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On Cyber-enabled investigations of turbulent mixing and dispersion on a periodic domain[1]

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Direct numerical simulation (DNS) of homogeneous isotropic turbulence on a 3D periodic domain is an important benchmark problem in developments towards Petascale computing. Advanced cyberinfrastructure resources are expected to allow simulations using 12288^3 grid points by the year 2011. Subject to a careful choice of parameters and adherence to appropriate accuracy requirements, simulations of such size (or larger) can be expected to provide great opportunities for fundamental studies of turbulence, mixing, and dispersion, including the role of intermittency, viscous-convective scaling, Lagrangian Kolmogorov similarity, and Richardson scaling. However, as the problem sizes considered continue to grow, a number of highly nontrivial challenges arise. Effective use of $O(10^4)$ to $O(10^6)$ processors requires a highly scalable domain decomposition scheme with efficient interprocessor communication. Large volume I/O is very demanding on the system hardware and can become a new bottleneck especially for post-processing which is vital for contributions to physical understanding and science impact. In this talk we will discuss recent progress and experiences with a 2D domain decomposition scheme which has been tested to perform very well in both strong scaling and weak scaling up to 4096^3 on 32768 processors. We also make the case for developing collaborative strategies in making data and algorithms available to the research community, with help from leading supercomputer centers.

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