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SYMMETRY-PRESERVING APPROXIMATE DECONVOLUTIONS

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Summary. Reconciling accuracy, physical fidelity and stability is not an easy task in CFD. We (the community) usually opt for numerical techniques that provide stable solutions regardless of the working conditions. A clear example thereof is he modelization of the subgrid-scales (SGS) in large-eddy simulation (LES). On one hand, the most popular models rely on the eddy-viscosity (eddy-diffusivity for the transport of active/passive scalars) assumption despite their well-known lack of accuracy in *a priori* studies. On the other hand, the gradient model, which is the leading term of the Taylor series of the SGS flux, is much more accurate *a priori* but cannot be used as a standalone model since it produces a finite-time blow-up. Another example is the construction of (high-order) numerical schemes on unstructured grids: since stability is a must, we usually choose between (local) accuracy (*e.g.* high-order numerical schemes for the flux reconstruction) or physical fidelity (*e.g.* second-order symmetry-preserving discretization). In this context, we firstly aim to reconcile accuracy and stability for the gradient model. To do so, it is expressed as a linear combination of regularized (smoother) forms of the convective operator, $\mathcal{C}(\boldsymbol{u}, \phi) \equiv (\boldsymbol{u} \cdot \nabla)\phi$, as follows

$$\nabla \cdot \tau_{\phi}^{grad} = \mathcal{C}(\boldsymbol{u}, \phi) + \overline{\mathcal{C}(\boldsymbol{u}, \phi)} - \mathcal{C}(\overline{\boldsymbol{u}}, \phi) - \mathcal{C}(\boldsymbol{u}, \overline{\phi}). \quad (1)$$

deconvolution of the exact SGS flux, $\tau_{\phi} \equiv \overline{\boldsymbol{u}\phi} - \overline{\boldsymbol{u}}\overline{\phi}$. Moreover, it facilitates the mathematical analysis of the gradient model, neatly identifying those terms that may cause numerical instabilities, leading to a new unconditionally stable non-linear model that can be viewed as a stabilized version of the gradient model. In this way, we expect to combine the good *a priori* accuracy of the gradient model with the stability required in practical simulations. Finally, we also show that (high-order) symmetry-preserving discretizations can be derived in the same vein.

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. Therefore, we may turn to large-eddy simulation (LES) to predict the large-scale behavior of turbulent flows: namely, the large scales are

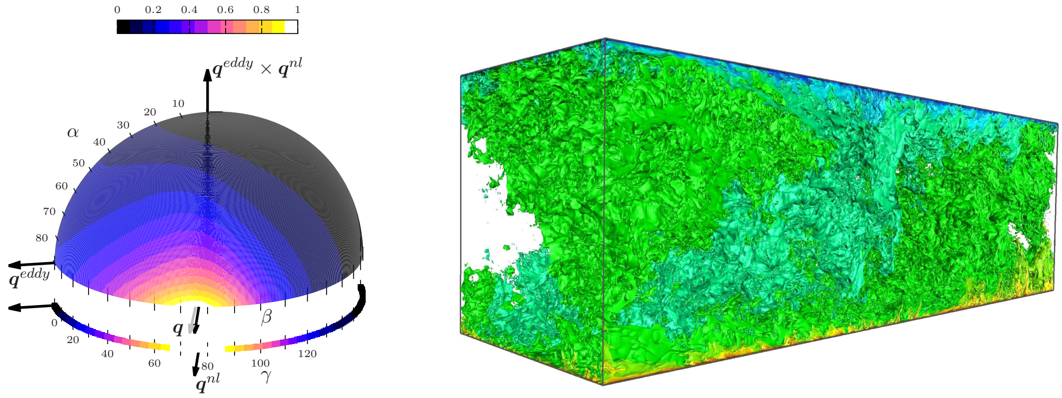

Figure 1: Left: alignment trends of the actual SGS heat flux. For details the reader is referred to our work [3]. Right: DNS of the air-filled RBC at $Ra = 10^{10}$ studied in Refs. [3, 7].

