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Large eddy simulation with sub-grid stress determined by molecular simulation and its applications for turbulent channel flows

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Abstract

In this paper, a novel simulation method of turbulence by solving filtered Navier-Stokes equations based on LES methodology and calculating the sub-grid scale stress with D-IP method is developed. Compared to the sub-grid scale models used in LES method with Boussinesq assumption, the sub-gird scale stress of the LES-DIP method is directly estimated based on statistics of molecule motions. To validate the LES-DIP method, turbulent channel flow at different Reynolds numbers of Re_τ =180, 390 and 590 are simulated. The results are found to be in agreement with those of DNS with much smaller computational cost.

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Keywords: Turbulent channel flow, large eddy simulation, molecular statistics, diffusive information preservation

1. Introduction

Large eddy simulation (LES) of turbulence solves the large scale motions with filtered Navier-Stokes equation, and the small scales are modeled by sub-grid stress model. The sub-grid scale (SGS) model represents effects of small turbulence scales on the flow and has been developed since early of 1990's and applied. to simulate different turbulence problems in engineering [1-4]. Most of the SGS models take the Boussinesq hypothesis assuming that sub-grid stress is coaxial with velocity strain rate tensor and the concept of turbulent viscosity is adopted. However, the Boussinesq assumption may not be valid for many of turbulent flow with complicated geometrical or external effects in engineering problems. Therefore, it is imperative to develop a novel method to determine the sub-grid stress without Boussinesq hypothesis.

Diffusive information preservation method (D-IP) is a recently developed molecular simulation method [5]. With description of molecular motion with Langevin equation and IP quantities (T_{IP} ,$\vec{u}_{IP}$), which are averaged to obtain the macroscopic temperature and velocity, the D-IP method can be used to simulate turbulent flow at low Reynolds

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numbers [6, 7]. Compared to direct numerical simulation (DNS), the cell sizes of D-IP method are as fine as that of DNS, the computational cost, however, is much more expensive than DNS because D-IP needs to solve evolutions of hundreds of molecules in each cell. Therefore, it is very expensive and not feasible to apply the D-IP method for simulation of turbulence at high Reynolds numbers.

In the present work, we develop a novel method of combining LES and D-IP (as so called LES-DIP) to decrease the computational cost of D-IP and to directly calculate the sub-grid scale stress based on the solutions of molecule motions. Specifically, we solve the box-filtered incompressible Navier-Stokes equations by finite difference method as used by LES. However, the sub-grid stress $\overline{u_i u_j} - \overline{u}_i \overline{u}_j$ is obtained by molecular statistics of IP quantities instead of previous SGS models. The algorithm will be described in detail in the next section, that is followed by application of the LES-DIP method to simulate turbulent channel flow at varied Reynolds numbers.

2. Methodology

2.1. LES

In LES, the flow variables are divided into grid scale and sub-grid scale components. The grid scale component is obtained by

$$\overline{f}(\mathbf{x}) = \int_D f(\mathbf{x}')G(\mathbf{x},\mathbf{x}')d\mathbf{x}' \tag{1}$$

where D denotes the computational domain and G is the grid filter function. And box filter means an average of the flow variables in the box. Applying the filter operation to the continuity and Navier-Stokes equation yields the filtered equations of motions

$$\frac{\partial \overline{u}_i}{\partial x_i} = 0 \tag{2}$$

$$\frac{\partial \overline{u}_i}{\partial t} + \frac{\partial \overline{u}_i \overline{u}_j}{\partial x_j} + \frac{\partial \tau_{ij}}{\partial x_j} = -\frac{\partial \overline{p}}{\partial x_i} + \nu \frac{\partial^2 \overline{u}_i}{\partial x_j^2} + \overline{f}_i \tag{3}$$

In Eq. (3), the sub-grid stresses, $\tau_{ij} = \overline{u}_i \overline{u}_j - \overline{u_i u_j}$, must be determined to close the equations.

