The Improvement of Parallel Predict-Correct Gmres(m) Algorithm and it's Application for Thin Plate Structures

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***Abstract*—Through the research of the parallel computational model based on the principal and subordinate mode and the basic theory of Gmres Algorithm in Krylov subspace, this essay raises a improvement parallel Predict-Correct Gmres(m) algorithm which posses Predict-Correct pattern, and shows the computing examples for linear equations. After the comparison with the result from the new parallel Predict-Correct GMRES(m) algorithm, at last one application is given for thin plate structures, it shows that this designed parallel algorithm can reduce the iteration frequency, shorten the computing time and obtain**

***IndexTerms*—Predict-Correct GMRES(m) Algorithm; Parallel Algorithm; thin plate structures; speedup-ratio**

I. INTRODUCTION

With the rapid development of the technology of the network, the parallel computation has become the main technology to solving the large-scale calculation, and cluster system has become a main platform cluster system for parallel algorithm, which using high-speed universal network to dispatch a group of high-performance working stations or PCs integrally, assigned relevant supporting software, such as MPI, PVM, etc., constitutes a high efficient parallel processing system. But the algorithm used in the cluster system only applies to the parallel of medium grain and above, which makes it necessary to design coarse grain parallel algorithm suitable to the network parallel.

Generalized Minimal Residual algorithm (Gmres) is a kind of projective algorithm in Krylov subspace to solve large-scale unsymmetry linear equations, which was proposed by Y.Saad andM.H.chltz in 1986. Because the Gmres algorithm is based on the wholly orthogonalization of the Krylov vectors, it has the dominance of few calculative amount and few storage, and it is widely used in the engineering domains of mechanics, numerical dynamics and numerical mathematics at present. In order to increase the calculative efficiency of the algorithm, it is a quite exective way to adopt the beforehand conditional subtechnology. Xiaoming Liu used Gmres algorithm to compute and simulate numerically in the oil deposit questions, in which the cofficient matrix was proceeded pretreatment based on the technology of dividing matrix and PE way. Chunxiao Yu and Aimin Yang [1, 2] proposed a beforehand conditional way to improve the astringency of the Gmres(m) algorithm, and proved its accuracy. By using divide and rule strategy ,Yiming Chen and Aimin Yang [3, 4] conducted parallel process of the Gmres algorithm to accelerate the calculation in matrix and vector, matrix and matrix. Except for the methods listed above, a parallel Predict-Correct Gmres(m) algotithm will be proposed to quicken convergency speed and bring down storage space, and the new parallel algorithm is based on the way to measure cmmunicative expenses of B.K.Schmidt [5], and is a parallel projective method in Krylov subspace. Through using predict-correct strategy, the parallel Predict-Correct Gmres(m) algorithm can reduce the iteration number; shorten the computational time; improve the

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computational efficiency, and increased the speedup-ratio. In this paper, the improvement of Predict-Correct Gmres(m) is given and it's application is shown for thin plate structures.

II. Predict-Correct Gmres(m) algorithm

A. Galerkin theory of linear equations in Krylov subspace

Suppose the system of equations is $Ax = b$, in which A is a nonsingular large matrix, $b \in R^n$ is a known vector and the norm herein after is 2-norm. K_m and L_m are m dimensional subspaces, which are generated from $\{v_i\}_{i=1}^m$ and $\{w_i\}_{i=1}^m$. Supposing $x_0 \in R^n$ is a random vector and $x = x_0 + z$, $Ax = b$ is equivalent to $Az = r_0$, in which $r_0 = b - Ax_0$ .Galerkin Theory used in $Az = r_0$ can be stated that approximate result z_m is sought in the subspace K_m so as to get the residual vectors $r_0 - Az_m$ and all vectors in L_m reach orthogonality. That is to say, if $z_m \in K_m$ and $\forall w \in L_m$, we will get $(r_0 - Az_m, w) = 0$ [6~9] .

Suppose $V_m = (v_1, v_2, \cdots v_m)$ and $W_m = (w_1, w_2, \cdots w_m)$, in which $\{v_i\}_{i=1}^m$ and $\{W_i\}_{i=1}^m$ are the bases of K_m and L_m separately. So we can express z_m into $z_m = V_m y_m$, in which $y_m \in R^m$. Then $(r_0 - Az_m, w) = 0$ can be shown $(W_m^T AV_m) y_m = W_m^T r_0$. Supposing $W_m^T AV_m$ is a nonsingular matrix, we can get an approximate result

$$z_m = V_m (W_m^T AV_m)^{-1} W_m^T r_0$$

B. The Gmres (m) algorithm

If we choose $L_m = K_m$, we call this Galerkin Method Arnoldi Algorithm; if we choose $L_m = AK_m$, we call this Galerkin Method as GMRES Algorithm. GMRES Algorithm has been improved greatly with the efforts from many professionals. It also has become the main method to solve large asymmetrical linear system equations through being integrated with various pretreatment technologies [10, 11].