explicitly computed, whereas effects of small scale motions are modeled. Since the advent of CFD many subgrid-scale (SGS) 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 models fail to properly approximate of the actual SGS flux since they are strongly misaligned [1, 2]. This was shown in our previous works [3, 4] where the SGS features were studied *a priori* for a Rayleigh–Bénard convection (RBC) at Ra-number up to 10^{11} (see $\boldsymbol{q}^{eddy}$ in Figure 1). This leads to the conclusion that nonlinear (or tensorial) models are necessary to provide good approximations of the SGS heat flux (see $\boldsymbol{q}$ in Figure 1). In this regard, the nonlinear Leonard model [5] (or gradient model), which is the leading term of the Taylor series of the SGS flux, provides a very accurate *a priori* approximation (see $\boldsymbol{q}^{nl}$ in Figure 1). However, the local dissipation introduced by the model can take negative values (see Section 3); therefore, the Leonard model (also other similar structural models) cannot be used as a standalone SGS flux model, since it has a finite-time blow-up [6]. In this context, we aim to shed light to the following research question: *can we find a simple approach to reconcile accuracy and stability for the gradient model?*

2 DECONSTRUCTING THE GRADIENT MODEL

Let us firstly consider the following transport equation

$$\partial_t \phi + \mathcal{C}(\boldsymbol{u}, \phi) = \mathcal{D}\phi, \tag{2}$$

where $\boldsymbol{u}$ denotes the advective velocity and ϕ represents a generic (transported) scalar field. The non-linear convective term is given by $\mathcal{C}(\boldsymbol{u}, \phi) \equiv (\boldsymbol{u} \cdot \nabla)\phi$ whereas the diffusive terms reads $\mathcal{D}\phi \equiv \Gamma \nabla^2 \phi$. Shortly, LES equations arises from applying a spatial commutative filter, $\overline{(\cdot)}$, with filter length, δ,

$$\partial_t \overline{\phi} + \mathcal{C}(\overline{\boldsymbol{u}}, \overline{\phi}) = \mathcal{D}\overline{\phi} - \nabla \cdot \tau_\phi, \tag{3}$$

where $\tau_\phi \equiv \overline{\boldsymbol{u}\phi} - \overline{\boldsymbol{u}}\overline{\phi}$ is the subgrid scalar flux. Then, the gradient model follows from considering a Taylor-series expansion of the filter

$$\phi = \overline{\phi} + \phi' = \overline{\phi} - \frac{\delta^2}{24}\nabla^2\phi + \mathcal{O}(\delta^4), \tag{4}$$

where ϕ' is the filter residual. Then, applying this to $\overline{\boldsymbol{u}\phi}$ and $\overline{\boldsymbol{u}}\overline{\phi}$ leads to

$$\overline{\boldsymbol{u}\phi} \approx \boldsymbol{u}\phi + \frac{\delta^2}{24}\nabla^2(\boldsymbol{u}\phi) = \boldsymbol{u}\phi + \frac{\delta^2}{24}(\nabla^2\boldsymbol{u})\phi + \frac{\delta^2}{12}\nabla\boldsymbol{u}\nabla\phi + \frac{\delta^2}{24}\boldsymbol{u}\nabla^2\phi,$$
$$\overline{\boldsymbol{u}}\overline{\phi} \approx \left(\boldsymbol{u} + \frac{\delta^2}{24}\nabla^2\boldsymbol{u}\right)\left(\phi + \frac{\delta^2}{24}\nabla^2\phi\right) = \boldsymbol{u}\phi + \frac{\delta^2}{24}(\nabla^2\boldsymbol{u})\phi + \frac{\delta^2}{24}\boldsymbol{u}\nabla^2\phi + \frac{\delta^4}{24^2}\nabla^2\boldsymbol{u}\nabla^2\phi.$$

Finally, plugging this into the definition of τ_ϕ and discarding high-order terms yields

$$\tau_\phi \approx \tau_\phi^{grad} = \frac{\delta^2}{12}\nabla\boldsymbol{u}\nabla\phi, \tag{5}$$

which is the standard form of the gradient model. Alternatively, it can be expressed in terms of regularized (smoother) forms of the convective operator as follows

$$\nabla \cdot \tau_\phi^{grad} = \mathcal{C}(\boldsymbol{u},\phi) + \widetilde{\mathcal{C}(\boldsymbol{u},\phi)} - \mathcal{C}(\widetilde{\boldsymbol{u}},\phi) - \mathcal{C}(\boldsymbol{u},\widetilde{\phi}), \tag{6}$$

