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Using Highly-Resolved Direct Numerical Simulations to Analyse the Universality of Small-Scale Turbulence

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The universality of a passive scalar advected in homogeneous isotropic turbulence is studied by scale-by-scale budget equations for higher order moments. Based on an analytical development of structure functions in the dissipative range, a scaling for higher order structure functions is proposed. A similarity scale analysis is used to show the validity of the proposed scaling in the dissipative range and the inertial range. The analysis is based on highly resolved direct numerical simulations (DNS) with different Reynolds numbers. To this end, a comprehensive DNS data base of turbulence has been created. To resolve all relevant scales of turbulence the grid size is as high as 68 billion grid points. This data base allows a consistent analysis of small-scale turbulence and scaling laws of turbulent flows.

1 Introduction

The motion of turbulent flows is a complex, non-linear multi-scale phenomenon, posing some of the most fundamental problems in classical physics. A precise prediction of the statistical properties of turbulence based on the governing equations would be of tremendous practical importance for a wide field of applications ranging from geophysics to combustion science. In these disciplines the transport and mixing of a passive scalar species by turbulence is of special interest. A passive scalar is advected by the velocity field but has itself a negligible effect on the flow. The scalar species can be a concentration field, a pollutant, or it can be interpreted as a temperature field in the case that buoyancy forces are small compared to inertial forces. The dynamic of the scalar field exhibits complex behaviour due to the non-linear coupling with the velocity field. The dominant process for turbulent mixing is the stretching and folding mechanism imposed by the velocity field on regions of locally homogeneous concentration. Stretching and folding increases local concentration gradients until molecular diffusion becomes significant and dissipates local variations of the scalar. This process generates a cascade of different scales and has two important implications. Firstly, turbulence dramatically enhances the rate of mixing, but secondly, stretching and folding creates locally confined strong bursts in the scalar field. The occurrence of very large but relatively rare events affects the statistics of the scalar field and results in a deviation from Gaussianity. In the literature this phenomenon is called internal intermittency. Despite decades of research, the physical mechanism behind internal intermittency is still unresolved, see Sreenivasan and Antonia[1].

Direct numerical simulations (DNS) has become a profound and well established tool to fundamentally investigate scaling properties of turbulence. DNS solves the governing equations, namely the Navier-Stokes equations, for all relevant scales and provides access

to spatially and temporally resolved three-dimensional fields. However, numerical approaches to solve the Navier-Stokes equations are very challenging, since one has to cope with a tremendous number of degrees of freedom. Using the scale separation between large and small scales, the number of required grid points N^3 to resolve all relevant degrees of freedom can be expressed as a function of the Reynolds number, i.e.

$$N^3 \propto Re_\lambda^{9/2}\,, \tag{1}$$

where Re_λ is the Reynolds number based on the Taylor length scale. Eq. 1 reveals that the computational cost increases dramatically with Reynolds number. However, the growing capabilities of recent supercomputers have enabled DNS of turbulent flows at adequately high Reynolds numbers close to experiments at laboratory scale.

The remainder of the paper is as follows. In Sec. 2 we present the direct numerical simulations on which the analysis is based. In Sec. 3 the impact of intermittency on scalar structure functions is studied in the context of universality and self-similarity.

2 Direct Numerical Simulations

In order to tackle the turbulence problem, we developed a massive-parallel DNS code named *psOPEN*. The DNS code solves the three-dimensional incompressible Navier-Stokes equations in the vorticity formulation together with an advection-diffusion equation for a passive scalar ϕ. A uniform mean gradient Γ is imposed on the scalar field in x_2-direction and injects continuously energy into the scalar field to keep statistics in a statistically steady state. We consider a passive scalar with unity Schmidt number $Sc = \nu/D$, so that the kinematic viscosity ν equals the molecular diffusivity D.

