Parallel Numerical Algorithm for Simulation of a Three-Dimensional Lid-Driven Cavity Flow Problem with the Use of Compact Schemes

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Abstract

The parallel algorithm for simulation of the three-dimensional lid driven cavity flow problem with Reynolds numbers up to 10000 on a grid 128x128x128 was developed and implemented in the research. The problem is solved by numerical method where momentum equation is solved by a modified fractional step method with the use of compact scheme and pressure equation is solved by Fourier method in combination with the matrix sweep. The technique of the domain decomposition for parallelization of the proposed numerical method is described. In the process of computing and comparative experiment the dependency of the resulted acceleration and the coefficient of the calculation scalability on number of processors was found.

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1 Introduction

The turbulent motion is the most common form of the motion of fluids, gases in nature and in many technical devices. Therefore, the main issue for the studies of turbulent flows is development or improvement of the known numerical methods allowing to make the most effective and accurate complex calculations of turbulence and their applications in the solving of major practical problems of turbulent flows [1], [2], [3]. Known analytical methods are restricted in describing of the turbulence dynamics due to neglect of the influence of pressure and other forces. Nowadays numerical simulation with the use of parallel techniques is the only method for the turbulence dynamics simulation.

In this research the effective parallel numerical algorithm for solving a three-dimensional problem of a moving cavity [4] with large Reynolds numbers implemented on the multiprocessing system.

2 Statement of problem

The three-dimensional test problem on the lid-driven cavity flow at different Reynolds numbers: Re=400, Re=1000, Re=5000, Re=10000 is considered. The cavity lid (wall 6 in fig. 1) moves to the right with the constant speed of $u_1 = 1$. No slip boundary conditions have been employed on the remaining walls (walls 1, 2, 3, 4, 5 in fig. 1). To determine the turbulent characteristics it is necessary to numerically simulate the changes in all parameters at different Reynolds numbers.

![Figure 1: Computational domain](image)

The numerical simulation of the problem is performed on the basis of solving of non-stationary filtered Navier-Stokes equations within equation of con-
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Continuity in Cartesian coordinate system:

\[
\begin{aligned}
\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial (\bar{u}_i \bar{u}_j)}{\partial x_j} &= -\frac{1}{\rho} \frac{\partial \bar{p}}{\partial x_i} + \frac{1}{Re} \frac{\partial^2 \bar{u}_i}{\partial x_j \partial x_j} - \frac{\partial \tau_{ij}}{\partial x_j}, \\
\frac{\partial \bar{u}_i}{\partial x_i} &= 0,
\end{aligned}
\]

(1)

where \(\bar{u}_i\) – velocity components, \(\bar{p}\) – pressure, \(t\) – time, \(\nu\) – coefficient of kinematic viscosity, \(\tau_{ij}\) – subgrid tensor responsible for small-scale structures, \(i, j = 1, 2, 3\).

The idea of the large eddy simulation is to present exactly of motions of subgrid turbulence scales. This effect of the subgrid turbulence scales influence is expressed by the subgrid member.

For simulation of subgrid tensor we used the viscous model which appears in the form of:

\[
\tau_{ij} - \frac{\delta_{ij}}{3} \tau_{kk} = -2\nu_T \bar{S}_{ij},
\]

where \(\nu_T = C_S \Delta^2 \left(2\bar{S}_{ij}\bar{S}_{ij}\right)^{1/2}\) – turbulent viscosity; \(C_S\) – empirical coefficient; \(\Delta = \left(\Delta_i \Delta_j \Delta_k\right)^{1/3}\) – strainer screen width; \(\bar{S}_{ij} = \frac{1}{2} \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i}\right)\) – velocity strain tensor [5],[6].

3 Numerical method

For the numerical solution of the Navier-Stokes equation (1) we used the scheme of splitting by physical parameters which consist of three stages. At the first stage, Navier-Stokes equation is solved without taking into account the pressure. The compact extended-precision scheme [7],[8],[9] is used for the approximation of convective and diffusive members of the equation.

The intermediate velocity field is found with the use of the fractional step method [10] within the sweep method. The intermediate values of velocities are calculated by three processors in parallel.

Compact approximation of convective term of momentum equations is the third order of accuracy, and for diffusion terms - of the forth order of accuracy.

