Proper SGS heat flux models and numerical methods for LES

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1 Introduction

In the last decades, many engineering/scientific applications have benefited from the advances in the field of Computational Fluid Dynamics (CFD). Unfortunately, most of practical turbulent flows cannot be directly computed from the Navier-Stokes equations because not enough resolution is available to resolve all the relevant scales of motion. Therefore, practical numerical simulations have to resort to turbulence modeling. We may therefore turn to large-eddy simulation (LES) to predict the large-scale behavior of turbulent flows. In LES, the large scales of motions are explicitly computed, whereas effects of small scale motions are modeled. Since the advent of CFD many subgrid-scale models have been proposed and successfully applied to a wide range of flows. Eddy-viscosity models for LES is probably the most popular example thereof. Then, for problems with the presence of active/passive scalars (*e.g.* heat transfer problems, transport of species in combustion, dispersion of contaminants,...) the (linear) eddy-diffusivity assumption is usually chosen. However, this type of approximation systematically fails to provide a reasonable approximation of the actual SGS flux because they are strongly misaligned [1, 2]. This was clearly shown in our previous works [3, 4] where SGS features were studied a priori for a RBC at Ra-number up to 10^{11}. This leads to the conclusion that nonlinear (or tensorial) models are necessary to provide good approximations of the actual SGS heat flux. In this regard, the nonlinear Leonard model [5], which is the leading term of the Taylor series of the SGS heat flux, provides a very accurate *a priori* approximation. However, the local dissipation introduced by the model can take negative values; therefore, the Leonard model cannot be used as a standalone SGS heat flux model, since it produces a finite-time blow-up. A similar problem is encountered with the nonlinear tensorial model proposed by Peng and Davidson [6]. An attempt to overcome these instability issues is the so-called mixed model [1], where the Leonard model is combined with an eddy-diffusivity model.

2 On a proper tensorial SGS heat flux model

In this context, we planned to shed light to the following research question: *can we find a nonlinear subgrid-scale heat flux model with good physical and numerical properties, such that we can obtain satisfactory predictions for buoyancy-driven turbulent flows?* To that end, we consider nonlinear SGS heat flux models that can adequately represent the dynamics of the smallest (unresolved) scales, overcoming the above-mentioned inherent limitations of the eddy-diffusivity models [3, 4]. The specific SGS models that we consider consist of a linear eddy-viscosity term for momentum supplemented by a nonlinear model for the SGS heat flux. Firstly, we have firstly studied and confirmed the suitability of the eddy-

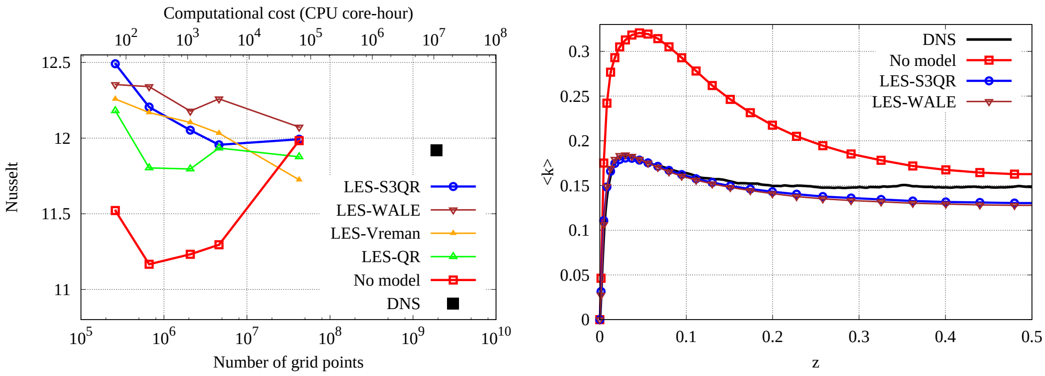

Figure 1: Comparison of LES (and no-model) versus DNS results of liquid-sodium ($Pr = 0.005$) RBC at $Ra = 7.14 \times 10^7$. Left: average Nusselt for different meshes. Computational costs at the MareNostrum 4 supercomputer are shown in the top of the plots. Right: LES results at $Ra = 7.14 \times 10^6$ of turbulent kinetic energy at the cavity mid-width for a $96 \times 52 \times 52$ mesh compared with the DNS results obtained with a mesh of $488 \times 488 \times 1280 \approx 305M$.

