Towards Lagrangian dynamic SGS model for SCALES of isotropic turbulence

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1 Introduction

Although turbulence is common in engineering applications, a solution to the fundamental equations that govern turbulent flow still eludes the scientific community. Due to the prohibitively large disparity of spatial and temporal scales, direct numerical simulation (DNS) of turbulent flows of practical engineering interest are impossible, even on the fastest supercomputers that exist or will be available in the foreseeable future. Large eddy simulation (LES) is often viewed as a feasible alternative for turbulent flow modelling, *e.g.*, [1]. The main idea behind LES is to solve only large-scale motions, while modelling the effect of the unresolved subgrid scale (SGS) eddies.

When dealing with complex turbulent flows, current LES methods rely on, at best, a zonal grid adaptation strategy to attempt to minimize the computational cost. While an improvement over the use of regular grids, these methods fail to resolve the high wavenumber components of spatially intermittent coherent eddies that typify turbulent flows, thus, neglecting valuable physical information. At the same time, the flow is over-resolved in regions between the coherent eddies, consequently wasting computational resources. Another important drawback of LES, which is often overlooked, is that *a priori* decided grid resolution distorts the spectral content of any vortical structure by not supporting its small-scale contribution.

Recently, a novel approach to turbulent complex flow simulation, called stochastic coherent adaptive large eddy simulation (SCALES) has been introduced [2, 3]. This method addresses the above mentioned shortcomings of LES by using a wavelet thresholding filter to dynamically resolve and “track” the most energetic coherent structures during the simulation. The less energetic unresolved modes, the effect of which must be modeled, have been shown to be composed of a minority of coherent modes that dominate the total SGS dissipation and a majority of incoherent modes that, due to their decorrelation with the resolved modes, add little to the total SGS dissipation [2, 4]. The physical coherent/incoherent composition of the SGS modes is reflected in the naming of the SCALES methodology, yet as pointed out in [4] this physical coherent/incoherent composition of the SGS modes is also present in classical LES implementations. For this work, as in much of classical LES research, only the coherent part of the SGS modes will be modeled using a deterministic SGS stress model. The use of a stochastic model to capture the effect of the incoherent SGS modes will be the subject of future work.

The first step towards the construction of SGS models for SCALES was undertaken in [3], wherein a dynamic eddy viscosity model based on Germano's classical dynamic procedure redefined in terms of two wavelet thresholding filters was developed. The main drawback of this formulation is the use of a global (spatially non-variable) Smagorinsky model coefficient. The use a global dynamic model unnecessarily limits the SCALES approach to flows with at least one homogeneous direction. This is unfortunate since the dynamic adaptability of SCALES is ideally suited to fully non-homogeneous flows. In this paper a localized dynamic model is developed to allow the application of the SCALES methodology to inhomogeneous flows. The proposed model is based on the Lagrangian formulation introduced in [5].

2 Stochastic coherent adaptive large eddy simulation

2.1 Wavelet thresholding filter

Let us very briefly outline the main features of the wavelet thresholding filter. More details can be found, for instance, in [6]. A velocity field $u_i(\mathbf{x})$ can be represented in terms of wavelet basis functions as

$$u_i(\mathbf{x}) = \sum_{\mathbf{l}\in\mathcal{L}^0} c^0_{\mathbf{l}}\phi^0_{\mathbf{l}}(\mathbf{x}) + \sum_{j=0}^{+\infty}\sum_{\mu=1}^{2^n-1}\sum_{\mathbf{k}\in\mathcal{K}^{\mu,j}} d^{\mu,j}_{\mathbf{k}}\psi^{\mu,j}_{\mathbf{k}}(\mathbf{x}) \, , \tag{1}$$

where $\phi^0_{\mathbf{k}}(\mathbf{x})$ and $\psi^{\mu,j}_{\mathbf{l}}$ are n-dimensional scaling functions and wavelets of different families and levels of resolution, indexed with μ and j, respectively. One may think of a wavelet decomposition as a multilevel or multiresolution representation of u_i, where each level of resolution j (except the coarsest one) consists of a family of wavelets $\psi^{\mu,j}_{\mathbf{l}}$ having the same scale but located at different positions. Scaling function coefficients represent the averaged values of the field, while the wavelet coefficients represent the details of the field at different scales.

