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LES USING A SPECTRAL ELEMENT METHOD AND EDDY-VISCOSITY TYPE SUBGRID MODELS

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We have successfully applied the Rocketdyne *UniFlo* code to the simulation of a turbulent channel flow at Re_τ of 180 and 1050, respectively. *UniFlo* uses a spectral element spatial discretization and second order accurate time marching method for the solution of the Navier-Stokes equations. The results for under-resolved direct numerical simulation (DNS), and subgrid scale models based on Smagorinsky and Renormalization Group theory, respectively, have been compared. Both models predicted results that are in reasonable agreement with DNS and experimental data. The magnitude of the predicted subgrid scale dissipation is about half of that of the molecular dissipation. The effect of time step size on turbulence statistics has also been investigation. Numerical results indicate that the chosen time step size must be smaller than the Kolmogorov time scale for numerical convergence and it must be ten times smaller to obtain accurate turbulence statistics.

1 Introduction

Computational modeling techniques, primarily computational fluid dynamics (CFD), together with select ground and flight testing, provide the best potential to be the engineering tools of choice in the new Air Force and NASA advanced propulsion programs. Currently one of the biggest hindrances to the more extensive use of computational tools in engineering is the lack of reliable physical process models (e.g. turbulence, transition, chemistry). Turbulence is the pacing item and has the most bearing on the fidelity of the calculations. The current work horse turbulence models used in engineering are of the 1- and 2- equation variety designed for Reynolds Averaged Navier-Stokes equations. The performance of these models appear to be application dependent and range from fair to poor for complex geometries. Higher order phenomenological models such as algebraic stress and full Reynolds stress models are yet to be demonstrated conclusively on realistic 3D problems. The initial results on benchmark problems appear to be not very encouraging about the potential of these models as the future engineering turbulence models of choice for propulsion applications. While this assessment is continuing, may be the time has come to take a closer look at LES type of models. In principle, small scale turbulence is less sensitive to different boundary conditions so by directly capturing the larger and more energetic scales and model the effect of small scale one can develop a predictive method that can be applied to a variety of flow conditions.

To realize the capability of LES for engineering analyses, Rocketdyne has initiated a multi-year effort to develop a spectral element method that provides the necessary high numerical accuracy and flexibility for modeling complex flow paths. As a building block to acquire experience and expertise in using LES, we have decided to start with eddy-viscosity type subgrid models due to their simplicity. Two have been chosen; the first one is the Smagorinsky [1] model with Van Driest damping near the wall while the second one is the RNG model of Yakhot and Orszag [2]. In what follows, we provide a brief description of the numerical method, results of turbulent channel flow simulations using both subgrid scale models, and the sensitivity of prediction on time step size. Although many papers have been published in the LES area, the detailed procedures in setting up the problem and analyzing the results are still very sketchy. So it is our attempt to provide all the necessary details in our paper and hopefully promote the interests of other engineers in applying LES to analyze practical flow problems.

2 Numerical Method and Subgrid Scale Models

By applying an appropriate spatial filter to the Navier-Stokes equations, one can derive a set of governing equations for the resolvable flow field as

$$\frac{\partial u_i}{\partial t} + \frac{\partial u_i u_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \delta_{1i} + \frac{1}{Re_\tau}\frac{\partial^2 u_i}{\partial x_j \partial x_j} - \frac{\partial \tau_{ij}}{\partial x_j}$$

$$\frac{\partial u_j}{\partial x_j} = 0$$

where u_i is the resolved velocity, p is the fluctuating pressure, x_i represents the Cartesian coordinate vector, with x_1, x_2 and x_3 (or x, y and z) being the streamwise, spanwise and wall-to-wall direction, respectively, δ_{1i} is the Kronecker delta, τ_{ij} is the subgrid scale stress tensor, and Re_τ is the Reynolds number based on wall frictional velocity, u_τ, channel half-height, H and dynamic viscosity, ν. In these equations the velocity is scaled by u_τ, the pressure is scaled by ρu_τ^2 and physical dimensions are scaled by H, where ρ is the density. A pressure gradient of one in the streamwise direction maintains a constant through flow in that direction. In this work, the computational grid plays the role of a filter and no explicit filtering procedures are required.

