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COMPARISON OF FOUR EDDY-VISCOSITY SGS MODELS IN LARGE-EDDY SIMULATION OF FLOWS OVER ROUGH WALLS

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ABSTRACT

Large Eddy Simulation (LES) has become an increasingly attractive option for turbulence modeling due to the rise in computing power and the improvement in sub-grid scale (SGS) parameterizations. This study tests the improvements in simulations of wall-bounded flows over heterogeneous surfaces attained by the implementation of three improvements in the eddy-viscosity SGS closure: the dynamic model by Germano *et al.* [1], the Lagrangian model by Meneveau *et al.* [2], and the scale-dependent approach by Porté-Agel *et al.* [3]. The dynamic model consists of using the resolved scales to 'measure' the model coefficient during the simulation; therefore, no a-priori knowledge of the coefficient or the flow physics is needed. The traditional dynamic approach averages the coefficient over statistically homogeneous directions to numerically stabilize the simulations. The Lagrangian model relaxes the need for homogeneous directions by averaging the coefficient over pathlines, hence allowing local determination of the coefficient and facilitating applications to complex-geometry flows. The scale-dependent approach uses the dynamic formulation but does not assume that the SGS coefficients are scale-invariant, as is the case in traditional dynamic formulations.

The deficiencies of the traditional Smagorinsky model are confirmed. Implementation of a dynamic model treats some of these deficiencies but is found to be under-dissipative close to the wall in high Reynolds number LES that does not resolve the viscous layer. The sensitivity of the model coefficient to the wall roughness is demonstrated thus confirming the need for a local SGS model such as the Lagrangian model used here. Finally, when the Lagrangian-dynamic model is implemented with the scale-dependent formulation, the results improve significantly.

INTRODUCTION

The Large-Eddy Simulation (LES) approach originated in meteorological modeling [4-6] but its scope has broadened and it is currently a very appealing technique for a wide range of engineering applications as well. The filtering of the Navier-Stokes equations that yields the LES equations gives rise to a subgrid-scale (SGS) stress term that represents the effect of the small unresolved scales of motion on the resolved scales. Modeling of this term is needed to close the system of equations and solve it numerically. The sensitivity of LES results to the specific SGS closure used was appreciated only gradually and continues to be a current research topic. Early studies [5-6] attempted to optimize the coefficients of the eddy-viscosity model proposed by Smagorinsky [4] and to adapt this model to geophysical and engineering flows. However, as the shortcomings of the classic Smagorinsky parameterization became apparent (as detailed later in this paper), the need for new models became obvious. In the last 15 years, several new SGS formulations appeared; the understanding of SGS physics improved due to numerical and experimental studies; verification, validation, and comparison of SGS models expanded; and the relation between filtering and SGS closure became clearer [7-9].

Eddy-viscosity models continue to be widely used and good results can be obtained with such models for a great variety of flows. This paper will focus on the effect of some SGS modeling improvements on eddy-viscosity SGS models. Simulations over homogeneous and heterogeneous surfaces will be performed using: the simple Smagorinsky or Smagorinsky-Lilly model with a wall damping function

(SMAG), the planar-averaged scale-invariant model (PASI), the Lagrangian-averaged scale-invariant model (LASI), the planar-averaged scale-dependent model (PASD), and the Lagrangian-averaged scale-dependent model (LASD).

LARGE EDDY SIMULATION

Underlying the eddy-viscosity models is the notion that the small eddies often do not significantly contribute to the transport of momentum or scalars and that their main effect is to dissipate the energy that cascades from larger scales. The large-eddy simulation technique utilizes this feature of turbulent flows and resolves only the large scales of motion that are responsible for most of the transport of momentum and scalars.

Formally, eliminating the small scales is equivalent to filtering the Navier-Stokes equation. The effect of the unresolved scales appears as a subgrid-scale (SGS) flux term $\sigma_{ij} = \widetilde{u_i u_j} - \widetilde{u}_i \widetilde{u}_j$. A homogeneous filter is used so that filtering commutes with differentiation and the resulting system of equations is:

$$\frac{\partial \tilde{u}_i}{\partial t} + \tilde{u}_j \left(\frac{\partial \tilde{u}_i}{\partial x_j} - \frac{\partial \tilde{u}_j}{\partial x_i} \right) = -\frac{1}{\rho} \frac{\partial \tilde{p}^*}{\partial x_i} - \frac{\partial}{\partial x_j} \tau_{ij} + \widetilde{F}_i$$
$$\frac{\partial \widetilde{u_i}}{\partial x_i} = 0. \qquad (1)$$

This is the rotational form of the LES equation used to ensure conservation of kinetic energy and mass [10]. F_i is the mean streamwise pressure forcing and τ_{ij} is the deviatoric part of the SGS stress tensor σ_{ij} defined as

$$\tau_{ij} = \sigma_{ij} - \frac{1}{3} \sigma_{kk} \delta_{ij}. \qquad (2)$$

Note that in the above equations, the viscous term is neglected because the paper focuses on very high Reynolds number flows and the wall layer is modeled (as opposed to resolving the viscous sublayer, see [11]).

The solution of the filtered Navier-Stokes equations yields the filtered (resolved) velocity vector $\tilde{u}(\boldsymbol{x},t)$, the tilde ($\tilde{}$) will be used throughout this paper to indicate the filtering operation at the grid scale Δ or refer to a filtered variable. The pressure term $\tilde{p}^* = \tilde{p} + (1/3)\rho\sigma_{kk} + (1/2)\rho\tilde{u}_j\tilde{u}_j$ represents a dynamic variable that is deduced so that the velocity field remains divergence free. Taking the divergence of the above equation and using continuity results in a Poisson equation for pressure that can be solved for $\tilde{p}^*$.

