Rotated Alternative LU Decomposition Method and Its Preconditioner for Periodic Block Pentadiagonal Linear Systems on Vector Processor.

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Abstract

In this paper, a new method "Rotated Alternative LU (Rotated ALU) decomposition" for solving block pentadiagonal linear systems is proposed, that makes vector processing more efficient. And a new way to apply the Rotated ALU decomposition to periodic pentadiagonal linear systems is proposed. A few numerical experiments show that these methods are more faster than the conventional LU decomposition.

1 Introduction

Applying the fourth order accuracy's approximate factorization (AF) method to compressive three-dimensional computational fluid dynamics (CFD), a lot of linear systems (1.1) must be solved.

$$\hat{A}_{j,k} \boldsymbol{x}_{j,k} = \boldsymbol{b}_{j,k} \tag{1.1}$$

In the case of Dirichlet boundary conditions, its coefficient matrix is block pentadiagonal matrices $\hat{A}_{i,k}$ (*i* makes row direction) [6].

When vector processor is used, the direct method, the LU decomposition (Gaussian elimination), is more often used for solving a lot of linear systems like (1.1) than the iterative methods. Then the matrices $\hat{A}_{j,k}$ can be factorized by the LU decomposition, with vectorizing for j or k direction to compute at the same time. However, the conventional LU decomposition is afford to improve its calculating performance on the vector processors.

In this paper, a new effective method on vector processor the "Rotated Alternative LU (Rotated ALU) decomposition method" for block pentadiagonal systems is proposed. This method makes the vector-length (the number of the elements that are simultaneously computed) twice with the linear algebra.

In the case of periodic boundary systems, this method can not be applied directly. And the Sherman-Morrison-Woodbury formula is used as a preconditioner for the Rotated ALU decomposition.

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2 Solving block pentadiagonal linear systems

In this case, the coefficient matrix is as follows.:

where $A_{j,k}^i, B_{j,k}^i, C_{j,k}^i, D_{j,k}^i, E_{j,k}^i (i=1,...,l; j=1,...,m; k=1,...,n)$ are 5×5 block matrix.

2.1 The conventional LU decomposition method

Usually, $\hat{F}_{j,k}$ is factored as the product of the lower block tridiagonal matrices and the upper block tridiagonal matrices with the conventional LU decomposition.

Here, I means the unit matrix, $\hat{L}_{j,k}$ is the forward elemination matrices, $\hat{U}_{j,k}$ is the backward substitution matrices. And block matrices with tilde $(ex. \tilde{C}_{j,k}^2)$ are updated by the factorization.

When vector processor is used, the vector-length is m with vectorizing for j-direction or n with vectorizing for k-direction.

Program1 roughly shows the forward elemination step. In this program, j-direction is vectorized.

Program1 The conventional LU decomposition.

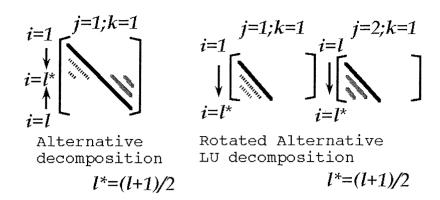


Figure 1: Illustrations of the Alternative decomposition and the Rotated ALU decomposition.

2.2 The Rotated Alternative LU decomposition method

On the other hand, the Alternative decomposition[8] (Another name: A twisted factorization[7]) method has been proposed. This method is algebraically equivalent to the conventional LU decomposition except for the both-sides' decomposition. Applied the Alternative decomposition, $\hat{F}_{j,k}$ is factored as (2.3).

Block matrices with tilde in (2.3) are updated by the factorization, too. Here the LU decomposition can be computed simultaneously from the both-sides of diagonal elements to the middle of row $(\frac{l+1}{2})$. This computation is vectorizable for j-direction. And the backward-substitution can be computed from the middle element to the each side.

In this paper, the procedure of decomposition is given attention to.

Generally, vector processors perform superbly as the vector-length is sufficiently long. From other point of view, the double vector-length makes the performance improve. Concerning this property on vector architecture, the Altenative decomposition can be further improved with keeping the algebraically equivalence. This new proposed method is named the "Ratated Alternative LU (Rotated ALU) decomposition method" [4] .

Fig.1 is the illustration of the Alternative decomposition and the Rotated ALU decomposition for single matrix $\hat{P}_{1,1}$ (m=1,n=1). In this figure, the black solid lines, the gray solid lines and the broken lines are corresponding to the both figures, and the arrows shows the order of the LU decomposition. The Rotated ALU decomposition is done as follows.

