WORKSHOP
Direct and Large-Eddy Simulation 12
June 5th-7th 2019, Madrid, Spain

ON A PROPER TENSOR-DIFFUSIVITY MODEL FOR LARGE-EDDY SIMULATIONS OF BUOYANCY DRIVEN FLOWS

F.X.Trias[1], **F.Dabbagh**[1,2], **A.Gorobets**[1,3], **A.Oliva**[1]
[1] Heat and Mass Transfer Technological Center, Technical University of Catalonia
C/Colom 11, 08222 Terrassa (Barcelona) xavi@cttc.upc.edu
[2] Christian Doppler Laboratory for Multi-Scale Modeling of Multiphase Processes,
Johannes Kepler University, Altenbergerstraße 69, 4040 Linz, Austria
[3] Keldysh Institute of Applied Mathematics, 4A, Miusskaya Sq., Moscow 125047, Russia.

In this work, we plan to shed light on the following research question: *can we find a nonlinear 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 findings showing that the classical (linear) eddy-diffusivity assumption fails to provide a reasonable approximation for the SGS heat flux. This was shown in our work [1] where SGS features have been studied *a priori* for a Rayleigh-Bénard convection. We have also concluded that nonlinear (or tensorial) models can give good approximations of the actual SGS heat flux. Briefly, the large-eddy simulation (LES) equations arise from applying a spatial commutative filter, with filter length δ, to the incompressible Navier-Stokes and thermal energy equations,

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

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

where $\overline{\boldsymbol{u}}$, $\overline{T}$ and $\overline{p}$ are respectively the filtered velocity, temperature and pressure, and the incompressibility constraint reads $\nabla \cdot \overline{\boldsymbol{u}} = 0$. The SGS stress tensor, $\tau = \overline{\boldsymbol{u} \otimes \boldsymbol{u}} - \overline{\boldsymbol{u}} \otimes \overline{\boldsymbol{u}}$, and the SGS heat flux vector, $\boldsymbol{q} = \overline{\boldsymbol{u}T} - \overline{\boldsymbol{u}}\overline{T}$, represent the effect of the unresolved scales, 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 assumed to be aligned with the local rate-of-strain tensor, $\mathsf{S} = 1/2(\nabla \overline{\boldsymbol{u}} + \nabla \overline{\boldsymbol{u}}^t)$, *i.e.* $\tau \approx -2\nu_e \mathsf{S}(\overline{\boldsymbol{u}})$. By analogy, the SGS heat flux, $\boldsymbol{q}$, is usually approximated using the gradient-diffusion hypothesis (linear modeling), given by

$$\boldsymbol{q} \approx -\kappa_t \nabla \overline{T} \qquad (\equiv \boldsymbol{q}^{eddy}). \quad (3)$$

Then, the Reynolds analogy assumption is applied to evaluate the eddy-diffusivity, κ_t, via a constant turbulent Prandtl number, Pr_t, *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 [1]. Namely, *a priori* analysis showed that the eddy-diffusivity assumption, $\boldsymbol{q}^{eddy}$ (Eq. 3), is completely misaligned with the actual subgrid heat flux, $\boldsymbol{q}$ (see Figure 1, top). In contrast, the tensor diffusivity (nonlinear) Leonard model [2], which is obtained by taking the leading term of the Taylor series expansion of $\boldsymbol{q}$,

$$\boldsymbol{q} \approx \frac{\delta^2}{12} \mathsf{G} \nabla \overline{T} \qquad (\equiv \boldsymbol{q}^{nl}), \quad (4)$$

provides a much more accurate *a priori* representation of $\boldsymbol{q}$ (see Figure 1, top). Here, $\mathsf{G} \equiv \nabla \overline{\boldsymbol{u}}$ represents the gradient of the resolved velocity field. 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 [1, 3]). Then, the dominant anti-symmetric tensor, $\Omega = 1/2(\mathsf{G} - \mathsf{G}^T)$, rotates the thermal gradient vector, $\nabla \overline{T}$, to be almost perpendicular to $\boldsymbol{q}^{nl}$ (see Eq.4). Therefore, the eddy-diffusivity paradigm is only applicable in the not-so-frequent strain-dominated areas.