The code used in the present simulations of channel-flow like geometries uses a pseudo-spectral approach in the horizontal directions. A second-order accurate centered-differences scheme, requiring a staggered grid, is used in the vertical direction. This entails storing the variables at heights *ndz* or *(n–1/2)dz*; where *n* goes from 0 to N_z (the number of vertical grid points). The fully explicit second-order accurate Adams-Bashforth scheme is used for time advancement. Aliasing errors can be detrimental to the accuracy of the SGS parameterization since they affect the smallest resolved scales used to compute the dynamic Smagorinsky coefficient (see below). To overcome this problem, the 3/2 rule [Orszag, 1970] is used to fully dealias the convective terms and the SGS terms. More details about the code can be found in Albertson and Parlange [12-13] and Porté-Agel *et al.* [3])

EDDY-VISCOSITY SGS MODEL

The past 15 years have brought considerable improvement in SGS modeling and increased the understanding of SGS physics. The first SGS model used for LES is the Smagorinsky model [4]; it uses the eddy-viscosity model and the mixing length approach to express the SGS flux as a function of the resolved strain rate tensor $\tilde{S}_{ij} = 0.5(\partial_j \tilde{u}_i + \partial_i \tilde{u}_j)$ using

$$\tau_{ij}^{smag} = -2\nu_T \tilde{S}_{ij} = -2(c_{s,\Delta}\,\Delta)^2 \left|\tilde{S}_{ij}\right| \tilde{S}_{ij}, \qquad (3)$$

where Δ is the grid width and ν_T is the eddy viscosity. The only unknown in the above expression is the Smagorinsky coefficient $c_{s,\Delta}$. The model postulates that the SGS stress and strain-rate tensors are aligned (eigenvector alignment) and can be related through the eddy viscosity. This assumption is almost never accurate because the scale separation allowing a linear relation between stress and strain-rate for molecular viscosity does not hold for turbulent eddy viscosity [9]. Experimental studies [14-15] confirm that the SGS stress and strain rate tensors indeed are not aligned in turbulent flows.

If the further assumption that the filter scale Δ is contained well inside an ideal inertial range of locally isotropic and homogeneous turbulence is made, $c_{s,\Delta}$ is expected to have a constant average that was estimated by Lilly to be about 0.17 [5].

However, in most flows of practical interest, Δ does not fall inside a range of inertial, isotropic and homogeneous turbulence. Most importantly for wall-bounded flows, the Smagorinsky model fails when the grid-scale approaches the limits of the inertial range, such as in the vicinity of solid boundaries. It is precisely in such areas that sub-grid scale fluxes contribute a significant share of the total fluxes and where an accurate model is needed. The Smagorinsky coefficient has to decrease close to the surface. To replicate this reduction in c_s in the vicinity of walls, a wall damping function was proposed by Mason and Thompson [16] where the SGS mixing length $\lambda = c_s\Delta$ is decreased close to the surface to merge smoothly with the expected $\lambda \sim z$ behavior. The damping function used is

$$\frac{1}{\lambda^n} = \frac{1}{\lambda_0^n} + \frac{1}{\left[\kappa(z+z_o)\right]^n}, \qquad (4)$$

where κ is the von-Karman constant (=0.4) and $\lambda_0 = c_{s,0}\Delta$ is the mixing length away from the wall (in a region of homogeneous isotropic turbulence). In this study, $c_{s,0}$ is taken

as 0.16 and a value of 2 is assigned to n, which fixes the damping function shape. An alternative value of 1 was tested for n; this did not change the results of the model presented later in the paper. Despite the use of this wall-damping function, the Smagorinsky–Lilly model remains overdissipative [16].

The shortcomings of the traditional Smagorinsky model with the Lilly coefficient prompted the development of other eddy-viscosity type models using Smagorinsky coefficients specifically adapted for the application at hand. However, the eddy viscosity of the model is always constrained to be positive, i.e. the model is purely dissipative and energy always flows from the resolved to the SGS scales. In practice, allowing a negative eddy viscosity might yield negative overall diffusion (it certainly will in codes that neglect molecular diffusion like the code used in this study to simulate very high-Reynold number flows). Negative overall diffusion is numerically destabilizing to many time-advancement schemes; therefore, energy backscatter (flow of kinetic energy from small to large scales) cannot be included in the model by allowing negative c_s values. Several approaches to include backscatter through different mechanisms, random force for example, have been developed [16-19].

Despite these shortcomings, eddy-viscosity models are widely used and can yield good results. This good performance can be attributed to the success of the eddy-viscosity model in reproducing the correct average SGS energy dissipation if an appropriate value of c_s is used. SGS energy dissipation remains the most important function of the SGS model in well resolved turbulence simulations [9, 20].

THE DYNAMIC MODEL

The dynamic model proposed by Germano *et al.* [1] was arguably one of the most significant improvements in SGS modeling. The approach consists of using the smallest resolved scales to 'measure' the model coefficient during the simulation. The model is based on a relation between SGS stresses at different scales expressed by the following identity

$$L_{ij} = T_{ij} - \hat{\sigma}_{ij} = \widehat{\widetilde{u}_i \widetilde{u}_j} - \hat{\widetilde{u}}_i \hat{\widetilde{u}}_j , \qquad (5)$$

where the caret (^) denotes filtering at a test filter scale $\alpha\Delta$ (α=2 in this sturdy). T_{ij} is the SGS stress at the scale $\alpha\Delta$ and L_{ij} is the SGS stress defined from scales intermediate between Δ and $\alpha\Delta$. L_{ij} is the resolved stress tensor and can be computed exactly from the resolved velocity field (Eq. (5)). Using the Smagorinsky model to express the deviatoric parts of SGS stresses at the scale Δ and $\alpha\Delta$ and assuming that the c_s coefficient does not fluctuate strongly in space to justify extracting it from the test-filtering operation [2, 21] results in the following expressions

$$\hat{\tau}_{ij} = -2c_{s,\Delta}^2 \Delta^2 \widehat{|\widetilde{S}|\widetilde{S}_{ij}}, \qquad T_{ij}^D = -2c_{s,\alpha\Delta}^2 (\alpha\Delta)^2 |\hat{\widetilde{S}}|\hat{\widetilde{S}}_{ij} . \qquad (6)$$

