LARGE EDDY SIMULATION OF TURBULENT MIXING BY USING 3D DECOMPOSITION METHOD

Alibek Issakhov
al-Farabi Kazakh National University, Almaty, Kazakhstan
E-mail: aliisahov@mail.ru

Abstract. Parallel implementation of algorithm of numerical solution of Navier-Stokes equations for large eddy simulation (LES) of turbulence is presented in this research. The dynamic Smagorinsky model is applied for sub-grid simulation of turbulence. The numerical algorithm was worked out using a scheme of splitting on physical parameters. At the first stage it is supposed that carrying over of movement amount takes place only due to convection and diffusion. Intermediate field of velocity is determined by method of fractional steps by using Thomas algorithm (tridiagonal matrix algorithm). At the second stage the determined intermediate field of velocity is used for determination of the field of pressure. Three dimensional Poisson equation for the field of pressure is solved using over relaxation method.

1. Introduction

Most flows occurring in nature and in engineering applications are turbulent. Turbulent flow is a fluid motion that possesses complex and seemingly random structure at some macroscopic scale of dynamical importance. The most important physical consequence of turbulence is the enhancement of transport processes. In turbulent flow, momentum, energy and particle transport rates greatly exceed the corresponding molecular transport rates. Currently, there are three basic and commonly used approach for simulation of turbulent flows. First approach direct numerical simulation (DNS) consists in solving Navier - Stokes equations, resolving all the scales of motion, with initial and boundary conditions appropriate to the flow considered. Each simulation produces a single realization of the flow. The DNS approach was infeasible until the 1970s when computers of sufficient power became available. In DNS whole range of spatial and temporal scales of the turbulence must be resolved. All the spatial scales of the turbulence must be resolved in the computational mesh, from the smallest dissipative scales (Kolmogorov microscales), up to the integral scale L, associated with the motions containing most of the kinetic energy. Second approach large eddy simulation (LES), the larger three-dimensional unsteady turbulent motions are directly represented, whereas the effects of the smaller-scale motions are modelled. In computational expense, LES lies between Reynolds-stress models and DNS. Because the large-scale unsteady motions are represented explicitly, LES can be expected to be more accurate and reliable than Reynolds-stress models for flows in which large-scale unsteadiness is significant - such as the flow over bluff bodies, which involves unsteady separation and vortex shedding. The computational cost of DNS is high, and it increases as
the cube of the Reynolds number, so that DNS is inapplicable to high Reynolds number flows. Nearly all of the computational effort in DNS is expended on the smallest, dissipative motions, whereas the energy and anisotropy are contained predominantly in the larger scales of motion. (Chung, 2002; Hinze, 1959; Pope, 2000; Tennekes, 1972)

2. Mathematical model

Under the assumption of incompressible flow, the dimensionless governing equations are as follows:

\[
\frac{\partial u_i}{\partial t} + \frac{\partial u_j u_i}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{1}{Re} \frac{\partial}{\partial x_j} \left( \frac{\partial u_i}{\partial x_j} \right) - \frac{\partial \tau_{ij}}{\partial x_j} \tag{1}
\]

\[
\frac{\partial u_j}{\partial x_j} = 0 \quad (i = 1, 2, 3). \tag{2}
\]

where \( \tau_{ij} = u_i u_j - u_k u_k \)

In this work considered solving spread of flow in three dimensional areas. \( u_i \) velocity, \( p \) represented the total pressure. The Reynolds number is defined as \( Re = DV/\nu \) (\( \nu \) dynamic viscosity). A Cartesian coordinate system is employed, in which \( z \) is stream wise direction, \( x, y \) are in the lateral directions. As model of turbulence used dynamic model of Smagorinsky. The underlying principle of the dynamic model is to extract information concerning a given eddy-viscosity model via a double filtering in physical space. Most of the historical developments have been done with Smagorinsky’s model (Lesieur, 2005; Sagaut, 2000)

\[
\tau_{ij} - \frac{1}{3} \delta_{ij} \tau_{kk} = -2\nu_{sgs} \tilde{\tau}_{ij}
\]

\[
\delta_{ij} = \begin{cases} 1, & i = j \text{ Kronekersymbol} \\ 0, & i \neq j \end{cases}
\]

where \( \nu_{sgs} = (C_s \Delta)^2 \sqrt{2s_{ij} s_{ij}} \).

\[
\tilde{\tau}_{ij} = \frac{1}{2} \left( \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right), \quad \Delta = (\Delta x \Delta y \Delta z)^{1/3}
\]

\[
C_s = \frac{1}{3} \left( \frac{3C_k}{2} \right)^{-3/4}, \quad C_s = 0.18 \text{ for a Kolmogov constant of 1,4.}
\]

But the dynamic procedure applies in fact to the types of eddy viscosities such as those used in the structure-function model.