Wavelet filtering is performed in wavelet space using wavelet coefficient thresholding, which can be considered as a nonlinear filter that depends on each flow realization. The wavelet thresholding filter is defined by,

$$\overline{u_i}^{>\epsilon}(\mathbf{x}) = \sum_{\mathbf{l}\in\mathcal{L}^0} c^0_{\mathbf{l}}\phi^0_{\mathbf{l}}(\mathbf{x}) + \sum_{j=0}^{+\infty}\sum_{\mu=1}^{2^n-1}\sum_{\substack{\mathbf{k}\,\in\,\mathcal{K}^{\mu,j}\\ |d^{\mu,j}_{\mathbf{k}}|\,>\,\epsilon U_i}} d^{\mu,j}_{\mathbf{k}}\psi^{\mu,j}_{\mathbf{k}}(\mathbf{x})\,, \tag{2}$$

where $\epsilon > 0$ stands for the non-dimensional (relative) threshold value, U_i being the (absolute) dimensional velocity scale. The latter can be specified, for instance, as the norm $U_i = \|\mathbf{u}\|_2$.

2.2 Wavelet-filtered Navier-Stokes equations

When applying the wavelet thresholding filter to the Navier-Stokes equations, each variable should be filtered, according to Eq. (2), with a corresponding absolute scale. However, this would lead to numerical complications due to the one-to-one correspondence between wavelet locations and grid points. In particular, each variable would be solved on a different numerical grid. In order to avoid this difficulty, in the present study, the coupled wavelet thresholding strategy is used. Namely, after constructing the masks of significant wavelet coefficients for each primary variable, the union of these masks results in a global thresholding mask that is used for filtering each term. Note that other additional variables, like vorticity or strain rate, can be used for constructing the global mask.

Once the global mask is constructed, one can view the wavelet thresholding as a local low-pass filtering, where the high frequencies are removed according to the global mask. Such interpretation of wavelet threshold filtering highlights the similarity between SCALES and classical LES approaches. However, the wavelet filter is drastically different from the LES filters, primarily because it changes in time following the evolution of the solution, which, in turn, results in an adaptive computational grid that tracks the areas of locally significant energy in physical space.

Therefore, the SCALES equations for incompressible flow, which describe the evolution of the most energetic coherent vortices in the flow field, can be formally obtained by applying the wavelet thresholding filter to the incompressible Navier-Stokes equations:

$$\frac{\partial \overline{u_i}^{>\epsilon}}{\partial x_i} = 0\,, \tag{3}$$

$$\frac{\partial \overline{u_i}^{>\epsilon}}{\partial t} + \frac{\partial(\overline{u_i}^{>\epsilon}\,\overline{u_j}^{>\epsilon})}{\partial x_j} = -\frac{1}{\rho}\frac{\partial \overline{p}^{>\epsilon}}{\partial x_i} + \nu\frac{\partial^2 \overline{u_i}^{>\epsilon}}{\partial x_j \partial x_j} - \frac{\partial \tau_{ij}}{\partial x_j}\,, \tag{4}$$

where ρ, ν are the constant density and kinematic viscosity, and p stands for the pressure. As a result of the filtering process the unresolved quantities

$$\tau_{ij} = \overline{u_i u_j}^{>\epsilon} - \overline{u}_i^{>\epsilon}\,\overline{u}_j^{>\epsilon}\,, \tag{5}$$

commonly referred to as SGS stresses, are introduced. They represent the effect of unresolved (less energetic) coherent and incoherent eddies on the resolved (energetic) coherent vortices. As usual in a LES approach, in order to close equations (4), a SGS model is needed to express the unknown stresses in terms of the resolved field.

From a numerical viewpoint, the SCALES methodology is implemented using the dynamically adaptive wavelet collocation (DAWC) method, *e.g.*, [7]. The DAWC method is ideal for the actual approach as it combines the resolution of the energetic coherent modes in a turbulent flow with the simulation of their temporal evolution. The wavelet collocation method employs wavelet compression as an integral part of the numerical algorithm such that the solution is obtained with the minimum number of grid points for a given accuracy.

