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BUILDING A PROPER TENSOR-DIFFUSIVITY MODEL FOR LARGE-EDDY SIMULATION OF BUOYANCY-DRIVEN FLOWS

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Abstract. In this work, we plan to shed light on the following research question: *can we find a nonlinear tensorial subgrid-scale (SGS) heat flux model with good physical and numerical properties, such that we can obtain satisfactory predictions for buoyancy driven turbulent flows?* This is motivated by our recent findings showing that the classical (linear) eddy-diffusivity assumption, $\boldsymbol{q}^{eddy} \propto \nabla\overline{T}$, fails to provide a reasonable approximation for the SGS heat flux, $\boldsymbol{q} = \overline{\boldsymbol{u}T} - \overline{\boldsymbol{u}}\overline{T}$. This has been shown in our recent work [Dabbagh *et al.*, Phys. Fluids 29, 105103 (2017)] where SGS features have been studied *a priori* for a Rayleigh-Bénard convection (RBC). We have also concluded that nonlinear (or tensorial) models can give good approximations of the actual SGS heat flux. The nonlinear Leonard model, $\boldsymbol{q}^{nl} \propto \nabla\overline{\boldsymbol{u}}\nabla\overline{T}$, is an example thereof. However, this model is unstable and therefore it cannot be used as standalone SGS heat flux model. Apart from being numerically stable we also want to have the proper cubic near-wall behavior. Corrections in this regard will be presented together with *a priori/posteriori* studies of nonlinear SGS heat flux models for RBC. Results from LES simulations will be compared with the DNS results obtained in the on-going PRACE project *"Exploring new frontiers in Rayleigh-Bénard convection"*.

1 INTRODUCTION

Turbulent flows driven by thermal buoyancy are present in many technological applications, such as governing flows in nuclear reactors, solar thermal power plants, indoor space heating and cooling, electronic devices, and convection in the atmosphere, oceans and deep mantle. Most of these flows are ruled by turbulent regime purely sustained by buoyancy, the reason that imparts a significant complexity into the flow system. Mainly, the chief dynamics therein such as the vortical structures and thermal plumes are essentially associated with immanent unsteadiness, energy nonequilibriums, strong pressure fluctuations and hardly interacted different size scales of motions [1]. Following the self-sustained cycle of the plumes, they produce alternative nonequilibriums between the buoyant production and the viscous dissipation, which are mainly compensated by the pressure transport mechanisms [2]. As a consequence, predicting the complex coherent dynamics in a turbulent buoyancy-driven flow derives formidable challenges, particularly within the scope of turbulence modeling.

Direct numerical simulations (DNS) have provided a fruitful knowledge about the problem in the fields of coherent dynamics and turbulence physics [3, 4]. Apart from overcoming the uncertainties pertaining to the experimental studies, DNS has allowed to investigate and resolve many queries in Rayleigh-Bénard convection (RBC) at relatively high Rayleigh (Ra) numbers [5, 6]. However, the full resolution of every generated vortical filament in DNS requires increasing computational demands with Ra. Therefore, in the foreseeable future, the numerical simulations of hard turbulent RBC will have to resort to turbulence modeling. We therefore turn to large-eddy simulation (LES) to predict the large-scale behavior of incompressible turbulent flows driven by buoyancy. In LES, the large scales of motions in a flow are explicitly computed, whereas effects of small-scale motions are modeled. Since the advent of computational fluid dynamics many subgrid-scale models have been proposed and successfully applied to a wide range of flows (see, for instance, the encyclopedic work of Sagaut [7]). The main goal of the current project is to improve the diffusive (linear) description of turbulent flows that is provided by eddy-diffusivity models for the subgrid-scale (SGS) heat flux. To that end, we will consider nonlinear SGS heat flux models that can properly represent the dynamics of the smallest (unresolved) scales, overcoming the inherent limitations of the eddy-diffusivity models [8]. Related with this, we also aim to find a proper definition of the subgrid characteristic length scale for simulations on anisotropic or unstructured grids. This is particularly important for highly anisotropic grids, on which the smallest grid spacing may start dominating the usually chosen characteristic length scale.

