On a proper tensorial subgrid heat flux model for LES

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Abstract. In this work, we aim to shed light on the following research question: *can we find a subgrid-scale (SGS) heat flux model with good physical and numerical properties, such that we can obtain satisfactory predictions for buoyancy-driven turbulence at high Rayleigh numbers?* This is motivated by our previous findings showing the limitations of existing SGS heat flux models for LES. On one hand, the most popular models rely on the eddy-diffusivity 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. 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. The new alternative form can indeed be viewed as an approximate deconvolution of the exact SGS flux. 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 indeed 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 numerical simulations.

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} (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 actual SGS

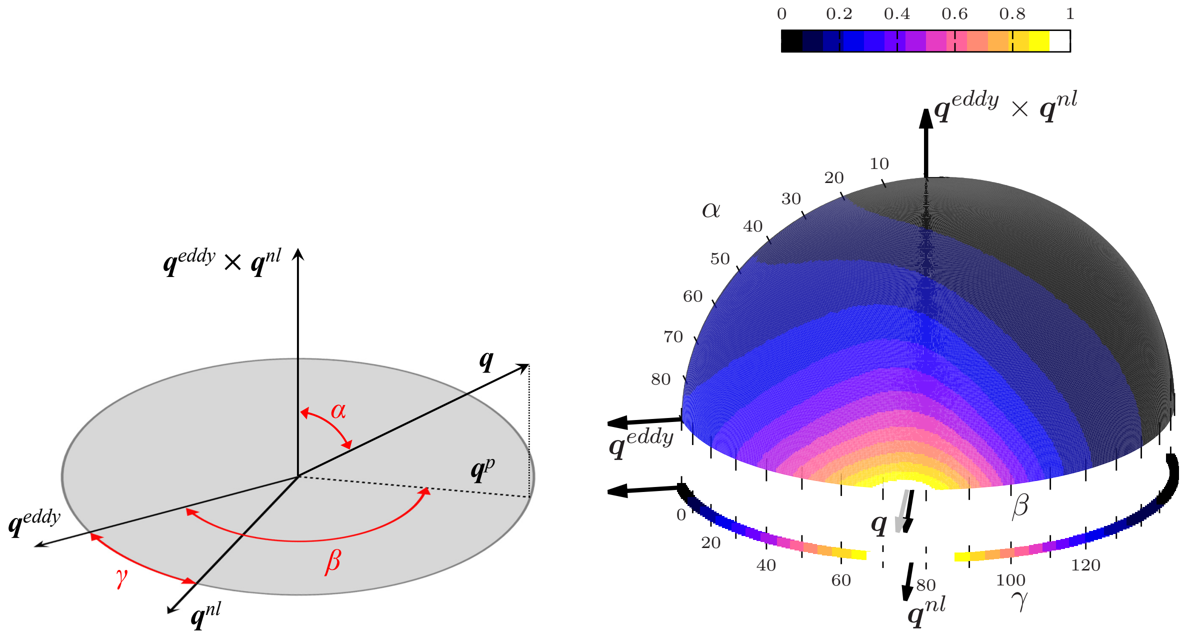

Figure 1. Alignment trends of the actual SGS heat flux for an air-filled Rayleigh–Bénard convection at Rayleigh 10^{10}. For details the reader is referred to our work [3].

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; therefore, the Leonard model cannot be used as a standalone SGS flux model, since it produces a finite-time blow-up. In this context, we aim to shed light to the following research question: *can we 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

$$\partial_t \phi + \mathcal{C}(\boldsymbol{u}, \phi) = \mathcal{D}\phi, \tag{1}$$

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,

$$\partial_t \overline{\phi} + \mathcal{C}(\overline{\boldsymbol{u}}, \overline{\phi}) = \mathcal{D}\overline{\phi} - \nabla \cdot \tau_\phi, \tag{2}$$

