Anomalous Scaling of Structure Functions and Dynamic Constraints on Turbulence Simulations

Victor Yakhot[1] and Katepalli R. Sreenivasan[2]

[1]Department of Aerospace and Mechanical Engineering

Boston University, Boston 02215

[2]International Center for Theoretical Physics, Trieste, Italy

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Abstract

The connection between anomalous scaling of structure functions (intermittency) and numerical methods for turbulence simulations is discussed. It is argued that the computational work for direct numerical simulations (DNS) of fully developed turbulence increases as Re^4, and not as Re^3 expected from Kolmogorov's theory, where Re is a large-scale Reynolds number. Various relations for the moments of acceleration and velocity derivatives are derived. An infinite set of exact constraints on dynamically consistent subgrid models for Large Eddy Simulations (LES) is derived from the Navier-Stokes equations, and some problems of principle associated with existing LES models are highlighted.

1 Background

The theory of turbulence and the development of calculation methods for high-Reynolds-number flows became an active research topic around the beginning of the twentieth century. This effort yielded many important results of general interest in statistical physics. For instance, Kolmogorov's work [1]-[3] on turbulence theory formulated the scaling ideas for the first time, and Kraichnan [4] proposed the mode coupling approach. However, the "turbulence problem", lacking a small parameter characterizing the strong nonlinear interactions, has turned out to be remarkably difficult—and it remains so today.

The revolutionary realization of Osborne Reynolds that turbulence theory is a subject of statistical hydrodynamics rather than classical hydrodynamics, led almost hundred years ago to various elegant and useful phenomenological models based on ideas of kinetic theory (Prandtl [5], Richardson [6], Kolmogorov [3]), which strongly impacted the engineering profession. These heuristic semi-empirical models, based on low-order closures of various perturbation expansions, had a somewhat limited range of success and needed adjustable parameters, often varying from flow to flow. Nevertheless, the role of these models was—and still is—so immense that one can hardly imagine processes in mechanical and chemical engineering, aerodynamics and meteorology which do not have their input.

With the advent of powerful computers, the possibility of accurate numerical simulations, directly based on the Navier-Stokes equations, became a reality. Since the introduction of spectral methods in the end of sixties [7]-[8], direct numerical simulations (DNS) have become a new tool to attack the "turbulence problem". A strategic goal of the DNS has been to complement expensive and complicated physical experiments, and their dream is to dispense with them altogether.

The computational power required for DNS is estimated on the basis of Kolmogorov's phenomenology that describes turbulent fluctuations filling the interval of wavenumbers $1/L \ll k \ll 1/\eta_K$, where L and $\eta_K = LRe^{-\frac{3}{4}}$ are the integral and dissipation scales, respectively, and $Re = u_{rms}L/\nu$ is the Reynolds number based on L and the root-mean-square velocity u_{rms}. If we assume that the velocity fluctuations on scales $r << \eta_K$ are highly damped and cannot contribute to the inertial range dynamics, the effective number of degrees of freedom [9] is then $(L/\eta_K)^3 = Re^{9/4}$. This is the minimum number of grid points required in DNS for a cubic box of linear dimension L. The required number of time steps in the computation is usually proportional to the spatial grid points, so the total computational work increases as Re^3. This means that a mere doubling of the Reynolds number requires almost an order of magnitude increase of computational work.

The accuracy of numerical methods is traditionally estimated as follows. The dissipation contribution to the equation for turbulent kinetic energy is given by

$$\mathcal{E} = -\nu\overline{\mathbf{u}\cdot\frac{\partial^2\mathbf{u}}{\partial x_i^2}} = -\nu\ lim_{r\to\eta}\frac{\partial^2}{\partial r^2}\overline{u_i(x)u_i(x+r)} = \nu\ lim_{r\to\eta}\frac{1}{2}\frac{\partial^2}{\partial r^2}S_{2,0}(r) \propto \nu\mathcal{E}^{\frac{2}{3}}\eta^{\xi_2-2},$$

where the order of magnitude estimate in the last step comes from Kolmogorov's phenomenology. For this case, $\xi_2 = 2/3$ and we have $\eta_K = (\frac{\nu^3}{\mathcal{E}})^{\frac{1}{4}}$. We then have the familiar estimate $\eta_K \approx LRe^{-\frac{3}{4}}$, mentioned earlier. Thus, to accurately describe the flow, one has to simply account for fluctuations on the scales $r \geq \eta_K$ by choosing the computational mesh size to be

$$\Delta = a\eta_K \approx aLRe^{-\frac{3}{4}}, \tag{1}$$

where $a = const = O(1)$. On this mesh, the velocity derivative is defined as

$$\frac{u(x+\Delta)-u(x)}{\Delta} = \frac{\partial u(x)}{\partial x} + \sum_{n=2}\frac{1}{n!}\frac{\partial^n u(x)}{\partial x^n}\Delta^{n-1}. \tag{2}$$

Now, in Kolmogorov's turbulence, $(\partial_x u)_{rms} = \sqrt{\overline{(\partial_x u)^2}} \approx (\frac{\mathcal{E}Re}{u_{rms}L})^{\frac{1}{2}} = O(Re^{\frac{1}{2}})$, and, since $\frac{\partial^n u(x)}{\partial x^n} \approx \partial_x u(x)/\eta_K^{n-1}$, using the mesh size Δ from the relation (1), we arrive at the estimate

$$\frac{1}{n!}(\frac{\partial^n u(x)}{\partial x^n})_{rms}\Delta^{n-1} \approx \frac{1}{n!}(\partial_x u)_{rms}(\frac{\Delta}{\eta_K})^{n-1} \approx \frac{a^{n-1}}{n!}Re^{\frac{1}{2}}. \tag{3}$$

The relation (3) is essentially the basis for all numerical finite difference schemes used for the DNS of turbulence [9]. Indeed, we see that if $a < 1$, the first-order finite difference accurately represents the velocity derivatives.

