DNS and LES of buoyancy-driven turbulence at high Rayleigh numbers: numerical methods and subgrid-scale models

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1 Introduction

Buoyancy-driven flows have always been an important subject of scientific studies with numerous applications in environment and technology. The most famous example thereof is the thermally driven flow developed in a fluid layer heated from below and cooled from above, *i.e.* the Rayleigh-Bénard convection (RBC). It constitutes a canonical flow configuration that resembles many natural and industrial processes, such as solar thermal power plants, indoor space heating and cooling, flows in nuclear reactors, electronic devices, and convection in the atmosphere, oceans and the deep mantle.

In the last decades significant efforts, both numerically and experimentally, have been directed at investigating the mechanisms and the detailed scaling behavior of the Nusselt number as a function of Rayleigh and Prandtl numbers in the general form $Nu \propto Ra^{\gamma} Pr^{\beta}$ [1]. In this regard, Figure 1 shows the predictions of the Nu-number based on the classical Grossmann-Lohse (GL) theory [2] and its subsequent corrections [3, 4] where different scaling regimes, characterized by their corresponding exponents γ and β, are identified. Assuming this power-law scalings and following the same reasoning as in Ref. [5] leads to the estimations for the number of grid points shown in Figure 2 (top). This corresponds to mesh resolution requirements for DNS and it clearly explains why nowadays DNS of RBC is still limited to relatively low Ra-numbers [1]. However, many of the above-mentioned applications are governed by much higher Ra numbers, located in the region of the

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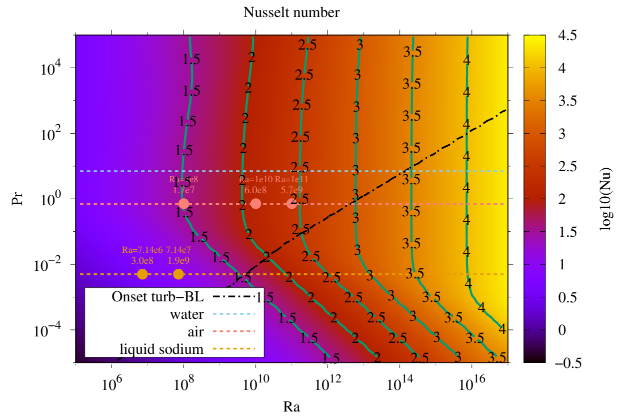

Fig. 1 Estimation of the Nusselt number of a RBC in the $\{Ra, Pr\}$ phase space given by the classical GL theory [2] and its subsequent corrections [3]. Green solid isolines represent the $log10$ of the Nusselt. Three dashed horizontal lines correspond to three different working fluids: water ($Pr = 7$), air ($Pr = 0.7$) and liquid sodium ($Pr = 0.005$). Dots displayed in the top figure correspond to the DNS simulations carried out in previous studies [5, 7, 8]. Black dash-dotted line is an estimation for the onset of turbulence in the thermal boundary layer.

$\{Ra, Pr\}$ phase space where the thermal boundary layer becomes turbulent (*i.e.* below the black dash-dotted line in Figure 2). This region corresponds to the so-called asymptotic Kraichnan or ultimate regime of turbulence [6], with $\gamma = 1/2$. On the other hand, reaching such Ra-numbers experimentally while keeping the basic assumptions (Boussinesq approximation, adibaticity of the closing walls, isothermal horizontal walls, perfectly smooth surfaces...) is a very hard task; therefore, the observation of the Kraichnan regime also remains elusive [3, 4].