UniFlo has two different time marching schemes for solving the Navier-Stokes equations. The first one is the least-squares spectral element formulation developed by Chan [3] and applied by Chan and Mittal [4] to predict the turbulent flow behind a backward facing step. The second method employs the fractional step procedure due to Kim and Moin [5] and has been extended by Chan [6] in the framework of a Fourier-Legendre Galerkin spectral element approach. The least-squares approach is a generalized method, which operates exclusively in physics space, and can handle a variety of boundary conditions and complex geometries in the expense of higher computational cost, i.e. about ten times more expensive than the Fourier-Legnedre fractional step method. In light of the simple geometry and boundary conditions involved in the channel flow simulation, we opted to use the fractional step method for this work and briefly describe the method here for completeness. Since the flow in the x_1 and x_2 directions are assumed to be homogeneous, it is possible to use Fourier series to approximate the flow field in these directions and obtain a set of discrete modal equations that change only in the x_3 direction. The Galerkin procedure is then applied and with the weak formulation the equations are reduced from second to first order. Therefore, only C^0 continuity is required for the selected basis function which is represented by Legendre polynomials. This idea was first proposed by the MIT group led by Patera and additional details were provided by Rønquist and Patera [7] as well as the references therein. The governing equations are integrated in three different steps. The first step uses Jameson's [8] four-stage Runge Kutta scheme to integrate both the convective terms and subgrid scale terms. To minimize the aliasing errors and alleviate the need of dealiasing, we employ the skew-symmetric form of the convective terms as proposed by Horiuti [9]. The subgrid stresses are evaluated in a weak formulation, for instance, in the streamwise momentum equation the variation of the subgrid stress in the vertical direction is evaluated as $-\int \frac{\partial \tau_{13}}{\partial x_3} W\, dx_3 = \sum_{n=0}^{N} g_n \left(\frac{\partial W}{\partial \xi_3}\right)_{ni} (\tau_{13})_n$, where N is the degree of Legendre polynomials employed, W is the shape function of the Legendre basis, g_n is the Gauss quadrature weighting factor and ξ_3 is the transformed coordinate in the vertical direction with the distribution of Legendre-Gauss-Lobatto collocation points. The second step integrates the viscous step using the Crank-Nicholson scheme with the extrapolated boundary conditions [5] imposed along the walls to minimize the splitting error. The predicted velocity field at the walls is not divergence free and in most cases the error is about 10^{-4}. The last step enforces the continuity equation and results in solving a Poisson equation for pressure, and with the weak formulation no ad-hoc boundary condition is required for the pressure. The pressure value at the lower wall is set to zero for the zero wave number. This is equivalent to setting a reference value for the pressure. The last two steps also use the Jacobi preconditioned conjugate gradient method to seek the solution to a set of algebraic equations. Since the first step is explicit, it is important to keep the CFL number below $2\sqrt{2}$ to achieve numerical stability.