3 Lagrangian dynamic SGS model

The primary objective of the current work is to develop a local SGS model for SCALES of inhomogeneous turbulent flows. In previous work a dynamic Smagorinsky model with a global (spatially non-variable) coefficient has been developed and successfully tested for decaying isotropic turbulence [3]. In this work this idea is further extended by exploring the use of a local Lagrangian dynamic model [5]. Following [3], where it was shown that when a wavelet thresholding filter is applied to the velocity field, the resulting SGS stresses scale like ϵ^2, the following Smagorinsky-type eddy viscosity model is used for simulating the deviatoric part (hereafter noted with a star) of the SGS stress tensor (5):

$$\tau^*_{ij} \cong -2 C_S \Delta^2 \epsilon^2 \left| \overline{S}^{>\epsilon} \right| \overline{S_{ij}}^{>\epsilon} , \tag{6}$$

where $\overline{S_{ij}}^{>\epsilon} = \frac{1}{2}\left(\frac{\partial \overline{u_i}^{>\epsilon}}{\partial x_j} + \frac{\partial \overline{u_j}^{>\epsilon}}{\partial x_i} \right)$ is the resolved rate-of-strain tensor and $\Delta(\mathbf{x}, t)$ is the local characteristic vortical lengthscale implicitly defined by wavelet thresholding filter. Note that Δ is distinctively different from the classical LES, where the local filter width is used instead. Also note that despite its implicit definition, Δ can be extracted from the actual thresholding mask during the simulation.

Following the modified Germano's dynamic procedure redefined in terms of two wavelet thresholding filters, originally introduced in [3], the SGS stress corresponding to the wavelet test filter at twice the threshold, noted $\overline{(\cdot)}^{>2\epsilon}$, is defined as

$$T_{ij} = \overline{u_i u_j}^{>2\epsilon} - \overline{u_i}^{>2\epsilon} \, \overline{u_j}^{>2\epsilon} . \tag{7}$$

Note that, the wavelet filter being a projection operator, by definition, it holds $\overline{\overline{(\cdot)}^{>\epsilon}}^{>2\epsilon} \equiv \overline{(\cdot)}^{>2\epsilon}$. Filtering (5) at the test filter level and combining with (7) results in the following modified Germano identity for the Leonard stresses:

$$L_{ij} \equiv T_{ij} - \overline{\tau_{ij}}^{>2\epsilon} = \overline{\overline{u_i}^{>\epsilon} \overline{u_j}^{>\epsilon}}^{>2\epsilon} - \overline{u_i}^{>2\epsilon} \, \overline{u_j}^{>2\epsilon} . \tag{8}$$

Exploiting the model (6) and the analogous relation for the test filtered SGS stresses

$$T^*_{ij} \cong -2C_S \Delta^2 (2\epsilon)^2 \left|\overline{S}^{>2\epsilon}\right| \overline{S_{ij}}^{>2\epsilon} , \tag{9}$$

one obtains

$$\overline{2C_S \Delta^2 \epsilon^2 \left|\overline{S}^{>\epsilon}\right| \overline{S_{ij}}^{>\epsilon}}^{>2\epsilon} - 2C_S \Delta^2 (2\epsilon)^2 \left|\overline{S}^{>2\epsilon}\right| \overline{S_{ij}}^{>2\epsilon} = L^*_{ij} . \tag{10}$$

A least square solution to (10) leads to the following local Smagorinsky model coefficient definition:

$$C_S(\mathbf{x}, t)\epsilon^2 = \frac{L^*_{ij} M_{ij}}{M_{hk} M_{hk}} , \tag{11}$$

where

$$M_{hk} \equiv 2\Delta^2 \left[\overline{\left|\overline{S}^{>\epsilon}\right| \overline{S_{hk}}^{>\epsilon}}^{>2\epsilon} - 4 \left|\overline{S}^{>2\epsilon}\right| \overline{S_{hk}}^{>2\epsilon} \right] . \tag{12}$$

The coefficient C_S can be actually positive or negative, that allows for local backscatter of energy from unresolved to resolved modes. However, it has been found that negative values of C_S cause numerical instabilities. To avoid this fact, for homogeneous flow, one can introduce an average over homogeneous directions. This procedure results in the global dynamic model proposed in [3].