2 LES of buoyancy-driven turbulence

In this context, we may turn to LES to predict the large-scale behavior of incompressible turbulent flows driven by buoyancy at very high Ra-numbers. In LES, the large-scale motions are explicitly computed, whereas the 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. However, there still exist inherent difficulties in the proper modelization of the SGS heat flux. This was analyzed in detail in the PRACE project entitled ”Exploring new frontiers in Rayleigh-Bénard convection” (33.1 millions of CPU hours on MareNostrum 4 in 2018-2019), where DNS simulations of air-filled ($Pr = 0.7$) RBC up to $Ra = 10^{11}$ were carried out using meshes up to 5600M grid points (see dots displayed in Figures 1 and 2, top). These results shed light into the flow topology and the small-scale dynamics, which are crucial in constructing the turbulent wind and energy budgets [7]. Moreover, it also provided new insights into the preferential alignments of the SGS and its dependence with the *Ra*-numbers [8], highlighting that the modelization of the SGS heat flux is the main difficulty that (still) precludes reliable LES of buoyancy-driven flows at (very) high Ra-numbers. This inherent difficulty can be by-passed by carrying out simulations at low-Prandtl numbers. In this case, the ratio between the Kolmogorov length scale and the Obukhov-Corrsin length scale (the smallest scale for the temperature field) is given by $Pr^{3/4}$; therefore, for instance, at $Pr = 0.005$ (liquid sodium) we have a separation of more than one decade. Hence, it is possible to combine an LES simulation for the velocity field (momentum equation) with the numerical resolution of all the thermal scales. Results obtained in Ref. [8] suggest that accurate predictions of the overall Nu can be obtained with meshes significantly coarser than those needed for a DNS (*e.g.* in practice for $Pr = 0.005$ we can expect mesh reductions in the range 10^2-10^3 for the total number of grid points leading to computational cost reductions in the range 10^3-10^4). This can be clearly observed in Figure 2 (bottom), where estimations of the mesh size for LES are given with the assumption that thermal scales are fully resolved. This opens the possibility to reach the ultimate regime carrying out LES at low-Pr using meshes of ”only” 10^{10}-10^{11} grid points. Nevertheless, to do so, we also need to combine proper numerical techniques for LES (also DNS) with an efficient use of modern high-performance computing (HPC) systems.

3 Numerical methods and algorithms for large-scale simulations on modern supercomputers

The essence of turbulence are the smallest scales of motion. They result from a subtle balance between convective transport and diffusive dissipation. Mathematically, these terms are governed by two differential operators differing in symmetry: the convective operator is skew-symmetric, whereas the diffusive is symmetric and negative semi-definite. At discrete level, operator symmetries must be retained to preserve the analogous (invariant) properties of the continuous equations: namely, the convective operator is represented by a skew-symmetric matrix, the diffusive operator by a symmetric, negative semi-definite matrix and the divergence is minus the transpose of the gradient operator. In our opinion, this is a basic requirement for reliable DNS and LES simulations. Furthermore, these (large-scale) simulations should run efficiently on the variety of modern HPC systems (CPUs, GPUs, ARM,...) while keeping the code easy to port, optimize and maintain.

In this regard, a fully-conservative discretization for collocated unstructured grids was proposed [9]. It exactly preserves the symmetries of the underlying differential operators and is based on only five discrete operators (*i.e.* matrices): the cell-centered and staggered control volumes (diagonal matrices), Ω_c and Ω_s, the face normal vectors, N_s, the cell-to-face interpolation, $\Pi_{c\rightarrow s}$ and the cell-to-face divergence operator, M. Therefore, it constitutes a robust approach that can be easily

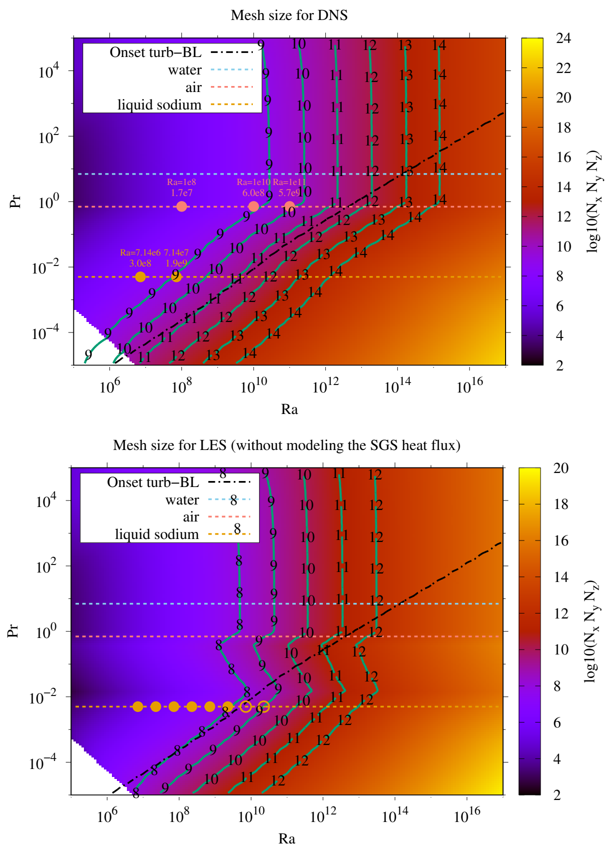

Fig. 2 Estimation of the mesh sizes for DNS (top) and LES (bottom) simulations of RBC in the $\{Ra, Pr\}$ phase space. LES estimations assume that thermal scales are fully resolved, *i.e.* no SGS heat flux model is needed. Green solid isolines represent the $log10$ of the total number of grid points. Three dashed horizontal lines correspond to three different working fluids: water ($Pr = 7$), air ($Pr = 0.7$) and liquid sodium ($Pr = 0.005$). Dots displayed in the top figure correspond to the DNS simulations carried out in previous studies [5, 7, 8] whereas the dots shown in the bottom figure are the set of LES simulations (being) carried out in the present work. Black dash-dotted line is an estimation for the onset of turbulence in the thermal boundary layer.

