Optimal sub-grid-scale models for inertial range turbulence

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Turbulent flows are ubiquitous in nature and in engineering applications and they are characterized by the presence of intense non-Gaussian fluctuations on a wide range of inertial scales and frequencies. The main mechanism that needs to be controlled and, eventually, modeled is the energy transfer from the large-scale, $L$, where the flow is stirred, to the small-scale, $\eta$, where viscous effects are dominant. The Reynolds number is a measure of the separation between the two scales, $Re \sim (L/\eta)^4/3$. For most applications, $Re$ is too large to allow the problem to be attacked by direct numerical simulations (DNS). Similarly, fundamental problems connected to the presence of anomalous scaling in the limit $Re \to \infty$ cannot be easily studied using numerical tools. In such a deadlock, the applied community resorts to Large Eddy Simulations (LES), a numerical scheme that restricts the Navier-Stokes equations to a range of scales (or wavenumbers) larger (smaller) than a given cut-off, $r \gg r_c$ ($k \ll k_c$), and modeling all sub-grid-scale (SGS) degrees of freedom with ad-hoc closures in configuration space, or Fourier space. The aim is to achieve a good accuracy for the dynamics of the energy-containing modes, without necessarily paying too much attention to the those (inertial) scales that are fully resolved, but also unavoidably affected by the sub-grid-scale closure. As a matter of fact, most LES implementation that reproduce successfully the large-scale dynamics, $k \ll k_c$, are inaccurate for what concerns the statistical properties of the highest resolved wavenumber modes, $k \sim k_c$. This fact, prevents the possibility to use LES models to improve our understanding of multi-scale velocity fluctuations and/or the feedback of extreme small-scale fluctuations on global mean profiles. In particular, too simple SGS-models perform very poorly concerning the reproduction of the inertial-range scaling of velocity structure functions (SF):

$$S_n(r) = \langle |\delta_r u|^n \rangle \sim \left( \frac{r}{L} \right)^{\zeta_n}$$

where we have introduced the longitudinal increments $\delta_r u = u(r+x) - u(x)$, and we have assumed isotropy and homogeneity. The scaling exponents $\zeta_n$ are the key quantities that need to be measured in order to predict the asymptotic statistics for large Reynolds numbers, where $r/L$ can be arbitrarily small. On one side, experiments and numerical simulations have provided a wealth of evidence that the scaling of $S_n(r)$ is anomalous, i.e. different from the Kolmogorov 1941 (K41) prediction $\zeta_n = n/3$. On the other hand, we do not have any first-principle derivations of the $\zeta_n$. Furthermore, it is extremely difficult to get accurate measurements of the exponents, due to the concurrent requirements of having a large scaling range and large statistical ensembles. As a result, we also lack the numerical and experimental accuracy to distinguish among different phenomenological models. Finally, few assessments exist concerning the robustness of the exponents with respect to the small-scale dissipative mechanism.

In this paper, we study a class of sub-grid models with the aim to minimize the impact of the SGS closure on the inertial-range turbulent scale: a sort of optimal energy-cascade sink that permits to achieve a much higher effective numerical resolution to study the inertial-range scaling properties in turbulence. The idea was already presented in but never applied and developed in the way we do here. In practice, we introduce a self-similar buffer close to the highest resolved mode, such as to have an ultraviolet boundary condition for the energy cascade at high $k$ which is consistent with the existence of an infinitely extended inertial range. The advantages with respect to other closures are many. First, our model is time-reversible, allowing the formation of backscatter events also. Second, it is a minor modification of the high-wave numbers dynamics, without touching the Fourier-phases and therefore with a minimal impact on the formation of those spatial intermittent events that are believed to be the responsible of anomalous scaling. Un-
like in [31], here we focus on high Reynolds applications in order to assess the impact of the closure on the inertial range turbulent properties. Furthermore, we expand the protocol by considering also a new Fourier modulation in the wave-numbers range where the closure acts such as to improve its efficiency in providing an ideal adsorbing boundary for the energy cascade.

In the following, we show that our LES protocol is able to obtain the same inertial-range extension of a fully resolved viscous DNS while saving roughly one order of magnitude of resolution per each direction. As a result, considering also the gain due to the possibility to relax the time step, the improvement in the computational resources is larger than a factor 1000, opening the way to make a quantum leap in the accuracy to measure scaling exponents in turbulence, concerning the scaling range extension and the statistical accuracy. Moreover, the agreement between the scaling obtained with our SGS-model with the ones measured in DNS and experiments [8, 9, 17] allow to make a strong statement about universality of inertial range properties with respect to the ultraviolet small-scales dissipative mechanism. Another by-product, is to provide a LES model that is accurate for what concerns the small-scale evolution, something that is becoming important for engineering applications interested in controlling extreme non-Gaussian events close to the sub-grid cut-off [32, 33]. Finally, we stress that our approach is fully general and of broad applicability, it can be easily extended to other flow configuration as for the case of rotating or stratified turbulence, conducting flows, as well as along the homogeneous directions of wall-bounded flows.

