RESOLUTION EFFECTS AND EXTREME EVENTS IN PETASCALE TURBULENCE SIMULATIONS

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EXECUTIVE SUMMARY

Substantial advances have occurred in both domain science and computing for fluid turbulence since access to the Blue Waters resource began. Recent analyses have focused on a critical examination of the effects of insufficient or limited resolution in both space and time for the study of intermittency, which often is expressed via intense but localized fluctuations. Two important indicators of the fine-scale turbulence structure are the dissipation rate and enstrophy (the integral of the vorticity), both of which tend to exhibit extreme events at thousands of the mean value or more. Recently, we have obtained a new understanding of how the probability distributions of these two variables compare, both of which are of stretched-exponential form but with different parameters. Further, we have obtained some data for short periods of time at resolutions beyond 1 trillion grid points.

RESEARCH CHALLENGE

Intermittency, or the occurrence of intense fluctuations localized in time and space, is a fundamental but still not well-understood property of turbulence at high Reynolds number that is used to help predict flow patterns in different fluid flow situations and arises in numerous fields of science and engineering [1]. For an intermittent flow variable, such as energy dissipation rate, a basic question is how large the fluctuations can be, with what likelihood, and whether the dependence on Reynolds number can be quantified reliably. In principle, reliable answers can be obtained from direct numerical simulations of the instantaneous turbulent flow in simplified geometries, such as periodic domains in three-dimensional space. While attaining a high Reynolds number is always desirable, theoretical models have also suggested a need to resolve the small scales better than is often practiced [2].

Although direct numerical simulations based on exact equations for the basic physical laws of conservation of mass and momentum are, in principle, closest to the truth, the physical fidelity of the results is sensitive to the effects of errors of a numerical or statistical nature. In addition, it is unavoidable that, in each given simulation, some statistics are highly accurate while others are less reliable. For example, high accuracy for extreme events in the energy dissipation rate are very difficult to achieve if the Reynolds number is to be at least moderately high. A critical examination of requirements for accuracy is also especially timely in the transition toward the next generation of multi-petaflop architectures.

METHODS & CODES

In our simulations we integrated the Navier–Stokes equations over a large number of timesteps using Fourier pseudospectral methods in space and finite differencing in time. The probability distribution of fluctuations of energy dissipation rate (quadratic measure of strain rates) and enstrophy (likewise, of the rotation rate), can be computed by postprocessing of large data sets archived on mass-storage systems, or calculated on the fly at many time-instants during the simulation. We have found the latter approach to be beneficial for the purpose of studying high-intensity, small-scale fluctuations that evolve on very short time scales. Besides computing the probability distribution, which can be averaged in time, we also extracted peak values (of intermittent variables), which serve as a simple diagnostic of how strong any extreme events can be.

If a particular quantity in a given simulation is significantly contaminated by numerical errors, it is expected to change substantially when a new and larger simulation at improved resolution is performed. However, before conducting a more expensive simulation with finer grid spacing or shorter timesteps, it is useful to first identify which quantities are more problematic. We have developed an approach to obtain this information by progressively filtering out spectral content at high wavenumbers where aliasing errors associated with nonlinear terms in the equations of motion may not be fully removed.

RESULTS & IMPACT

We have recently conducted a detailed study [3] of the effects of errors due to insufficient spatial and temporal resolutions using a combination of filtering and short simulations where statistics of dissipation and enstrophy are sampled very frequently. Although dissipation is less intermittent than the enstrophy, results show conclusively that, because of the role of incompressibility, dissipation is more sensitive to errors caused by insufficient or limited resolution. The expectation that higher resolution allows larger gradients (hence more intense dissipation and enstrophy) to be captured is clearly demonstrated only if the resolution in time is sufficiently good to suppress the influence of aliasing errors. Because of the advective nature of momentum transport, the proper measure of temporal resolution is not in terms of the time scales of the small-scale motion, but instead of the Courant number, which is usually interpreted as a criterion for numerical stability of the time-integration procedure.

The observation that dissipation is affected by resolution effects more than enstrophy suggests past statements [4,5] concerning comparative behaviors of extreme events in these quantities may require revision. In [3] we came to the conclusion that the probability density functions (PDFs) of these two variables do not coincide in the range where extreme events occur. However, these two PDFs do possess a remarkable degree of similarity, with both being well described by stretched-exponential fitting functions differing in only one parameter. This result is seen in Fig. 1, where the PDF of normalized enstrophy agrees very closely with that of twice the dissipation for reasons that can be investigated using the theory of multifractals [6]. Furthermore, a parallel investigation [7] suggests that the time scale of the extreme events in dissipation rate behaves similarly as a power law in the Reynolds number.

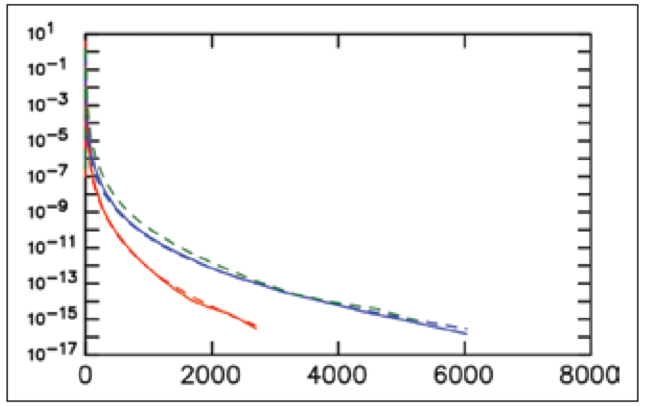

Figure 1: Probability density functions of normalized dissipation (red) and enstrophy (blue) in isotropic turbulence, at higher spatial and temporal resolution than in previous work. Dashed lines show very close fits with stretched exponentials. Line in green shows results for twice the dissipation.

WHY BLUE WATERS

The highest grid resolutions reported in [4,5,7] were all at the level of $8,192^3$. Although not included in our original project plans, we have also obtained some results at $12,288^3$ (which exceeds 1 trillion grid points) with good resolution in time. Further analyses are expected to lead to more publications.

PUBLICATIONS & DATA SETS

Yeung, P.K., X.M. Zhai, and K.R. Sreenivasan, Extreme events in computational turbulence. *Proceedings of the National Academy of Sciences*, 112 (2015), pp. 12633–12638.

Iyer, K.P., K.R. Sreenivasan, and P.K. Yeung, Reynolds number scaling of velocity increments in isotropic turbulence. *Physical Review E*, 95 (2017), p. 021101R.

Yeung, P.K., K.R. Sreenivasan, and S.B. Pope, Effects of finite spatial and temporal resolution on extreme events in direct numerical simulations of incompressible isotropic turbulence. *Physical Review Fluids*, 3 (2018), p. 064603.

Buaria, D., A. Pumir, E. Bodenschatz, and P.K. Yeung, Extreme velocity gradients in turbulent flows. Submitted to *Physical Review X* (2018).