Extreme events, resolution and a new parallel algorithm for turbulent mixing on Blue Waters

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Disorderly fluctuations: unsteady, 3D, multiscale, nonlinear
  — prevalent in many fields of science and engineering
  — effective mixing (coupling with molecular diffusion)

Higher Reynolds no \( (UL/\nu) \): wider range of scales, more uncertainty, larger number of degrees of freedom; \( \Rightarrow \) more CPU power needed
A Two-Part Presentation

1. Extreme events and resolution effects in simulation of high Reynolds no. turbulence, on world-leading scale
   - Fundamentals of wide implication, despite idealized geometry
   - Fourier pseudo-spectral, benefits from favorable network topology
   - $8192^3$ and $16384^3$ grid resolution

2. Turbulent mixing at low molecular diffusivity, with novel algorithm that achieves 6% of peak on BW
   - A multi-resolution problem, suggesting hybrid approaches
   - Velocity on coarser grid, passive scalar on finer grid
   - Compact finite difference, nested OpenMP parallelism
Extreme Events and Turbulence

- High intensity, rare, localized in space and/or short-lived in time
- Fluid elements experiencing extreme local deformation
  - rate of strain (change in shape)
  - rate of rotation (change in orientation)
- Search for self-similarity: scaling exponents of dissipation rate are central in turbulence theory addressing fine-scale intermittency
- Very sensitive to Reynolds number, and more:
  - small-scale resolution and sampling are both important
- On Blue Waters: first $8192^3$ simulation of homogeneous isotropic turbulence on a periodic domain, focus on fundamental issues
- A short simulation at $16384^3$ has also been performed
The Computational Approach

- Direct numerical simulation (DNS): use exact equations of motion
  (Navier-Stokes; $\nabla \cdot u = 0$ for constant density)

\[
\frac{\partial u}{\partial t} + u \cdot \nabla u = -\nabla \left( \frac{p}{\rho} \right) + \nu \nabla^2 u + f
\]

- Fourier pseudo-spectral: high accuracy, but communication-intensive
  - massive parallelism: 2D (pencils) domain decomposition

- BW: MPI, Co-Array Fortran, $8192^3$ w/ favorable topology:
  - 8.897 secs/step on 262,144 cores; 30 secs on 65,536
  - I/O is usually fast: 4 TB in a minute or less
  - postprocessing and on-the-fly processing
  - VISIT for 3D scientific visualization

- To span several large-eddy time scales: $O(10^5)$ time steps
Intermittency and Local Averaging

- Dissipation rate and enstrophy as quadratic measures of local strain and rotation rates (vorticity):

\[ \epsilon \equiv 2\nu s_{ij} s_{ij} \quad ; \quad \Omega \equiv \omega_i \omega_i \]

- Kolmogorov (1941): averaged \( \langle \epsilon \rangle \) represents rate of energy transfer (cascade) from large scales to small scales

- Kolmogorov Refined Similarity (1962): average locally over a volume of space of linear dimension \( r \) at inertial (intermediate) scales

\[ \epsilon_r(x, t) = \frac{1}{\text{Vol}} \int_{\text{Vol}} \epsilon(x + r', t) \, dr' \]

- Although 3D averages are important, they are not often reported:
  - averaging along a line (1D) is much easier
  - 1D surrogate \( (\partial u/\partial x)^2 \) often used in experiments
  - DNS: also, nontrivial due to domain decomposition
At smallest scales, very large higher-order moments, such as $\langle (\epsilon_r/\langle \epsilon \rangle)^m \rangle \ (m > 1)$ are expected, as a result of intermittency and extreme events (Yeung et al. JFM 2012, PNAS 2015):

Data from high $Re 8192^3$ simulation: $\epsilon$ (solid) and $\Omega$ (dashed)

The importance of 3D averages: strong indication of an “inertial” scaling range around $60 \leq r/\eta \leq 600$; both $\epsilon$ and $\Omega$
Higher-order Scaling Exponents (Preliminary)

- Inertial: $\langle \epsilon_r^q \rangle / \langle \epsilon \rangle^q \propto (r/\eta)^{-\tau_q}$

- Find $\tau_q$: look for best fit of flat region for $\langle \epsilon_r^q \rangle / \langle \epsilon \rangle^q (r/\eta)^{\tau_q}$.