In spectral simulations of isotropic and homogeneous turbulence, one prescribes a suitable number of the Fourier modes to represent the velocity field. Usually, this number is chosen on the basis of the magnitude of the expected Kolmogorov scale η_K or the largest wavenumber

$k_{max} = 2\pi/\eta_K$. In the state-of-the-art simulations [10],[11], the cut-off is usually chosen such that $k_{max} = \sqrt{2}N/3$ on a grid of size N^3.

In summary, the principal elements of Kolmogorov's phenomenology which have enabled these traditional estimates are the following: (a) the scaling exponents of the structure functions $S_{n,0} \propto r^{\xi_n}$ are given by the Kolmogorov values $\xi_n = n/3$; (b) the mean dissipation rate $\mathcal{E} = \nu\overline{(\partial_i u_j)^2}$ is constant and $O(1)$, as are the moments of the dissipation rate $\overline{\mathcal{E}^n}$ for all n; if the latter were not the case, one can define different Kolmogorov scales on the basis of different moments of $\mathcal{E}$; and (c) the "skewness" factors $\overline{(\partial_x u)^n}/\overline{(\partial_x u)^2}^{\frac{n}{2}} = O(1)$, independent of the Reynolds number; for, if this were not so, one can again define different Kolmogorov scales through odd moments of different order.

The main point of the present paper is that there is a need to reexamine the traditional estimates in the light of modern developments in turbulent theory and experiment. We concentrate on isotropic and homogeneous turbulence but expect that the considerations hold for more general flows as well.

2 Results for Intermittent Turbulence

We are interested in the Navier-Stokes dynamics of incompressible fluids. In 1941, Kolomogorov derived the few exact relation of turbulence theory, presented here for an arbitrary space dimensionality d, as

$$\frac{1}{r^{d+1}}\frac{\partial}{\partial r}r^{d+1}S_{3,0} = (-1)^d\frac{12}{d}\mathcal{E},$$

giving $S_{3,0} = -\frac{12}{d(d+2)}\mathcal{E}r$ and $S_{3,0}/S_{1,2} = 3$. A dimensional generalization of this result, without however the analytical support, yields the Kolomogorov's (normal) scaling $\xi_n = n/3$. Recently [12],[13], some additional exact consequences of the Navier-Stokes equations have been derived. In combination with recent experimental results, we consider their consequences for intermittent turbulence.

a. Dissipation scale as a random field We consider the moments of velocity difference (also called structure functions). Choosing the displacement vector $\mathbf{r}$ parallel to the "x-axis", we can define the structure functions $S_{n,m}(r) = \overline{(u(\mathbf{x}+r\mathbf{i}) - u(\mathbf{x}))^n(v(\mathbf{x}+r\mathbf{i}) - v(\mathbf{x}))^n} \equiv$

$\overline{(\delta_r u)^m(\delta_r v)^n}$, where u and v are the components of velocity vector parallel and normal the x-axis, respectively. In the inertial range the velocity structure functions are Re-independent; that is, if the displacement r belongs to the interval $\eta \ll r \ll L$, then $S_{n,m}(r)$ do not involve any information about the dissipation scale.

Modern experiments have revealed that Kolmogorov's result $\xi_n = n/3$ is almost certainly incorrect and that ξ_n is a concave function of n—or the ratio ξ_n/n is a decreasing function of the moment number n. (See for example Refs. [14] for reviews and Ref. [15] for the most recent data.) Further, the form of structure functions is given by $S_{2n}(r) = \overline{(u(x+r)-u(x))^{2n}} \approx (2n-1)!!(\epsilon L)^{\frac{2n}{3}}(\frac{r}{L})^{\xi_{2n}}$. The factor $(2n-1)!!$, ensuring Gaussian statistics at the integral scale L, is a subject of a forthcoming paper, but it suffices here to say here that it has been recently verified in experiments and numerical simulations [16]. On the other hand, in the limit $r \to 0$, the analytic structure function is approximately equal to $S_{2n}(r) \approx \overline{(\partial_x u(0))^{2n}} r^{2n}$. Combining the two, we can define a natural dissipation scale of the $2n^{th}$-order structure function [17]-[18] as

$$\eta_{2n} = (\overline{(\partial_x u)^{2n}})^{\frac{1}{\xi_{2n}-2n}}((2n-1)!!\epsilon^{\frac{2n}{3}} L^{\frac{2n}{3}-\xi_n})^{\frac{1}{2n-\xi_{2n}}}. \qquad (4)$$

According to (4), the dissipation scales, which are expressed in terms of the moments of velocity derivatives, define a random field η. By a random field we mean here that the value of the length scale η depends on the order of the moment considered. It will be shown below that (4) is an approximation to a more accurate representation. Similar ideas were proposed earlier in Refs. [19]-[21] within the framework of multifractal theories. Writing $i_{2n} = [(2n-1)!!]^{\frac{1}{2n-\xi_{2n}}}$, and using the Stirling formula ($n \gg 1$), one obtains $i_{2n} \approx (\frac{n}{2e})^{\frac{3}{4}}$ for $\xi_n = n/3$. This means that the effect of the factor $(2n-1)!!$ can be safely neglected. For anomalous exponents $\xi_n < n/3$, this factor is even closer to unity and does not modify the conclusions obtained below.

b. Dissipation anomaly If the velocity field is differentiable, we obtain $S_3(r) \propto r^3$ and $\partial_r S_3(r) \to 0$ in contradiction with the Kolmogorov relation. This implies that the velocity field is singular in the limit of $\nu \to 0$ and $r \to 0$ (in that order), leading to the so-called dissipation anomaly. Here we first reproduce some details of Polyakov's derivation [22] of the dissipation anomaly for turbulence governed by Burgers equation and then outline similar procedure for the Navier-Stokes equations. Consider the one-dimensional Burgers equation

