A Priori and A Posteriori Evaluations of Subgrid Stress Models with the Burgers’ Equation

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In large eddy simulations (LES) of turbulent flow, large scale motions are resolved by the numerical simulation while the impact of the small scale motions is represented as subgrid stresses (SGS), which are computed with SGS models. In the present study, we performed a priori and a posteriori evaluations of five SGS models for the one dimensional Burgers’ equation discretized with the correction procedure via reconstruction method (CPR). The evaluation compares the modeled SGS with the true SGS computed from the direct numerical simulation (DNS) in both a priori and a posteriori tests. Solutions computed from different models including implicit LES (ILES) are also compared with the filtered DNS solution. The scale similarity model (SSM) showed good performance after a long term simulation. We are investigating why. In addition, we conducted two real-world three dimensional simulations, the decaying isotropic turbulence with the Taylor micro-scale Reynolds number $Re_{\lambda} \approx 25$ and the turbulent channel flow with a Reynolds number of 5,930. LES instantaneous and statistical results were compared with the DNS results. The 1D and 3D studies appear to show that none of the SGS models, except the SSM, demonstrated any definite advantage over the ILES approach, in which the numerical dissipation serves as the stabilizing mechanism in the context of the CPR approach.

Nomenclature

\[\begin{align*}
u & = \text{the state variable} \\
\nu & = \text{molecular viscosity} \\
\tau_{SGS} & = \text{subgrid stress} \\
G & = \text{filter kernel} \\
\Delta x & = \text{cell size} \\
F & = \text{filter width} \\
\nu_{SGS} & = \text{subgrid viscosity} \\
S_{ij} & = \text{rate of strain} \\
c_s & = \text{the Smagorinsky model coefficient} \\
c_{ssm} & = \text{the scale-similarity model coefficient} \\
T_{ij} & = \text{Germano identity} \\
L_{ij} & = \text{resolved stress} \\
\Delta & = \text{LES filter width} \\
\tilde{\Delta} & = \text{test filter width} \\
\gamma & = \text{ratio of the test filter width over the LES filter} \\
\alpha & = \text{lifting coefficient} \\
C & = \text{LES cell size}
\end{align*}\]

I. Introduction

Large eddy simulations (LES) have been used substantially for the computation of turbulent flows in recent decades. As a comparison, the Reynolds-averaged Navier-Stokes (RANS) methods model all scales of turbulence impacts, while the direct numerical simulation (DNS) methods resolve all scales of turbulent fluid dynamics. Although RANS models have been effective for many problems, they cannot handle complex massively

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separated unsteady flows. The usage of DNS in computing high Reynolds number flow is also, for the foreseeable future, limited by computing power [1]. LES is a compromise of the two approaches, and offers the best promise for vortex dominated separated flows. In LES, large scales and small scales are separated by low-pass filters. Conventionally, the large scale motions are resolved while the impact of small scale motions is represented by an explicit subgrid stress (SGS) model. As a result, vortex structures are visible and some separated flows are handled well while the required computer resource is far less demanding than DNS [2].

Many different SGS models have been developed in last three decades. This paper focuses on five of them: the static Smagorinsky model (SS) [3, 4], the dynamic Smagorinsky model (DS) [5], the scale-similar model (SSM) [10], the mixed model [25], and the linear unified RANS-LES model (LUM) [34]. Among explicit models, the Smagorinsky model is the most popular. The effects of SGS upon the resolved scales are modeled as an eddy viscosity. The eddy viscosity is expressed in the mixing length form with a dimensionless empirical coefficient. However, it has been found that the empirical coefficient depends on the flow. It also adds too much dissipation to the large scale motions if we keep the coefficient the same as we approach wall boundaries. To solve these problems, the dynamic Smagorinsky model was developed and is described in [5]. In the dynamic Smagorinsky model, the coefficient is calculated based on the Germano identity, which involves two levels of filtering and relates the resolved stress to the SGS. The coefficient is locally decided and no longer a prescribed constant, and it goes to zero as a wall boundary is approached. The dynamic Smagorinsky model fixes some problems of the Smagorinsky model due to the constant coefficient and has been applied to a large variety of flow simulations [6,7,8,9].

An alternative way to model the SGS is offered by the scale similarity model [10]. As the name indicates, it assumes similarity between two scales of stresses, the resolved stress and the subgrid stress. Numerical tests show that energy accumulates at small scales with this model [11]. To remedy the problem, the Smagorinsky model is added to dissipate the energy, which leads to the mixed model. The coefficient in the Smagorinsky model is also found dynamically.

Recently, hybrid RANS-LES models have become popular. They combine RANS with LES equations so that for the wall-bounded turbulent flows at high Reynolds number, the near wall region is solved by RANS equations while the in the outer region LES equations are used. These models give more reasonable solutions near the wall while permitting the large scale eddies to develop in the LES region and, at the same time, reduce the computational cost when compared to the same level pure LES simulations. The linear unified RANS-LES model (LUM) has been developed and shows promising properties [34]. In the present work, we also evaluate the LUM model.

Because of the disparate length scales in a turbulent flow, high order methods are a good choice to compute the large scale dynamics because of their high accuracy. The correction procedure via reconstruction (CPR) was recently developed in [12], and extended to hybrid meshes in [13]. The CPR formulation is among the most efficient discontinuous methods. Thus in the present work, we employ the CPR method.

