Parallel Algorithm for Symmetric Positive Definite Banded Linear Systems: A Divide and Conquer Approach

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Abstract—The WZ factorization for the solution of symmetric positive definite banded linear systems when combined with a partitioned scheme, renders a divide and conquer algorithm. The WZ factorization of the coefficient matrix in each block has the properties: the vector \([a_1, \ldots, a_\beta, 0, \ldots, 0, a_{n-\beta+1}, \ldots, a_n]^T\) is invariant under the transformation \(W\) where \(\beta\) is the semibandwidth of the coefficient matrix and the solution process with the coefficient matrix \(Z\) proceeds from the first and the last unknowns to the middle. These properties of WZ factorization help us to decouple the partitioned system for the parallel execution once the 'reduced system' is solved.

Keywords: WZ factorization, banded linear systems, parallel computing.

1. Introduction

Consider the parallel solution of the linear system

\[Ax = f\]  \hspace{1cm} (1)

where \(A\) is an \(N \times N\) symmetric positive definite matrix with \(A = (a_{ij}), \ i, j = 1, 2, \ldots, N\) and \(a_{ij} = 0\) if \(|i - j| > \beta\), where \(\beta\) is an integer such that \(\beta << N\), called semi bandwidth of \(A\). \(x, f\) are \(N\)-component unknown and known vectors given by \(x = x^T_{1\rightarrow N}, f = f^T_{1\rightarrow N}\). They occur frequently in the numerical solution of partial and ordinary differential equations. To solve narrow banded systems in parallel divide and conquer, single width separator and double width separator approaches are available in the literature ([15],[11],[3],[16],[2]). Divide and conquer ([15]) and single width separator ([12],[4]) approaches are suitable for diagonally dominant and positive definite matrices, while double width separator approach ([16],[2]) is suitable for arbitrary (nonsingular) matrices. With the increasing availability and use of parallel computers much effort had been spent on the development of algorithms for the solution of banded systems. Survey on parallel solution of linear systems was given in [5]. Conroy [2] discussed the generalization of Wang's partition method [15] and one way dissection was applied to band matrices. These algorithms are comparable with Gaussian elimination and cyclic reduction. Wright [16] described and analyzed partitioned Gaussian elimination algorithm which was based on Dongarra and Johnsson [3]. Polizzi and Sameh [13] gave narrow banded system solvers based on SPIKE algorithm.

For the parallel algorithm based on modified Q.I.F. which was given in [8] the number of processors required for the algorithm was in terms of semibandwidth and the size of the system; on the other hand the number of processors required for the present parallel algorithm is in terms of number of blocks into which the system is partitioned. In the present work, the WZ factorization for the solution of symmetric positive definite banded linear systems is combined with a partitioned scheme. This renders a divide and conquer algorithm. The WZ factorization of the coefficient matrix in each block has the properties: the vector \([a_1, \ldots, a_\beta, 0, \ldots, 0, a_{n-\beta+1}, \ldots, a_n]^T\) is invariant under the transformation \(W\) where \(\beta\) is the semibandwidth of the coefficient matrix and the solution process with the coefficient matrix \(Z\) proceeds from the first and the last unknowns to the middle. These properties of WZ factorization help us to decouple the partitioned system for the parallel execution once the 'reduced system' is solved.

The outline of the paper is as follows. Section 2 describes the WZ factorization, partitioning of the symmetric banded linear system and the method of solution. The Algorithm is presented in section 3. Section 4 contains numerical experiments.

2. The Present Method

First we describe the WZ factorization, then consider the partitioning of the system and decoupling the partitioned subsystems. Finally, the method is discussed. The resulting algorithm is given in section 3.