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = \nu\frac{\partial^2 u}{\partial x^2}, \tag{5}$$

for which the energy balance reads as

$$\frac{1}{2}\frac{\partial u^2}{\partial t} + \frac{1}{3}\frac{\partial}{\partial x}u^3 = \nu u(x)\frac{\partial^2 u}{\partial x^2}.$$

Introducing $x_{\pm} = x \pm \frac{y}{2}$, so that, $\frac{1}{2}\frac{\partial}{\partial x_{\pm}} = \pm\frac{\partial}{\partial y}$, we can represent the energy balance equation as

$$lim_{y\to 0}[\frac{\partial u(x_+)u(x_-)}{\partial t} + \frac{1}{2}\frac{\partial}{\partial x_+}u(x_+)^2u(x_-) + \frac{1}{2}\frac{\partial}{\partial x_-}u(x_-)^2u(x_+) = \nu(\frac{\partial^2}{\partial x_+^2} + \frac{\partial^2}{\partial x_-^2})u(x_+)u(x_-))]. \tag{6}$$

We also have the identities:

$$\frac{\partial}{\partial y}(u(x_+) - u(x_-))^3 = \frac{1}{2}[\frac{\partial u(x_+)^3}{\partial x_+} + \frac{\partial u(x_-)^3}{\partial x_-}] - \frac{3}{2}[\frac{\partial u(x_+)^2u(x_-)}{\partial x_+} + \frac{\partial u(x_-)^2u(x_+)}{\partial x_-}], \tag{7}$$

and

$$\nu[u(x_+)\frac{\partial^2 u(x_-)}{\partial x_-^2} + u(x_-)\frac{\partial^2 u(x_+)}{\partial x_+^2}] = \nu[(u(x_+) - u(x_-))\frac{\partial^2}{\partial y^2}(u(x_+) - u(x_-))] + D, \tag{8}$$

where D, the dissipation contribution to the energy balance, is given by

$$D = \nu[u(x_+)\frac{\partial^2}{\partial x_+^2}u(x_+) + u(x_-)\frac{\partial^2}{\partial x_-^2}u(x_-)]. \tag{9}$$

Substituting these identities into the equation (6) and taking account of the fact that $lim_{y\to 0}\frac{\partial u(x_{\pm})^3}{\partial x_{\pm}} = \frac{\partial u(x)^3}{\partial x}$, so that in the limit $y \to 0$ all non-singular terms disappear by virtue of the energy equation (5), we are left with the balance between the singular (anomalous) contributions

$$\lim_{y\to 0}\frac{1}{6}\frac{\partial}{\partial y}(u(x_+) - u(x_-))^3 = \nu[(u(x_+) - u(x_-))\frac{\partial^2}{\partial y^2}(u(x_+) - u(x_-))]. \tag{10}$$

This is Polyakov's expression for the dissipation anomaly derived for the Burgers equation [22]. Averaging (10) gives the exact relation $\overline{(\delta_y u)^3} = -12\mathcal{E}y$ where the dissipation rate $\mathcal{E} = \nu\overline{(\frac{\partial u}{\partial x})^2}$.

We are interested in the Navier-Stokes dynamics of incompressible fluids, for which the energy balance equation (with the density $\rho = 1$) is written as

$$\frac{1}{2}\frac{\partial u^2}{\partial t} + \frac{1}{2}\mathbf{u}\cdot\nabla u^2 = -\nabla p\cdot\mathbf{u} + \nu\mathbf{u}\cdot\frac{\partial^2\mathbf{u}}{\partial x_i^2},$$

and that for the scalar product $\mathbf{u}(\mathbf{x}+\frac{\mathbf{y}}{\mathbf{2}})\cdot\mathbf{u}(\mathbf{x}-\frac{\mathbf{y}}{\mathbf{2}}) \equiv \mathbf{u}(+)\cdot\mathbf{u}(-)$ can be written as

$$\frac{\partial\mathbf{u}(+)\cdot\mathbf{u}(-)}{\partial t} + \mathbf{u}(+)\cdot\frac{\partial}{\partial\mathbf{x}_+}\mathbf{u}(+)\cdot\mathbf{u}(-) + \mathbf{u}(-)\cdot\frac{\partial}{\partial\mathbf{x}_-}\mathbf{u}(-)\cdot\mathbf{u}(+) =$$
$$-\frac{\partial p(+)}{\partial x_{+,i}}u_i(-) - \frac{\partial p(-)}{\partial x_{-,i}}u_i(+) + \nu[\mathbf{u}(-)\cdot\frac{\partial^2}{\partial x_{+,j}^2}\mathbf{u}(+) + \mathbf{u}(+)\cdot\frac{\partial^2}{\partial x_{-,j}^2}\mathbf{u}(-)]. \qquad (11)$$

It is clear that in the limit $y\to 0$, for which $\mathbf{x}_\pm\to\mathbf{x}$, this equation gives the energy balance. Following Polyakov's procedure outlined above, let us consider the two identities:

$$\frac{\partial}{\partial y_i}(u_i(+)-u_i(-))(u_j(+)-u_j(-))^2 =$$
$$\frac{1}{2}\frac{\partial}{\partial x_{+,i}}u_i(+)u_j^2(+) + \frac{1}{2}\frac{\partial}{\partial x_{+,i}}u_i(+)u_j^2(-) - \frac{\partial}{\partial x_{+,i}}u_i(+)u_j(+)u_j(-) +$$
$$\frac{1}{2}\frac{\partial}{\partial x_{-,i}}u_i(-)u_j^2(-) + \frac{1}{2}\frac{\partial}{\partial x_{-,i}}u_i(-)u_j^2(+) - \frac{\partial}{\partial x_{-,i}}u_i(+)u_j(-)u_j(+) \qquad (12)$$

and

$$u_i(+)\frac{\partial^2}{\partial x_{-,j}^2}u_i(-) + u_i(-)\frac{\partial^2}{\partial x_{+,j}^2}u_i(+) =$$
$$-4(u_i(+)-u_i(-))\frac{\partial^2}{\partial y_j^2}(u_i(+)-u_i(-)) + u_i(+)\frac{\partial^2}{\partial x_{+,j}^2}u_i(+) +$$
$$u_i(-)\frac{\partial^2}{\partial x_{-,j}^2}u_i(-). \qquad (13)$$

