Available online at http://scik.org
J. Math. Comput. Sci. 5 (2015), No. 3, 280-296
ISSN: 1927-5307

FAST FINITE ELEMENT SOLVER FOR INCOMPRESSIBLE NAVIER-STOKES EQUATION BY PARALLEL GRAM-SCHMIDT PROCESS BASED GMRES AND HSS

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Abstract. After finite element discretization of incompressible Navier-Stokes equation, a sparse linear system is obtained in every iteration, and GMRES provides an efficient approach to solve this system. However, if the size of the original PDE model is large, the solution speed of the incompressible Navier-Stokes equation is still slow. Since the linear system from the incompressible Navier-Stokes equation is saddle point problem, we find that large portion of computational efforts for solving the linear system is occupied by the vector projection in GMRES. In this paper, by our parallel Gram-Schmidt process based GMRES and newly developed preconditioner Hermitian/Skew-Hermitian Separation (HSS), we develop a fast solver HSS-pGMRES for the saddle point problem from incompressible Navier-Stokes Equation. Theoretical analysis shows that, HSS-pGMRES decreases the computational complexity of finite element solver for incompressible Navier-Stokes equation from O(m^2n) to O(mn), where m is the grid size. Computational experiments show that, the fast solver HSS-pGMRES significantly increases the solution speed for the saddle point problem of incompressible Navier-Stokes equation than the conventional solvers.

Keywords: fast solver; vector projection; parallel GMRES; Hermitian/Skew-Hermitian Separation; finite element method; incompressible Navier-Stokes equation.

2010 AMS Subject Classification: 76M10.

1. INTRODUCTION

The incompressible Navier-Stokes equation is a mass conservation and momentum conservation based mathematical equation. Besides the fluid density ρ is fixed, the incompressible Navier-Stokes decides two fundamental properties of a flow: the velocity u and the pressure p in a flow

Received December 11, 2014

field along with the time *t*, and the boundary condition of the flow field and the initial condition for the time *t* provide the uniqueness of the two variables.

Incompressible Navier-Stokes equation is usually solved by numerical methods such as finite difference method or finite element method: Anderson studied the numerical solution of Navier-Stokes equation by finite difference method in [1], and Elman *et al*. studied finite element solution of incompressible Navier-Stokes equation in [2].

Numerically solving incompressible Navier-Stokes equation is slow when the grid size is large, acceleration methods for Navier-Stokes equation are developed to accelerate the solution speed, and these approaches include high-order discretization [3-5], preconditioning, parallel computing [6-13], GPU computing, *etc*.

The linear system from the discretization of incompressible Navier-Stokes equation is often solved by sparse solvers such as GMRES, and GMRES stands for Generalized Minimal Residual Method [14]. Performance improvement of GMRES is studied in [15, 16], and parallel GMRES is one of possible approaches to accelerate the solution speed of incompressible Navier-Stokes equation.

Preconditioner is another approach to accelerate the solution speed of incompressible Navier-Stokes equation. Elman *et al*. developed kinds of preconditioners in [17-21], and Benzi *et al*. developed preconditioners for the system [22, 23].

If the size of the original PDE model is large, the solution speed of the incompressible Navier-Stokes equation is still slow. Since the linear system from the incompressible Navier-Stokes equation is the saddle point problem, we find that large portion of computational efforts of solving the linear system is invested on the vector projection in GMRES. In this paper, by our parallel Gram-Schmidt process based GMRES and newly developed preconditioner Hermitian/Skew-Hermitian Separation (HSS) for the saddle point problem, we develop a fast solver HSS-pGMRES for incompressible Navier-Stokes equation.

2. METHODS

In this section, we firstly discuss the preconditioner Hermitian/Skew-Hermitian Separation, then we develop parallel GMRES, and we develop the fast solver HSS-pGMRES for the saddle point problem. Finally, HSS-pGMRES is applied to incompressible Navier-Stokes equation for a fast solution.