2.1 The WZ Factorization

Consider an \(n \times n\) symmetric positive definite matrix \(A\) with \(n = 2m - 2\). Then there exists a matrix \(W\) (see[14]) such that

\[A = WW^T\]  \hspace{1cm} (2)
where

\[
W = \begin{bmatrix}
    w_{1,1} & w_{1,2} & \ldots & \ldots & w_{1,n} \\
    0 & w_{2,2} & \ldots & \ldots & \ldots \\
    \vdots & \vdots & \ddots & \ddots & \vdots \\
    \vdots & \vdots & \ddots & \ddots & \vdots \\
    0 & 0 & \ldots & 0 & w_{n,n} \\
\end{bmatrix}
\]

Note that the structure of $W$ here, appears as transpose of $W$ structure of Evans [6].

When $A$ is a symmetric band matrix with semibandwidth $\beta$, for example, for $n = 10, \beta = 2$; the matrix $W$ in (2) is given by

\[
W = \begin{bmatrix}
    w_{1,1} & w_{1,2} & w_{1,3} & 0 & 0 & 0 & 0 & w_{1,9} & w_{1,10} \\
    0 & w_{2,2} & w_{2,3} & w_{2,4} & 0 & 0 & 0 & w_{2,7} & 0 \\
    0 & 0 & w_{3,3} & w_{3,4} & w_{3,5} & 0 & w_{3,7} & w_{3,8} & 0 \\
    0 & 0 & 0 & w_{4,4} & w_{4,5} & w_{4,6} & w_{4,7} & 0 & 0 \\
    0 & 0 & 0 & 0 & w_{5,5} & w_{5,6} & w_{5,7} & w_{5,8} & 0 \\
    0 & 0 & 0 & 0 & 0 & w_{6,6} & w_{6,7} & w_{6,8} & 0 \\
    0 & 0 & 0 & 0 & 0 & 0 & w_{7,7} & w_{7,8} & 0 \\
    0 & 0 & 0 & 0 & 0 & 0 & 0 & w_{8,8} & 0 \\
    0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & w_{9,9} \\
    0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & w_{10,10} \\
\end{bmatrix}
\]

In order to design a multiprocessor algorithm for symmetric banded linear system when solved by divide and conquer technique, we introduce the $WZ$ factorization in which the inner $(n - 2) \times (n - 2)$ submatrices of $W$ and $Z$ are same as that of $W$ and $W^T$ in (3) respectively, and the vector $[a_1, a_2, 0, \ldots, 0, a_{n-\beta+1}, \ldots, a_n]^T$ is invariant under the transformation $W$.

The factorization of $A$ into $WZ$ is defined as follows $(n = 2m - 2)$:

\[
A = WZ.
\]

Let $w_i$ and $z_i$ be the $i^{th}$ column of $W$ and $Z$ respectively.

Each $w_i$, $i = 1, 2, \ldots, n$ is of the following form.

\[
w_i = \begin{cases}
    [0, \ldots, 0, 1, 0, \ldots, 0]^T, & \text{for } i = 1 \text{ to } \beta \\
    [0, \ldots, 0, 0, \ldots, 0, 0, \ldots, 0]^T, & \text{for } i = n - \beta + 1 \text{ to } n.
\end{cases}
\]

and each $z_i$, $i = 1, 2, \ldots, n$ is of the following form.

\[
z_i = \begin{cases}
    [w_{1,i}, \ldots, w_{i,i}, w_{i+1,i}, \ldots, w_{\beta,i}, w_{i+\beta+1,i}, \ldots, w_{i,n}, 0, \ldots, 0, w_{i,n-i+1}, 0, \ldots, 0]^T, & \text{for } i = 1 \text{ to } \beta, \\
    [0, \ldots, 0, 0, \ldots, 0, 0, \ldots, 0]^T, & \text{for } i = n - \beta + 1 \text{ to } n.
\end{cases}
\]