Similar identities for the pressure terms can be written easily. Substituting them into (11) and, as in the case of Burgers equation considered above, accounting for the energy balance, one has

$$lim_{y\to 0}[-\frac{\partial}{\partial y_i}(u_i(+)-u_i(-))(u_j(+)-u_j(-))^2 + \frac{1}{2}(\frac{\partial}{\partial x_{+,i}}u_i(+)u_j(-)^2 + \frac{\partial}{\partial x_{-,i}}u_i(-)u_j(+)^2) =$$
$$-4\nu(u_i(+)-u_i(-))\frac{\partial^2}{\partial y_j^2}(u_i(+)-u_i(-)) + (\frac{\partial p(+)}{\partial\mathbf{x}_+} - \frac{\partial p(-)}{\partial\mathbf{x}_-})\cdot(\mathbf{u}(+)-\mathbf{u}(-))]. (14)$$

This equation can be written in a compact form as

$$lim_{y\to 0}[-\frac{\partial}{\partial y_i}\delta u_i|\delta_{\mathbf{y}}\mathbf{u}|^2 + \frac{1}{2}(\frac{\partial}{\partial x_{+,i}}u_i(+)u_j(-)^2 + \frac{\partial}{\partial x_{-,i}}u_i(-)u_j(+)^2) = -2\delta_{\mathbf{y}}\mathbf{u}\cdot\delta_{\mathbf{y}}\mathbf{a}],$$

where $\mathbf{a} = -\nabla p + \nu\nabla^2\mathbf{u}$ is the Lagrangian acceleration. The equation (14) is exact. Choosing the displacement vector along one of the coordinate axes and averaging (14), one obtains

$$\frac{\partial}{\partial y}\overline{\delta u|\delta\mathbf{u}|^2} = 8\overline{\delta u_i\frac{\partial^2}{\partial y^2}\delta u_i} = 2\overline{(\delta_y u_i)\partial_x^2(\delta_y u_i)} = -\frac{4}{3}\mathcal{E},$$

where $\delta_y u = \delta_{\mathbf{y}}\mathbf{u}\cdot\mathbf{y}/y$. The pressure terms in and the second contribution to the left side of (14) disappeared by the averaging procedure. In general, we can choose a sphere of radius $y << R \to 0$ around a point $\mathbf{x}$ and average (14) over this sphere. This causes the all scalar-velocity contributions to (14) disappear and the resulting equation can be perceived as a local form of the 4/3 Kolmogorov law. This fact has been realized before. Introducing the angular averaging, Robert and Duchon [23] and Eyink [24] locally expressed the relation (14) in terms of longitudinal and transverse velocity differences. We are interested in the order of magnitude estimates (see below), and restrict ourselves to (14).

c. Relations between the moments In the isotropic and homogeneous turbulence, the Navier-Stokes equations lead to the following exact relations for structure functions. They were derived in [12] and [13] and experimentally investigated in some detail in Ref. [25]; see also Ref. [26]. The relations for different values of n are

$$\frac{\partial S_{2n,0}}{\partial r} + \frac{d-1}{r}S_{2n,0} = \frac{(2n-1)(d-1)}{r}S_{2n-2,2} + (2n-1)\overline{\delta_r a_x(x)(\delta_r u)^{2n-2}}. \qquad (15)$$

Similar equations for all structure functions $S_{n,m}$ can easily be obtained from the equation for generating functions derived in [12].

d. The closure problem Equation (15), which includes both velocity and Lagrangian acceleration increments, is not closed and cannot be solved unless the relation between acceleration and velocity differences is established. It has been proposed in Ref. [17] that the local expression (14) written for the displacement magnitudes corresponding to the bottom of inertial range, i.e. in the limit $y \to \eta \to 0$ can be used as a closure. At the present time, this can be done only approximately. Since at the values of displacement $y \ll \eta \to 0$, the difference $\delta_y u \approx \frac{\partial u(0)}{\partial x}y$, we can modify the *lim* operation in (14) as

$$\lim_{y\to 0} \approx \lim_{y\to\eta\to 0}, \qquad (16)$$

leading to the order-of-magnitude estimate

$$lim_{y\to\eta} A\frac{\partial(\delta_y u)^3}{\partial y} + B\frac{\partial}{\partial y}\delta_y u(\delta_y v)^2 \propto \nu\delta_y u\frac{\partial^2}{\partial y^2}\delta_y u - \frac{\partial\delta_y p(x)}{\partial y}\delta_y u \approx \delta_\eta u\delta_\eta a_x, \tag{17}$$

where A and B are undetermined constants. On extrapolating to the dissipation scale η where all terms in the right side of (18) are of the same order, we derive the estimate [17] as

$$\nu \approx \eta\delta_\eta u \equiv \eta(u(x+\eta) - u(x)). \tag{18}$$

The relation (18) tells us that each velocity fluctuation $\delta_\eta u$ is dissipated on its 'own' dissipation scale η and the local value of the Reynolds number $Re_l = O(1)$. This allows a simple physical interpretation that the dissipation processes at all levels n happen on "quasi-laminar structures" where the inertial and viscous terms are of the same order. In general, the higher the moment order, the more the intense events contribute, and the smaller the value of the corresponding dissipation scale.

e. Dissipation scales and moments of derivatives The theory gives for the moments of Lagrangian acceleration $\mathbf{a} = -\nabla p + \nu\nabla^2\mathbf{u}$ the result that

$$a_x \approx \frac{\delta_\eta u}{\tau_\eta} \approx \frac{(\delta_\eta u)^2}{\eta} \approx \frac{(\delta_\eta u)^3}{\nu} = (\delta_\eta u)^3\frac{Re}{u_{rms}L}, \tag{19}$$

where the turn-over time $\tau_\eta \approx \eta/\delta_\eta u$.