The system of equations is solved by a standard Fourier pseudo-spectral method in a triply periodic cubic box with size 2π by following an approach similar to that of Mansour and Wray[2]. An integrating factor technique is used for an exact integration of the viscous and diffusive terms. Temporal integration is performed by a low-storage, stability preserving, third-order Runge-Kutta scheme. The non-linear term is computed in physical space and a truncation technique with a smooth spectral filter is applied to remove aliasing errors. An external stochastic forcing[3] is applied to the velocity field to maintain a statistically steady state. The forcing is statistically homogeneous and isotropic, and limited to a low wave-number range so that the small scales are not affected by the forcing scheme. For optimal performance on the BlueGene/Q system, the code *psOPEN* has been parallelised by a hybrid MPI/OpenMP technique. To improve the parallel efficiency a novel parallel pencil-FFT library has been developed. The library utilises an asynchronous approach with the aim to overlap communication and computation. With this technique, the strong scaling of *psOPEN* on JUQUEEN reveals an excellent efficiency up to 458,752 cores.

In the frame of this project, we have created a comprehensive DNS data base of turbulence at various Reynolds numbers. The DNS has been conducted on the supercomputer JUQUEEN. The Reynolds number is varied between $Re_\lambda = 88$ and $Re_\lambda = 754$ by solely adjusting the kinematic viscosity ν, while keeping all other parameters constant. Characteristic parameters are summarised in Tab. 1, where N denotes the number of grid points along one coordinate axis, $\langle k \rangle$ the mean kinetic energy, $\langle \varepsilon \rangle$ the mean energy dissipation, $\langle \phi^2 \rangle$ the mean scalar variance, and $\langle \chi \rangle$ the mean scalar dissipation. Ensemble-averages are denoted by angular brackets and are computed over the whole computational domain

	R0	R1	R2	R3	R4	R5	R6
N	512^3	1024^3	1024^3	2048^3	2048^3	4096^3	4096^3
Re_λ	88	119	184	215	331	529	754
ν	0.01	0.0055	0.0025	0.0019	0.0010	0.00048	0.00027
$\langle k \rangle$	11.15	11.20	11.42	12.70	14.35	23.95	24.41
$\langle \varepsilon \rangle$	10.78	10.52	10.30	11.87	12.55	28.51	26.71
$\langle \phi^2 \rangle$	1.95	1.89	1.94	2.47	2.25	2.41	2.43
$\langle \chi \rangle$	3.92	3.90	4.01	5.00	4.76	6.78	6.14
t_{avg}/τ	100	30	30	10	10	2	3
M	189	62	61	10	10	6	9
$\kappa_{\max}\eta$	3.93	4.99	2.93	4.41	2.53	2.95	1.95

Table 1. Summary of different DNS cases. Reynolds number variation between $\mathrm{Re}_\lambda = 88$ and $\mathrm{Re}_\lambda = 754$.

due to homogeneity and over a time frame t_{avg} due to stationarity. To improve the accuracy of statistics, averages are computed over M statistically independent ensembles, with M between 6 for case R5 and 189 for case R0.

An adequate resolution of relevant length and time scales is of primary importance for the accuracy of the DNS. To ensure an appropriate resolution of the smallest scales in the present DNS, the number of grid points has been increased to as high as $4096 \times 4096 \times 4096$. Following Ishihara *et al.*[4], a resolution condition of $\kappa_{\max}\eta > 2.0$ is maintained for all cases, where $\kappa_{\max}$ is the highest resolved wave-number mode and $\eta = (\nu^3/\langle\varepsilon\rangle)^{1/4}$ is the Kolmogorov length scale. Recent theoretical studies have pointed out the need for high spatial resolution. This is especially important for the computation of higher-order moments, which are relevant for the study of intermittency. Further details about the DNS are presented by Gauding *et al.*[5], Peters *et al.*[6], and Goebbert *et al.*[7].

3 Universality of Higher Order Statistics in Small-Scale Turbulence

Fully developed turbulence is characterised by a large range of length scales, varying from the so-called integral length scale l_t, at which large velocity fluctuations occur on average, down to the smallest scale, the so-called Kolmogorov or dissipation scale η, at which turbulent fluctuations are dissipated. Before turning to a quantitative analysis of turbulence we present a visualisation of the data obtained from DNS. Fig. 1 shows the iso-surface of the enstrophy. The enstrophy is a small-scale quantity, that is characterised by a high level of intermittency. Fig. 1 reveals an enormous number of degrees of freedom represented by the interaction of vortices that tend to cluster in coherent structures.