Grinstein et al. [14] introduced another approach of large eddy simulation, which is called the implicit large eddy simulation (ILES). In ILES, the numerical algorithm has its numerical dissipation which serves as the subgrid dissipation. No explicit subgrid models are involved at all. The first advantage of ILES is its lower computational cost compared with the conventional LES. However, it is still a mystery whether the SGS effects can be replaced by the numerical dissipation and how well ILES behaves compared with the SGS models.

In order to answer this question, this paper compares the different approaches mentioned above. For the sake of simplicity, different models are tested with the one dimensional Burgers’ equation first, rather than the full Navier Stokes equations. To imitate turbulence, we initialize the simulations following the turbulence energy spectrum in fourier space with random phase angles. The CPR method is used to discretize the Burgers’ equation and the explicit three-stage SSP Runge Kutta scheme for time integration. In DNS, we start the computation directly from the initial condition. In LES, we use the same grid as that in DNS to minimize the numerical truncation error’s impact and start from a filtered initial condition which is filtered by a box filter. Two different filter widths are tested. We evaluate the models behavior on coarse meshes as well to take the numerical dissipation into count. Both the a priori and a posteriori tests were performed for all the five models and ILES.

To test the evaluations in 1D, two canonical three-dimensional turbulence simulations are also presented: the decaying homogeneous isotropic turbulence and the turbulent channel flow. Both static and dynamic Smagorinsky models were implemented in an unstructured three-dimensional CPR solver. A discretized filter developed by Guido Lodato et al. [35] was used as the test filter of the dynamic Smagorinsky model to avoid searching for neighbors to build the stencil. All the results are compared with DNS results.

This paper is organized as follows. In the second section, the governing equation for the one-dimensional Burgers’ equation is given and the subgrid stress models are briefly reviewed and derived for the one dimensional Burgers’ equation. In section 3, the numerical method is briefly reviewed. In Section 4, the one-dimensional results

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are presented and discussed. In Section 5, the three-dimensional cases are presented and discussed. The conclusions are given in Section 6.

II. Governing equation and subgrid models

The governing equations for three dimensional turbulence are the three dimensional Navier-Stokes equations. As a simpler counterpart, we consider the one dimensional Burgers’ equation,

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = \nu \frac{\partial^2 u}{\partial x^2},$$

where $u$ is the state variable such as velocity, $\nu$ is the viscosity.

To derive the LES governing equation, we apply a low-pass spatial filter, $G(x, \xi)$, to Eq (1) to obtain

$$\frac{\partial \hat{u}}{\partial t} + \hat{u} \frac{\partial \hat{u}}{\partial x} = \nu \frac{\partial^2 \hat{u}}{\partial x^2} - \frac{1}{2} \frac{\partial (\frac{1}{2} \hat{u}^2 - \frac{1}{2} \hat{u}^2)}{\partial x}.$$  

The filtering process is defined mathematically in the physical space as a convolution product. The filtered variable $\hat{u}$ of a space-time variable in 1D is defined as

$$\hat{\phi}(x, t) = \int_{-\infty}^{\infty} G(x - \xi) \phi(x, t) d\xi,$$

where $G$ is the convolution kernel and $\int_{-\infty}^{+\infty} G(\xi) d\xi = 1$. The filtering process is linear, i.e. $\hat{\phi} + \phi = \hat{\phi} + \phi$. Normally, we assume $\frac{\partial \hat{\phi}}{\partial x} = \hat{\phi}$. In practice, instead of Eq. (3), we only do the integral on a finite domain,

$$\hat{\phi}(x, t) = \int_{x-\Delta/2}^{x+\Delta/2} G(x - \xi) \phi(x, t) d\xi,$$

where $\Delta$ represents the filter width. The subgrid stress arises due to the filtering of the nonlinear convection term,

$$\tau_{SGS} = \frac{1}{2} \hat{u} \hat{u} - \frac{1}{2} \hat{u} \hat{u},$$

which is the unclosed term in the governing equation.

LES methods use models to replace the impact of the subgrid stress. Many models were developed in recent decades. In this section we review those ideas and translate them to work for the one dimensional Burgers’ equation.

A. Smagorinsky model

The Smagorinsky model in the eddy viscosity form, in three dimensions, for incompressible flow is

$$\tau_{SGS} = -2 \nu_{SGS} \hat{S},$$

where $\hat{S}_{ij}$ is the resolved rate of strain tensor, and

$$\hat{S}_{ij} = \frac{1}{2} \left( \partial_i \hat{u}_j + \partial_j \hat{u}_i \right).$$

And the subgrid viscosity, $\nu_{SGS}$, is modeled following the mixing length form:

$$\nu_{SGS} = (c_s \Delta)^2 \sqrt{2 |\hat{S}|^2},$$

where $|\hat{S}|^2 = \hat{S}_{ij} \hat{S}_{ji}$, $c_s$ is the prescribed coefficient. By comparing the mean SGS dissipation from DNS and the modeled SGS dissipation, $c_s$ can be determined to make those to be equal. Lilly used this procedure for isotropic turbulence to obtain $c_s = 0.16$.

The Smagorinsky model was described by Moin & Kim[15], Rogallo & Moin[16], Lesieur & Metais[17] and Pope[18]. The deficiency of this model first showed up in the comparison of the modeled subgrid stress and the true subgrid stress computed from the DNS solution by Clark et al.[19], McMillan & Ferziger[20], and Bardina et al.[10]. The comparisons imply that the model does not capture the subgrid physics adequately. In [11], Meneveau et al. give an explain of this problem. Another weakness of this model is that it gives non-zero eddy viscosity in laminar-flow regions. Therefore a wall function is needed to damp the SGS viscosity in a wall-bounded flow.