In this study we follow a Lagrangian dynamic model formulation [5] and take the following statistical averages over the trajectory of a fluid particle:

$$\mathcal{I}_{LM}(\boldsymbol{x}, t) = \frac{1}{T} \int_{-\infty}^{t} e^{\frac{\tau - t}{T}} L_{ij}(\boldsymbol{x}(\tau), \tau) M_{ij}(\boldsymbol{x}(\tau), \tau) \, d\tau , \tag{13}$$

$$\mathcal{I}_{MM}(\boldsymbol{x}, t) = \frac{1}{T} \int_{-\infty}^{t} e^{\frac{\tau - t}{T}} M_{hk}(\boldsymbol{x}(\tau), \tau) M_{hk}(\boldsymbol{x}(\tau), \tau) \, d\tau , \tag{14}$$

which leads to the following local Smagorinsky model coefficient

$$C_S(\mathbf{x}, t)\epsilon^2 = \frac{\mathcal{I}_{LM}}{\mathcal{I}_{MM}}. \tag{15}$$

To avoid the computationally expensive procedure of Lagrangian pathline averaging, following [5], Eqs. (13) and (14) are differentiated with respect to time leading to the following evolution equations for $\mathcal{I}_{LM}$ and $\mathcal{I}_{MM}$:

$$\frac{\partial \mathcal{I}_{LM}}{\partial t} + \overline{u}_l^{>\epsilon} \frac{\partial \mathcal{I}_{LM}}{\partial x_l} = \frac{1}{T}(L_{ij} M_{ij} - \mathcal{I}_{LM}), \tag{16}$$

$$\frac{\partial \mathcal{I}_{MM}}{\partial t} + \overline{u}_l^{>\epsilon} \frac{\partial \mathcal{I}_{MM}}{\partial x_l} = \frac{1}{T}(M_{hk} M_{hk} - \mathcal{I}_{MM}). \tag{17}$$

As in [5] the relaxation time scale T is defined as $T(\mathbf{x}, t) = \theta \Delta \, (\mathcal{I}_{LM} \mathcal{I}_{MM})^{-1/8}$, θ being a dimensionless parameter of order unity.

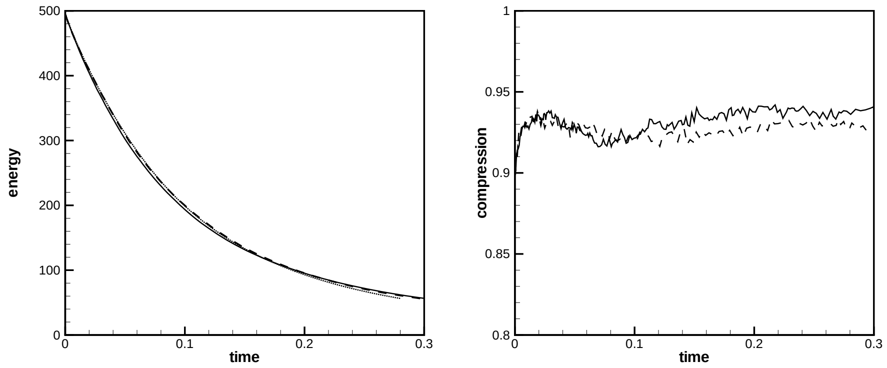

Fig. 1. Kinetic energy decay (left) and grid compression (right) for GDM (dashed line) and LDM (solid line). The reference energy decay for DNS is also reported (dotted line).

The equations (16) and (17) should be solved together with the SCALES equations, (3) and (4). It should be noticed that both $\mathcal{I}_{LM}$ and $\mathcal{I}_{MM}$ have higher frequency content when compared to the velocity field. This is due to two main factors: the quartic character of nonlinearity of $\mathcal{I}_{LM}$ and $\mathcal{I}_{MM}$ with respect to velocity and the creation of small scales due to chaotic convective mixing. Thus, in order to adequately resolve both $\mathcal{I}_{LM}$ and $\mathcal{I}_{MM}$, one needs to have a substantially finer computational mesh than the one required by the velocity field, which is impractical. To by-pass this problem, an artificial diffusion term is added to Eqs. (16) and (17):

$$\frac{\partial \mathcal{I}_{LM}}{\partial t} + \overline{u}_l^{>\epsilon} \frac{\partial \mathcal{I}_{LM}}{\partial x_l} = \frac{1}{T}(L_{ij}M_{ij} - \mathcal{I}_{LM}) + \mathcal{D}_{\mathcal{I}} \frac{\partial^2 \mathcal{I}_{LM}}{\partial x_l \partial x_l}, \tag{18}$$

$$\frac{\partial \mathcal{I}_{MM}}{\partial t} + \overline{u}_l^{>\epsilon} \frac{\partial \mathcal{I}_{MM}}{\partial x_l} = \frac{1}{T}(M_{hk}M_{hk} - \mathcal{I}_{MM}) + \mathcal{D}_{\mathcal{I}} \frac{\partial^2 \mathcal{I}_{MM}}{\partial x_l \partial x_l}. \tag{19}$$

