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Grid-Size Dependence in the Large-Eddy Simulation of Kolmogorov Flow

S. L. Woodruff*
Florida State University, Tallahassee, Florida 32306-4120
J. M. Seiner†
University of Mississippi, University, Mississippi 38677
and
M. Y. Hussaini‡
Florida State University, Tallahassee, Florida 32306-4120

Through the use of both an a priori analysis of direct numerical simulation data and experiments with large-eddy simulations, a non-Smagorinsky grid-size dependence is established for the Smagorinsky subgrid scale model for low numbers of resolved scales. It is shown that an increase in the Smagorinsky constant as the grid size is increased permits successful large-eddy simulations for cutoffs approaching the energy-containing range of length scales. A detailed comparative analysis is made of the second-order turbulence quantities as determined by the differently resolutioned large-eddy simulations.

Introduction

THE basic idea behind a large-eddy simulation (LES) is that the largest turbulent scales will be resolved numerically, and only the universal and self-similar smallest scales will be modeled. Provided one truly can resolve all of the scales of the energy-containing range of the turbulent flow as well as of the large-scale portion of the inertial range, the model used may be a simple and efficiently computed one: the Smagorinsky model, for example, for all its faults, has been remarkably successful in LES computations of many basic flows.[1] The reality, of course, is that only for the very simplest flows can this ideal even be approached, and for moderately complex flows, let alone flows of practical interest, current computational resources permit, at best, resolution only into the transitional region between the energy-containing range and the inertial range.[2]

Given this reality, and given that the faster computers of the near future will make but a small dent in the problem (we will only use them to try to solve even more complicated flows, anyway), it is reasonable to ask what are the consequences of this inadequate resolution and what might be done to ameliorate them. In the present investigation, we ask the specific question, can an alternative, non-Δ^2, grid-size dependence for the Smagorinsky model improve LES results conducted with what would ordinarily be considered inadequate numerical resolution? The possibility of alternative grid-size dependencies and, more generally, subgrid scale models designed to handle the modeling of turbulence in the lower inertial range and the upper energy-containing range has been raised by Speziale[3] and Woodruff et al. (S. L. Woodruff, C. G. Speziale, M. Y. Hussaini, and G. Erlebacher, "Continuous Modeling for Isotropic Turbulence," personal communication, 1998).

In this paper, alternative grid-size dependencies for the Smagorinsky model are considered for the large-eddy simulation of Kolmogorov flow. Kolmogorov flow arises when a fluid, in this case incompressible, is subjected to an artificial, sinusoidal, body force. The flow is periodic and shares many properties with common shear flows, but lacks many of the computational difficulties presented by homogeneous shear flow or such wall-bounded shear flows as channel flow or boundary-layer flow. Kolmogorov flow was originally proposed by Kolmogorov to his students as a simple flow for the study of stability problems in shear flows and has since been subjected to a number of stability analyses.[4,5] Turbulent Kolmogorov flow in two dimensions was studied by She[6,7]; three-dimensional direct numerical simulations of turbulent Kolmogorov flow employing the physical viscous stresses were performed by Shebalin and Woodruff.[8] Three-dimensional hyperviscosity simulations were performed by Borue and Orszag.[9] Some preliminary results from the present investigation have been presented earlier,[10] and the present results have been recently presented.[11]

The question of possible alternative grid-size dependencies for the Smagorinsky model is here approached in two ways. First, an a priori analysis of a 64^3 direct numerical simulation (DNS) data set is conducted. The fully resolved velocity field from the DNS is filtered over a wide range of filter widths; for each filter width, both the Smagorinsky model formula and the Reynolds stress it is supposed to predict are evaluated. Comparing the two permits the filter width (or grid size) dependence of the Smagorinsky model to be assessed. The second approach to assessing the grid-size dependence of the Smagorinsky model is by LES experimentation: at each of a number of numerical resolutions, simulations are run with different values of the Smagorinsky constant. Determining which value of the Smagorinsky constant leads to the best results at a given resolution yields an empirically determined grid-size dependence.

