Anomalous scaling of structure functions and sub-grid models for large eddy simulations of strong turbulence.

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The original goal of Large Eddy Simulations of fully developed turbulent flows was to accurately describe large-scale flow features \( u(\Delta) \) at the scales \( r \geq \Delta \) where \( \Delta \) is a size of computational mesh. The effect of small-scale velocity fluctuations \( r < \Delta \) was to be accounted for by effective transport coefficients (subgrid models) in the coarse-grained Navier-Stokes equations. It is shown in this paper that, due to anomalous inertial range scaling (intermittency) of the moments of velocity difference, the existing subgrid models are intrinsically incapable of quantitatively describing flow features at the scales \( r < N\Delta \) with \( N \approx 10 \). This increases computational work approximately by a factor \( 10^3 - 10^4 \). The breakdown of the widely used Smagorinsky relation for the subgrid viscosity on the scales \( \Delta/L < 1 \) is demonstrated and a modification accounting for intermittency of the filtered out small-scale fluctuations is proposed.

Introduction. In 1969 S. Orszag introduced spectral methods as a tool for direct numerical simulations (DNS) of strong turbulence [1] which were implemented in simulations of three-dimensional isotropic flow in 1970-1971 and published in his paper with Patterson in 1972 [2]. Thus, a new field of numerical experimentations on turbulent flows was born. Based on Kolmogorov’s theory Orszag estimated the scaling of computational work \( W \) with the large-scale Reynolds number \( Re = u_{rms}L/\nu_0 \): \( W = O(Re^3) \). Here \( L \) and \( \nu_0 \) stand for the integral scale corresponding to the top of inertial range and molecular viscosity, respectively. Although it became clear recently [3] that, due to intermittency, the scaling of computational work required for full simulations of developed turbulence can be as bad as \( W = O(Re^4) \), this work, defining computation as an alternative experimental tool for turbulence studies, was a major breakthrough.

It became clear immediately that due to the unfavorable Reynolds number scaling of computational work, the DNS of high Reynolds number flows of engineering interest were impractical and derivation of coarse-grained equations (models) for prediction of the large-scale flow features, theoretically accounting for the small-scale fluctuations were of crucial importance. The aim was to eliminate the small-scale velocity fluctuations, describing structures on the scales \( r < \Delta \), from the Navier-Stokes equations, express their effect in terms of the resolved field and reduce the computational work to \( W = O(Re^\gamma) \) with \( \gamma \approx 0 - 1 \).

The problem is formulated as follows. The Reynolds stress can be decomposed as:

\[
RS = \mathbf{u} \cdot \nabla \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u}_{SG} + \mathbf{u}_{SG} \cdot \nabla \mathbf{u} + \mathbf{u}_{SG} \cdot \nabla \mathbf{u}_{SG}
\]

where \( \mathbf{u} \) and \( \mathbf{u}_{SG} \) are the resolved and subgrid velocity fields describing flow structures on the scales \( r \geq \Delta \) and \( r \leq \Delta \), respectively. To fully simulate velocity fluctuations on the length-scale \( r \) varying in the interval \( L \geq r \geq \eta_K \approx LRe^{-\frac{3}{4}} \), one needs a computational mesh at least as small as \( \Delta \approx \eta_K \). If due to computational limitations the practically available mesh size \( \Delta \gg \eta_K \), one needs equations for velocity field \( \mathbf{u}(\Delta) \equiv \mathbf{u} \) defined on the resolved scales \( r \geq \Delta \). The rapidly varying terms involving the computationally unaccessible small-scale subgrid fluctuations \( \mathbf{u}_{SG} \) on the scales \( \eta_K < r < \Delta \) are to be averaged out and their effect represented in terms of the resolved field \( \mathbf{u} \).