The standard paradigm of turbulence is that under the condition of sufficiently high Reynolds numbers, the small scales of the flow decouple from the large scales. While the large scales are non-universal and depend on the initial and boundary conditions, the small scales should reveal in a statistical sense universal properties. The notion of small-scale universality was first put forward by Kolmogorov in 1941. In Kolmogorov[8], the velocity increment $\Delta u_i = u_i(\boldsymbol{x} + \boldsymbol{r}) - u_i(\boldsymbol{x})$ was introduced as the difference of the velocity fluctuations $u_i(\boldsymbol{x}; t)$ separated by a distance $\boldsymbol{r}$. The statistical moments of the velocity

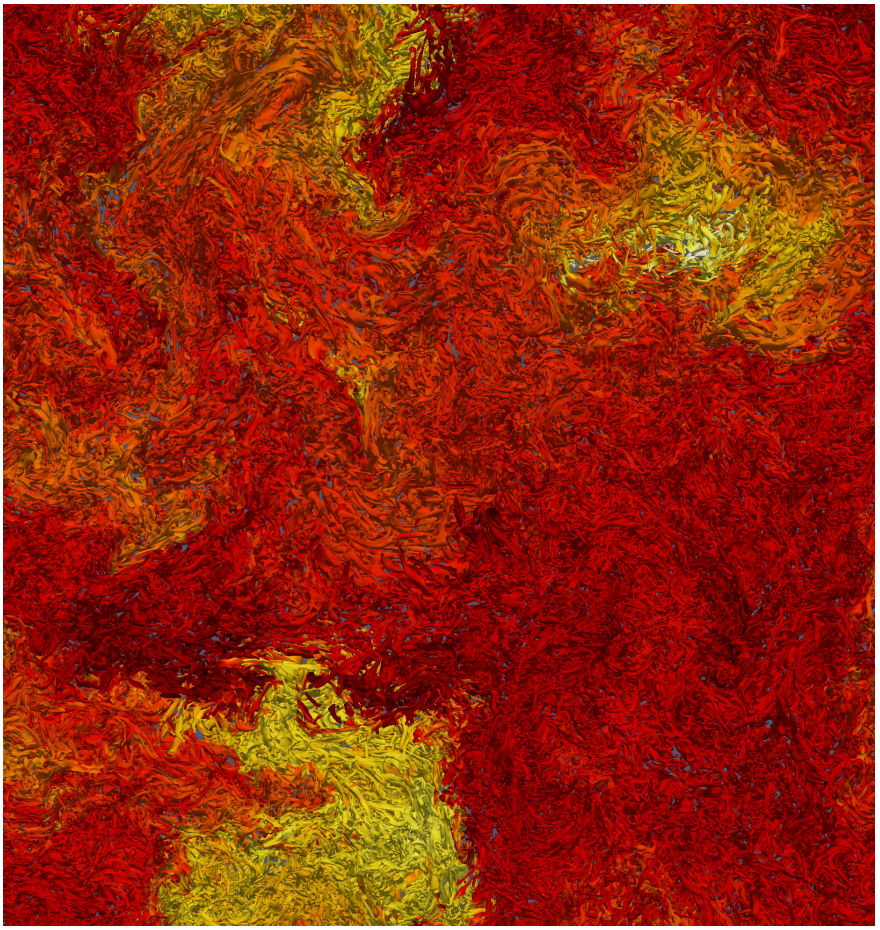

Figure 1. Iso-surface of the enstrophy obtained from case R4 coloured by the value of the passive scalar. The turbulent field exhibits coherent structures that represent the interaction of vortices of different size and intensity.

increment are known as structure functions, where

$$D_{p,0}(r) = \langle (u_1(x_1 + r, x_2, x_3) - u_1(x_1, x_2, x_3))^p \rangle \,, \tag{2}$$

is the longitudinal velocity structure function of order p, which is independent of position $\boldsymbol{x}$ and the direction of $\boldsymbol{r}$. Kolmogorov hypothesised that in the dissipative range for small values of r, the distribution function of Δu should depend only on two parameters, namely the viscosity ν and the mean energy dissipation rate $\langle \varepsilon \rangle$. Because only two quantities with different physical units are involved, this was viewed as a claim of universality. However, Landau[15] argued that universality would be violated due to the intermittent character of the dissipation.

