsilon_{n+1}}{\rho_{n+1}} - \gamma_{n+1}\mu_{n+1}. \end{aligned}$$

Algorithm 1 Improved Lanczos Process

$p_0 = q_0 = u_0 = 0, \gamma_1 = (\tilde{v}_1, \tilde{v}_1), \xi_1 = (\tilde{w}_1, \tilde{w}_1), s_1 = A^T\tilde{w}_1,$
$\rho_1 = (\tilde{w}_1, \tilde{v}_1), \varepsilon_1 = (s_1, \tilde{v}_1), \mu_1 = 0, \tau_1 = \frac{\varepsilon_1}{\rho_1};$
for n= 1,2,... **do**
  $q_n = \frac{1}{\xi_n}s_n - \frac{\gamma_n\mu_n}{\xi_n}q_{n-1};$
  $\tilde{w}_{n+1} = q_n - \frac{\tau_n}{\xi_n}\tilde{w}_n;$
  $s_{n+1} = A^T\tilde{w}_{n+1};$
  $t_n = A\tilde{v}_n;$
  $u_n = \frac{1}{\gamma_n}t_n - \mu_n u_{n-1};$
  $\tilde{v}_{n+1} = u_n - \frac{\tau_n}{\gamma_n}\tilde{v}_n;$
  $p_n = \frac{1}{\gamma_n}\tilde{v}_n - \mu_n p_{n-1};$
  $\gamma_{n+1} = (\tilde{v}_{n+1}, \tilde{v}_{n+1});$
  $\xi_{n+1} = (\tilde{w}_{n+1}, \tilde{w}_{n+1});$
  $\rho_{n+1} = (\tilde{w}_{n+1}, \tilde{v}_{n+1});$
  $\varepsilon_{n+1} = (s_{n+1}, \tilde{v}_{n+1});$
  $\mu_{n+1} = \frac{\gamma_n\xi_n\rho_{n+1}}{\gamma_{n+1}\tau_n\rho_n};$
  $\tau_{n+1} = \frac{\varepsilon_{n+1}}{\rho_{n+1}} - \gamma_{n+1}\mu_{n+1};$
end for

Now we are able to (re)schedule the operations of in the Lanczos process, in such a way that the numerical stability are maintained and all inner products and matrix-vector multiplications of a single iteration step are independent and subsequently communication time required for inner product can be overlapped efficiently with computation time. The framework of this improved Lanczos process based on two-term recurrences is described above. In the following, we consider the parallelism of the operations in a single iteration step implemented as follows:

- The inner products of a single iteration step (11), (12), (13) and (14) are independent.
- The matrix-vector multiplications of a single iteration step (6) and (7) are independent.
- The communications required for the inner products (11), (12), (13) and (14) can be overlapped with the update for p_n in (10).

Therefore, the cost of communication time on parallel distributed memory computers can be significantly reduced.

Since the biorthogonality relationship (2) and (3) are used to derive the algorithm. We can conversely show that, in exact arithmetic, the vectors $\tilde{v}_i$ and $\tilde{w}_i$ generated by the above algorithm are still biorthogonal.

Theorem 2.1 *Assume that no breakdown occurs, the vectors $\tilde{v}_i$ and $\tilde{w}_i$ generated by the Improved Lanczos Process satisfy*

$$\tilde{w}_i^T\tilde{v}_j = \begin{cases} 0 & i \neq j, \\ \rho_i \neq 0 & i = j. \end{cases}$$

3 The Improved BiConjugate Gradient Method

The following derivation is mainly based on [5, 6]. The improved Lanczos process now is used as a major component to a Krylov subspace method for solving a system of linear equations

$$Ax = b, \quad \text{where} \quad A \in \Re^{n\times n} \quad x, b \in \Re^n. \tag{4}$$

In each step, it produces approximation x_n to the exact solution of the form

$$x_n = x_0 + \mathcal{K}_n(r_0, A), \quad n = 1, 2, ... \tag{5}$$

Here x_0 is any initial guess for the solution of linear systems, $r_0 = b - Ax_0$ is the initial residual, and $\mathcal{K}_n(r_0, A) = span\{r_0, Ar_0, \ldots, A^{n-1}r_0\}$, is the n-th Krylov subspace with respect to r_0 and A.

Given any initial guess x_0, the n-th iterate is of the form

$$x_n = x_0 + V_n z_n, \tag{6}$$

where V_n is generated by the improved unsymmetric Lanczos process, and z_n is determined by the property described later.

