Large Eddy Simulation of Internal Turbulent Flows

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Introduction

Modern distributed memory parallel computers are characterized by a very high computational potential. Therefore they are very attractive for the solution of time-consuming non-steady three-dimensional (3D) computational fluid dynamics (CFD) problem. The contribution of CFD has several aspects. These are cost effectiveness, reduced design times and ability to examine flow properties in cases were an experimental technique is not feasible. The cost effectiveness of CFD stems from fact that computational methods take advantage of computer power. Therefore all costs associated with the construction of models, maintenance and operation of experimental configurations are spared. The time spent on design or optimization of engineering applications is substantially reduced. Once a CFD model has been successfully set-up, it can provide results, design guidelines in a very short time.

The introduction of new models and improved computer power allows making more accurate computations performed with less empiricism than before. The technique is supposed to make possible studying of the physical phenomena that occurs in more complex engineering-like applications. Large eddy simulation (LES) methodology corresponds to those purposes [1]. The type of used grid, grid density, mathematical approach, discretization schemes, solution procedure and process modelling influence success and sound of LES approach.

The application of LES for computation of turbulent flows in the ducts with fluid injection is considered in this paper. Investigation of such flows has a great significance for the designing and perfection of heat exchangers and solid rocket motors. In these applications exact computation of field of fluid flow plays an important role because it serves as a background for simulation of condensed particles formed during the combustion of solid fuel, their interaction and separation on wall of duct [2].

Governing equations and closure model

The instantaneous properties of a turbulent flow of incompressible fluid are described with the governing equations which include continuity equation, momentum equation and equation for temperature.

LES uses filtered governing equations. The filter operation is defined as the following

$$\bar{f}(\mathbf{x},t) = \int_{D} f(\boldsymbol{\xi},t) g(\mathbf{x}-\boldsymbol{\xi}) d\boldsymbol{\xi},$$

where $g(\mathbf{x})$ is a filtering function, D is a computational domain. The computational domain is shown in the figure 1.

Then, filtered Navier-Stokes equations are written as

 $\nabla \overline{\mathbf{v}} = 0;$

$$\frac{\partial \overline{\mathbf{v}}}{\partial t} + (\nabla \cdot \overline{\mathbf{v}})\overline{\mathbf{v}} = -\nabla \overline{p} + \nabla [(\nu + \nu_t)\nabla \overline{\mathbf{v}}];$$

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$$\frac{\partial \overline{T}}{\partial t} + (\nabla \cdot \overline{\mathbf{v}})\overline{T} = \nabla \left[(a + a_t) \nabla \overline{T} \right].$$

Here t is time, v is velocity, p is pressure, T is temperature, v and a are kinematic viscosity and temperature conductivity correspondingly. Index t is related with turbulent properties of fluid flow.



Fig. 1. Computational domain.

LES concept allows to exclude the computation of turbulent eddies which have smaller sizes than adjusted value Δ named the filter length. The filter length separates eddies which are resolved from those which are simulated.

The subgrid terms representing the cascade of energy from large to small scales are modeled based on the assumption that the small scales are universal and contain only a small amount of energy. The non-resolvable small scales turbulence can be represented by a subgrid scale model. Subgrid turbulent viscosity is computed using the Smagorinsky's formula with damping on the wall

$$v_t = f_v (C_S \Delta)^2 |\overline{\varepsilon}|, \qquad |\overline{\varepsilon}| = \left(2\overline{\varepsilon}_{ij}\overline{\varepsilon}_{ij}\right)^{1/2}, \qquad \overline{\varepsilon}_{ij} = \frac{1}{2} \left(\frac{\partial \overline{v}_i}{\partial x_j} + \frac{\partial \overline{v}_j}{\partial x_i}\right)$$

Subgrid turbulent temperature conductivity is connected with the subgrid viscosity

$$a_t = v_t / \Pr_t$$

Here C_S is Smagorinsky's constant, f_v is Van Driest damping function. The subgrid turbulent Prandl's number is constant ($Pr_t = 0.6$). The subgrid length is assumed to be proportional to the filter width Δ , which then is related to the volume of grid mesh in three dimensions

$$\Delta = \left(\Delta x \Delta y \Delta z\right)^{1/3},$$

where Δx , Δy , Δz are the size of grid mesh in directions *x*, *y*, *z* correspondingly. The present LES implicity applies a box filter in each direction.