2.1 The Hermitian/Skew-Hermitian Separation

Saddle point matrix is a matrix with the form:

$$\begin{bmatrix} F & D^T \\ D & -E \end{bmatrix} \begin{bmatrix} du \\ dp \end{bmatrix} = \begin{bmatrix} R_d \\ r_d \end{bmatrix}, \tag{1}$$

where *F* and *E* are usually symmetric matrices [24], *du* and *dp* are unknown variables, and R_d and r_d are right-hand-side. Saddle point problems appear in high-frequency in scientific and engineering applications. Golub reviewed solution methods for saddle point problem in [24], and the solution methods for saddle point problem include Schur complement reduction, null space methods, coupled direct solvers, stationary iterations, Krylov subspace methods, preconditioner and multilevel methods [24].

Newly developed matrix splitting based methods such as HSS provide an efficient way to solve saddle point problems [25-27]. Golub *et al*. developed HSS in [28], parameter optimization for HSS is proposed in [29], and preconditioned HSS is studied in [30-35].

To efficiently solve a linear system with the structure of saddle point problem of equation (1) with the symmetric part *H* and the skew-symmetric part *S*, we firstly solve an uncoupled linear system:

$$(H + \alpha I_n) \cdot du^{k+\frac{1}{2}} = f_{uc}^k, \tag{2.1}$$

$$(E + \alpha I_m) \cdot dp^{k+\frac{1}{2}} = g_{uc}^k. \tag{2.2}$$

where $f_{uc}{}^k$ and $g_{uc}{}^k$ are right-hand-side. Then we solve a coupled linear system:

$$(\alpha I_n + S) \cdot du^{k+1} + D^T \cdot dp^{k+1} = f_c^k, \tag{3.1}$$

$$-D \cdot du^{k+1} + \alpha p^{k+1} = g_c^k. \tag{3.2}$$

where f^k and g^k are right-hand-side. By Schur complement reduction, we obtain:

$$[D(I_n + \alpha^{-1}S)^{-1}D^T + \alpha^2 I_m] \cdot dp^{k+1} = D(I_n + \alpha^{-1}S)^{-1}f^k + \alpha g^k. \tag{4}$$

Since the coefficient matrix $[D(I_n + \alpha^{-1}S)^{-1}D^T + \alpha^2 I_m]$ of equations (4) is large and sparse matrix, GMRES is applied to solve dp^{k+1}, then we obtain du^{k+1}. The details of HSS are described in Algorithm 1:

Algorithm 1: The Hermitian/Skew-Hermitian Separation

Initialization of HSS

while $R < tol_{HSS}$

Solve the couple system equations (2)

Solve the uncoupled system equations (3)

end while

Convergence analysis of HSS (Algorithm 1) can be found in [30], and the convergence speed of HSS (Algorithm 1) is decided by tol_{HSS}. However, the linear systems are unnecessary to be solved exactly, and the tolerance of the iterative solver for the linear systems can be loosened to increase the solution speed, which leads to inexact HSS.

2.2 Parallel GMRES

As we discussed, the uncoupled system equations (4) in HSS (Algorithm 1) can be solved by sparse solvers such as GMRES, and the details of GMRES are described in Algorithm 2:

Algorithm 2: GMRES

Initialization of GMRES

while $R_k < tol_{GMRES}$

$w_0^{k+1} = A \cdot v^k$

$v_{i+1}^{k+1} = v_i^{k+1} - \sum_{i=1}^{k-1} P\left(w_i^{k+1}, v_i\right)$

Calculate y_k such that $R_k = min\|R_0 e_1 - H_k y_k\|$

end while

$u^k = u^0 + V_k y_k$

In GMRES (Algorithm 2), Gram-Schmidt process is chosen to build the orthogonal set u. In details of Gram-Schmidt process, the vector projection is defined as:

$$P(u, v) = \frac{\langle u,v \rangle}{\langle u,u \rangle} u. \tag{5}$$

Gram-Schmidt process works as:

$$u_1 = v_1,$$
$$u_k = v_k - \sum_{i=1}^{k-1} P(u_i, v_i). \tag{6}$$

In GMRES (Algorithm 2), large portion of computational efforts is spent on building the orthogonalization basis in Gram-Schmidt process, and statistics from computational experiments show that the ratio of computational cost of Gram-Schmidt process to GMRES (Algorithm 2) is about 1/4. To further increase the solution speed of GMRES (Algorithm 2), the process of building the orthogonalization basis can be parallelized for higher efficiency, and the parallel strategy for Gram-Schmidt process based GMRES (pGMRES) is illustrated in **Figure 1**.