The first $\beta$ and the last $\beta$ columns of $W$ contain unit element on the diagonal position and zero elsewhere and $W$ is transpose of $Z$, except for the first $\beta$ and the last $\beta$ columns. For example, for $n=10, \beta = 2$

\[
W = \begin{bmatrix}
    1 & 0 & w_{1,3} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
    0 & 1 & w_{2,3} & w_{2,4} & 0 & 0 & 0 & 0 & 0 & 0 \\
    0 & 0 & w_{3,3} & w_{3,4} & w_{3,5} & 0 & w_{3,7} & w_{3,8} & 0 & 0 \\
    0 & 0 & 0 & w_{4,4} & w_{4,5} & w_{4,6} & w_{4,7} & 0 & 0 & 0 \\
    0 & 0 & 0 & 0 & w_{5,5} & w_{5,6} & w_{5,7} & w_{5,8} & 0 & 0 \\
    0 & 0 & 0 & 0 & 0 & w_{6,6} & w_{6,7} & w_{6,8} & 0 & 0 \\
    0 & 0 & 0 & 0 & 0 & 0 & w_{7,7} & w_{7,8} & 0 & 0 \\
    0 & 0 & 0 & 0 & 0 & 0 & 0 & w_{8,8} & 0 & 0 \\
    0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & w_{9,9} & 0 \\
    0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & w_{10,10}
\end{bmatrix}
\]

and

\[
Z = \begin{bmatrix}
    w_{1,1} & w_{1,2} & 0 & 0 & 0 & 0 & 0 & w_{1,9} & w_{1,10} \\
    w_{2,1} & w_{2,2} & 0 & 0 & 0 & 0 & 0 & w_{2,9} & w_{2,10} \\
    w_{3,1} & w_{3,2} & w_{3,3} & 0 & 0 & 0 & 0 & w_{3,9} & w_{3,10} \\
    0 & w_{4,2} & w_{4,3} & w_{4,4} & 0 & 0 & 0 & w_{4,8} & w_{4,9} \\
    0 & 0 & w_{5,2} & w_{5,3} & w_{5,4} & w_{5,5} & 0 & w_{5,8} & w_{5,9} \\
    0 & 0 & 0 & w_{6,3} & w_{6,4} & w_{6,5} & w_{6,6} & w_{6,8} & w_{6,9} \\
    0 & 0 & 0 & 0 & w_{7,4} & w_{7,5} & w_{7,6} & w_{7,7} & w_{7,8} \\
    0 & 0 & 0 & 0 & 0 & w_{8,5} & w_{8,6} & w_{8,7} & w_{8,9} \\
    0 & 0 & 0 & 0 & 0 & 0 & w_{9,6} & w_{9,7} & w_{9,8} \\
    0 & 0 & 0 & 0 & 0 & 0 & 0 & w_{10,8} & w_{10,9} \\
\end{bmatrix}
\]

2.2 Partitioning of the System

Consider the linear system $Ax = f$, $A \in \mathbb{R}^{N \times N}$, $x^T A x > 0$, $f \in \mathbb{R}^N$.

\[
A = (a_{ij}), \quad i, j = 1, 2, \ldots, N \text{ and } a_{ij} = 0 \text{ if } |i-j| > \beta
\]

where $\beta$ is an integer such that $\beta < N$, called semibandwidth of $A$. Partition $A$ along the diagonal into $r$ blocks each of size $n \times n$ (i.e. $N = rn$, we assume for simplicity that all blocks are of same size). Assume that $2\beta < n$. Partition the vectors $x$ and $f$ accordingly. Now each diagonal block has the same structure and the same bandwidth of $A$.

\[
B^{(j)} x^{(j-1)} + A^{(j)} x^{(j)} + C^{(j)} x^{(j+1)} = f^{(j)} \quad 1 \leq j \leq r
\]

with $B^{(1)} = 0, C^{(r)} = 0; B^{(r+1)} = C^{(1)}; j = 1, \ldots, r-1$; $x^{(0)} = 0, x^{(r+1)} = 0$; and

\[
B^{(j)} = \begin{bmatrix}
    0 & B^{(j)} \\
    0 & 0
\end{bmatrix}, \quad C^{(j)} = \begin{bmatrix}
    0 & 0 \\
    C^{(j)} & 0
\end{bmatrix};
\]