First attempts to achieve this goal were made by Durst [4] who applied the model previously derived by Lilly and Smagorinsky [5] to simulations of wall flows. This model is based on an assumption that the effect of small-scale velocity fluctuations on the large-scale ones can be represented in terms of effective viscosity. It will become clear below that while this assumption is accurate when \( \Delta/L \approx 1 \), due to the anomalous scaling of the inertial range structure functions, it is grossly incorrect when the cut-off \( \Delta \) is small, i.e. \( \Delta/L \ll 1 \). The essence of the Lilly-Smagoronsky construction can be formulated as follows. Consider a length-scale \( \Delta \) in the inertial range. Then, according to Kolmogorov’s theory, the scale-independent energy flux

\[
\bar{\mathcal{E}} = \bar{\mathcal{E}}(\Delta) \equiv 2\nu(\Delta)\bar{S}^2(\Delta) \approx \frac{1}{(u(x+\Delta) - u(x))^2}/\Delta = \frac{\bar{S}^2(\Delta)b^2}{\Delta} \tag{1}
\]

where \( S(\Delta) \equiv \sqrt{S_{ij}(\Delta)S_{ij}(\Delta)} \), with \( S_{ij}(\Delta) = \frac{1}{2}(\partial_i u_j + \partial_j u_i) \), is the rate of strain evaluated on the resolved scales \( r \geq \Delta \) and the effective viscosity \( \nu(\Delta) \) accounts for the contribution of the small-scale velocity fluctuations acting on the scales \( r \leq \Delta \). The filtering of the small-scale velocity fluctuations from the interval of scales \( r < \Delta \) generates the resolved field which is smooth...
on the scales \( r \geq \Delta \) and, as a result, the spatial derivatives \( \partial_j u_i(\Delta) \approx (u_i(x+\Delta,j) - u(x))/\Delta_j \) are expressed in terms of velocity increments of the scale \( \Delta \). From here, we have for the well-known relation for turbulent viscosity \( \nu(\Delta) \approx \Delta^2 |S(\Delta)|/S^2(\Delta) \).

This global argument, dealing with the mean properties of a flow, is relatively safe. To develop a numerical method, one needs local differential equations for the numerically resolved velocity field with a local expression for turbulent viscosity in terms of this resolved field. A dimensionally correct possibility is the following: based on (1), write \( E(\Delta) = 2\nu(\Delta)S_{ij}(\Delta)S_{ij}(\Delta) + \Psi(\Delta) \) where \( \Psi \) is an unknown function satisfying a global constraint \( \Psi = 0 \). Evaluation of this function which is an extremely difficult task will be discussed below. The simplest and crudest way to develop a model is by dropping the averaging symbols in (1), setting \( \Psi = 0 \) and, interested in isotropic turbulence, taking for simplicity \( \Delta_i = \Delta \) obtain:

\[
\nu_S(\Delta) = aS\Delta^2 \approx a|u(x+\Delta) - u(x)|/\Delta
\]  

(2)

which is basically a mixing length model well-known from Prandtl’s works. The derivation of this model directly from the Navier-Stokes equation, based on the one-loop renormalization perturbation expansion led to the expression for effective viscosity \( \nu_{eff} = \nu_S(1 - e^{-\frac{\Delta}{\eta_K}}) \) where \( \eta_K \approx LRe^{-\frac{1}{3}} \) is the Kolmogorov dissipation scale [6]. Typically, in the LES the cut-off \( \Delta \gg \eta_K \), so that \( \nu_{eff} \approx \nu_S \). This expression for effective viscosity, combined with the Navier-Stokes equations for the resolved velocity field, is a celebrated Smagorinsky model for the large-eddy-simulations of turbulence (LES). The expression (2) is the basis of majority of modern LES schemes postulating the length-scale \( \Delta \) identical to the size of a cell of computational mesh. We can see that since \( \nu(\Delta) \gg \nu_0 \), the role of this increased viscosity is to reduce the Reynolds number and, consequently, the number of degrees of freedom necessary for description of the large-scale flow features. In general fluctuating parameter \( a \), which is constant in isotropic and homogeneous turbulence cannot be derived from this qualitative argument.