where

$$\widetilde{\mathcal{C}(\boldsymbol{u},\phi)} - \mathcal{C}(\boldsymbol{u},\phi) = \frac{\tilde{\delta}^2}{24}\nabla^2\nabla\cdot(\boldsymbol{u}\phi) = \frac{\tilde{\delta}^2}{24}\nabla\cdot(\nabla^2(\boldsymbol{u}\phi)), \tag{7}$$

$$\mathcal{C}(\widetilde{\boldsymbol{u}},\phi) - \mathcal{C}(\boldsymbol{u},\phi) = \frac{\tilde{\delta}^2}{24}\nabla\cdot((\nabla^2\boldsymbol{u})\phi), \tag{8}$$

$$\mathcal{C}(\boldsymbol{u},\widetilde{\phi}) - \mathcal{C}(\boldsymbol{u},\phi) = \frac{\tilde{\delta}^2}{24}\nabla\cdot(\boldsymbol{u}\nabla^2\phi). \tag{9}$$

Here $\widetilde{(\cdot)}$ denotes an explicit filter with filter length $\tilde{\delta}$. Notice that in practice we usually assume that the filter length of the gradient model is equal to the local grid size, *i.e.* $\tilde{\delta} = \delta = \Delta x$. The alternative form given in Eq.(6) is simply based on the non-linear convective operator and the linear filter; therefore, its implementation is straightforward. Moreover, it avoids the interpolations required if the standard gradient model given in Eq.(5) is directly implemented. Finally, it facilitates the analysis of the gradient model, neatly identifying those terms that may cause numerical instabilities. This is addressed in the following section.

3 STABILIZING THE GRADIENT MODEL

Following the notation used in Ref. [8], the novel form of the gradient model given in Eq.(6) would be discretized as follows

$$\mathsf{M}\boldsymbol{\tau}_{\phi,h}^{grad} = \mathsf{C}(\boldsymbol{u}_s)\boldsymbol{\phi}_c + \mathsf{F}\mathsf{C}(\boldsymbol{u}_s)\boldsymbol{\phi}_c - \mathsf{C}(\mathsf{F}\boldsymbol{u}_s)\boldsymbol{\phi}_c - \mathsf{C}(\boldsymbol{u}_s)\mathsf{F}\boldsymbol{\phi}_c, \tag{10}$$

where $\boldsymbol{u}_s$ and $\boldsymbol{\phi}_c$ are respectively the discrete velocity field defined at the faces and the cell-centered scalar field. Moreover, M, $\mathsf{C}(\boldsymbol{u}_s)$ and F are matrices representing the discrete divergence, convective and filter operators. For details, the reader is referred to Ref. [8]. Then, the

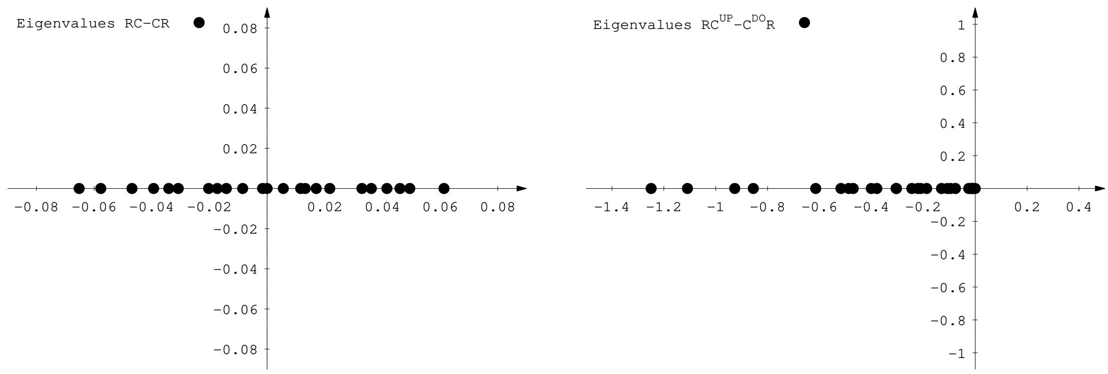

Figure 2: Location of the eigenvalues for the matrix $\mathsf{CF} - \mathsf{FC}$ (left) and $\mathsf{RC}^{\mathsf{UP}} - \mathsf{C}^{\mathsf{DO}}\mathsf{R}$ (right). Results correspond to a 5×5 Cartesian with a random divergence-free velocity field.