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 [2] given in Eq.(4) can provide a very accurate *a priori* representation of the SGS heat flux (see Figure 1, 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, $\lambda_1^{\mathsf{S}} + \lambda_2^{\mathsf{S}} + \lambda_3^{\mathsf{S}} = 0$, 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 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 $\boldsymbol{q}^{PD}$ proposed by Peng and Davidson [5],

$$\boldsymbol{q} \approx C_t \delta^2 \mathsf{S} \nabla T \qquad (\equiv \boldsymbol{q}^{PD}), \quad (5)$$

$$\boldsymbol{q} \approx -\mathcal{T}_{SGS} \tau \nabla T = -\frac{1}{|\mathsf{S}|} \frac{\delta^2}{12} \mathsf{G} \mathsf{G}^T \nabla T \qquad (\equiv \boldsymbol{q}^{DH}), \quad (6)$$

whereas the nonlinear model $\boldsymbol{q}^{DH}$ proposed by Daly and Harlow [4] relies on the positive semi-definite tensor $\mathsf{G}\mathsf{G}^T$. Here, $\mathcal{T}_{SGS} = 1/|\mathsf{S}|$ is the SGS timescale. Notice that the model proposed by Peng and Davidson, $\boldsymbol{q}^{PD}$, 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, especially the DH model (see Figure 1, middle). Moreover, the DH is numerically stable since the tensor $\mathsf{G}\mathsf{G}^T$ is positive semi-definite. Hence, it seems appropriate to build models based on this tensor. However, the DH model does not have the proper near-wall behaviour, *i.e.* $\boldsymbol{q} \propto \langle v'T' \rangle = \mathcal{O}(y^3)$ where y is the distance to the wall. An analysis of the DH model leads to $\mathsf{G}\mathsf{G}^T \nabla \overline{T} \propto \mathcal{O}(y^1)$. Therefore, the

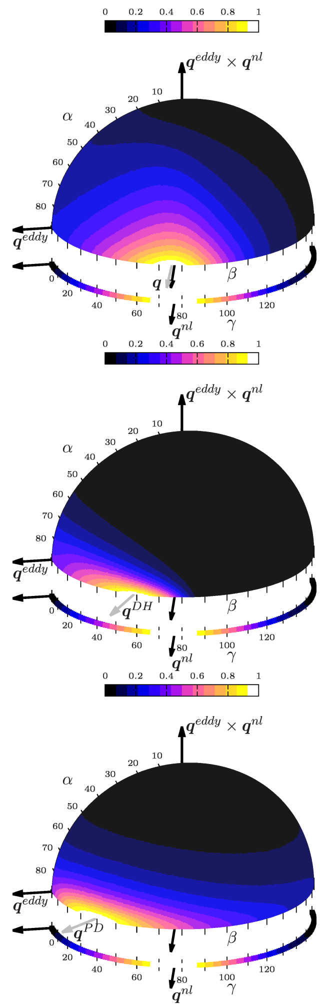

Figure 1: Joint probability distribution functions (PDF) of the angles (α, β) plotted on a half unit sphere to show the orientation in the space of the mixed model. From top to bottom, alignment trends of the actual SGS heat flux, $\boldsymbol{q}$, the Daly and Harlow [4] model (Eq. 6) and the Peng and Davidson model [5] (Eq. 5). For simplicity, the JPDF and the PDF magnitudes are normalized by its maximal. For details the reader is referred to [1].

near-wall cubic behaviour is recovered if $\mathcal{T}_{SGS} \propto \mathcal{O}(y^2)$. This is not the case of the timescale used in the Daly and Harlow [4] model, *i.e.* $\mathcal{T}_{SGS} = 1/|\mathsf{S}| = \mathcal{O}(y^0)$.