As follows from (2) the moments of fluctuating resolved dissipation rate are:

\[
\mathcal{E}^n(\Delta) = [\nu_S S^2]^{\xi_n} \propto a^n |(\Delta u)|^{3n}/\Delta^n \propto (\xi L) \frac{\Delta}{L}^{\frac{n}{3}}\xi_n^{-n}
\]  

(3)

with "anomalous" scaling exponents \( \xi_n \) consistent with the so called Kolmogorov’s refined similarity hypothesis. The relation (2) is a result of a general small-scale filtering procedure or, equivalently, the scale elimination methods developed for the dynamic renormalization group. All existing sub-grid models are based on an assumption that the filtering leads to the equation for the resolved velocity field (for state-of-the-art review, see Ref.[7])

\[
\partial_t u + u \nabla u = -\nabla p + \nu_S(\Delta) \partial_{ij} u + EN + f \quad (4)
\]

where \( \nu(\Delta) \) originates from the \( u_{SG} \cdot \nabla u_{SG} \) contributions to the Reynolds stress and \( EN \) stands for the back scattering term ("eddy noise") leading to a small fraction of energy the large-scale eddies receive from interactions with the small-scale ones. Interested in three-dimensional turbulence dominated by the direct cascade we, for a time being, can neglect the \( EN \)-contribution. The large-scale forcing function \( f \) in the right side of (4) is not modified by the coarse-graining (filtering) procedure described below. Multiplying (4) by \( u \), the energy balance for the resolved velocity field is calculated readily:

\[
P = \nabla \cdot f = \Delta^2 \left| \frac{\partial u_i}{\partial x_j} \right|^2 = O \left( \frac{|u(x+\Delta) - u(x)|^2}{\Delta} \right)^2
\]

which, by choosing a proper magnitude for the constant \( a \), is consistent with the Kolmogorov’s 4/5 law. Since by construction, the arbitrary cut-off \( \Delta \) is chosen in the inertial range, the equation (4) with the Smagorinsky viscosity (2) is expected to produce approximately accurate results for the resolved energy spectrum and the second moment \( S_2 = (u(x+\Delta) - u(x))^2 \).

However, if consistent, the local equation (4) with subgrid model (2) is supposed to describe the resolved velocity field, including all structure functions \( S_n(\Delta) = (u(x+r) - u(x))^n \) and moments of resolved dissipation rate on all scales \( r \geq \Delta \).

Scale by scale comparison of LES with DNS. To assess the scale-by-scale performance of a subgrid model we have introduced the displacement \( r = N\Delta \) where \( N > 1 \) are the integers, and evaluated the modified structure functions \( S_p(N\Delta) = \frac{|u(x+N\Delta) - u(x)|^p}{\Delta^p} \) using the DNS (resolution 256³ ) and variational LES (resolution 32³) described in detail in the Ref. [8]. For \( p = 2 \) this parameter gives \( \sqrt{S_2} = (\delta_{N\Delta} u)^{rms} \) and for an arbitrary \( p \) it is a useful tool for analyzing quality of prediction of the most intense small-scale events. The energy spectra \( E(k) \), evaluated using both methods in Ref.[8], were in a good agreement with each other [8]. On Fig.1 we show the ratio \( S_{p,LES}/S_{p,DNS} \) as a function of displacement \( r = N\Delta \). As expected, even for this low Reynolds number flow for which \( \Delta/L \approx 0.1 \), the "small-scale" results rapidly deteriorate with increase of power \( p \). This drawback of all existing subgrid models (for different examples see an excellent review [7]) , which cannot be cured by introducing the scale-dependent
where, to simplify notation, we set $r/L < \Delta$, one has to use (5) - (6) as a filter applied to the Navier-Stokes equations which is not a simple task.

To illustrate the role of intermittency (anomalous scaling) in the LES modeling we, can use an approach leading to derivation of turbulence models from a kinetic equation for some artificial “particles” forming a “fluid” characterized by the relaxation time $\tau$ reflecting dynamic properties of a system. For example, choosing $\tau = \text{const}$ leads in the first order of the Chapman-Enskog expansion to the Navier-Stokes equations with viscosity $\nu_0 = \tau u_{rms}^2/3$ with non-linear corrections appearing from the higher order terms. The same procedure but with the relaxation time $\tau \propto K/E$ yields the well-known linear and non-linear $K - E$ models for the large-scale velocity field [14]. Repeating the procedure, presented in Refs.[14], it is easy to see that the LES, Smagorinsky-like, models are generated by the same equations with $\tau(\Delta) = 1/[S_{ij}(\Delta)]$. In the second order of perturbation expansion in powers of dimensional rate of strain the procedure gives:

$$
\sigma_{ij} = 2\nu_S(\Delta)S_{ij} - 2\nu_S(\Delta)(\partial_t + u \cdot \nabla)(\tau S_{ij})/3
- 4\nu_S(\Delta)\tau[S_{ik} S_{kj} - \frac{1}{7} \delta_{ij} S_{kk} S_{ii}]
+ \nu_S(\Delta)\tau[S_{ik} \Omega_{kj} + S_{jk} \Omega_{ik}]
$$

(7)

with $\nu_S = \tau u_{rms}^2(\Delta) = \Delta^{-\nu_s} u_{rms}^2 / \nu_s$, which is a probability density of single-point velocity field.