2.2. Sub-grid stresses determined by D-IP

In D-IP, every molecule carries IP velocity $\mathbf{u}_{IP}$ (and T_{IP} if necessary), which is much less scattered than the molecular thermal velocity $\mathbf{c}$, and the macroscopic velocity $\mathbf{u}(\mathbf{x})$ based on $\mathbf{u}_{IP}$ is given by $\mathbf{u}(\mathbf{x}) = \lim_{V \to 0} \langle \mathbf{u}_{IP} \rangle_{\mathbf{x},V}$, with '$\langle\ \rangle_{\mathbf{x},V}$' denotes the average of all the molecules in a volume V centered at $\mathbf{x}$. And the sub-grid stresses can be determined by second order statistics of $\mathbf{u}_{IP}$.

The evolution of $u_{IP,i}$ in incompressible flow is governed by

$$\frac{\partial}{\partial t} u_{IP,i} + \frac{\partial}{\partial x_j}\left(u_{IP,i} u_{IP,j}\right) = -\frac{\partial p}{\partial x_i} - \frac{\partial}{\partial x_j}\left(u_{IP,i} c_j\right) + \text{collisions} + f_i \tag{4}$$

where, pressure p can be solved by Poisson equation based on incompressible flow conditions. The second term

in the left of Eq. (4) corresponds to the convective effect.

Taking an average of $u_{IP,i}u_{IP,j}$ and $u_{IP,i}$ in a filtered box will lead to the term $\overline{u_i u_j}$ and $\overline{u_i}$ respectively, therefore, the sub-grid stresses in D-IP can be determined by

$$\bar{u}_i\bar{u}_j - \overline{u_i u_j} = \langle u_{IP,i}\rangle_{x,V}\langle u_{IP,j}\rangle_{x,V} - \langle u_{IP,i}u_{IP,j}\rangle_{x,V} \tag{5}$$

The viscosity effect appears in the second and third terms on the right side of Eq. (4).
On the other hand, the motion of a molecule is determined by considering convective and diffusive motions,

$$r_i(t+\Delta t) = r_i(t) + u_{IP,i}\times\Delta t + \Delta r_i^D \tag{6}$$

where, Δr_i^D denotes the diffusive motion, which is determined by Langevin equation [8].

2.3. Procedure of the LES-DIP method

In the combination of LES and D-IP, the LES calculates Eq. (2) and (3) and the D-IP determines molecular motions and the time evolution of IP velocity. The procedure of the algorithm is illustrated as below.

1) Initialize the filtered velocity field $\bar{\mathbf{u}}$ and IP velocity $\mathbf{u}_{IP}$, thermal velocity $\mathbf{c}$ and position $\mathbf{r}$ of the molecules.
2) Calculate the sub-grid stresses according to Eq. (5).
3) Based on the obtained filtered field and sub-grid stresses, update the filtered field by solving Eq. (2) ~ (3).
4) Solve molecules motion according to Eq. (6).
5) Simulate molecules collisions and accelerations due to pressure gradient and external forces [7].
6) Go to the second step for time advancement or end the program.

3. Simulation of turbulent channel flow

To validate the LES-DIP method, turbulent channel flows at $\mathrm{Re}_\tau = 180, 390, 590$ are simulated. The results are compared with those obtained by DNS [9,10] and LES using dynamic SGS model [2] with the calculated eddy viscosity kept nonnegative.

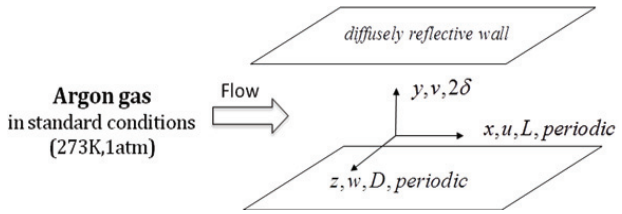

Fig 1. Schematic of turbulent channel flow and computational conditions

Figure 1 shows the flow geometry, the coordinate system and the boundary conditions. Based on the flow characteristics, the computational domain is divided in cells which are uniform in streamwise and spanwise directions and stretched in normal (y) direction.

