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Turbulent flow simulation using large eddy simulation combined with characteristic-based split scheme

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ABSTRACT

A numerical method of large eddy simulation (LES) combined with a characteristic-based split scheme (CBS) is proposed. The CBS scheme is introduced to discretize the motion equation in the time domain along the characteristic line, and the space domain is discretized by the split algorithm, which calculates the velocity and pressure separately. Turbulent flow simulations in a lid-driven cubical cavity and two circular section 90° pipes are conducted, and the results are validated by comparison with experimental data and other direct numerical simulation results. For a circular section 90° pipe, an additional pair of vortexes that is near the curved section inner side has been observed, and their rotational direction is the same as that of the main vortex. To the author's knowledge, this type of four-vortex structure has not been previously reported.

1. Introduction

Large eddy simulation (LES) directly calculates the large and energetic vortical structures in turbulent flows, while modeling the smaller-scale eddies. Therefore, compared to Reynolds-averaged Navier–Stokes (RANS) models, the advantages of LES are significant. RANS is effective for steady simulations of fluid flow, but there are some theoretical imperfections when RANS equations are used to simulate unsteady flows. Solutions from the RANS equations usually deteriorate when the flow field of interest involves large-scale separations.

Nevertheless, generalization of LES methods to industry is still problematic. Industrial flows are usually physically complex, highly unsteady, and have large Reynolds numbers. The key challenges that LES models must meet for overall success in industrial applications include accurate flow averaging reflecting the true flow, minimization of discretization errors, performance of the simulation in a time and cost-effective manner [1]. Although the number of LES models has increased almost exponentially in recent years, the original Smagorinsky model is being favored in a large majority of cases. Due to the intricate and natural coupling between numerical discretization and LES modeling, the performance of simulation is solely dependent on the numerical framework. As noted in the work of Geurts [2] and Chow and Moin [3], low-order numerical discretization can be as influential as the subgrid scale (SGS) model. The finite volume method is widely used for LES because it is easy to compose high-order schemes [4].

The finite element method is not used as widely as that of finite volume in computational fluid dynamics (CFD), although it is an important numerical procedure in the area of numerical simulations. Over the past thirty years, some advanced finite element schemes have been developed in order to solve convection dominated flow problems, such as the streamline upwind Petrov–Galerkin method [5], the Taylor–Galerkin method [6], the Galerkin least square (GLS) method [7], and the characteristic Galerkin (CG) method [8]. Among these methods, the CG method discretizes the time domain along the characteristic line, and it is especially effective at solving convection dominated flow problems. Donea et al. [9] extended the fractional step method proposed by Chorin [10] into a finite element context, and the fractional step algorithm was used as a stabilization technique to restrain spurious pressure interpolations violating the so-called Ladyzhenskaya–Babuška–Breezi condition. Zienkiewicz and Codina [11] presented the well-known characteristic-based split (CBS) algorithm by introducing Taylor expansion and combining it with a split algorithm into the CG method. The CBS procedure combines the advantages of the characteristic method and the split algorithm, and it is effective and flexible due to many additional improvements that raise stability and accuracy for incompressible flows in complex geometries. Codina et al. [12,13] compared CBS procedures with other formulations, such as GLS and SGS, to solve the incompressible Navier–Stokes equations. The comparisons showed that all these

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formulations are similar, and are stable for the convective term and the pressure interpolation. Over more than ten years of development, the CBS procedure has been applied to simulate different flow problems, including turbulent incompressible flows [14].

The present work concentrates on the incorporation of a semi-implicit CBS method to LES. The finite element discrete equations for incompressible flows are derived using the framework of LES, and these equations are applied to solve three dimensional flow problems. Numerical simulations of the flows in a lid-driven cubical cavity and circular section 90° pipes are conducted. The results are compared with experimental data and direct numerical simulation (DNS) results. The comparisons show that the proposed scheme can simulate turbulent flows accurately, although the formulae of second order accuracy both in time and space have been used. Furthermore, for a circular section 90° pipe, an additional pair of vortexes has been observed, which, to the author's knowledge, has been not reported before.

2. Mathematical model and numerical algorithm

2.1. LES mathematical algorithm

For incompressible flow, by applying the grid filter to the continuity and momentum equations, the following expressions can be obtained:

$$\frac{\partial \bar{u}_i}{\partial x_i} = 0, \tag{1}$$

$$\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial(\bar{u}_i\bar{u}_j)}{\partial x_j} = -\frac{1}{\rho}\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j}\left[\nu\left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i}\right)\right] - \frac{\partial \tau_{ij}}{\partial x_j}, \tag{2}$$

where variables accompanied by a macron ("‒") here, as elsewhere, are resolved scale variables after filtration and τ_{ij} is the subgrid stress. Based on the widely used subgrid eddy viscosity model, the subgrid stress can be written as

$$\tau_{ij} = -2\nu_{sgs}\bar{S}_{ij} + \frac{1}{3}\delta_{ij}\tau_{kk}. \tag{3}$$

In Eq. (3) above, $\bar{S}_{ij}$ is the strain rate tensor in resolved scale and ν_{sgs} is the subgrid eddy viscosity coefficient having the following format:

$$\nu_{sgs} = (C_S\Delta)^2(2\bar{S}_{ij}\bar{S}_{ij})^{0.5}, \tag{4}$$

where C_S is the Smagorinsky coefficient, which can be dynamically determined by the dynamic Smagorinsky model (DSM) [15].