Through Boussinesq approximation, one can relate the subgrid scale stress tensor to the resolved velocity field as $\tau_{ij} = -2\nu_t S_{ij} = -\nu_t \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$, where ν_t is the eddy viscosity and S_{ij} is the strain rate. For the Smagorinsky model ν_t takes the form $\nu_t = (C_s f_s \Delta)^2 \sqrt{2 S_{ij} S_{ij}}$, where Δ is the length scale determined by the local grid spacings as $(\Delta x_1 \Delta x_2 \Delta x_3)^{1/3}$, C_s has a value of 0.1 and f_s is the Van Driest damping with $f_s = 1.0 - exp(-x_3^+/25)$ and $x_3^+ = x_3 u_\tau/\nu$ or $x_3^+ = (x_3/H) Re_\tau$, where x_3 is the vertical distance from the wall. For the RNG model, we solve the quartic form of the equation as $\nu_T^4 - \nu_T \nu^3 - \mathcal{H}\left(a\tau^2 L_f^4 - \nu_T C_c \nu^3\right) = 0$, where ν_T is the effective viscosity and is equal to the sum of ν and ν_t, $\mathcal{H}$ is the Heaviside function which behaves like $\mathcal{H}(a) = a$ if $a \geq 0$ and $\mathcal{H}(a) = 0$ otherwise. This model has many different varieties which are given in several articles that appeared in the proceedings by Galperin and Orszag [10]. We chose to use $C_c = 75$, $\tau = \nu_T \sqrt{S_{ij} S_{ij}}$, $L_f = f_s \Delta$ and $a = 0.0062$ and solve the equation using the Newton-Raphson method. Unfortunately, the model causes numerical divergence without the incorporation of the Van Driest damping term in determining the length scale. This restriction took away the possibility of applying this model to an unstructured grid arrangement commonly employed for analyzing complex flow paths. Further fine tuning in this area is needed.

To evaluate turbulence statistics, we compute the time average value of the product of two different fluctuating components such as $\overline{\phi_1' \phi_2'}$ which can be evaluated on the fly as

$$\overline{(\phi_1 - \overline{\phi_1})(\phi_2 - \overline{\phi_2})} = \overline{\phi_1 \phi_2} - \overline{\phi_1}\,\overline{\phi_2}$$

where ϕ_1 and ϕ_2 are instantaneous field values. In this case the running sums for $\overline{u_1 u_1}$, $\overline{u_2 u_2}$, $\overline{u_3 u_3}$, $\overline{u_1 u_2}$ $\overline{u_2 u_3}$, $\overline{u_1}$, $\overline{u_2}$ and $\overline{u_3}$, must be accumulated at each time step.

3 Results and Conclusions

We first computed the case with $Re_\tau = 180$ using a grid that comprises of $32 \times 32 \times 65$ points in the x, y, and z, respectively, and with dimensions $4\pi H \times 2\pi H \times 2H$. The initial flow field was interpolated from the instantaneous DNS solution of Gilbert and Kleiser [11]. Starting from this initial velocity field, the governing equations were integrated forward in time with five different time step sizes, $\Delta t^+ = \Delta t u_\tau^2/\nu = 0.18$, 0.36, 0.54, 1.08 and 1.8, until the numerical solutions reached a statistically steady state which we determined by monitoring the normalized wall shear stress. Once the velocity field had reached the statistically steady state, we integrated the equations further in time for another $4000\nu/u_\tau^2$ to obtain the planewise average of various statistical quantities. Choi and Moin [12] estimated the Kolmogorov time to be about 2.4 which appears to be the largest time size allowed, since whenever we employed a time step size that exceeded this value, the code diverged. Figure 1 shows when the flow reaches the statistical stationary state, the mean value of the wall shear stress has a value of approximately one. The instantaneous streamwise velocity in Figure 1 also shows the near wall streaky structures which are consistent with experimental observations. Figure 2 shows too large of a time step size can incur significant error in both mean flow and turbulence statistics predictions. The optimal value is approximately 0.18 which is about one-tenth of the Kolmogorov time scale. Therefore in selecting the time step size, accuracy (not numerical stability) is the determining factor for the numerical scheme employed here. Figure 3 shows the subgrid dissipation prediction by the RNG model is three times smaller than that predicted by the Smagorinsky model which predicted a peak subgrid dissipation about half of the molecular dissipation. Both models seem to predict turbulence statistics that generally agree with DNS and experimental data [13]. Figure 4 shows the results for $Re_\tau = 1050$ obtained with $48 \times 64 \times 65$ points and a domain size of $2.5\pi H \times 0.5\pi H \times 2H$. The RNG model did not work for this case and caused to flow to relaminarize. In addition to the experimental data, we also compare to the results of Piomelli [14] who applied the dynamic model. The Smagorinsky model appears to perform just as well as the dynamic model. The predicted eddy viscosity is higher than the previous case by a factor of two.

