INTERMITTENCY, RESOLUTION EFFECTS AND HIGH SCHMIDT NUMBER MIXING IN TURBULENCE

Allocation: NSF PRAC/9,547.165 Knh
PI: P.K Yeung[1]
Collaborator: T. Gotoh[2]

[1]Georgia Institute of Technology
[2]Nagoya Institute of Technology, Japan

EXECUTIVE SUMMARY

Substantial advances have been made in both science and computing for fluid turbulence using Blue Waters. Simulations on grids of up to 4 trillion points show clear differences between energy dissipation rates averaged locally in three versus one dimension (the latter being common in the literature). Resolution effects on extreme events are examined critically using a multi-resolution approach. We have also developed a new algorithm for turbulent mixing at low diffusivity, where scalar fluctuations arise at scales much smaller than in the velocity field. We use a dual communicator approach where different groups of MPI processes compute the velocity and scalar field at different resolutions and using different numerical schemes. Through careful use of inter-communicator communication, as well as multithreading via nested OpenMP constructs, the code scales well up to 524,288 cores at close to six percent of theoretical peak performance.

RESEARCH CHALLENGE

Turbulent flows with disorderly fluctuations over a wide range of scales are an important agent of efficient mixing in many fields of science and engineering. An enduring challenge in the theory of this subject is to understand the nature of intermittency [1] in terms of fluctuations of the energy dissipation rate (a measure of local straining) and enstrophy (a measure of local rotation) over a wide range of domain sizes. Direct numerical simulations of the scale enabled by Blue Waters are the best source of data for this purpose, but the complexity of the flow physics requires a critical examination of the accuracy and reliability of the results. Accordingly, in addition to analyzing data from a 0.5-trillion-grid-points simulation [2] we have also performed a short simulation using as many as 4 trillion grid points. Massive datasets at this level allow us to investigate the effects of differences in the local averaging procedure as well as the effects of finite resolution.

A second focus area is the development and application of a new parallel algorithm that is uniquely suited to the study of turbulent mixing at high Schmidt number, where low molecular diffusivity leads to fluctuations at scales smaller than those in the velocity field. Our objective includes checking a scaling relation proposed in classical theory for which confirmation via either simulation or experiment has been limited by grid resolution and/or Schmidt number. Our new simulation uses a new dual-resolution parallel paradigm to make the calculation practical.

METHODS & CODES

Our technical approach is direct numerical simulation (DNS), which is based on exact physical laws and can be carried out efficiently in simplified geometries. We use Fourier pseudo-spectral methods for the velocity field, and perform local averaging both along a line (one dimension) and over a cube (three dimensions). To study resolution effects via filtering we apply successive truncations in wavenumber space before transforming to physical space coordinates. Results that differ greatly after truncation may indicate substantial errors.

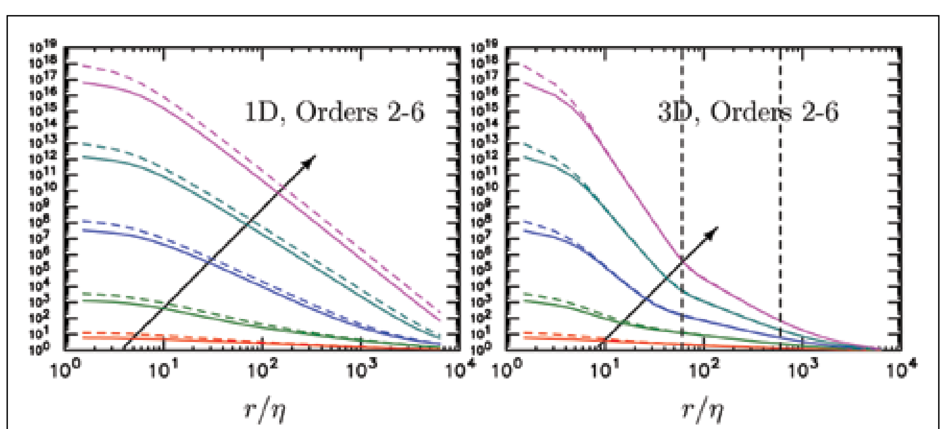

Figure 1: Moments of orders 2 to 6 (in direction of arrows) of normalized and locally averaged dissipation (solid lines) and enstrophy (dashed lines) versus scale size normalized by the Kolmogorov scale. Frames (a) and (b) show data obtained from 1D and 3D averages, respectively.