To test the Smagorinsky model for the 1D Burgers’ equation, we adjust the formula. The rate of strain in 1D is

$$\hat{S} = \hat{\partial}_x \hat{u}.$$  

The subgrid viscosity,

$$\nu_{SGS} = (c_s \Delta)^2 |\partial_x \hat{u}|,$$

Eventually the subgrid stress becomes

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\[ \tau^{SGS} = -\nu_{SGS} \hat{S}. \]  

(11)

**B. Dynamic Smagorinsky model**

The coefficient, \( c_s \), in Smagorinsky model is prescribed. However, it is found empirically that \( c_s \) depends on the flow, being 0.1 for plane channel flow and 0.2 for isotropic turbulence [2]. The dynamic Smagorinsky model (DS) makes it a variable spatially and temporally. It introduces a test filter to the resolved scales and uses the assumption of scale invariance to compute the model coefficient. The model is self-sustained and depends on the flow. As the model for three dimensional turbulence is available in many resources, we will not repeat it here but only give the derivation for the 1D Burgers’ equation instead.

Following Eq.(5), consider the filter, \( \tilde{\Delta} \), defined as \( \tilde{\Delta} = \gamma \Delta \). By applying this filter to the subgrid stress, we get

\[ \tilde{\tau}^{SGS} = \frac{1}{2} \tilde{u} \tilde{u} - \frac{1}{2} \tilde{u} \tilde{u}. \]  

(12)

By applying the filter to the LES solution, we get the resolved stress,

\[ L = \frac{1}{2} \tilde{u} \tilde{u} - \frac{1}{2} \tilde{u} \tilde{u}. \]  

(13)

The Germano identity, \( T \), can be written as

\[ T = \tilde{\tau}^{SGS} + L, \]  

(14)

where \( T = \tilde{u} \tilde{u} - \tilde{u} \tilde{u} \). \( T \) is treated as the subgrid stress by the filter, \( \tilde{\Delta} \). We apply the Smagorinsky model to both \( T \) and \( \tau \) and assume they share the same coefficient, \( c_s \), which gives

\[-(c_s \tilde{\Delta})^2 | \frac{\partial \tilde{u}}{\partial x} | \frac{\partial \tilde{u}}{\partial x} - (c_s \Delta)^2 | \frac{\partial \tilde{u}}{\partial x} | \frac{\partial \tilde{u}}{\partial x} + L.\]  

(15)

We define

\[ M = \Delta^2 | \frac{\partial \tilde{u}}{\partial x} | \frac{\partial \tilde{u}}{\partial x} - \Delta^2 | \frac{\partial \tilde{u}}{\partial x} | \frac{\partial \tilde{u}}{\partial x}. \]  

(16)

Thus \( c_s^2 = \frac{L}{M} \). It is assumed that \( c_s \) is spatially uniform so that it can be extracted from under the test-filtering operation (Ghosal et al 1995)[21]. In the 1D test, we follow the most common choice of \( \gamma = 2 \).

In three dimensions, this is an overdetermined system. To minimize the square error, Lilly used the following approach:

\[ c_s^2 = \frac{\langle L_{ij} M_{ij} \rangle}{\langle M_{ij} M_{ij} \rangle} \]  

(17)

The DS gives a highly variable eddy viscosity field [22] including negative values which makes the simulation unstable. Averaging over homogeneous directions was used by Germano et al. [5] to prevent this problem. Ghosal et al. [21] show that this procedure minimizes the total error in the homogeneous region over which the averaging is operated. With these modifications, the eddy viscosity still can be negative. So the value of \( c_s^2 \) is clipped to be non-negative. In 1D, we don’t have these problems. Thus we don’t use a least square averaging operation, but still we set \( c_s^2 \) to be non-negative.

**C. Scale-similarity model**

The scale-similarity model (SSM) was first introduced by Bardina et al. [10]. It assumes the scale invariance of the computable stress \( L \) and the subgrid stress \( \tau^{SGS} \). This comes from an empirical basis from bandpass-filtered PIV measurements by Liu et al. [23]. It suggests that \( \tau^{SGS} \) is similar to a stress constructed from the resolved scales,

\[ \tau^{SGS} = c_{ssm} L \]  

(18)

where \( L \) is the resolved stress, which is the same as that in Eq.(13).

There are many different forms of the SSM. The Bardina’s model uses the same filter width for the two filters, \( \Delta = \tilde{\Delta} \), and \( \gamma = 1 \). Liu et al used \( \gamma = 2 \) and Akhavan et al use \( \gamma = \frac{4}{3} \) [24]. The coefficient \( c_{ssm} \) is empirical and found to be near to 1. In the 1D test, \( c_{ssm} \) is adjusted to 0.25.

The true and modeled stresses show high correlation in Bardina et al’s a priori tests. And the SSM allows for the energy backscatter. However, this model is found to be not sufficiently dissipative with energy accumulating at small scales, thus this model might lead to numerical instability.

