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Parameter-free symmetry-preserving regularization modeling of a turbulent differentially heated cavity

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ABSTRACT

Since direct numerical simulations of buoyancy driven flows cannot be computed at high Rayleigh numbers, a dynamically less complex mathematical formulation is sought. In the quest for such a formulation, we consider regularizations (smooth approximations) of the non-linearity: the convective term is altered to reduce the production of small scales of motion by means of vortex stretching. In doing so, we propose to preserve the symmetry and conservation properties of the convective terms exactly. This requirement yielded a novel class of regularizations [Comput Fluids 2008;37:887] that restrain the convective production of smaller and smaller scales of motion in an unconditionally stable manner, meaning that the velocity cannot blow up in the energy-norm (in 2D also: enstrophy-norm). The numerical algorithm used to solve the governing equations preserves the symmetry and conservation properties too. In the present work, a criterion to determine dynamically the regularization parameter (local filter length) is proposed: it is based on the requirement that the vortex stretching must stop at the scale set by the grid. Therefore, the proposed method constitutes a parameter-free turbulence model. The resulting regularization method is tested for a 3D natural convection flow in an air-filled ($Pr = 0.71$) differentially heated cavity of height aspect ratio 4. Direct comparison with DNS results at Rayleigh number $6.4 \times 10^8 \leq Ra \leq 10^{11}$ shows fairly good agreement even for very coarse grids. Finally, the robustness of the method is tested by performing simulations with Ra up to 10^{17} . A $2/7$ scaling law of Nusselt number has been obtained for the investigated range of Ra .

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1. Introduction

Natural convection in parallelepipedic enclosures has been the subject of numerous studies over the past decades. Most of them can be classified in three main groups: cavities where the flow is due to internal heat generation, cavities heated from below (Rayleigh–Bénard configuration), and those heated from the sides. The configuration of the latter class, namely differentially heated cavity (DHC), is considered here. This configuration models many engineering applications such as ventilation of rooms, cooling of electronic devices or air flow in buildings. Simultaneously, since the pioneering work by Vahl Davis [1], where the original benchmark formulation was established, this configuration has served as a prototype for the development of numerical algorithms (see [2] and references therein, for instance).

An accurate prediction of the flow structure and the heat transfer in such a configuration is of great interest and despite the effort devoted (see for instance [3–8]) for an accurate turbulence modeling of this configuration, it still remains as a great challenge. This is mainly due to the complex behavior exhibit (see Fig. 1): the boundary layers remain laminar in their upstream part up to the point where the waves traveling downstream grow up enough to disrupt the boundary layers ejecting large unsteady eddies to the core of the cavity. The mixing effect of these eddies, that throw hot and cold fluid respectively, tends to result in almost isothermal hot upper and cold lower regions. This mixing effect at the top and bottom areas of the cavity forces the temperature drop in the core of the cavity to occur in a smaller region. Therefore, an accurate prediction of the transition point is crucial to determine correctly the flow structure in the cavity [8]. However, the high sensitivity of the thermal boundary layer to external disturbances makes it difficult to predict. Moreover, the 3D effects play an important role and therefore they must be considered; in [2] it was observed that the energy of 3D large eddies is rapidly passed down the cascade to smaller eddies. This leads to a manifest reduction of the mixing effect at the hot upper and cold lower regions and consequently the stratified cavity core remains motionless. In contrast the 2D

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Fig. 1. Top: Several instantaneous temperature fields at $Ra = 10^{11}$ and $Pr = 0.71$ (air). Bottom: Zoom around the point where the vertical boundary layer becomes totally disrupted and large eddies are ejected.

simulation results display increasingly large top and bottom regions of disorganization that reduce the area of uniform temperature stratification. This causes the transition point in the vertical boundary layers to move downstream in the 2D simulations. These differences become more pronounced when the Rayleigh number is increased. In conclusion, the DHC is a challenging configuration for turbulence modeling since areas with completely different regimes coexist and interplay.

The Navier–Stokes (NS) equations form an excellent mathematical model for turbulent flows. Preserving the (skew-)symmetries of the continuous differential operators when discretizing [9] them has been shown to be a very suitable approach for direct numerical simulation (DNS). Doing so, certain fundamental properties such as the inviscid invariants – kinetic energy, enstrophy (in 2D) and helicity (in 3D) – are exactly preserved in a discrete sense. However, direct simulation at high Rayleigh (Ra) numbers is not feasi-

ble. Therefore, a dynamically less complex mathematical formulation is needed. In the quest for such a formulation, we consider regularizations [10,11] (smooth approximations) of the non-linearity. The first outstanding approach in this direction goes back to Leray [12]; the Navier–Stokes- α model also forms an example of regularization modeling (see [11], for instance). The regularization methods basically alter the convective terms to reduce the production of small scales of motion. In doing so, we proposed to preserve the symmetry and conservation properties of the convective terms exactly [13]. This requirement yielded a family of *symmetry-preserving regularization* models: a novel class of regularizations that restrain the convective production of smaller and smaller scales of motion in an unconditionally stable manner, meaning that the velocity cannot blow up in the energy-norm (in 2D also: enstrophy-norm). The numerical algorithm used to solve the governing equations preserves the conservation properties too [9] and is

therefore well-suited to test the proposed simulation model. The regularization makes use of a normalized self-adjoint filter. In our previous works [13,14], we kept the ratio filter length/grid width constant. Thus, this parameter had to be prescribed in advance and therefore a convergence analysis was needed. In the present work, we propose to determine the regularization parameter (the local filter length) dynamically from the requirement that the vortex stretching must be stopped at the scale set by the grid. Thus, the proposed method constitutes a parameter-free turbulence model.

The rest of the paper is arranged as follows. In Section 2, the symmetry-preserving regularization modeling is presented and analyzed. Its relation with the Large-Eddy Simulation (LES) concept is also discussed. In Section 3, a new criteria to determine the regularization parameter (i.e., the local filter length) is proposed. It is based on the requirement that the vortex stretching must stop at the smallest grid scale. Then, the numerical approximations needed to apply the method in a discrete setting are addressed in Section 4. The important role of the discretization of the operators and the linear filter is discussed. In Section 5, the performance of the proposed method is evaluated for a 3D natural convection flow in an air-filled ($Pr = 0.71$) DHC of height aspect ratio 4. Results are compared with previous DNS data [2,15,16] for a wide range of Rayleigh numbers $6.4 \times 10^8 \leq Ra \leq 10^{11}$. Thereafter, simulations with Ra up to 10^{17} are also performed showing a very good agreement with the 2/7 power-law scaling of the Nusselt as a function of Ra . Finally, relevant results are summarized and conclusions are given.

2. Restraining the production of small scales: C_n -regularization method

2.1. Problem definition

We consider a differentially heated cavity of height L_3 , width, L_2 and depth L_1 , filled with an incompressible Newtonian viscous fluid of kinematic viscosity ν , thermal diffusivity α and density ρ . The Rayleigh number, Ra , (based on the cavity height) and the Prandtl number, Pr , are $g\beta L_3^3(T_h - T_c)/(\nu\alpha)$ and ν/α , respectively. To model the buoyancy term, the Boussinesq approximation is used. The thermal radiation is neglected. Under these conditions, the velocity, u , and the temperature, T , are governed by the following set of dimensionless partial differential equations

$$\partial_t u + \mathcal{C}(u, u) = PrRa^{-1/2} \Delta u - \nabla p + f, \quad (1)$$

$$\partial_t T + \mathcal{C}(u, T) = Ra^{-1/2} \Delta T, \quad (2)$$

where the convective term is given by $\mathcal{C}(u, v) = (u \cdot \nabla)v$, the body force vector is given by $f = (0, 0, Pr T)$ and the incompressibility constraint reads $\nabla \cdot u = 0$. The reference length, time, velocity, temperature and dynamic pressure are, L_3 , $(L_3^2/\alpha)Ra^{-1/2}$, $(\alpha/L_3)Ra^{1/2}$, $T_h - T_c$ and $\rho(\alpha^2/L_3^3)Ra$. The cavity (see Fig. 2) is subjected to a temperature difference, $T_h - T_c$, across the vertical isothermal walls while the top and bottom walls are adiabatic. The temperature and the velocity are assumed to be periodic in the x_1 -direction. The no-slip boundary condition is imposed on the velocity at the four closing walls. The cavity is filled with air ($Pr = 0.71$) and its height aspect ratio (L_3/L_2) is set equal to 4; hence, the configuration depends on the Ra only. For further details, the reader is referred to [2] and references therein.