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. The model terms are designed to preserve important mathematical and physical properties, such as symmetries of the Navier-Stokes equations, and the near-wall scaling and the dissipative nature of the SGS. The desired properties are already included in existing models for the SGS stresses. Examples of eddy-viscosity models that exhibit the proper near-wall behavior are given by the WALE model [9], the σ-model [10] and the S3PQR model proposed in our previous work [11]. However, the (linear) eddy-diffusivity assumption fails to provide a reasonable approximation for the SGS heat flux. This has been clearly shown in our very recent work [8] where the SGS features have been studied *a priori* for a RBC at $Ra = 10^{10}$. We have also conclude that nonlinear (or tensorial) models can give a good approximation of the actual SGS heat flux. Among them, the models proposed by Daly and Harlow [12] (for RANS modeling) and Peng and Davidson [13] will be considered together with the new approach recently proposed on the basis of our *a priori* studies [8].

The rest of the paper is organized as follows. In the next section, the theoretical background of LES simulation of buoyancy-driven flows is presented. Then, in Section 3 different nonlinear SGS heat flux models are discussed and analyzed. Finally, conclusions are given in Section 4.

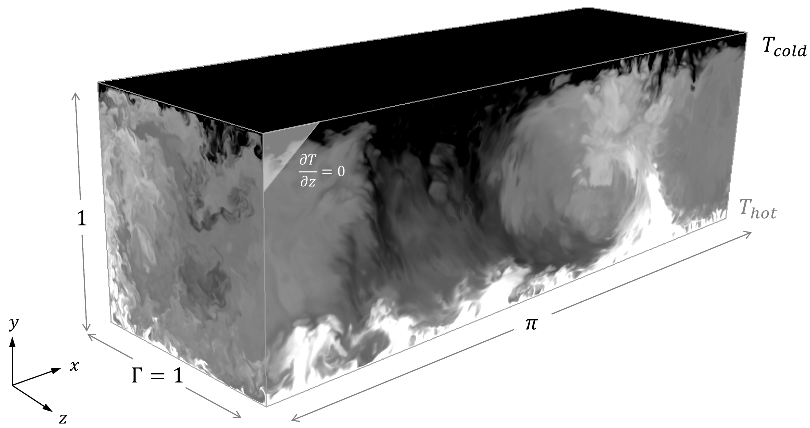

Figure 1: Schema of the Rayleigh-Bénard configuration studied in Refs. [4, 8]. Displayed together with a developed instantaneous temperature field taken of the DNS at $Ra = 10^{10}$.

2 BACKGROUND

2.1 Large-eddy simulation of buoyancy-driven flows

In large-eddy simulation, a filtering or coarse-graining operation is employed to distinguish between large and small scales of motion. This operation is denoted by an overbar in what follows. The evolution of the incompressible large-scale velocity, $\overline{\boldsymbol{u}}$, and temperature, $\overline{T}$, fields can be described by the filtered Navier-Stokes and thermal energy equations, supplemented by the incompressibility constraint,

$$\partial_t \overline{\boldsymbol{u}} + (\overline{\boldsymbol{u}} \cdot \nabla)\overline{\boldsymbol{u}} = (Pr/Ra)^{1/2} \; \nabla^2 \overline{\boldsymbol{u}} - \nabla \overline{p} + \overline{\boldsymbol{f}} - \nabla \cdot \tau \, ; \qquad \nabla \cdot \overline{\boldsymbol{u}} = 0, \tag{1}$$

$$\partial_t \overline{T} + (\overline{\boldsymbol{u}} \cdot \nabla)\overline{T} = (Ra/Pr)^{-1/2} \nabla^2 \overline{T} \qquad\qquad - \nabla \cdot \boldsymbol{q}, \tag{2}$$

