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Advancing understanding of turbulence through extreme-scale computation[1]

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Since its beginnings in the early 1970s, direct numerical simulation of turbulence in canonical geometries has always been the computational approach that is physically the most accurate, a massive source of data, and a grand challenge in high-performance computing, whose definition has evolved by many orders of magnitude since then. In particular, challenges driving the need for ever-larger simulations on a 3D periodic domain include, to name a few, fine-scale intermittency at high Reynolds number with stringent resolution requirements, the mixing of a passive scalar of low molecular diffusivity, and the motion of fluid and inertial particles in a Lagrangian framework. Most known state-of-the-art simulations have employed massive CPU-based parallelism, which is ultimately limited by communication costs traceable to the multi-dimensional nature of the Navier-Stokes equations. However, current trends in pre-Exascale leadership computing are pointing to the growing importance of heterogeneous platforms, whose principal advantage is accelerated computation and whose full exploitation requires a new paradigm in code development. In this talk, we will discuss the major features of a new pseudo-spectral code which has been shown to scale satisfactorily up to a problem size of 18432^3 resolution on the currently world's fastest GPU-based "Summit" supercomputer located at the Department of Energy Oak Ridge National Laboratory. We show that new simulations at this resolution are enabling significant advancements in studies of small-scale turbulence, with emphasis on extreme events where fluctuations of energy dissipation rate and enstrophy (vorticity squared) can reach $O(10^3)$ times of the mean value or higher. We also discuss briefly how recent simulations at resolution 8192^3 or higher are contributing to progress in the study of turbulent mixing, for both passive and active scalars in non-unity Schmidt number regimes.

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