2.2. Regularization modeling

At high Ra , the velocity and the temperature cannot be computed numerically from Eqs. (1) and (2), because the solution possesses far too many scales of motion. The computationally almost

Fig. 2. Differentially heated cavity problem.

numberless small scales result from the non-linear, convective terms $\mathcal{C}(u, u)$ and $\mathcal{C}(u, T)$ that allow the transfer of energy from the scales as large as the flow domain to the smallest scales that can survive viscous dissipation. In the quest for a dynamically less complex mathematical formulation, we consider smooth approximations (regularizations) of the non-linearity,

$$\partial_t u_\epsilon + \tilde{\mathcal{C}}(u_\epsilon, u_\epsilon) = PrRa^{-1/2} \Delta u_\epsilon - \nabla p_\epsilon + f_\epsilon, \quad (3)$$

$$\partial_t T_\epsilon + \tilde{\mathcal{C}}(u_\epsilon, T_\epsilon) = Ra^{-1/2} \Delta T_\epsilon, \quad (4)$$

where the variable names are changed from u and T to u_ϵ and T_ϵ , respectively, to stress that the solution of (3) and (4) differs from that of Eqs. (1) and (2).

The regularized system (3) and (4) should be more amenable to be solved numerically (that is, the regularization should limit the production of small scales of motion), while the leading modes of u_ϵ , T_ϵ have to approximate the corresponding modes of the solution u , T of Eqs. (1) and (2). The regularized system (3) and (4) may also be seen in relation to Large-Eddy Simulation (LES). In LES, Eqs. (1) and (2) are filtered spatially, and the resulting non-linear terms involving residual velocities and temperatures are modeled in terms of the filtered velocity and temperature:

$$\partial_t \bar{u}_\epsilon + \mathcal{C}(\bar{u}_\epsilon, \bar{u}_\epsilon) = PrRa^{-1/2} \Delta \bar{u}_\epsilon - \nabla \bar{p}_\epsilon + \bar{f}_\epsilon + \mathcal{M}_1(\bar{u}_\epsilon), \quad (5)$$

$$\partial_t \bar{T}_\epsilon + \mathcal{C}(\bar{u}_\epsilon, \bar{T}_\epsilon) = Ra^{-1/2} \Delta \bar{T}_\epsilon + \mathcal{M}_2(\bar{u}_\epsilon, \bar{T}_\epsilon), \quad (6)$$

where the model terms are approximately given by

$$\mathcal{M}_1(\bar{u}_\epsilon) \approx \mathcal{C}(\bar{u}_\epsilon, \bar{u}_\epsilon) - \overline{\mathcal{C}(u_\epsilon, u_\epsilon)},$$

$$\mathcal{M}_2(\bar{u}_\epsilon, \bar{T}_\epsilon) \approx \mathcal{C}(\bar{u}_\epsilon, \bar{T}_\epsilon) - \overline{\mathcal{C}(u_\epsilon, T_\epsilon)}.$$

The regularization described by Eqs. (3) and (4) falls in with this concept if

$$\overline{\mathcal{C}(u_\epsilon, u_\epsilon)} = \mathcal{C}(\bar{u}_\epsilon, \bar{u}_\epsilon) - \mathcal{M}_1(\bar{u}_\epsilon),$$

$$\overline{\mathcal{C}(u_\epsilon, T_\epsilon)} = \mathcal{C}(\bar{u}_\epsilon, \bar{T}_\epsilon) - \mathcal{M}_2(\bar{u}_\epsilon, \bar{T}_\epsilon). \quad (7)$$

Indeed under this condition, Eqs. (3) and (4) are equivalent to (5) and (6): we can filter (3) and (4) first and thereafter compare the filtered version of (3) and (4) term-by-term with (5) and (6)

to identify the closure models $\mathcal{M}_1(\bar{u}_\epsilon)$ and $\mathcal{M}_2(\bar{u}_\epsilon, \bar{T}_\epsilon)$. Finally, it may be noted that Eq. (7) relates the regularization $\mathcal{C}$ one-to-one to the closure models $\mathcal{M}_1$ and $\mathcal{M}_2$ for any invertible filter.

2.3. Symmetry-preserving regularization models

The regularization method basically alters the non-linearity to restrain the production of small scales of motion, (see e.g., [11]). In doing so, one can preserve certain fundamental properties of the convective operator $\mathcal{C}$ in Eqs. (1) and (2) exactly. We propose to preserve the symmetry properties that form the basis for the conservation of energy, enstrophy (in 2D) and helicity. The skew-symmetry (with respect to v and w) of the trilinear form $(\mathcal{C}(u, v), w)$

$$(\mathcal{C}(u, v), w) = -(v, \mathcal{C}(u, w)), \quad (8)$$

ensures the conservation of energy and helicity. Additionally, the following identity

$$(\mathcal{C}(u, v), \Delta v) = (u, \mathcal{C}(\Delta v, v)), \quad (9)$$

must be satisfied to conserve enstrophy in 2D. Therefore, we aim to regularize the convective operator $\mathcal{C}$ in such a manner that the underlying symmetries (given by Eqs. (8) and (9)) are preserved. In other words, we require that the approximation $\tilde{\mathcal{C}}$ of $\mathcal{C}$ satisfies

$$(\tilde{\mathcal{C}}(u, v), w) = -(v, \tilde{\mathcal{C}}(u, w)), \quad (10)$$

and in 2D,

$$(\tilde{\mathcal{C}}(u, v), \Delta v) = (u, \tilde{\mathcal{C}}(\Delta v, v)). \quad (11)$$

This criterion yields the following class of regularizations proposed in [13],

$$\mathcal{C}_2(u, v) = \overline{\mathcal{C}(\bar{u}, \bar{v})}, \quad (12a)$$

$$\mathcal{C}_4(u, v) = \mathcal{C}(\bar{u}, \bar{v}) + \overline{\mathcal{C}(\bar{u}, v')} + \overline{\mathcal{C}(u', \bar{v})}, \quad (12b)$$

$$\mathcal{C}_6(u, v) = \mathcal{C}(\bar{u}, \bar{v}) + \mathcal{C}(\bar{u}, v') + \mathcal{C}(u', \bar{v}) + \overline{\mathcal{C}(u', v')}, \quad (12c)$$

where a prime indicates the residual of the filter, e.g., $u' = u - \bar{u}$, which can be explicitly evaluated, and $\overline{(\cdot)}$ represents a normalized self-adjoint linear filter with filter length ϵ . The difference between $\mathcal{C}_n(u, u)$ and $\mathcal{C}(u, u)$ is of the order ϵ^n (where $n = 2, 4, 6$) for symmetric filters with filter length ϵ . Note that for a generic, symmetric filter: $u' = \mathcal{O}(\epsilon^2)u$ [17].