For improved Lanczos process, the n-th iteration step generates

$$V_{n+1} = [v_1, v_2, \cdots, v_{n+1}] \text{ and } P_n = [p_1, p_2, \cdots, p_n],$$

that are connected by

$$P_n = V_n U_n^{-1}, \qquad AP_n = V_{n+1}L_n, \tag{7}$$

where L_n and U_n are the leading principal $(n+1)\times n$ and $n\times n$ submatrices of the bidiagonal matrices L and

U generated by the improved Lanczos process. Note that L_n has full rank since we assume no breakdown occurs. The setting of $y_n = U_n z_n$ can be used to reformulate the iterate in term of y_n instead of z_n giving

$$x_n = x_0 + P_n y_n. \tag{8}$$

The corresponding residual vector in term of y_n is obtained by the above scenario, namely

$$\begin{aligned} r_n &= b - Ax_n = r_0 - V_{n+1} L_n y_n \qquad (9)\\ &= V_{n+1}(\gamma_1 e_1^{(n+1)} - L_n y_n), \end{aligned}$$

where the improved Lanczos process starts with $v_1 = \frac{1}{\|r_0\|_2} r_0$ and $e_1^{(n+1)} = (1, 0, \ldots, 0)^T$. By using the Lanczos process to generate the Krylov subspace and fixing y_n, and so implicitly z_n by $y_n = U_n z_n$, we can easily derive the iterative method. Let $\widehat{y}_i$ denote the ith component of y_n, i.e., $y_n = (\widehat{y}_1, \widehat{y}_2, \ldots, \widehat{y}_n)^T$. We can derive r_n to the zero vector by

$$\widehat{y}_i = \begin{cases} \frac{\gamma_1}{\tau_1} & \text{if } i = 1, \\ -\frac{\gamma_i}{\tau_i}\widehat{y}_{i-1} & \text{if } i = 2, 3, \ldots, n. \end{cases} \tag{10}$$

This choice of y_n is observed by the special structure of L_n given in [5] and zeros out the first n components of the vector $\gamma_1 e_1^{(n+1)} - L_n y_n$ in (9). The residual vector is then expressed by

$$r_n = V_{n+1} \begin{pmatrix} 0 \\ \vdots \\ 0 \\ -\gamma_{n+1}\widehat{y}_n \end{pmatrix} \tag{11}$$

We can observe that the process of fixing y_n is easily updated in each iteration step because y_{n-1} coincides with the first $n-1$ components of y_n. The corresponding recursion can be described as follows:

$$y_n = \begin{pmatrix} y_{n-1} \\ 0 \end{pmatrix} + \kappa_n e_n \ , \tag{12}$$

where $e_n = (0, \ldots, 0, 1)^T \in \Re^n$ and

$$\kappa_n = -\frac{\gamma_n}{\tau_n}\kappa_{n-1} \tag{13}$$

with $\kappa_0 = -1$. By substitutating (12) into (8), it yields

$$\begin{aligned} x_n &= x_0 + P_{n-1} y_{n-1} + \kappa_n p_n \qquad (14)\\ &= x_{n-1} + \kappa_n p_n \ . \qquad (15) \end{aligned}$$

Note that $\|r_n\|$ is immediately available because, at every iteration step, the last component of y_n is κ_n by (12). Hence, from (11) the following relation can be derived

$$\|r_n\| = \|v_{n+1}\| \cdot |\gamma_{n+1}\kappa_n|. \tag{16}$$

By properly reorganizing (13) and (15) into the improved Lanczos process characterized by equations (6), we can derive results described in Algorithm 2. Note that the underlying Lanczos process operates with unit scaling of both sequences of Lanczos vectors, and is explicitly presented in [2]. In this case, (16) simplifies to

$$\|r_n\| = |\gamma_{n+1}\kappa_n|. \tag{17}$$

Correspondingly, we can use it as a simple stopping criterion.

If looking carefully the the above iterative process for the solution of linear systems, you can see that Algorithm 2 is just a new variant of the BiConjugate Gradient method (BiCG) [10, 14]. The detailed description and corresponding discussion can be found in [5, 6].