Eq. (2) and Eq. (3) are solved by the numerical schemes as addressed in literature [11]. The spatial discretization has 2nd-order accuracy and the temporal terms related to the external body and the non-linear terms are explicitly discretized by Runge-Kutta third-order scheme with linear terms discretized by implicit Crank-Nicolson scheme.

Parameters of test cases, including domain size, number of cells at al. are listed in Table 1. Re_m is defined by the mean bulk velocity U_m and the channel half-width. As shown in Table 1, three cases with Reynolds number of 2800, 7000 and 11000 are simulated and results obtained with the LES-DIP, LES and DNS methods are compared.

Table 1. Calculation parameters of all the simulations. Parameters of the DNS are extracted from the literature[9, 10].

Re_m	2800			~7000			~11000		
Numerical method	LES-DIP	LES	DNS	LES-DIP	LES	DNS	LES-DIP	LES	DNS
Re_τ	176	167	178	406	374	392	599	546	587
$L:2\delta:D$	$2\pi:2:\pi$	$2\pi:2:\pi$	$4\pi:2:1.33\pi$	$2\pi:2:0.75\pi$	$2\pi:2:0.75\pi$	$2\pi:2:\pi$	$\pi:2:0.5\pi$	$\pi:2:0.5\pi$	$2\pi:2:\pi$
Cells	$32\times64\times32$	$32\times64\times32$	$128\times128\times128$	$48\times64\times64$	$48\times64\times64$	$256\times192\times192$	$48\times72\times48$	$48\times72\times48$	$384\times256\times384$

In the present simulation, the initial filtered velocity is set to be a laminar velocity profile imposed with random perturbations with magnitude of 20% of the laminar velocity. 100 molecules are randomly distributed in each cell. The IP velocity is equal to the locally filtered velocity and the thermal velocity is Maxwellian distributed. The simulation process includes two stages. In the first stage, the initial perturbed laminar flow field evolves to a fully developed turbulent flow. After that, the turbulent flow is simulated for a period of $600\,\delta/U_m$ to obtain accurate statistics of flow properties.

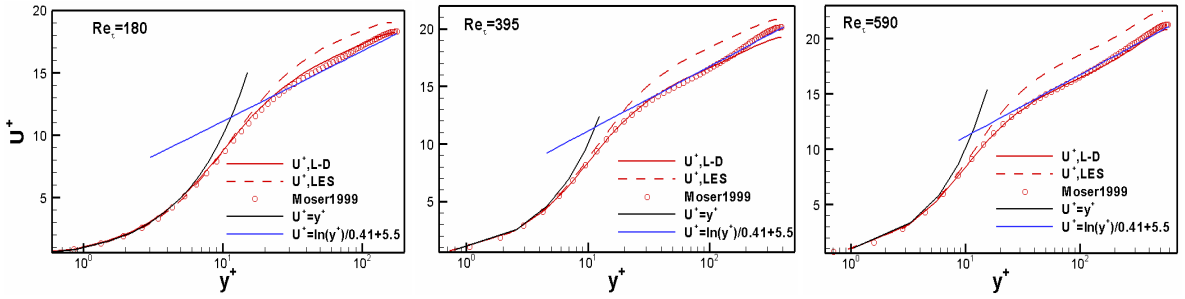

Fig 2. The mean velocity profiles for the three cases obtained by LES-DIP, LES and DNS method

The profiles of mean velocity U obtained with LES-DIP, LES and DNS (Moser's results [10]) are compared in Fig. 2, where the superscript '+' denotes dimensionless quantities scaled by wall units, specifically, the friction velocity u_τ $\left(=\nu\sqrt{dU/dy|_w}\right)$ and viscous length scale ν/u_τ. It is shown that LES with dynamic model yields larger B constant in log-law region. It attributes to the stronger dissipation caused by nonnegative eddy viscosity used in the SGS model. However, the results obtained by the present LES-DIP method, with sub-grid stress determined by molecule statistics, agree very well with the DNS results for all the three cases with varied Reynolds numbers.