discrete form of $\nabla \cdot \tau_{\phi}^{grad}$ can be expressed in matrix-vector form as follows

$$\mathsf{M}\boldsymbol{\tau}_{\phi,h}^{grad} = \begin{pmatrix} \mathsf{I} \\ \mathsf{R} \end{pmatrix}^T \begin{pmatrix} \mathsf{C}(\boldsymbol{u}_s) - \mathsf{C}(\mathsf{F}\boldsymbol{u}_s) & \mathsf{C}(\boldsymbol{u}_s) \\ -\mathsf{C}(\boldsymbol{u}_s) & 0 \end{pmatrix} \begin{pmatrix} \mathsf{I} \\ \mathsf{R} \end{pmatrix} \boldsymbol{\phi}_c. \tag{11}$$

where R is the filter residual, *i.e.* $\mathsf{F} = \mathsf{I} - \mathsf{R}$. Recalling that the discrete convective and filter operator should be respectively represented by a skew-symmetric matrix, $\mathsf{C} = -\mathsf{C}^T$, and a symmetric matrix, $\mathsf{F}{=}\mathsf{F}^T$, the contribution of the gradient model to the time-evolution of the L2-norm of $\boldsymbol{\phi}_c$ is given by

$$-\boldsymbol{\phi}_c \cdot \mathsf{M}\boldsymbol{\tau}_{\phi,h}^{grad} = \boldsymbol{\phi}_c \cdot (\mathsf{RC} - \mathsf{CR})\, \boldsymbol{\phi}_c. \tag{12}$$

Hereafter, for simplicity, $\mathsf{C} = \mathsf{C}(\boldsymbol{u}_s)$. Therefore, stability of the gradient model is determined by the sign of the Rayleigh quotient of the matrix $\mathsf{RC} - \mathsf{CR}$. Therefore, if $\mathsf{C} = -\mathsf{C}^T$, as it should be from a physical point-of-view,

$$\boldsymbol{\phi}_c \cdot \mathsf{RC}\boldsymbol{\phi}_c = \boldsymbol{\phi}_c \cdot (\mathsf{RC})^T \boldsymbol{\phi}_c = \boldsymbol{\phi}_c \cdot \mathsf{C}^T \mathsf{R}^T \boldsymbol{\phi}_c = -\boldsymbol{\phi}_c \cdot \mathsf{CF}\boldsymbol{\phi}_c. \tag{13}$$

In this case, there is no guarantee that the eigenvalues of the matrix $\mathsf{RC} - \mathsf{CR}$ lie on stable half-side and, therefore, the gradient model will be eventually unstable. This is clearly shown in Figure 2 (left) where the location of the eigenvalues is displayed for a 5×5 stretched Cartesian mesh with a random divergence-free velocity field.

Nevertheless, at this point, we have neatly identified the discrete operators that lead to unstable modes. Hence, they must be modified if we aim to solve the problem. A very simple solution consists on replacing C by C^{UP} (lower diagonal) and C^{DO} (upper diagonal) in the off-diagonal terms in Eq.(11), leading to an overall contribution to the time-evolution of the L2-norm of $\boldsymbol{\phi}_c$ given by

$$-\boldsymbol{\phi}_c \cdot \mathsf{M}\boldsymbol{\tau}_{\phi,h}^{grad} = \boldsymbol{\phi}_c \cdot \left(\mathsf{RC}^{\mathsf{UP}} - \mathsf{C}^{\mathsf{DO}}\mathsf{R}\right) \boldsymbol{\phi}_c, \tag{14}$$

where $\mathsf{C}^{\mathsf{UP}}/\mathsf{C}^{\mathsf{DO}}$ correspond to a first-order upwind/downwind discretization of the convective term. In this way, all the eigenvalues lie on the stable half-side (see Figure 2, right).