**D. Mixed model**

To resolve the problem of the scale-similarity model, the dynamic Smagorinsky model is included in the formulation to add dissipation. In three dimensions,

\[ \tau_{ij}^{SGS} = c_{ssm} L_{ij} - 2\nu_{SGS} \hat{S}_{ij}. \]  

(19)

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Liu et al. show that the magnitude of the similarity term is much higher than that of the dissipative Smagorinsky term. Hence, the high correlation of the SSM is not degraded by the viscosity. Zang et al. used this model for recirculating flows with $\gamma = 1$. Wu & Squires applied this model successfully with Lagrangian averaging in simulations of 3D boundary layers [25]. For $c_{ssem}$, there are dynamic ways to determine it, as well. Vreman et al. proposed a two-parameter dynamic mixed model in which $c_s$ and $c_{ssem}$ are both calculated dynamically with $\gamma = 1$. And Liu et al. analyzed it with $\gamma = 2$.

In one dimension, the values $c_{ssem} = 1$ and $\gamma = 2$ are used. The SGS is defined as

$$\tau = c_{ssem} \left( \frac{1}{2} \frac{d\vec{u}}{dt} - \frac{1}{2} \vec{u} \frac{d\vec{u}}{dt} \right) - \nu_{SGS} \vec{u}.$$

### E. Linear unified RANS-LES model

The wall-bounded turbulent flows at high Reynolds number are a big challenge for LES. The near region requires a high resolution grid to resolve the energetic scales. The linear unified RANS-LES model (LUM) combines RANS with LES to solve this problem. The incompressible formula is

$$\frac{D\vec{U}_i}{Dt} = -\frac{\partial \left( \rho \vec{u}_i \right)}{\partial x} + 2 \frac{\partial (\nu \vec{u}) S_{ik}}{\partial x_k} + \frac{\partial \left( \nu + \nu_t \right) S_{ik}}{\partial x_k}$$

$$\frac{Dk}{Dt} = -\frac{\partial \left( \nu + \nu_t \right) \frac{\partial k}{\partial x_i}}{\partial x_i} + \nu_t S^2 - 2 \frac{(1 - c_0)k}{\tau_L},$$

$$\frac{D\omega}{Dt} = C_{w1} \frac{\omega}{k} \nu_t S^2 - C_{w2} \frac{\omega}{\nu_t} \omega^2 + \frac{\partial \left( \nu + \nu_t \right) \frac{\partial \omega}{\partial x_j}}{\partial x_j} + \frac{C_{w3} \omega}{k} \nu_t \frac{\partial k}{\partial x_j}$$

where $C_{w1}, C_{w2}, C_{w3}, C_k, c_0$ and $\sigma_0$ are all model constants, $\vec{U}_i$ is the filtered velocity, $k$ is the turbulent kinetic energy, $\omega$ is the specific dissipation, $\tau_L$ is the time scale and $\nu_t$ is the modeled viscosity. In this work, we only focus on the LES side of the model. So $\tau_L$ is calculated by $\tau_L = l_s \Delta / k^{\frac{1}{2}}$, where $l_s = 1/3$. To sum up, for the one-dimensional Burgers’ equation, we solve

$$\frac{D\vec{u}}{Dt} = -\frac{\partial (\nu + \nu_t) \frac{\partial \vec{u}}{\partial x}}{\partial x}$$

$$\frac{Dk}{Dt} = -\frac{\partial \left( \nu + \nu_t \right) \frac{\partial k}{\partial x}}{\partial x} + 2 \nu_t \left( \frac{\partial \vec{u}}{\partial x} \right)^2 - 2 \frac{(1 - c_0)k}{\tau_L}$$

where $\nu_t = \frac{k \tau_L}{3}, \tau_L = l_s \Delta / k^{\frac{1}{2}}$.

### III. Numerical method

#### A. Spatial discretization

Huynh [12] developed a high-order CPR formulation, which was later employed for the Navier-Stokes equations on hybrid 3D meshes [26]. It has been used for 1D, 2D and 3D laminar and turbulent flows. Validations and successful applications can be found in [27-33]. In this study, we apply the scheme to the 1D Burgers’ equation and evaluate its performance with the subgrid stress.

The detailed CPR formulation can be found in [13]. The resulting scheme for a hyperbolic equation

$$\frac{\partial \vec{u}}{\partial t} + \nabla \cdot \vec{F}(\vec{u}) = 0,$$

is given as

$$\frac{\partial u_{i,j}}{\partial t} + \Pi_i (\nabla \cdot \vec{F}(u_{i,j})) + \frac{1}{|V_i|} \sum_{f \in \partial V_i} \sum_{l} a_{j,l} \Pi_f [F^n u_{i,j}] = 0,$$

where $u_{i,j}$ is the degree of freedom, $\Pi_i (\nabla \cdot \vec{F}(u_{i,j}))$ denotes the projected derivative of flux on the solution point, $a_{j,l}$ are the lifting constants independent of the solution variables. The last term on the left hand side
of the equation represents the influence of the neighboring cells. In CPR, solution is discontinuous across cell interfaces. \([F^n]_i\) is the difference between the local flux, which is reconstructed based on local cell solution points, and the common flux at the interface. The common flux is calculated using the Godunov flux, which makes the scheme dissipative and stable by itself.

The 1D CPR formulation is

$$\frac{\partial u_{i,j}}{\partial t} + \Pi_j \left( \frac{\partial F(u_i)}{\partial x} \right) + \frac{1}{|\Delta x_i|} \left( \alpha_{R,j}[F^n]_R + \alpha_{L,j}[F^n]_L \right) = 0,$$

where \(\Delta x_i\) is the length of element \(i\), which has two interfaces, the left one and right one, with unit face areas and unit face normals of -1 and 1. For the viscosity term on the right hand side of Burgers’ equation, we take

$$R(x) = \nabla u(x).$$

We apply the CPR scheme on \(\nabla R\), as well by following the so called BR2 approach [38].