1. $\hat{P}_{1,1}$ is partitioned into two-parts by the middle row. And the matrix $\hat{Q}_{1,1}$ is also partitioned

same way.

2. The latter part is rotated by 180 degrees like Fig.1 and joined to the first part in the direction of the vectorization(in this case, j). Then the first part is j=1; k=1, the latter part is j=2; k=1. Eventually the number of the j-direction's element is double. And the matrix $\hat{Q}_{1,1}$ is also rotated same way.

The Rotated ALU decomposition computes the first and latter part at the same time.

For the matrices $\hat{P}_{j,k}$ (here, j=1,...,m; k=1,...,n), the first part forms j=1,...,m, the latter part elements are rotated by 180 degrees and formed j=(m+1),...,2m. And j-direction is vectorized. Finally the vector-length increases twice (2m). These processes are done for k=1,...,n. And the matrices $\hat{Q}_{j,k}$ is also done same way.

Program2 shows the forward elemination by the Rotated Alternative LU decomposition. The details are same as Program1.

```
\begin{array}{l} \text{parameter } (\text{ix=}(l+1)/2, \, \text{iy=}2m, \, \text{iz=}n) \\ \text{dimension } (\text{A}(\text{iy,iz,ix,}5,5), \, \text{B}(\text{iy,iz,ix,}5,5), \\ \text{c} \quad \text{C}(\text{iy,iz,ix,}5,5), \, \text{D}(\text{iy,iz,ix,}5,5), \, \text{E}(\text{iy,iz,ix,}5,5)) \\ \text{do 2 i=}1, \text{ix} \\ \text{do 2 k=}1, \text{iz} \\ \text{do 2 j=}1, \text{iy} \\ \tilde{B}^{i}_{j,k} = B^{i}_{j,k} - A^{i}_{j,k} \times \tilde{D}^{i-2}_{j,k} \\ \tilde{C}^{i}_{j,k} = C^{i}_{j,k} - A^{i}_{j,k} \times \tilde{E}^{i-2}_{j,k} - \tilde{B}^{i}_{j,k} \times \tilde{D}^{i-1}_{j,k} \\ \tilde{D}^{i}_{j,k} = (\tilde{C}^{i}_{j,k})^{-1} \times (D^{i}_{j,k} - \tilde{B}^{i}_{j,k} \times \tilde{E}^{i-1}_{j,k}) \\ \tilde{E}^{i}_{j,k} = (\tilde{C}^{i}_{j,k})^{-1} \times E^{i}_{j,k} \\ \tilde{b}^{i}_{j,k} = (\tilde{C}^{i}_{j,k})^{-1} \\ \times (b^{i}_{j,k} - A^{i}_{j,k} \times \tilde{b}^{i-2}_{j,k} - B^{i}_{j,k} \times \tilde{b}^{i-1}_{j,k}) \\ 2 \quad \text{continue} \end{array}
```

Program2 The Rotated Alternative LU decomposition method.

2.3 Numerical Experiments-1

In this section, a few numerical results are presented, that is comparing the conventional LU decomposition to the Rotated ALU decomposition. In experiments, the computing against some various vector-length that had been based on the CFD problems was done.

2.3.1 Methods

Testing model was as follows. Block matrices composing the coefficient matrix $\hat{F}_{j,k}$ was generated with based on Frank matrix, and with being able to factor by the LU decomposition. The exact solution $x_{j,k}$ was generated by random numbers. The right hand side $b_{j,k}$ was generated by multiplying $\hat{F}_{j,k}$ and $x_{j,k}$. To keep the number of the elements $(l \times m \times n)$ being constant, the number of the row-direction's elements (l), the LU decomposition direction, was fixed (l = 63), and the number of other directions' elements were varied to be satisfied with $m \times n = 2400$ (Constant) (Tab. 1). And j-direction was vectorized.

The computing time and the accuracy for the solving linear systems are measured and evaluated between the conventional LU decomposition and the Rotated ALU decomposition. Experiment was carried out in single precision and executed on Fujitsu VPP500/1PE vector processor.