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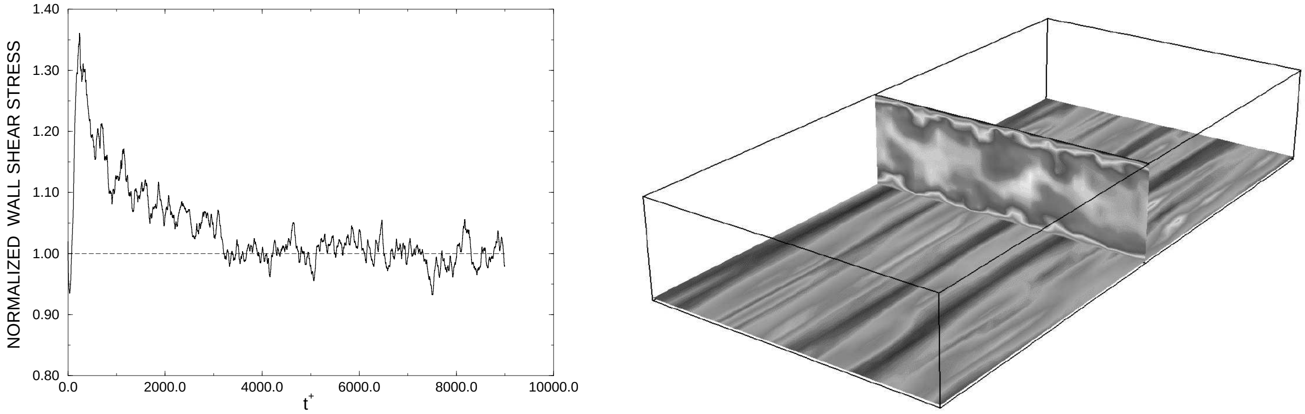

Figure 1: Turbulent channel flow LES for $Re_\tau = 180$ using Smagorinsky model; on the left is the time variation of spanwise averaged wall shear stress and on the right is the magnitude of instantaneous streamwise velocity showing streaky near wall flow structure.