Kolmogorov's scaling theory was extended to scalar turbulence by Obukhov[9] and Corrsin[10] (in the following referred to as KOC theory). Similar to Eq. 2, a scalar struc-

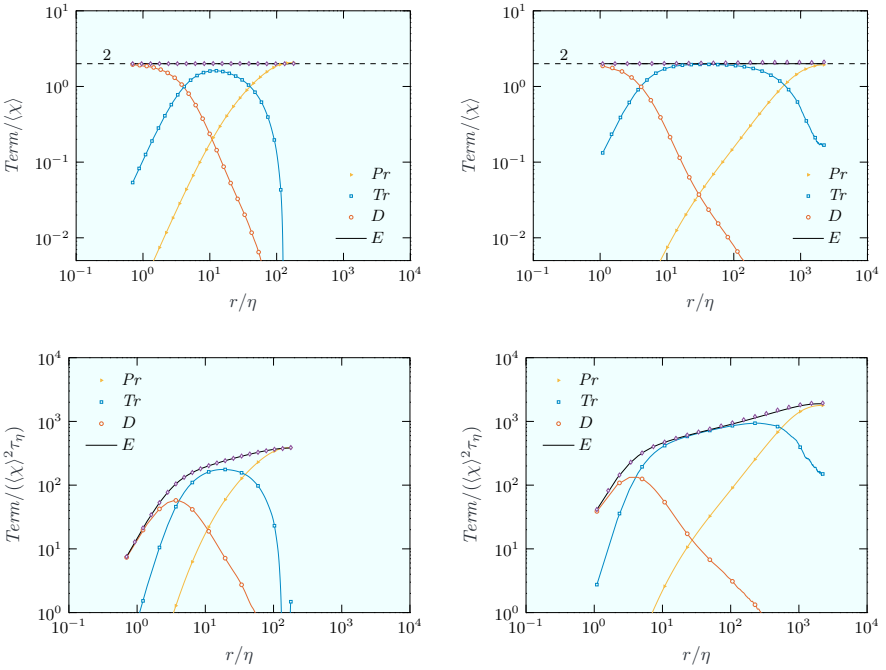

Figure 2. Terms in Eqs. 4 and 5 for the second (top) and fourth (bottom) order scalar structure function equation for case R0 (left) and for case R5 (right). The diamond symbols represent the sum $Tr_{2n}(r)+Pr_{2n}(r)+D_{2n}(r)$, which balances the term $E_{2n}(r)$ for all scales. This indicates that the budget is satisfied.

ture function of order p is defined by

$$S_p(r) = \langle(\phi(x+r) - \phi(x))^p\rangle = \langle(\Delta\phi)^p\rangle\,. \tag{3}$$

Transport equations for the even moments of the scalar increment $\Delta\phi$ can be derived as presented in Danaila *et al.*[11] and Gauding *et al.*[12] and read

$$\frac{\partial}{\partial t}\big\langle(\Delta\phi)^{2n}\big\rangle(\boldsymbol{r}) + \underbrace{\frac{\partial}{\partial r_i}\big\langle(\Delta u_i)(\Delta\phi)^{2n}\big\rangle(\boldsymbol{r})}_{-Tr_{2n}} + \underbrace{2n\Gamma\big\langle(\Delta u_2)(\Delta\phi)^{2n-1}\big\rangle(\boldsymbol{r})}_{-Pr_{2n}} = J_{2n}(\boldsymbol{r})\,, \tag{4}$$

where J_{2n} collects all terms that contain the molecular diffusivity D, i.e.

$$J_{2n}(\boldsymbol{r}) = \underbrace{2D\frac{\partial^2}{\partial r_i^2}\langle(\Delta\phi)^{2n}\rangle}_{D_{2n}} - \underbrace{n(2n-1)\langle(\Delta\phi)^{2n-2}\left(\chi(\boldsymbol{x})+\chi(\boldsymbol{x}+\boldsymbol{r})\right)\rangle}_{E_{2n}}\,, \tag{5}$$

with χ being the scalar dissipation. Eq. 4 is exact, which means that it is derived from first-principles without any approximation beside of incompressibility and homogeneity.