The superscript ^{D} denotes the trace free part of the tensor. Replacing in Eq. (5) yields an error induced by the use of the Smagorinsky model. This error is

$$e_{ij} = L_{ij}^D - (T_{ij}^D - \hat{\tau}_{ij}) = L_{ij}^D - c_{s,\Delta}^2 M_{ij} , \qquad (7)$$

where $M_{ij} = 2\Delta^2 \left[\widehat{|\widetilde{S}|\widetilde{S}_{ij}} - \alpha^2 \beta |\hat{\widetilde{S}}|\hat{\widetilde{S}}_{ij} \right]$ and $\beta = c_{s,\alpha\Delta}^2 / c_{s,\Delta}^2$ is a scaling factor for c_s. Usually, the use of this model makes the assumption of scale-invariance in the Smagorinsky coefficient, i.e. $c_{s,\Delta} = c_{s,\alpha\Delta}$ or $\beta = 1$ [9], by applying the coefficient measured from the resolved scales to the subgrid-scale range.

To obtain the optimal value of c_s, an error minimization approach is used. However, Eq. (7) expanded over all terms is in fact an overdetermined system of 5 equations with only one unknown. The original work [1] contracted Eq. (7) with $\tilde{S}_{ij}$ to compute a single value for c_s, thus making the error orthogonal to the strain rate tensor. A more widely used approach, proposed by Lilly [22], consists of minimizing the error in a least square sense; this was shown to give a better conditioned system where the error is orthogonal to M_{ij}.

This local determination of c_s yields a highly variable coefficient that is numerically unstable mainly due to a high frequency of negative values. Ghosal [21] showed that averaging over homogeneous spatial directions yields a system that is consistent with the extraction of c_s from the filter operation and that is equivalent to Lilly's expression averaged over homogeneous directions.

$$c_{s,\Delta}^2 = \frac{\langle L_{ij} M_{ij} \rangle}{\langle M_{ij} M_{ij} \rangle} \qquad (8)$$

Note that the contraction of L_{ij} with M_{ij} eliminates the need to distinguish between L_{ij} and L_{ij}^D, since M_{ij} is a deviatoric (traceless) tensor in incompressible flows.

THE LAGRANGIAN SGS MODEL

The requirement for homogeneous directions in the flow field limits the use of the dynamic model to flows with at least one homogeneous direction excluding many practical flows. Local formulations of the model have been developed [21, 23]. Nevertheless, the models impose a poorly justifiable constraint forcing c_s to remain positive or relax that constraint by allowing backscatter and solving the SGS kinetic energy. Moreover, it is not obvious that the eddy-viscosity analogy would hold in a local sense. Some averaging is needed to recover the statistical basis of the eddy-viscosity model [2, 9].

An alternative approach, combining features from the local and averaged formulations, was developed by Meneveau *et al.* [2]. The model averages the coefficient in time following fluid pathlines and hence is called the Lagrangian model. The Lagrangian averaging recovers the statistical basis that supports the use of an eddy-diffusion model. Furthermore, the averaging is physically justifiable since turbulent eddies with

sizes about the grid scale are likely to be convected along fluid pathlines. Meneveau and Lund [24] also showed that energy cascade is most apparent when viewed in a Lagrangian frame of reference. The model is very well suited for the applications with heterogeneous spatial conditions since it preserves local variability, preserves Galilean invariance, and does not require homogeneous directions.

In the Lagrangian SGS model, the coefficient c_s is obtained by minimizing the weighted time average of the squared local error (Eq. (7)) over pathlines; this weighted time average can be written as

$$E = \int_{-\infty}^{t} e_{ij}(\boldsymbol{z}(t'),t')\, e_{ij}(\boldsymbol{z}(t'),t')\, W(t-t')dt' \ . \tag{9}$$

where $\boldsymbol{z}(t')$ are the previous positions of the fluid elements. Setting the variation of E with respect to $c^2_{s,\Delta}$ to zero,

$$\frac{\partial E}{\partial c_s^2} = \int_{-\infty}^{t} 2e_{ij}\, \frac{\partial e_{ij}}{\partial c_s^2} W(t-t')dt' = 0 \ , \tag{10}$$

results in the following expression for $c^2_{s,\Delta}$:

$$c^2_{s,\Delta} = \frac{\mathcal{J}_{LM}}{\mathcal{J}_{MM}} \tag{11}$$

where

$$\mathcal{J}_{LM} = \int_{-\infty}^{t} L_{ij}M_{ij}(\boldsymbol{z}(t'),t')W(t-t')dt', \tag{12}$$

$$\mathcal{J}_{MM} = \int_{-\infty}^{t} M_{ij}M_{ij}(\boldsymbol{z}(t'),t')W(t-t')dt', \tag{13}$$

and $W(t)$ is a relaxation function that allocates a higher weight to the recent history of the coefficients. A choice of an exponential form, $W(t-t')=(1/T)e^{-(t-t')/T}$, allows replacing cumbersome evaluations of backward time integrals with forward relaxation-transport equations. Based on DNS results and dimensional self-consistency [2], the time scale T is chosen as $T=1.5\Delta(\mathcal{J}_{LM}\mathcal{J}_{MM})^{-1/8}$. This choice of the time scale offers the practical advantage of allocating less weight to recent history (i.e. increasing the model's memory) if the current values of L_{ij} and M_{ij} are driving the equations toward small c_s. The time scale is effectively infinite if $\mathcal{J}_{LM}$ is negative thus preventing negative values of c_s . The relaxation transport equations thus obtained for $\mathcal{J}_{\mathrm{LM}}$ and $\mathcal{J}_{\mathrm{MM}}$ are

$$\frac{\mathrm{D}\mathcal{J}_{LM}}{Dt} = \frac{\partial \mathcal{J}_{LM}}{\partial t} + \tilde{\boldsymbol{u}}\cdot\nabla\mathcal{J}_{LM} = \frac{1}{T}(L_{ij}M_{ij} - \mathcal{J}_{LM}) \tag{14}$$

$$\frac{\mathrm{D}\mathcal{J}_{MM}}{Dt} = \frac{\partial \mathcal{J}_{MM}}{\partial t} + \tilde{\boldsymbol{u}}\cdot\nabla\mathcal{J}_{MM} = \frac{1}{T}(M_{ij}M_{ij} - \mathcal{J}_{MM}) \tag{15}$$