Algorithm 2 Improved Biconjugate Gradient Method

$p_0 = q_0 = 0\,, \widetilde{v}_1 = \widetilde{w}_1 = b - Ax_0$
$\gamma_0 = \xi_0 = 0\,, \tau_0 = \rho_0 \neq 0\,, \kappa_0 = -1$
$a_0 = A^T q_0, b_0 = Ap_0, s_0 = A^T \widetilde{w}_1$
$\gamma_1 = \|\widetilde{v}_1\|, \xi_1 = \|\widetilde{w}_1\|\,, \varrho_1 = \widetilde{w}_1^T v_1\,, \varepsilon_1 = s_1^T \widetilde{v}_1$
for n = 1, 2, 3, ... **do**
  $\mu_n = \frac{\gamma_{n-1}\xi_{n-1}\varrho_n}{\gamma_n \tau_{n-1}\varrho_{n-1}}$
  $\tau_n = \frac{\varepsilon_n}{\varrho_n} - \gamma_n \mu_n$
  $\kappa_n = -\frac{\gamma_n}{\tau_n}\kappa_{n-1}$
  $p_n = \frac{1}{\gamma_n}\widetilde{v}_n - \mu_n p_{n-1}$
  $q_n = \frac{1}{\xi_n} s_n - \frac{\gamma_n \mu_n}{\xi_n} q_{n-1}$
  $a_n = A^T q_n$
  $b_n = Ap_n$
  $s_{n+1} = a_n - \frac{\tau_n}{\xi_n} s_n$
  $\widetilde{v}_{n+1} = b_n - \frac{\tau_n}{\gamma_n}\widetilde{v}_n$
  $\widetilde{w}_{n+1} = q_n - \frac{\tau_n}{\xi_n}\widetilde{w}_n$
  $\gamma_{n+1} = \widetilde{v}_{n+1}^T \widetilde{v}_{n+1}$
  $\xi_{n+1} = \widetilde{w}_{n+1}^T \widetilde{w}_{n+1}$
  $\varrho_{n+1} = \widetilde{w}_{n+1}^T \widetilde{v}_{n+1}$
  $\varepsilon_{n+1} = s_n^T \widetilde{v}_{n+1}$
  $x_n = x_{n-1} + \kappa_n p_n$
  if $(|\gamma_{n+1}\kappa_n| < tol)$ **then**
    STOP
  end if
end for

Under the assumptions, the Improved BiConjugate gradient (IBiCG) method using improved Lanczos process as underlying process can be efficiently parallelized as follows:

- The inner products of a single iteration step (16), (17), (18), and (19) are independent.
- The matrix-vector multiplications of a single iteration step (11) and (12) are independent.

- The vector updates (13), (14) and (15) are independent.
- The vector updates (9) and (10) are independent.
- The communications required for the inner products (16), (17), (18) and (19) can be overlapped with the update for p_n in (20).

Therefore, the cost of communication time on parallel distributed memory computers can be significantly reduced.

4 Parallel Implementation

4.1 Data distribution

The efficient storage schemes should be considered differently if we are working on different computer system architectures or dealing with different algorithms or data when the coefficient matrices of the linear systems are large and sparse. One of the most common format called CRS format (compressed row storage) is used in the paper because this type of storage scheme is very suitable for both regularly and irregularly structured large and sparse matrices. There are many available description in the literature. In several words, the non-zeros of large and sparse matrix are stored in rowwise in three one-dimensional arrays. The values of the non-zeros are contained in array *value*. The corresponding column indices are contained in array *col_ind*. The elements of *row_ptr* point to the position of the beginning of each row in *value* and *col_ind*.

In order to efficiently parallelize the IBiCG algorithm, in particularly, on a distributed memory architecture, we first need to decide the data distribution of matrix and vector arrays, hopefully optimally, to each processor and then determine an efficient communication scheme by taking into account different sparsity patterns, not only for matrix-vector multiplication but also for inner products, to minimize the overall execution time. In this paper, we will mainly follow the approach has been used in [1] for data distribution and communication scheme which do not require any knowledge about the matrix sparsity pattern. Also the communication scheme are automatically determined by the analysis of the indices of the non-zero matrix elements.

