

## COMPLEXITIES OF HIGH-REYNOLDS-NUMBER TURBULENCE

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### EXECUTIVE SUMMARY:

We study the complexities of turbulent fluid flow at high Reynolds number, where resolution of fluctuations over a wide range of scales requires sustained petascale computation. Using 262,144 cores of Blue Waters in a favorable node-topology configuration, we have performed the first 8,192<sup>3</sup> production simulation of isotropic turbulence (8,192<sup>3</sup> results in over half a trillion cells in the simulation). Both the dissipation rate and entropy, representing deformation and rotation of local fluid elements, take values as large as on the order of 10<sup>5</sup> times the mean at nearly the same locations in space. Regions of most extreme vorticity are not worm-like as commonly thought. These results have important implications for phenomena such as stretching of flame surfaces and preferential concentration of particles of finite inertia. An active algorithmic effort is under way to improve our ability to study the dispersion of tens of millions of fluid particles and other entities in a Lagrangian framework. Turbulent mixing at high Reynolds number will also be addressed.

### INTRODUCTION

Fluid motions in many fields of science and engineering are typically turbulent, with disorderly fluctuations over a range of scales. One of our fundamental objectives is to understand the nature of intense fluctuations that are highly localized in time and space, and to use this understanding to address the effects of fine-scale intermittency [1] in applications. For example, extremely high strain rate can break a flame surface and lead to local extinction, while high rotation rate has a strong influence on the local concentration of inertial particles and vapor droplets in multiphase flows and cloud physics problems. The likelihood and the intensity of large fluctuations increase with the range of scales present, which can be expressed as a positive power of a Reynolds number, defined as the product of turbulence velocity and length scales divided by the kinematic viscosity. The study of extreme fluctuations at the small scales in high-Reynolds-number turbulence is thus of great importance.

A very important effect of turbulence is enhanced mixing and dispersion of fluid elements of distinct properties or other entities such as heat, chemical species, and pollutants carried in the flow. Predictions of rates of mixing between fuel and oxygen in jet engines and the rate of growth of pollutant plumes in the environment depend on understanding of small-scale turbulence, sometimes coupled with other physico-chemical processes. Continuing work will mostly focus on studies of turbulent mixing and dispersion [2,3], including molecular diffusivity and (in part) in a reference frame moving with the flow. In most cases, quality data at high Reynolds number with proper resolution of the small scales in space are necessary for definitive answers [4].

### METHODS & RESULTS

The only technical approach capable of truly capturing extreme events localized in both time and space is direct numerical simulation (DNS) in which we solve exact equations for conservation of mass and momentum. Because of the focus on small scales, we consider isotropic turbulence on a 3D periodic domain. Although Fourier pseudo-spectral codes are communication intensive, the overall performance benefits substantially from remote memory addressing and favorable

network topologies. The first production simulation had 8,192 grid points in each direction (over half a trillion total points), at a Reynolds number slightly higher than recent work, and with better scale resolution as well.

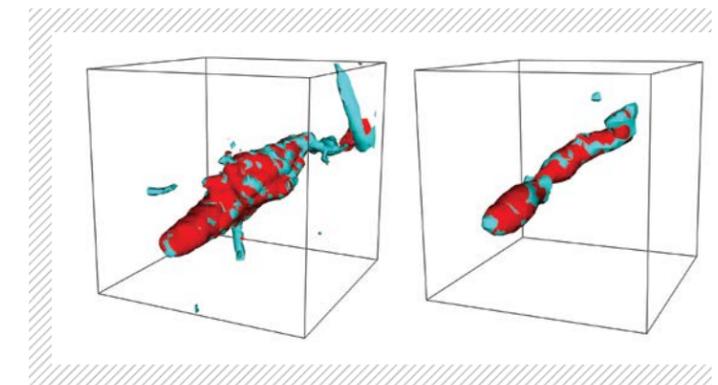
The new simulation data have been analyzed from probabilistic, spatial, and temporal viewpoints. Both dissipation and enstrophy (which are quadratic measures of local strain and rotation rates) exhibited values as large as 10<sup>5</sup> times the mean. This was well beyond that usually called intense in the literature, where high-dissipation regions are seen as sheet-like and high-enstrophy regions as filament- or worm-like. Extreme events at this intensity likely have a spatial structure different from those at moderately intense amplitude two to three orders of magnitude lower. Indeed, 3D visualization at various viewing resolutions and thresholds (fig. 1) showed that the most extreme events of high enstrophy appeared not as narrow filaments but instead as chunky, slightly elongated regions wrapped by curved sheets of almost equally intense dissipation (fig. 2). Numerous instantaneous snapshots of velocity fields supported a robust observation that peak values of dissipation and enstrophy were nearly coincident (one or two grid points apart). These extreme events apparently maintained their intensity for about two or three small-eddy time scales. The evolution of instantaneous enstrophy was also studied through an exact transport equation.

Our results to date suggest strongly that conventional descriptions of organized vortical motions should be revisited to truly account for the effects of extreme fluctuations in the present data (which may be only partly captured if the small scales are not as well resolved). Similar considerations for extreme dissipation are also central to much-needed improvements in the modeling of effects of intermittency in turbulent combustion, pollutant transport, and other problems. We note that although extreme events are inherently rare, they can have a first-order effect on physical phenomena of great concern to society (such as tornadoes, explosions, and extreme weather events).

### WHY BLUE WATERS?

In general, a 8,192<sup>3</sup> simulation is almost 16 times as expensive as one at 4,096<sup>3</sup>, but it is necessary since otherwise (as verified by numerical tests)

we would not be able to reach sufficiently high Reynolds number and sufficient small-scale resolution at the same time. A large allocation on a multi-petaflop computer such as Blue Waters is thus vital. We have also found high-quality and dedicated support through NSF's PRAC program to be essential. In particular, Cray personnel worked on remote memory addressing, and the Blue Waters staff made arrangements for reserved partitions of up to 8,192 nodes with favorable network topology to improve productivity and time to solution. Possible future targets on the next Track-1 system include simulations at similar rigor for turbulent flows subjected to other external influences such as buoyancy, solid-body rotation, or electromagnetic forces.



**FIGURE 2:**

Close-ups of sub-region inside the sub-domain in fig. 1, zoomed in to the most extreme values of dissipation (red) and enstrophy (cyan): (left) 51<sup>3</sup> viewing box at a threshold 300 times the mean, and (right) a 31<sup>3</sup> viewing box at a threshold 4,800 times the mean. The global maxima are located near the bottom left in both frames.

**FIGURE 1:**

Perspective view of 3D contour surfaces at ten times the mean value of dissipation (red) and enstrophy (cyan), in a 768<sup>3</sup> sub-domain extracted from an instantaneous snapshot of a 8,192<sup>3</sup> simulation. The intricate detail of small-scale turbulence is evident; many worm-like vortex filaments can be seen in cyan.