\[
x^{(j)} = \begin{bmatrix}
    x_1^{(j)} \\
    \vdots \\
    x_{n}^{(j)}
\end{bmatrix}, \quad f^{(j)} = \begin{bmatrix}
    f_1^{(j)} \\
    \vdots \\
    f_{n}^{(j)}
\end{bmatrix}.
\]
All $B^{(j)}, A^{(j)}, C^{(j)}$ are $n \times n$ matrices and $x^{(j)}$ and $f^{(j)}$ are $n \times 1$ vectors. $B^{(j)}$ and $C^{(j)}$ are $\beta \times \beta$ upper and lower triangular matrices respectively.

From (5) it follows that

$$A^{(j)}x^{(j)} = f^{(j)} - \begin{bmatrix} \hat{B}^{(j)}x_L^{(j-1)} \\ 0 \\ \vdots \\ 0 \\ \hat{C}^{(j)}x_F^{(j+1)} \end{bmatrix} = f^{(j)} \text{ say, } j = 1, \ldots, r. \quad (6)$$

where

$$x_F^{(j)} = [x_1^{(j)}, \ldots, x_\beta^{(j)}]^T, x_L^{(j)} = [x_{n-\beta+1}^{(j)}, \ldots, x_n^{(j)}]^T.$$

Note that $f^{(j)}$ in (6) differs from $f^{(j)}$ only in its first $\beta$ and last $\beta$ components. For the purpose we need a factorization of submatrices $A^{(j)}$ into $W^{(j)}Z^{(j)}; 1 \leq j \leq r$, with the properties that vector $[a_1, \ldots, a_\beta, 0, \ldots, 0, a_{n-\beta+1}, \ldots, a_n]^T$ is invariant under the transformation $W^{(j)}$ and the solution process with coefficient matrix $Z^{(j)}$ proceeds from the first and the last unknowns to the middle. The WZ factorization which we introduced has these properties.

### 2.3 The Method

We now consider the solution of the systems (5). This consists of finding $x^{(j)}$ from

$$W^{(j)}y^{(j)} = f^{(j)}, \quad j = 1, \ldots, r$$

and then solving for $x^{(j)}$

$$Z^{(j)}x^{(j)} = y^{(j)}, \quad j = 1, \ldots, r. \quad (7)$$

Let $y^{(j)} = [y_1^{(j)}, \ldots, y_n^{(j)}]^T$ and consider

$$W^{(j)}y^{(j)} = f^{(j)}, \quad j = 1, \ldots, r.$$

Because the vector $[a_1, \ldots, a_\beta, 0, \ldots, 0, a_{n-\beta+1}, \ldots, a_n]^T$ is invariant under the transformation $W^{(j)}$, and from the definition of $f^{(j)}$, it immediately follows that

$$y^{(j)} = y^{(j)} - \begin{bmatrix} \hat{B}^{(j)}x_L^{(j-1)} \\ 0 \\ \vdots \\ 0 \\ \hat{C}^{(j)}x_F^{(j+1)} \end{bmatrix}, \quad j = 1, \ldots, r. \quad (8)$$

Once $y^{(j)}$ are determined, the subsystem (7) can be replaced by

$$Z^{(j)}x^{(j)} = y^{(j)} - \begin{bmatrix} \hat{B}^{(j)}x_L^{(j-1)} \\ 0 \\ \vdots \\ 0 \\ \hat{C}^{(j)}x_F^{(j+1)} \end{bmatrix}, \quad j = 1, \ldots, r. \quad (9)$$

From the definition of $W^{(j)}$ it is now clear that among the subsystems in (9) we can extract a relatively small (for $r \ll N$) subsystem involving only the first $\beta$ and the last $\beta$ unknowns of each block. Accordingly, collecting together the first and the last $\beta$ equations of each block, we obtain a linear system called ‘reduced system’ of order $2\beta r \times 2\beta r$ of semi bandwidth $2\beta - 1$.