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

$$\overline{\phi} = \phi - \phi' = \phi + \frac{\delta^2}{24} \nabla^2 \phi + \mathcal{O}(\delta^4), \tag{3}$$

where $\phi' \approx -(\delta^2/24)\nabla^2\phi$ is the filter residual. Then, applying this to $\overline{\overline{\boldsymbol{u}}\overline{\phi}}$ leads to

$$
\begin{aligned}
\overline{\overline{\boldsymbol{u}}\overline{\phi}} &\approx \overline{\boldsymbol{u}}\overline{\phi} + \frac{\delta^2}{24}\nabla^2(\overline{\boldsymbol{u}}\overline{\phi}) \\
&= \overline{\boldsymbol{u}}\overline{\phi} + \frac{\delta^2}{24}(\nabla^2\overline{\boldsymbol{u}})\overline{\phi} + \frac{\delta^2}{12}\nabla\overline{\boldsymbol{u}}\nabla\overline{\phi} + \frac{\delta^2}{24}\overline{\boldsymbol{u}}\nabla^2\overline{\phi},
\end{aligned} \tag{4}
$$

and

$$
\begin{aligned}
\overline{\overline{\boldsymbol{u}\phi}} &\approx \overline{\left(\boldsymbol{u} + \frac{\delta^2}{24}\nabla^2\boldsymbol{u}\right)\left(\phi + \frac{\delta^2}{24}\nabla^2\phi\right)} = \overline{\boldsymbol{u}\phi} + \frac{\delta^2}{24}\overline{\boldsymbol{u}\nabla^2\phi} + \frac{\delta^2}{24}\overline{(\nabla^2\boldsymbol{u})\phi} + \frac{\delta^4}{24^2}\overline{\nabla^2\boldsymbol{u}\nabla^2\phi} \\
&\approx \overline{\boldsymbol{u}\phi} + \frac{\delta^2}{24}\overline{\boldsymbol{u}}\nabla^2\overline{\phi} + \frac{\delta^2}{24}(\nabla^2\overline{\boldsymbol{u}})\overline{\phi} + \mathcal{O}(\delta^4).
\end{aligned} \tag{5}
$$

Notice that $(\delta^2/24)\overline{a\nabla^2 b} \approx (\delta^2/24)\overline{a}\nabla^2\overline{b} + \mathcal{O}(\delta^4)$. Finally, combining eqs.(4) and (5) and discarding high-order terms leads to the standard form of the gradient model

$$
\tau_\phi \approx \tau_\phi^{grad} = \frac{\delta^2}{12}\nabla\overline{\boldsymbol{u}}\nabla\overline{\phi}. \tag{6}
$$

Hereafter all the overbars, $\overline{(\cdot)}$, are dropped for the sake of simplicity. Alternatively, τ_ϕ^{grad} can be expressed in terms of regularized (smoother) forms of the convective operator as follows

$$
\nabla\cdot\tau_\phi^{grad} = \mathcal{C}(\boldsymbol{u},\phi) + \widetilde{\mathcal{C}(\boldsymbol{u},\phi)} - \mathcal{C}(\widetilde{\boldsymbol{u}},\phi) - \mathcal{C}(\boldsymbol{u},\widetilde{\phi}), \tag{7}
$$

where

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

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

$$
\mathcal{C}(\boldsymbol{u},\widetilde{\phi}) - \mathcal{C}(\boldsymbol{u},\phi) = \frac{\tilde{\delta}^2}{24}\nabla\cdot(\boldsymbol{u}\nabla^2\phi). \tag{10}
$$

Notice that $\widetilde{(\cdot)}$ represents an explicit filter with filter length $\tilde{\delta}$ that is not necessarily equal to the filter length δ of the LES filter, $\overline{(\cdot)}$. The alternative form given in eq.(7) 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.(6) 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 next section.

3. Stabilizing the gradient model

Following the notation used in ref. [6], the novel form of the gradient model given in eq.(7) would be discretized as follows

$$
\mathsf{M}\boldsymbol{\tau}_{\phi,h}^{grad} = \mathsf{C}\left(\boldsymbol{u}_s\right)\boldsymbol{\phi}_c + \mathsf{F}\mathsf{C}\left(\boldsymbol{u}_s\right)\boldsymbol{\phi}_c - \mathsf{C}\left(\mathsf{F}\boldsymbol{u}_s\right)\boldsymbol{\phi}_c - \mathsf{C}\left(\boldsymbol{u}_s\right)\mathsf{F}\boldsymbol{\phi}_c, \tag{11}
$$