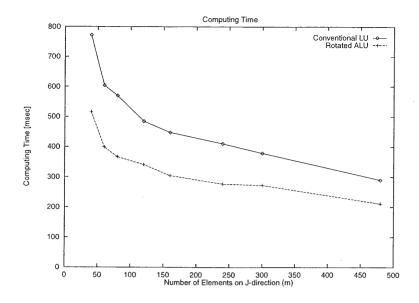


Figure 2: Comparison of computing time between the conventional LU decomposition and the Rotated ALU deomposition.

2.3.2 Results

Fig.2 shows the computing time plot corresponding to Tab.1. The abscissa indicates the number of j-direction's elements (m) and the ordinate indicates the computing time [msec]. Fig.3 shows the computing time ratio, (the Rotated ALU/the conventional LU)×100[%].

From these results, the Rotated ALU decomposition is faster nearly 30[%] than the conventional LU decomposition. On the accuracy, both algorithms are the same for this testing model, and the relative 2-norm error is as follows:

$$\frac{\|\boldsymbol{x}_{j,k} - \bar{\boldsymbol{x}}_{j,k}\|_2}{\|\boldsymbol{x}_{j,k}\|_2} \sim O(10^{-6})$$
(2.4)

where $x_{j,k}$ is the exact solution, and $\bar{x}_{j,k}$ is the numerical solution.

Table 1: Testing sizes.

\overline{l}	63	63	63	63 120 20	63	63	63	63
m	40	60	80	120	160	240	300	480
n	60	40	30	20	15	10	8	5

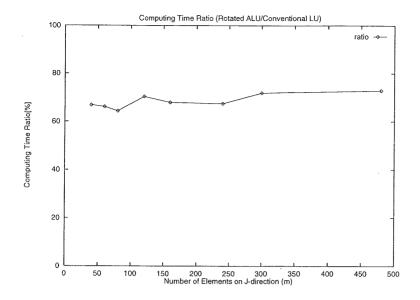


Figure 3: The ratio of computing time between the conventional LU decomposition and the Rotated ALU decomposition.

3 Solving periodic block pentadiagonal linear systems

In this case, the coefficient matrix is as follows.:

where $A_{j,k}^1, B_{j,k}^1, A_{j,k}^2, E_{j,k}^{l-1}, D_{j,k}^l, E_{j,k}^l$ are periodic boundary elements (PBE: the matrix's elements generated from periodic boundary conditions by discretizing of partial differential equation).

3.1 Difficulty of applying the Rotated Alternative LU decomposition method

The conventional LU decomposition factors (3.1) into (3.2).