The approximations $\mathcal{C}_n(u_\epsilon, u_\epsilon)$ are stable by construction, meaning that the convective terms do not contribute to the evolution of $|u_\epsilon|^2$ and $|T_\epsilon|^2$; in other words, in absence of body forces, i.e., $f_\epsilon = 0$, the evolution of both $|u_\epsilon|^2$ and $|T_\epsilon|^2$ is governed by a dissipative process. Replacing the convective term in the NS equations by the $\mathcal{O}(\epsilon^n)$ -accurate smooth approximation $\mathcal{C}_n(u_\epsilon, u_\epsilon)$ results into

$$\partial_t u_\epsilon + \mathcal{C}_n(u_\epsilon, u_\epsilon) = PrRa^{-1/2} \Delta u_\epsilon - \nabla p_\epsilon + f_\epsilon, \quad (13)$$

$$\partial_t T_\epsilon + \mathcal{C}_n(u_\epsilon, T_\epsilon) = Ra^{-1/2} \Delta T_\epsilon. \quad (14)$$

At this point, it must be recalled that the inviscid invariants follow directly from the symmetries of the governing equations. Actually, for each symmetry there is a corresponding invariant [18]. Hence, in the case of adding a new invariant that follows from different symmetry properties, the regularization model should be adapted to preserve the underlying new symmetry. For further details about the symmetry-preserving regularization modeling the reader is referred to [13].

2.4. Non-linear transport mechanism

To see how the above defined regularizations restrain the production of small scales of motion, we take the curl of Eq. (3), with $\mathcal{C}$ as in Eqs. 12a, 12b and 12c,

$$\partial_t \omega_\epsilon + \mathcal{C}_n(u_\epsilon, \omega_\epsilon) = PrRa^{-1/2} \Delta \omega_\epsilon + \nabla \times f_\epsilon + \mathcal{C}_n(\omega_\epsilon, u_\epsilon). \quad (15)$$

This equation resembles the vorticity equation that results from the NS equations: the only difference is that $\mathcal{C}$ is replaced by its regularization $\mathcal{C}_n$. If it happens that the vortex stretching term $\mathcal{C}_n(\omega_\epsilon, u_\epsilon)$ in Eq. (15) is so strong that the dissipative term $PrRa^{-1/2} \Delta \omega_\epsilon$ cannot prevent the intensification of vorticity, smaller vortical structures are produced. The NS equations lead to the source term

$$\mathcal{C}(\omega, u) = S\omega = \bar{S}\bar{\omega} + \bar{S}\omega' + S'\bar{\omega} + S'\omega', \quad (16)$$

where $S = (\nabla u + \nabla u^T)/2$ is the deformation tensor. The regularization reduce the high frequencies in the vortex stretching term:

$$\mathcal{C}_2(\omega, u) = \bar{S}\bar{\omega}, \quad (17a)$$

$$\mathcal{C}_4(\omega, u) = \bar{S}\bar{\omega} + \bar{S}\omega' + S'\bar{\omega}, \quad (17b)$$

$$\mathcal{C}_6(\omega, u) = \bar{S}\bar{\omega} + \bar{S}\omega' + S'\bar{\omega} + S'\omega'. \quad (17c)$$

Qualitatively, vortex stretching leads to the production of smaller and smaller scales, i.e., to a continuous, local increase of both S' and ω' . Consequently, at the positions where vortex stretching occurs, the terms with S' and ω' will eventually amount considerably to $\mathcal{C}(\omega, u)$. Since the regularizations $\mathcal{C}_n(\omega, u)$ diminish these terms, they counteract the production of smaller and smaller scales by means of vortex stretching and may eventually stop the continuation of the vortex stretching process. In this way, the symmetry-preserving regularization method restrains the convective production of smaller and smaller scales of motion by means of vortex stretching, while ensuring that convection makes no contribution to the dynamics of both $|u_\epsilon|^2$ and $|T_\epsilon|^2$.

2.5. LES-interpretation of $\mathcal{C}_n$ -regularizations

In Section 2.2, regularization modeling was related to LES concept via Eq. (7). In our case, the model term results into

$$\mathcal{M}_1(\bar{u}_\epsilon) = -\frac{\epsilon^2}{12} \nabla \cdot (\nabla \bar{u}_\epsilon : \nabla \bar{u}_\epsilon) + \mathcal{O}(\epsilon^4, \epsilon^n) \quad (18)$$

The generic, second-order term in the right-hand side is referred as gradient or tensor diffusivity [19,20]. In general, the gradient model does not lead to a stable LES (see [21], for instance). To overcome this, in the original form by Clark et al. [19], the gradient model was combined with an eddy-viscosity model, i.e., by adding a dissipative $\mathcal{O}(\epsilon^2)$ term. This mix effectively stabilizes the gradient model [21]. In our case, the gradient model forms the leading-order term of the closure models resulting from the fourth- and sixth-order approximations $\mathcal{C}_4$ and $\mathcal{C}_6$. Since the $\mathcal{C}_n$ -regularizations are unconditionally stable (in the energy-norm), from a LES point-of-view, we can interpret them as higher-order, anisotropic stabilizations of the gradient model. The second-order approximation $\mathcal{C}_2$ adds $-\frac{1}{12}\epsilon^2 \nabla^2 \mathcal{C}(\bar{u}_\epsilon, \bar{u}_\epsilon) + \mathcal{O}(\epsilon^4)$ to the gradient model.

3. On the dynamic determination of the filter length

In the initial tests, the performance of the $\mathcal{C}_4$ approximations was tested keeping the ratio ϵ/h (filter length to the grid width) constant. Therefore, only one parameter is needed to be prescribed in advance. In [14], a differentially heated cavity with height aspect ratio 4 and $Ra = 10^{10}$ was analyzed in detail. Comparison with DNS reference results showed significant improvements in capturing the general pattern of the flow even for very coarse meshes. A fairly good agreement with the DNS mean flow was observed for a wide range of ϵ/h ratios (see Fig. 3). Here, h denotes the local grid width. Moreover, the smoothed solutions exhibited the ability to capture the basic patterns of turbulent statistics only for a short range of ϵ/h values. Those preliminary results, together with results for a turbulent channel flow at $Re_\tau = 180$ and $Re_\tau = 395$ [13], illustrated

Fig. 3. The overall averaged Nusselt number (left) and the maximum of the averaged vertical velocity at the horizontal mid-height plane (right) as a function of the ratio of the filter length ϵ to the average grid width h .

the potential of the method as a new simulation shortcut and suggested that symmetry-preserving regularization modeling possesses the ability to predict correctly the flow structure even for very coarse grids. However, since the ϵ/h had to be prescribed in advance, a convergence analysis was needed. Even more important, for many configurations completely different regimes may coexist and interplay (Figs. 4 and 5 in Section 4.4 exemplify this); therefore, a homogeneous ϵ/h does not seem to be the optimal solution. With this in mind, in the present work, we propose to determine ϵ dynamically with the requirement that the vortex stretching must be stopped at the scale set by the grid.

