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Impact of unresolved smaller scales on the scalar dissipation rate in direct numerical simulations of wall bounded flows

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ABSTRACT

Passive scalar dynamics in a turbulent channel flow is studied with Direct Numerical Simulation at friction Reynolds number $Re_\tau = 160$ and Prandtl number $Pr = 1$. The goal of the study is to assess the grid spacing requirement for an accurate estimation of various integral turbulent statistics, with a special focus on the scalar dissipation rate. The implemented spatial resolutions span from the resolution comparable to the similar Direct Numerical Simulations (DNS) studies in the past, to the very fine resolution implemented by Galantucci and Quadrio (2010). All scalar fields are computed in parallel using a single velocity field resolved with the finest resolution, thus reducing the statistical variability. In addition, to confidently assess the grid spacing requirement, we also evaluate the statistical uncertainty. The "standard" resolution of the DNS studies (resolution used by Kim et al. (1987)) is usually sufficient for predictions of first and second-order integral turbulence scalar field statistics. Non-negligible corrections of the fourth-order integral statistics, especially the scalar dissipation variance profile, are observed with enhancement of the scalar resolution from the one used in the "standard" DNS studies to the resolution recommended by Vreman and Kuerten (2014), which is roughly two times finer in each spatial direction. Further resolution enhancements produce only marginal differences.

1. Introduction

Since the pioneering efforts of Obukhov (1968), Corrsin (1951), Batchelor (1959) and Batchelor et al. (1959), passive scalars in turbulent flows have been the focus of a number of studies. As summarized in the review by Warhaft (2000), experiments and simulations are challenging classical descriptions of passive scalars derived from the Kolmogorov cascade phenomenology. Evidences suggest a strong coupling between large and small scales and no local isotropy at inertial and dissipation scales. They also suggest that passive scalars are associated with a stronger intermittency compared with the velocity.

Following Batchelor (1959) and Batchelor et al. (1959), for a unit Prandtl number as herein, the smallest spatial scale for scalar mixing is the Kolmogorov scale $\eta = (\nu^3/\bar{\varepsilon})^{1/4}$, where ν is the dynamic viscosity and $\bar{\varepsilon}$ the mean dissipation rate of the turbulent kinetic energy. Similarly, the smallest time scale is the Kolmogorov time scale $\tau_\eta = \sqrt{\nu/\bar{\varepsilon}}$. As the passive scalar is intermittent, locally, structures with a spatial (temporal) span shorter than η (τ_η) appear in a flow. Suspecting those fine structures to be related to highly dissipative events, a number of DNS have been performed with sub-Kolmogorov scales resolved (Schumacher et al., 2005; Donzis and Yeung, 2010; Galantucci and Quadrio, 2010).

One of the central quantity in those studies is ε_θ, the scalar dissipation rate, defined by

$$\varepsilon_\theta = 2\alpha\,|\nabla\theta|^2 = 2\alpha\left[\sum_{i=1}^{3}(\partial_i\theta)^2\right] \tag{1}$$

where α is the thermal diffusivity. According to Pope (2013), this quantity he calls the all-important dissipation rate matters in combustion models. It is also a central quantity in Reynolds Averaged Navier-Stokes (RANS) turbulence models as it appears in the budget equation of the scalar variance. Lately, Flageul et al. (2017) showed that the dissipation rate associated with the temperature variance is discontinuous at the fluid-solid interface in case of conjugate heat transfer. This is prominent for industrial applications where thermal fatigue is a concern.

Studying homogeneous isotropic turbulence, Schumacher et al. (2005) showed that the improved resolution matters when investigating the tails of the Probability Density Function (PDF) of ε_θ, which correspond to low probability events associated with high or low dissipation rates. More specifically, they show that a poorer resolution has a stronger impact on regions of low ε_θ than on those of high ε_θ. On a similar configuration, Donzis and Yeung (2010) showed accurate estimation of advanced statistics (scalar dissipation intermittency

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exponent, structure functions at moderately high orders and PDF of ε_θ up to 200 $\overline{\varepsilon_\theta}$) with a grid spacing equal to the Batchelor scale, which is exactly the Kolmogorov scale in the present study.

Studying a turbulent channel flow ($Re_\tau = 160$, $Pr = 1$), Galantucci and Quadrio (2010) extended the analysis to wall-bounded flows. They showed resolution effects on the profiles of the mean ε_θ and its variance, but also on the PDF of ε_θ and recommended a very fine spatial resolution ($\Delta_x^+ = \Delta_z^+ = 1$ and $0.43 < \Delta_y^+ < 2$). In the streamwise (spanwise) direction, this is 6 (4) times finer than what is necessary for the velocity according to Vreman and Kuerten (2014). The authors of the present study estimate that the resolution proposed by Vreman and Kuerten is sufficient for accurate predictions of the key integral turbulent statistics of the passive scalar field at $Pr = 1$, including the average scalar dissipation rate and its variance. The main objective of the present paper is to assess this claim.

The structure of the paper is as follows. In the second section, the governing equations and the computational setup are described alongside with the procedure to estimate the sampling error. In the third section, preliminary investigation on coarser grids is presented. In the fourth section, the DNS results are presented. Discussion and conclusions are collected in the last section.

2. Governing equations, computational setup and sampling error

Dimensionless equations of the incompressible turbulent channel flow with transport of a passive scalar can be found in various sources (Kasagi et al., 1991; Kawamura et al., 1998):

$$\nabla.\ u \ = 0 \tag{2}$$

$$\partial_t u \ = \ -\nabla.\ (u.\ u) + \frac{1}{Re_\tau}\nabla^2 u - \nabla(p) + \overrightarrow{1_x} \tag{3}$$

$$\partial_t \theta \ = \ -\nabla.\ (u.\ \theta) + \frac{1}{Re_\tau Pr}\nabla^2 \theta \tag{4}$$

Eqs. (3) and (4) are normalized with the channel half width h, the kinematic viscosity ν and the friction velocity u_τ. Low friction Reynolds number $Re_\tau = 160$ and Prandtl number $Pr = 1$ were selected in order to replicate the conditions of the simulations performed by Galantucci and Quadrio (2010). As the Prandtl number is unity, Kolmogorov and Batchelor length-scales are identical.