At the second stage Poisson equation is solved. Poisson equation is derived from the equation of continuity taking into account the velocity field of the first stage. The original solution algorithm was developed to solve three-dimensional Poisson equation. It is the spectral transformation in combination with the matrix sweep which is applied for the determination of Fourier coef-
ficients and appears in the following finite-difference form:

\[
\frac{\bar{p}_{i+1,j,k}-2\bar{p}_{i,j,k}+\bar{p}_{i-1,j,k}}{\Delta x_1^2} + \\
\frac{\bar{p}_{i,j+1,k}-2\bar{p}_{i,j,k}+\bar{p}_{i,j-1,k}}{\Delta x_2^2} + \\
\frac{\bar{p}_{i,j,k+1}-2\bar{p}_{i,j,k}+\bar{p}_{i,j,k-1}}{\Delta x_3^2} = -F_{i,j,k}
\]  

(2)

The pressure field appears in the form of Fourier’s series [11]:

\[
\bar{p}_{i,j,k} = \frac{2}{N_3} \sum_{l=0}^{N_3} \rho_l a_{i,j,l} \cos \frac{\pi kl}{N_3},
\]

\[
F_{i,j,k} = \frac{2}{N_3} \sum_{l=0}^{N_3} \rho_l b_{i,j,l} \cos \frac{\pi kl}{N_3}
\]

(3)

where

\[
a_{i,j,l} = \sum_{k=0}^{N_3} \rho_k \bar{p}_{i,j,k} \cos \frac{\pi kl}{N_3},
\]

\[
b_{i,j,l} = \sum_{k=0}^{N_3} \rho_k F_{i,j,k} \cos \frac{\pi kl}{N_3}
\]

(4)

\[
\rho_i = \begin{cases} 
1, & 1 \leq i \leq N_3 - 1 \\
0.5, & i = 0, N_3.
\end{cases}
\]

After substituting (3) in the equation (2) and several arithmetical transformations the equation (2) is of the form:

\[-\frac{1}{\Delta x_2^2} a_{i,j-1,l} + \\
\left[ \frac{2}{\Delta x_1^2} + \frac{2}{\Delta x_2^2} - \frac{1}{\Delta x_1^2} \left( 2 \cos \frac{\pi l}{N_3} - 2 \right) \right] a_{i,j,l} - \\
-\frac{1}{\Delta x_2^2} a_{i,j+1,l} = b_{i,j,l} \]

(5)

In vector form the equation (5) is written for each fixed value \( l = k, k = 0, N_3 \) as follows:

\[-A_j \vec{a}_{j-1} + B_j \vec{a}_j - C_j \vec{a}_{j+1} = \vec{F}_j, \]

(6)

where matrices \( A_j, B_j, C_j \) and vectors \( \vec{F}_j, \vec{a}_j \) are of the following form:

\[
A_j = \begin{bmatrix} 
\frac{1}{\Delta x_2^2} & 0 \\
\vdots & \ddots \\
0 & \frac{1}{\Delta x_2^2}
\end{bmatrix}, \quad C_j = \begin{bmatrix} 
\frac{1}{\Delta x_2^2} & 0 \\
\vdots & \ddots \\
0 & \frac{1}{\Delta x_2^2}
\end{bmatrix}
\]
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\[ B_j = \begin{bmatrix}
\frac{2}{\Delta x^2} + \frac{2}{\Delta y^2} - \frac{1}{\Delta x^2} \left(2 \cos \frac{\pi j}{N_3} - 2\right) & \cdots & \frac{2}{\Delta x^2} \\
\cdots & \ddots & \cdots \\
0 & \cdots & -\frac{1}{\Delta x^2} \left(\frac{2}{\Delta x^2} + \frac{2}{\Delta y^2} - \frac{1}{\Delta x^2} \left(2 \cos \frac{\pi j}{N_3} - 2\right)\right)
\end{bmatrix}_{(N_3+1)\times(N_3+1)} \]  

(7)

\[ \vec{a}_j = \begin{bmatrix} a_{0,j} \\ \vdots \\ a_{N_3,j} \end{bmatrix}, \quad \vec{F}_j = \begin{bmatrix} b_{0,j} \\ \vdots \\ b_{N_3,j} \end{bmatrix} \]

The equation (5) is solved by the matrix sweep method with parallelizing at each fixed value - \( l \), and on each processor there is additional condition for \( l \):

\[ \left\lfloor \frac{(N_3+1) \cdot \text{rank}}{N_{\text{proc}}} \right\rfloor \leq l \leq \left\lfloor \left(\frac{(N_3+1)}{N_{\text{proc}}} - 1\right) \cdot (\text{rank} + 1) \right\rfloor. \]

The equation (5) is solved on each processor, where \( \text{rank} \) – is the processor number, and \( N_{\text{proc}} \) – number of processors.