4 TOWARDS HIGH-ORDER SYMMETRY-PRESERVING SCHEMES

Within a finite-volume framework the diffusive term is discretized on a 1D uniform mesh as follows

$$\left.\frac{\partial^2 \phi}{\partial x^2}\right|_{x_i} = \frac{1}{h}\left(\left.\frac{\partial \phi}{\partial x}\right|_{x_{i+1/2}} - \left.\frac{\partial \phi}{\partial x}\right|_{x_{i-1/2}} \right) + \mathcal{O}(h^2), \tag{15}$$

where h is the grid spacing. Notice that this expression is indeed exact in integral form. Nevertheless, it can also be viewed as applying a box filter with filter length equal to h

$$\overline{\phi}(x) = \frac{1}{h}\int_{x-h/2}^{x+h/2} \phi dx, \tag{16}$$

Namely,

$$\left.\overline{\frac{\partial^2 \phi}{\partial x^2}}\right|_{x_i} = \frac{1}{h}\left(\left.\frac{\partial \phi}{\partial x}\right|_{x_{i+1/2}} - \left.\frac{\partial \phi}{\partial x}\right|_{x_{i-1/2}} \right). \tag{17}$$

Moreover, the partial derivatives are discretized using a second-order approximation

$$\left.\frac{\partial \phi}{\partial x}\right|_{x_{i+1/2}} \approx \frac{\phi_{i+1} - \phi_i}{h} + \mathcal{O}(h^2) \tag{18}$$

Notice that this discretization can also be written as follows

$$\left.\overline{\frac{\partial \phi}{\partial x}}\right|_{x_{i+1/2}} = \left.\frac{\partial \overline{\phi}}{\partial x}\right|_{x_{i+1/2}} = \frac{\phi_{i+1} - \phi_i}{h}. \tag{19}$$

Notice that both Eqs.(17) and (19) are exact expressions. Hence, the standard second-order finite-volume discretization can be viewed as

$$\left.\frac{\partial^2 \phi}{\partial x^2}\right|_{x_i} \approx \left.\overline{\frac{\partial^2 \overline{\phi}}{\partial x^2}}\right|_{x_i} + \mathcal{O}(h^2) \qquad \text{where} \qquad \left.\overline{\frac{\partial^2 \overline{\phi}}{\partial x^2}}\right|_{x_i} = \frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{h^2}. \tag{20}$$

This analysis can be extended to multidimensional problems leading to

$$\nabla^2 \phi \approx \overline{\nabla^2 \overline{\phi}} + \mathcal{O}(h^2), \tag{21}$$

At this point, we recall the Taylor-series expansion of the filter given in Eq.(4) to obtain the following expression

$$\nabla^2 \phi = \overline{\nabla^2 \overline{\phi}} + \overline{\nabla^2 \phi'} + (\nabla^2 \overline{\phi})' + (\nabla^2 \phi')'. \tag{22}$$

Therefore, the order of accuracy can be improved by considering additional terms as follows

$$\nabla^2 \phi \approx \overline{\nabla^2 \overline{\phi}} + \overline{\nabla^2 \phi'} + (\nabla^2 \overline{\phi})' + \mathcal{O}(h^4). \tag{23}$$

Let us apply this to the above 1D case

$$\frac{\partial^2 \phi}{\partial x^2} \approx \overline{\frac{\partial^2 \overline{\phi}}{\partial x^2}} + \overline{\frac{\partial^2 \phi'}{\partial x^2}} + \left(\frac{\partial^2 \overline{\phi}}{\partial x^2}\right)' + \mathcal{O}(h^4). \tag{24}$$

where the filter residual can be computed as

$$\phi_i' \approx -\frac{1}{24}(\overline{\phi}_{i+1} - 2\overline{\phi}_i + \overline{\phi}_{i-1}) + \mathcal{O}(h^2). \tag{25}$$

This corresponds to a second-order approximate deconvolution. Combining this with the Eq.(20) leads to

$$\begin{aligned} \left.\frac{\partial^2 \phi}{\partial x^2}\right|_{x_i} &\approx \frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{h^2} + 2\frac{-\phi_{i+2} + 4\phi_{i+1} - 6\phi_i + 4\phi_{i-1} - \phi_{i-2}}{24h^2} \\ &= \frac{-\phi_{i+2} + 16\phi_{i+1} - 30\phi_i + 16\phi_{i-1} - \phi_{i-2}}{12h^2} + \mathcal{O}(h^4), \end{aligned} \tag{26}$$

which is the classical 5-point fourth-order approximation of the second derivative. We may alternatively consider all the terms in the right-hand-side of Eq.(22) leading, in 1D, to the following expression