Using first-order numerical approximations in space and time, these equations can be discretized and included in the numerical LES model. The resultant formulation is very simple and numerically efficient

$$\left.\begin{aligned}
&\mathcal{J}^{n+1}_{MM}(\boldsymbol{x}) = \varepsilon\,[M_{ij}M_{ij}]^{n+1}(\boldsymbol{x}) + (1-\varepsilon)\mathcal{J}^{n}_{MM}(\boldsymbol{x}-\tilde{\boldsymbol{u}}^{n}\Delta t),\\
&\mathcal{J}^{n+1}_{LM}(\boldsymbol{x}) = \mathrm{H}\left\{\varepsilon\,[L_{ij}M_{ij}]^{n+1}(\boldsymbol{x}) + (1-\varepsilon)\mathcal{J}^{n}_{LM}(\boldsymbol{x}-\tilde{\boldsymbol{u}}^{n}\Delta t)\right\},\\
&\text{where}\quad \varepsilon = \frac{\Delta t/T^n}{1+\Delta t/T^n}, \qquad T^n = 1.5\Delta(\mathcal{J}^{n}_{LM}\mathcal{J}^{n}_{MM})^{-1/8},\\
&\text{and,}\quad \mathrm{H}\{\mathrm{x}\} = \text{ramp function} = \begin{cases} x & \text{if} \quad x \ge 0\\ 0 & \text{otherwise.}\end{cases}
\end{aligned}\right| \tag{16}$$

Δt is the time step. The ramp function is needed to ensure that numerical inaccuracies (mainly due to the discretization of the equations) do not yield a slightly negative c_s despite the choice of the time scale to avoid such occurrences. Periodic boundary conditions for $\mathcal{J}_{LM}$ and $\mathcal{J}_{MM}$ are used in the horizontal directions. At the lower and upper boundaries, zero-gradient (homogeneous Neumann) boundary conditions are imposed, i.e., the values at the boundary are set equal to the values at the closest node inside the domain.

A SCALE-DEPENDENT FORMULATION

As previously discussed, the traditional applications of the dynamic model assumed scale-invariance near the grid-filter scale Δ, i.e. $c_{s,\Delta} = c_{s,2\Delta}$ or $\beta = 1$. However, scale-invariance does not always hold. Examples of flows where scale invariance breaks down include: high Reynolds number flows with solid boundaries [3], finely resolved LES [25], shear flows [26, 27], and stably stratified flows [27, 28].

To account for scale effects, two well-posed and practical approaches exist. If prior knowledge of the scale effect is available, the coefficient β could be prescribed a-priori. This is a semi-dynamic approach; however, note that the scale-invariant formulation imposes β equals to 1 and is equally not a fully dynamic approach. The other option is to implement a fully dynamic formulation where the scaling coefficient β is measured. The latter approach has been successfully implemented for atmospheric boundary-layer (ABL) flows by Porté-Agel *et al.* [3]. A power-law behavior was assumed for the scale dependence of c_s: $c_{s,\Delta} \sim \Delta^{\Phi}$ or $c_{s,2\Delta} \sim 2^{\Phi}\Delta^{\Phi} = \beta\Delta^{\Phi}$. This is a much weaker assumption than the scale-invariance assumption which corresponds to $\Phi=0$ or $\beta=1$. The coefficient β itself was measured dynamically through an additional filtering operation at a scale 4Δ. Porté-Agel *et al*. [3] also showed that the use of the scale-dependent dynamic model for simple LES of a neutrally stable ABL gives substantial improvements over both the traditional Smagorinsky model with wall-damping functions and the scale-invariant dynamic model. In this work, the semi-dynamic approach is used instead and β is prescribed a-priori as a function of z/Δ (where z is the distance to the wall and Δ is the filter size) using the fully dynamic simulations of Porté-Agel *et al*. [3]. Neutral ABL simulations in that work are effectively simulations of a channel flow over a rough wall. Fig. 1 depicts the smooth fit describing the already computed dependence of β upon z/Δ.

An approach that allows a dynamic computation of β in SGS models with Lagrangian averaging is currently under development. The problem with using the approach presented in Porté-Agel et al. [2000] is that the Lagrangian model uses a weaker averaging than the planar averaged model which could result in significant oscillations in β and c_s.

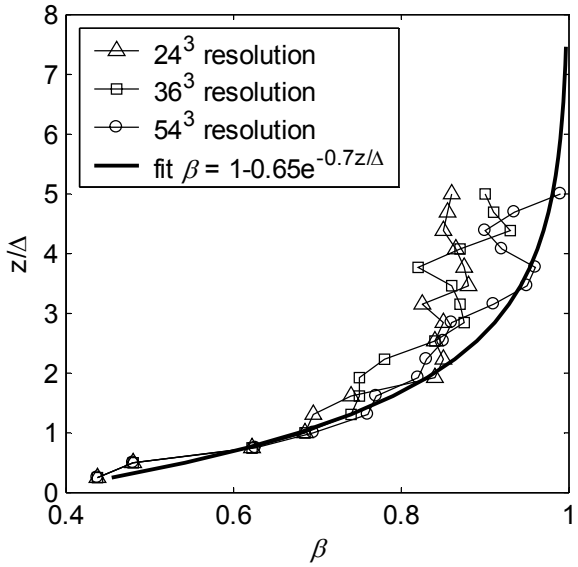

Figure 1. Scaling factor *β*, from Porté-Agel *et al.* [3] and the fit used in this work to impose *β*.

SIMULATIONS

In order to investigate the sensitivity of LES simulations to different SGS formulations, simulations were run with different SGS models and with homogeneous and heterogeneous surface conditions. Fig. 2 presents the main parameters used in the simulations and depicts the simulation domain for the heterogeneous surface case where the wall consists of 2 patches of different roughness.