On the basis of the analysis of the upward section, we choose $K_m = span\{r_0, Ar_0, \cdots A^{m-1} r_0\}$, so we can find a set of standard orthogonal bases in K_m. Then

$$\|r_0 - Az\| = \|r_0 - AV_m y\| = \|r_0 - AV_{m+1}\overline{H}_m y\| = \|V_{m+1}(\beta e_1 - \overline{H}_m y)\|$$

is got.

Because $V_{m+1}^T V_{m+1} = I$, $\|r_0 - Az\| = \|\beta e_1 - \overline{H}_m y\|$. So minimizing $\|r_0 - Az\|$ in R^n equals to minimizing $\|\beta e_1 - \overline{H}_m y\|$ in K_m, which can be eventually concluded into solve least squares equation $\min\|\beta e_1 - \overline{H}_m y\|$.

The calculation process of GMRES Method can be concluded into:

(1) Select x_0, then calculate $r_0 = f - A x_0$ and $v_1 = r_0 / \| r_0 \|$;

(2) Iterate $For \quad j = 1, 2, \cdots, k, \cdots$ till meeting the needs of do

$$h_{ij} = (Av_j, v_i) \quad (i = 1, 2, \cdots, j);$$

$$\hat{v}_{j+1} = Av_j - \sum_{i=1}^{j} h_{ij} v_i;$$

$$h_{j+1,j} = \|\hat{v}_{j+1}\|; \quad v_{j+1} = \hat{v}_{j+1} / h_{j+1,j}$$

(3) Construct an approximate solution $x_k = x_0 + V_k y_k$ in which y_k satisfies $\min J(y)$ ($J(y) = \|\beta e_1 - \overline{H}_k y_k\|$).

C. The Gmre(m)s Algorithm in the predict-correct system

Theoretically speaking, if $\{A^i r_0\}_{i=0}^{n-1}$ near independence, while $m = n$, GMRES(m) algorithm should offer the accurately solution, but when m is very big, all the $(v_i)_{i=1}^m$ must be saved in the calculation, which will cause memory empty more larger to large scale problem, so it is unpractical. And when $k \to \infty$, not only internal memory and the amount of calculating are increasing, but also the orthogonalily of each array in the matrix V_k becomes relatively poor, this time the solution will oscillation in a small domain. While, after the original algorithm is predicted and corrected, the difficulty is overcome when the technology of over again opening is supplied through changing the original count, then the Predict-Correct Gmres(m) algorithm in the predict-correct system is obtained.

The concrete realized steps of the Predict-Correct Gmres(m) algorithm are:

(1) Let: $x_0 = 0$, $r_0 = b - Ax_0$, $\beta = \| r_0 \|$, $v_1 = r_0 / \beta$, $V_1 = \{v_1\}$;

（2）Iteration：$For \quad j = 1, 2, \cdots, m \quad do$

$$h_{ij} = (Av_j, v_i)\,(i = 1, 2, \cdots, j), \quad \hat{v}_{j+1} = Av_j - \sum_{i=1}^{j} h_{ij} v_i$$

$$h_{j+1,j} = \|\hat{v}_{j+1}\|, \quad v_{j+1} = \hat{v}_{j+1} / h_{j+1,j},$$

$$V_{j+1} = (V_j, v_{j+1}), \quad \overline{H}_j = \begin{pmatrix} \overline{H}_{j-1} & h_{ij} \\ 0 & h_{j+1,j} \end{pmatrix}_{(j+1)\times j}$$

$\overline{H}_j$ is a upper Hessenberg matrix，when $j = 1$, the first array is omission, and $AV_m = V_{m+1}\overline{H}_m$.