B. Grid and spatial filter

The computational domain is \([-1, 1]\). A mesh refinement study indicates that 2560 cells with the 3rd order CPR method is capable of resolving all the scales, which are embedded in the DNS solution. For the LES simulation, first the same grid is used in order to minimize the effects of the numerical truncation error in the solution. However, a filter which is much wider than the cell size, say 16 or 256 times of \(\Delta x\), is applied to the initial condition before the simulations. A coarse mesh in which \(C = 2\) is tested as well to take the truncation error into consideration.

The box filter is used in this study, which means \(G(x - \xi) = \frac{1}{\Delta}\) for any \(\xi \in \left[ x - \frac{\Delta}{2}, x + \frac{\Delta}{2} \right]\). Thus the filtered variable is

$$\phi(x, t) = \int_{x-\Delta/2}^{x+\Delta/2} G(x - \xi) \phi(\xi, t) d\xi = \frac{1}{\Delta} \int_{x-\Delta/2}^{x+\Delta/2} \phi(\xi, t) d\xi$$

We call the filter used on the initial condition the first filter. The first filter width is 16 or 256 times of the cell size \(\Delta x\). For the family of the dynamic models, the test filter width is 2 times the width of the first filter, which makes \(\gamma = 2\).

C. Initial and boundary conditions

To imitate turbulence, the initial energy spectrum is given in the Fourier space \(k\). In the present work, the following initial spectrum is used:

$$E_0(k) = \begin{cases} 
5^{-\frac{5}{3}} & 1 \leq k \leq 5 \\
5^{-\frac{5}{3}} & k > 5
\end{cases},$$

where \(k\) is integer varing from 1 to 1280. For each \(k\), the velocity \(u\) has a random phase angle, \(\beta\), varying in \([-\pi, \pi]\).
The explicit three-stage SSP Runge Kutta scheme is used for temporal discretization. The two boundaries are set to be periodic due to the periodicity of the initial condition.

IV. Numerical results

In this section, the results for the a priori and a posteriori tests are presented. The viscosity of the Burgers’ equation is 0.004. Due to the nonlinear convection term, shock waves start to appear after a certain time. Thus all results are obtained before the shock waves develop, \( t_1 = 0.004 \) and \( t_2 = 5e-02 \), to ensure that the results are not polluted by the shocks. Figure 2 shows the energy spectrum at three different times, \( t = t_0, t = t_1 \) and \( t_2 \) of the DNS computation. We can see that as time goes by, the high frequencies are damped out by the physical viscosity while the lower frequencies sustain. This behavior is very important in evaluating and understanding the models performance later.

![Figure 2. The energy spectrum](image)

A. A priori tests

Figure 3 shows the SGSs computed using different models based on the filtered-DNS data at \( t = t_1 \) and \( t = t_2 \). The filter size is 16 times that of the cell size. In Figure 2a and 2b, the same fine mesh for DNS is used for LES, while in 2c and 2d, the cell size used in LES is the same as that of the filter. Therefore the results in Figures 2c and 2d include the effects of the truncation error. For the static Smagorinsky model, \( c_s \) is set to the default value of 0.2 for all of the comparisons. For ILES, the subgrid stress is 0 everywhere.

According to Figure 3a, no model shows good results. From the results at \( t = t_1 \), the static model shows some agreement with the true SGS, but for the most part, it gives the opposite sign. The dynamic Smagorinsky model fixes the incorrect sign problem and yields zero at those regions. It also misses much of the true SGS. The SSM has a better correlation with the true SGS but it overshoots the peaks and has phase errors. The mixed model is a combination of the dynamic Smagorinsky model and SSM. Thus it keeps the phase errors of SSM and makes the overshoots worse. The LUM model shows the maximum overshoots, sometimes with an opposite sign. After a longer dissipation time, at \( t = t_2 \), the SS, DS and SSM performs better. Especially the SSM agrees very well with the true SGS. With the truncation error being included, in 3c and 3d, we observe the same performance.
(a) $t = t_1$, on the fine mesh

(b) $t = t_2$, on the fine mesh

(c) $t = t_1$, on the coarse mesh
Figure 3. The a priori subgrid stress comparison ($F = 16\Delta x$)

(a) $t = t_1$, on the fine mesh

(b) $t = t_2$, on the fine mesh

(d) $t = t_2$, on the coarse mesh
Next, we try a much wider filter, 256 times the cell-size and the results are shown in Figure 4. Note that the models computed more energetic high-frequency oscillations, and the simulated SGSs again are far away from the true SGS. The DS, SSM and mixed models are able to predict the correct sign sometimes and catch some peaks but, still, are far from satisfactory. The LUM model shows some agreement with the SS. Results improve at $t = t_2$. The SS and DS were able to catch some of the peaks but unfortunately, DS failed to predict the correct sign either. SSM and the mixed model showed the best correlation with the true SGS, but instead of overshooting, they undershoot and missed quite a lot of peaks. The LUM agree more with the SS but is still far away from the true SGS. In the coarse mesh LES, we obtain the same performance except that the LUM overshoots much more.

From the a priori test, we see that for a given filtered DNS solution, no model was able to correctly predict the SGS, no matter how much is left for the model. However some models are closer than others. The SSM and the mixed model show better agreement consistently. To evaluate the behavior of these models in computation, we perform a posteriori tests next.