**The model.** Let us consider the Fourier-space evolution of the three dimensional Navier-Stokes equations in a periodic box of size $L = 2\pi$ and resolved with $N$ grid points per direction and maximum wavenumber in all direction given by $k_{max} = N/2$:

$$\left(\partial_t + \nu k^2\right)\hat{u}_k(t) = \hat{T}_k(t) + \hat{f}_k(t)$$

(2)

where $\nu$ is the viscosity, $\hat{f}_k(t)$ is the Fourier transform of the external forcing and $\hat{T}_k(t) = -ik \cdot \left(\mathbb{1} - \frac{k \otimes k}{|k|^2}\right)\sum_{k'} \hat{u}_{k'}(t) \otimes \hat{u}_{k'-k}(t)$ is the non-linear term. We follow [31] and we replace the viscous term on the lhs of (2) with a non-linear inertial closure that imposes a perfect self-similar Kolmogorov-like spectrum in a k-window close to the ultraviolet cut-off, $k_{max}$:

$$E_k(t) = \left(\frac{k}{k_c}\right)^{-\frac{5}{2}} E_k(t); \quad k_c \leq k \leq k_{max},$$

(3)

where $E_k(t) = \frac{1}{2} \sum_{|k|=k} |\hat{u}_k(t)|^2$. The LES equation for the resolved velocity field equipped with the fixed-spectrum SGS-model can be written using a Lagrangian multiplier $\lambda_k(t)$ [30],

$$\partial_t \hat{u}_k(t) = \hat{T}_k(t) + \hat{f}_k(t) - \gamma_k \lambda_k(t) \hat{u}_k(t)$$

(4)

where we have removed the viscosity and $\gamma_k$ is a projector which selects the range of scales where the sub-grid closure acts: $\gamma_k = 0$ if $k \leq k_c$ and $\gamma_k = 1$ if $k_c < k < k_{max}$ (SGSM-sharp). It is easy to realize that in order to satisfy (2) we can impose $dE_k/dt = (k_c/k)^{5/3} dE_k/dt$ and choose $\lambda_k(t)$ to be:

$$\lambda_k(t) = \frac{1}{2} \frac{T_k(t) - (k/k_c)^{-5/3} T_{k_c}(t)}{E_k(t)},$$

(5)

where $T_k(t)$ is the transfer function: $T_k(t) = \sum_{k'=k} \hat{u}_{k'}(t) \hat{T}_k(t)$. In order to mitigate the sharp transition across the SGS, $k_c$, we also explored another protocol where the percentage of constrained modes grows linearly from 0 at $k_c$ to 1 at $k_{max}$. To do that, with define a (quenched) probability to apply the SGS model at any given wavenumber as follows (SGSM-smooth):

$$\gamma_k = \begin{cases} 0 & \text{if } k \leq k_c \\ 1 & \text{with prob. } P_k = \frac{k-k_c}{k_{max}-k_c} & \text{if } k_c < k \leq k_{max} \end{cases}$$

In this way, only a fraction of modes $(k-k_c)/(k_{max}-k_c)$ will be affected by the constraint for any given shell $k$, such that we move from fully unconstrained dynamics (for $k < k_c$) to a fixed spectrum dynamics (for $k = k_c$) with continuity (see inset of Fig. [1] for a graphical scheme of the Fourier space support of the projector $\gamma_k$ for both sharp and smooth SGSM cases).

**Results.** In the following we will compare the results of the LES obtained at a resolution of $1024^3$ grid points with that from two different DNS resolutions: one identical to the LES (DNSx1) and one taken from a state-of-the-art study at $8192^3$ collocation points [3] which will be denoted (DNSx8). All runs are forced with a white-in-time Gaussian forcing acting at $k_f \in [1, 1.5]$ for DNSx1 resolution and a $k_f \in [1, 3]$ for DNSx8. More details on the numerical set up can be found in Table I. In Fig. [1] we show the spectral properties of the three data-sets. Our closure is able to reproduce the same extension of the scaling range of the DNSx8 data set and extend considerably the one obtained with the DNSx1. Without recourse to the whole layer of scales required in the DNSx8

| $N$ | $k_c$ | $k_{max}$ | $\varepsilon$ | $\nu$ | $T$ | Re |
|-----|-------|-----------|---------------|-------|-----|-----|
| SGSM-sharp | 1024 340 512 | 3.0 | $8.0 \cdot 10^{-5}$ | 8.5 | 2.1 $\cdot 10^5$ |
| SGSM-smooth | 1024 340 512 | 3.0 | $4.0 \cdot 10^{-5}$ | 8.5 | 4.2 $\cdot 10^5$ |
| DNSx1 | 1024 – 340 | 2.5 | $8.0 \cdot 10^{-4}$ | 12 | 2.0 $\cdot 10^4$ |
| DNSx8 | 8192 – 3861 | 1.5 | $4.4 \cdot 10^{-5}$ | 3.4 | 3.0 $\cdot 10^5$ |
to adsorb the energy cascade with standard viscosity, we obtain an inertial behavior for all $k$ in the LES model.