The same notations introduced in [1] are used for illustrations in the rest of section. Let n_k and e_k denote the number of rows and no-zeros of processor k, where $k = 0, \ldots, p-1$, respectively. e and n are the total number of corresponding numbers. g_k is the index of the first row of processor k, and z_i is the number of non-zeros of row i. Easily we can get the following relations from [1]: $n = \sum_{k=0}^{p-1} n_k, e = \sum_{k=0}^{p-1} e_k, g_k = 1 + \sum_{i=0}^{k-1} n_i, e_k(g_k, n_k) = \sum_{i=gk}^{gk+nk-1} z_i$ Based on the analysis, the total costs of each iteration can be described as $c_1\ s\ e + c_2\ n + c_3$ where the first term corresponds to the number of operations for s matrix-vector multiplications, the second term corresponds to the number of vector updates. Since we are mainly dealing with large and sparse matrices, the constants can be neglected. Now we can estimate the contribution of the operations executed on processor k to the total number of operations by

$$\zeta \approx \frac{c_1\ s\ e_k + c_2\ n_k}{c_1\ s\ e + c_2\ n} = \frac{s\ e_k + \xi\ n_k}{s\ e + \xi n},$$

where $\xi = c_2/c_1$ depends on both the iterative methods and also the processor architecture. Ideally, the computational load balance should be distributed in such a way that each processor only gets p-th fraction for the total number of operations. Based on this, we can use the following strategy to distribute the rows of the matrix and the vector components [1]:

$$n_k = \begin{cases} \min\limits_{1 \le t \le n - g_k + 1} \{t | \frac{s\ e_k(t) + \xi\ t}{s\ e + \xi\ n} \ge \frac{1}{p}\} & k = 0, 1, \ldots, q \\ n - \sum_{i=0}^{q} n_i & k = q+1 \\ 0 & k = q+2, \ldots, p-1 \end{cases}$$

Since our main target is large and sparse matrices and we assume $p \ll n$, the relation $q = p-1$ or $q+1 = p-1$ always hold. It can be shown that for $\xi = c_2/c_1 \to 0$, each processor will get nearly the same number of non-zeros which means that the execution time of the vector updates in negligible with the execution of matrix-vector multiplications. It also can be shown that for $\xi = c_2/c_1 \to \infty$ each processor will get nearly the same number of rows which means that the execution time of the matrix-vector multiplications only contribute to a very small part of the total execution time.

4.2 Communication schemes

After discussing the first phase, data distribution, we also need to investigate a suitable communication scheme by preprocessing the distributed column index arrays for efficient matrix-vector multiplications since on a distributed memory systems, its computation requires communication due to the partial vector on each processor. Similarly we will use the approach proposed in [1] for our communication schemes.

If we decide to implement the matrix vector multiplication row-wisely, components of the vector x of $y = Ax$ are communicated. We firstly analyze the arrays *col_ind* on each processor to determine which elements result in access to non-local data. Then, the processors exchange information to decide which local data must be sent to which processors. Based on the above analysis, we will reorder these two arrays *col_ind* and *value* in such a way that the data that results in

access to processor l is collected in block l, called *local block*. The motivation behind this reordering is to perform computation and communication overlapped. The elements of block l succeed one another row-wise with increasing column index per row. The detailed description can be found in [1].

For the parallel implementation of this operation, each processor executes asynchronous receive-routines to receive necessary non-local data. Then all components of the vector x that are needed on other processors are sent asynchronously. After the required data are available, each processor will perform operations with it local block. After that, as soon as non-local data arrive, processor continue the matrix vector operation by accessing the elements of the corresponding blocks. It will be repeated until the whole operation is completed. According to the communication scheme described above, the communication and computation are performed overlapped so that waiting time can be reduced.

5 Numerical Experiments

The parallel variant of the improved BiCG (IBiCG) using the improved Lanczos process as the underlying Lanczos process is compared with the modified version of BiCG (MBiCG) proposed by Bücker et al. [5, 6] and the original BiCG based on coupled two-term recurrences on a massively distributed memory Patsytec computer in this section.

Similarly the partial differential equation is tested which taken from [3, 5, 6]

$$Lu = f, \qquad \text{on} \qquad \Omega = (0,1) \times (0,1),$$

with Dirichlet boundary condition $u = 0$ where

$$Lu = -\Delta u - 20(x\frac{\partial u}{\partial x} + y\frac{\partial u}{\partial y}),$$

and the right-hand side f is chosen so that the solution is

$$u(x,y) = \frac{1}{2}\sin(4\pi x)\sin(6\pi y).$$

First of all, we discretize the above differential equation using second order centered differences on a 400×400 with mesh size $1/441$, leading to a system of 193600 linear equations with a unsymmetric coefficient matrix of 966240 nonzero entries. Diagonal preconditioning is used to speed up the convergence. $x_0 = 0$ as initial guess and $tol = 10^{-5}$ as stopping parameter are chosen for the numerical tests.