where $\overline{\boldsymbol{u}}$, $\overline{T}$ and $\overline{p}$ are respectively the filtered velocity, temperature and pressure. The SGS stress tensor, τ, and the SGS heat flux vector, $\boldsymbol{q}$, represents the effect of the unresolved scales,

$$\tau = \overline{\boldsymbol{u} \otimes \boldsymbol{u}} - \overline{\boldsymbol{u}} \otimes \overline{\boldsymbol{u}}, \tag{3}$$

$$\boldsymbol{q} \; = \overline{\boldsymbol{u}T} - \overline{\boldsymbol{u}}\overline{T}, \tag{4}$$

and they need to be modeled in order to close the system. The most popular approach is the eddy-viscosity assumption, where the SGS stress tensor is computed in alignment with the local rate-of-strain tensor, $\mathsf{S} = 1/2(\nabla\overline{\boldsymbol{u}} + \nabla\overline{\boldsymbol{u}}^t)$, *i.e.*

$$\tau \approx -2\nu_e \mathsf{S}(\overline{\boldsymbol{u}}). \tag{5}$$

In analogy to τ, the SGS heat flux is often approximated employing the gradient-diffusion hypothesis (linear modeling), given by

$$\boldsymbol{q} \approx -\kappa_t \nabla \overline{T} \qquad (\equiv \boldsymbol{q}^{eddy}). \tag{6}$$

Then, the Reynolds analogy assumption is applied to evaluate the eddy-diffusivity, κ_t: the heat flux is assumed to be analogous to the momentum flux and its ratio therefore, is constant. In this case, the eddy-diffusivity, κ_t, is derived from the eddy-viscosity, ν_e, by a constant turbulent Prandtl number, Pr_t, independent of the instantaneous flow conditions, *i.e.* $\kappa_t = \nu_e/Pr_t$. These assumptions have been shown to be erroneous to provide accurate predictions of the SGS heat flux in our recent work [8]. Namely, *a priori* analysis has shown that the eddy-diffusivity assumption, $\boldsymbol{q}^{eddy}$ (Eq. 6), is completely misaligned with the actual subgrid heat flux, $\boldsymbol{q}$ (see Figure 2, top left). In conclusion, one can corroborate the failure of the isotropic eddy-diffusivity parametrization ($\boldsymbol{q}^{eddy}$) in turbulent buoyancy driven flows. In contrast, the tensor diffusivity (nonlinear) Leonard model [14], which is obtained by taking the leading term of the Taylor series expansion of $\boldsymbol{q}$,

$$\boldsymbol{q} \approx \frac{\delta^2}{12}\mathsf{G}\nabla\overline{T} \qquad (\equiv \boldsymbol{q}^{nl}), \tag{7}$$

provides a much more accurate *a priori* representation of $\boldsymbol{q}$ (see Figure 2, top left). Here, G represents the gradient of the resolved velocity field, *i.e.* $\mathsf{G} \equiv \nabla\overline{\boldsymbol{u}}$. Then, the rate-of-strain, S, and the rate-of-rotation, Ω, tensors are respectively given by the symmetric and anti-symmetric parts,

$$\mathsf{S} = \frac{1}{2}(\mathsf{G}+\mathsf{G}^T) \qquad \Omega = \frac{1}{2}(\mathsf{G}-\mathsf{G}^T). \tag{8}$$

It can be argued that the rotational geometries are prevalent in the bulk region over the strain slots, *i.e.* $|\Omega| > |\mathsf{S}|$ (see Refs [4, 8]). Then, the dominant anti-symmetric tensor, Ω, rotates the thermal gradient vector, $\nabla\overline{T}$ to be almost perpendicular to $\boldsymbol{q}^{nl}$ (see Eq.7). Therefore, the eddy-diffusivity paradigm is only applicable in the not-so-frequent strain-dominated areas. This also matches with the observations of Chumakov [15], who performed *a priori* study of the SGS flux of a passive scalar in isotropic homogeneous turbulence.