**ANOMALOUS SCALING OF HIGH ORDER SF.** In order to assess the scaling properties in a quantitative way, we refrain from doing a log-log fit and we directly measure local scaling exponents, defined in terms of the logarithmic local slopes:

$$\xi_n(r) = \frac{d \log S_n(r)}{d \log(r)}$$

where, of course, in the presence of pure power-laws we must have $\xi_n(r) = \text{const.} = \xi_n$.

In Fig. (2) we show $\xi_2(r)$ for our two SGSM closures and compare them with the same quantity measured on DNSx1 and on DNSx8. As already shown for the spectral case, the LES data have a much larger extension of the scaling properties than DNSx1, being able to match quite well the DNS obtained with a 8-times larger resolution (DNSx8).

Despite that an inertial-range region with a plateau for $\xi_2(r)$ develops for all data-sets, the tendency for all curves to reach the differentiable behavior $\xi_2(r) \to 2$ for $r \to 0$ makes very difficult to quantitatively distinguish the Kolmogorov 1941 (K41) scaling from the phenomenological She-Leveque (SL) value [22] which is taken here as a proxy of previous numerical and experimental results at high Reynolds numbers. To be more accurate, in Fig. (3) we show the scaling of the Flatness and of the scale-by-scale ratio $\Delta(r) + 2 = \xi_4(r)/\xi_2(r)$ (see inset).

FIG. 1. Energy spectra for the simulations described in Table 1. The curves are shifted vertically for the sake of data presentation. The grey area marks the range of wavenumbers where the closure acts. Inset: 2d sketch of the Fourier space support where $\gamma_k = 1$. Left and right panels represent respectively SGSM-sharp and SGSM-smooth cases.

FIG. 2. Log-lin plot of $\xi_2(r)$ vs $r$. Solid line indicates the SL prediction, $\xi_2 = 0.69$. The dashed line is the K41 value $\xi_2 = 2/3$. In grey, we indicate the range of scales where the power-law constraint (5) is acting. Notice the important improvement in the scaling-range extension comparing the DNSx1 and our LES data (blue and red symbols). Error bars are comparable with symbols’ size.

FIG. 3. Log-lin plot of the local exponent, $\xi_4(r)/\xi_2(r)$, for both SGSMs and DNSs, here dashed horizontal line represents the K41 prediction, 2, the solid line is the SL value, 1.839, which almost coincides with the average of the one obtained from the SGSM-smooth model, 1.843 ± 0.009 (see also table II). In grey, we indicate the range of scales where the SGS power-law model (5) is applied. Inset: log-log plot of Flatness vs $r$ with same symbols of the main panel. The SL scaling, $\xi_4 - 2\xi_2 = -0.11$, and the K41 prediction are given by the solid and the dashed lines, respectively. In all figures, errors are evaluated from the scatter of 40 configurations taken equispaced in time.

The advantage with respect to a simple log-log fit of (1) is evident: by measuring where $\xi_2(r)$ is constant we have an unbiased definition of the inertial range extension and we can assess scale-by-scale the quality of our data. In particular, scale-dependent deviations from a Gaussian behavior can be measured by the deviation from zero of $\Delta(r) = \xi_4(r)/\xi_2(r) - 2$ as can be seen from the definition of the Flatness in terms of the 2nd order SF:

$$F(r) = \frac{S_4(r)}{(S_2(r))^2} \sim r^{\xi_4(r) - 2\xi_2(r)} \sim [S_2(r)](\frac{\xi_4(r)}{\xi_2(r)})^2.$$  

In Fig. (2) we show $\xi_2(r)$ for our two SGSM closures and compare them with the same quantity measured on DNSx1 and on DNSx8. As already shown for the spectral case, the LES data have a much larger extension of the scaling properties than DNSx1, being able to match quite well the DNS obtained with a 8-times larger resolution (DNSx8).
on the scale separation $k_c/k_{max}$). Finally, we found that it might also be important to preserve a very small viscous term together with the SGSM closure, in order to smooth the transition across $k_c$. This is indeed implemented in our approach, where we keep a term $\nu k^2 \hat{u}_k(t)$ in Eq. (2) but with a very small $\nu$ as shown in Table I. Before concluding we also discuss the comparison with two other popular ways to enhance the Reynolds numbers. In particular, in Fig. 4 we compare the Flatness obtained from a DNS with hyper-viscosity [28, 37] or from a Smagorinsky SGS model [10, 11, 35] with the one proposed in this paper. Notice that the hyperviscous data are only qualitatively as good as the SGSM-smooth case as can be seen from the fact that the former has a less extended plateau wrt to the latter. There are no doubts that the closure (i) is superior to both Smagorinsky and hyperviscous models. Finally, we mention that from our closure (i) one can also define a Galilean-invariant SGS energy transfer: $\Pi(x) = \partial_t u_j(x) \int dk \gamma_k \lambda_k c_k x \hat{u}_k / k^2 \hat{u}_j k$, which is non-positive definite and therefore able to reproduce back-scatter events too.