**B. A posteriori tests**

In this test, the filtered 1D Burgers’ equation is solved together with different models. The results at the same physical time is compared. Figure 5 shows the subgrid stress comparisons with (a) $t = t_3$, $F = 16\Delta x$, (b) $t = t_1$, $F = 16\Delta x$. (c) and (d) corresponds to (a) and (b) but with the LES cell size being the same as the filter size.
In Figure 5, the SS shows good correlation with the true SGS at some of the peaks. However, for the rest, it yields the opposite sign for the stress. The DS keeps the advantage of SS and fixes the wrong sign of SS. The SSM gives the most satisfactory results for both fine and coarse mesh LES. The coefficient $c_{sm}$ here is adjusted to be 0.25 to obtain the best results which is almost on top of the true SGS. The mixed model combines the original SSM, in which $c_{sm} = 1$, with the DS. It overshoots at the peaks. The LUM catches several peaks of the true SGS with large overshoots. For the most part, it yields wrong sign with large magnitude.

The excellent behavior of the adjusted SSM model is surprising. It might mean that the true SGS can be predicted. But unfortunately, it is not the case. At $t = t_2$, the high-frequency contents are damped out and the filter is too narrow to filter out any low frequency spectrum. The first filter and test filter have very good correlation with a scale of $\left(\frac{1}{2}\right)^2 = 4$. That’s why $c_{sm} = 0.25$ is chosen for this test. This relation only exists at a late stage. The comparison at $t = t_3$ is shown next to demonstrate this claim. From Figure 5 (b) and (d), we can see clearly that the SSM is far less satisfactory. It undershoots and misses most of the peaks. The SS and DS also lose their good performance compared with the results at $t = t_2$. The LUM’s phase agrees with SS, but the magnitude is much bigger.

Figure 6 shows the comparison for a 256-cell-size filter at $t = t_2$, with a (left) fine mesh and (right) coarse mesh. In this case, a wider spectrum is left for the models to take care of than the case with a narrower filter width. Similar to Figure 5(b), none of the models shows satisfactory results. The LUM model diverged, thus it is not shown here.
Figure 5. Subgrid stress comparison \((F = 16\Delta x)\)

Figure 6. Subgrid stress comparison \((t = t_2, F = 256\Delta x)\)

(c) \(t = t_2\), on the coarse mesh

(d) \(t = t_1\), on the coarse mesh
Figure 7. Solution comparison ($t = t_2, F = 16\Delta x$)

Figure 8. Solution comparison ($t = t_2, F = 256\Delta x$)

Figure 7 shows the comparison of the solution, $\hat{u}$, with $F = 16\Delta x$ and Figure 8 shows the comparison with $F=256\Delta x$ at $t = t_2$. The solutions agree with the filtered DNS solution quite well for $F = 16\Delta x$. More details are shown in Figure 8. The solution computed with the true SGS is right on top of the filtered DNS solution on the fine mesh. The solutions computed with models and ILES all have off sets, to different extents. With a large truncation error, the LES results are farther away from DNS results. Table 1 shows the comparison quantitatively. From Table 1 we can see that none of the models show obvious advantage over ILES. Especially on the coarse mesh LES, differences between different models and ILES are very small. The truncation error is dominant. However, much more computing resources are necessary for the models, especially the dynamic family, the DS, the SSM and mixed model.

Table 1. L2 norm error of the solution

<table>
<thead>
<tr>
<th>Model</th>
<th>True SGS</th>
<th>ILES</th>
<th>SS</th>
<th>DS</th>
<th>SSM</th>
<th>Mixed</th>
<th>LUM</th>
</tr>
</thead>
<tbody>
<tr>
<td>$F=16\Delta x$</td>
<td>8.11e-08</td>
<td>5.97e-04</td>
<td>8.77e-04</td>
<td>4.56e-04</td>
<td>1.18e-04</td>
<td>1.82e-03</td>
<td>1.06e-02</td>
</tr>
<tr>
<td>$F=256\Delta x$</td>
<td>2.44e-07</td>
<td>1.27e-02</td>
<td>1.38e-02</td>
<td>1.19e-02</td>
<td>1.24e-02</td>
<td>1.10e-02</td>
<td>---</td>
</tr>
<tr>
<td>$C=F=256\Delta x$</td>
<td>1.10e-02</td>
<td>1.45e-02</td>
<td>1.82e-02</td>
<td>1.48e-02</td>
<td>1.53e-02</td>
<td>1.45e-02</td>
<td>2.17e-02</td>
</tr>
</tbody>
</table>
V. Three dimensional simulations

In this section, we apply the SS and the DS models to two real-world turbulence problems, the decaying homogenous isotropic turbulence and the channel flow. Instantaneous and statistical results are used to evaluate the models’ behavior.