3.1. Triadic interactions

To study the inter-scale interactions in more detail, we continue in the spectral space. The spectral representation of the convective term in the NS equations is given by

$$\mathcal{C}_k = i\Pi(k) \sum_{p+q=k} \hat{u}_p q \hat{v}_q, \quad (19)$$

where $\Pi(k) = I - k k^T / |k|^2$ denotes the projector onto divergence-free velocity fields in the spectral space. Taking the Fourier transform of 12a, 12b and 12c, we obtain the evolution of each Fourier-mode $\hat{u}_k(t)$ of $u_\epsilon(t)$ for the $\mathcal{C}_n$ approximation¹

$$\left(\frac{d}{dt} + \frac{Pr}{\sqrt{Ra}} |k|^2 \right) \hat{u}_k + i\Pi(k) \sum_{p+q=k} f_n(\hat{g}_k, \hat{g}_p, \hat{g}_q) \hat{u}_p q \hat{v}_q = F_k, \quad (20)$$

where $\hat{g}_k$ denotes the k th Fourier-mode of the kernel of the convolution filter, i.e., $\bar{u}_k = \hat{g}_k \hat{u}_k$. The mode $\hat{u}_k$ interacts only with those modes whose wave vectors p and q form a triangle with the vector k . Thus, compared with (19), every triad interaction is multiplied by

$$f_2(\hat{g}_k, \hat{g}_p, \hat{g}_q) = \hat{g}_k \hat{g}_p \hat{g}_q, \quad (21a)$$

$$f_4(\hat{g}_k, \hat{g}_p, \hat{g}_q) = \hat{g}_k \hat{g}_p + \hat{g}_k \hat{g}_q + \hat{g}_p \hat{g}_q - 2\hat{g}_k \hat{g}_p \hat{g}_q, \quad (21b)$$

$$f_6(\hat{g}_k, \hat{g}_p, \hat{g}_q) = 1 - (1 - \hat{g}_k)(1 - \hat{g}_p)(1 - \hat{g}_q). \quad (21c)$$

¹ Here, for simplicity, the sub-index ϵ is dropped.

Fig. 4. Two instantaneous snapshots at $Ra = 10^{10}$. Zoom around the top half of the cavity. For each of them the instantaneous isotherms are in the left and the corresponding spatial distribution of $\lambda_{\max}(S)$ on the right. Isotherms are uniformly distributed from 0 to 1. Results correspond to a 2D section of the DNS simulation presented in [2].

Fig. 5. Time evolution of $\lambda_{\max}(S)$ during 20 temporal units at three different (x_2, x_3) -locations: A (0.00625, 0.5), B (0.025, 0.9375) and C (0.125, 0.5), respectively. Results have been obtained for the mesh RM1 at $Ra = 10^{10}$.

Moreover, since for a generic, symmetric convolution filter (see [17], for instance)

$$\hat{g}_k = 1 - \alpha^2 |k|^2 + \mathcal{O}(\alpha^4) \quad \text{with} \quad \alpha^2 = \epsilon^2/24, \quad (22)$$

damping functions f_n can be approximated by

$$f_2 \approx 1 - \alpha^2 (|k|^2 + |p|^2 + |q|^2), \quad (23a)$$

$$f_4 \approx 1 - \alpha^4 (|k|^2 |p|^2 + |k|^2 |q|^2 + |p|^2 |q|^2), \quad (23b)$$

$$f_6 \approx 1 - \alpha^6 |k|^2 |p|^2 |q|^2. \quad (23c)$$

Therefore, the interactions between large scales of motion ($\epsilon |k| < 1$) approximate the NS dynamics up to $\mathcal{O}(\epsilon^n)$, with $n=2, 4, 6$, respectively. Hence, the triadic interactions between large scales are only slightly altered. All interactions involving longer wavevectors (smaller scales of motion) are reduced. The amount by which the interactions between the wavevector-triple (k, p, q) are lessened depends on the length of the legs of the triangle $k = p + q$. In case $n=4$, for example, all triadic interactions for

which at least two legs are (much) longer than $1/\epsilon$ are (strongly) attenuated, whereas interactions for which at least two legs are (much) shorter than $1/\epsilon$ are reduced to a small degree only.

3.2. Stopping the vortex stretching mechanism

The evolution of $|\omega|^2$ can be obtained by left-multiplying the vorticity transport Eq. (15) by ω . Doing so, the vortex-stretching and dissipation term contributions to $(1/|\omega|^2) \partial_t |\omega|^2$ for the original NS equations ($\epsilon=0$) result

$$\frac{\omega \cdot \mathcal{C}(\omega, u)}{\omega \cdot \omega} = \frac{\omega \cdot S\omega}{\omega \cdot \omega} \quad \text{and} \quad \frac{Pr}{\sqrt{Ra}} \frac{\nabla \omega : \nabla \omega}{\omega \cdot \omega}, \quad (24)$$

respectively. At the smallest grid scale, $k = \pi/h$, it can happen that the vortex stretching is so strong that the dissipative term cannot prevent a local intensification of vorticity,

$$\frac{\omega_k \cdot \mathcal{C}(\omega, u)_k}{\omega_k \cdot \omega_k} > \frac{Pr}{\sqrt{Ra}} k^2. \quad (25)$$

Therefore, in the present work we propose to determine dynamically the local filter length, ϵ , from the criteria that the vortex stretching must be stopped at the scale set by the grid, i.e., the following inequality must be satisfied locally

$$\frac{\omega_k \cdot \mathcal{C}_n(\omega, u)_k}{\omega_k \cdot \omega_k} \leq \frac{Pr}{\sqrt{Ra}} k^2. \quad (26)$$

Note that $\mathcal{C}_n(\omega, u)$ depends on the filter length ϵ . Assuming that local interactions are dominant, this dependence becomes

$$\frac{\omega_k \cdot \mathcal{C}_n(\omega, u)_k}{\omega_k \cdot \omega_k} \approx f_{n,k}(\epsilon) \frac{\omega_k \cdot S \omega_k}{\omega_k \cdot \omega_k} = f_{n,k}(\epsilon) \lambda_k, \quad (27)$$

where $\lambda_k = \omega_k \cdot S \omega_k / (\omega_k \cdot \omega_k)$ is the Rayleigh quotient of the vortex stretching at the grid scale and $f_{n,k}$ is the k th Fourier-mode of the damping function f_n . In our case, the value of λ_k has been bounded by the largest (positive) eigenvalue of the strain tensor S ,

$$\lambda_k \leq \lambda_{\max}(S). \quad (28)$$

For the $\mathcal{C}_n$ -approximation, the damping function, $0 < f_{n,k} \leq 1$, at the highest frequency is approximately given by $f_n(\hat{g}_k, \hat{g}_k, \hat{g}_k)$, where $0 < \hat{g}_k(\epsilon) \leq 1$ is the transfer function of the linear filter. Therefore, it suffices that the following inequality holds

$$f_{n,k}(\epsilon) \leq \frac{Pr}{\sqrt{Ra}} \frac{k^2}{\lambda_{\max}(S)} \stackrel{(21)}{\rightarrow} \hat{g}_k(\epsilon) \stackrel{(22)}{\rightarrow} \epsilon, \quad (29)$$

to guarantee that the vortex-stretching mechanism stops at the smallest scale set by the mesh.

4. Numerical approximations

To evaluate the performance of the proposed regularization models, numerical results are compared with reference data in the following sections. In such *a posteriori* tests modeling errors and discretization errors are mixed together. At this point, it must be noted that discretization is also a regularization. Consequently, the discretization of the governing equations is a very important point when dealing with *a posteriori* performance tests for LES-like models. The regularizations $\mathcal{C}_n$ given by Eqs. 12a, 12b and 12c are constructed in a way that the symmetry properties (8) and (9) are exactly preserved. Of course, the same should hold for the numerical approximations that are used to discretize them. For this, the basic ingredients are twofold: (i) a symmetry-preserving discretization of the original NS equations and (ii) a normalized self-adjoint linear filter. These two crucial points, together with the time-integration procedure, are addressed in the next subsections.