### TABLE II. Averaged scaling exponent $\Delta_{avg}$

| SGS closure  | $\Delta_{avg}$ | $r_{min}/L$ | $r_{max}/L$ |
|-------------|----------------|--------------|-------------|
| SGSM-sharp  | 1.836 ± 0.013  | 0.03         | 0.9         |
| SGSM-smooth | 1.843 ± 0.009  | 0.03         | 0.9         |
| DNSx1       | 1.826 ± 0.015  | 0.09         | 0.9         |
| DNSx8       | 1.824 ± 0.011  | 0.03         | 0.9         |

TABLE II. Averaged scaling exponent $\Delta_{avg}$ where the value is obtained as a fit of $\xi_{avg}(r)$ shown in the inset of Fig. (5) in the range $r \in [r_{min} : r_{max}] L$. Errors refers to the combination of statistical fluctuations plus the maximum variations considered by taking the fit in the first or second half of the scaling range indicated in the table. The SL prediction for the same quantity is 1.389.

A few comments are now in order. First, although the results are extremely good, it is clear from Fig. (3) that even for the SGMS data sets there is a pseudo-viscous range (extended over a few grid points) where the anomalous scaling breaks down. This is somehow unavoidable because our closure is acting in the Fourier space and does not enforce any pure scaling for the high order SFs in the configuration space. On the other hand, the efficiency in extending the anomalous scaling-range is a good evidence that to capture intermittency the SGS must maintain the correct phase-correlations [34], which is one of the main added value of (5). Second, the recipe given by the smooth projector is of course not unique and one can imagine many different ways to enforce the transition from modes that evolve according to their Euler dynamics ($k < k_c$) to those that feel the spectral constraint. In particular, once the controlled buffer is introduced and it is large enough, one might imagine to even avoid the de-aliasing protocol. Indeed the SGSM data shown in all figures have been obtained without any de-aliasing, i.e. with $k_{max} = N/2$. We tested the effects of introducing a de-aliasing and we did not observe any important change (a detailed and systematic report about this issues will be published elsewhere, together with the dependency of the results scaling is now evident and much more importantly- our SGS closures are able to develop an inertial scaling range as extended as the DNSx8 case, if not even larger. Moreover, the SGSM-smooth closure is a bit better than the SGSM-sharp case. We consider these results a clear demonstration that the SGS model developed here can be considered a sort of quasi-optimal infinite-Reynolds closure. A rough estimate of the gaining factor must consider a multiplier $8^3$ for the spatial resolution between the SGSM-smooth and the DNSx8, which together with the less stringent CFL condition for the time integration leads to a final estimate for the gain close to a factor 1000, if not higher. In Table II we present a summary for the averaged scaling properties of the Flatness from where it is clear that our SGS model reproduces the SL value with the same accuracy, if not a bit higher, of the DNSx8 fully resolved data.

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![Figure 4](image-url) FIG. 4. Comparison of $\xi_4(r) / \xi_2(r)$ for (i) SGSM-smooth, (ii) Smagorinsky-LES and (iii) hyper-viscous simulations. In the latter the dissipative term is given by $\nu \Delta^2 \mathbf{u}$ with $\nu = 2.0 \cdot 10^{-8}$. All simulations are performed with $1024^3$ collocation points. The SL anomalous scaling and the K41 prediction are given by the solid and the dashed lines, respectively. The corresponding $F(r)$ is shown in the inset. Error bars are comparable to the ones shown in Fig. (3).
absorbing mechanism at small scales. At the same time, our model considerably outperforms other common closures such as the Smagorinsky model or DNS with hyper-viscous dissipation. Fully time-reversible models are also of theoretical interest, being natural candidates for a formally pure inertial closure and for the application of the chaotic hypothesis [39]. The main advantage of our SGS closure is that the phase dynamics is left untouched. Because of its generality, the closure can be applied to a broad set of other flow configurations such as rotating, stratified or MHD turbulence, including stiff problems as the kinematic dynamo in the limit of small Prandtl numbers [40], or to any wall bounded flow in the homogeneous directions.

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