The algorithm of the realization of the matrix sweep method for solving the equation (5) is of the following form:

\[ \alpha_{j+1} = (C_j - A_j \alpha_j)^{-1} B_j, \quad j = 1, 2, \ldots N_2 - 1, \quad \alpha_1 = C_0^{-1} B_0, \]

\[ \vec{b}_{j+1} = (C_j - A_j \alpha_j)^{-1} \left( \vec{F}_j + A_j \vec{b}_j \right), \quad j = 1, 2, \ldots N_2, \quad \vec{b}_1 = C_0^{-1} \vec{F}_0, \]

\[ \vec{a}_j = \alpha_{j+1} \vec{a}_{j+1} + \vec{b}_{j+1}, \quad j = N_2 - 1, \ldots 0, \quad \vec{a}_{N_2} = \vec{b}_{N_2 + 1}. \]

After computing \( a_{i,j,l} \) on several processors their values are collected to the main processor. Thereafter on the main processor pressure field values are found from (3). The method of fast Fourier transformation is used to calculate sum (3) in \( O(N_3 \ln N_3) \) actions allowing reducing of the calculation time. The obtained pressure field at the third stage is used for obtaining divergence free velocity field [11].

4 Results of simulation

In the research we considered the lid-driven cavity flow problem with Reynolds numbers: \( \text{Re}=400, \text{Re}=1000, \text{Re}=5000, \text{Re}=10000 \). Grid resolution is 128x128x128.

Fig. 2 shows the average velocity profile of the three-dimensional problem of a lid-driven cavity. Fig. 3 presents dynamics of change of flow functions in time for the three-dimensional problem on a lid-driven cavity.
5 Computing experiment and analysis of results

Speedup obtained by using of the parallel algorithm for \( p \) processors as compared with the successive variant of performing calculations, is determined by value:

\[
S_p (N) = \frac{T_1 (N)}{T_p (N)},
\]

where value \( N = N_3 \) is used for parameterization of the computational complexity of the current task. Efficiency of processors using a parallel algorithm for solving the problem is given by:

\[
E_p (N) = \frac{T_1 (N)}{(p \cdot T_p (N))} = \frac{S_p (N)}{p},
\]

the efficiency value determines the average share of time of execution of a parallel algorithm in which processors are really used to solve the problem. Cost of calculations: \( C_p = pT_p \) – indicator of a parallel algorithm efficiency. To evaluate speedups, the cost of calculations and the efficiency we consider several parallel variants allowing to simulate in three-dimensional area measuring of \( 128\times128\times128=2097152 \) calculation points on URSA cluster (al-Farabi Kazakh National University). Table 1 shows real values of speedups, the cost of calculations, the efficiency and time for calculations, obtained in the computational experiment in various cases. As follows from consideration of table 1, the
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Figure 3: Dynamics of current streamline changes in time: (a) $t = 0.5$; (b) $t = 0.75$; (c) $t = 1.5$

speedup linearly depends on the number of used processors, i.e. the parallel program is scalable.

Where $T_p(N)$ – time of calculations, $C_p(N)$ - cost of calculations, $E_p(N)$ - efficiency and $S_p(N)$ - speedup depending on $N_{proc}$ - number of processors used in different cases.

The problem was solved by decomposition of computational domain into subdomains for each processor. The exchange of required calculation values between the processors is implemented by MPI library [12],[13].

Table 1: Computational experiment on paralleling three-dimensional Navier-Stokes equations and Poisson equation.

<table>
<thead>
<tr>
<th>Grid size</th>
<th>$N_{proc}$</th>
<th>$T_p(N)$</th>
<th>$S_p(N)$</th>
<th>$E_p(N)$</th>
<th>$C_p(N)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>N=128</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
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<tr>
<td>16</td>
<td>10.79</td>
<td>6.487</td>
<td>0.648</td>
<td>107.9</td>
<td></td>
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<tr>
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<td></td>
</tr>
<tr>
<td>64</td>
<td>3.93</td>
<td>17,811</td>
<td>0.356</td>
<td>196.5</td>
<td></td>
</tr>
</tbody>
</table>
6 Conclusion

In the research by way of example of the numerical simulation of a three-dimensional lid-driven cavity flow problem, process aspects of the development of scalable parallel calculations with the use of MPI library are given. Parallel algorithm scalability and implementation evaluated by obtaining values of speedups, efficiency and computation time. These results show that the algorithm has considerable volume of potential parallelism and high quality structure from the parallelizing point of view.

The presented comparative results show that developed parallel numerical algorithm adequately describes the dynamics of turbulent flows in closed area. Some variances with numerical results are the consequences of the fact that simple Smagorinskiy viscous model was used in this research.

New parallel algorithm of Fourier method with the use of the matrix sweep for Fourier coefficients was developed and implemented for solving the three-dimensional Poisson equation for the pressure. The results were found on the basis of the large eddy simulation and sufficiently fully describe of the real physical process.

Thus the efficient parallel numerical algorithm of solving non-stationary three-dimensional Navier-Stokes equations by the large eddies method developed. Parallel numerical algorithm tested on lid-driven cavity flow problem at different Reynolds numbers. The increase in accuracy of calculations was achieved by using of compact extended-precision schemes. The proposed method may be used for solving a wide range of problems related to the turbulence.
References


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