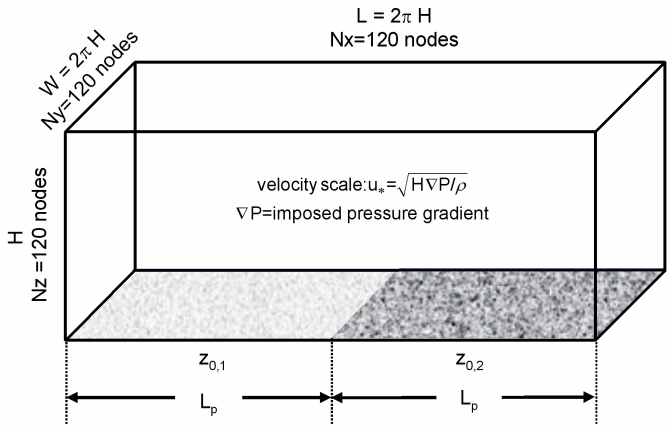

Figure 2. Simulation domain, the 2-patches case.

The homogeneous surface simulations used a wall roughness height of 10^{-5}H while the two consecutive patches had roughness heights of 0.25×10^{-5}H and 2.5×10^{-5}H. The equivalent roughness of the 2-patch configuration is very close to roughness of the homogeneous surface [29].

The boundary conditions in the horizontal directions are periodic. Hence, the flow that exits at the downstream boundary of the domain is fed back at the upstream boundary. This implies that the domain simulated actually is an infinite surface (or an infinite number of alternating patches) in the stream-wise direction (x). Similarly, the periodic boundary conditions in the cross-stream direction imply that the domain is of infinite width in the cross-stream direction (y). The transition between patches is abrupt. A stress free condition is imposed at the top of the domain by setting

$$\partial_3 \tilde{u}_{1,2} = \tilde{u}_3 = 0\,, \tag{17}$$

where 1, 2, and 3 (or x, y, z in other parts of the paper) refer to the stream-wise, cross-stream and vertical direction, respectively. At the bottom of the domain, the vertical velocity is set to 0 at the surface. As a consequence of the staggered grid formulation, no boundary conditions are needed for the horizontal velocities since they are only stored at *dz/2* above the surface. Stresses at the surface are imposed through a local law-of-the-wall formulation ([6]; see Piomelli and Balaras [30] for a review of wall-modeling in LES and Bou-Zeid *et al.* [29] for the details of the wall-model used in this study). However, velocities filtered at twice the grid scale are used to compute the surface stress; this is needed to ensure that the average of the imposed wall stress is not erroneously high due to the local formulation. This is done using

$$\tau_w(x,y) = -\left[\frac{\kappa}{\ln(z/z_o)}\right]^2 \left(\left[\hat{\tilde{u}}(x,y,dz/2)\right]^2 + \left[\hat{\tilde{v}}(x,y,dz/2)\right]^2\right). \tag{18}$$

Subsequently, the stress is partitioned into its stream-wise and cross-stream components in the usual manner,

$$\tau_{i,3}^{wall}(x,y) = \tau_w \left[\frac{\hat{\tilde{u}}_i(x,y,dz/2)}{\sqrt{\hat{\tilde{u}}_1^{\,2} + \hat{\tilde{u}}_2^{\,2}}}\right], \qquad i = 1,2\,. \tag{19}$$

The planar-averaged model is given by Eq. (8). β is set to 1 throughout the domain for the scale-invariant version (PASI) while for the scale-dependent version (PASD), β is imposed from Fig. 1. A problem was detected with the planar-averaged SGS models close to the top boundary. The stress free boundary condition imposed at that boundary is not very realistic and is not expected to yield physical flow patterns. This was causing large negative values of the dynamically computed numerator of Eq. (8) at some points. When averaged over the plane, the resulting c_s was either very small or negative. This was not dissipating enough energy causing the flow velocity to increase incorrectly; the disturbance was propagating into the flow field. To remedy this problem, the negative values of $L_{ij}M_{ij}$ were clipped to zero before averaging

for the computation of c_s; this was only done at the topmost plane. For all other planes, the usual approach for the planar averaged model was used, i.e. $L_{ij}M_{ij}$ was plane averaged and the resulting c_s, if negative, was then clipped to zero. The Lagrangian model is given by Eq. (16). For the scale-invariant model β is set to 1 while for the scale-dependent formulation β is imposed from Porté-Agel *et al.* [3] as illustrated in Fig. 1.

SMAGORISNKY COEFFICIENT PROFILES

The c_s coefficients computed by different models (or imposed for the SMAG model) for the homogeneous surface simulations were compared (Fig. 3). Close to the surface, all the dynamic formulations predict a lower value for c_s than the one imposed by the Mason-Thompson formulation. The planar averaged formulation predicts higher c_s than the equivalent Lagrangian formulation. However, when the Lagrangian model is allowed to be scale dependent, the computed c_s is increased. In the middle of the domain, the planar averaged c_s is lower than the Lagrangian c_s and the scale-dependence clearly increases the value of c_s throughout the domain.