(3) Solve the least square problem $\|r_m\| = \min_{y_m \in R^m} \|\beta e_1 - \overline{H}_m y_m\|$, and y_m is obtained;

(4) Conform the proximately solution

$$x_m = x_0 + V_m y_m;$$

(5) Calculate the modulo of the residual vector $\| \boldsymbol{r_m} \| = \| \boldsymbol{b} - \boldsymbol{A}\, \boldsymbol{x_m} \|$;

(6) Predict-Correct: if $\| \boldsymbol{r_m} \| \le \boldsymbol{\varepsilon}$, then $\boldsymbol{x} = \boldsymbol{x_m}$; and if $\| \boldsymbol{r_m} \| > \boldsymbol{\varepsilon}$, the result doesn't satisfy the error demand, then let $\boldsymbol{x_0} = \boldsymbol{x_m}$, predict the original count over again and return step(1) to calculate correctively (can be proceeded time and time again), in which $\boldsymbol{m}$ is the number of times in iteration of predict-correct system, $\boldsymbol{\varepsilon}$ is the established reliance of convergent judgment, and often recommendable $\varepsilon = 1.0 \times 10^{-6}$.

In (3), $\overline{\boldsymbol{H}}_{\boldsymbol{m}}$ must be changed into $\boldsymbol{F_i}$ $(\boldsymbol{i = 1, 2, \cdots, m+1})$ through plane rotation transformation in order to get y_m, in other words the QR decomposition must be proceeded to $\overline{\boldsymbol{H}}_{\boldsymbol{m}}$, that is

$$\boldsymbol{Q_m \overline{H}_m = R_m}$$

in which $\boldsymbol{Q_m = F_1 F_2 \cdots F_{m+1}}$ is a $(\boldsymbol{m+1}) \times (\boldsymbol{m+1})$ matrix, $\boldsymbol{R_m}$ is a $(\boldsymbol{m+1}) \times \boldsymbol{m}$ upper triangular matrix (the elements of the last line are all zero), then

$$\min \| \boldsymbol{\beta e_1 - \overline{H}_m y_m} \| = \| \boldsymbol{Q_m (\beta e_1 - \overline{H}_m y_m)} \| = \| \boldsymbol{g_m - R_m y_m} \|$$

in which $\boldsymbol{g_m = Q_m \beta e_1}$. That is

$$\| \boldsymbol{r_m} \| = \| \boldsymbol{b - A\, x_m} \| = \left| \boldsymbol{\bar{e}_m^T g_m} \right|$$

in which $\bar{e}_m^T$ is a $m+1$ dimension unit vector.

III. The improvement of Parallel Predict-Correct GMRES(M) algorithm

The conformation of element in Hessenberg matrix and vector in Krylov subspace both use long recurrence relation formula in Arnoldi algorithm and Gmres algorithm, which cause large storage amount and long time, but the shortcomings are overcome by the parallel Gmres algorithm in predict-correct system. Predict-Correct Gmres(m) algorithm mainly includes: the calculation of inner product for vectors, the calculation of matrix timing vector, the calculation of matrix timing matrix, the calculation of QR decomposition to solve the least square problem, predict-correct restart and etc. To the large-scale linear questions, the parallel design of these parts in the algorithm is necessary and feasible. Fundamentally basing on divide and algorithm strategy, relying on principal and subordinate mode, then design the rough grit parallel algorithm. It is a much better proposal to the cluster system which has no more nodes.

In large linear problem, it is the foremost segment of the Predict-Correct Gmres(m) algorithm to establish the test condition matrixes, to calculate the test conditions, and to solve the least square problem using QR decomposition and to restart the predict-correct system. So it is necessary to make them parallel. The parallel Predict-Correct Gmres(m) algorithm is organic combination of these segments, and through change the iteration coefficient to improve the original parallel algorithm.

If let $\boldsymbol{A = (A_1^T, A_2^T, \cdots, A_p^T)^T}$, $\boldsymbol{b = (f_1^T, f_2^T, \cdots, f_P^T)^T}$, which is the form of dividing blocks, each block will be distributed various node, the parallel iterate algorithm will be accomplished under the parallel Predict-Correct Gmres(m) algorithm in predict-correct system. In order to get the convergent solution of the linear equations more quickly, the matrix $\overline{\boldsymbol{H}}_{\boldsymbol{k}}$ will be formed over again, in every step, but its exponent will be increasing continuously. The particularly calculative steps are:

(1) $\forall \boldsymbol{X_0}$, setup parameter $\boldsymbol{\xi, \alpha, \beta, m}$ 。

(2) calculate $\boldsymbol{r_0^{(i)} = b - A_i X_0}$ in each CPU $\boldsymbol{P_i (i = 1, 2, \cdots, P)}$, get $\boldsymbol{r_0 = \sum_{i=1}^{P} r_0^{(i)}}$ and $\|\boldsymbol{r_0}\|$ through communication relying on principal and subordinate mode, then sent out r_0 and $\|r_0\|$ to P_i, and $v_1 = r_0 / \| r_0 \|$ is calculated.