We start with regular LES corresponding to a “bar-filter” of width \( \Delta x \), an operator associating an function \( \tilde{f}(x, t) \). We then define a second “test filter” tilde of large width \( 2\Delta x \) associating \( \tilde{f}(\tilde{x}, t) \). Let us first apply this filter product to the Navier-Stokes equation. The subgrid-scale tensor of the field \( \tilde{u}_i \) is obtained from equation (3) with the replacement of the filter bar by the double filter and tilde filter:

\[
\tau_{ij} = \tilde{u}_i \tilde{u}_j - \tilde{u}_k \tilde{u}_k \tag{3}
\]

\[
l_{ij} = \tilde{u}_i \tilde{u}_j - \tilde{u}_k \tilde{u}_k \tag{4}
\]

We now apply the tilde filter to equation (3), which leads to

\[
\tilde{\tau}_{ij} = \tilde{u}_i \tilde{u}_j - \tilde{u}_k \tilde{u}_k \tag{5}
\]
Adding equations (4) and (5) and using equation (3), we obtain

\[ l_{ij} = \tau_{ij} - \tilde{\tau}_{ij} \]

We use Smagorinsky’s model expression for the subgrid stresses related to the bar filter and tilde-filter it to get

\[ \tilde{\tau}_{ij} - \frac{1}{3} \delta_{ij} \tilde{\tau}_{kk} = -2C A_{ij} \] \hspace{1cm} (6)

where \( A_{ij} = (\Delta x)^2 |S| S_{ij} \)

We now have to determine \( \tau_{ij} \), the stress resulting from the filter product. This is again obtained using the Smagorinsky model, which yields

\[ \tau_{ij} - \frac{1}{3} \delta_{ij} \tau_{kk} = -2C B_{ij} \] \hspace{1cm} (7)

where \( B_{ij} = (2\Delta x)^2 |S| S_{ij} \)

Subtracting (6) from (7) yields with the aid of Germano’s identity

\[ l_{ij} - \frac{1}{3} \delta_{ij} l_{kk} = 2CB_{ij} - 2CA_{ij} \]

\[ l_{ij} - \frac{1}{3} \delta_{ij} l_{kk} = 2CM_{ij} \]

where \( M_{ij} = B_{ij} - A_{ij} \) \hspace{1cm} (8)

All the terms of equation (8) may now be determined with the aid of \( \overline{\tau} \). Unfortunately, there are five independent equations for only one variable \( C \), and thus the problem is overdetermined. A first solution proposed by Germano is to multiply (8) tensorially by \( S_{ij} \) to get

\[ C = \frac{1}{2} \frac{l_{ij} S_{ij}}{M_{ij} S_{ij}} \]

This provides finally dynamical evaluation of \( C \), which can be used in the LES of the bar field \( \overline{\tau} \).

3. Boundary conditions

In performed computations we only considered the rectangular box \( H \times H \times 2H \) where at the inlet plane we specified the jet velocity profile

\[ u_3(x, y, 0, t) = -U_0 \ast (1 - tanh(2.8 \ast (\frac{r}{R} - \frac{R}{r}))) \ast (1 + 0.0025 \ast \sin(2 \ast \pi \ast St_a \ast t \ast 2 \ast U_0/2 \ast R)) \]

The Strouhal number of axial forcing was equal to 0.45. The lateral boundaries of the computational domain are assumed like this

\[ \frac{\partial u_i}{\partial x_i} = 0 \hspace{1cm} i = 1, 2, 3 \]
4. Numerical Simulation

The numerical solution of system is built on the staggered grid with use of the scheme against a stream of the second type (Anderson, 1995, 1984; Fletcher vol.1 , 1988; Fletcher vol. 2, 1988; Peyret, 1983; Roache, 1972; Tannehill, 1997)

\[
\frac{\partial u_\zeta}{\partial x} = \frac{u_R \xi_R - u_L \xi_L}{\Delta x} \text{ where } \zeta \text{ can be } u, v, w
\]

\[
u L = \frac{u_i + u_{i-1}}{2}, \quad u_R = \frac{u_{i+1} + u_i}{2}
\]

\[
\xi_L = \begin{cases} 
\xi_i, & u_L > 0 \\
\xi_{i+1}, & u_L < 0 
\end{cases}
\]

\[
\xi_R = \begin{cases} 
\xi_i, & u_R > 0 \\
\xi_{i+1}, & u_R < 0 
\end{cases}
\]

and compact approximation for convective member. (Lely, 1992; Tolstykh, 1990)

\[
f(x) = \frac{du}{dx}
\]

\[
\alpha f_{i-1} + \beta f_i + \gamma f_{i+1} = \frac{u_j - u_{j-1}}{h}
\]

Factorizing the \( f(x) \) and \( u(x) \) to Taylor series we can determine \( \alpha, \beta, \gamma \)