$$\frac{\partial^2 \phi}{\partial x^2} = \overline{\frac{\partial^2 \overline{\phi}}{\partial x^2}} + \overline{\frac{\partial^2 \phi'}{\partial x^2}} + \left(\frac{\partial^2 \overline{\phi}}{\partial x^2}\right)' + \left(\frac{\partial^2 \phi'}{\partial x^2}\right)'. \tag{27}$$

instead of Eq.(24). Notice that this extra term is $\mathcal{O}(h^4)$. Nevertheless, we can only compute an approximation using Eq.(25), *i.e.*

$$\left(\frac{\partial^2 \phi'}{\partial x^2}\right)_i' \approx \frac{\phi_{i+3} - 6\phi_{i+2} + 15\phi_{i+1} - 20\phi_i + 15\phi_{i-1} - 6\phi_{i-2} + \phi_{i-3}}{576h^2}, \tag{28}$$

leading to the following 7-point fourth-order approximation

$$\left.\frac{\partial^2 \phi}{\partial x^2}\right|_{x_i} \approx \frac{\phi_{i+3} - 54\phi_{i+2} + 783\phi_{i+1} - 1460\phi_i + 783\phi_{i-1} - 54\phi_{i-2} + \phi_{i-3}}{576h^2} + \mathcal{O}(h^4) \tag{29}$$

Compared with the 5-point approximation given in Eq.(26), the order of accuracy remains the same, *i.e.* fourth-order. However, this expression requires more memory, more data traffic and more floating-point operations, whereas the order of accuracy remains the same.

At discrete level, and using the same notation used in previous sections, it basically consist on replacing the standard second-order approximation of the discrete Laplacian, $\mathsf{L} \equiv \mathsf{MG}$, by the following expression

$$\mathsf{L}^{\mathsf{HO}} = (\mathsf{I} + \mathsf{R})\mathsf{L}(\mathsf{I} + \mathsf{R}), \tag{30}$$

where the discrete filter residual is defined as follows

$$\mathsf{R} \equiv -\frac{1}{24}\mathsf{T}^T\mathsf{T}, \tag{31}$$

and T is the cell-to-face incidence matrix (see [9] for details). Notice that L^{HO} is also a symmetric negative semi-definite matrix, as it should be from a physical point-of-view. The accuracy of the non-linear convective term can be improved in a similar manner as follow

$$\mathsf{C}^{\mathsf{HO}} = (\mathsf{I} + \mathsf{R})\mathsf{C}(\mathsf{I} + \mathsf{R}). \tag{32}$$