Encouragingly, both approaches lead to similar conclusions about grid-size dependence. In both cases, an intermediate range of wave numbers (or grid sizes) was found where the standard Δ^2 grid-size dependence worked well. Beyond the low-wave number (coarse resolution) end of this range, an enhanced grid-size dependence is found to be necessary to give the best possible results, both in the a priori analysis of the DNS data set and for the LES experiments. Satisfactory LES results were achieved at suprisingly low resolutions, when an appropriate grid-size dependence was used, though there was deterioration in the predictions, particularly of the turbulent shear stress.

The investigation outlined in this paper has sought to establish in a simple way that there is merit to the idea of altering the grid-size dependence of a subgrid-scale model (in this case, the Smagorinsky model, with its traditional grid-size dependence based on inertial-range dynamics) to compensate for limited underresolution in an LES. In keeping with this goal, a simple criterion for selecting the best Smagorinsky constant has been chosen (comparing the kinetic energies in different simulations) and simple criteria for

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*Visiting Associate Professor, Department of Mathematics and School for Computational Science and Information Technology.

†Associate Director for Applied Research and Research Professor, National Center for Physical Acoustics.

‡Director, School for Computational Science and Information Technology.

assessing the adequacy of the underresolved simulations (comparing several second-order statistical quantities) were employed in this preliminary investigation. More sophisticated approaches to fixing the Smagorinsky constant (including a theoretical discussion of its grid-size dependence as the energy-containing range is approached from above) and to assessing the usefulness of underresolved LES are the subject of current investigation.

Following the problem statement and notational definitions of the next section, the a priori analysis of the DNS data set and the LES experiments are discussed. The paper concludes with a discussion of the results and their implication for the LES of complex flows.

Problem Statement and Numerical Considerations

Kolmogorov flow is described by the Navier–Stokes equations subject to an artificial periodic body force with wave number k_f and amplitude $k_f v_0^2$. An appropriate nondimensionalization consists of using $1/k_f$ for the reference length and $1/k_f v_0$ for the reference time; the Reynolds number is then $v_0/k_f \nu$. Taking the force vector to be in the positive x direction, the Navier–Stokes equations for an incompressible flow become

$$\frac{D\boldsymbol{v}}{Dt} = -\frac{1}{\rho}\nabla p + \frac{1}{Re}\nabla^2\boldsymbol{v} + \hat{\boldsymbol{\imath}}\sin z \tag{1}$$

Periodic boundary conditions are imposed in all three directions, so that the forcing wave number k_f reappears in the formulation in the ratio of the forcing wave number to the wave number of the longest wave contained in the box; this ratio will hereafter be denoted simply k_f.

The simulations examined in the present investigation have a Reynolds number of 28 and a forcing wave number of 6. This Reynolds number is sufficiently high to give fully developed turbulence (transition to turbulence occurs at $Re = 12$–13 in this nondimensionalization).[6,7] Previous experience with this flow[12] indicates the flow attains a statistically steady state more rapidly as the forcing wave number is increased; the use here of $k_f = 6$ provides fairly brief initial transients.

In the DNS that provides the data set employed in the a priori analysis, the code of Shebalin[13] was used as configured for the earlier DNS found in Ref. 8. This code is pseudospectral with Fourier modes in the three spatial directions. A predictor–corrector time stepping algorithm is employed, with the viscous terms handled implicitly and the nonlinear terms handled explicitly.

The LES were performed with the same code, as adapted for LES for the simulations discussed in Ref. 12. The subgrid-scale stresses τ_{ij} are incorporated as an explicit contribution to the time stepping; in this case the traditional Smagorinsky expression is used[14]:

$$\tau_{ij} = -C_S\Delta^2\sqrt{S_{mn}S_{mn}}S_{ij} \tag{2}$$

where C_S is the Smagorinsky constant, Δ^2 is a measure of the grid size, and S_{ij} is the rate-of-strain tensor. As has been customary with LES using the Smagorinsky model and Fourier modes, the grid size (relative to the length of the sides of the box) is taken as $2\pi/N$, with N the number of modes in each coordinate direction. (All simulations considered here have the same number of modes in each coordinate direction.)