As we have already discussed that the vectors are distributed over the processor grid, the inner products usually are computed in two steps. All processors start

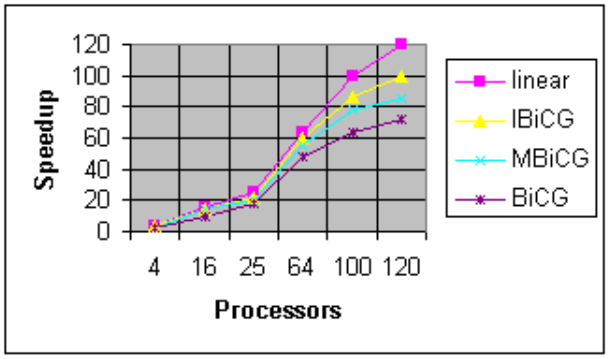

Figure 1. Experimental results of speed-up

to compute in parallel the local inner products. After that, the local inner products are accumulated on one central processor and broadcasted. The communication time of an accumulation or a broadcast increases proportionally with the diameter of the processor grid. That means if the number of processors increases then the communication time for the inner products increases as well, and hence this is a potential threat to the scalability of the algorithm.

With regards to the convergence, the proposed improved BiCG (IBiCG) is almost the same as the modified BiCG (MBiCG) suggested by Bücker et al. [5] and original BiCG version based on two-term recurrences where $\|r_n\|_2$ is computed recursively. A similar numerical behavior to these variants is observed. There is hardly any difference with respect to the true residual norm $\|b - Ax_n\|_2$ in those versions. The parallel performance are given in Fig. 1 where linear is the theoretical linear speedup, IBiCG is the speedup of the improved BiCG method, MBiCG is the speedup of the modified BiCG method suggested by Bücker et al. [5, 6] and BiCG is the speedup of the original BiCG method with two-term recurrences. These results are based on timing measurements of a fixed number of iterations. Since we do not know exactly the implemention details of the modified BiCG method [5, 6], we only take their published data as the experimental data for comparison. The speedup is computed as the ratio of the parallel execution time and the execution time using one processor. From the results, we can see clearly that the modified BiCG (MBiCG) suggested by Bücker et al. [5, 6] is faster than the original one. Meanwhile the new approach can achieve much better parallel performance with a higher scalability than the modified one. In comparison to the two other approaches, the reduction in execution time by the IBiCG increases with the number of processors. More precisely, the quantity is $1 - T_A(p)/T_B(p)$, where $T_A(p)$ and $T_B(p)$ are the execution times on p processors of approach A and B respectively. In Fig. 2, first curve shows the percentage

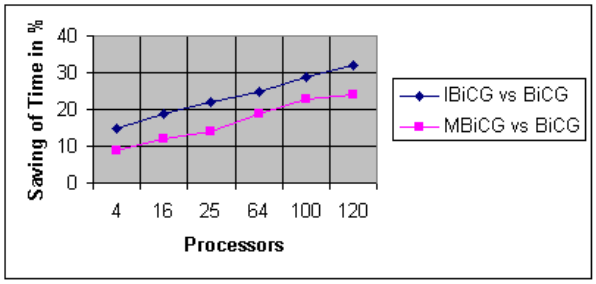

Figure 2. Execution time reduction

of reduction in execution time by our improved BiCG (IBiCG) approach compared to the original one. Another curve shows the percentage of reduction of time for the modified BiCG (MBiCG) proposed by Bücker et al. [5, 6] compared to the original BiCG method.

6 Conclusions

An improved version of the BiConjugate Gradient method (IBiCG) method is proposed by using the Lanczos process as a major component combining elements of numerical stability and parallel algorithm design for the solution of large and sparse linear systems of equations with unsymmetric coefficient matrices. The algorithm is derived in such a way that all inner products, matrix-vector multiplications and vector updates of a single iteration step are independent and subsequently communication time required for inner product can be overlapped efficiently with computation time of vector updates. Therefore, the cost of global communication on parallel distributed memory computers can be significantly reduced. The resulting IBiCG algorithm maintains the favorable properties of the Lanczos process while not increasing computational costs. Data distribution suitable for both irregularly and regularly structured matrices based on the analysis of the non-zero matrix elements has been presented. Communication scheme can be supported by overlapping execution of computation and communication to reduce waiting times. High scalability of the approach has been demonstrated as well.

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