The small-scale ($r/L < 1$) strong fluctuations are well described by the expression following from the steepest descent evaluation of the integral (5) (for details see [10]-[11]):

$$
P(\delta_r u) = \mathcal{P}(\delta_r u) \int_{-\infty}^{\infty} e^{x^2} dx \int_{-\infty}^{\infty} e^{i n \left[ \frac{x^2}{2 \sqrt{\ln \frac{n^2}{\nu_s}}} - n^2 \ln r \right]} dn
$$

(5)

where, to simplify notation, we set $r \equiv r/L$ and $\delta_r u \equiv \delta_r u / u_{rms}$. In the limit $r \to 1$, this expression gives Gaussian PDF $P \propto e^{-(\delta_r u)^2/2} = e^{-(\delta_r u)^2/2}$ which is a probability density of single-point velocity field.

The small-scale ($r/L < 1$) strong fluctuations are well described by the expression following from the steepest descent evaluation of the integral (5) (for details see [10]-[11]):

$$
P(\delta_r u) = \frac{2}{\pi(\delta_r u) \sqrt{4 \ln r}} \int_{-\infty}^{\infty} e^{-x^2} \frac{1}{\nu_s} \left[ \frac{\ln \frac{\delta_r u}{\sqrt{4 \ln r}}} {4b \ln r} \right] dx
$$

(6)

The constants in (5)-(6) tested in various flows [11]-[13], are $a \approx 0.383$ and $b \approx 0.01667$. As $\Delta/L \to 0$, the PDF (6) is an extremely shallow function stressing the importance of strong small-scale fluctuations not accounted for by Smagorinsky-like models. Thus, to eliminate small-scale fluctuations $r < \Delta$, one has to use (5) - (6) as a filter applied to the Navier-Stokes equations which is not a simple task.

algebraic relations $a = a(r/\Delta)$, is quite costly: the model which is capable of accurately describing the flow on the scales from the interval $r/\Delta \geq 10$ only, is at least by the factor 1000 more expensive than the one valid in the entire interval $L \geq r \geq \Delta$.

The Smagorinsky model has been derived in Ref. [6] directly from the Navier-Stokes equations from the one-loop renormalized perturbation expansion in powers of the Reynolds number $Re_{eff} = u_{rms} L / \nu(L) = O(1)$ which can be reformulated as a series in powers of dimensionless rate -of-strain proportional to the velocity increments with displacement $r$ in the inertial range. As well-known from experimental data, at the large scales $r \approx L$, the velocity fluctuations obey Gaussian statistics and, therefore, all contributions to the expansion are of the same order and a few first contributions to the series give quantitatively accurate results. As $r/L << 1$ this is not so high-order-contributions to the series become dominant and must be taken into account. The severity of this problem, stressed in [9], becomes clear from a general expression for the probability density of velocity fluctuations (increments) [10]:

$$
P(\delta_r u) = \frac{1}{\sqrt{\pi} \delta_r u} \int_{-\infty}^{\infty} e^{x^2} dx \int_{-\infty}^{\infty} e^{i n \left[ \frac{x^2}{2 \sqrt{\ln \frac{n^2}{\nu_s}}} - n^2 \ln r \right]} dn
$$

(5)

where, to simplify notation, we set $r \equiv r/L$ and $\delta_r u \equiv \delta_r u / u_{rms}$. In the limit $r \to 1$, this expression gives Gaussian PDF $P \propto e^{-(\delta_r u)^2/2} = e^{-(\delta_r u)^2/2}$ which is a probability density of single-point velocity field.
obtained in the lowest order of expansion in powers of dimensionless rate of strain. Now, we will discuss the limits of its validity.