At this point it is interesting to observe that new timescales can be derived by imposing restrictions on the differential operators they are based on. For instance, let us consider models that are based on the invariants of the tensor GG^T

$$\boldsymbol{q} \approx -C_M \left(P^p_{\mathsf{GG}^T} Q^q_{\mathsf{GG}^T} R^r_{\mathsf{GG}^T} \right) \frac{\delta^2}{12} \mathsf{GG}^T \nabla T \qquad (\equiv \boldsymbol{q}^{S2}) \quad (7)$$

where P_{GG^T}, Q_{GG^T} and R_{GG^T} are the first, second and third invariant of the GG^T tensor. This tensor is proportional to the gradient model [6] given by the leading term of the Taylor series expansion of the subgrid stress tensor $\tau(\overline{\boldsymbol{u}}) = (\delta^2/12)\mathsf{GG}^T + \mathcal{O}(\delta^4)$. Then, the exponents p, q and r in Eq.(7), must satisfy the following equations

$$-6r - 4q - 2p = 1; \qquad 6r + 2q = s, \qquad (8)$$

to guarantee that the differential operator has units of time,

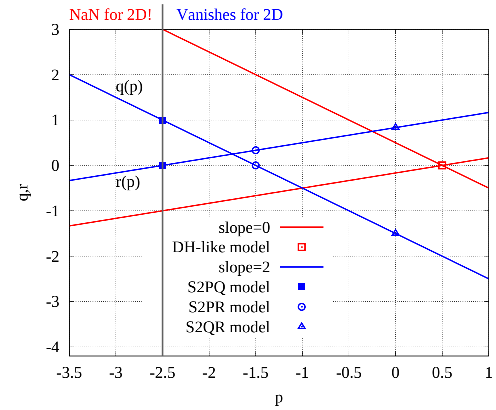

Figure 2: Solutions of the linear system of Eq.(8) for $s = 0$ (red lines) and $s = 2$ (blue lines). Each (r, p, q) represents an tensor-diffusivity model with the form of Eq.(7).

i.e. $[P^p_{\mathsf{GG}^T} Q^q_{\mathsf{GG}^T} R^r_{\mathsf{GG}^T}] = [T^1]$ and a slope s for the asymptotic near-wall behavior, *i.e.* $\mathcal{O}(y^s)$. Solutions for $q(p, s) = -(1 + s)/2 - p$ and $r(p, s) = (2s+1)/6 + p/3$ are displayed in Figure 2. It we restrict ourselves to solutions with the proper near-wall scaling, *i.e.* $s = 2$ (blue lines in Figure 2), a family of p-dependent models follows. Restricting ourselves to solutions involving only two invariants of GG^T three models are found. Namely,

$$\boldsymbol{q}^{S2PQ} = -C_{s2pq} P^{-5/2}_{\mathsf{GG}^T} Q_{\mathsf{GG}^T} \frac{\delta^2}{12} \mathsf{GG}^T \nabla \overline{T}, \qquad (9)$$

$$\boldsymbol{q}^{S2PR} = -C_{s2pr} P^{-3/2}_{\mathsf{GG}^T} R^{1/3}_{\mathsf{GG}^T} \frac{\delta^2}{12} \mathsf{GG}^T \nabla \overline{T}, \qquad (10)$$

$$\boldsymbol{q}^{S2QR} = -C_{s2qr} Q^{3/2}_{\mathsf{GG}^T} R^{5/6}_{\mathsf{GG}^T} \frac{\delta^2}{12} \mathsf{GG}^T \nabla \overline{T}, \qquad (11)$$

for $p = -5/2$, $p = -1.5$ and $p = 0$, respectively. These three solutions are represented in Figure 2. Apart from being unconditionally stable, these models display very good *a priori* alignment trends in the bulk (similar to the PD model; see Figure 1, middle) but also in the near-wall region. Hence, we consider that they are very good candidates for *a posteriori* LES simulations of buoyancy-driven flows. Results from LES simulations will be compared with the DNS data obtained in the PRACE project *"Exploring new frontiers in Rayleigh-Bénard convection"*.

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