2.2 Nonlinear SGS heat flux models for large-eddy simulation

Since the eddy-diffusivity, $\boldsymbol{q}^{eddy}$, cannot provide an accurate representation of the SGS heat flux, we turn our attention to nonlinear models. As mentioned above, the Leonard model [14] given in Eq.(7) can provide a very accurate *a priori* representation of the SGS heat flux (see Figure 2, top left). However, the local dissipation (in the L2-norm sense) is proportional to $\nabla T \cdot \mathsf{G}\nabla T = \nabla T \cdot \mathsf{S}\nabla T + \nabla T \cdot \Omega\nabla T = \nabla T \cdot \mathsf{S}\nabla T$. Since the velocity field is divergence-free, $\lambda_1^{\mathsf{S}} + \lambda_2^{\mathsf{S}} + \lambda_3^{\mathsf{S}} = 0$, and the eigensystem can be ordered $\lambda_1^{\mathsf{S}} \geqslant \lambda_2^{\mathsf{S}} \geqslant \lambda_3^{\mathsf{S}}$ with $\lambda_1^{\mathsf{S}} \geqslant 0$ (extensive eigendirection) and $\lambda_3^{\mathsf{S}} \leqslant 0$ (compressive eigendirection), and λ_2^{S} is either positive or negative. Hence, the local dissipation introduced by the model can take on 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 [13],

$$\boldsymbol{q} \approx C_t\delta^2\mathsf{S}\nabla T \qquad (\equiv \boldsymbol{q}^{PD}). \tag{9}$$