implemented in existing codes such as OpenFOAM® [10]. Then, for the sake of cross-platform portability and optimization, CFD algorithms should rely on a very reduced set of (algebraic) kernels [11] (*e.g.* sparse-matrix vector product, SpMV; dot product; linear combination of vectors). In this implementation approach, the basic kernels of the code shrink to dozens of lines; therefore, the portability becomes natural, and maintaining multiple implementations for different HPC architectures takes minor effort.

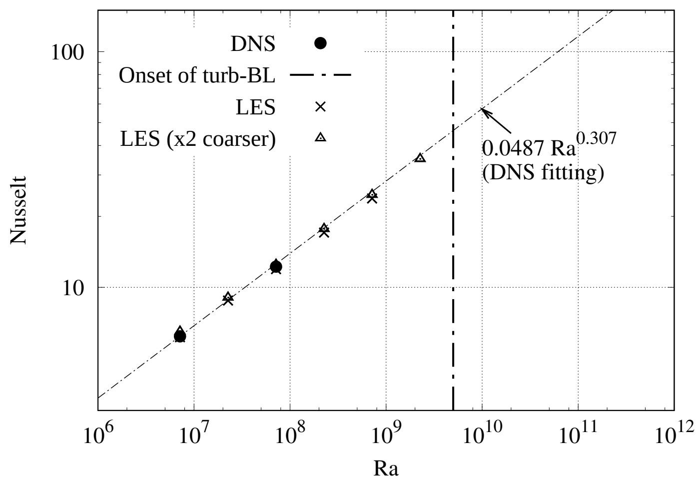

Fig. 3 Nu-vs-Ra results obtained with LES simulations at $Pr = 0.005$ using the same RBC configuration as in Ref.[8] where the two DNS results (solid black dots) were computed. The vertical dash-dotted line corresponds to the estimated Ra (for this particular Pr) where the thermal boundary layer becomes turbulent.

4 First results and conclusions

The above explained numerical techniques are being used to carry out a set of LES simulations of RBC at $Pr = 0.005$ for a wide range of Ra numbers (see dots in Figure 2, bottom). The configuration is the same as in Ref.[8] where two DNS simulations (solid black dots in Figure 3) were computed using meshes with $488 \times 488 \times 1280 \approx 305M$ ($Ra = 7.14 \times 10^6$) and $996 \times 996 \times 2048 \approx 1911M$ ($Ra = 7.14 \times 10^7$) grid points, respectively. For the LES simulations, two levels of mesh refinement are being used: namely, a fine level that approximately corresponds to estimations shown in Figure 2 (bottom) and a coarse level which is approximately twice coarser in each spatial direction. For instance, LES meshes at $Ra = 7.14 \times 10^7$ have respectively $44 \times 44 \times 96 \approx 0.19M$ and $90 \times 90 \times 160 \approx 1.3M$ grid points, *i.e.* ≈ 10000 and ≈ 1500 coarser compared with the DNS mesh. Meshes are designed to properly resolve the boundary layer whereas the much coarser bulk region is fine enough to guarantee that thermal scales are fully resolved, *i.e.* no SGS heat flux model is needed. Then, the SGS stress tensor is modelled using the S3PQ model [12] which was already tested for this RBC configuration in Ref. [8].

Results of the overall Nusselt number are displayed in Figure 3. LES simulations up to $Ra = 7.14 \times 10^{10}$ (for the coarse level) and $Ra = 2.26 \times 10^{10}$ (for the fine level) are still being computed on MareNostrum 4 supercomputer. These points are located beyond the transition point for this Pr-number (see Figure 2, bottom). Nevertheless, these simulations are not statistically converged yet and, therefore, results are not shown here. At first sight, we can observe an accurate agreement with previous DNS results. Furthermore, there is a rather good agreement with the Nu-vs-Ra scaling predicted using the DNS data. In any case, these preliminary results show the capability to obtain accurate predictions of the Nu-number using LES simulations. Accordingly to the classical GL theory, on-going LES simulations at higher Ra-number should possibly show a change in the Nu-vs-Ra scaling indicating that we are finally hitting the ultimate regime of thermal turbulence.

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