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# On discretization errors and subgrid scale model implementations in large eddy simulations

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#### ABSTRACT

We analyze the impact of discretization errors on the performance of the Smagorinsky model in large eddy simulations (LES). To avoid difficulties related to solid boundaries, we focus on decaying homogeneous turbulence. It is shown that two numerical implementations of the model in the same finite volume code lead to significantly different results in terms of kinetic energy decay, time evolutions of the viscous dissipation and kinetic energy spectra. In comparison with spectral LES results, excellent predictions are however obtained with a novel formulation of the model derived from the discrete Navier–Stokes equations. We also highlight the effect of discretization errors on the measurement of physical quantities that involve scales close to the grid resolution.

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#### 1. Introduction

The aim of large eddy simulations is to reproduce with accuracy the large scale properties of a turbulent flow at a much lower computational cost than required by direct numerical simulations (DNS). By definition, LES are thus performed on coarse meshes that do not capture the small scales which are present in the actual flow. These *subgrid scales* are nevertheless important and strongly influence the dynamics of the large *resolved scales*. The main challenge of LES is then to appropriately model the influence of the subgrid scales on the resolved scales through a *subgrid scale (SGS) model*. On these grounds, SGS modeling is largely a physics problem that needs to take into account the nature of turbulence and in particular the cascade of energy from large to small scales through the inertial range. This viewpoint is supported by Kolmogorov's universality theory which implies that the statistical properties of turbulence are universal in the inertial range at large Reynolds numbers.

The numerical method that is most faithful to the LES paradigm is of course the spectral method. Focusing on homogeneous turbulence, the resolved velocity field can indeed be developed on the basis of Fourier modes limited to wave vectors up to a given cut-off. Hence, the neglected modes unambiguously define the subgrid scales. The LES equations are also perfectly well defined since all spatial derivatives can be computed exactly by multiplication of the Fourier modes with the appropriate powers of the wave vector. In the absence of explicit filtering (for example with a Gaussian or top-hat filter), the physical problem of subgrid scale modeling is then completely free of discretization errors.

In practice, the flow configurations are usually much more complex. For problems in wall-bounded or complex geometries, one usually resorts to other spatial discretizations of the Navier–Stokes equations. Here, the attention is restricted to finite volume methods, although the present arguments can be applied to other techniques like finite elements or finite difference schemes. Ultimately, the flow is simulated using a finite number of discrete variables located at a given set of grid

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points. For finite volume schemes, these variables represent the velocity and pressure fields averaged over control volumes of typical size  $\Delta$ . In LES,  $\Delta$  is obviously quite large in order to limit the computer requirements. If we exclude explicit filtering, the filtering operation which requires subgrid scale modeling can then be identified with the volume averaging on the coarse mesh (this averaging is responsible for the destruction of small scale information). However, because the mesh is coarse, the discrete operators needed for differentiations and interpolations introduce further errors that might be very significant. For differentiation operators, the severity of this problem increases with the order of the derivative taken. In that case, the physical relevance of the numerical results becomes questionable.

Several previous studies highlighted the interplay between discretization errors and subgrid modeling. The first systematic analyses of discretization errors in large eddy simulations are due to Vreman et al. [1] and Ghosal [2]. In the latter, the author analyzed finite difference operators in homogeneous isotropic turbulence and showed that discretization errors could be of equal importance as the subgrid scale model's contribution. To overcome this problem, the author recommends the use of higher-order discretization schemes or the explicit filtering of the LES field to damp scales close to the grid size. This study was extended to the case of stratified sheared turbulence where LES discretization errors were analyzed using data obtained from high resolution DNS [3].

The use of high-order methods is very demanding in terms of implementation and computational costs. For this reason, many studies have focused on the application of explicit filters in low-order methods with the aim of minimizing the influence of numerical errors. As explained in [4], the distinction between discretization and explicit filtering is then essential. Discretization is responsible for a loss of information and ultimately leads to a closure problem (this is made clear by considering the discretizing operators as "filters" [5]). This contrasts with explicit filters that can be formally taken into account by using a power series in the filter width (at least for a certain class of filters). The benefit provided by explicit filtering still remains unclear [6]. In particular, Lund [7] showed that a grid refinement with traditional models (i.e. without explicit filtering) may lead to better results than the use of an explicit filter in two directions. Furthermore, explicit filtering introduce difficulties related to the commutation error between the filter and differentiation operators [8]. Nevertheless, a revived interest in explicit filters has appeared in relation to "variational multiscale models" in which scales close to the grid size are separated from the rest of the resolved scales to determine the subgrid scale model [9,10].

Other studies have focused on the minimization of the total error (i.e. sum of modeling and discretization errors) and its dependence on numerical and physical settings [11–14]. As also observed by [15], the reduction of one component (or both) of the error may not necessary lead to a decrease of the total error. Hence, this may yield counter-intuitive effects and poses the question of quality and reliability of LES predictions [14].

The purpose of this paper is twofold. We first compare two implementations of the Smagorinsky subgrid scale model in a finite volume code. These implementations differ only in terms of the model discretization and we use a spectral LES (without explicit filtering) as the benchmark case. It is found that the performance of the model largely depends on the discretization adopted and we advocate the use of a discretization which is derived from the discrete implementation of the Navier–Stokes equations. Some filtered DNS results are also presented but only for illustrative purposes. They are deliberately not used as the main benchmark since we do not focus on the intrinsic performance of the Smagorinsky model but only on how to implement the analytical form as faithfully as possible in a numerical code. In that respect, comparison with a spectral LES is more appropriate whereas comparison with a filtered DNS is more suitable to test the physical content of a model.

The second objective of this work is to bring the attention on the ambiguity, resulting from discretization errors, of physical results extracted from LES on coarse meshes. We stress that the conclusions of this study are applicable to finite element or finite difference schemes without any significant changes. Also, to avoid having to deal with the resolution of boundary layers, we limit our attention to homogeneous turbulence. This further allows a detailed comparison with an accurate spectral solver.

The manuscript is organized as follows. The second-order finite volume LES solver is presented in Section 2. Using kinetic energy budgets, the performance of two implementations of the Smagorinsky subgrid scale model is compared in Section 3. In Section 4, we comment on the importance of discretization errors in the measurement of physical quantities involving length-scales close to the grid size. Finally, our conclusions are presented in Section 5.

#### 2. Numerical method and subgrid modeling

#### 2.1. Numerical discretization

The computations are performed using the CDP code developed at the Center For Turbulence Research (Stanford/ NASA Ames). This code uses a collocated discretization of the incompressible Navier–Stokes equations in a node-based formulation. A typical grid element is illustrated in Fig. 1. The label C corresponds to the location of the centroid of the element in the original volume-based grid. In the dual mesh, the node-based control volumes are centered around each of the vertices (nodes) of this original mesh. In the figure, P represents such a node of the dual mesh. The velocity and pressure fields are stored at these nodes and the (independent) face normal velocity  $U_F$  are stored at the centroid of the dual volume's faces.

The details of the code are described extensively in [16–18], and therefore, only the information relevant to the present study is reported here. The LES equations derived from the incompressible Navier–Stokes equations are solved using the following fractional step method:

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