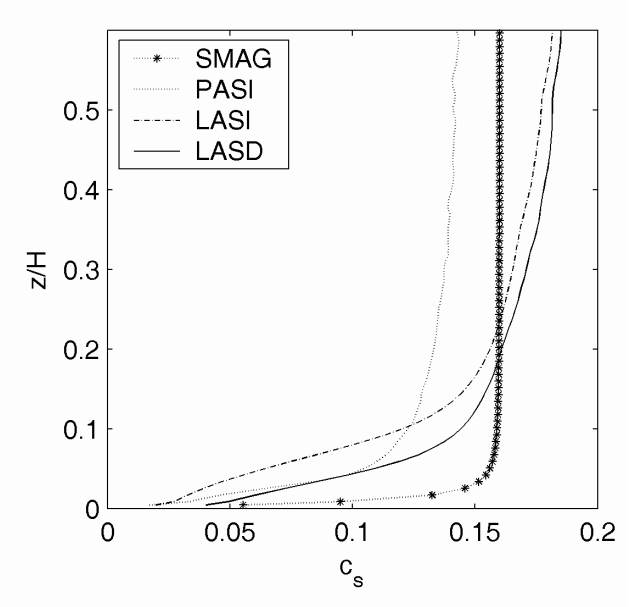

Figure 3. Profiles of the Smagorinsky coefficient computed (imposed for the SMAG model) for the different SGS models

VELOCITY PROFILES AND LOG LAW PREDICTION

For the homogeneous surface simulations, the velocity profile is expected to be logarithmic close to the surface. This can be checked by plotting the non dimensional streamwise velocity gradient $(\kappa z/u)\partial u/\partial z$; the value has to be about 1 near the surface, increasing further up. Fig. 4 depicts $(\kappa z/u)\partial u/\partial z$ obtained using the different SGS models. The Smagorinsky model results in a high gradient near the wall. This is in agreement with the previous findings [3, 16] suggesting that the model overdissipates energy close to solid boundaries. The two scale-invariant formulations (PASI and LASI) both produce a low value of the velocity gradient suggesting that the dissipation produced by these SGS models is insufficient. On the other hand, the scale-dependent formulation yields a value of $(\kappa z/u)\partial u/\partial z$ very close to 1 near the surface suggesting that it is dissipating energy at the correct rate and hence reproducing the log-law region successfully.

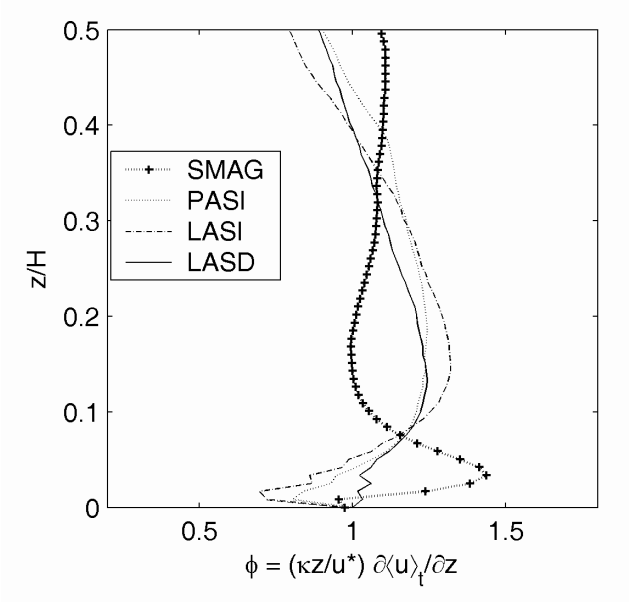

Figure 4. Profiles of the non-dimensional velocity gradients

VELOCITY SPECTRA

Reproducing the log-law region is intrinsically linked to the ability of the SGS model to provide the correct dissipation rate. However, a more complete insight to the energy dissipation characteristics of the SGS closure can be obtained by examining the streamwise velocity spectra. In the inertial subrange ($k_1 z>1$), the effects of viscosity, boundary conditions, and large scale structures are not important and the turbulence is essentially isotropic. The energy cascade in this subrange follows the Kolmogorov spectrum yielding a slope of -5/3. In the production range ($k_1 z <1$), energy cascade is affected by the flow configuration. In wall-bounded flows with neutral stability, the energy spectrum in the production range has often been shown to follow a slope of -1 from scaling arguments and experimental results [31, 32]. Fig. 5 depicts the *u* spectra produced by the different SGS models in the homogeneous surface simulations. The conclusions are similar to what was discussed for the log-law prediction. With the Smagorinsky model, too much energy is dissipated and the spectra lines decay too fast at high wavenumbers. The Lagrangian scale-invariant and the plane-averaged scale-invariant formulations give spectra that are too flat indicating insufficient energy dissipation and a buildup of energy at the

smallest resolved scales. The spectra for the SMAG, LASI, and PASI models are most obviously in error close to the wall, where the assumption of isotropic homogeneous turbulence and the assumption of scale-invariance are clearly violated. The spectra obtained with the scale-dependent Lagrangian model follow the -1 and -5/3 slopes well in the two ranges. This confirms that a dynamic scale-dependent formulation for LES is important in the vicinity of walls.