Below we will mainly discuss the equations for even-order structure functions, for which, if the displacement r is in the inertial range, the dissipation contribution to the increment of Lagrangian acceleration is negligibly small [17],[18]. For this case, we have

$$\frac{\partial S_{2n,0}}{\partial r} + \frac{d-1}{r}S_{2n,0} = \frac{(2n-1)(d-1)}{r}S_{2n-2,2} - (2n-1)\overline{\delta_r p_x(\delta_r u)^{2n-2}}, \tag{20}$$

where $p_x = \partial_x p(x)$ and d denotes, as before, the space dimensionality.

The relation (15) is valid for all magnitudes of displacement $r \ll L$, including $r \to \eta$. Below, to simplify the notation, we will omit the subscript x in the x-component of acceleration a_x. In this limit, treating (19) as $a = \lim_{r\to\eta}(\delta_r u)^3/\nu$ and substituting it in (15) gives $\frac{S_{2n}(r)}{r} \approx \frac{S_{2n+1}(r)}{\nu}$. On a scale $r = \eta_{2n}$, writing $S_{n,0} \propto A_n\eta_n^{\xi_n}$, equation (15) gives

$$\eta_n \propto LRe^{\frac{1}{\xi_n - \xi_{n+1} - 1}}. \tag{21}$$

For Kolmogorov turbulence with $\xi_n = n/3$ the formula (21) reads, as expected, as $\eta_n \equiv \eta_K = LRe^{-\frac{3}{4}}$ which is n-independent. In intermittent turbulence, where the exponents can be well-described [12],[17] by the relation $\xi_n \approx 0.383 * n/(1+0.05n)$, the relation (21) defines the Reynolds-number-dependent dissipation scales. As $n \to \infty$, $\eta_n \to LRe^{-1}$. Thus, to resolve all fluctuations including the strongest, the computational work need to increase as Re^4, as already noted in Ref. [27]. In general, in the limit $n \to \infty$, the relation (21) can be written as

$$\eta_n \approx LRe^{-\frac{1}{\frac{d\xi_n}{dn}+1}},$$

so one may get a somewhat different estimate for the computational work than Re^4, but the principal conclusion is inescapable that intermittency makes DNS more expensive than previously thought.

Using the relations (18), (20) and (21), obtained by balancing various terms in the exact dynamic equations (14), (15), we can develop the multi-scaling algebra. For example,

$$\overline{a^{2n}} \approx (\frac{Re}{u_{rms}L})^{2n} S_{6n}(\eta_{6n}) \propto (\frac{Re}{u_{rms}L})^{2n} \eta_{6n}^{\xi_{6n}} \approx (\frac{u_{rms}^2}{L})^{2n} Re^{a_{2n}}, \tag{22}$$

with $a_{2n} = 2n + \frac{\xi_{6n}}{\xi_{6n}-\xi_{6n+1}-1}$. With $\xi_6 = 2$ and $\xi_7 = 7/3$, we recover Yaglom's result [28] $\overline{a^2} \approx \frac{u_{rms}^{\frac{9}{2}}}{\sqrt{\nu}}$. The intermittency corrections are readily found from (22). Recent experiments by Reynolds et al. [29] have lent strong support to this result. The formula (22) shows that the second moment of Lagrangian acceleration is expressed in terms of the sixth-order structure function evaluated on its dissipation scale η_6. To extract information about the fourth moment $\overline{a^4}$, we should have accurate data on $S_{12}(\eta_{12})$ which is very difficult to obtain in high-Reynolds-number flows.

The moments of velocity derivatives are evaluated easily. In accordance with (18), we have

$$\overline{(\partial_x u)^{2n}} \approx \overline{(\frac{\delta_\eta u}{\eta})^{2n}} \approx \overline{(\frac{(\delta_\eta u)^2}{\nu})^{2n}} \approx Re^{d_{2n}}, \tag{23}$$

where $d_{2n} = 2n + \frac{\xi_{4n}}{\xi_{4n}-\xi_{4n+1}-1}$.

It is important to stress that the first equality in (23) involves the averaging over two random fields u and η. To perform this averaging, we have to either know the joint probability $p(u, \eta, r)$ or use the functional relation between the fields given by (18). This leads to the second equation in (23) and the final result. Since $\overline{(\partial_x u)^2} \propto Re$, the relation (3) leads to a new relation between exponents

$$2\xi_4 = \xi_5 + 1$$

which agrees extremely well with experimental data. The relation (23) differs from proposals reviewed in Ref. [14].

f. The role of the fluctuations of the dissipation scale Let us reexamine the relation (4). In the limit $r \to 0$, the velocity field is analytic and can be expanded by Taylor series so that $\frac{\partial u}{\partial x} \approx \delta_r u/r$. This gives $\overline{(\frac{\partial u}{\partial x} r)^{2n}} \approx S_{2n}(r)$. When $r \to \eta \to 0$, we have to evaluate the mean of the ratio $\overline{(\delta_\eta u/\eta)^{2n}}$ which is not a trivial task, since we are dealing here with the ratio of two random fields—unless the relation (18), which expresses the dissipation scale in terms of velocity field, is used. If, however, we *incorrectly* assume that the dissipation scale fluctuations are independent of those of the velocity field and neglect the step leading to the last equations in the right hand side of (23), it is possible to write the moments of velocity derivative as

$$\overline{(\partial_x u)^{2n}} \approx \overline{(\frac{\delta_\eta u}{\eta})^{2n}} \approx S_{2n}(\eta_{2n})/\eta_{2n}^{2n} \propto Re^{p_{2n}}, \tag{24}$$