4.1. Spatial discretization

A Cartesian structured mesh has been chosen to discretize the equations. Grid spacing in the periodic x_1 -direction is uniform and the wall-normal points in the x_2 - and x_3 -directions are distributed using a hyperbolic-tangent function with concentration factors γ_2 and γ_3 , respectively. For the x_2 -direction it reads

$$(x_2)_j = \frac{L_2}{2} \left(1 + \frac{\tanh\{\gamma_2(2(j-1)/N_2 - 1)\}}{\tanh\gamma_2} \right). \quad (30)$$

On the other hand, the regularizations $\mathcal{C}_n$ given by Eqs. 12a, 12b and 12c are constructed in a way that symmetry properties (10) and (11) are preserved. Of course, the same should hold for the numerical approximations that are used to discretize $\mathcal{C}$. To do so, symmetry-preserving schemes [9] have been used here to discretize the NS equations. They preserve the symmetry properties of the underlying differential operators: the convective operator is represented by a skew-symmetric matrix and the diffusive operator by a symmetric positive-definite matrix. In short, the temporal evolu-

tion of the spatially discrete staggered velocity, u_h , and centered temperature, T_h , vectors is governed by the following finite-volume discretization of Eqs. (13) and (14)

$$\Omega_s \frac{du_h}{dt} + C_s(u_h)u_h + D_s u_h - M^T p_h = f_h, \quad (31)$$

$$\Omega_c \frac{dT_h}{dt} + C_c(u_h)T_h + D_c T_h = 0_h, \quad (32)$$

where the discrete incompressibility constraint reads $M u_h = 0_h$ and the subindices s and c refer to whether the operators are applied to staggered or centered discrete vectors. The diffusive matrix, D_s , is symmetric and positive semi-definite; it represents the integral of the diffusive flux $-\nabla u \cdot n / Re$ through the faces. The diagonal matrix, Ω_s , describes the sizes of the control volumes and the approximate, convective flux is discretized as in [9]. The resulting convective matrix, $C_s(u_h)$, is skew-symmetric

$$C_s(u_h) + C_s^T(u_h) = 0. \quad (33)$$

In a discrete setting, the skew-symmetry of $C_s(u_h)$ implies that

$$C_s(u_h) v_h \cdot w_h = v_h \cdot C_s^T(u_h) w_h = -v_h \cdot C_s(u_h) w_h, \quad (34)$$

for any discrete velocity vectors u_h (if $M u_h = 0_h$), v_h and w_h . Note that Eq. (34) is the discrete analogue of Eq. (8). Then, the evolution of the discrete energy, $\|u_h\|^2 = u_h \cdot \Omega_s u_h$, is governed by

$$\frac{d}{dt} \|u_h\|^2 = \underbrace{-u_h \cdot (D_s + D_s^T) u_h}_{<0} + 2f_h \cdot \Omega_s u_h, \quad (35)$$

where the convective and pressure gradient contributions cancels because of Eq. (33) and incompressibility constraint $M u_h = 0_h$, respectively. Therefore, even for coarse grids, the energy of the resolved scales of motion is convected in a stable manner: that is, the discrete convective operator transports energy from a resolved scale of motion to other resolved scales without dissipating any energy, as it should do from a physical point-of-view. This forms a good starting point for LES-like simulations. For a detailed explanation, the reader is referred to [9]. The temporal evolution of T_h (32) is discretized in the same vein.

4.2. Time-integration method

The governing equations are integrated in time using a classical fractional step projection method [22,23]. In the projection methods, solutions of the unsteady NS equations are obtained by first time-advancing the velocity field, u^n , without regard for its solenoidality constraint, then recovering the proper solenoidal velocity field, u^{n+1} ($\nabla \cdot u^{n+1} = 0$). For the temporal discretization, a fully second-order-explicit one-leg scheme [9] is used. Thus, the resulting fully-discretized problem reads

$$\frac{(\kappa + 1/2)u_h^n - 2\kappa u_h^n + (\kappa - 1/2)u_h^{n-1}}{\delta t} = R((1 + \kappa)u_h^n - \kappa u_h^{n-1}), \quad (36)$$

where $R(u_h) = -C_s(u_h)u_h - D u_h$ and u_h^p is a predictor velocity that can be directly evaluated from the previous expression. The time-integration parameter, κ , is computed to adapt the linear stability domain of the time-integration scheme to the instantaneous flow conditions in order to use the maximum time-step, δt , possible. For further details about the time-integration method the reader is referred to [2]. Finally, u_h^p must be projected onto a divergence-free space

$$u_h^{n+1} = u_h^p + \Omega_s^{-1} M^T \tilde{p}_h^{n+1}, \quad (37)$$

by adding the gradient of the pseudo-pressure, $\tilde{p}_h = \delta t / (\kappa + 1/2) p_h$, satisfying the following Poisson equation

$$-M\Omega_s^{-1}M^T p_h^{n+1} = Mu_h^p. \quad (38)$$

Here, this equation, that results from taking the divergence of Eq. (37), is solved by a direct method. Details about the Poisson solver can be found in [24,25].

4.3. Normalized self-adjoint filtering

Our filtering operation is based upon a Gaussian filter,

$$\begin{aligned} \bar{\phi}(x) &= \int_{-\infty}^{+\infty} G(x - \xi) \phi(\xi) d\xi \quad \text{with} \\ G(x - \xi) &= \sqrt{\frac{6}{\pi\Delta^2}} \exp\left(-\frac{6|x - \xi|^2}{\Delta^2}\right), \end{aligned} \quad (39)$$

where $\bar{\Delta} = \epsilon h$ is the characteristic cut-off length-scale. The filter length, defined by $\epsilon = \bar{\Delta}/h$, need not to be restricted to integer multiples of the grid width, h . The boundary conditions that supplement the NS equations are also applied to (39). The filter commutes with the gradient operator, i.e., $\nabla \bar{\phi} = \bar{\nabla} \phi$ for any (sufficiently differentiable) scalar ϕ . This implies that the approximations $\mathcal{C}_n$ are exact for potential flows. More important, if we decompose the velocity field u into a gradient part and a rotational part, $u = \nabla \phi + \nabla \times \Psi$, we see that the fluctuating part u' of u is purely rotational: $u' = \nabla \times \Psi'$. Thus, the fluctuating velocity captures a characteristic property of turbulence: it consists of fluctuating rotational flow.

In practice, a fourth-order accurate approximation [26] has been chosen to compute the Gaussian filter (39) on a Cartesian structured grid. In 1D it reads

$$\begin{aligned} \bar{u}_i &= \frac{\epsilon^4 - 4\epsilon^2}{1152} (u_{i+2} + u_{i-2}) + \frac{16\epsilon^2 - \epsilon^4}{288} (u_{i+1} + u_{i-1}) \\ &\quad + \frac{\epsilon^4 - 20\epsilon^2 + 192}{192} u_i. \end{aligned} \quad (40)$$

This results into the following linear operator

$$\bar{u}_h \approx \tilde{F} u_h, \quad (41)$$

where the same boundary conditions of u_h are applied to the filtered velocity, $\bar{u}_h$. In order to ensure that all the symmetry and conservation properties hold exactly a normalized self-adjoint filter [27] is needed. In general, this is not satisfied by $\tilde{F}$, therefore, we define our linear filter F as follows

$$2S = \Omega_s^{-1} \{ \Omega_s \tilde{F} + (\Omega_s \tilde{F})^T \}, \quad (42)$$

$$F = S - \text{diag}(S1 - 1). \quad (43)$$

The linear map $u_h \mapsto u_h$ defined by Eqs. (42) and (43) possesses the following basic properties: (i) symmetry, $\Omega_s F = (\Omega_s F)^T$, (ii) a constant velocity vector is unaffected, i.e., $F1 = 1$ and (iii) it reduces the high-frequency components of the discrete velocity vector u_h . This means that F constitutes a suitable filter for our application.