- Orders 2-6, 8192³ datasets
  0.23, 0.70, 1.40, 2.35, 3.40

  Close to Log-normal theory:
  $\tau_q = \mu q (q - 1)/2$
  0.23, 0.69, 1.38, 2.30, 3.45

- To compare with past 1D results (Sreenivasan & Antonia 1997)

- Same exponents for $\epsilon_r$ (solid) and $\Omega_r$ (dashed)
Are these results accurate and reliable?

8192³ DNS: a decent match in $Re$ for many experiments, but showing much more “extreme” fluctuations than in past literature.

How do we assess adequacy of small-scale resolution?

- Refine the grid spacing, run again with same physical parameters
  - perform a yet-larger simulation: expensive, may be unfeasible
  - comparisons contaminated by statistical variability

- Take existing dataset, coarsen grid spacing, compare the results
  - if discrepancies are small, then solution is accurate enough
  - can quantify, e.g. what fraction of extreme events would be missed if resolution were degraded
  - a post-processing task at modest cost, that allows us to isolate effects of truncation error from statistical sampling
Tests of accuracy, up to 16384$^3$

Compensated plots using same exponents as found for
(a) 8192$^3$ ensemble-averaged scaling of 3D averages, $k_{max}\eta \approx 2$
(b) single 16384$^3$ snapshot, by grid refinement, $k_{max}\eta \approx 3.8$
(c) filter from (b) to 8192$^3$ resolution, $k_{max}\eta \approx 1.9$

- $q = 6$
- $q = 4$
- $q = 2$

- Great variability at small $r$ (dominated by extreme events)
- But relatively robust scaling in inertial range
Why Blue Waters

- Turbulence as a Grand Challenge in Science:
  - unsteady, 3D, nonlinear, stochastic, wide range of scales
  - smaller simulations often compromised in physics or accuracy needed for applications where turbulence is the critical process

- Turbulence as a Grand Challenge in Computing:
  - first $4096^3$ simulation was performed in Japan (2002)
  - on BW: the first production $8192^3$ (16X more expensive)

- Would be impossible if not for BW:
  - very large resource allocation on multi-Pflop machine
  - dedicated and expert staff assistance (even late nights!)
  - generous storage capacity (2 PB)
Temperature or concentration fields in a turbulent flow
- Dynamically passive scalars governed by advection-diffusion equation
- The Schmidt number \((Sc = \nu/D)\) varies over a wide range
  - \(Sc\): \(O(0.01)\) liquid metals, \(O(1)\) gas-phase, \(O(1000)\) salinity in ocean

Low diffusivity is more difficult in both experiment and DNS
- Fluctuations arise at scales smaller than those in velocity field
- Fundamental differences in shape of spectrum, intermittency, etc.

A dual-resolution, dual-numerical-scheme code
- Velocity on coarser grid, scalar on finer grid
- Compact finite differences for scalar (Gotoh et al. JCP 2012)
- How do we design a parallel algorithm for best efficiency?
Computational Challenges: Range of Scales

Broad range of scales in scalar field at high $Sc$ (low diffusivity)

- Small scales for velocity field on the order of the Kolmogorov scale $\eta$
- Small scales in scalar field given by the Batchelor scale $\eta_B = \eta Sc^{-1/2}$

Figure: Scalar (left, $1024^3$) $Sc = 8$ and (middle, $8192^3$) $Sc = 512$ at $R_\lambda = 140$. 
Equations and Dual Numerical Scheme

- Velocity field on coarser grid: Navier-Stokes equations, via usual Fourier pseudo-spectral method (3D FFTs)
- Scalar fluctuations on finer grid (Gotoh et al., JCP 2012), with uniform mean scalar gradient:

\[
\frac{\partial \theta}{\partial t} + \mathbf{u} \cdot \nabla \theta = D \nabla^2 \theta - \mathbf{u} \cdot \nabla \langle \Theta \rangle
\]

- Eighth-order combined compact finite differences (Mahesh, JCP 1998)
- Computes first and second derivatives in all 3 directions
- Much less communication than typical FPS codes

Diagram:

- Velocity Field
- Interpolation
- Scalar Field
Algorithm for $Sc \gg 1$ on Blue Waters

Want high $Sc$, while ensuring accuracy at moderate Reynolds no.