(3) Iteration: DO $k = 1,\ n$

Calculate $\boldsymbol{A_i v_k}$ in $\boldsymbol{P_i}$, get $\boldsymbol{Av_k = \sum_{i=1}^{P} A_i v_k}$ through communication.

Such calculation will be run in P_i as

$$h_{ik} = (Av_k, v_i),\ i = 1, 2, \cdots, k$$

$$\hat{v}_{k+1} = Av_k - \sum_{i=1}^{k} h_{ik} v_i$$

$$h_{k+1,k} = \| \hat{v}_{k+1} \|$$

$$v_{k+1} = \hat{v}_{k+1} / h_{k+1,k}$$

Let

$$\alpha_0 = \max_i \left\{ \| v_{k+1} \|, \| v_i \| \right\} \quad i = 1, 2, \cdots, k$$

$$\boldsymbol{f_k = \left| \bar{e}_m^T g_m \right|} \quad \text{(To}$$

Predict-Correct Gmres(m) algorithm)

IF $(f_k < \xi)$ THEN

$$X_k = X_0 + V_k y_k$$

GOTO (4)

END IF

IF $(k = m \quad and \quad \alpha_0 > \alpha)$ THEN (Predict)

$$X_k = X_0 + V_k y_k$$

令 $X_0 = X_k$

GOTO (2)

END IF

Let $\beta_0 = f_k - \min_i f_i \quad (i = 1, 2, \cdots, k)$

IF $(\beta_0 > \beta)$, THEN

Let $l:\ \min_i f_i = f_l$

$$X^{(l)} = X_0 + V_l y^{(l)}$$

$$X_0 = X_l$$

（Correct）

GOTO (2)

END IF

END DO

(4) The calculation will be independently accomplished in P_i.

In the calculative process, the uppercase letter express matrix except Z_k, the lowercase letter express vector. When $n \to \infty$, $\| r_m \| < \xi$ (insure the precision requisition), $\max\limits_{1 \le i \le m} \| v_i \| \le \alpha$ (insure the orthogonalily of v_i), $\max \left| \| r_k \| - \| r_i \| \right| \le \beta$ (insure the stability of process).

The ensemble generalization of the parallel algorithm is:

(1) In the orthogonal process of forming the V and H matrixes, the parallel methods of calculating inner product and matrix timing vector will be transferred;

(2) In the process of solving the least square problem, the parallel methods of QR decomposition, matrix timing matrix, and matrix timing vector will be transferred.

(3) In the whole calculative process the divide and conquer strategy, principal and subordinate mode both are relied on. Prediction firstly and correction secondly are proceeded in the iteration process of the parallel calculation.

These are the basic calculative style and projectional thought, and relied on the divide technology and the reciprocal technology of internal and outside memory, then the scale to solve problems is improved; the calculative speed is accelerated, and time of analysis and communication is decreased, espacialy the iterational coeffecient is often adjusted to fit for reality, and then the parallel algorithm is improved. So the new parallel Predict-Correct Gmres(m) algorithm is more suitable for calculating the large-scale engineering questions, and provides a better way to make the linear equations in a broad application than original mothed.

IV. THE APPLICATION OF THE IMPROVEMENT PARALLEL PREDICT-CORRECT GMRES(M) ALGORITHM TO SOLVE THE LARGE-SCALE LINEAR EQUATIONS

Use MPI to simulate the above algorithm in the internet of 1000Mbps, choose the equity model configuration ,and realize it using Fortran. In the 8-hodes cluster system, we separately use 2 nodes ,4nocks and 8nodes to simulate the improvement parallel Predict-Correct Gmres(m) algorithm, then compare it with serial runtime and the original parallel algorithm's runtime. In the cluster each node is p_4 2.6GHZ×2. Assure the child takes of the QR decomposition is separately 2 , 4 and 8.

If $\boldsymbol{n = 800}$, $\boldsymbol{k = 3, p = 4}$, give $\boldsymbol{m}$ some values which is the iterationa's number of times in predict-correct system, and to compute using the new parallel Predict-Correct Gmres(m) algorithm, then the graph of relation is obtained about $\boldsymbol{m}$ and $\boldsymbol{l}$ (the predict-correct's number of times), such as fig. 1.