At this point, it must be noted that, in general, an incompressible velocity field, u_h ($Mu_h = 0_h$), does not automatically imply that $\bar{u}_h$ ($u'_h = u_h - \bar{u}_h$ also) is also divergence-free. Although no 'real' mass is lost in terms of the u_h field, $M\bar{u}_h \neq 0_h$ and $Mu'_h \neq 0_h$ have series implications: the skew-symmetry of the convective operator (34) and consequently the conservation properties that follow from it would be lost. For instance, because of this, the convection term would not be a pure re-distributor of energy any more; instead, it becomes an active source or sink of kinetic energy and therefore the stability of the method is lost. This problem becomes especially relevant in the near-wall regions where the non-slip boundary conditions may cause significant compressibility effects on the filtered velocity. This question has been addressed before for a Leray- α model in [28]. One possible solution to this problem

could be to project the filtered velocity onto a divergence-free space,

$$\tilde{u}_h = Fu_h, \quad (44)$$

$$\bar{u}_h = \tilde{u}_h + \Omega_s^{-1} M^T q_h \quad \text{with} \quad M\bar{u}_h = 0_h. \quad (45)$$

However, an additional Poisson equation, $M\Omega_s^{-1} M^T q_h = M\tilde{u}$, needs to be solved each time-step. A computationally less demanding approach relies on explicitly forcing the diagonal term of the discrete convective operators, $C_s(\bar{u}_h)$ and $C_c(\bar{u}_h)$, to be equal to zero,

$$[C_s(\bar{u}_h)]_{k,k} = 0; \quad [C_c(\bar{u}_h)]_{k,k} = 0, \quad \forall k. \quad (46)$$

In this way, the skew-symmetry of the convective operator (34) is restored irrespective whether the advective velocity is exactly divergence-free. Both approaches have been tested. Since no significant differences have been observed, in the view of lower cost, the second approach has been chosen.

4.4. Does the discrete linear filter need to be recomputed at each time-step?

In practice, the computational cost to determine the local filter length, ϵ , by the sequence (29) may be not negligible. Firstly, the local strain tensor, S , must be computed and its maximum eigenvalue, $\lambda_{\max}(S)$, evaluated. Then, $\hat{g}_k(\epsilon)$ follows from the limiting value obtained for $f_{n,k}$. For instance, for the $\mathcal{C}_4$ approximation, $f_{4,k} = 3\hat{g}_k^2(\epsilon) - 2\hat{g}_k^3(\epsilon)$, and consequently a cubic equation, with only one real root, for $\hat{g}_k$ must be solved. Finally, ϵ follows straightforwardly from (22).

In the view of lower costs, the question now is whether it is necessary to recompute the local filter length, ϵ , and, if it is needed, how often. In Fig. 4, the spatial distributions of $\lambda_{\max}(S)$ corresponding to two different instants are displayed. These results correspond to a 2D section of the DNS simulation at $Ra = 10^{10}$ presented in [2]. As expected, we can observe that regions with completely different regimes co-exists. More importantly, we also observe areas where the changes of $\lambda_{\max}(S)$ are significant. Therefore, we conclude that the discrete filter need to be recomputed during the simulation. Then, the following question is how often to do so. To answer this, the time evolution of $\lambda_{\max}(S)$ at three different locations is displayed in Fig. 5. These monitoring points correspond to three positions in the cavity where completely different regimes are observed. At first sight, we can observe that once a statistically stationary steady state has been reached, the values of $\lambda_{\max}(S)$ oscillate around a mean value. More importantly, the difference between consecutive time-steps remains minimal. Therefore, these results, combined with the fact that the final solution is not strongly dependent on the precise value of ϵ , suggest that the local filter length is not needed to be updated so often. Direct comparison between results obtained updating ϵ at each time-step and results updating up to every temporal unit revealed no significant differences. Therefore, for the remainder of this paper all the parameter-free $\mathcal{C}_n$ -simulations have been carried out updating ϵ every 0.5 temporal units (for the simulation shown in Fig. 5, it represents around 40 time-steps, that is 40 times cheaper!).

5. Results for a turbulent differentially heated cavity at $Ra = 10^{10}$

The performance of the proposed method to dynamically determine the regularization parameter, ϵ , of the $\mathcal{C}_n$ approximations has been tested for the DHC problem defined in Section 2.1. Here, we restrict ourselves to the $\mathcal{C}_4$ because it outperforms $\mathcal{C}_2$ and no significant difference has been observed with respect to the results obtained with $\mathcal{C}_6$, which is computationally more demanding.

Table 1

Description of meshes: the spanwise (N_1), the wall-normal horizontal (N_2), and the vertical (N_3) resolutions for the tested cases. Further details about the meshing can be found in [2].

	DNS	RM1	RM2
$N_1 \times N_2 \times N_3$	$128 \times 190 \times 462$	$16 \times 34 \times 80$	$8 \times 17 \times 40$
γ_2	2.0	2.2	2.2
γ_3	1.0	1.0	1.0

Averages over the three statistically invariant transformations (time, x_1 -direction and central point symmetry around the center of the cavity) have been carried out. The standard averaging notation, $\langle \cdot \rangle$, is used here. The total integration period is 1000 time units for all the simulations irrespective of the Ra . In order to be sure that the statistically steady state had been reached, which usually requires around 100–200 time units, statistical values have been obtained for a time interval corresponding to the last ≈ 500 time units of simulation. Further details about the averaging procedure can be found in [29].

As an initial test, two very coarse meshes consisting of $8 \times 17 \times 40$ and $16 \times 34 \times 80$ grid points respectively (see Table 1) have been used to solve the DHC problem at $Ra = 10^{10}$. These are the same meshes used in [14] where the method was tested keeping the ratio ϵ/h constant. The coarse meshes RM1 and RM2 have approximately the same grid points distribution as the DNS grid but with much less spatial resolutions. The domain size in the periodic direction was taken equal to the size used for the DNS simulations, i.e., $L_1/L_2 = 1$. The first results displayed in Fig. 3 exhibit the great potential of this method. Note that in the parameter-free $\mathcal{C}_4$ cases, the results do not depend on ϵ/h . The results that are being obtained here are at least as good as the those ones that were obtained in [14] using the optimal ϵ/h ratio determined by trial-and-error procedure.

5.1. Mean fields

The corresponding vertical temperature profile at mid-width is displayed in Fig. 6. At first sight we can observe a significant improvement for the smoothed solutions. At the top and bottom areas, where the flow is more turbulent, some discrepancies regarding the reference solution are still observed for both meshes. The fairly good prediction at the cavity core even for the coarsest

mesh is especially relevant. As it was pointed out in Section 1, an accurate prediction of thermal stratification of this configuration is a challenge for turbulence modeling. This is due to the high sensitivity exhibit: small disturbances in the location of the transitional point at the vertical boundary layers or a sudden ‘artificial’ stop of the energy cascade at large scales of motion can dramatically affect the structure of the stratified cavity core (notice the large dispersion for non-smoothed results in Fig. 11, top). In Fig. 6, we can see that without smoothing ($\epsilon = 0$), the thermal stratification is clearly under-predicted, especially for the coarsest mesh.

Let us focus now on the vertical boundary layer. It remains laminar in its upstream part up to the point where the Tollmien–Schlichting waves traveling downstream grow up enough to disrupt the boundary layer. Its high sensitivity to external disturbances makes it difficult to predict. The corresponding temperature and vertical velocity profiles at the cavity mid-height plane, $x_3 = 0.5$, are displayed in Figs. 7 and 8, respectively. As expected, we can observe a strong correlation between the quality of the solutions for $\langle T \rangle$ and $\langle u_3 \rangle$. For the results corresponding to $\epsilon = 0$ (labeled ‘No Model’), the vertical boundary layer is too thick, whereas with the parameter-free $\mathcal{C}_4$ -smoothing, the solutions for the two coarse meshes agree very well with the DNS reference solution. Fig. 9 depicts essentially the same for the horizontal velocity profile. It must be noted that values of $\langle u_2 \rangle$ are significantly smaller than $\langle u_3 \rangle$ and therefore more difficult to predict.