- Velocity: $R_\lambda = 140, N_v = 1024, k_{max,v}\eta = 5.6$ (512 cores)
- Scalar: $Sc = 512, N_\theta = 8192, k_{max,\theta}\eta_B = 2.0$ (262,144 cores)

Use disjoint groups of processors for velocity and scalar fields

- To form advective term, send well-resolved velocity field to scalar communicator, and perform tricubic interpolation
- Overlap inter-communicator transfer with CCD operations on scalar
Scheme is implicit: all points along grid line coupled. Must solve linear system \( Ax = b \) for each grid line in all three coordinate directions.

To avoid memory transposes, adopt a static 3D domain decomposition:
- Implies that no processor ever has data in-core to solve CCD system
- Adopt parallel algorithm (Nihei et al.) to solve system

### Operation Summary

<table>
<thead>
<tr>
<th>Op.</th>
<th>Operation Summary</th>
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<tbody>
<tr>
<td>A</td>
<td>Fill ghost layers for scalar field with SEND and RECV operations</td>
</tr>
<tr>
<td>B</td>
<td>Form right-hand-side of linear system and obtain solution</td>
</tr>
<tr>
<td>C</td>
<td>Pack and distribute data for reduced system with MPI_ALLTOALL</td>
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<tr>
<td>D</td>
<td>Unpack data and solve reduced linear system</td>
</tr>
<tr>
<td>E</td>
<td>Pack and distribute data for final solution with MPI_ALLTOALL</td>
</tr>
<tr>
<td>F</td>
<td>Unpack data and finalize solution of CCD linear system</td>
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Operations for three coordinate directions are independent
- Try to overlap communication with computation
Overlapping Communication with Computation

Achieve overlap by interleaving communication and computation operations for all three coordinate directions in one subroutine.

1. Use non-blocking communication calls from MPI
   - Post communication call for next coordinate direction (e.g., $x_2$) before proceeding with computations for current direction (e.g., $x_1$)
   - Use MPI\_WAIT to ensure results are ready, when needed

2. Using dedicated communication threads in a MPI/OpenMP approach
   - Goal: one thread per NUMA domain to communicate, while others compute
   - Thread synchronization: use OpenMP locks
     - Use one lock for each coordinate direction
     - Thread must obtain lock for a given coordinate direction before doing work
   - Work-sharing the computations: use nested OpenMP parallelism
     - Initial comput. thread spawns nested parallel region to use rest of threads
     - Loops cannot be partitioned evenly: explore GUIDED and DYNAMIC scheduling
Using Dedicated Communication Threads

CALL OMP_SET_LOCK(x2)  CALL OMP_SET_LOCK(x3)

! Spin until the x1 lock is set.
test= .TRUE.
DO WHILE(test)
    test=OMP.TEST_LOCK(x1)
    IF (test) CALL OMP_UNSET_LOCK(x1)
END DO

COMMUNICATE x2 [A2]
CALL OMP_UNSET_LOCK(x2)

COMMUNICATE x3 [A3]
CALL OMP_UNSET_LOCK(x3)

CALL OMP_SET_LOCK(x1)
COMMUNICATE x1 [C1]
Figure: Scalability of scalar field computation using different versions of the CCD routines: □ single-threaded, blocking; △▽○ (2,4,8 threads) multi-threaded, blocking; ■ single-threaded, overlapped; ▲▼● multi-threaded, overlapped; ★ one dedicated communication thread per NUMA domain.
Spectrum of Passive Scalar at High Schmidt Number

- Theory predicts $k^{-1}$ in the viscous-convective range ($1/\eta \ll k \ll 1/\eta_B$).
- Kraichnan: exponential, not Gaussian (Batchelor), in diffusive range

$$E_\theta(k) = C_B \langle \chi \rangle (\langle \epsilon \rangle / \nu)^{-1/2} k^{-1} (1 + \sqrt{6} C_B k \eta_B) \exp(-\sqrt{6} C_B k \eta_B)$$

- Considerable scatter in $C_B$ (Donzis et al. FTC 2010, Gotoh et al. 2014)
Simulations of turbulence at $8192^3$ grid resolution conducted using PRAC allocation of BW resources:

- isotropic turbulence at high Reynolds number w/ good scale resolution
- study of turbulent dispersion under the same conditions (reported at BW Symposium last year)
- turbulent mixing at high Schmidt number, using a newly-developed advanced parallel algorithm (Clay et al. CPC 2017)

Ongoing and future work (re: PRAC renewal award)

- A penultimate Petascale computational turbulence laboratory
- Magnetohydrodynamic turbulence (at low magnetic Reynolds no.)