Because the fast-Fourier transform algorithm in the code expects the number of modes to be a power of two, runs with intermediate numbers of modes are performed by zeroing out the excess modes at each time step. For example, 24^3 runs are performed with the code set for 32^3 and with modes with wave numbers of 13–16 zeroed out.

All DNS and LES runs reported here were initialized with a random initial velocity field with an exponential energy spectrum. Time series for the total kinetic energy, dissipation, etc., were used to establish that a statistically steady state had been reached.

A Priori Analysis

The goal of the a priori analysis is to determine what grid-size dependence gives the best fit between the subgrid-scale turbulent stresses predicted by the Smagorinsky model and the true subgrid-scale stresses when both are determined from a DNS data set. A 64^3 simulation was run as described in the preceding section until a statistically steady state was reached, then the instantaneous velocity field from this simulation was used in the analysis.

The instantaneous velocity field was first filtered into super- and subgrid components by means of a spectral cutoff filter (denoted $\langle\cdot\rangle$); that is, the velocity field was decomposed according to

$$u_i = \langle u_i\rangle + u_i' \tag{3}$$

with $\langle u_i\rangle$ containing all Fourier modes with wave number less than the cutoff k_c and $u_i' = u_i - \langle u_i\rangle$ containing all Fourier modes with wave number greater than k_c. This decomposition was performed for all integer values of k_c running from 32 (no filtering, with all modes contained in the supergrid velocity $\bar{u}_i$) down to 2 (nearly complete filtering, with only the zero and $k = 1$ modes contained in the supergrid velocity and all of the others contained in the subgrid velocity u_i').

At each of the cutoff wave numbers k_c, the Smagorinsky representation of the subgrid-scale stresses was computed, as well as the true stresses it is supposed to predict. The two tensors $A_{ij} = \sqrt{(S_{mn}S_{mn})}S_{ij}$ and $\tau_{ij} = -\langle u_i'u_j'\rangle$ that result are, according to the Smagorinsky model [Eq. (2)], supposed to be proportional, with proportionality factor $C_S\Delta^2$. An empirical value of the proportionality factor may be determined by reducing these second-rank tensor fields varying in x, y, and z to single numbers and taking their ratio.

Each of the components of these two tensors is a function of x, y, and z; in this work, this function is reduced to a single number by taking the L^2 norm. Such a norm seems appropriate for this problem, given the statistical homogeneity of the flow in the x and y directions. The flow is not statistically homogeneous in the z direction, but even there flow features do not cluster in particular regions of the flow domain and a norm that weights equally all parts of the flow seems reasonable. A more specialized norm will probably be necessary to get useful results when such an analysis is applied to, for example, turbulent boundary-layer flow or turbulent channel flow.

In summary, for each filter cutoff wave number the velocity field is decomposed into supergrid and subgrid parts, the true subgrid-scale stress and the Smagorinsky subgrid-stress are formed, the L^2 norms are taken of each of the six independent components of the tensors, and the ratios are taken. In the results presented, these ratios have been further divided by Δ^2, so that the result of the calculation is a grid-size dependent Smagorinsky constant C_S.

Figure 1 gives C_S as a function of $k_c = 2\pi/\Delta$ as determined from the xy tensor component. (The results of the LES experiments discussed in the next section are also included in Fig. 1.) Note the plateau at intermediate wave numbers (where LES is traditionally carried out), the gradual rise as the forcing wave number ($k_f = 6$) is approached from above and the rapid rise at the forcing wave number. This behavior provides some hope that LES with an enhanced grid-size dependence could be successful, primarily for those values

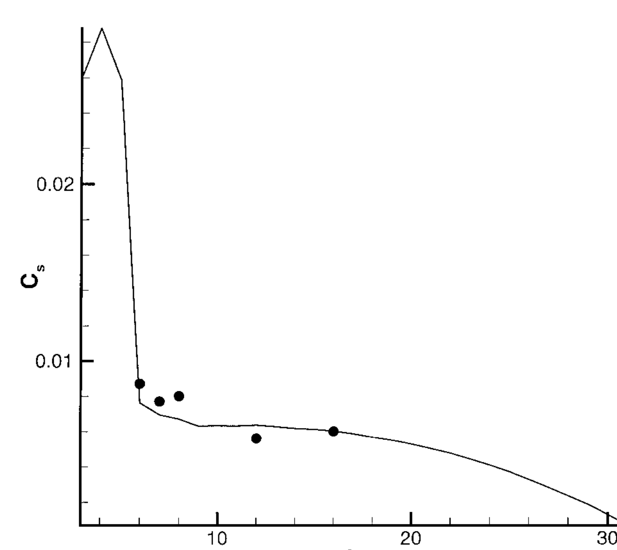

Fig. 1 Smagorinsky constant C_S as function of grid-size, as determined by ——, a priori analysis, and •, LES experiments.