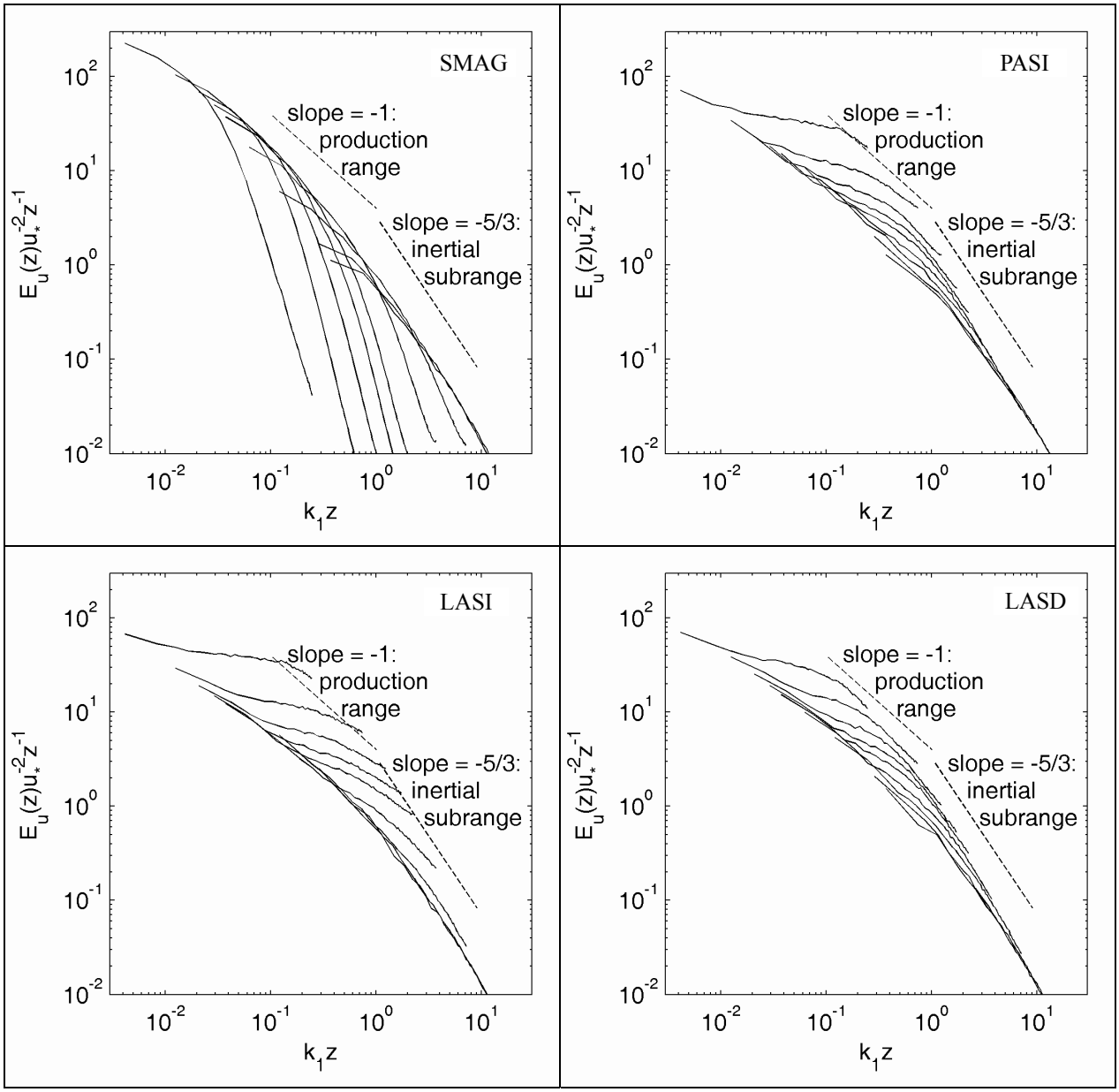

Figure 5. Streamwise velocity spectra versus k_1z; k_1 is the stream-wise wave number and z is the height. The lines represent the data at heights z/H of 0.0042, 0.0126, 0.0210, 0.0294, 0.0378, 0.0630, 0.122, 0.290, or 0.374.

THE EFFECT OF LOCAL COEFFICIENT DETERMINATION

The previous discussion focused mainly on the homogeneous surface simulations and compared the dissipation characteristic of the SGS models. It was clear that the scale-dependent approach yields better results than the ad-hoc Smagorinsky or the scale-invariant formulations. Nevertheless, the fully dynamic version used in Porté-Agel *et al.* [3] and the planar-averaged scale-dependent (PASD) model tested here generate dissipation characteristics similar to the

Lagrangian scale-dependent (LASD) formulation. Hence the advantages of using a Lagrangian model have not yet been established.

A local model is really needed when homogeneous directions are not available for averaging. In the simulations over heterogeneous walls presented here, averaging over horizontal planes is possible; however, the x-direction is not homogeneous and hence the variability of the coefficient in that direction would be suppressed by planar averaging. The failure to account for c_s variability might be significant in wall bounded flows mainly because the wall layer controls many features of the outer flow. It certainly would be problematic in studies that specifically consider surface heterogeneity effects (e.g. Bou-Zeid *et al.,* [29]).

More importantly, in many practical flows with complex geometries, no spatial averaging of the coefficient is feasibly at all. In such complex flows, a local SGS model is indispensable. The Lagrangian model has been used (in a scale-invariant formulation) for LES of complex geometry flows in internal combustion engines [33], flow over wavy walls [34], flow of impinging jets [35], and flow in thrust-reversers [36].

In flows where some spatial averaging is possible if variability in the coefficient is ignored, the question remains whether the variability is great enough to justify the extra cost of the Lagrangian averaging. Moreover, one should consider whether the variability actually affects relevant parameters such as fluid velocities and stresses. These two questions are addressed here.

COEFFICIENT VARIABILITY

In Fig. 6, the value of c_s averaged in the cross-stream direction is plotted versus x and z for the 2-patch simulation with the LASD model. The coefficient is divided by its average over horizontal planes to remove the effect of vertical variations and detect the sensitivity to horizontal variations. The value of the coefficient varies by up to 50 percent between the high-roughness and low-roughness patches near the ground and the effect of surface heterogeneity extends well into the lowest 5 percent of the domain. This very high variability is caused by a change of one order of magnitude in the surface roughness.

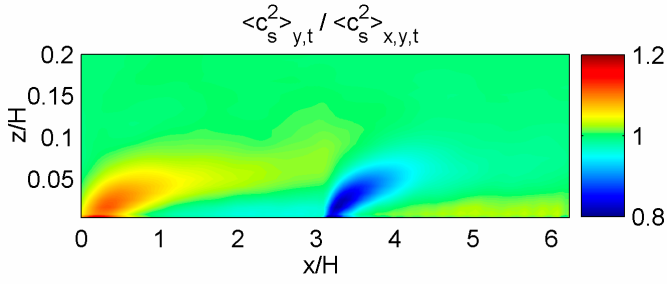

Figure 6. Sensitivity of the c_s coefficient to surface roughness for the LASD model

EFFECT OF COEFFICIENT VARIABILITY ON FLOW VELOCITIES AND STRESSES

Fig. 7 presents the ratio of the LASD streamwise velocity over the PASD streamwise velocity at the plane closest to the surface (z/H = 0.0042). The maximum difference between the two models is about 4 percent and occurs close to the roughness change. More significant is the difference between the predicted SGS stresses. The ratio of the SGS stress predicted by the LASD model over the SGS stress predicted by the PASD model is also depicted in Fig. 7 (for z/H = dz = 0.0084, the first grid node where the SGS model is used to compute the stress). The difference can reach up to 32 percent. These results indicate that the variability in the Smagorinsky coefficient has a strong influence on velocities and stresses predicted in the model, thus suggesting that a local model should be used where the flow physics will result in strong variations in the Smagorinsky coefficient.

