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A multiple-resolution strategy for Direct Numerical Simulation of scalar turbulence

R. Ostilla-Monico [a,*,1], Yantao Yang [a,1], E.P. van der Poel [a], D. Lohse [a], R. Verzicco [a,b]

[a] Physics of Fluids, MESA+ Institute, University of Twente, Enschede, The Netherlands
[b] Department of Industrial Engineering, Università di Roma "Tor Vergata", Roma, Italy

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ABSTRACT

In this paper a numerical procedure to simulate low diffusivity scalar turbulence is presented. The method consists of using a grid for the advected scalar with a higher spatial resolution than that of the momentum. The latter usually requires a less refined mesh and integrating both fields on a single grid tailored to the most demanding variable produces an unnecessary computational overhead. A multiple resolution approach is used also in the time integration in order to maintain the stability of the scalars on the finer grid. The method is the more advantageous the less diffusive the scalar is with respect to momentum, therefore it is particularly well suited for large Prandtl or Schmidt number flows. However, even in the case of equal diffusivities the present procedure gives CPU time and memory occupation savings, due to the increased gradients and more intermittent behaviour of the scalars when compared to momentum.

1. Introduction

Countless phenomena in Nature and technology involve one or more scalar fields that are advected and diffused by a turbulent flow. The dilution of pollution in the atmosphere [1], the transport of nutrients in oceans [2], the cooling or heating of devices [3] and the buoyancy-driven currents generated by natural- [4,5] and double-diffusive [6,7] convection are just few examples among many. Scalars have also be used to capture interfaces in multiphase flows [8] or to determine the dynamical properties of turbulent flows [9].

Scalars can be classified as either passive or active, depending on whether they couple back to the velocity field or not. Many studies of simulations of passive scalars in incompressible homogeneous isotropic turbulence (HIT) have been performed during the years [10–15]. For a comprehensive overview, we refer the reader to the review by Warhaft [16] and the references therein. For active scalars, especially in the context of natural convection, numerical simulations have also been proven to be very helpful in unravelling the complex physics behind these phenomena [17] even if the calculations have shown to be more demanding than expected, taking up to millions of CPU hours in recent studies [18,19].

The common understanding of the problem is that in three-dimensional turbulent flows, there is a cascade from the largest towards the small spatial scales up to a lower limit that is determined by the diffusivity. As each field has its own diffusivity, these scales can have different magnitudes. In direct numerical simulation (DNS) the mesh size must be smaller

* Corresponding author.
E-mail address: r.ostillamonico@utwente.nl (R. Ostilla-Monico).
[1] Both these authors have made an equal contribution to the manuscript.

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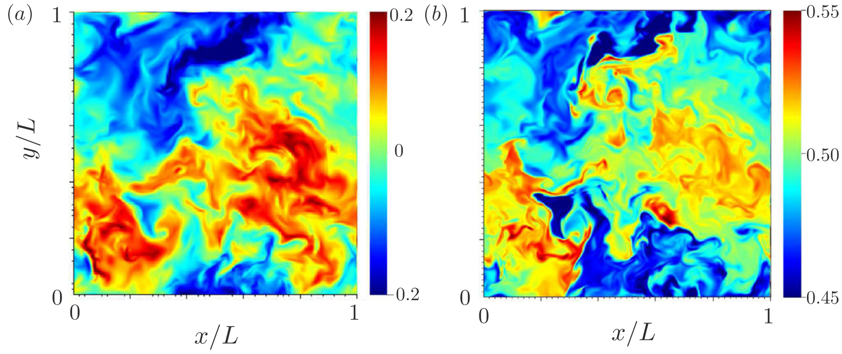

Fig. 1. A horizontal plane halfway between the plates for a Rayleigh–Bénard simulation in a Cartesian geometry at $Ra = 10^{10}$ and Prandtl number $Pr = 1$. (a) Vertical velocity, red indicating rising fluid while blue indicates falling fluid, (b) temperature, red indicating hot fluid and blue indicating cold fluid. Even though the Prandtl number is one, much sharper gradients can be seen in the right panel. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