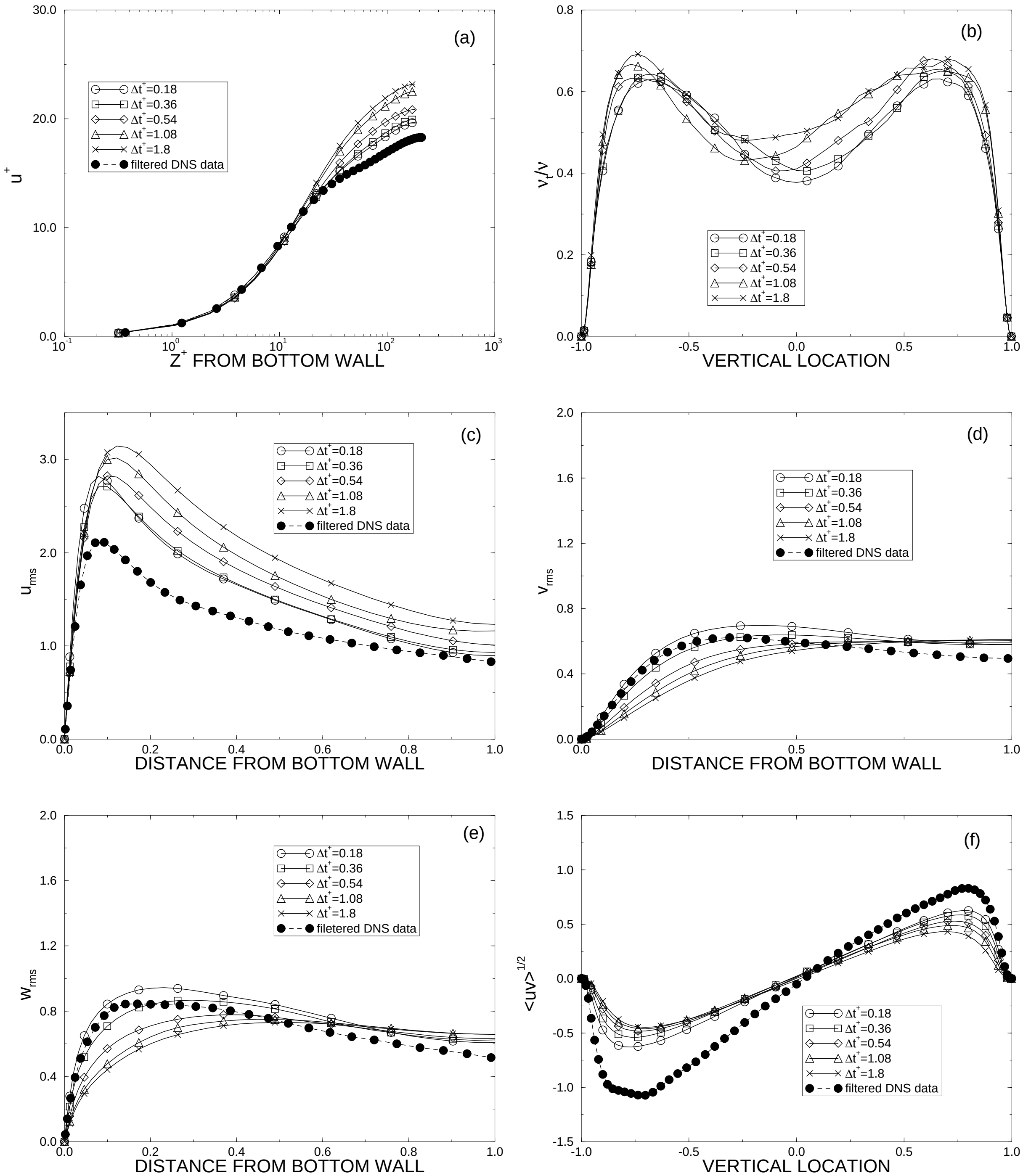

Figure 2: Turbulent channel flow LES for $Re_\tau = 180$ using Smagorinsky model and different time step sizes; (a) mean streamwise velocity in wall units, (b) profile of instantaneous eddy viscosity normalized by molecular viscosity (c) streamwise velocity turbulence intensity, (d) spanwise velocity turbulence intensity, and (e) turbulence intensity of the velocity component in the wall-to-wall direction and (f) turbulence intensity of $u_1 u_2$