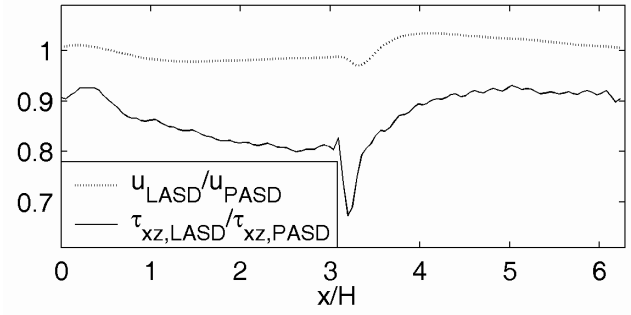

Figure 7. Ratios of the streamwise velocity at z/H = 0.0042 and the SGS stress at z/H = 0.0084 predicted by the LASD and PASD models.

COMPUTATIONAL COST COMPARISON

With the advent of more sophisticated SGS models, the computational cost and complexity of LES is significantly increasing [8]. If the cost of implementing and testing an SGS model are set aside, models should be compared based on equal CPU times. For example, results from a model that increases the overall computational cost by 50 percent over the Smagorinsky model should be compared to results obtained with the Smagorisnky model run at $1.5^{1/4}$ times the resolution. The ¼ factor accounts for the increased resolution in 3 directions and the reduced time step based on the Courant-Friedrich-Lévy (CFL) stability condition. Noting that $1.5^{1/4}$ is roughly 1.1, it is often true that the improvements obtained by using better SGS models are greater than improvements obtained by increasing resolution. However, an a priori evaluation is often valuable to assess whether a better SGS model is worthwhile for a given application.

In this study, the maximum increase in overall computational cost over the simple Smagorinsky is 11 percent, equivalent to an increase in resolution of 2.75 percent. This comparison is based on the total CPU time required by the LES code when it is run with different SGS model. Noting the high base-resolution used (120^3), increasing the resolution of

the Smagorinsky simulation by 2.75 percent was deemed unnecessary. Therefore, all the SGS models were run at the same resolution and their computational cost (in CPU time) was compared. For dynamic simulations, the dynamic Smagorinsky coefficient computations can be performed every time-step; alternatively, c_s could be update less frequently. Porté-Agel *et al.* [3] updated the dynamic coefficient every 10 time-steps without any effect on the results. With the Lagrangian model, the coefficient needs to be update more frequently. Hence, the Lagrangian c_s computations were performed every 5th time step. Results were compared with a test run where the coefficient is updated every single time-step to ensure results are insensitive to the update frequency; no significant differences in the results were detected.

Fig. 8 shows a comparison of the computational cost (CPU time) normalized so that the Smagorinsky model cost is 1 unit. If the coefficient is to be update every time step the plane averaged dynamic model cost exceeds the cost of the Smagorinsky model by 28 percent. The Lagrangian model includes all the computations of the dynamic coefficient (very similar to the plane-averaged dynamic); in addition, the relaxation transport equations (Eqs. 16) have to be advanced in time requiring additional computational resources. The Lagrangian model updated every single time step increases the computational cost by 58 percent over the simple Smagorinsky. When the coefficient is updated every 5th time step, the additional costs are reduced to 5 percent and 12 percent for the plane-averaged and Lagrangian model, respectively.

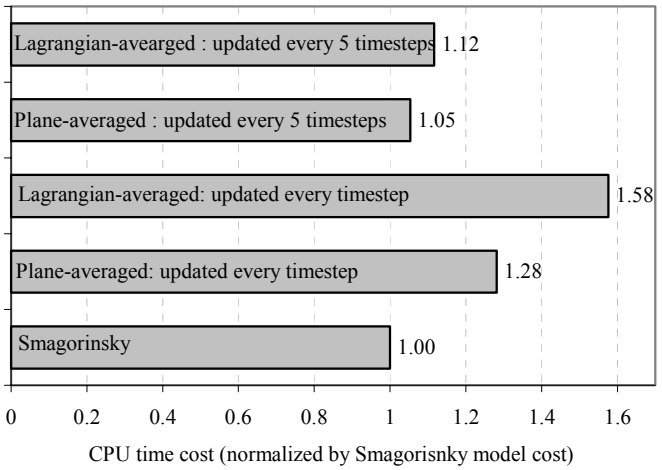

Figure 8. Total computational cost of the LES code run with the different SGS models, normalized by the cost of the code with the Smagorinsky model

CONCLUSION

Several eddy-viscosity SGS formulations have been tested in high-Reynolds number, non-wall resolving, LES of turbulent flow over rough walls. The classic Smagorinsky model with imposed c_s was found to be overdissipative close to the solid boundary. The dynamic model with planar-averaging and Lagrangian-averaging was under-dissipative close to the solid boundary, mainly due to the erroneous assumption of scale similarity for the coefficient c_s in the near-wall region where the grid scale Δ tends to the integral scale. A scale-dependent version of the dynamic model was found to give better dissipation characteristics hence reproducing the log-law region more successfully.

The sensitivity of the c_s coefficient to the wall roughness was assessed. High variability in the coefficient was detected in the near-wall region. The coefficient varied by up to 50 percent between the low-roughness and high roughness regions. The effect of this variability on the velocities produced by the LES was about 4 percent close to the wall. The effect on the SGS stress in that region was much higher reaching up to 32 percent. This suggests that a local SGS formulation is essential in complex flows. Spatial averaging of c_s can only be performed over truly homogeneous directions. Finally, the additional computational cost associated with this improved Lagrangian dynamic scale-dependent SGS model was found to be on the order of 10 percent (compared to the simple Smagorinsky model) when the c_s coefficient is updated every 5th time step. This is a very modest increase that is justifiable in view of the significant improvements in the results.

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