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, $\mathsf{C}\left(\boldsymbol{u}_s\right)$ and F are matrices representing the discrete

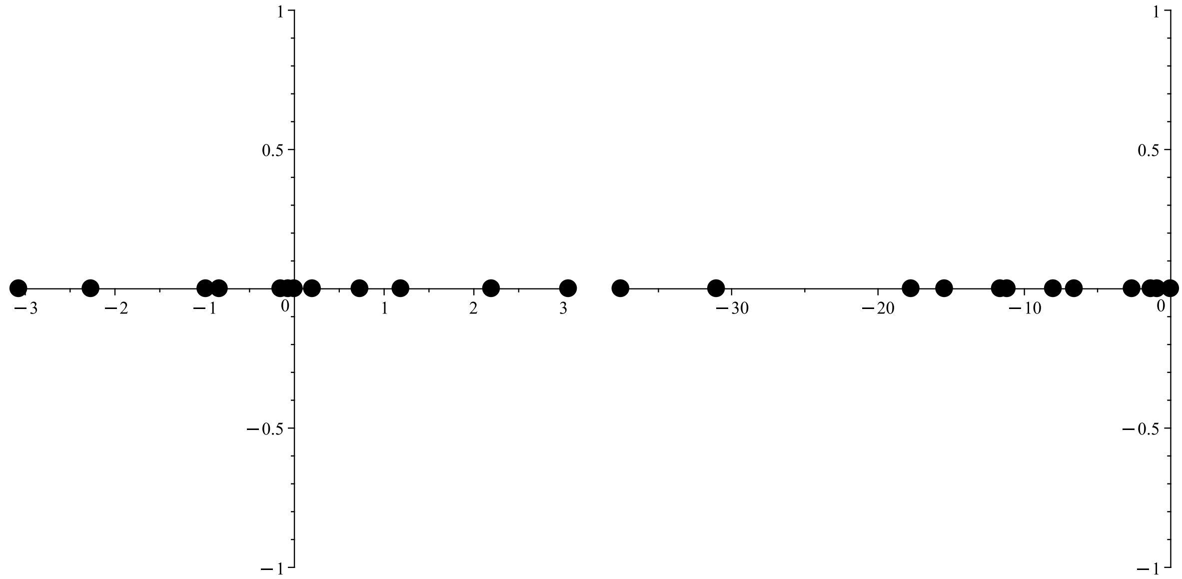

Figure 2. Location of the eigenvalues for the matrix $\mathsf{CF}-\mathsf{FC}$ (left) and $\mathsf{C}^{UP}\mathsf{F}-\mathsf{FC}^{UP}$ (right). Results correspond to a 4×3 Cartesian with a random divergence-free velocity field.

divergence, convective and filter operators. For details, the reader is referred to ref. [6]. This discrete form of τ_{ϕ}^{grad} can be expressed in matrix-vector form as follows

$$\mathsf{M}\boldsymbol{\tau}_{\phi,h}^{grad} = \begin{pmatrix} \mathsf{I} \\ \mathsf{F} \end{pmatrix}^T \begin{pmatrix} \mathsf{C}\left(\boldsymbol{u}_s\right) - \mathsf{C}\left(\mathsf{F}\boldsymbol{u}_s\right) & -\mathsf{C}\left(\boldsymbol{u}_s\right) \\ \mathsf{C}\left(\boldsymbol{u}_s\right) & 0 \end{pmatrix} \begin{pmatrix} \mathsf{I} \\ \mathsf{F} \end{pmatrix} \boldsymbol{\phi}_c. \tag{12}$$

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, F=F^T, the contribution of the gradient model to the time-evolution of the L2-norm of $\boldsymbol{\phi}_c$ is given by

$$-\boldsymbol{\phi}_c \cdot \mathsf{M}\boldsymbol{\tau}_{\phi,h}^{grad} = \boldsymbol{\phi}_c \cdot \left(\mathsf{CF}-\mathsf{FC}\right)\boldsymbol{\phi}_c. \tag{13}$$

For details regarding the construction of symmetric linear filter F, the reader is referred to our previous works [7, 8].