To avoid the creation of small scales, the diffusion time scale, $\Delta^2/\mathcal{D}_{\mathcal{I}}$, should be smaller than the convective time scale associated with local strain, $\left|\overline{S}^{>\epsilon}\right|^{-1}$, which results in $\mathcal{D}_{\mathcal{I}} = C_{\mathcal{I}}\Delta^2 \left|\overline{S}^{>\epsilon}\right|$, where C_I is a dimensionless parameter of order unity.

4 Results

In this paper, the preliminary results of the application of SCALES method together with Lagrangian dynamic modeling (for discussion: LDM) to incompressible isotropic decaying turbulence simulation are presented. The LDM solution is compared to SCALES with global dynamic model (for discussion: GDM) [3]. The initial velocity field is a realization of a statistically stationary turbulent flow at $Re_\lambda = 48$, as provided by a pseudo-spectral DNS database, *e.g.* [4]. In both SCALES cases the wavelet thresholding parameter is set to $\epsilon = 0.5$. For a deep discussion of the way this choice can be made one can see in [2]. The additional SGS modeling variables are initialized as $\mathcal{I}_{MM} = M_{hk}M_{hk}$ and $\mathcal{I}_{LM} = \bar{C}_s\epsilon^2\mathcal{I}_{MM}$, $\bar{C}_s$ being the volume averaged value. For the time relaxation scale definition, the suggested value $\theta = 1.5$ is chosen. For a discussion of the model sensitivity to this parameter, one can see the original work [5]. As to the artificial diffusion coefficient, several experiments have been performed, leading to the choice of $C_{\mathcal{I}} = 5$ for this preliminary test, in order to have a stable solution.

In Figure 1 the kinetic energy decay and grid compression for LDM are compared to GDM. The energy decay for a pseudo-spectral DNS solution is also reported for reference. The compression is always evaluated with respect to the maximum field resolution, that is 128^3 for both SCALES cases. The LDM case appears initially slightly over dissipative in comparison to DNS. Though both SCALES use the same relative ϵ, yet the compression for the LDM run is slightly better. In fact, a very interesting aspect of the SCALES methodology is that the dynamic grid evolution is closely coupled to the flow physics and is therefore affected by the SGS stress model forcing.

Figure 2 shows the energy density spectra at a given time instant, that is $t = 0.104$. The spectral DNS and wavelet-filtered DNS solutions are also shown for reference. It can be seen that, at this point in the decay, both the LDM and the GDM models show excess energy in the small scales, leading to the conclusion that the model is either not damping out small scales or is itself introducing excess small scale motions. This again highlights the strong coupling between the dynamically adapting grid and the flow physics.

In conclusion, we want to emphasize that the work on local Lagrangian model is ongoing. However, from these limited initial results, one can conclude that the local model works as well as the global one. Further work will pursue a more computationally efficient formulation as well as improve the model behavior at small scales level. It is worth reporting that SCALES with GDM at higher Reynolds number have provided better agreement with DNS solution [3]. The same good results are expected for the LDM case. Moreover, once a cost effective model implementation is developed, the LDM approach will allow to study non-homogeneous flows.

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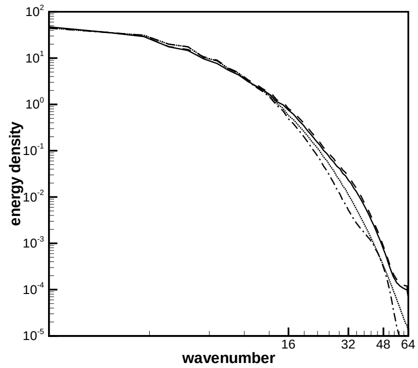

Fig. 2. Energy density spectra at a given time instant ($t = 0.104$) for DNS (dotted line), wavelet filtered DNS (dash-dotted line), GDM (dashed line) and LDM (solid line).

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