of the cutoff wave number where the increase is gradual in Fig. 1. (The jump in C_S at the forcing wave number indicates that things are changing dramatically and that an LES is less likely to be successful; one would not expect to be able to conduct traditional LES with forcing in the subgrid scales.) The utility of an enhanced grid-size dependence in LES can be properly tested only in actual simulations, which is the topic of the next section.

LES Experiments

To test the concept of a variable grid-size dependence in actual LES computations, simulations conducted as described in the second section were carried out with different resolutions and different values of the Smagorinsky constant. Each simulation began with the same initial condition and was continued until a statistical steady state was reached. All comparisons of results from simulations with different resolutions and different values of the Smagorinsky constant were made for that steady state.

Simulations were performed with resolutions ranging from 32^3 to 12^3 (the latter resolution being the smallest that permits the forcing at $k_f = 6$ to be in the numerically resolved scales). Those resolutions not a whole number power of two are performed as whole number powers of two simulations with excess modes zeroed out at each time step, as described in the second section.

For each resolution, several simulations were carried out at different values of the Smagorinsky constant; the two simulations closest to the true results are presented here. The variation of these values of the Smagorinsky constant with resolution may then be examined. To carry out this program, a baseline for comparison must be established to give the true values, and a measure of how close the results of any given simulation are to the true values must be chosen. Previous experience[12] indicates that a 32^3 LES is adequate to properly simulate a Kolmogoroff flow with the present Reynolds number and k_f. The 32^3 results will, thus, be used as the baseline for comparison with all other simulations. A simple way to compare the lower-resolution LES with the baseline is to compare the steady-state values of the total kinetic energy in the periodic box. The mere fact of agreement of the values of the kinetic energy obviously by no means guarantees agreement of any other features of the flow, and extensive comparisons are made hereafter of some of those other features to see what agreement does exist. However, at this early stage of this research program, this measure of agreement provides a simple and surprisingly effective means of comparison.

In addition to the 32^3 reference simulations, LESs were carried out at resolutions of 24^3, 16^3, 14^3, and 12^3. Time histories of results are shown in Figs. 2–6; Table 1 contains parameters for the individual simulations and time averages of representative quantities over the statistically steady portion of the simulations' time histories.

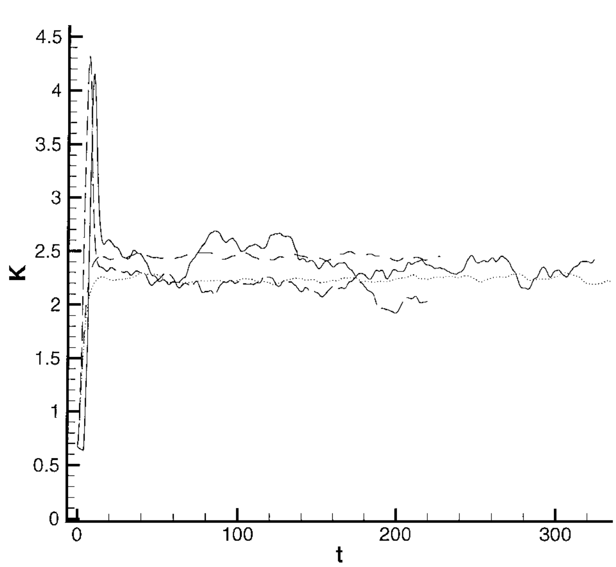

Fig. 2 Kinetic energy vs time for ——, 32^3 simulation with $C_S = 0.006$; – – –, 32^3 simulation with $C_S = 0.008$; - - - -, 12^3 simulation with $C_S = 0.0087$; and · · · ·, 12^3 simulation with $C_S = 0.0096$.