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

$$\boldsymbol{\phi}_c \cdot \mathsf{CF}\boldsymbol{\phi}_c = \boldsymbol{\phi}_c \cdot \left(\mathsf{CF}\right)^T\boldsymbol{\phi}_c = \boldsymbol{\phi}_c \cdot \mathsf{F}^T\mathsf{C}^T\boldsymbol{\phi}_c = -\boldsymbol{\phi}_c \cdot \mathsf{FC}\boldsymbol{\phi}_c. \tag{14}$$

In this case, there is no guarantee that the eigenvalues of the matrix $\mathsf{CF}-\mathsf{FC}$ will lie on stable half-side and, therefore, the gradient model will be eventually unstable. This is clearly shown in figure 2 (left) where the locations of the eigenvalues is displayed for a 3×4 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. To do so, we need firstly to re-write the expression given in eq.(11) as follows

$$\mathsf{M}\boldsymbol{\tau}_{\phi,h}^{grad} = \mathsf{C}\left(\boldsymbol{u}_s\right)\boldsymbol{\phi}_c - \mathsf{RC}\left(\boldsymbol{u}_s\right)\boldsymbol{\phi}_c - \mathsf{C}\left(\mathsf{F}\boldsymbol{u}_s\right)\boldsymbol{\phi}_c + \mathsf{C}\left(\boldsymbol{u}_s\right)\mathsf{R}\boldsymbol{\phi}_c, \tag{15}$$

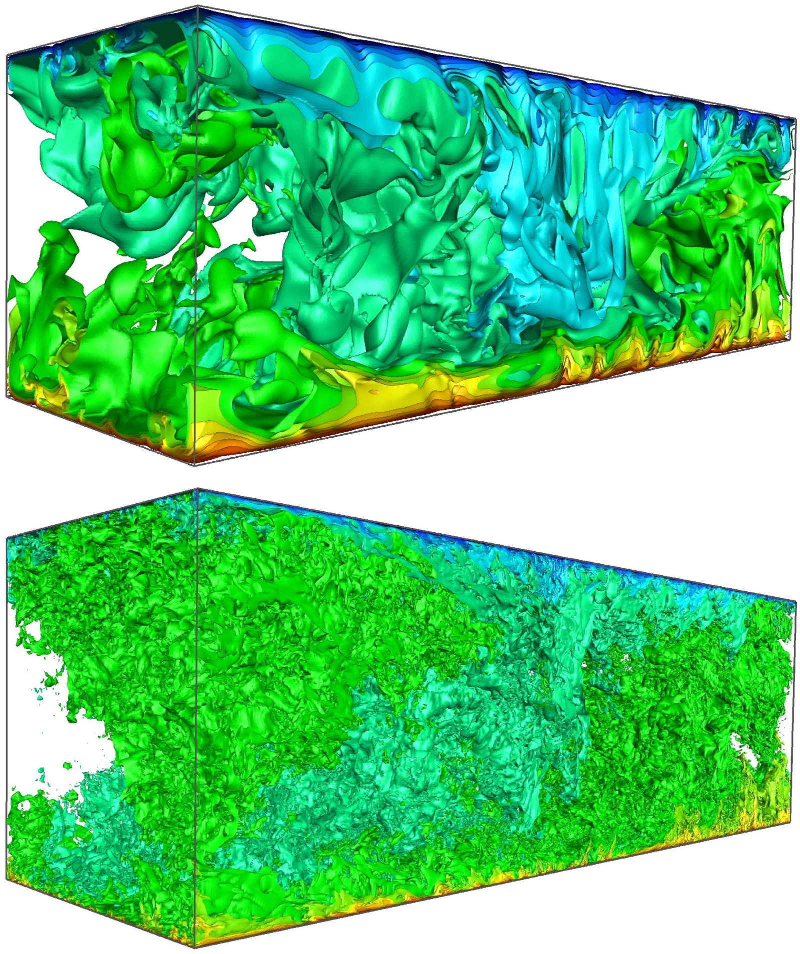

Figure 3. DNS of the air-filled RBC at $Ra = 10^8$ (top) and $Ra = 10^{10}$ (bottom) carried out on the MareNostrum 4 supercomputer using 17M (400x206x206) and 600M (1024x766x766) grid points, respectively.