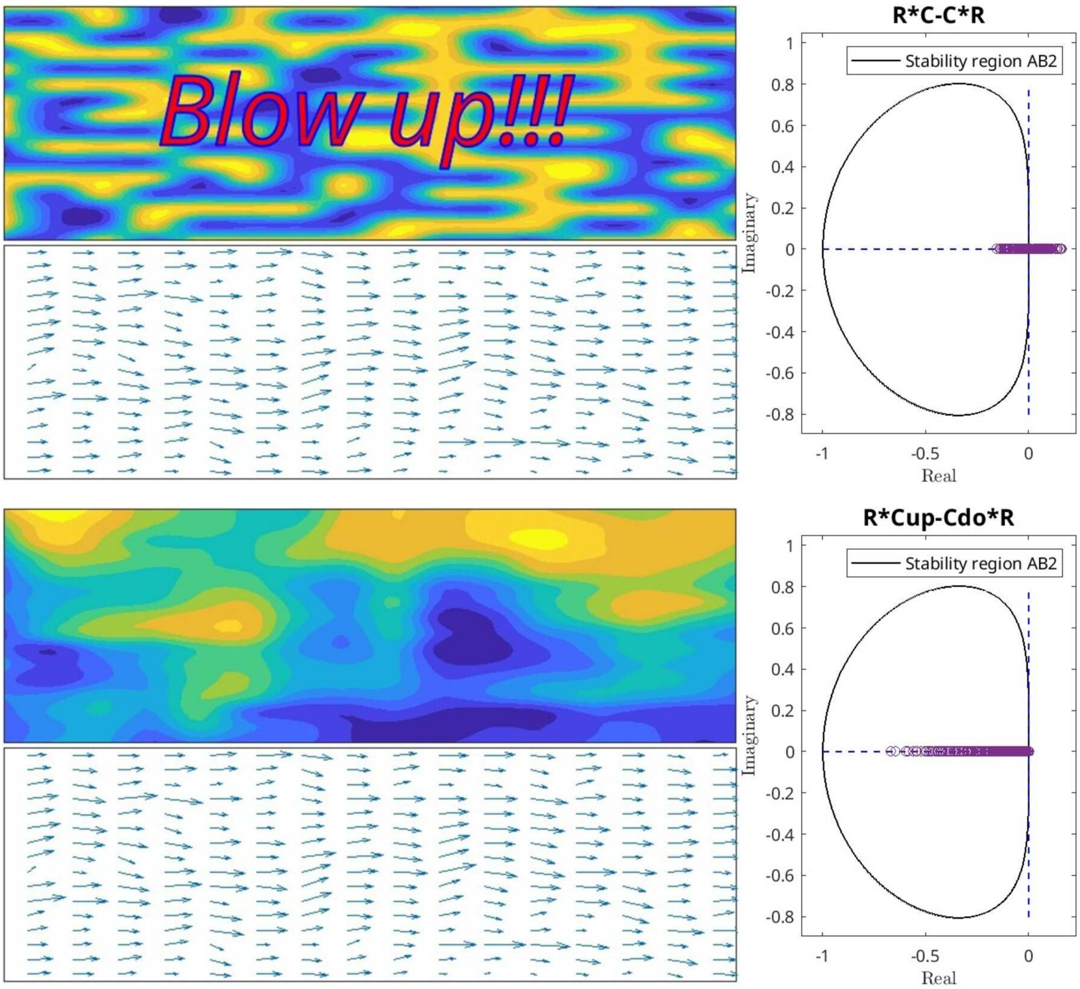

Figure 3: Top: transport of a passive scalar in a turbulent channel flow at $Re_\tau = 180$ and $Sc = 0.71$ using the standard gradient model given in Eq.(33) on a mesh of 16×16 control volumes (see the velocity field). In this case, the matrix $\mathsf{CF} - \mathsf{FC}$ contains unstable modes that eventually blow up the simulation. Bottom: exactly the same but using the alternative form given in Eq.(34). In this case, all the eigenvalues of the matrix $\mathsf{RC}^{\mathsf{UP}} - \mathsf{C}^{\mathsf{DO}}\mathsf{R}$ lie on the stable half side.

5 NUMERICAL RESULTS AND CONCLUSIONS

In this work, we have shown that the gradient model can be easily implemented as follows

$$\mathsf{M}\boldsymbol{\tau}^{grad}_{\phi,h} = \mathsf{C}\left(\boldsymbol{u}_s\right)\boldsymbol{\phi}_c - \mathsf{RC}\left(\boldsymbol{u}_s\right)\boldsymbol{\phi}_c - \mathsf{C}\left(\mathsf{R}\boldsymbol{u}_s\right)\boldsymbol{\phi}_c + \mathsf{C}\left(\boldsymbol{u}_s\right)\mathsf{R}\boldsymbol{\phi}_c, \tag{33}$$

where M, $\mathsf{C}\left(\boldsymbol{u}_s\right)$ and R are matrices representing the discrete divergence, convective and filter residual operators. This form is the discrete counterpart of Eq.(6), and the main advantages are twofold: (i) it reduces the number of interpolations, *i.e.* explicit *ad hoc* filtering operations, respect to the direct implementation of the standard form of the gradient model given in Eq.(5), and (ii) it can be straightforwardly implemented since it is based on already existing discrete operators. Nevertheless, it still contains unstable modes that may eventually blow up your numerical simulations; namely, the symmetric matrix $\mathsf{RC} - \mathsf{CR}$ contains positive eigenvalues. This is clearly observed in Figure 3 (top) where a passive scalar is transported in a turbulent channel flow at $Re_\tau = 180$ and $Sc = 0.71$ using a very coarse mesh of 16×16 control volumes. The scalar field blows up due to the above-mentioned presence of positive eigenvalues in the matrix $\mathsf{RC} - \mathsf{CR}$. To remedy this problem, we have proposed the following alternative approximation

$$\mathsf{M}\boldsymbol{\tau}^{grad}_{\phi,h} = \mathsf{C}\left(\boldsymbol{u}_s\right)\boldsymbol{\phi}_c - \mathsf{RC}^{\mathsf{UP}}(\boldsymbol{u}_s)\boldsymbol{\phi}_c - \mathsf{C}\left(\mathsf{R}\boldsymbol{u}_s\right)\boldsymbol{\phi}_c + \mathsf{C}^{\mathsf{DO}}(\boldsymbol{u}_s)\mathsf{R}\boldsymbol{\phi}_c. \tag{34}$$