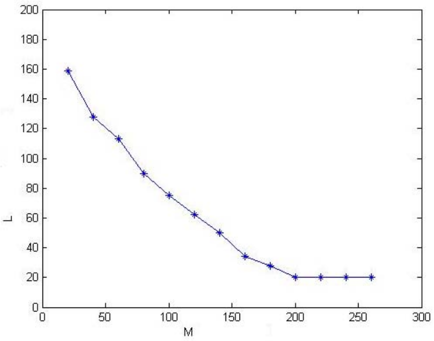

Fig.1 Inflence of iteration number on predict-correct number

If let the iterative number of times $m = 195$ in predict-correct system, part of calculative result are given as table 1.

In the table $\boldsymbol{n}$ expresses the rank of the matrix, P expresses the number of CPU, K expresses the number of the divided assignment.

We can see from the table that under the loom cluster environment, when p=2, the parallel algorithm gets a certain acceleration will also increase, but the acceleration ratio when k=4 is less than the acceleration ratio when k=8 .this is because when k increase, the date that transported also increase, so it causes the increasing of the communication. This is fit to the theoretical and practical analysis.

Table 1 The calculative consecutive comprison of Predict-Correct Gmres(m) algorithm and it's improvement

n	Algorithm	Serial time (s)	K=2 P=2		
			Parallel time (s)	Speed-up ratio	Efficiency
600	The Improvement	90.66	49.36	1.84	0.94
	Predict-Correct Gmres(m)	90.66	50.03	1.81	0.91
1200	The Improvement	190.53	93.21	1.88	0.94
	Predict-Correct Gmres(m)	190.53	102.35	1.86	0.93
n	Algorithm	Serial time (s)	K=4 P=4		
			Parallel time (s)	Speed-up ratio	Efficiency
600	The Improvement	90.66	39.11	2.67	0.62
	Predict-Correct	90.66	40.68	2.23	0.56

	Gmres(m)				
1200	The Improvement	190.53	58.02	3.22	0.81
	Predict-Correct Gmres(m)	190.53	60.33	3.16	0.79
n	Algorithm	Serial time (s)	K=8 P=8		
			Parallel time (s)	Speed-up ratio	Effic-iency
600	The Improvement	90.66	35	2.55	0.32
	Predict-Correct Gmres(m)	90.66	35.79	2.53	0.32
1200	The Improvement	190.53	70.33	2.72	0.40
	Predict-Correct Gmres(m)	190.53	72.34	2.63	0.33

V. THE APPLICATION FOR THIN PLATE STRUCTURES

A plate with the size of 1920×1920×120 shown as below is fixed on both sides. Its upper surface has a 100 uniform load. The elastic coefficient is $E = 2.0 \times 10^9, v = 0.25$. Now the upper and bottom suffaces are divided into 16×16 small unites and the sides are divided into 16×4 small unites. The model nodes number is 2306; the freedom degree is 6918; the units number is 768. Using the BEM from Parallel new algorithm in this papper, if $m = 195$, the comparsion with the traditional BEM is as Fig. 2.

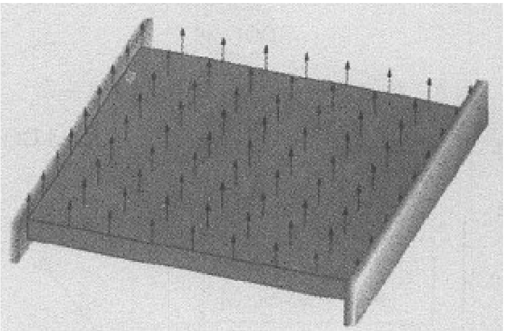

Fig.2 Thin pane fixed at two lateral surface

Table 2 Comparison of New Algorithm and Traditional BEM

	New Algorithm (P=2)	Traditional BEM
Error/%	<0.53	<9
Iteration Number	195	75
Computation Time/s	893	921
One-step Time/s	8.91	12.28
Forming Matrix Time/s	234	299

We can see from Fig. 2 that, the convergence speed happened in the improved parallel algorithm is much faster than that in the traditional BEM. And the error happened in the improved parallel algorithm is much reduced.

VI. CONCUSION AND OUTLOOK

The improvement of parallel Predict-Correct Gmres(m) algorithm put forward in this text has the traits of little communication and high level parallel degree. From the theoretical analysis and the experiment, we can say that it is fit to compute under the cluster environment, and that it has faster calculative speed and higher calculative efficiency. The researchable conculsion in this paper has very vasty applicative foreground in computational mathematics and computational mechanics.

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