where $p_{2n} = \frac{\xi_{2n}-2n}{\xi_{2n}-\xi_{2n+1}-1}$. Equating expressions (23) and (24), we have

$$\frac{\xi_{2n} - 2n}{\xi_{2n} - \xi_{2n+1} - 1} = 2n + \frac{\xi_{4n}}{\xi_{4n} - \xi_{4n+1} - 1}, \tag{25}$$

subject to the constraints $\xi_0 = 0$ and $\xi_3 = 1$. The only solution to (25) is $\xi_n = n/3$. Since equation (25) is based on the first equality (23), which in general is incorrect, we can conclude that the source of anomalous scaling in hydrodynamic turbulence is the fluctuation of the dissipation scale field η, which itself is strongly correlated the velocity field fluctuations via expression (18). This does not preclude a different situation from arising in other forms of turbulence, e.g., scalar turbulence generated by white-noise forcing [30].

It follows that $\overline{(\frac{\partial u}{\partial x})^2} = \lim_{r\to\eta_2} \overline{\frac{\partial u(x)}{\partial x}\frac{\partial u(x')}{\partial x'}} = -\lim_{r\to\eta_2} \frac{\partial^2}{\partial r^2}\overline{u(x)u(x')} \propto (2-\xi_2)\eta_2^{\xi_2-2}$. The higher-order derivatives are evaluated in a similar way to yield

$$(\frac{\partial^n u}{\partial x^n})_{rms} = lim_{r\to\eta_2}\sqrt{\frac{\partial^{2n}}{\partial r^{2n}} S_2(r)} \approx \eta_2^{\frac{\xi_2-2n}{2}} \approx Re^{\frac{\xi_2-2n}{2(\xi_2-2)}} = Re^{\frac{1}{2}} Re^{\frac{n-1}{\xi_2-2}}. \tag{26}$$

3 Implications for Numerical Methods

According to experimental data (see Refs. [25,15] for recent results), the exponent $\xi_2 \approx 0.70 - 0.71 > 2/3$ and as $n \to \infty$, the terms in the expansion (2) for simulating the "typical" velocity derivatives can be estimated via

$$(\frac{\partial^n u}{\partial x^n})_{rms}\Delta^{n-1} \propto Re^{\frac{1}{2}} Re^{\gamma(n-1)}, \tag{27}$$

with $\gamma = (-\frac{3}{4} - \frac{1}{\xi_2 - 2})) > 0$. For $\xi_2 \approx 0.71$, we find $\gamma \approx 0.025$. The accuracy of the numerical method in calculating the most intense velocity fluctuations can be estimated if, in the limit $n \to \infty$, the expression

$$\overline{(\frac{\partial u}{\partial x})^{2n}}^{\frac{1}{2n}} (\frac{\Delta}{\eta_{2n}})^{n-1} \propto Re^{\frac{1}{2}} Re^{\frac{n+1}{4}} \tag{28}$$

is used instead of $(\partial_x u)_{rms}$. In the above equation, the mesh size Δ is defined by (1) and the expressions (23) for the moments of velocity derivative have been used. We see that when the Reynolds number is large, the high-order derivatives in the expression (2) dominate. This means that the DNS based on the mesh equal to the Kolmogorov scale becomes quite inaccurate. It is easy to check that accurate simulations of the largest fluctuations requires the resolution of the smallest scales which are $O(1/Re)$. This means that the computational resolution scales as Re^3 and the computational work grows as Re^4.

In Refs. [19], it has argued that the intermittent nature of turbulence makes the size of the attractor smaller than the conventionally estimated, so the computational power needed becomes correspondingly smaller than the conventional estimate—not larger as just claimed. The rationale is roughly that the "interesting" parts of the flow occupy small volumes of space so any reasonable computational effort that focuses on those volumes is likely to be less expensive. This is also the spirit of adaptive meshing [31]. Even if the interesting parts of a turbulent flow are not space-filling, as discussed at length in Ref. [20], we do not yet know how to track them efficiently in hydrodynamics turbulence. We also do not know if the part of the flow that contains the less interesting parts can be computed with greater economy. Nevertheless, it must be said that the present estimates apply to uniform meshing, which has been the most successful of the computing schemes until now. It should also be mentioned that there is a specific suggestion [32] on the most singular structure in turbulence, which yields $Re^{3.6}$, which is slightly different from Re^4 estimated in this paper.

4 Dynamic Constraints on Sub-Grid Models for LES

If the Reynolds number is large, the computational work involved in the numerical simulation of a flow is huge. It is interesting that at about the same time that DNS came into being, the idea of the Large Eddy Simulations (LES) was proposed by Deardorff [33]. The idea is very simple. Consider the Navier-Stokes equations

$$\partial_t \mathbf{u} + u_i \partial_i \mathbf{u} = -\nabla p + \nu \partial^2 \mathbf{u}; \quad \partial_i u_i = 0. \tag{29}$$

We choose the mesh size Δ and define the so-called "sub-grid" velocity fluctuations $u^>(k) \neq 0$ for $k \geq \pi/\Delta$. The Fourier-transform of velocity field is defined as

$$u(\mathbf{k}) = u^<(\mathbf{k}) + u^>(\mathbf{k}), \tag{30}$$

so that

$$u^>(\mathbf{x}) = \int_{|k|>\frac{2\pi}{\Delta}} e^{i\mathbf{k}\cdot\mathbf{x}} u^>(\mathbf{k}) d^3k; \qquad u^<(\mathbf{x}) = \int_{|k|\leq\frac{2\pi}{\Delta}} e^{i\mathbf{k}\cdot\mathbf{x}} u^<(\mathbf{k}) d^3k. \tag{31}$$

The goal is to obtain the correct equation for the resolved scales $u^<(k) \neq 0$ in the interval $0 \leq k \leq \pi/\Delta$. We decompose the field and write the equation for only the resolved scales as

$$\partial_t \mathbf{u}^< + u_i^< \cdot \partial_i \mathbf{u}^< = \mathcal{SG} - \nabla p^< + \nu \partial^2 \mathbf{u}^<, \tag{32}$$

where, for this particular formulation, the subgrid contribution is $\mathcal{SG} = -u_i^< \cdot \partial_i \mathbf{u}^> - u_i^> \cdot \partial_i \mathbf{u}^< - u_i^> \cdot \partial_i \mathbf{u}^>$. The LES equations are considered a success if the large-scale velocity fields (i.e., for $k \leq 1/\Delta$) given by the Navier-Stokes equations (30) and by a model (33) are identical or close enough for all Reynolds numbers.