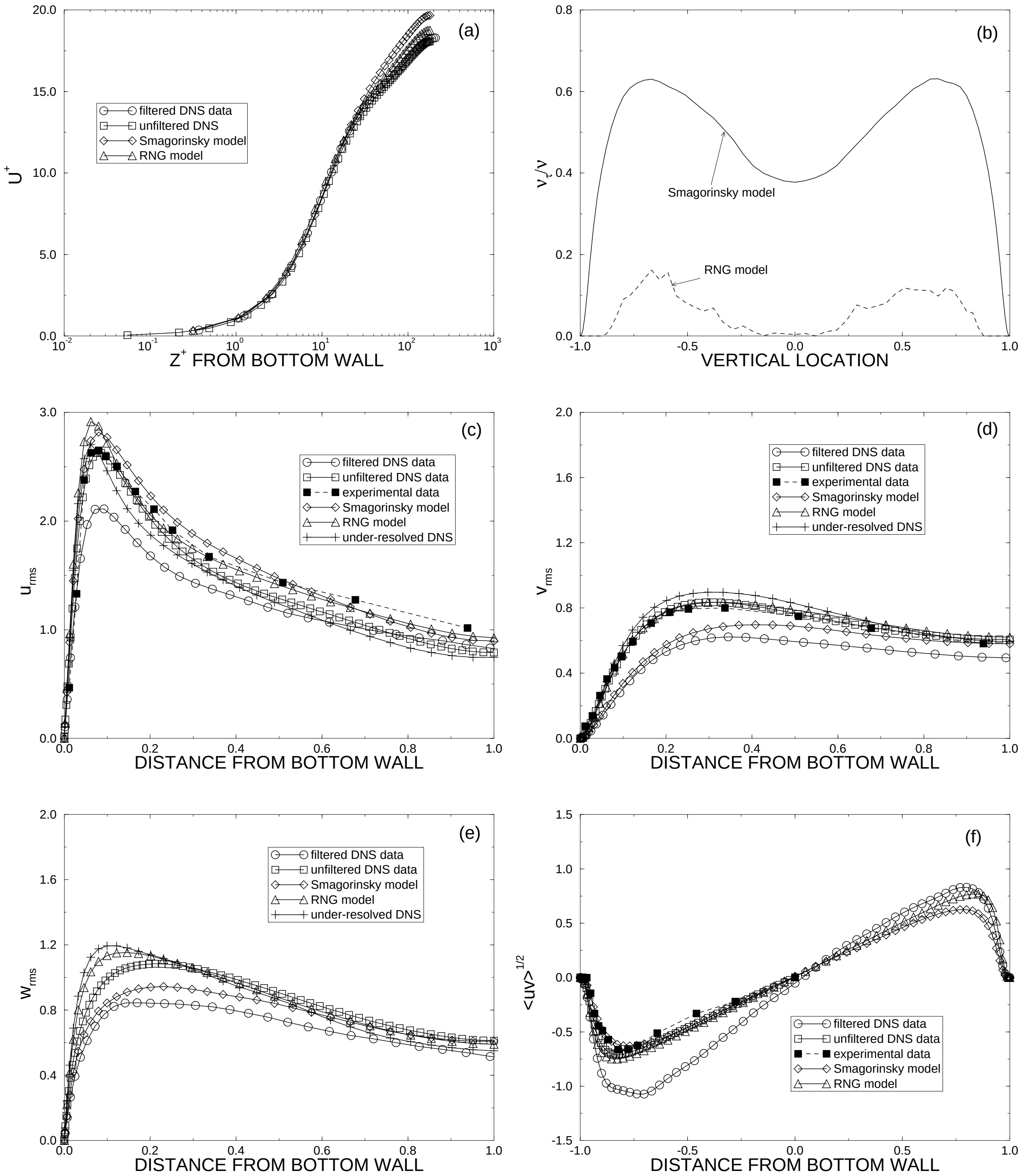

Figure 3: Turbulent channel flow LES for $Re_\tau = 180$ using different subgrid scale models and a time step size of $\Delta t^+ = 0.18$; (a) mean streamwise velocity in wall units, (b) profile of instantaneous eddy viscosity normalized by molecular viscosity (c) streamwise velocity turbulence intensity, (d) spanwise velocity turbulence intensity, and (e) turbulence intensity of the velocity component in the wall-to-wall direction and (f) turbulence intensity of $u_1 u_2$