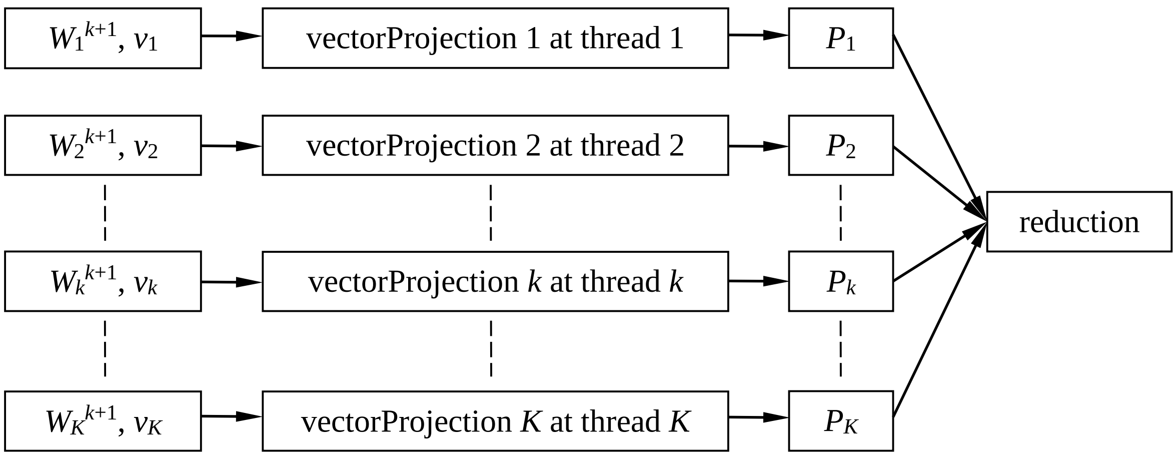


Figure 1. Parallel Strategy for Gram-Schmidt Process based GMRES

pGMRES is designed to simultaneously calculate the vector projection $P(u, v)$ of equation (5). From **Figure 1** we can see, every thread is responsible for calculating a the vector projection $P(u, v)$ of equation (5), and a reduction is followed to calculate the summation in equation (6). The number of the vector projection $P(u, v)$ of equation (5) increases in the summation of equation (6) along with pGMRES iterations. However, the number of threads for pGMRES must keep the same in **Figure 1**. To settle this conflict, the redundant threads calculate vectors with all zero elements to keep the load balance of threads.

Algorithm 3: Parallel Gram-Schmidt Process based GMRES

Initialization of GMRES

while $R_k < tol_{GMRES}$

$$w_0^{k+1} = A \cdot v^k$$

Calculate v_{i+1}^{k+1} by parallel Gram-Schmidt Process

Calculate y_k

end while

$u^k = u^0 + V_k y_k$

In the conventional Gram-Schmidt Process, we need *k* times computation of the vector projection *P*(*u*, *v*) of equation (5) in *k* iteration of GMRES. Therefore, we need total $\frac{m(m+1)}{2}$ computation of the vector projection *P*(*u*, *v*) of equation (5) with time complexity O(m^2) to build the orthogonal set *u*. In parallel Gram-Schmidt Process of **Figure 1** and Algorithm 3, we calculate the vector projection *P*(*u*, *v*) of equation (5) simultaneously in *k* iteration of GMRES, and we only need *m* computation of the vector projection *P*(*u*, *v*) of equation (5) with time complexity O(*m*) to build the orthogonal set *u*.