$$\hat{G}_{j,k} =$$

$$\begin{bmatrix} C^{1}_{j,k} & & & & & & \\ B^{2}_{j,k} & \tilde{C}^{2}_{j,k} & & & & & \\ A^{3}_{j,k} & \tilde{B}^{3}_{j,k} & \tilde{C}^{3}_{j,k} & & & & \\ & \cdots & \cdots & & & & & \\ & \vdots & \ddots & \cdots & \vdots & \vdots & & \\ O & & A^{l-2}_{j,k} & \tilde{B}^{l-2}_{j,k} & \tilde{C}^{l-2}_{j,k} & \tilde{C}^{l-1}_{j,k} \\ D^{l}_{j,k} & \tilde{E}^{l}_{j,k} & \star & \cdots & \star & \star & A^{l-1}_{j,k} & \tilde{B}^{l}_{j,k} & \tilde{C}^{l}_{j,k} \\ D^{l}_{j,k} & \tilde{E}^{l}_{j,k} & \star & \cdots & \star & \star & A^{l-1}_{j,k} & \tilde{B}^{l}_{j,k} & \tilde{C}^{l}_{j,k} \\ D^{l}_{j,k} & \tilde{E}^{l}_{j,k} & \star & \cdots & \star & \star & A^{l}_{j,k} & \tilde{B}^{l}_{j,k} & \tilde{C}^{l}_{j,k} \\ D^{l}_{j,k} & \tilde{E}^{l}_{j,k} & \star & \cdots & \star & \star & A^{l}_{j,k} & \tilde{B}^{l}_{j,k} & \tilde{C}^{l}_{j,k} \\ D^{l}_{j,k} & \tilde{E}^{l}_{j,k} & \star & \cdots & \star & \star & A^{l}_{j,k} & \tilde{B}^{l}_{j,k} & \tilde{C}^{l}_{j,k} \\ D^{l}_{j,k} & \tilde{E}^{l}_{j,k} & \star & \cdots & \star & \star & A^{l}_{j,k} & \tilde{B}^{l}_{j,k} & \tilde{C}^{l}_{j,k} \\ D^{l}_{j,k} & \tilde{E}^{l}_{j,k} & \star & \cdots & \star & \star & A^{l}_{j,k} & \tilde{B}^{l}_{j,k} & \tilde{C}^{l}_{j,k} \\ D^{l}_{j,k} & \tilde{E}^{l}_{j,k} & \star & \cdots & \star & \star & A^{l}_{j,k} & \tilde{B}^{l}_{j,k} & \tilde{C}^{l}_{j,k} \\ D^{l}_{j,k} & \tilde{E}^{l}_{j,k} & \star & \cdots & \star & \star & A^{l}_{j,k} & \tilde{B}^{l}_{j,k} & \tilde{C}^{l}_{j,k} \\ D^{l}_{j,k} & \tilde{E}^{l}_{j,k} & \tilde{E}^{l}_{j,k} & \tilde{E}^{l}_{j,k} & \tilde{E}^{l}_{j,k} & \tilde{E}^{l}_{j,k} \\ D^{l}_{j,k} & \tilde{E}^{l}_{j,k} & \tilde{E}^{l}_{j,k} & \tilde{E}^{l}_{j,k} & \tilde{E}^{l}_{j,k} & \tilde{E}^{l}_{j,k} \\ D^{l}_{j,k} & \tilde{E}^{l}_{j,k} & \tilde{E}^{l}_{j,k} & \tilde{E}^{l}_{j,k} & \tilde{E}^{l}_{j,k} & \tilde{E}^{l}_{j,k} \\ D^{l}_{j,k} & \tilde{E}^{l}_{j,k} & \tilde{E}^{l}_{j,k} & \tilde{E}^{l}_{j,k} & \tilde{E}^{l}_{j,k} & \tilde{E}^{l}_{j,k} \\ D^{l}_{j,k} & \tilde{E}^{l}_{j,k} & \tilde{E}^{l}_{j,k} & \tilde{E}^{l}_{j,k} & \tilde{E}^{l}_{j,k} & \tilde{E}^{l}_{j,k} \\ D^{l}_{j,k} & \tilde{E}^{l}_{j,k} & \tilde{E}^{l}_{j,k} & \tilde{E}^{l}_{j,k} & \tilde{E}^{l}_{j,k} & \tilde{E}^{l}_{j,k} \\ D^{l}_{j,k} & \tilde{E}^{l}_{j,k} & \tilde{E}^{l}_{j,k} & \tilde{E}^{l}_{j,k} & \tilde{E}^{l}_{j,k} & \tilde{E}^{l}_{j,k} \\ D^{l}_{j,k} & \tilde{E}^{l}_{j,k} & \tilde{E}^{l}_{j,k} & \tilde{E}^{l}_{j,k} & \tilde{E}^{l}_{j,k} & \tilde{E}^{l}_{j,k} \\ D^{l}_{j,k} & \tilde{E}^{l}_{j,k} & \tilde{E}^{l}_{$$

By using the conventional decomposition, the PBEs occur fill-in¹ that is showed by \star in Eq.(3.2). On the other hand, the Rotated ALU decomposition would be able to solve faster, but this method cannot be applied directly to such like the periodic block pentadiagonal linear systems. Because this method to $\hat{G}_{i,k}$ invited fill-in, that makes the applying the Rotated ALU decomposition difficult.

To solve with the Rotated ALU decomposition, the coefficient matrix must be factorized with the Alternative decomposition (2.3). However, the Alternative decomposition occurs the fill-in showed in (3.3) by the \star , and the number of the unknowns are much more than the number of the equations.

$$\hat{G}_{j,k} =$$

Therefore, it is impossible to solve the linear systems of (3.1).

3.2 Applying the Sherman-Morrison-Woodbury formula

Against this point of issue, the Sherman-Morrison-Woodbury(SMW) formula [3]

$$(P + UV^{T})^{-1} = P^{-1} - P^{-1}U(I + V^{T}P^{-1}U)^{-1}V^{T}P^{-1}$$
(3.4)

is used as a preconditioner for the Rotated ALU decomposition.

For applying to the SMW formula, the coefficient matrix $\hat{G}_{j,k}$ should be splitted into two-matrices, block pentadiagonal matrices(P) and the matrices composed of the PBEs, and the latter term should be transform into two block matrices' multiplying. Here, P is adaptable form for the Rotated ALU decomposition. This preconditioner has been named "Split/SMW" [9].