Numerical scheme

The filtered Navier-Stokes equations are solved numerically with the help of a finite difference method. Variables are sampled using a staggered grid with non-uniform cell size in a 3D rectangular domain. Velocity components are specified at the cell faces, while the scalar variables such as pressure and temperature are located at the center of cell.

The numerical procedure employs a Chorin type projection method for the decoupling of momentum and continuity equations resulting to the Poisson equation for pressure. A second order Adams-Bashforth time integration scheme is used to advance the velocity and scalar fields. The discretization of diffusive flux is based on the second order central difference scheme in Cartesian coordinates.

Concerning numerical method, the most important component is the discretization of the non-linear convective fluxes. Higher order resolution schemes are used for discretization of convective flux. The classical lower order schemes such as upwind difference scheme, central difference scheme and hybrid central/upwind scheme are unconditionally bounded and highly stable but highly diffusive when the flow direction is skewed relative to the grid lines. A simple remedy to overcome the false diffusion is to use a fine enough grid. However, such approach is not practical due to the requirement of excessive computer storage and computational efforts, especially in the complex three-dimensional calculations. Higher order discretization schemes provide results of increased accuracy in less computational time [3]. The quadratic upwind interpolation for convective kinematics (QUICK), hybrid-linear parabolic approximation (HLPA), sharp and monotonic algorithm for relative transport (SMART) are used. The choice of these schemes is based on the good and stable convergence behavior.

The accuracy of numerical results are evaluated for each scheme. The relative performances among the schemes are examined through applications to the several test problems. Test problems include the flow in a lid-driven cavity and the test convection problem. The computed results for the lower order schemes are also included for better comparison with the existing popular schemes.

The Poisson equation is solved globally in the entire domain on every time step. Iterative procedure is used to solve the difference equations, which is produced by the discretization of Poisson equation for pressure. The system of adifference equations is solved by successive over relaxation method (SOR), symmetric successive over relaxation method (SSOR), conjugate gradients method (CG) and bi-conjugate gradients stabilized method (BiCGStab) with preconditioning [4]. The efficiency and speed of convergence for these methods are compared.

Parallelization procedure

The computational domain is divided into several rectangular subdomains for the parallelization. Each process holds some ghost cells which overlap inner cells of the adjacent process. Values are copied from these to the ghost cells when necessary. To minimize communications, the program divides computational domain in a way that minimizes the area of the touching faces and equilibrates the number of cells in the different subdomains [5].

The program code is written in C++ programming language. The library MPI is used for organization of communication between processors.

Performance and parallelization efficiency for different distributed memory machines (massive parallel computers and SMP-clusters) are established. The evolution of parallelization efficiency of the developed code for different number of processors and problem sizes in comparison with the measured computational and communication characteristics are fixed.

Results

The main results of the investigation are the following. Some problematic issues concerning the methodological base of LES were investigated. These issues include

- a) elaboration of convergence criteria of LES (in other words, how filter length influences computational results and how filter kernel influences treatment of computational results);
- b) development of numerical schemes ensuring necessary accuracy;
- c) near wall simulation (in future we plan to use detached eddy simulation as one acceptable variant for decreasing the number of grid nodes near wall);
- d) development of LES for computation of turbulent flows on the basis of general curvilinear grid structures;
- e) construction of parallel numerical algorithm for high performance computer systems both with shared and with distributed memory.

Fluid flow pattern was investigated depending on intensity of fluid injection. The formation of recycling regions and reverse flow in the duct was discovered with the some of initial data.

The computed results are compared with the approximate solutions, the available benchmark solutions and experimental data. The obtained results have a good agreement with the results computed on the base Reynolds averaged Navier-Stokes equations [2].

Conclusion

Successful application LES for computation of fluid properties in the duct with fluid injection makes possible computations taking into account more complex physical and chemical effects. It requires development subgrid scale models for compressible fluid, connection combustion model to LES concept and elaboration corresponding computational tools.

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