where R is the filter residual, *i.e.* $\mathsf{F} = \mathsf{I} - \mathsf{R}$. Previous analysis can be easily redone leading to the following matrix-vector form

$$\mathsf{M}\boldsymbol{\tau}_{\phi,h}^{grad} = \begin{pmatrix} \mathsf{I} \\ \mathsf{R} \end{pmatrix}^T \begin{pmatrix} \mathsf{C}(\boldsymbol{u}_s) - \mathsf{C}(\mathsf{F}\boldsymbol{u}_s) & \mathsf{C}(\boldsymbol{u}_s) \\ -\mathsf{C}(\boldsymbol{u}_s) & 0 \end{pmatrix} \begin{pmatrix} \mathsf{I} \\ \mathsf{R} \end{pmatrix} \boldsymbol{\phi}_c. \tag{16}$$

and the following contribution to the L2-norm of $\boldsymbol{\phi}_c$

$$-\boldsymbol{\phi}_c \cdot \mathsf{M}\boldsymbol{\tau}_{\phi,h}^{grad} = \boldsymbol{\phi}_c \cdot (\mathsf{RC} - \mathsf{CR})\,\boldsymbol{\phi}_c. \tag{17}$$

At this point, a very simple solution consists on using an upwind/downwind for the convective terms in eq.(17); namely, replacing C by C^{UP} and C^{DO} in the off-diagonal terms in eq.(16), leading to an overall contribution to the time-evolution of the L2-norm of $\boldsymbol{\phi}_c$ given by

$$-\boldsymbol{\phi}_c \cdot \mathsf{M}\boldsymbol{\tau}_{\phi,h}^{grad} = \boldsymbol{\phi}_c \cdot \left(\mathsf{RC}^{\mathsf{UP}} - \mathsf{C}^{\mathsf{DO}}\mathsf{R}\right) \boldsymbol{\phi}_c, \tag{18}$$

where C^{UP} (C^{DO}) corresponds 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). A formal proof will be presented in the conference.

4. Concluding remarks

A new form of the standard gradient model has been proposed in eq.(7). Apart from being easier to implement than its standard form (see eq.6), it facilitates the mathematical analysis of the gradient model, neatly identifying those terms that may cause numerical instabilities leading to (details will be presented in the conference) to a new unconditionally stable non-linear model given by

$$\mathsf{M}\boldsymbol{\tau}_{\phi,h}^{grad} = \mathsf{C}\left(\boldsymbol{u}_s\right)\boldsymbol{\phi}_c - \mathsf{RC}\left(\boldsymbol{u}_s\right)^{\mathsf{UP}}\boldsymbol{\phi}_c - \mathsf{C}\left(\mathsf{F}\boldsymbol{u}_s\right)\boldsymbol{\phi}_c + \mathsf{C}\left(\boldsymbol{u}_s\right)^{\mathsf{DO}}\mathsf{R}\boldsymbol{\phi}_c, \tag{19}$$

where $\mathsf{C}\left(\boldsymbol{u}_s\right)^{\mathsf{UP}}$ and $\mathsf{C}\left(\boldsymbol{u}_s\right)^{\mathsf{DO}}$ correspond to a first-order upwind and downwind discretization of the convective term, respectively. This new form can indeed be viewed as a stabilized version of the gradient model than preserves good alignment trends (see figure 1, left). We plan to study *a posteriori* the performance of these models. In this case, LES simulations will be carried out with the same code (for details see refs.[9, 10]) and results compared with the DNS data corresponding to an air-filled ($Pr = 0.7$) RBC at Rayleigh number up to 10^{10} (see figure 3).

Acknowledgments

F.X.T. and A.O. are supported by SIMEX project (PID2022-142174OB-I00) of *Ministerio de Ciencia e Innovación* and the RETOtwin project (PDC2021-120970-I00) of *Ministerio de Economía y Competitividad*, Spain. Calculations were carried out on MareNostrum 4 supercomputer at BSC. The authors thankfully acknowledge these institutions.

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