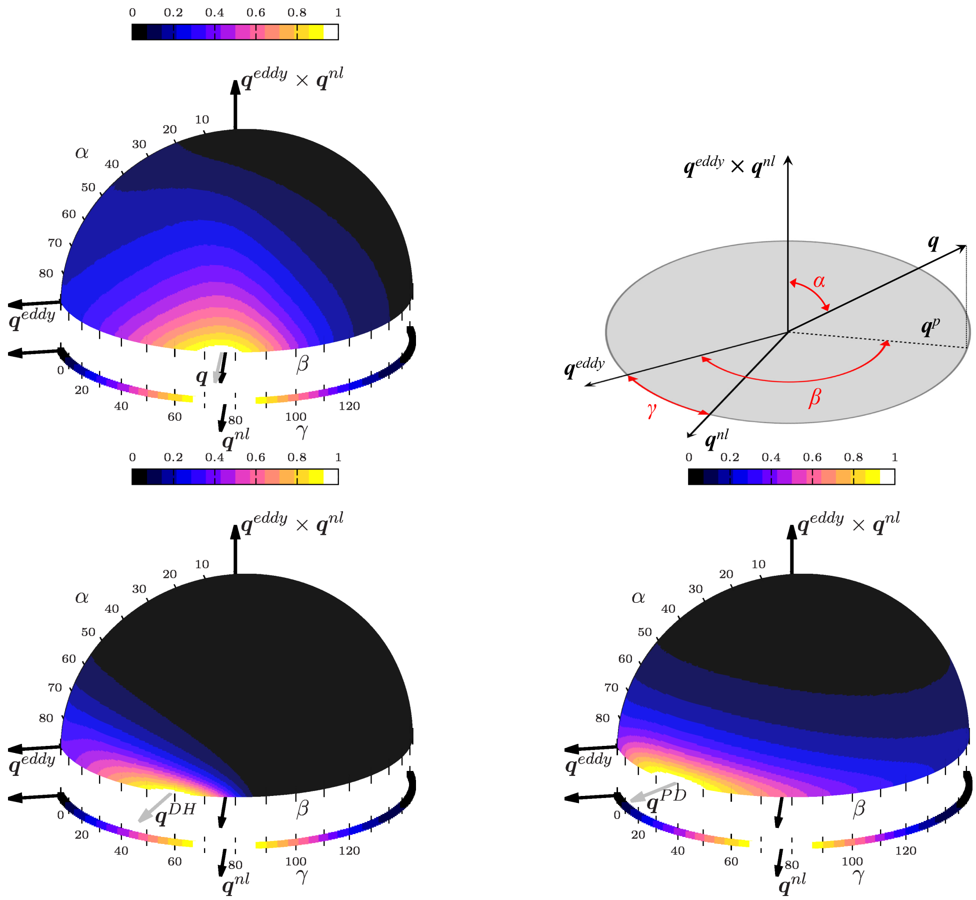

Figure 2: Joint probability distribution functions (PDF) of the angles (α, β) defined in the top right figure and plotted on a half unit sphere to show the orientation trends in the space of the mixed model. The PDF of γ is shown along the bottom strip of each chart. Alignment trends of the actual SGS heat flux, $\boldsymbol{q}$ (top, left), the Daly and Harlow [12] model (see $\boldsymbol{q}^{DH}$ in Eq. 11) (bottom, left) and the Peng and Davidson model [13] (see $\boldsymbol{q}^{PD}$ in Eq. 9) (bottom, right). For comparative and simplicity reasons, the JPDF and the PDF magnitudes are normalized by its maximal. For further details the reader is referred to our recent paper [8].

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An attempt to overcome these instability issues is the so-called mixed model [16], where the Leonard model (Eq. 7) is linearly combined with an eddy-diffusivity model (Eq. 6),

$$\boldsymbol{q} \approx \frac{\delta^2}{12}\left(\mathsf{G}\nabla T - \Lambda|\mathsf{S}|\nabla T\right) \qquad (\equiv \boldsymbol{q}^{mix}), \tag{10}$$

where Λ is the ratio of the corresponding model coefficients. Another interesting nonlinear model was proposed by Daly and Harlow [12] for modeling the SGS heat flux for RANS,

$$\boldsymbol{q} \approx -\mathcal{T}_{SGS}\tau\nabla T = -\frac{1}{|\mathsf{S}|}\frac{\delta^2}{12}\mathsf{G}\mathsf{G}^T\nabla T \qquad (\equiv \boldsymbol{q}^{DH}), \tag{11}$$

where $\mathcal{T}_{SGS} = 1/|\mathsf{S}|$ is an appropriate SGS timescale [15] and the SGS stress tensor, τ, is approximated with the gradient model [17], *i.e.* $\tau \approx (\delta^2/12)\mathsf{G}\mathsf{G}^T$. Notice that the model

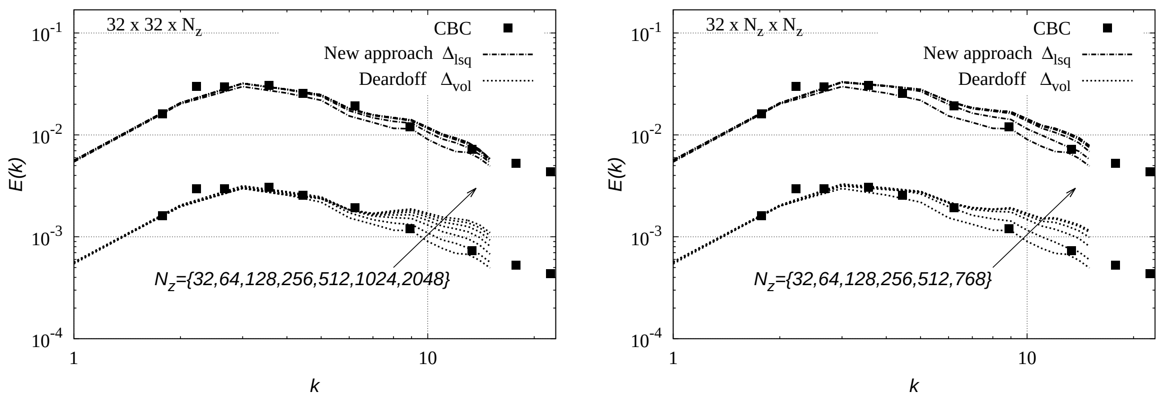

Figure 3: Energy spectra for decaying isotropic turbulence corresponding to the experiment of Comte-Bellot and Corrsin [18]. Results obtained with the new definition δ_{lsq} proposed in Eq.(12) are compared with the classical definition proposed by Deardorff given in Eq.(14). For clarity, latter results are shifted one decade down. For details the reader is referred to our recent paper [19].