There is, however, one problem. To derive the equation of motion containing only the resolved fields, one has to express all contributions to $\mathcal{SG}$, involving the sub-grid velocity fluctuations $\mathbf{u}^>$, in terms of $\mathbf{u}^<$, which is basically equivalent to solution of the proverbial "turbulence problem". The model equation (33) is written in a generic form, but a similar difficulty arises if, instead of the Fourier-space decomposition introduced above, the filtering or any other kind is used.

The accurate LES model must satisfy the following dynamic constraints. The method developed in the Ref. [17] can be literally applied to the Navier-Stokes equations with an arbitrary right hand side and, defining the coarse-grained structure functions $S^{<}_{n,0}(r) = \overline{(\delta_r u^{<})^n}$, we obtain, from (21), the result

$$\frac{\partial S^{<}_{2n,0}}{\partial r} + \frac{d-1}{r} S^{<}_{2n,0} = \frac{(2n-1)(d-1)}{r} S^{<}_{2n-2,2} + (2n-1)\overline{(\delta_r(\mathcal{SG}_x) - \delta_r p^{<}_x)(\delta_r u^{<})^{2n-2}}. \quad (33)$$

The large-scale velocity fields obtained from DNS and LES can be identical $S_{n,0}(r) = S^{<}_{n,0}(r)$ if and only if

$$\overline{(\delta_r(\mathcal{SG}_x) - \delta_r p^{<}_x)(\delta_r u^{<})^{2n-2}} = -\overline{\delta_r p_x (\delta_r u)^{2n-2}}. \quad (34)$$

Similar constraints, coming from the equations for various structure functions $S_{n,m}$ can be readily obtained. It is impossible to demand equality of two random fields $\mathbf{u}$ and $\mathbf{u}^{<}$ obtained from two different equations. The only criterion we can impose is that of statistical equality or, equivalently, constraint on all moments, namely $S^{<}_n(r) = S_n(r)$. The relations (34), reflecting this necessary condition of the LES validity, must be satisfied.

We wish to stress that these constraints are not dissimilar to $S^{LES}_{n,m} \approx S^{<}_{n,m}$, often implied in the literature. Here $S^{LES}_{n,m}(r)$ are the structure functions evaluated from the velocity field obtained from LES. The velocity increment can be written as $\delta_r u = \int u(k) e^{ikx}(e^{ikr} - 1)$, so that

$$S_2 \propto \int E(k)(1 - \cos kr) dk.$$

It is easy to see that if $r << L$, where L is the integral scale, and the energy spectrum decreases with k fast enough, the main contribution to the integral comes from the range where $kr \approx 1$. Thus the structure functions $S_{n,0}(r)$ probe structures on the scales of the order r and cannot differ strongly from the one obtained from the filtered field.

Various model considerations, leading to expressions for $\mathcal{SG}$, have been suggested in the last forty years. Consider the example that follows from Kolmogorov's theory. If the role of the small scale fluctuations in the large-scale dynamics can be expressed in terms of effective viscosity ν_{SG}, then $\nu_{SG} \approx (\overline{\epsilon}\Delta^4)^{\frac{1}{3}}$. Then, dropping the averaging sign (quite an assumption!) and substituting a simple estimate coming from the energy balance, namely, $\epsilon = \nu_{SG} S^<_{ij} S^<_{ij} \equiv \nu_{SG} S^2_{ij}$, we derive the Smagorinsky formula [34] given by $\nu_{SG} = \alpha\sqrt{S^<_{ij} S^<_{ij}}\Delta^2$, where $\alpha = O(1)$. It is important that the resolved rate of strain is evaluated in terms of velocity differences on the computational mesh

$$S^<_{ij}(x) = \frac{1}{2}\left(\frac{u^<_i(x+\Delta_j) - u^<_i(x)}{\Delta_j} + \frac{u^<_j(x+\Delta_i) - u^<_j(x)}{\Delta_i}\right), \tag{35}$$

where $i, j = 1, 2, 3$. In this approximation, the Reynolds stress $\tau_{ij} = -\overline{u_i u_j} \approx \nu S_{ij} \approx \nu_{SG} S^<_{ij}$. Equation (36) with the model for $\mathcal{SG}$ defines a closed set of equations which can be used for LES. The analytically evaluated coefficient from Yakhot and Orszag [35] gives $\alpha \approx 0.2$, while the so-called dynamic method [36] gives something different. In all approaches, since the large-scale fields $\delta_r \mathbf{u}^<$ and $\delta_r \mathbf{u}$ are statistically independent upon Reynolds number, the parameter $\alpha = O(Re^0)$. Thus, this simple model is

$$\mathcal{SG} \approx a\Delta^2 \nabla |S^<_{ij}| \nabla u^< = O(1). \tag{36}$$

Examining the relations (34) and (36), an interesting conclusion can be reached. If $\Delta \ll r$, one can assume statistical independence of all velocity differences $\delta_r u^<$ and $\delta_\Delta u^<$. Since $\mathcal{SG}$ given by (34) and (35) depends on the velocity differences defined on the mesh size Δ as

$$\overline{\delta_r \mathcal{SG} (\delta_r u^<)^{2n-2}} \approx \overline{\delta_r \mathcal{SG}}\ \overline{(\delta_r u^<)^{2n-2}} = 0, \tag{37}$$

we see that the Smagorinsky model satisfies the dynamic constraints, provided the pressure gradient differences in the filtered and unfiltered fields are close to each other. The validity of the dynamic Smagorinsky models in the range $k << 1/\Delta$ has been verified by large eddy simulations (A. Oberai, private communication 2005). However, as $r \to \Delta$, $\delta_r \mathcal{SG}$, $\delta_r p_x$ and $\delta_r u^<$ are strongly correlated and, as a result, the model becomes invalid. This consideration is applicable to all low-order closures.