2.3 Hermitian/Skew–Hermitian Separation–parallel GMRES

pGMRES (Algorithm 3) developed in the subsection 2.2 can be applied to HSS (Algorithm 1) in the subsection 2.1 to construct a fast solver HSS-pGMRES for the saddle point problem. HSS-pGMRES consists of two loops: the outer loop for HSS and the inner loop for pGMRES, and the details of HSS-pGMRES are described in Algorithm 4:

Algorithm 4: HSS-pGMRES

Initialization of HSS

while $R < tol_{HSS}$

Solve the couple system equation (1)

Solve the uncouple system equation (2)

Initialization of pGMRES

while $R_k < tol_{GMRES}$

$w_0^{k+1} = A \cdot v^k$

Calculate v_{i+1}^{k+1} by parallel Gram-Schmidt Process

Calculate y_k

end while

$u^k = u^0 + V_k y_k$

end while

In the conventional GMRES (Algorithm 2), we need k times computation of the vector projection $P(u, v)$ of equation (5) in k iteration of GMRES and n iteration of HSS (Algorithm 1). Therefore, we need total $\frac{m(m+1)n}{2}$ computation of the vector projection $P(u, v)$ of equation (5) with time complexity $O(m^2n)$ to build all orthogonal sets. In HSS-pGMRES (Algorithm 4), we calculate the vector projection $P(u, v)$ of equation (5) simultaneously in k iteration of GMRES and n iteration of HSS (Algorithm 1), and we only need mn computation of the vector projection $P(u, v)$ of equation (5) with time complexity $O(mn)$ to build the orthogonal set u.

2.4 HSS-pGMRES for Incompressible Navier-Stokes equation

In this subsection, we apply HSS-pGMRES (Algorithm 4) to fast solve the saddle point problem from incompressible Navier-Stokes equation, which is discretized by finite element method. The time-independent incompressible Navier-Stokes equation is:

$$-k\Delta u + u \cdot \nabla u + \nabla p = f, \tag{6.1}$$

$$\nabla \cdot u = 0, \tag{6.2}$$

where k is kinematic viscosity, u is velocity, p is pressure and f is the force term.

Firstly we approximate u by velocity basis function φ_i and p by pressure basis function ψ_j, and we obtain:

$$k \int \nabla\varphi_i \cdot \nabla\varphi_j + \int \left(u^* \cdot \nabla\varphi_j\right)\varphi_j + \int \left(\varphi_j \cdot \nabla u^*\right)\varphi_j - k \int \nabla\varphi_i \cdot \nabla\varphi_j = R_d,$$

$$\int \varphi_k \cdot \nabla\varphi_j = r_d,$$

where R_d and r_d is the right-hand-side. Setting

$$A = \int \nabla\varphi_i \cdot \nabla\varphi_j,$$

$$B = \int \nabla\varphi_i \cdot \nabla\varphi_j,$$

$$C = \int \nabla\varphi_i \cdot \nabla\varphi_j,$$

$$D = \int \nabla\varphi_i \cdot \nabla\varphi_j,$$

we obtain the linear system of the saddle point problem of equation (1). A posteriori error estimate is used for error analysis, and the estimated error is plotted based on grid used in the specific problem [2].

In the conventional GMRES (Algorithm 2) for incompressible Navier-Stokes equation, we need k times computation of the vector projection $P(u, v)$ of equation (5) in k iteration of GMRES and n iteration of HSS (Algorithm 1). Therefore, we need total $\frac{m(m+1)n}{2}$ computation of the vector projection $P(u, v)$ of equation (5) with time complexity $O(m^2n)$ to solve incompressible Navier-Stokes equation. In HSS-pGMRES (Algorithm 4) for incompressible Navier-Stokes equation, we calculate the vector projection $P(u, v)$ of equation (5) simultaneously in k iteration of GMRES and n iteration of HSS (Algorithm 1), and we only need mn computation of the vector projection $P(u, v)$ of equation (5) with time complexity $O(mn)$ for solving incompressible Naiver-Stokes equation. Meanwhile, m usually means the grid size for discretization of incompressible Navier-Stokes equation, either by finite element method or finite difference method.

3. COMPUTATIONAL RESULTS

3.1 The Problem

To test the performance of HSS-pGMRES (Algorithm 4) for incompressible Navier-Stokes equation, we set $f = 0$ in equation (6.1) in the square $-1 \leq x \leq 1$ and $-1 \leq y \leq 1$. The inflow boundary is set as the Dirichlet condition $x = -1$, and the outflow boundary is set as the Neumann condition:

$$\frac{\partial u_x}{\partial x} - p = 0,$$
$$\frac{\partial u_y}{\partial y} = 0.$$

We coded HSS-pGMRES (Algorithm 4), and the discretization of incompressible Navier-Stokes equation is based on IFISS [36]. The server is Intel Core 2 2.66 GHz CPU and 4G ECC 800MHz memory (DELL XPS 410). We test the performance of HSS-pGMRES (Algorithm 4), and all numerical experiments are repeated for three times.