proposed by Peng and Davidson (Eq. 9) can be viewed in the same framework if the SGS stress tensor is estimated by an eddy-viscosity model, *i.e.* $\tau \approx -2\nu_e \mathsf{S}$ and $\mathcal{T}_{SGS} \propto \delta^2/\nu_e$. These two models have shown a much better *a priori* alignment with the actual SGS heat flux (see Figure 2, bottom).

2.3 Choice of the characteristic length scale

As is clear from the definition of all the model coefficients, we need a specification of the subgrid characteristic length scale, δ. The subgrid characteristic length is usually associated with the local grid size. That is, for isotropic grids, δ is taken equal to the mesh size, $\delta = \Delta x = \Delta y = \Delta z$. However, for anisotropic or unstructured grids, a consensus has not been reached yet. In this context, and with the aim to overcome the limitation of the Deardorff definition [20] (cube root of the cell volume), the following definition for δ was proposed and studied in a recent paper [19],

$$\delta_{\text{lsq}} = \sqrt{\frac{\mathsf{G}_\delta \mathsf{G}_\delta^T : \mathsf{G}\mathsf{G}^T}{\mathsf{G}\mathsf{G}^T : \mathsf{G}\mathsf{G}^T}}, \tag{12}$$

where $\mathsf{G} \equiv \nabla \overline{\boldsymbol{u}}$, $\mathsf{G}_\delta \equiv \mathsf{G}\Delta$ and $\Delta \equiv \text{diag}(\Delta x, \Delta y, \Delta z)$ (for a Cartesian grid). This definition of δ fulfills a set of desirable properties. Namely, it is locally defined and well bounded, $\Delta x \leq \delta_{\text{lsq}} \leq \Delta z$ (assuming that $\Delta x \leq \Delta y \leq \Delta z$). Moreover, it is sensitive to flow orientation and applicable to unstructured meshes (by simply replacing the tensor Δ by the Jacobian of the mapping from the physical to the computational space). This definition (12) is obtained minimizing (in a least-squares sense) the difference between the leading terms of the Taylor series of the SGS tensor, $\tau(\overline{\boldsymbol{u}})$, for an isotropic and an anisotropic filters lengths; namely,

$$\tau(\overline{\boldsymbol{u}}) = \frac{\delta^2}{12}\mathsf{G}\mathsf{G}^T + \mathcal{O}(\delta^4)\ ; \quad \tau(\overline{\boldsymbol{u}}) = \frac{1}{12}\mathsf{G}_\delta \mathsf{G}_\delta^T + \mathcal{O}(\delta^4), \tag{13}$$

Results displayed in Figure 3 correspond to the classical experimental results obtained by Comte-Bellot and Corrsin [18]. LES results have been obtained using the Smagorinsky model, for a set of (artificially) stretched meshes. In contrast with the results obtained using the Deardorff definition [20],

$$\delta_{\mathrm{vol}} = (\Delta x \Delta y \Delta z)^{1/3}, \tag{14}$$

the proposed definition of the subgrid characteristic length, δ_{lsq}, significantly minimizes the effect of mesh anisotropies on the performance of SGS stress tensor models. For further details the reader is referred to our recent paper [19].

3 BUILDING A PROPER SGS HEAT FLUX MODEL

3.1 Exploring nonlinear SGS heat flux models

In this work we focus on finding a nonlinear SGS heat flux model with good physical and mathematical properties, that provides both accurate *a priori* representation of the actual SGS heat flux, $\boldsymbol{q}$, and satisfactory *a posteriori* predictions for turbulent buoyancy driven flows.