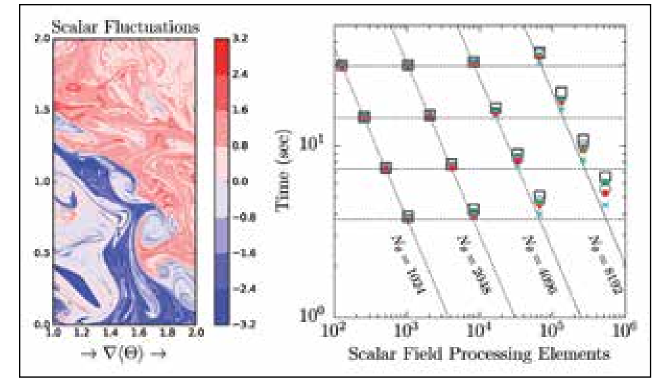

Figure 2: Left—Isocontours of normalized scalar fluctuations in a local region within a two-dimensional plane. Right—Scalability of scalar field computation for different grid resolutions using different versions of the CCD routines, from the baseline single-threaded nonoverlapped version (open squares) to the best version with dedicated communication threads (stars).

For high Schmidt number mixing we retain pseudo-spectral methods for the advecting velocity field but use combined compact finite differences (CCD) on a finer grid to satisfy stringent resolution requirements for the scalar [3]. We have devised a new dual-communicator parallel algorithm [4] where distinct groups of MPI parallel processes work on the velocity and scalar fields at different resolutions. This particular setup is less communication-intensive than full pseudo-spectral codes. Rigorous efforts have been made to improve performance by overlapping communication with computation. The best performance is obtained by dedicating one OpenMP thread to communication and dividing computational work among the other threads using nested OpenMP parallelism.

RESULTS & IMPACT

In the study of intermittency in high Reynolds number turbulence there is great interest in whether higher-order moments of the local averages of dissipation and enstrophy exhibit power law behaviors at intermediate scale sizes. Most past data in the literature were based on one-dimensional averaging, which is conceptually not ideal. Fig. 1 shows data on logarithmic scales with a clear scaling range (between the two vertical dashed lines) but only for averages taken in three dimensions, in a long simulation with $8,192^3$ grid points in each direction. Dissipation and enstrophy scale in the same manner, as well. A short simulation at an even higher resolution has further confirmed these results. The values of "scaling exponents" deduced from the data are helpful in allowing intermittency theories to be evaluated more definitively than in the past.

For turbulent mixing at high Schmidt number, Fig. 2 shows the delicate fine-scale structure of a scalar field at Schmidt number 512 (comparable to the salinity of the ocean), and the high scalability of the dual-communicator hybrid algorithm over a wide range of problem sizes and Cray XE6 core counts on Blue Waters. Careful observation aided by the color annotations in the figure suggests the presence of sharp interfaces where large fluctuations of the scalar gradients exist. In the right frame of Fig. 2, different symbols represent different coding implementations of the hybrid algorithm, differing mostly in the manner and degree in which overlapping between computation and communication is implemented. Horizontal and sloping lines indicate limits of perfect weak and strong scaling, respectively. At the largest problem size ($8,192^3$), strong scaling efficiency from 65,536 to 262,144 cores is as high as 94 percent. This highly scalable code enables studies of turbulent mixing in this previously unreachable Schmidt number regime.

WHY BLUE WATERS

The $8,192^3$ grid resolution of our production simulations requires access to a world-class machine such as Blue Waters, and the memory capacity of Blue Waters has enabled us to obtain data at 16,3843 resolution, the highest known worldwide in the turbulence community. Other important machine characteristics include support for Co-Array Fortran, topologically aware scheduling, and a large number of cores per node, which is conducive to nested OpenMP parallelism in our high-Schmidt-number algorithm.

PUBLICATIONS AND DATA SETS

Clay, M. P., Strained turbulence and low-diffusivity turbulent mixing. Ph.D. thesis, Georgia Institute of Technology (2017).

Clay, M. P., D. Buaria, T. Gotoh, and P. K. Yeung, A dual communicator dual grid-resolution algorithm for petascale simulations of turbulent mixing at high Schmidt number. *Computer Physics Communications*, in press (2017), DOI: 10.1016/j.cpc.2017.06.009).

Iyer, K. P., K. R. Sreenivasan, and P. K. Yeung, Reynolds number scaling of velocity increments in isotropic turbulence. *Physical Review E*, 95:2 (2017), DOI: 10.1103/PhysRevE.95.021101.

Yeung, P.K. Turbulence in fluid dynamics: the science, and the need for exascale. *First International Symposium on Research and Education for Computational Science*, Tokyo, Japan, November 29–30, 2016.