It basically consists on replacing the matrix $\mathsf{RC}-\mathsf{CR}$ by $\mathsf{RC}^{\mathsf{UP}}-\mathsf{C}^{\mathsf{DO}}\mathsf{R}$, where $\mathsf{C}^{\mathsf{UP}}/\mathsf{C}^{\mathsf{DO}}$ correspond to a first-order upwind/downwind discretization of the convective term. It can be formally proved that, in this case, all the eigenvalues lie in the stable half side (see Figure 3, bottom) and, therefore, the simulation runs stably even for extremely coarse meshes. The proposed method is not limited to any type of mesh provided that the (skew-)symmetries of the discrete operators are preserved. This emphasizes even more the delicate entanglement between the numerical discretization and the modelization of the subgrid-scales. Future research plans include running *a posteriori* tests for more complex configurations.

Apart from this, we have explored a novel approach to developed high-order symmetry-preserving schemes. It basically consists on replacing the standard second-order approximation by an approximate deconvolution of both the convective and diffusive terms (see Eqs. 30 and 32). The main potential advantages of this new approach are twofold: (i) it is suitable for both structured and unstructured meshes, leading to a fourth-order symmetry-preserving discretization on those regions where the mesh is Cartesian (similarly to schemes proposed in Ref. [10] for structured Cartesian meshes), and (ii) it leads to matrices with a significantly higher number of non-zeros per rows, which leads to higher arithmetic intensity and, therefore, to a potentially higher performance [11].

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References

[1] C. W. Higgins, M. B. Parlange, and C. Meneveau. The heat flux and the temperature gradient in the lower atmosphere. *Geophysical Research Letter*, 31:L22105, 2004.

[2] S. G. Chumakov. "*A priori* study of subgrid-scale flux of a passive scalar in isotropic homogeneous turbulence. *Physical Review E*, 78:036313, 2008.

[3] F. Dabbagh, F. X. Trias, A. Gorobets, and A. Oliva. A priori study of subgrid-scale features in turbulent Rayleigh-Bénard convection. *Physics of Fluids*, 29:105103, 2017.

[4] F. Dabbagh, F. X. Trias, A. Gorobets, and A. Oliva. Flow topology dynamics in a three-dimensional phase space for turbulent Rayleigh-Bénard convection. *Physical Review Fluids*, 5:024603, 2020.

[5] A. Leonard. Large-eddy simulation of chaotic convection and beyond. *AIAA paper*, 97-0304, 1997.

[6] M. Klein, S. Ketterl, L. Engelmann, A. Kempf, and H. Kobayashi. Regularized, parameter free scale similarity type models for Large Eddy Simulation. *International Journal of Heat and Fluid Flow*, 81, 2020.

[7] F.X. Trias, F.Dabbagh, A.Gorobets, and C.Oliet. On a proper tensor-diffusivity model for large-eddy simulation of buoyancy-driven turbulence. *Flow, Turbulence and Combustion*, 105:393–414, 2020.

[8] F. X. Trias, O. Lehmkuhl, A. Oliva, C.D. Pérez-Segarra, and R.W.C.P. Verstappen. Symmetry-preserving discretization of Navier-Stokes equations on collocated unstructured meshes. *Journal of Computational Physics*, 258:246–267, 2014.

[9] F. X. Trias, X. Álvarez-Farré, À. Alsalti-Baldellou, A. Gorobets, and A. Oliva. An efficient eigenvalue bounding method: CFL condition revisited. *Computer Physics Communications*, 305:109351, 2024.

[10] R. W. C. P. Verstappen and A. E. P. Veldman. Symmetry-Preserving Discretization of Turbulent Flow. *Journal of Computational Physics*, 187:343–368, 2003.

[11] À. Alsalti-Baldellou, X. Álvarez-Farré, F. X. Trias, and A. Oliva. Exploiting spatial symmetries for solving Poisson's equation. *Journal of Computational Physics*, 486:112133, 2023.