Table 1 Simulation parameters and temporal averages of results

Number of modes	C_S	K	$\|\|\bar{u}\|\|$	$\|\|u'\|\|$	$\|\|v'\|\|$	$\|\|w'\|\|$	C_{zx}
32	0.006	2.33	0.93	1.24	0.89	1.21	0.41
32	0.008	2.08	0.74	1.20	0.82	1.22	0.44
24	0.0045	2.48	0.88	1.36	0.96	1.19	0.40
24	0.0056	2.33	0.85	1.32	0.90	1.17	0.41
16	0.008	2.49	0.96	1.28	0.88	1.28	0.25
16	0.012	2.26	1.04	1.21	0.71	1.20	0.27
14	0.0077	2.38	0.85	1.26	0.82	1.33	0.27
14	0.010	2.18	0.82	1.15	0.69	1.37	0.28
12	0.0087	2.44	1.75	0.97	0.81	0.45	0.32
12	0.0096	2.25	1.69	0.92	0.78	0.42	0.34

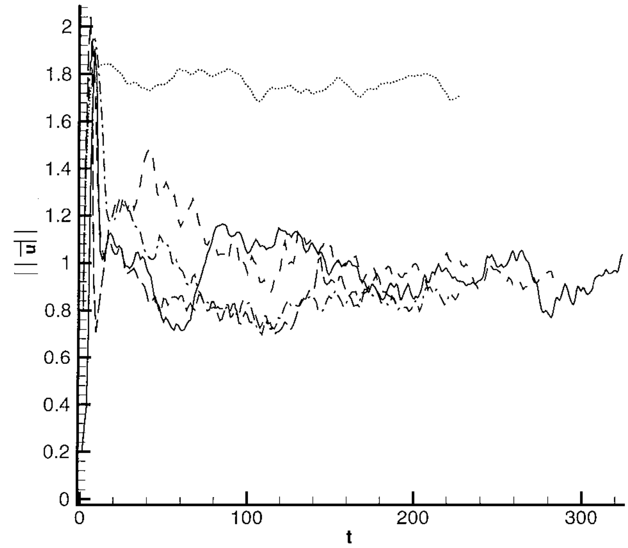

Fig. 3 Time for ——, 32^3 simulation vs $\|\bar{u}\|$ with $C_S = 0.006$; – – –, 24^3 simulation with $C_S = 0.0045$; - - - -, 16^3 simulation with $C_S = 0.008$; – · –, 14^3 simulation with $C_S = 0.010$; and · · · ·, 12^3 simulation with $C_S = 0.0087$.

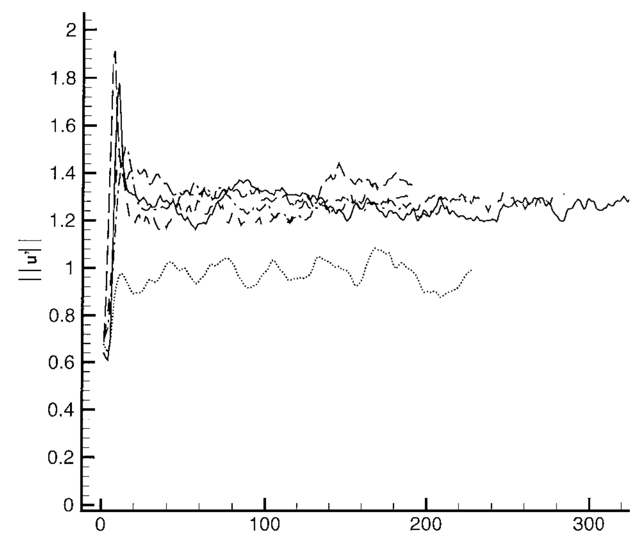

Fig. 4 Time for ——, 32^3 simulation vs $\|u'\|$ with $C_S = 0.006$; – – –, 24^3 simulation with $C_S = 0.0045$; - - - -, 16^3 simulation with $C_S = 0.008$; – · –, 14^3 simulation with $C_S = 0.010$; and · · · ·, 12^3 simulation with $C_S = 0.0087$.