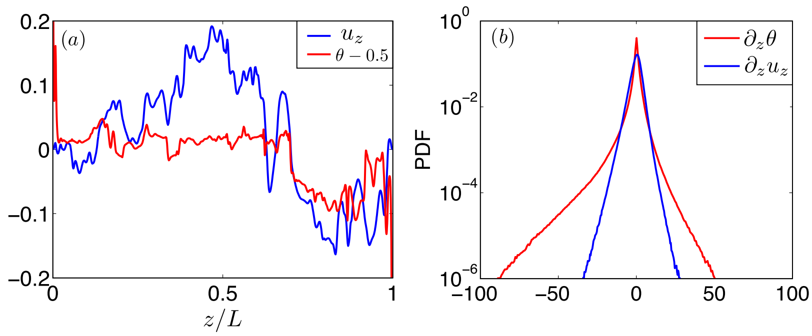

Fig. 2. (a) Instantaneous θ and u_z profiles as a function of the vertical coordinate z/L for $Ra = 10^{10}$, $Pr = 1$ RB simulation. (b) PDF of $\partial_z\theta$ and $\partial_z u_z$ for the same simulation in the bulk.

than the smallest among them: This requirement quickly renders DNS infeasible. Denoting as η_K the smallest (Kolmogorov) scale of the momentum field, we can calculate the analogous quantity for a scalar field S as $\eta_B = \eta_K / Sc^{1/2}$, also called the Batchelor scale, with $Sc = \nu/\kappa_S$ the Schmidt number defined as the ratio of the kinematic viscosity ν and the scalar diffusivity κ_S, respectively. In some cases, like sugar in water, the Schmidt number exceeds 10^3 resulting in a Batchelor scale of $\eta_B \simeq \eta_K/30$. With equal grid resolutions for the scalar and the momentum fields, this entails that the momentum field is overresolved by a factor of approximately 30 in each spatial direction. The problem is exacerbated by the fact that a scalar is described by only a single quantity, while momentum is a vector field satisfying the incompressibility condition or other related constraints. This implies that the solution of the momentum alone generally takes an order of 90% of the total CPU time of a simulation and therefore resolving it on an unnecessary fine mesh is not desirable.

The above scenario, essentially derived from dimensional analysis, does not give the complete picture since it does not account for the structure of the equations. In fact, the naïve comparison between the Kolmogorov and Batchelor scales suggests that for $Sc \approx 1$, $\eta_K \simeq \eta_B$ although in practice the resolution requirements for the momentum and the scalar fields are not the same. Visual evidence of the latter statement can be obtained from the instantaneous snapshots of Fig. 1 showing horizontal cross-sections of temperature and vertical velocity in a thermally driven turbulent flow, the Rayleigh–Bénard (RB) problem, i.e. the flow between two parallel plates heated from above and cooled from below. In RB flow, the fluid hotter than the average temperature (0.5 in nondimensional units) generates upward buoyancy and therefore positive vertical velocity (and vice versa). Although the two fields are very well correlated on the large scales, the sharp fronts of the scalar field do not have an analogous counterpart in the momentum distribution and this results in a different resolution requirement for scalar and momentum fields.

For a fully resolved DNS, the momentum gradients must be adequately captured so that the dissipative scale (and thus vorticity) is adequately resolved. Analogously, the scalar (temperature) gradients must be correctly captured so that the diffusive scale (and thus the scalar variance) is adequately resolved. We quantify the difference in gradients between scalars and momentum in Fig. 2(a) by showing instantaneous temperature θ and vertical velocity u_z profiles across a vertical line from a doubly periodic Rayleigh–Bénard simulation: much steeper gradients can be seen in the temperature (scalar) field. These steep gradients are smoother in the vertical velocity and this lowers the resolution requirements of momentum with respect to those of scalars. This observation is further corroborated by Fig. 2(b) showing the probability density functions of $\partial_z\theta$ and $\partial_z u_z$ computed in the bulk of the flow without the boundary layers. Extreme gradients can be seen to be more likely for θ thus evidencing a more intermittent behaviour. This behaviour has been extensively studied in experiments