A. Governing equations for three dimensional simulations

The governing equations are the unsteady three-dimensional compressible filtered Navier-Stokes equations. They are summarized briefly here for completeness.

\[
\frac{\partial \bar{Q}}{\partial t} + \nabla \cdot (F(\bar{Q}) - \bar{F}'(\bar{Q})) = S,
\]

where \( \bar{Q} = [\bar{\rho} \bar{u} \bar{v} \bar{w} \bar{\rho}' \bar{\rho}' \bar{\rho}']^T \) is the filtered conservative state vector, \( \bar{\rho} \) the density, \( u, v, w \) are the cartesian velocity components, and \( E \) is the total energy. It is filtered by the grid filtering function \( \int \) and Favre-averaging, \( \int \). However, in real simulation, no explicit filtering was applied to the initial condition before running the simulation. The solution variables are treated as the filtered values. \( F \) is the convective flux and \( \bar{F}' \) is the viscous flux. In LES, SGS models are added to the viscous flux. \( S \) is the source term. It is zero for the decaying homogenous isotropic turbulence case. It serves as driving force for the turbulent channel flow. Since the three-dimensional subgrid models are not the focus of the present study, more details are available in [4, 5, 21].

B. Decaying homogenous isotropic turbulence

The decaying homogeneous isotropic turbulence (DHIT) problem is a canonical problem in turbulence theory [36]. It has been used as a standard test to validate numerical schemes for DNS. In the present work, it is used to evaluate the static and dynamic models in LES compared with ILES.

The computational domain is a three-dimensional cube of the size \( L^3 = (2\pi)^3 \). In all three directions, the boundary conditions are set to be periodic. The initial energy spectrum is given in Fourier space \( \bar{k} \), with the following initial spectrum:

\[
E_{\bar{k}}(k) := A k^4 e^{-0.14k^2}, \quad k \in [k_a, k_b],
\]

where the magnitude \( A \) and the range of the initial energy spectrum \([k_a, k_b]\) determine the initial total kinetic energy \( K_0 \). \( A = 1.4293 \times 10^{-4}, k_a = 3, k_b = 8 \) are used in the study. Thus the initial kinetic energy is \( K_0 \approx 1.08 e - 02 \). The initial velocity field \( u_0 \) is generated in Fourier space according to Rogallo’s procedure. Then the velocity field is transferred to physical space. The detailed process can be found in [36]. \( u' \) is the root-mean-squared turbulent fluctuating velocity value, \( u' := \frac{1}{\sqrt{3}} \sqrt{\langle u \cdot u \rangle} \). In the present work, \( u' = 0.12 \), corresponding to \( Ma \approx 0.13 \), the initial dissipation rate \( e_0 = 7.40 e - 04 \).

We compare instantaneous turbulent kinetic energy spectrum obtained from the DNS and LES, which is defined as:

\[
E(k, t) := \frac{1}{2} \langle u(k, t) \cdot u(k, t) \rangle.
\]

We also calculate other statistical quantities pertinent to DHIT:

\[
K(t) := \frac{1}{2} \langle u \cdot u \rangle, \quad \Omega(t) := \langle (\nabla u)^2 \rangle, \quad \epsilon(t) := 2
\]

\[
\eta(t) := \frac{s}{\sqrt{\epsilon(t)}}
\]

where \( K(t), \Omega(t) \) and \( \epsilon(t) \) are the total kinetic energy, the entropy and the dissipation rate; \( \eta(t) \) is the Kolmogorov length scale. The Taylor microscale Reynolds number \( Re_{\lambda} \) is used to characterize the flow:

\[
Re_{\lambda} := \frac{u' \lambda}{v}
\]

Where \( \lambda \) is the transverse Taylor micro-scale length, \( \lambda := \frac{15}{2\pi} u' \).

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Three grids, \(64^3\), \(32^3\) and \(16^3\) cells, are used with the 3rd order CPR scheme. The explicit 3rd order Runge-Kutta scheme is used for time marching. The non-dimensional time step, \(dt' = \frac{dt}{t_0}\), is set to be 8.56e-05, where \(t_0\) is the turbulence turnover time, \(t_0 = K_0/e_0\). All the simulations start with the same initial velocity field mentioned above with constant density and pressure.

The mesh refinement study is shown in Figure 9. Our results computed on \(32^3\) and \(64^3\) grids show clear convergence and they agree well with the pseudo spectral method [36], thus we take the \(64^3\) results as the DNS results. We first show the statistical quantities comparison in Figure 10. All the LES simulations are computed on the \(16^3\) cell grid. From the total kinetic energy, the models show more dissipation than the ILES. As the dissipation rate here is a function of the vorticity, less vorticity is shown in the results that are computed with models. The Kolmogorov lengths computed with the models are larger than ILES, which means that the effective viscosity is so big that the turbulent kinetic energy is dissipated into heat at a larger scale than it should be. All the three statistical quantities show that the models add too much dissipation to the flow, which is not necessary and very expensive.

Figure 11 shows the instantaneous energy spectra \(E(k, t')\) at two different times, \(t' = 0.25t_0\) and \(t' = 4t_0\). The LES results show good agreement with DNS results at low-frequencies but much lower energy at high-frequencies than the DNS results. However, this difference decreases with time. The reason is that the energy is decaying while time goes by and the high-frequencies dissipate first for both LES and DNS. As the machine zero is approached, it is reasonable to have a decreasing difference. The results computed with the models still are further away from the DNS results than the ILES results.

![Figure 9. The H refinement study: (a) Evolution of the normalized total kinetic energy \(K(t')/K_0\), (b) the normalized dissipation rate \(\varepsilon(t')/\varepsilon_0\) and (c) the normalized Kolmogorov length \(\eta(t')/\Delta x\).](image-url)
Figure 10. (a) Evolution of the normalized total kinetic energy $K(t')/K_0$, (b) the normalized dissipation rate $\varepsilon(t')/\varepsilon_0$ and (c) the normalized Kolmogorov length $\eta(t')/\Delta x$.