5.2. Heat transfer

In Fig. 3 (top), the total Nusselt number as a function of ϵ/h is displayed (see Table 2, for exact results). The reference value $Nu = 101.94$ has been obtained from our DNS simulation [15,16] with $\epsilon = 0$. We see that both $\mathcal{C}_4$ simulations, RM1 and RM2, predict fairly well the reference value. Moreover, in Fig. 11, we observe that the heat transfer is also well captured for all randomly generated meshes whereas the solutions obtained without smoothing ($\epsilon = 0$) are incomparably worse. Results of the distribution of Nusselt number in the hot wall are shown in Fig. 10. A change in the shape is observed at nearly $x_3 = 0.2$ for the non-smoothed results, indicating a much too early transition toward turbulence. In contrast, the $\mathcal{C}_4$ results are able to capture well most of the profile except for the most upstream part where the heat transfer is slightly under-predicted.

Fig. 6. Averaged vertical temperature profile at mid-width.

Fig. 7. Averaged temperature profile at the horizontal mid-height plane.

Fig. 8. Averaged vertical velocity profile at the horizontal mid-height plane.

In Table 2, the maximum and the minimum values of the local Nusselt number are also shown. These two quantities are of interest because they occur in two clearly different parts of the vertical boundary layers. Maximum values are in the upstream part of the boundary layer where it is still almost laminar whereas minimum values are observed at the most downstream part of the boundary layer where it has become fully turbulent (see Fig. 1). For both coarse grids, the significant improvements are achieved for the smoothed solutions.

5.3. Grid (in)dependence analysis

A reliable modeling of turbulence at (very) coarse grids is a great challenge. The coarser the grid the more convincing model quality is perceived. However, it might happen that the solution is strongly dependent on meshing parameters and thus some particular combinations could ‘accidentally’ provide good results. An example of this behavior has been observed in [30] for a turbulent channel flow. In order to elucidate this point, the same DHC prob-

lem has been solved on a series of 50 randomly generated meshes: with (N_1, N_2, N_3) -values limited by those given by meshes RM1 and RM2 (see Table 2), i.e., $8 \leq N_1 \leq 16$, $17 \leq N_2 \leq 34$, and $40 \leq N_3 \leq 80$. The concentration parameters, γ_2 and γ_3 are kept equal to values given in Table 1. It must be noted that for this test the number of grid points in one direction was randomly generated irrespective of the number of points in the other two directions. Therefore, some of the numerical experiments displayed in Fig. 11 correspond to highly skewed grids.

Results for the overall Nusselt and the centerline stratification values are displayed in Fig. 11 (top). At first sight, we can observe that the parameter-free $\mathcal{C}_4$ modeling predicts results well irrespective of the meshing whereas very poor and dispersed results are obtained when the model is switched off. The fairly good prediction of the stratification (note the dispersion obtained without model!) is especially important. In the Fig. 11 (bottom), the results for the maximum vertical velocity and the wall shear stress scaled by $Ra^{-1/4}$ at the horizontal mid-height plane, $x_3 = 0.5$, are displayed. These two quantities give valuable information about whether

Fig. 9. Averaged horizontal velocity profile at the horizontal mid-height plane.

Table 2

The overall, the maximum and the minimum of the averaged Nusselt number.

Mesh	DNS 128 × 190 × 462	RM1 16 × 34 × 80		RM2 8 × 17 × 40	
		No model	$\mathcal{C}_4$	No model	$\mathcal{C}_4$
Nu	101.94	121.93	100.81	128.14	102.17
Nu_{max}	454.86	437.78	451.12	342.02	459.59
Nu_{min}	8.50	10.92	10.18	27.77	7.03

the boundary layer is being correctly solved in our discrete setting. We observe that points corresponding to non-smoothed solutions are clustered around (0.3, 0.15) and therefore both quantities are clearly under-predicted whereas solutions obtained with the $\mathcal{C}_4$ method predict quite well the (0.422, 0.223) reference solution.

5.4. How many times cheaper is the $\mathcal{C}_4$ regularization?

The least to be expected from a turbulence model is a good prediction of the mean flow quantities at a significantly cheaper cost

than a (coarse) DNS. Of course, this will depend on many factors such as the configuration to be solved, the specific implementation of the method or the demanded level of accuracy. In this section, we shall try to elucidate this point with the help of the following test: a series of coarse DNS simulations have been carried out for the DHC problem at $Ra = 10^{10}$ starting from the RM2 grid and increasing the grid resolution homogeneously in each spatial direction. Results displayed in Fig. 12 show that meshes with at least 60 times more computational nodes than the RM2 are needed to achieve similar levels of accuracy. On the other hand, the cost required for the regularization compared with the cost of the no-model simulation on the same grid increases only around 30%. Since this additional cost is not significant compared with those of solving finer grids an analysis only in terms of mesh sizes suffices.

Solving finer grids makes a computation more expensive. The main factors that increase the computational cost are twofold: (i) the number of time-steps usually grows with $\mathcal{O}(N^{p/3})$, where $1 \leq p \leq 2$ and $N = N_1 N_2 N_3$ and (ii) the cost of solving one time-step grows with $\mathcal{O}(N^q)$, where $q \geq 1$. The two limiting values of p correspond to those cases where either convection ($p = 1$) or diffusion

Fig. 10. Local Nusselt number distribution.

Fig. 11. Top: The overall Nusselt number and the centerline stratification. Bottom: The maximum vertical velocity and the wall shear stress scaled by $Ra^{-1/4}$ at the horizontal mid-height plane. Results have been obtained for 50 randomly generated grids.

($p = 2$) are dominant. On the other hand, exponent q measures the scalability of the code; the limiting case, $q = 1$, corresponds to the ideal linear scalability. Therefore, the total computational cost increases with $\mathcal{O}(N^{p/3+q})$. Ideally, the exponent would be ‘only’ $4/3$ and therefore taking $N/N_{RM2} = 60$ would imply that, for this case, the $\mathcal{C}_4$ regularization is at least $60^{4/3} \approx 235$ times cheaper. Taking a more realistic exponent like $p/3 + q \approx 2$ then the method would be $60^2 \approx 3600$ times cheaper than just computing a coarse DNS providing the same levels of accuracy. According to the experience with our code [24] the latter is a more realistic approximation.

At this point it must be recalled that the numerical discretization itself is also a regularization (see Section 4.1). Since the numerical schemes used to discretize the governing equations are unconditionally stable and the discrete operators are constructed to mimic the underlying differential operators, their solution ($\epsilon = 0$) constitutes an excellent starting point for any turbulence model.

6. Performance at higher (and lower) Rayleigh numbers

The performance of the parameter-free $\mathcal{C}_4$ -regularization has also been tested at higher (and lower) Ra . This study covers a rel-

atively wide range, $6.4 \times 10^8 \leq Ra \leq 10^{11}$, from weak to fully developed turbulence. Within this range DNS results for five different configurations (at $Ra = 6.4 \times 10^8$, 2×10^9 , 10^{10} , 3×10^{10} and 10^{11} , respectively) are available [15,16]. The meshes used to carry out these simulations have been generated keeping the same number of points in the boundary layer as in the coarse mesh RM1 for $Ra = 10^{10}$. In this way, the meshes² for $Ra = 3 \times 10^{10}$ and 10^{11} become $10 \times 19 \times 46$ with $\gamma_2 = 2.26$ and $12 \times 26 \times 62$ with $\gamma_2 = 2.28$, respectively.

6.1. Boundary layer

For the sake of brevity, in this section we focus only on the two highest Ra , i.e., 3×10^{10} and 10^{11} . In Figs. 13 and 14, the temperature and the vertical velocity profiles at the horizontal mid-height plane, $x_3 = 0.5$, are displayed. Again, the parameter-free $\mathcal{C}_4$ method and non-smoothed results ($\epsilon = 0$) obtained using a mesh that it is twice finer in each direction are compared with DNS data. All plots

² Note that the grid stretching near the vertical walls has also been slightly increased with the Ra .