Even though Eq. 4 is exact, it cannot be solved directly, because it is not closed. Nonetheless, all terms can be obtained from DNS. This is displayed in Fig. 2, where the terms of the transport equations for the second and fourth order scalar structure functions

are shown for $Re_\lambda = 88$ and $Re_\lambda = 529$. The second order scale-by-scale budget equation has been widely studied in literature because it represents the inter-scale transport of scalar energy. Here, the sum of inter-scale transport Tr_2, production Pr_2 and diffusive transport D_2 is independent of r and equals $2\langle\chi\rangle$. Two separate analytical solutions can be derived for different range of scales. The first solution is obtained in the dissipative range for $r \to 0$, where the diffusive term D_2 and the mean scalar dissipation balance $\langle\chi\rangle$, i.e.

$$\langle(\Delta\phi)^2\rangle = \frac{\langle\chi\rangle}{6D}\, r^2\,. \tag{6}$$

The second solution is obtained in the inertial range, where the transport term Tr_2 balances the mean scalar dissipation, i.e.

$$\langle(\Delta u_L)(\Delta\phi)^2\rangle = -\frac{2}{3}\langle\chi\rangle r\,, \tag{7}$$

with Δu_L being the longitudinal velocity increment in the direction of $\boldsymbol{r}$. Note that Eq. 7 is only satisfied for sufficiently large Reynolds number, which is the case for $Re_\lambda = 529$ as shown in Fig. 2. Otherwise, finite Reynolds number contributions from the diffusive transport term and the large-scale production term are not negligible in the inertial range. The scale-by-scale budget for higher order structure function, i.e. $\langle(\Delta\phi)^4\rangle$, is significantly different from the second order as displayed by Fig. 2. For higher orders ($n \geq 2$), the so-called dissipative source term E_{2n} is a multi-scale correlation between the local scalar increments $(\Delta\phi)^{2n-2}$ and the local scalar dissipation χ. Thereby, E_{2n} is a function of r and represents the non-trivial coupling between intermittent fluctuations in the dissipative and the inertial range. Peters *et al.*[6] and Gauding *et al.*[12] showed that the dissipative source term plays an important role for the failure of classical theories to correctly describe the scaling of higher order structure functions.

A generalised theory for structure functions of arbitrary even order can be developed similar to Eq. 6 in the limit $r \to 0$ by

$$\langle(\Delta\phi)^{2n}\rangle = C_{2n}\langle\chi^n\rangle\tau_\eta^n\tilde{r}^{2n}\,, \tag{8}$$

with the normalised separation distance $\tilde{r} = r/\eta$, and the Kolmogorov time scale τ_η, defined as $\tau_\eta = (\nu/\langle\varepsilon\rangle)^{1/2}$. The constant C_{2n} is a function of the order, but not of the Reynolds number. Eq. 8 generalises the KOC scaling theory to higher orders and indicates a dependence of higher order structure functions on the corresponding moments of the scalar dissipation $\langle\chi^n\rangle$. A justification of Eq. 8 form DNS is given by Fig. 3, where the scalar structure functions $\langle(\Delta\phi)^{2n}\rangle$ are shown for different orders. It is clearly seen that an adequate collapse with the KOC scales $\langle\chi\rangle$ and τ_η applies only for the second order (and not for higher orders), while a normalisation according to Eq. 8 is reasonably supported also for higher orders. The collapse of the curves is not limited to the dissipative range, but reaches into the inertial range. This finding signifies that both dissipative and inertial range intermittency have the same Reynolds number dependence and reveal a scaling with $\langle\chi^n\rangle$. It is important to emphasise that it is not possible to derive Eq. 8 from pure dimensional arguments, because $\langle\chi\rangle^n$ and $\langle\chi^n\rangle$ have the same dimensions.