Figure 11. The energy spectra $E(k, t')$ at nondimensional time 0.25 and 4.
From all the comparisons, we see that for the three-dimensional decaying homogenous isotropic turbulence problem, on a given coarse mesh, ILES yields more accurate results than the SS or DS SGS models. It is worth mentioning that the DS model performs better than the SS model, but costs twice more than the SS, and even more than ILES.

C. Turbulent Channel flow with Re=5,930

The low-Reynolds number channel flow is another typical case for the LES. In the present work, we run the simulation for \( Re = 5930 \), \( Ma = 0.3 \). \( x, y, and z \) are taken as the streamwise, wall normal and spanwise directions. Periodic boundary conditions are used in \( y \) and \( z \) directions and the no slip iso-thermal condition is used at the walls. The computational domain size is \((L_1 \times L_2 \times L_3) = (4\pi \times 2 \times 2\pi)\) in \((x, y, z)\). Two grids are used, \(19^3\) and \(25^3\). The cell size is constant in the \(x\) and \(z\) directions and geometrically stretched in \(y\) from the walls, where the \(y^+ = 0.98\) for \(19^3\) mesh using the \(p2\) CPR scheme and \(y^+ = 0.35\) for \(25^3\) mesh using the \(p4\) CPR scheme. Because of the periodic streamwise boundary condition, the flow cannot sustain a streamwise pressure gradient. Thus we introduce an artificial source term as a driving force to imitate an imposed constant pressure gradient, thereby maintaining a fixed mass-flow rate. In particular, the source term \(s_x\) is determined at each time step to bring to equilibrium the instantaneous resultant shear at the wall \(F_w\). A relaxation term toward the expected mass flow rate \(\dot{m}_0\) is also included to accelerate convergence,

\[
s_x = \frac{F_w}{V} - \frac{\alpha}{\Delta t}(\dot{m} - \dot{m}_0), \tag{35}\]

where \(V = L_1 \times L_2 \times L_3\) is the volume of the computational domain and according to [35] the relaxation coefficient \(\alpha\) is set to be 0.3. The mass flow rate is computed as

\[
\dot{m} = \frac{1}{2\delta} \int_{-\delta}^{\delta} \langle pu \rangle \, dy, \tag{36}\]

where \(\langle \cdot \rangle\) means averaging in the streamwise and spanwise directions and \(\delta\) is half of the channel dimension in wall normal direction. A source term needs to be added to the energy equation as the product of \(s_x\) and the bulk velocity[37],

\[
s_e = u_b s_x, u_b = \frac{\dot{m}}{2\delta \int_{-\delta}^{\delta} \langle p \rangle \, dy}. \tag{37}\]

The initial velocity profiles is given as

\[
u(x) = 0.1u_0 \exp \left( -\left( \frac{x - L_1}{L_1} \right)^2 \right), \tag{38}\]

\[
u(x) = 0.1u_0 \exp \left[ -\left( \frac{x - L_1}{L_1} \right)^2 \right] \exp \left[ -\left( \frac{y}{2\delta} \right)^2 \right] \cos \left( 4\pi \frac{z}{L_3} \right), \tag{39}\]

where \(u_0\) is the reference velocity. The density and pressure are set to be uniform. The flow is left to evolve from transition to turbulence and eventually reach a statistically steady state. In the simulation computed with the static Smagorinsky model, the original Smagorinsky constant \(C_s\) is multiplied by the van Driest damping factor, 1 - \(\exp \left( -\frac{n^+}{\Delta} \right)\), at the near-wall regions to take the wall impact into consideration, where \(n^+\) is the normal distance from the wall in the law-of-the-wall coordinates and \(\Delta\) is set to be 25.

Figure 12 shows the evolution of the wall shear for all the simulations. We can see all the cases reached the statistically steady state. Figure 13 shows the ILES h and p refinement study, mean streamwise velocity and Reynolds stress \(\overline{uu}\). As the number of degrees of freedom increases, the results converge to the DNS results given in [15]. The LES comparisons are shown in Figure 14. The LES runs with \(19^3\) cells and uses the 3rd and 4th order CPR schemes. In the mean streamwise velocity comparison, the prediction with ILES is closer to the DNS result than that predicted with the DS model. Similarly, the ILES is also better than the DS model in predicting the Reynolds stress. Based on these comparisons, we can see that for three-dimensional turbulence problems with a wall boundary, ILES still produced more accurate results than the DS model, even though the latter costs more than twice in CPU time.
Figure 12. Evolution of wall shear

Figure 13. ILES convergence study: streamwise mean velocity(left) and Reynolds stress(right)

Figure 14. ILES and dynamic Smagorinsky comparison: streamwise mean velocity(left) and Reynolds stress(right)
VI. Conclusions

Five SGS models are evaluated using the 1D Burgers’ equation discretized with the CPR method. Filters with different width and solutions at different times are used to test the models’ performance. In both the a priori and a posteriori tests, none of the models predicts the SGS satisfactorily, except the adjusted SSM model, which showed excellent agreement with the true SGS after a long term simulation.

Two three-dimensional turbulent problems are tested for the SS and DS models, the decaying homogeneous isotropic turbulence and the turbulent channel flow. In the first case, both statistical and instantaneous results show that, neither SS nor DS shows any better results than ILES. Actually, they are even worse. The second case with a wall boundary gives the same conclusion. The SS and DS appear to add too much dissipation to the CPR method, which, degrades the results, instead of improving them in any way.

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