viscosity assumption for buoyancy-driven turbulent flows. To do so, we have carried out *a posteriori* tests for different LES models at very low Prandtl numbers (liquid sodium, $Pr = 0.005$) at $Ra = 7.14 \times 10^6$ and $Ra = 7.14 \times 10^7$. Recalling that the separation between the smallest scales of temperature and velocity, *i.e.* the ratio between the Kolmogorov and the Obukhov-Corrsin length scale is given by $Pr^{3/4}$ [7], it is then possible to combine an LES simulation for the velocity field with the numerical resolution of all the relevant scales of the thermal field. Regarding this, results shown in Figure 1 seem to confirm the adequacy of eddy-viscosity models for this kind of flows. For details the reader in referred to Ref. [8].

Then, in the quest for more accurate models, we recently proposed a new family of tensorial SGS heat flux models [8]. Among all possible candidates, we have chosen the so-called S2PR model given by

$$q^{S2PR} = -C_{s2pr} P_{\mathsf{GG}^T}^{-3/2} R_{\mathsf{GG}^T}^{1/3} \frac{\delta^2}{12} \mathsf{GG}^T \nabla \overline{T}, \tag{1}$$

with $C_{s2pr} \approx 12.02$, where P_{GG^T} and R_{GG^T} are the first and third invariants of the GG^T tensor, respectively. This tensor is proportional to the gradient model [9] given by the leading term of the Taylor series expansion of the subgrid stress tensor $\tau(\overline{u}) = (\delta^2/12)\mathsf{GG}^T + O(\delta^4)$. This model shows a very good representation of the SGS heat flux both in direction and magnitude. Moreover, apart from fulfilling a set of desirable properties (locality, Galilean invariance, numerical stability, proper near-wall behavior, and automatically switch-off for laminar and 2D flows), the proposed model is well-conditioned, and has a low computational cost and no intrinsic limitations for statistically in-homogeneous flows. Hence, it seems to be well suited for engineering applications.

3 Concluding remarks and future research

Nowadays, most of the CFD codes rely on the eddy-diffusivity assumption, $q^{eddy} \propto \nabla \overline{T}$, to model the SGS heat flux for LES simulations. Researchers' experience carrying out LES simulations of buoyancy-driven turbulence using this approach is, in general, quite frustrating. Namely, in many cases there is no relevant improvement compared with the results obtained without any SGS model. In other cases, the apparent improvement is simply due to the fact that the SGS model stabilizes the numerical simulation that otherwise (without model) would just blow up. The latter issue can be solved using numerical discretizations that are stable *per se* [10, 11]. In any case, very small improvements are actually observed [3] leading to the necessity to use very fine grids (sometimes similar to DNS) to obtain reliable solutions. Furthermore, *a priori* analysis using DNS data of RBC at high Ra-numbers clearly shows that the classical (linear) eddy-diffusivity assumption is completely misaligned with the actual SGS heat flux [3, 4]. In this regard, our near future research plans include testing *a posteriori* the new tensorial SGS heat flux model given in Eq.(1) for air-filled RBC problems at Ra up to 10^{11}. Prior to that, we also aim to properly discretize these models. As mentioned above, the underlying discretization can play a crucial role in the performance of SGS models. Discretizations that do not preserve the underlying symmetries of the continuous operators, *i.e.* the convective operator is skew-symmetric and the diffusive is symmetric and negative-definite, can easily overwhelm the effect of the SGS model itself. This can be especially difficult for complex configurations where unstructured meshes are needed. With this in mind, a fully conservative discretization method for unstructured collocated grids was proposed in Ref. [10]. However, any pressure-correction method on collocated grids suffer from the same drawbacks: the cell-centered velocity field is not exactly incompressible and some artificial dissipation is inevitable introduced. On the other hand, for staggered velocity fields, the projection onto a divergence-free space is a well-posed problem: given a velocity field, it can be uniquely decomposed into a solenoidal vector and the gradient of a scalar (pressure) field. This can be easily done without introducing any dissipation as it should be from a physical point-of-view. In this work, we will also explore the possibility to build up staggered formulations based on the easy-to-construct collocated operators.

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