Let us remark that the focus of this study is not on the eddy-viscosity part of the model (see Eq. 5), but on the nonlinear approximation of the SGS heat flux, $\boldsymbol{q}$ (see Eq. 4). We do, however, have to make a specific choice for the SGS stress tensor model. We can, for instance, take one of the previously mentioned models: the WALE model [9], the σ-model [10] or the S3PQR models [11] (with the same near-wall scaling as the true turbulent stresses). Aiming to include several of the desirable properties according to which these models have been designed, we suggest to take the S3QR model proposed in our work [11],

$$\nu_e^{S3QR} = (C_{s3qr}\delta)^2 Q_{\mathsf{GG}^T}^{-1} R_{\mathsf{GG}^T}^{5/6}, \tag{15}$$

where Q_{GG^T} and R_{GG^T}, are the second and the third invariants of the GG^T tensor, respectively. This model exhibits the same near-wall scaling behavior as the turbulent stresses and it vanishes in all two-component flows, as well as in states of pure shear and pure rotation. Moreover, from a numerical point-of-view, it is solely based on the local flow topology contained in the tensor of the resolved velocity field, G, it is well-conditioned and it always provides non-negative values for $\nu_e \geq 0$.

As mentioned before, (linear) eddy-diffusivity (see Eq. 6) assumption cannot provide an accurate representation of the SGS heat flux, $\boldsymbol{q}$; hence, we turn our attention to nonlinear models. The least to be expected from a SGS model is to keep the stability of the numerical solution. This is the case of the model proposed by Daly and Harlow [12] (see Eq. 11): the tensor GG^T is positive semi-definite. Moreover, this model has shown a rather good *a priori* alignment with the actual SGS heat flux (see Figure 2, bottom left). Apart from this, we also want to explore nonlinear models based on the tensor, $\mathsf{G}_\theta \mathsf{G}_\theta^T$, proposed in our recent work [8]. This tensor is also positive semi-definite and *a priori* studies of the SGS heat flux model given by

$$\boldsymbol{q} \approx -\frac{1}{2}\frac{1}{|\mathsf{S}|}\frac{\mathsf{G}_\theta \mathsf{G}_\theta^T}{|\nabla T|^2}\nabla T, \tag{16}$$

have displayed rather good alignment trends too. Furthermore, like the above-mentioned S3PQR models for the SGS stress tensor, τ, we also want that the SGS heat flux model have the proper cubic near-wall behavior. This is not the case of any of these two potential candidates. Corrections in this regard will be also explored.

4 CONCLUDING REMARKS AND FUTURE RESEARCH

Motivated by our recent findings showing that the classical (linear) eddy-diffusivity assumption, $\boldsymbol{q}^{eddy} \propto \nabla\overline{T}$, fails to provide a reasonable approximation for the SGS heat flux, $\boldsymbol{q} = \overline{\boldsymbol{u}T} - \overline{\boldsymbol{u}}\overline{T}$ (see Figure 2), in this work we plan to shed light on the following research question: *can we find a nonlinear SGS heat flux model with good physical and numerical properties, such that we can obtain satisfactory predictions for a turbulent Rayleigh-Bénard convection?* We aim to answer this question by first studying the capability of the eddy-viscosity assumption (see Eq. 5) to model the SGS stress tensor, τ, without any modelization of the SGS heat flux. To do so, we will carry out LES simulations for very low Pr numbers. In this case, the ratio between the Kolmogorov length scale and the Obukhov-Corrsin length scale is given by $Pr^{1/2}$ [7]; therefore, for a $Pr = 0.005$ (liquid sodium) we have a separation of more than one decade. Hence, it is possible to combine a LES simulation for the velocity field, $\overline{\boldsymbol{u}}$, with the numerical resolution of all the relevant scales of the thermal field, T. Furthermore, we will study the performance of the above-mentioned nonlinear SGS heat flux models. Results from LES simulations will be compared with those obtained from DNS. In this regard, it is expected to play an important role the results obtained from the on-going PRACE supercomputing project *"Exploring new frontiers in Rayleigh-Bénard convection"* awarded with 33.1Mh in last PRACE 15th call. Results will be presented during the conference.

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