For the solution of turbulence problem used the scheme of splitting on physical parameters:

1. \[ \vec{u}^n - \vec{u}^0 \tau = -(\vec{u}^n \nabla \vec{u}^n - \nu \Delta \vec{u}^0) \]

2. \[ \Delta p = \nabla \vec{u}^n \tau \]

3. \[ \vec{u}^{n+1} - \vec{u}^n \tau = -\nabla p \]

Second stage solved 3D Poisson equation for pressure field using an over - relaxation method. Three dimensional Poisson equation parallelized by using various geometrical decomposition (1D, 2D and 3D). As the basic approach of parallelization is selected geometric decomposition of the grid area. In this case, there are three different ways of sharing the values of the grid function on the compute nodes one-dimensional, two-dimensional and three-dimensional of the grid computing nodes. After a stage of decomposition, when performed on separate data blocks for the construction of a parallel algorithm, we proceed to phase linkage between the blocks, the calculations which will be run in parallel - communications planning. Because of the pattern used an explicit difference scheme for computing the next approximation in the border nodes of each subdomain is necessary to know the value of the grid function with bordering neighboring processor elements. To accomplish this, each compute node a fake cell for storing data from a neighboring computational node and arranged shipment of these boundary values needed to ensure the homogeneity of the calculations by explicit formulas (Figure 1). Data transmission is performed using procedures MPI. Calculations were performed on a cluster system URSKA KazNU after al-Farabi on grids of \( 128 \times 128 \times 128 \) and \( 256 \times 256 \times 256 \) by using up to 64 processors. Results of computational experiment showed the presence of a good speed in solving problems of this class. Focused on over-time shipments and time calculations for various methods of decomposition. In the first stage we used one overall program, the size of arrays from run to run have not changed, each processor element numbering of the array elements starting from scratch. Despite the fact that, in accordance with the theoretical analysis of the 3D decomposition is the best option for parallelization, computational experiments have shown that better results can be achieved using 2D decomposition when the number of processes from 25 to 144 (Figure 1, Figure 2)
5. Testing results of the numerical method

Consider a turbulent flow, which is located in the channel. Computations were performed for the Reynolds number \( Re = \frac{U_m D}{\nu} \) equal to 8000 defined based on the jet axis velocity. In the calculations, the following grid is taken \( N_x \times N_y \times N_z = 80 \times 80 \times 160 \).

In numerical solution describe spread of flow in three dimensional areas. Figure 3 show at different time scale isosurface of spread flow in three dimensional areas.

6. Conclusions

The results of numerical experiments showed that the constructed mathematical model of turbulence is able to reproduce the characteristic features of turbulent flow. Using dynamic Smagorinsky model allowed us to obtain good data for the study area. Application in the calculation of 2D decomposition gives 65% efficiency in the use of 25 compute nodes. With further increase in the number of compute nodes and 100 for the chosen mesh size, a characteristic was obtained for problems of this class efficiency value around 45%.

References

Anderson, J.D., Jr. 1995 Computational Fluid Dynamics. McGraw-Hill.
Anderson, D. A. & Tannehill, J. C. & and Pletcher, R.H. 1984 Computational Fluid Mechanics and Heat Transfer. McGraw-Hill.
Chung, T. J. 2002 Computational Fluid Dynamics. In Cambridge university press.
Fletcher, C. A. 1988 Computational Techniques for Fluid Dynamics. Vol 1: Fundamental and General Techniques. In *Springer-Verlag*.

Fletcher, C. A. 1988 Computational Techniques for Fluid Dynamics. Vol 2: Special Techniques for Differential Flow Categories. In *Springer-Verlag*.

Hinze, J. O. 1959 Turbulence. An introduction to its mechanism and theory. In *McGraw-Hill*.

Lely, S. K. 1992 Compact finite difference scheme with spectral-like resolution. In *J. Comp. Phys*. vol. 183, pp. 16-42

Lesieur, M. & Metais, O. & Comte, P. 2005 Large-eddy simulations of turbulence. In *Cambridge university press*.

Peyret, R. & Taylor, D. Th. 1983 Computational Methods for Fluid Flow. In *Springer-Verlag*.

Pope, S. B 2000 Turbulent Flows. In *Cambridge university press*.

Roache, P.J. 1972 Computational Fluid Dynamics. In *Hermosa Publications*.

Sagaut, P. 2000 Large eddy simulation for incompressible flows. In *Springer-Verlag. Physics and Astronomy*.

Tannehill, J.C. & Anderson, D.A. & and Pletcher, R.H. 1997 Computational Fluid Mechanics and Heat Transfer. 2nd ed. *McGraw-Hill*.

Tennekes, H. & Lumley, J.L. 1972 A first course in turbulence *The MIT Press*.

Tolstykh, A.I. 1990 Compact difference scheme and their applications to fluid dynamics problems *Nauka*. 