The time histories of the total kinetic energy for the most extreme case, the 12^3 simulations, are compared against the 32^3 reference simulations in Fig. 2. Time histories are shown for simulations with values of the Smagorinsky constant that bracket the 32^3 reference plots; the two time histories are shown to give a rough impression of the sensitivity of the results to the change in C_S at each resolution. Thus, at least as far as the kinetic energy is concerned, adjustment of the Smagorinsky constant permits successful simulations for

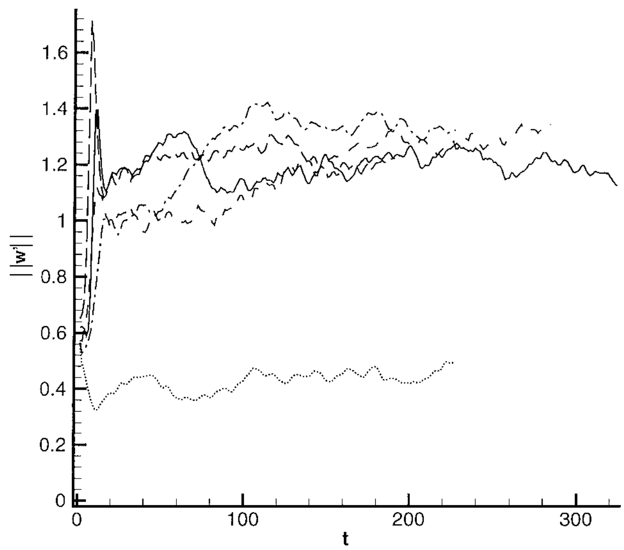

Fig. 5 Time for ——, 32^3 simulation vs $\|w'\|$ with $C_S = 0.006$; – – –, 24^3 simulation with $C_S = 0.0045$; - - - -, 16^3 simulation with $C_S = 0.008$; – ·–, 14^3 simulation with $C_S = 0.010$; and · · · ·, 12^3 simulation with $C_S = 0.0087$.

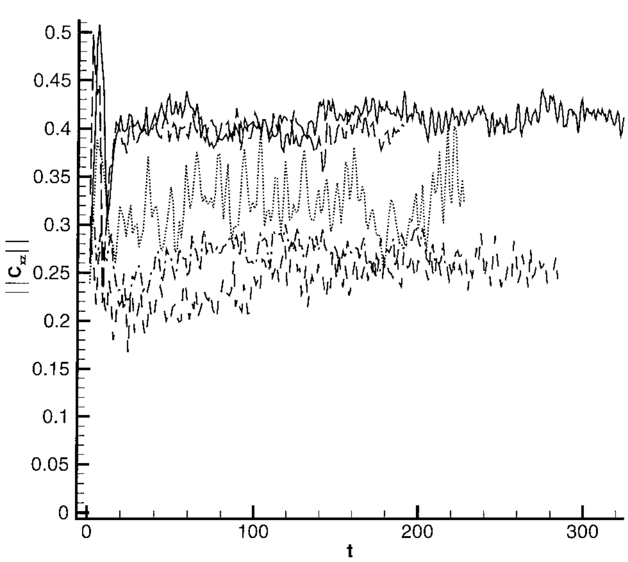

Fig. 6 Time for ——, 32^3 simulation vs $\|C_{xz}\|$ with $C_S = 0.006$; – – –, 24^3 simulation with $C_S = 0.0045$; - - - -, 16^3 simulation with $C_S = 0.008$; – ·–, 14^3 simulation with $C_S = 0.010$; and · · · ·, 12^3 simulation with $C_S = 0.0087$.

resolutions as low as 12^3. The extent to which other quantities are successfully simulated is examined in detail hereafter.

Interpolated values for C_S were plotted in Fig. 1 for comparison with the C_S values determined from the a priori analysis; it is seen that the LES experiments are consistent with the a priori results. The determination of similar variations in the Smagorinsky constant by these two independent means is strong evidence for the utility of alternative grid-size dependences in LES. Specifically, these results indicate that, not only is the enhanced grid-size dependence necessary for low-resolutioned LES (as indicated by the a priori analysis), but it is sufficient (at least as far as the kinetic energy is concerned.)