In a next step, we examine the conditions under which Eq. 4 satisfies universality. The universality we put forward is limited to a certain range of scales and is different from that first claimed by Kolmogorov, in the sense that we show exactly how the scales are to

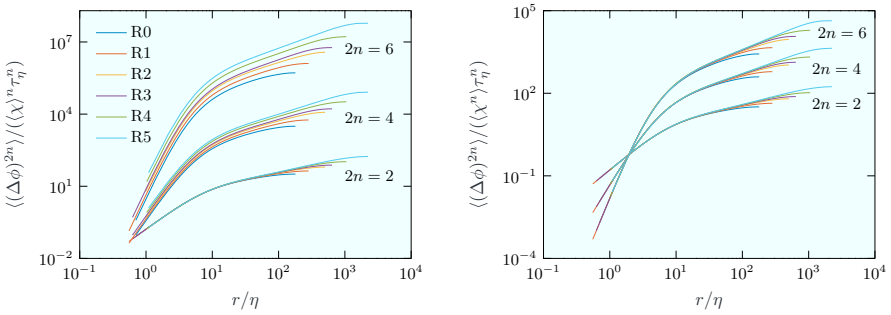

Figure 3. Higher order scalar structure function $\langle(\Delta\phi)^{2n}\rangle$, normalised with conventional KOC scaling (left) and the modified scaling according to Eq. 8.

be obtained from the hierarchy of structure functions. We define functional forms for the different terms, i.e.

$$\begin{aligned} S_{2n} &= \langle(\Delta\phi)^{2n}\rangle = \alpha_{2n} f_{2n}(\tilde{r}) \\ -Tr_{2n} &= \frac{\partial}{\partial r_i}\langle(\Delta u_i)(\Delta\phi)\rangle^{2n} = \beta_{2n} g_{2n}(\tilde{r}) \\ -Pr_{2n} &= 2n\Gamma\langle(\Delta u_2)(\Delta\phi)\rangle^{2n-1} = \gamma_{2n}\Gamma h_{2n}(\tilde{r}) \\ E_{2n} &= nD(2n-1)\langle(\Delta\phi)^{2n-2}\big[\chi(\boldsymbol{x}+\boldsymbol{r})+\chi(\boldsymbol{x})\big]\rangle = \delta_{2n} k_{2n}(\tilde{r})\,, \end{aligned} \tag{9}$$

and thereby have to distinguish between functions which are Reynolds number dependent (and do not depend on the scale r) and normalised structure functions which depend only on the normalised spatial increment $\tilde{r}$. Following Eq. 8, we introduced $\tilde{r} = r/\eta$, with η as the relevant characteristic length scale. Substituting Eq. 9 into Eq. 4 gives

$$\left[\frac{\beta_{2n}\eta^2}{D\alpha_{2n}}\right] g_{2n}(\tilde{r}) + \left[\frac{\gamma_{2n}\Gamma\eta^2}{D\alpha_{2n}}\right] h_{2n}(\tilde{r}) = [2]\, f''_{2n}(\tilde{r}) - \left[\frac{\delta_{2n}\eta^2}{D\alpha_{2n}}\right] k_{2n}(\tilde{r})\,. \tag{10}$$

For universality of Eq. 10, all terms within square brackets must evolve in exactly the same way. Since the first term on the right-hand is constant, all other terms are also required to be constant. This is easy to show for the normalised transport term (first term) and the normalised dissipation source term (last term), which turn into constants by defining a scaling with the moments of the scalar dissipation, i.e. $\beta_{2n} = \delta_{2n} = \langle\chi^n\rangle\tau_\eta^{n-1}$, and $\alpha_{2n} = \langle\chi^n\rangle\tau_\eta^n$, as proposed by Eq. 8. However, the second term in Eq. 10 corresponds to a production term due to the mean gradient Γ. As shown by Fig. 2 the production term is mainly active at large scales and drops quickly towards the inertial range. The energy injection mechanism is a non-universal phenomenon, that cannot be expressed by using only small-scale quantities like $\langle\chi^n\rangle$ and τ_η, see Lumley[13]. As a consequence, the scaling with $\langle\chi^n\rangle$ as indicated by Eq. 8 is only valid over a restricted range of scales limited to the dissipative range and parts of the inertial range. When the large-scale term comes into play, the scaling is changed and requires information about the non-universality at large scales.

In summary, we developed a theory that combines exact results from first principles to introduce a new scaling for higher-order scalar structure functions. The scaling was justified by using data from highly resolved DNS for a wide range of Reynolds numbers.

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