Let

$$W_1^{(j)} = \begin{bmatrix} w_{1,1}^{(j)} & \cdots & w_{1,\beta}^{(j)} \\ \vdots & \ddots & \vdots \\ w_{\beta,1}^{(j)} & \cdots & w_{\beta,\beta}^{(j)} \end{bmatrix},$$

$$W_2^{(j)} = \begin{bmatrix} w_{1,1-n-\beta}^{(j)} & \cdots & w_{1,n}^{(j)} \\ \vdots & \ddots & \vdots \\ w_{\beta,1-n-\beta}^{(j)} & \cdots & w_{\beta,n}^{(j)} \end{bmatrix},$$

$$W_4^{(j)} = \begin{bmatrix} w_{n-\beta+1,1-n-\beta}^{(j)} & \cdots & w_{n-\beta+1,n}^{(j)} \\ \vdots & \ddots & \vdots \\ w_{n,1-n-\beta}^{(j)} & \cdots & w_{n,n}^{(j)} \end{bmatrix},$$

where $W_2^{(j)}$ is symmetric.

Then the reduced system can be written as,

$$\begin{bmatrix} W_1^{(1)} & W_2^{(1)} & \hat{C}^{(1)} \\ W_3^{(1)} & W_4^{(1)} & \hat{C}^{(2)} \end{bmatrix} \begin{bmatrix} x_1^{(1)} \\ x_2^{(1)} \\ \vdots \\ x_r^{(1)} \\ \hat{C}^{(r-1)} \end{bmatrix} = \begin{bmatrix} y_1^{(1)} \\ y_2^{(1)} \\ \vdots \\ y_r^{(1)} \end{bmatrix}.$$

The reduced system (10) may be represented as

$$Rx_R = y_R \quad (11)$$

where

$$x_R = [x_F^{(1)}, x_L^{(1)}, \ldots, x_F^{(r)}, x_L^{(r)}]^T, y_R = [y_1^{(1)}, y_2^{(1)}, \ldots, y_F^{(r)}, y_L^{(r)}]^T,$$

and $R$ is the coefficient matrix of (10).

For a matrix $S = (s_{i,j})_{i,j=1}^{n-1}$ and a vector $q = (q_1, \ldots, q_{n-1})^T$, we introduce the notation:

$$S_{2\rightarrow n-1} = (s_{i,j})_{i,j=2}^{n-1} \quad \text{and} \quad q_{2\rightarrow n-1} = (q_2, \ldots, q_{n-1})^T.$$

Once the reduced system of order $2\beta r$ is solved for $x_F^{(j)}$ and $x_L^{(j)}$, $j = 1, \ldots, r$, the subsystems in (9), for $j = 1, \ldots, r$, are uncoupled into

$$Z_{\beta+1-n-\beta}^{(j)} - y_{\beta+1-n-\beta}^{(j)} - \begin{bmatrix} U_1^{(j)} & U_1^{(j)} & L_1^{(j)} \\ 0 & \ddots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \ddots & 0 \\ U_2^{(j)} & U_2^{(j)} & L_2^{(j)} \end{bmatrix}.$$
where

\[
U_1^{(j)} = \begin{bmatrix}
w_{1,\beta+1} & \cdots & w_{\beta,\beta+1} \\
0 & \ddots & \vdots \\
0 & 0 & w_{\beta,2}\beta
\end{bmatrix},
\]

\[
U_2^{(j)} = \begin{bmatrix}
w_{n-\beta+1,\beta+1} & \cdots & w_{\beta,\beta+1} \\
\vdots & \ddots & \vdots \\
w_{n-\beta+1,2\beta} & 0 & 0
\end{bmatrix},
\]

\[
L_1^{(j)} = \begin{bmatrix}
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & \ddots & \vdots \\
0 & 0 & w_{2,\beta}
\end{bmatrix},
\]

\[
L_2^{(j)} = \begin{bmatrix}
w_{n-\beta+1,1,\beta+1} & 0 & 0 \\
\vdots & \ddots & \vdots \\
w_{n-\beta+1,n-\beta} & \cdots & w_{n,n-\beta}
\end{bmatrix}.
\]