Our goal is to express the sub-grid contribution to the Reynolds stress in terms of the resolved field $u(r > \Delta)$. As one can see from (7), due to proliferation of the subscripts, with increase of the power of expansion each term becomes more and more complex. Some simplifications are based on the following: The resulting equation must be invariant under Galileo transformation. It is clear that the mean dissipation rate where the coefficients $\tau_\alpha \ll \tau_\omega$ is important for the flows rapidly varying on the time scale limit $\Delta \to L$. It has been shown [17]-[18] that expansion in powers of $\sigma$ effects, and $D$ constraints discussed above, choose an infinite subset of high-order terms in the expansion (7) we, based on the general expression for the Reynolds stress is $\sigma_{ij} = \sigma_{ij}(D_1, D_2)$.

It has been shown [17]-[18] that expansion in powers of $D_1$ results in the telegrapher equation with $O(\tau D_1^2)$-term in the left side of (4), responsible for the quasielastic response of turbulent flow to external high-frequency perturbations. In what follows, mainly interested in the intermittency contributions to $\sigma_{ij}$, we omit this term which is important for the flows rapidly varying on the time scale $\tau \ll \tau(\Delta)$. To simplify the treatment and to avoid dealing with an extremely complex tensorial structure of high-order terms in the expansion (7) we, based on the constraints discussed above, choose an infinite subset of leading contributions to each term in power series of $\sigma_{ij}$ similar to the "single-back-bone" diagrams of the Wyld’s expansion of the Navier-Stokes equations:

\[
\sigma_{ij} \approx \nu_S S_{ij}(\Delta) \sum_n \alpha_n \left( \frac{|S_{ij}(\Delta)|}{|S_{ij}(\Delta)|} \right)^n
\]

where the coefficients $\alpha_n$ can be evaluated only for the first few terms. Similar approach has been developed for the scalar problem in Ref. [19], where it was used for assessment of the accuracy of the $\epsilon$-expansion in turbulence theory. It is clear that the mean dissipation rate $\overline{\varepsilon} = -u_i \frac{\sigma_{ij}}{\tau \omega_j}$ and the sub-grid viscosity can be defined as:

\[
\nu_{SG}(\Delta) = \sigma_{ij} S_{ij}^{-1} = \nu_S \sum_n \alpha_n \left( \frac{|S_{ij}(\Delta)|}{|S_{ij}(\Delta)|} \right)^n
\]

This expression is easily understood if we notice that the expansion we are dealing with is in powers of dimensionless rate-of-strain $\eta = \tau(\Delta)/S$ similar to that discovered in derivation of the RNG $K - E$ model from the Navier-Stokes equations [20]. Adding to this expression contributions including $\Omega_{ij}$ does not change qualitative conclusions of the argument.

As we see, in case of normal scaling or in the large-scale limit $\Delta/L \to 1$, the ratios $\left( \frac{|S_{ij}(\Delta)|}{|S_{ij}(\Delta)|} \right)^n = \beta_n$ are $\Delta$-independent and the dissipation rate based on this sub-grid viscosity in the limit $\Delta \to L$ is proportional to

\[
\overline{\varepsilon}(L) \propto \nu_{SG}(\Delta) S^2(\Delta) \approx \frac{1}{L} \frac{1}{(\overline{\delta L u}(\overline{\delta L u})^2)} \sum_n \alpha_n \beta_n \approx \overline{\varepsilon} = \mathcal{P}(10)
\]

provided $\sum_n \alpha_n \beta_n$ is a finite number. This expression is equivalent to Smagorinsky model (2). In the large-scale limit $\Delta \to L \to \infty$, due to the Galileo invariance, the corrections to the non-linear term $u \cdot \nabla u$ in the coarse-grained equation (4) are equal to zero and, as $\Delta/L \approx 1$, the energy balance in the equation (4) with viscosity given by (9) is not violated.