Figure 3 shows profiles of turbulent intensities obtained by the present method versus those obtained by DNS and LES. It is seen that for all the Reynolds numbers, turbulent intensities obtained by L-D generally agree well with the DNS result, and the performance of L-D is better than that of LES. In the near-wall region, the rms. of fluctuation of streamwise velocity is slightly larger than that of DNS and the rms. velocity in spanwise and normal directions are slightly smaller than those of DNS . The discrepancy is believed to be caused partly by the low order of accuracy in the difference schemes used to solve Eq. (2) and Eq. (3)[12]. Figure 4 plots and compares the results of the turbulent stresses obtained by different methods. It shows that the Reynolds stresses calculated by LES-DIP agree well with DNS results.

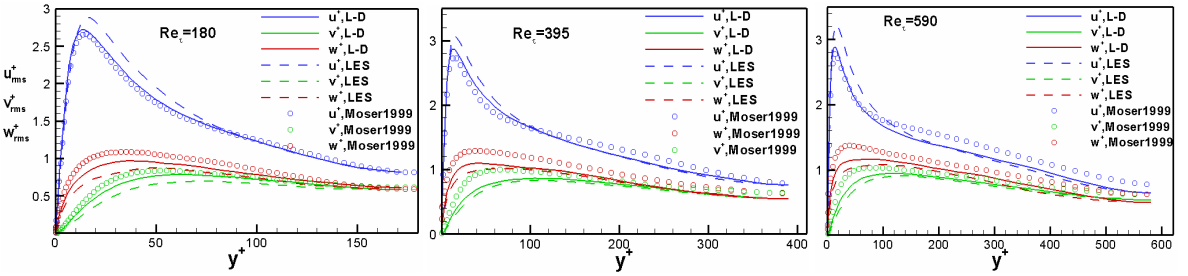

Fig 3. Turbulent intensities obtained by the present method versus DNS and LES results with dynamic sub-grid model.

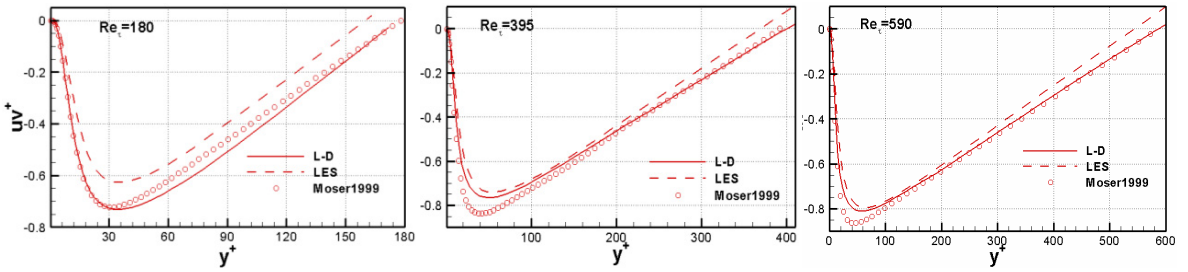

Fig 4. Reynolds stresses by the present method versus DNS and LES results with dynamic sub-grid model.

4. Conclusion

We developed a new method of turbulence simulation by solving the filtered Navier-Stokes equations based on LES methodology and calculating the sub-grid scale stress with D-IP method. Compared to the sub-grid scale models used in LES method with Boussinesq assumption, the sub-gird scale stress of the LES-DIP method is directly estimated based on statistics of molecule motions and is believed to have better universality in simulations of practical turbulent flows. The LES-DIP method is validated by simulating turbulent channel flows at three Reynolds number $\mathrm{Re}_\tau = 180,390,590$. Profiles of mean velocity obtained by LES-DIP agree very well with the DNS results of Moser (1999). Comparisons of first-order and second-order statistics of turbulent fluctuations show that the LES-DIP method performs better than LES with dynamic sub-grid model. It is worthy noticing that the computational cost of LES-DIP is significantly smaller than that of DNS for the same accuracy of results.

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