Substituting Eq. (3) into Eq. (2), we obtain

$$\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial(\bar{u}_i\bar{u}_j)}{\partial x_j} = -\frac{\partial}{\partial x_i}\left(\frac{\bar{p}}{\rho} + \frac{\tau_{kk}}{3}\right) + \frac{\partial}{\partial x_j}\left[(\nu + \nu_{SGS})\left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i}\right)\right]. \tag{5}$$

For concision, the total viscosity $(\nu + \nu_{sgs})$ can be written as ν' and the term $(\bar{p}/\rho + \tau_{kk}/3)$ as $\bar{p}$. Therefore, the governing equations of LES introducing the subgrid eddy viscosity coefficient for incompressible flow are

$$\frac{\partial \bar{u}_i}{\partial x_i} = 0, \tag{6}$$

$$\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial(\bar{u}_i\bar{u}_j)}{\partial x_j} = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j}\left[\nu'\left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i}\right)\right]. \tag{7}$$

Because the DSM is employed, C_S is not a constant value, and even a negative value is possible. A negative value for C_S means that the energy is transferred from small to large scales in the calculated region, and numerical instability may occur. Therefore, the following limitations are applied to C_S:

$$C_s^2 = 0, \text{ if } C_s < 0, \tag{8}$$

$$C_s^2 = C_{Limit}^2, \text{ if } C_s > C_{Limit}. \tag{9}$$

Here, C_{Limit} is defined according to the Courant–Friedrich–Levy condition

$$\nu + \nu_{Limit} = \frac{\Delta^2}{\Delta t}, \tag{10}$$

where Δt is the time step of the calculation and Δ is the grid filter width, which, in the present work, is determined by selecting the minimum of the three coordinate directions, $\Delta = \min(\Delta_x, \Delta_y, \Delta_z)$.

2.2. Time discretization

For simplification, the macron symbol is omitted in the following formulae. Consequently, the left term of Eq. (7) can be written in the form of the total derivative du_i/dt based on the characteristic method. In the characteristic method, the characteristic corresponds to the path line of a particle. An equation for these characteristics can be written as

$$\frac{dx_i}{dt} = u_i. \tag{11}$$

Here, $x_i (i = 1, 2, 3)$ is the trajectory and u_i the characteristic velocity of particle i, where the velocity is constant if a linear convection equation (negligible diffusion in Eq. (7)) is considered. Therefore, along the characteristics given by Eq. (11), Eq. (7) can be written as

$$\frac{du_i}{dt} = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j}\left[\nu'\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\right]. \tag{12}$$

The discretization of this equation yields

$$\begin{aligned} u_i^{n+1} = {} & u_i^n - \Delta t\widehat{u}_j\frac{\partial u_i^n}{\partial x_j} + \frac{\Delta t^2\widehat{u}_k}{2}\frac{\partial}{\partial x_k}\left(\widehat{u}_j\frac{\partial u_i^n}{\partial x_j}\right) \\ & + (1-\theta)\Delta t\left[Q^n - \Delta t\widehat{u}_j\frac{\partial Q^n}{\partial x_j}\right] + (1-\theta)\Delta t\left[E^n - \Delta t\widehat{u}_j\frac{\partial E^n}{\partial x_j}\right] \\ & + \theta\Delta t Q^{n+1} + \theta\Delta t E^{n+1}, \end{aligned} \tag{13}$$

where Q denotes $-\frac{\partial p}{\partial x_i}$ and E denotes $\frac{\partial}{\partial x_j}\left[\nu'\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\right]$, respectively. The above parameter θ ranges from 0 to 1 corresponding to different time discretization formulae. In the present work, we take $\theta = 1$ for the term $-\frac{\partial p}{\partial x_i}$ and $\theta = 0.5$ for the term $\frac{\partial}{\partial x_j}\left[\nu'\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\right]$. We therefore obtain

$$\begin{aligned} u_i^{n+1} = {} & u_i^n + \Delta t\left\{-u_j^n\frac{\partial u_i^n}{\partial x_j} - \frac{\partial p^{n+1}}{\partial x_i} + \frac{\partial}{\partial x_j}\left[\nu'\left(\frac{\partial u_i^n}{\partial x_j} + \frac{\partial u_j^n}{\partial x_i}\right)\right]\right\} \\ & + \frac{1}{2}\Delta t^2 u_k^n\frac{\partial}{\partial x_k}\left\{u_j^n\frac{\partial u_i^n}{\partial x_j} - \frac{\partial}{\partial x_j}\left[\nu'\left(\frac{\partial u_i^n}{\partial x_j} + \frac{\partial u_j^n}{\partial x_i}\right)\right]\right\}, \end{aligned} \tag{14}$$

where the third term on the right hand side is the stabilized term. The semi-implicit formulation given by Eq. (14) in time means that an explicit scheme is used to solve the velocity, and an implicit scheme is used to solve the pressure.

2.3. Split procedure and space discretization

The split procedure CBS operator is introduced to calculate the velocity and pressure separately. The general solution process consists of three steps: (1) prediction, (2) projection, and (3) correction. Because eight-noded-trilinear hexahedral elements are used in this study to discretize the space domain, the basic Lagrangian interpolation functions are three-order linear. Therefore, the accuracy of the space discretization is second order.