Petascale Simulation of High Reynolds Number Turbulence

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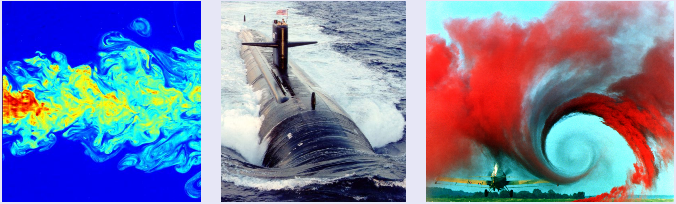
Introduction: Turbulence and Reynolds Number

Disorderly fluctuations: unsteady, 3D, multiscale, nonlinear
— and prevalent in many fields of science and engineering



(Images taken from Wikipedia page on Turbulence)

Higher Reynolds no (UL/ν): wider range of scales, more uncertainty, larger number of degrees of freedom; $\Longrightarrow$ more CPU power needed

Extreme Events and Turbulence

- High intensity, rare, localized in space and/or short-lived in time
  - strong enough to have first-order effects of importance (e.g., category-5 hurricane, F5 tornado, explosions)
- Turbulence: small scales are intermittent, fluid element may experience extreme local deformation
  - rate of strain (change in shape)
  - rate of rotation (change in orientation)

  Examples: flame surface breakup, cloud droplet clustering ...
- 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

Methods: Petascale DNS

- Direct numerical simulation: solve exact equations of motion (Navier-Stokes, with $\nabla\cdot\mathbf{u} = 0$ for incompressibility)

$$\partial\mathbf{u}/\partial t + \mathbf{u}\cdot\nabla\mathbf{u} = -\nabla(p/\rho) + \nu\nabla^2\mathbf{u} + \mathbf{f}$$

- Fourier pseudo-spectral: high accuracy, but communication-intensive (transposes in 2D 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

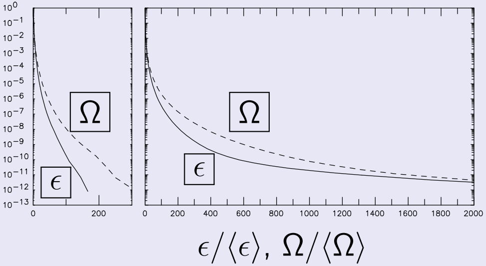
Dissipation and Enstrophy

- Dissipation: $\epsilon = 2\nu s_{ij} s_{ij}$, from strain rate $\mathbf{S} = (\nabla \mathbf{u} + \nabla \mathbf{u}^T)/2$
  - shape distortion of surfaces, spreading of pollutants
- Enstrophy: $\Omega = \vec{\omega} \cdot \vec{\omega}$ from vorticity $\vec{\omega} = \nabla \times \mathbf{u}$
  - vortical structure and swirling motions
- The basic questions, for high Reynolds number turbulence:
  - how intense, and how likely, are “extreme” fluctuations?
  - how do they form, evolve, and scale?
  - how do they affect turbulent mixing and dispersion?
- Require high Reynolds number, with small scales well resolved

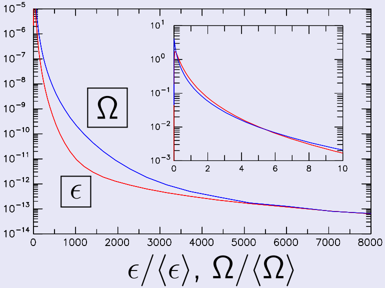
Likelihood: Probability Density Functions

- Low-probability extreme fluctuations seen in wide tails of PDF
- Long-standing question: is Ω more intermittent than ϵ? (both are measures of small scales, with different effects)

YDS JFM 2012, 4096^3, R_λ 240 & 1000



On BW: 8192^3, $R_\lambda \approx 1300$



- $R_\lambda \sim 400$ and up: far tails in the two PDFs almost coincide
- Tails stretch out wider yet if R_λ is higher