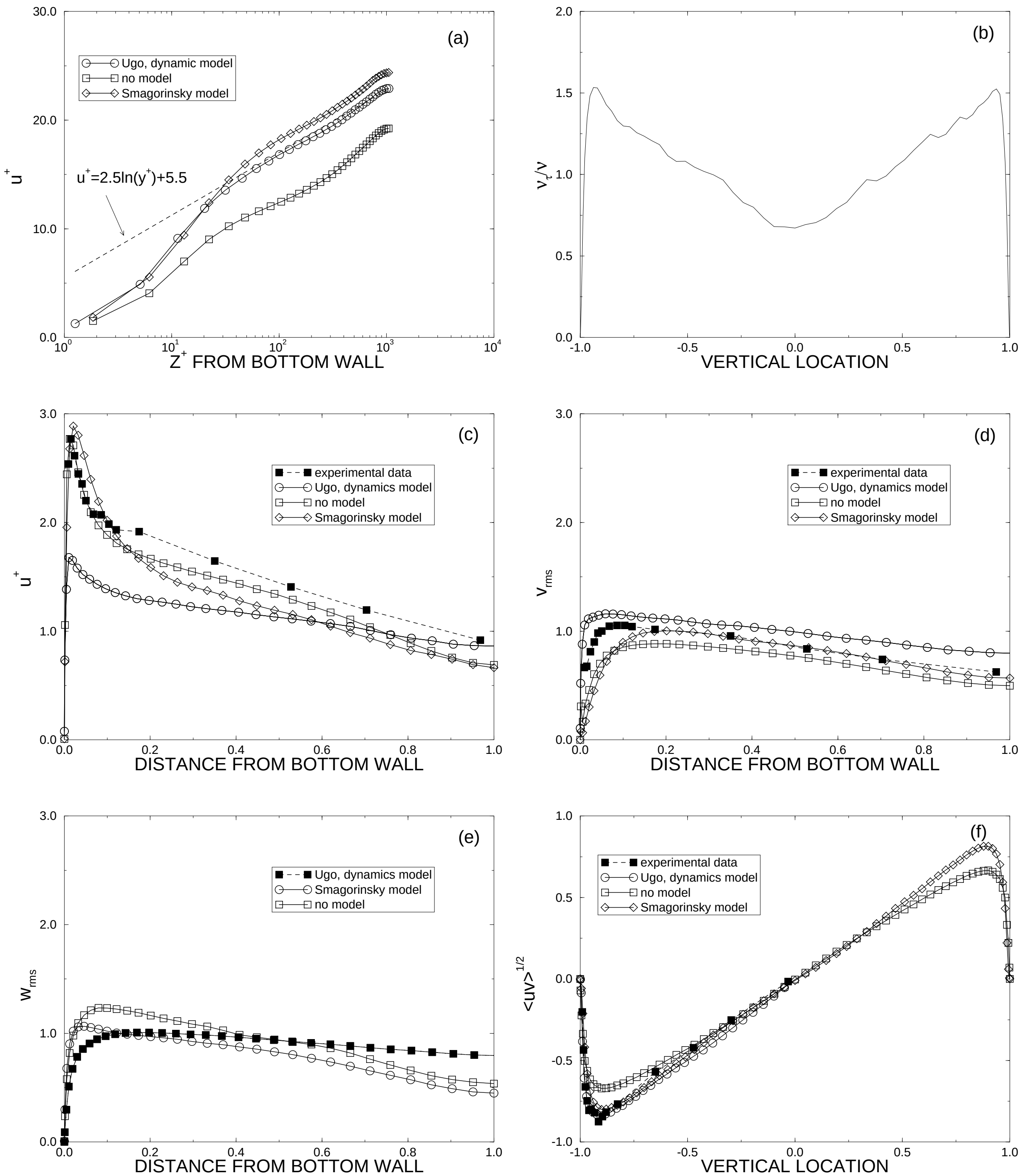

Figure 4: Turbulent channel flow LES for $Re_\tau = 1050$ using different subgrid scale models and a time step size of $\Delta t^+ = 0.18$; (a) mean streamwise velocity in wall units, (b) profile of instantaneous eddy viscosity predicted by the Smagorinsky model and normalized by molecular viscosity (c) streamwise velocity turbulence intensity, (d) spanwise velocity turbulence intensity, and (e) turbulence intensity of the velocity component in the wall-to-wall direction and (f) turbulence intensity of $u_1 u_2$