3.2 Performance of HSS-pGMRES

In this experiment, we compare time cost of three different solvers: Gauss Jordan Elimination (GJE), HSS-GJE and HSS-pGMRES (Algorithm 4) for incompressible Navier-Stokes equation. The grid in this experiment is 8×8. In HSS-pGMRES (Algorithm 4), we set $tol_{HSS} = 10^{-2}$ and

$tol_{GMRES} = 10^{-12}$. The time cost of all three solvers is tested for three times, average values and standard deviations are plotted in **Figure 2**.

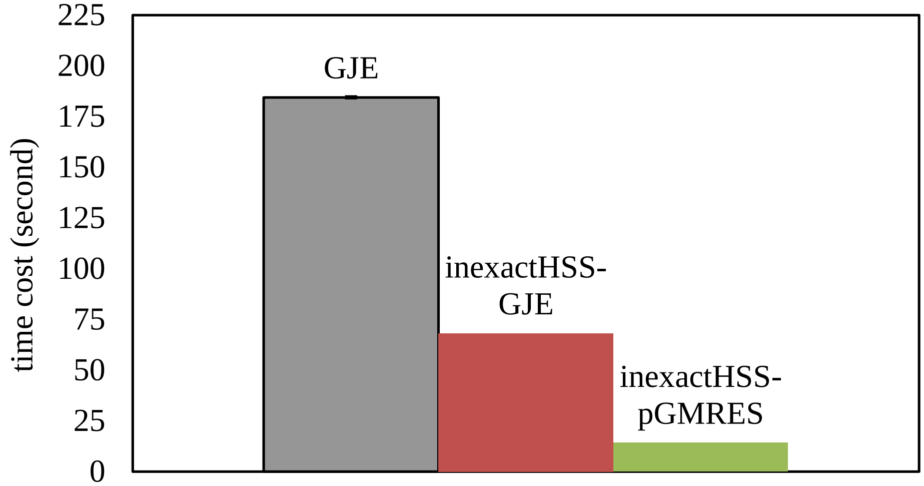


Figure 2. The time cost of the three solvers for incompressible Navier-Stokes equation: GJE, HSS-GJE and HSS-pGMRES

From **Figure 2** we can see, to solve a linear system with the same size, HSS-pGMRES (Algorithm 4) is the fastest, HSS-GJE is the middle, and GJE is the slowest. To quantitatively measure the acceleration of every solver, we define the acceleration rate as the following:

$$rate = \frac{t_{slowest}}{t_i},$$

where $t_{slowest}$ is the time cost of the slowest solver GJE, t_i is the time cost of a testing solver, and *rate* is the calculated acceleration rate. The calculated acceleration rates for the three solvers GJE, HSS-GJE and HSS-pGMRES (Algorithm 4) are listed in **Table 1**.

Table 1. Calculated acceleration rate for the three solvers: GJE, HSS-GJE and HSS-pGMRES

	GJE	HSS-GJE	HSS-pGMRES
Acceleration rate	1.00	2.71	12.93

From **Table 1** we can see, HSS-pGMRES (Algorithm 4) is about 12.93 times faster than GJE, and HSS-GJE is about 2.71 times faster than GJE. From **Figure 2** and **Table 1** we can see, HSS-pGMRES (Algorithm 4) significantly accelerates the solution speed of the saddle point problem from incompressible Navier-Stokes equation.

HSS-pGMRES (Algorithm 4) increases the solution speed of the saddle point problem from incompressible Navier-Stock equation, does HSS-pGMRES (Algorithm 4) produce the same results to GJE and HSS-GJE? To answer this question, we plot calculated velocity *u* from GJE, HSS-GJE and HSS-pGMRES (Algorithm 4) in **Figure 3**.