Time histories of some other first- and second-order statistical quantities are shown in Figs. 3–6. In each of Figs. 3–6, one simulation at each resolution is shown. (In all cases, the simulation is the one with the higher kinetic energy.) The statistical quantities are computed using averages in the x–y plane. Thus, $\bar{u}$ is a function of z; Fig. 3 shows the L^2 norms of these functions. The fluctuating velocities $u' = u - \bar{u}$ and $w' = w - \bar{w}$ are represented by their L^2 norms in Figs. 4 and 5. (Note these fluctuating velocities are different from the primed, fluctuating velocities defined in the preceding section.) The final plot, Fig. 6, is of the L^2 norms of the correlation coefficient, defined by

$$C_{xz} = \frac{\overline{u'w'}}{\sqrt{\overline{u'^2}\,\overline{w'^2}}} \tag{4}$$

Considering first the mean and fluctuating velocities of Figs. 3–5, it is clear that almost all of the simulations' predictions for these quantities cluster together quite well, once the initial transients have evolved into the statistical steady state. The exception is the 12^3 simulation, where it is clear that the limits of resolution have been exceeded. Note that the 12^3 simulation has achieved the correct total kinetic energy by significantly overestimating the plane-averaged mean velocity and underestimating the fluctuating velocities, indicating the low resolution is suppressing the fluctuations.

The time series of the L^2 norm of the correlation coefficient shown in Fig. 6 provide a more rigorous measure of the faithfulness of the simulations to the true turbulence physics, and their examination reveals weaknesses in the lower-resolutioned simulations. The C_{xy} and C_{yz} correlations (not shown) are reproduced fairly well by all simulations (even the 12^3 simulation); it is, however, the C_{xz} correlation, describing the Reynolds stress component that effects energy transfer from the mean to the fluctuating motion, where real breakdowns in the low-resolution simulations may be seen. Figure 6 shows that only the 24^3 simulation reproduces the steady-state value of C_{xz} correctly, with the 16^3 and 14^3 simulations giving values around half the true value. Curiously, and probably fortuitously, the 12^3 simulation does better here than the 14^3 and 16^3 simulations. Note as well (see Table 1) that the correlation coefficients are essentially unaffected by the changes in the Smagorinsky constant at a given resolution.

Conclusion

These results indicate that the low-resolution simulations not only correctly reproduce the total kinetic energy but, except for the lowest resolution, 12^3 simulation, correctly reproduce most of the other statistical quantities examined as well. The major failure of the low-resolution simulations was in the determination of the correlation coefficient C_{xz}, where only the 24^3 simulation came close to the correct value.

In addition to this failure of the low-resolution LES results in the prediction of the C_{xz} correlation, the results (as presented in Table 1) also show virtually no sensitivity of this correlation coefficient to changes in the value of the Smagorinsky constant. It may be concluded that, not only do the simulations performed with the Smagorinsky constant tuned to give the correct kinetic energy fail to give the right C_{xz}, but no simple tuning of the Smagorinsky constant will give good results for the correlation coefficient. A more drastic adjustment of the model is necessary and is being developed.

The breakdown of the underresolved simulations at 12^3 and the failure of the underresolved simulations to produce the correct correlation coefficient C_{xz} are likely related. Reducing the number of modes and the resolved scales inhibits the mechanism for the transfer of the energy from the mean to the fluctuating motion. At the 12^3 resolution, this inhibition has reached the point where insufficient energy flows into the fluctuating motion and so the mean energy is too high and the fluctuating energy is too low. Because, in this flow, as in other parallel flows, the energy transfer between the mean and fluctuating motion is mediated by the C_{xz} correlation, the inhibited energy transfer is reflected in incorrect values for that correlation.

The a priori results and the LES experiments described indicate that, when used with care, low-resolution simulations with an alternative grid-size dependence can give satisfactory results. Significant advances in the application of LES to complex turbulent flows of practical interest may, thus, be possible, provided reliable, general-purpose models are developed incorporating the concept of alternative grid-size dependencies. Research into such models is currently under way.

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P. Givi
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