Fig. 12. Grid convergence study. The abscissa represents the ratio of the total number of nodes, $N = N_1 \times N_2 \times N_3$, with respect to the number of nodes of the RM2 mesh.

depict essentially the same: the parameter-free $\mathcal{C}_4$ method is able to capture well the flow structure of the vertical boundary layer even for the coarsest meshes whereas the results of the non-smoothed simulations differ largely from the reference solution.

6.2. Heat transfer

The heat flux as a function of Rayleigh number is investigated in this section. In the last decades significant efforts, both numerically and experimentally, have been directed at investigating the mechanisms and the detailed scaling behavior on turbulent Rayleigh–Bénard (RB) problems. Classical theory predicts that $Nu \sim Ra^\xi$ with $\xi = 1/3$. Alternative scaling theories, encouraged by experimental observations, lead to $\xi = 2/7$ [31,32]. Finally, an asymptotic regime, the so-called Kraichnan regime, with $\xi = 1/2$ is presumed to exist at very high Ra . Experimentally, power-law dependencies of heat flux with exponents between $1/4$ and $1/3$ have been measured [33]. Regarding the Kraichnan regime, and despite the great efforts de-

voted, no clear evidence has been observed yet [34]. On the other hand, there is still controversy whether a simple power-law $Nu \sim Ra^\xi$ is adequate. For instance, Grossmann and Lohse [33,35] developed a theory based on the kinematic and thermal dissipation rates in the bulk and the boundary layers. They identified different regimes and the $Nu(Ra, Pr)$ follows from a superposition of the scaling laws from neighboring regimes. More recently, Hölling and Herwig [36], developed an alternative theory by matching temperature gradients in the overlap region of the wall layer and the core layer. A Nusselt number scaling with logarithmic corrections follows.

Comparatively, the DHC problem has received much less attention from the scientific community (see Yu et al. [37] and Pessoa and Piva [38], for instance). Nevertheless, both configurations share similar heat transfer scaling [37] and most of the ideas applied to RB configuration can be easily applied to the DHC problem. The classical theory also predicts a $Nu \sim Ra^{1/3}$ correlation for fully turbulent regime. It follows from the assumption that, at high

Fig. 13. Averaged temperature (top) and vertical velocity (bottom) profiles at the horizontal mid-height plane at $Ra = 3 \times 10^{10}$.

Rayleigh numbers, the heat flux becomes independent of the distance between active walls. This implies the $1/3$ exponent since $Nu \sim L_2$ and $Ra \sim L_2^3$. On the other hand, the classical theory also predicts a scaling exponent of $1/4$ for the laminar regime. Recently, Yu et al. [37] argued that turbulence may be not essential for the classical $1/3$ power-law scaling of Nu . Instead, they proposed that the large-scale circulation together with the resultant boundary layers and core stratification are sufficient to produce the classical $1/3$ exponent scaling, and that the role of turbulence is not essential in this regard. In [16], we found that

$$Nu \approx 0.182Ra^{0.275}, \quad (47)$$

was the power-law scaling that fitted best our DNS results. Actually, this exponent cannot be considered 'near' $1/3$; rather, it is closer to the $2/7 \approx 0.286$ proposed by alternative theories of turbulent natural convection flows [31,32].

6.2.1. Comparison with DNS results

Results for the overall Nusselt number corresponding to 56 simulations within the whole range of Rayleigh numbers studied by DNS, i.e., $6.4 \times 10^8 \leq Ra \leq 10^{11}$, are displayed in Fig. 15. At first

sight, we observe again a fairly good agreement with the DNS results (solid dots) and the correlation (47) obtained from the DNS data. It must be noted that the Nu – Ra dependence obtained with the parameter-free $\mathcal{C}_4$ is smooth suggesting again that the proposed model is performing well 'independently' of Ra and meshing parameters that may suddenly change for two consecutive points in the graph.

6.2.2. Nusselt number correlation with Ra up to 10^{17}

Since performing computations with the parameter $\mathcal{C}_4$ approximation is rather cheap we were tempted to perform simulations at very high Ra . Following the aforesaid criterion to keep the number of points at the vertical boundary layer constant leads to a $68 \times 142 \times 334$ mesh with $\gamma_2 = 3.48$ for $Ra = 10^{17}$. Of course, for the range $10^{11} < Ra \leq 10^{17}$ there is no DNS (or experimental) data to compare with. Anyhow, it is interesting to see that results displayed in Fig. 16 show a good agreement with a $2/7$ power-law scaling of Nusselt (Nu increases approximately from 10^2 to 10^4 , that is 2 orders of magnitude, when Ra is increased 7 orders, from 10^{10} to 10^{17}). This scaling law, predicted by alternative theories [31,32] of turbulent natural convection, has also been experimentally measured for RB configurations [34].

Fig. 14. Averaged temperature (top) and vertical velocity (bottom) profiles at the horizontal mid-height plane at $Ra = 10^{11}$.

Fig. 15. Overall Nusselt number for $6.4 \times 10^8 \leq Ra \leq 10^{11}$.

Fig. 16. Overall Nusselt number for Rayleigh numbers up to 10^{17} .

7. Concluding remarks

The $\mathcal{C}_4$ -regularization of the non-linear convective term has been considered as a simulation shortcut. The symmetries and conservation properties of the original convective term are exactly preserved. Doing so, the production of smaller and smaller scales of motion is restrained in an unconditionally stable manner. The numerical algorithm to solve the governing equations is also fully-conservative and is therefore well-suited to test the proposed simulation method. Here, a novel criterion to determine the local filter length dynamically from the requirement that the vortex stretching must be stopped at the scale set by the grid has been proposed. In this way, it becomes a parameter-free turbulence model, i.e., no constant needs to be tuned or prescribed in advance.

As a first step to test the performance of the parameter-free $\mathcal{C}_4$ -regularization method a 3D air-filled differentially heated cavity of aspect ratio 4 has been considered. This is a challenging configuration for turbulence modeling since areas with completely different regimes coexist and interplay. Direct comparison with DNS reference results within a relatively wide range of Rayleigh numbers, $6.4 \times 10^8 \leq Ra \leq 10^{11}$, has shown that the method is able to capture the general pattern of the flow correctly even for very coarse meshes. Results are in good agreement for the mean velocity and the temperature as well as for the heat flux. Especially significant is the fairly good prediction of the centerline thermal stratification. To investigate the independence of the method regarding the meshing parameters four relevant mean flow quantities (i.e., overall Nusselt number, centerline stratification, maximum vertical velocity and wall shear stress at the horizontal mid-height plane) have been monitored for a series of randomly generated grids. Even for highly skewed grids, all the results obtained with the parameter-free $\mathcal{C}_4$ method were clustered around the DNS reference solution, in contrast with the rather poor (with a large dispersion also) results obtained without modeling. Finally, to study the heat transfer scaling, simulations at higher Ra up to 10^{17} have also been computed. A fairly good agreement with a $2/7$ power-law scaling of Nusselt has been measured for the whole range, i.e., $10^{11} \leq Ra \leq 10^{17}$. This scaling law, also predicted by alternative theories of turbulent natural convection, has also been experimentally measured for Rayleigh–Bénard configurations.

Therefore, considering the inherent difficulty of modeling a buoyancy driven turbulent flow in a differentially heated cavity, we can conclude that the results displayed here illustrate the great potential of the parameter-free $\mathcal{C}_4$ smoothing method as a new simulation shortcut. Moreover, since no *ad hoc* phenomenological arguments that cannot be formally derived from the governing Navier–Stokes equations are used, it suggests that this method may be valid for any other configurations. Nevertheless, more simulations for a wide variety of cases and meshes will be necessary to confirm these preliminary conclusions.

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