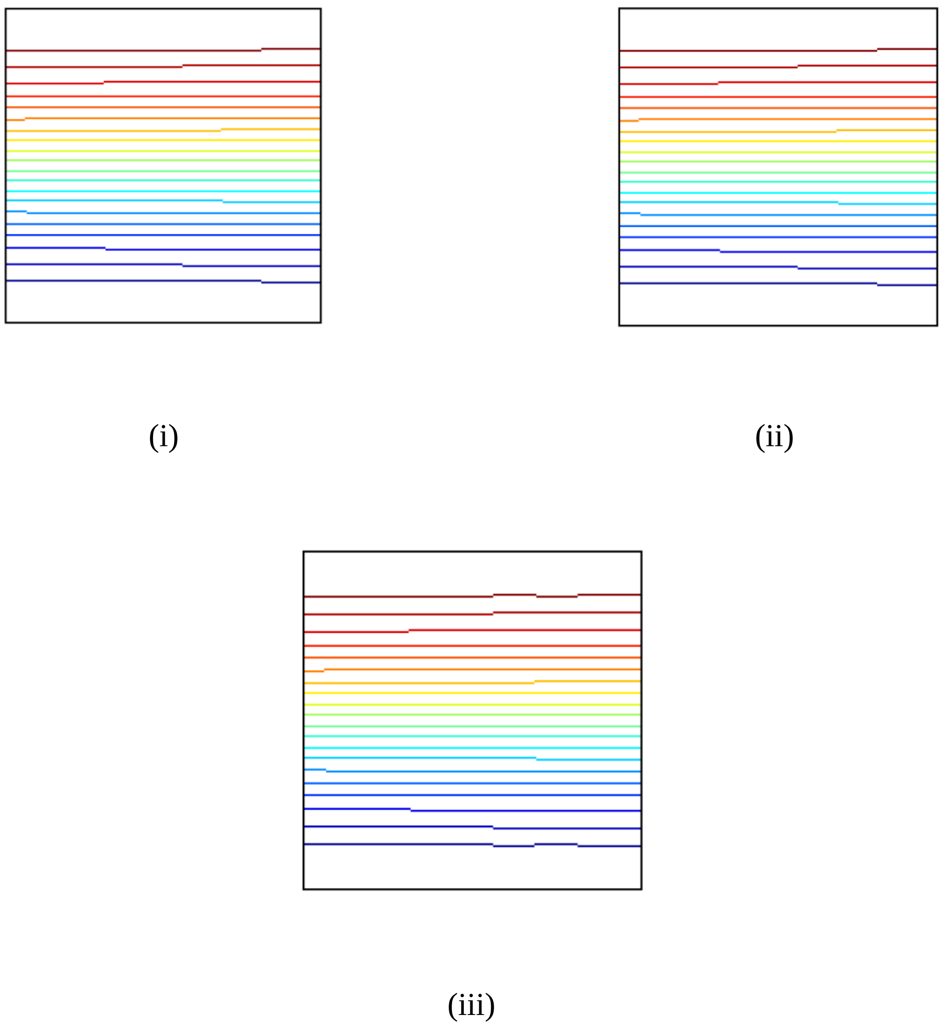
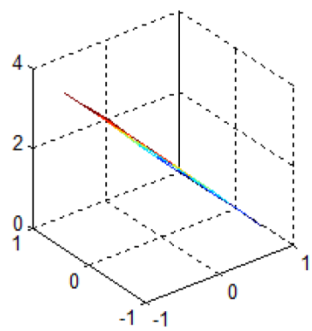
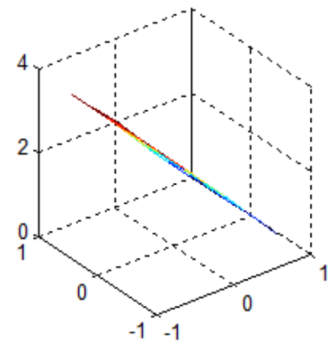


Figure 3. Calculated velocity *u* for incompressible Navier-Stokes equation by IFISS [36]: (i) GJE, (ii) HSS-GJE and (iii) HSS-pGMRES

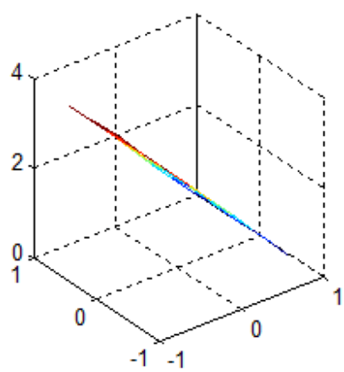
From **Figure 3** we can see, the three solvers, GJE, HSS-GJE and HSS-pGMRES (Algorithm 4) produce the same results of calculated velocity *u*. We also plot calculated pressure *p* from GJE, HSS-GJE and HSS-pGMRES (Algorithm 4) in **Figure 4**.