A completely different result is obtained when anomalous scaling is taken into consideration on the scales $\Delta < L$. It is clear from (9) that in this case the dissipation is not equal to (10) but is multiplied by an infinite sum:

\[
\overline{\varepsilon}(\Delta) \approx \nu_{SG}(\Delta) S^2(\Delta) \approx \overline{\varepsilon}(L) \sum_n \alpha_n \beta_n \left( \frac{\Delta}{L} \right)^{\xi_{n+3} - \frac{3}{2} - 1} \approx \mathcal{P}
\]

(11)

Since $\xi_{n+3} - \frac{3}{2} - 1 < 0$, for $\Delta/L \ll 1$ the dominating contributions from the high-order terms in (10) invalidate the Smagorinsky’s model in the range of scales $\Delta/L \ll 1$. As we see, since production $\mathcal{P}$ is a large-scale $\Delta$-independent property, when $\Delta/L \ll 1$, the energy balance in the LES equation (4) can be restored only by renormalization of the non-linear term, i.e. by accounting for the high-order non-linear contributions, disappearing in the limit $\Delta/L \to 1$. In this case the relation proportional to (9) is a possible candidate satisfying the above requirements. Thus, neglecting the “rapid-distortion” (memory) contribution, the LES models accounting for the inertial range intermittency is:

\[
\partial_t u + \Phi \{ S \frac{\Delta}{L} \} u_i \nabla \nu = -\nabla p + \nabla_\alpha \nu_{SG}(\Delta) \nabla_\alpha u + EN + f
\]

(12)

As $\Delta/L \to 1$ the functional $\Phi \to 1$. In the interval $\Delta < L$ it ensures cancellations leading to the cut-off -independent expression for the mean dissipation rate $\overline{\varepsilon}(\Delta) = \mathcal{E} = \mathcal{P}$.

To conduct numerical simulations using equations with transport coefficients given by infinite series in powers of dimensionless rate-of-strain $\tau S$ is not a simple task. One can attempt to qualitatively represent the sum in (9) in a compact form like $\nu_{SG}(\Delta) = \nu_S/(1 + \frac{S^2}{\tau \omega})$ which, by the averaging the expression for the dissipation rate using the probability density (5)-(6) is equivalent to the infinite series (11). This qualitative representation of an infinite series (9) proved to be very useful in the $K - E$ modeling emerging from a present theory in the limit $\tau(\Delta) \to \tau(L) \propto K/\mathcal{E}$ [21].
To summarize: in this paper we compare the LES based on Smagorinsky sub-grid model with the direct simulation of the same flow. It has been demonstrated that, while the LES gives a reasonably accurate representation of the large-scale flow features, it completely underestimates strong small-scale ($r < 10 < \Delta$) intermittent velocity fluctuations. The reason for this failure is traced to the inadequate account for the small-scale intermittency of the filtered out small-scale fluctuations in the Smagorinsky-class models. An improved model including the intermittent phenomena is proposed.

It is interesting to compare the outcomes of this work with the results presented in two important papers [22]-[23]. In these works the authors compared filtered and unfiltered experimental data on turbulent properties of a few flows (wakes, grid, decaying turbulence, etc). The filtering procedure of Refs.[22]-[23] was the same as the one used in the LES. Since no modeling was involved, and one would expect that the resolved velocity fluctuations on the scales $r \leq \Delta$ of the two fields must be identical. A completely different picture emerged: the strong small-scale features of the filtered field were grossly underpredicted compared with the raw, unfiltered, data. This important result indicates that large and small-scale velocity fluctuations strongly interact and one cannot obtain a reasonable representation of one by simply filtering out the other. This conclusion becomes clear if one recalls that in turbulent flows extremely thin and long geometrical structures, like pancakes, “worms” etc, consist of inseparable, strongly interacting large and small-scale flow features. Thus, smoothing the velocity field over length-scale $\Delta$ (filtering), distorts the entire field including the interval $\Delta < r < 10\Delta$. In short, the works [22]-[23] showed that the simple-minded filtering procedure is intrinsically flawed. The theory described in this paper, based on consistent procedure of small-scale elimination from the Navier-Stokes or Boltzmann-BGK equations, proposes a remedy for this drawback by strong modification of the equations of motion for the resolved scales. The resulting model, while at the large scale equivalent to the ordinary Smagorinsky model, at the small scales $r \approx \Delta$ does not resemble neither it nor the Navier-Stokes equations themselves.

Correctly accounting for the entire range of velocity fluctuations $L > \Delta > \eta K$ may substantially reduce cost of numerical simulations and improve quality of LES of mixing and sound generation by turbulence. This will be a subject of future communications.

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