Applying is as follows. Here,

$$\begin{array}{rcl} \tilde{C}_{j,k}^1 & = & C_{j,k}^1 - A_{j,k}^1, \\ \tilde{D}_{j,k}^1 & = & D_{j,k}^1 - B_{j,k}^1, \\ \tilde{C}_{j,k}^2 & = & C_{j,k}^2 - A_{j,k}^2, \\ \tilde{C}_{j,k}^{l-1} & = & C_{j,k}^{l-1} - E_{j,k}^{l-1}, \\ \tilde{B}_{j,k}^l & = & B_{j,k}^l - D_{j,k}^l, \\ \tilde{C}_{j,k}^l & = & C_{j,k}^l - E_{j,k}^l. \end{array}$$

¹The behavior that the elements of matrix is zero but not so in an exact factorization.

Then,

$$\hat{G}_{j,k} = \begin{bmatrix} \tilde{C}_{j,k}^{1} \tilde{D}_{j,k}^{1} E_{j,k}^{1} & \mathbf{0} \\ B_{j,k}^{2} \tilde{C}_{j,k}^{2} D_{j,k}^{2} E_{j,k}^{2} & \mathbf{0} \\ A_{j,k}^{3} B_{j,k}^{3} C_{j,k}^{3} D_{j,k}^{3} E_{j,k}^{3} & \\ \vdots & \vdots & \vdots \\ A_{j,k}^{l-2} B_{j,k}^{l-2} C_{j,k}^{l-2} D_{j,k}^{l-2} E_{j,k}^{l-2} \\ \mathbf{0} & A_{j,k}^{l-1} B_{j,k}^{l-1} \tilde{C}_{j,k}^{l-1} D_{j,k}^{l-1} \\ \mathbf{0} & A_{j,k}^{l} \tilde{B}_{j,k}^{l} \tilde{C}_{j,k}^{l} \end{bmatrix} + \begin{bmatrix} A_{j,k}^{1} B_{j,k}^{1} B_{j,k}^{1} \\ 0 & A_{j,k}^{2} B_{j,k}^{1} C_{j,k}^{0} \\ 0 & 0 \\ \vdots & \vdots \\ 0 & 0 \\ B_{j,k}^{l-1} 0 \\ D_{j,k}^{l-1} 0 \\ D_{j,k}^{l} E_{j,k}^{l} \end{bmatrix}$$

$$= P + [U_{1} U_{2}] \begin{bmatrix} V_{1}^{T} \\ V_{2}^{T} \end{bmatrix}$$

$$= P + UV^{T}. \tag{3.5}$$

By (3.5), the linear systems (1.1) is represented as follows.

$$\hat{G}_{j,k} x_{j,k} = (P + UV^T) x_{j,k} = b_{j,k}$$
(3.6)

therefore,

$$x_{j,k} = (P + UV^T)^{-1} b_{j,k}. (3.7)$$

By using (3.7) and the SMW formula, the solution $x_{i,k}$ is

$$x_{j,k} = \{P^{-1} - P^{-1}U(I + V^{T}P^{-1}U)^{-1}V^{T}P^{-1}\}b_{j,k}$$

$$= \{I - P^{-1}U(I + V^{T}P^{-1}U)^{-1}V^{T}\}P^{-1}b_{j,k}$$

$$= \left\{I - [Z_{1}Z_{2}]\left(I + \begin{bmatrix}V_{1}^{T}\\V_{2}^{T}\end{bmatrix}[Z_{1}Z_{2}]\right)^{-1}\begin{bmatrix}V_{1}^{T}\\V_{2}^{T}\end{bmatrix}\right\}y_{j,k}$$

$$= y_{j,k} - [Z_{1}Z_{2}]\begin{bmatrix}W_{1}^{T}\\W_{2}^{T}\end{bmatrix}y_{j,k}$$
(3.8)

where,

$$y_{j,k} = P^{-1}b_{j,k}, (3.9)$$

$$[Z_1 Z_2] = P^{-1} U$$

$$= P^{-1} [U_1 U_2]$$
(3.10)

$$y_{j,k} = P^{-1}b_{j,k},$$

$$[Z_1Z_2] = P^{-1}U$$

$$= P^{-1}[U_1U_2],$$

$$\begin{bmatrix} W_1^T \\ W_2^T \end{bmatrix} = \left(I + \begin{bmatrix} V_1^T \\ V_2^T \end{bmatrix} [Z_1Z_2] \right)^{-1} \begin{bmatrix} V_1^T \\ V_2^T \end{bmatrix}$$
(3.10)

By using (3.8), Eq.(3.7) comes to solving two linear systems (3.9)(3.10) which coefficient matrix is the block pentadiagonal matrices P. And these equations can be solved with the Rotated ALU decomposition.