(i)



(ii)



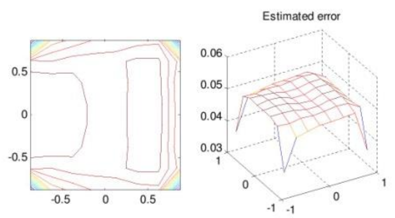
(iii)

Figure 4. Calculated pressure *p* for incompressible Navier-Stokes equation by IFISS [36]: (i) GJE, (ii) HSS-GJE and (iii) HSS-pGMRES

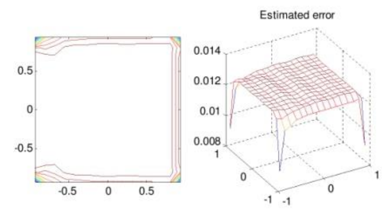
From **Figure 4** we can see, the three solvers, GJE, HSS-GJE and HSS-pGMRES (Algorithm 4) produce the same results of calculated pressure *p*. While **Figure 3** and **Figure 4** provide visual coincidence among results from GJE, HSS-GJE and HSS-pGMRES (Algorithm 4), quantitative coincidence among results from the three solvers can be compared by their estimated errors.

3.3 Scalability of HSS-pGMRES to the Grid Size

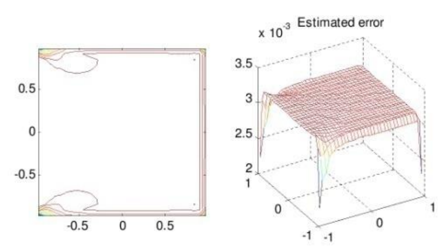
In this subsection, we compare the solution accuracy of HSS-pGMRES (Algorithm 4) in different grid size: 8×8, 16×16 and 32×32. We set $tol_{HSS} = 10^{-2}$ for 8×8, $tol_{HSS} = 10^{-3}$ for 16×16 and $tol_{HSS} = 10^{-4}$ for 32×32. Estimated error is plotted in **Figure 5**.



(i)



(ii)



(iii)

Figure 5. Estimated error by HSS-pGMRES for incompressible Navier-Stokes equation by IFISS: (i) $tol_{HSS} = 10^{-2}$ and grid = 8×8, (ii) $tol_{HSS} = 10^{-4}$ and grid = 8×8 and (iii) $tol_{HSS} = 10^{-4}$ and grid = 32×32

From **Figure 5** we can see, by HSS-pGMRES (Algorithm 4) for incompressible Navier-Stokes equation, the estimated error decreases along with increasing the tolerance of HSS tol_{HSS}, also the estimated error decreases along with increasing the grid size.

3.4 Scalability of HSS-pGMRES to Number of Threads

In this experiment, we test the acceleration of HSS-pGMRES (Algorithm 4) for incompressible Navier-Stokes equation along with increasing the number of threads. The grid in this experiment is 16×16. In inexactHSS, we set $tol_{HSS} = 10^{-3}$. In GMRES, we set $m = 10$ and $tol_{GMRES} = 10^{-12}$. The time cost of different number of threads is recorded for three times, average values and standard deviations are plotted in **Figure 6**.