This intrinsic failure of all **existing** LES models at scales comparable to the computational mesh is well-known. At sufficiently low Reynolds numbers, LES give accurate results. However, with increase of Re the quality of the simulations deteriorates starting from the vicinity of the cut-off, propagating toward the larger scales. At this point one is forced to increase the resolution. The reasons for this failure can be qualitatively understood as follows. Consider LES at a relatively low Re on a fixed mesh $\Delta/L_1 = \gamma_1$ where L_1 is an integral scale of this particular simulation. Now increase the length scale of the flow $L_2 >> L_1$, thus increasing the Reynolds number. If, in the first case, the number of the cascade steps for the energy flux to reach the mesh scale was say n_1, that in the second simulation is equal to $n_2 >> n_1$. Since the intermittency and deviation from the close-to-Gaussian statistics, experimentally observed at the integral scale, grows with the number of cascade steps, the contribution from the very strong velocity fluctuations at the "dissipation" scale Δ increases. As a result, the low order models that are successful in the close to Gaussian situations break down. In another scenario, let us increase the Reynolds number by increasing the mean velocity while keeping both the energy injection scale and the mesh size Δ constant. In this situation, the top of the "inertial" range will move into the range of scales which are larger than Δ, thus again invalidating the LES.

A recent paper by Kang et al. [37] has demonstrated that, at the scales close to those of the mesh size, the probability density function $p(\delta_r u)$ computed from LES was quite close to a Gaussian while the experimental PDF showed broader tails, typical of intermittency. This means that the contributions from strong velocity fluctuations obtained from LES are underpredicted. Since the intermittent effects becomes stronger with increasing Reynolds number, we expect this difference to grow, thus invalidating the LES if the mesh size is also not modified. A very interesting example is given by the LES of the flow in a simple cavity reported by Larcheveque et al. [38]. It was shown that to correctly reproduce the experimental data on pressure fluctuations in a frequency range $100 \leq f \leq 2000Hz$, the optimal cut-off of the large eddy simulations corresponded to $\Delta_f = 100KHz$. With decrease of Δ_f, the quality of the results rapidly deteriorated. The present theory explains the failure of LES schemes with fixed mesh to describe the high Reynolds number flows as originating from the failure of low-order models in an all-important range $r \approx \Delta$, this range being responsible for the energy cascade dissipation. At the present time, it is not clear how many constraints (35) must be satisfied to achieve accurate LES, but we believe that the number must grow with the Reynolds number.

5 Conclusions

For many years, intermittency and anomalous scaling in three-dimensional turbulence were considered major challenges for theorists. Recent developments of the multifractal theory and its dynamic formulation led to description of intermittency in terms of an infinite number of dissipation scales (ultraviolet cut-offs). It was shown that strong velocity fluctuations are dissipated on scales that are much smaller than that estimated from Kolomogorov's theory. In this paper, we have attempted to make a connection between the theory of anomalous scaling and numerical methods.

One conclusion that follows from this connection is that to simulate all fluctuations, including the strongest ones, the computational demands scale as Re^4, and not as Re^3 as traditionally deduced according to the Kolmogorov theory. To achieve the full DNS of turbulence, including the strongest small-scale velocity fluctuations, one has to use resolutions high enough to produce an analytic interval of structure functions, where $S_n \approx \overline{\partial_x u(0))^n} r^n$. Analyzing the results of various numerical state-of-the-art DNS, we have discovered that this criterion is satisfied only for $n \leq 4$. This is not sufficient to accurately simulate the velocity derivatives.

A second comment concerns the Large Eddy Simulations. An infinite number of dynamic constraints on a correct subgrid model has been derived from the exact relations for structure functions. Due to the Galilean invariance, the subgrid scales cannot influence the advective term in the Navier-Stokes equations, provided the subgrid scale $\Delta/r \to 0$. However, it is clear from analyzing the equations of Section 4 that the subgrid model cannot be reduced to a low-order viscosity expression, but must include high-order nonlinear contributions that do not vanish at the scales close to the mesh size.

Thus, while accurate DNS are possible if the resolution requirements are met and powerful enough computers are available. However, due to the basic theoretical problems, derivation of an accurate and theoretically justified subgrid model, valid at very high Reynolds numbers, remains a major challenge.

It is worth pointing out that we have considered homogeneous and isotropic turbulence.

The situation with wall flows is even more complex. There, turbulence is mainly produced in the vicinity of the wall where acceleration and turbulence production are highly intermittent. Recent DNS by Lee et al. [39] have demonstrated strong intermittency and the Reynolds number dependence of the few first moments of Lagrangian acceleration near the wall, sharply peaking at the reduced normalized distance $y_+ \approx 2.5$. At present, we do not know how to model this near-wall phenomenon that is largely responsible for turbulence production.

We wish to conclude on a “positive” note. The fact that the structure functions $S_{2n} \approx (2n-1)!!(\frac{r}{L})^{\xi_{2n}}$ means that the velocity distribution is close to the Gaussian near $r = L$, and the intermittency is weak or nonexistent. It follows that simple, semi-qualitative re-summations of the expansions in powers of the dimensionless rate-of-strain are much less problematic there. Thus, the derivation of the VLES or time-dependent RANS appears to have a brighter future.

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