3. Algorithm

Step 1. For \( j = 1, \ldots, r \) factorize in parallel

\[ A^{(j)} = W^{(j)} Z^{(j)}. \]

Step 2. For \( j = 1, \ldots, r \) compute \( y^{(j)} \) in parallel

\[ W^{(j)} y^{(j)} = f^{(j)}. \]

Step 3. Solve the reduced subsystem \((10)\) for \( x_1^{(j)}, \ldots, x_{\beta+1}^{(j)}, \ldots, x_n^{(j)}, j = 1, \ldots, r \) sequentially by band Cholesky factorization.

Step 4. For \( j = 1, \ldots, r \) compute \( x_{\beta+1-n,\beta}^{(j)} \) in parallel from (12).

Speedup, \( S_p \), of the parallel algorithm on \( r \) processor machine is given by

\[
S_p = \frac{\text{Time taken by the best sequential (\cite{7}) algorithm}}{\text{Time taken by the parallel algorithm on \( r \) processor machine}}.
\]

As \( N = nr \), if \( N \) is large enough and \( \beta \) is fairly large, speedup is approximately \( 0.25r \). If \( \beta \) is 2, the speedup is 0.5\( r \) and if \( \beta \) is 10 the speedup is approximately 0.33\( r \).

4. Numerical Experiments

Numerical experiments are conducted on a parallel machine; the Ultra SPARC III technology based Sunfire 6800 having 16 processors (each of 800 MHz and has 1 GB RAM) shared memory server. Full hardware redundancy and a variety of advances mainframe-class availability features such as CPU upgrades and dynamic reconfiguration, provide maximum uptime. The hard disk memory is 192 GB and the operating system is Solaris 8.0.

Total (computation and communication) time (in seconds) statistics of the proposed algorithm for the solution of symmetric positive definite banded linear systems of different orders with coefficient matrices having semibandwidth \( \beta = 10 \) against different number of processors is given in Table 1. In this table time for \( p=1 \), corresponds to the time taken by the best sequential algorithm (band Cholesky \cite{7}). From Table 1, we observe that the total time for the solution (for \( p=2 \) onwards) in each column decreases from top to bottom where as total time for the solution each row increases from left to right.

Speedup against different number of processors for symmetric positive definite banded linear systems of different orders with coefficient matrices having semibandwidth \( \beta = 10 \) is plotted in Figure 1. We observe from the Figure 1 that the speedup increases with the increase in the number of processors. Communication time against different number of processors in solving banded linear systems of different orders with coefficient matrices having semibandwidth \( \beta = 10 \) is plotted in Figure 2. We observe from the Figure 2 that the communication time on and after 6 processors is almost the same. This is because the semibandwidth \( \beta \) is same though the orders of symmetric positive definite banded linear systems are different and the dimension of the reduced system is \( 2\beta r \) where \( r \) is the number of processors. This is a main point of the algorithm which is illustrated through the leveling of the communication costs as the number of processors increases.

<table>
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<th>( N ) ( \rightarrow )</th>
<th>84000</th>
<th>168000</th>
<th>252000</th>
<th>336000</th>
<th>420000</th>
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<tbody>
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<td>|</td>
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Fig. 1: Speedup against different number of processors in solving banded linear systems of different orders with coefficient matrices having semibandwidth $\beta = 10$. The symbols ♦, ■, ▲, ∗, ■ correspond to linear systems of order 84000, 168000, 252000, 336000, 420000 respectively.

Fig. 2: Communication time against different number of processors in solving banded linear systems of different orders with coefficient matrices having semibandwidth $\beta = 10$. The symbols ♦, ■, ▲, ∗, ■ correspond to linear systems of order 84000, 168000, 252000, 336000, 420000 respectively.

References