This new proposed method is named the "Split/SMW+Rotated ALU decomposion method" [5].

Numerical Experiments-2 3.3

Here, a few numerical results are presented, that is comparing the conventional LU decomposition to the Split/SMW + Rotated ALU decomposition. In these experiments, the way of experiments and the processor had been same as the Numerical Experiments-1. And this experiments' own peculiar part is described.

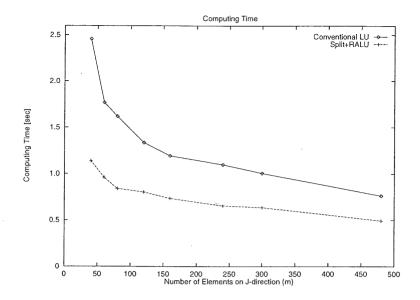


Figure 4: Comparison of computing time between the conventional LU decomposition and the Split/SMW+Rotated ALU deomposition.

3.3.1 Methods

Testing model was as follows. Block matrices composing the coefficient matrix $\hat{G}_{j,k}$ were generated with based on Frank matrix, and were sufficient nonsingularity of matrices P and $(I + V^T P^{-1} U)$. The exact solution $x_{j,k}$ was generated by random numbers. The right hand side $b_{j,k}$ was generated by multiplying $\hat{G}_{j,k}$ and $x_{j,k}$. The examination models have been showed as Tab.1. And j-direction was vectorized.

The computing time and the accuracy for the solving linear systems are measured and evaluated between the conventional LU decomposition and the Split/SMW+Rotated ALU decomposition.

3.3.2 Results

Fig.4 shows the computing time plot corresponding to Tab.1. The abscissa indicates the number of j-direction's elements (m) and the ordinate indicates the computing time [sec]. Fig.5 shows the computing time ratio. In these figures, "Split+RALU" means "Split/SMW+ Rotated ALU decomposition method".

From these results, the Split/SMW+ Ratated ALU decomposition is faster $35 \sim 40 [\%]$ than the conventional LU decomposition. On the accuracy, both algorithms are the same for this testing model, and the relative 2-norm error is as follows.:

$$\frac{\|\boldsymbol{x}_{j,k} - \bar{\boldsymbol{x}}_{j,k}\|_2}{\|\boldsymbol{x}_{j,k}\|_2} \sim O(10^{-6})$$
(3.12)

where $x_{j,k}$ is the exact solution, and $\bar{x}_{j,k}$ is the numerical solution.

4 Conclusion

In this paper, new methods are proposed and showed efficiency, those methods' application is block pentadiagonal linear systems appearing to the CFD problems.

In section 2, the detail of the Rotated ALU decomposition method are explained. This method is derived from improvement on the Alternative decomposition. From some numerical experiments,

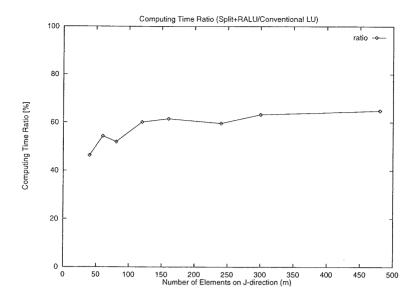


Figure 5: The ratio of computing time between the conventional LU decomposition and the Split/SMW+Rotated ALU decomposition.

the Rotated ALU decomposition is showed to effective for vector processors and kept up the accuracy against the conventional method. On the case of using vector processors, not only in the CFD problems but also in other problems, the coefficient matrix is structural symmetric matrices, the Rotated ALU decomposition method is useful.

In section 3, the theme is periodic block pentadiagonal matrices linear systems. This coefficient matrix is splitted into block pentadiagonal matrices and the matrices of the PBE, for using the Sherman-Morrison-Woodbury formula. From some numerical experiments, this Split/SMW+Rotated ALU decomposition is showed to effective and kept up the accuracy against the conventional method.

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