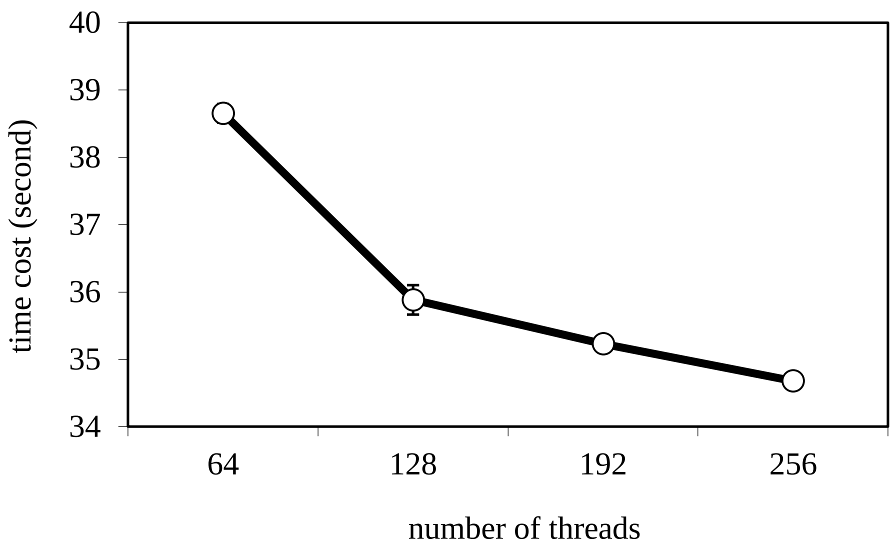


Figure 6. The time cost of different number of threads of HSS-pGMRES for incompressible Navier-Stokes equation

From **Figure 6** we can see, HSS-pGMRES (Algorithm 4) scales well with respect to the number of threads, and increasing the number of threads significantly decreases the time cost of HSS-pGMRES (Algorithm 4). In **Figure 6**, the time cost of HSS-pGMRES (Algorithm 4) does not linearly decrease, and the reason why this phenomenon happens is that parallel Gram-Schmidt process occupies a portion of computation of HSS-pGMRES (Algorithm 4).

4. CONCLUSIONS

In this paper, we find that large portion of computational efforts for solving the linear system is occupied by the vector projection in GMRES. By our parallel Gram-Schmidt process based GMRES and newly developed preconditioner Hermitian/Skew-Hermitian Separation, we develop a fast solver HSS-pGMRES (Algorithm 4) for the saddle point problem from incompressible Navier-Stokes equation. Theoretical analysis shows that, HSS-pGMRES (Algorithm 4) decreases the computational complexity of finite element solver for incompressible Navier-Stokes equation from $O(m^2n)$ to $O(mn)$, where m is the grid size. Computational results show that, HSS-pGMRES (Algorithm 4) significantly increases the solution speed of saddle point problem from incompressible Navier-Stokes equation than the conventional solvers.

5. DISCUSSION

In this paper, the fast solver HSS-pGMRES (Algorithm 4) is built by parallel Gram-Schmidt process. However, parallelization of Gram-Schmidt process is not the unique approach to accelerate GMRES, and other strategies are also possible to build parallel GMRES [37-41]. Also, the orthogonal set is built by Gram-Schmidt process in the fast solver HSS-pGMRES (Algorithm 4), and other orthonormalization algorithms are also suitable for this purpose.

In this paper, HSS-pGMRES (Algorithm 4) is implemented by CPU multi-threading programming. However, other parallel platforms such as GPU programming are also applicable. Recently, incompressible Navier-Stokes equation is widely accelerated in the platform of GPU computing. For example, Kelly *et al*. developed a GPU-accelerated mesh-less method in [42], Yidong *et al*. developed OpenACC-based GPU acceleration in [43], and Chandar *et al*. developed GPU-based solver on moving overset grids in [44].

HSS-pGMRES (Algorithm 4) has two loops: the outer loop of HSS and the inner loop of GMRES. The accuracy of HSS-pGMRES (Algorithm 4) is decided by the tolerances of the two loops: the tolerance of the outer loop HSS tol_{HSS} and the tolerance of the inner loop GMRES tol_{GMRES}: small tolerance means higher accuracy but more computation. Therefore, to obtain maximum accuracy of HSS-pGMRES (Algorithm 4) with the minimum computational burden, the selection of both tolerances should be careful.

In this paper, we apply the fast solver HSS-pGMRES (Algorithm 4) for the saddle point problem from incompressible Navier-Stokes equation. HSS-pGMRES (Algorithm 4) is also beneficial to saddle point problems from other equations such as computational solid mechanics, computational electromagnetic, linear elasticity and constrained quadratic optimization.

Conflict of Interests

The authors declare that there is no conflict of interests.

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