Periodic boundary conditions are used in the streamwise and spanwise directions, labelled x and z, respectively, while the wall-normal direction is labelled y. The forcing term $\overrightarrow{1_x}$ represents a constant pressure gradient in the streamwise direction and has a unit amplitude thanks to the normalization used. Boundary conditions for the passive scalar fields at the channel walls are $\theta = 1$ at $y = 1$, and $\theta = -1$ at $y = -1$ and were previously used in the simulations of Papavassiliou and Hanratty (1997), Johansson and Wikström (2000) and Galantucci and Quadrio (2010).

The equations are solved with a pseudo-spectral scheme. Fourier series are used in the x and z directions and Chebyshev polynomials are used in the y direction. Second-order accurate time differencing (Crank–Nicolson scheme for diffusive terms and Adams–Bashforth scheme for other terms) is used with maximum Courant number kept at approximately 0.1. The aliasing error is removed with computation of the nonlinear terms on a grid 1.5 times finer in all directions. The computer code is based on the code developed by Gavrilakis et al. (1986), which was later modified by Lam and Banerjee (1988). The code was used and verified in simulations of Tiselj et al. (2001), Tiselj and Cizelj (2012) and Tiselj (2014).

The extension of the computational domain, normalized with the channel half width h, was taken from the work of Galantucci and Quadrio (2010): $L_x = 4.19$, $L_y = 2$, and $L_z = 2.09$. Both in the streamwise and spanwise directions, this is about 3 times smaller than the domain used in Kasagi et al. (1991). Such a small computational domain neglects an important part of the large scale structures in the turbulent flow, however, it is known to be sufficient for special studies focused on small scale turbulent structures of the velocity field (Jiménez and Moin, 1991). The small domain offers a platform for simplified studies of the resolution requirements. It is often overlooked that in addition to obliterating large scale structures, small domain can be affected by a significant sampling error. For instance, Galantucci and Quadrio (2010) report up to 5% differences in the friction temperature values in their simulations performed on different resolutions and averaged over the time interval of 2400 viscous time units (statistics based on 60 instantaneous fields).

Table 1
Spatial resolution for the transported passive scalar fields.

Scalar field	$Nx*Ny*Nz$	Δ_x^+	$[\Delta_{y,min}^+, \Delta_{y,max}^+]$	Δ_z^+
1KMM	40*129*60	16.8	[0.048, 3.93]	5.57
2GQC	64*129*64	10.5	[0.048, 3.93]	5.23
3S	112*129*80	5.99	[0.048, 3.93]	4.18
4VK	112*181*80	5.99	[0.024, 2.78]	4.18
5GQM	360*129*180	1.86	[0.048, 3.93]	1.86
6S	360*181*180	1.86	[0.024, 2.78]	1.86

In the present study, the resolution requirement for the passive scalar field is examined with a single DNS run. The velocity field is calculated on the finest grid of $Nx*Ny*Nz = 360*181*180$ modes (Case 6S in Table 1). Six distinct passive scalar fields are simultaneously transported by this velocity field and resolved with different number of modes, see Table 1. The naming scheme for the passive scalar fields is inspired by the name of the authors who promoted certain resolution. For instance, in 1KMM, KMM stands for Kim et al. (1987). Similarly, in 4VK, VK stands for Vreman and Kuerten (2014). The number preceding the letters corresponds to a ranking of the grids: 1 for the coarsest, 6 for the finest. For the five scalar fields resolved with a lower resolution, all Fourier and Chebyshev modes above the indicated resolution are set to zero at the end of each time step.

This approach, which is comparable to the one in Brethouwer et al. (2003) or Gotoh et al. (2012), reduces the statistical variability and eases the separation of the sampling error from the error induced by a coarser spatial resolution. The separation of statistical uncertainty and resolution effects is of particular importance for the present work: the smaller extension of the domain in the homogeneous directions increases the sampling error, which easily exceeds the tiny differences induced by the variable resolution of the passive scalar field, except for simulations with a very long duration.

The finer resolution (case 6S in Table 1) used in the wall-normal direction follows (Vreman and Kuerten, 2014). In the streamwise and spanwise directions, case 6S corresponds to the resolution used by Galantucci and Quadrio (2010) in their “Medium” simulation. This is 2 to 3 times finer than the recommendation of Vreman and Kuerten (2014). Cases 5GQM and 2GQC correspond to the “Medium” and “Coarse” cases in Galantucci and Quadrio (2010), respectively. The case 4VK is using the resolution recommended by Vreman and Kuerten (2014). The case 3S is similar to 4VK except that it uses a coarser wall-normal grid. Lastly, the resolution in case 1KMM is comparable with most of the previous DNS simulations (Kim et al., 1987; Kasagi et al., 1991; Tiselj et al., 2001).

The present DNS is performed with a time step of 0.008 ν/u_τ^2 and one snapshot is taken every 1000 time steps. 700 snapshots are used to reconstruct the statistics, corresponding to an averaging time of 5600 ν/u_τ^2.

DNS is widely used to produce reference data. However, as pointed out by Oliver et al. (2014), statistics obtained from DNS contain nontrivial errors. Errors arise mainly from the discretization of the equations and from the finite statistical sampling. As our code is based on a pseudo-spectral method and we use a fine grid, the spatial