Spatial Structure: Local Averages

- Local averaging over a sub-volume of linear size $r \sim \mathcal{V}^{1/3}$:

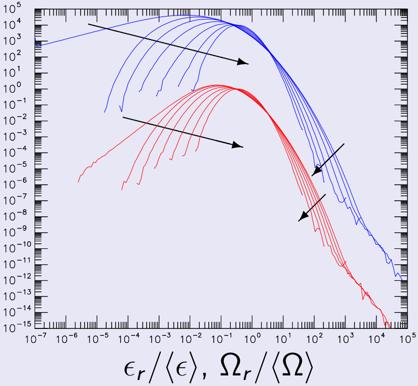
$$\epsilon_r = \frac{1}{\mathcal{V}} \iiint_{\mathcal{V}} \epsilon(\mathbf{x}') d\mathbf{x}'$$

  - $r \longrightarrow 0$: single-point fluctuation
  - $r \longrightarrow L_0$: global mean over domain of size L_0^3
  - Search for scale similarity: statistics as function of r? (the key to intermittency corrections for many classical results)

- Homogeneity in space: can sample ϵ_r and Ω_r anywhere. Same mean values for all r but moments and PDF vary $[\langle \epsilon^m \rangle \propto r^{-\mu_m}]$

Spatial Structure: Sub-Cubes

- 3D local averages from 2D decomposition:
  — subdivide within a pencil
  — merge from adjacent pencils
- Form PDF of averages over sub-cubes of 1, 2, 4, 8, 16, 32, 64 grid points in each direction



- Variability of ϵ_r and Ω_r drops as r increases (follow the arrows)
- Collapse onto power-law tail for smallest few sub-cube sizes (An indication that extreme events are localized in space)

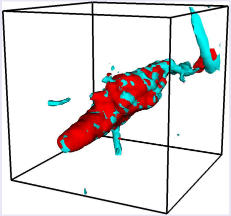
Spatial Structure: Visualization

- The challenge of intricate detail in massive turbulence datasets
  - 8192^3 image is hard to make, too much to look at
  - instead, focus on extreme events and their neighborhood (start by identifying grid-point location of peak ϵ and Ω)
  - raise contour thresholds while zooming in
- Conventional thought is that high intensity dissipation is in sheets while high enstrophy is in worm-like vortex filaments
  - does this hold for the truly extreme events where peak values of these variables appear to be co-located in space?

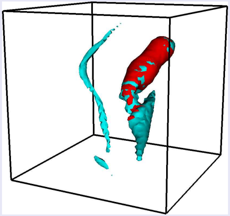
Zooming in neighborhoods of peak ϵ and Ω [Video]

Multiple snapshots and Reynolds no. dependence

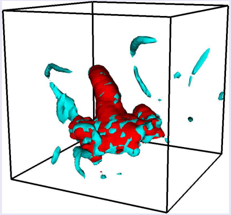
$R_\lambda \sim 1300$, #1



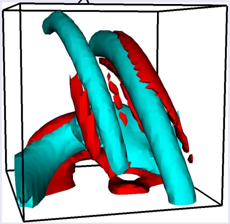
$R_\lambda \sim 1300$, #2



$R_\lambda \sim 1300$, #3



$R_\lambda \sim 390$



$R_\lambda \sim 1000$ is characteristically different from $R_\lambda \sim 390$

Temporal Evolution

Characterize/understand temporal properties of extreme events in several different ways:

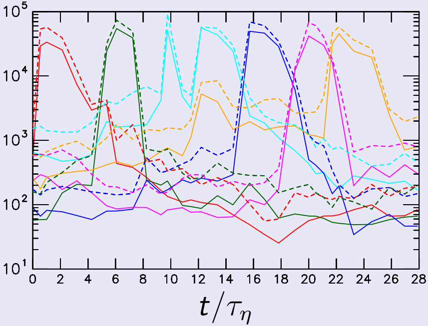
- Time history of the local maxima of $\epsilon/\langle\epsilon\rangle$ and $\Omega/\langle\Omega\rangle$ in subcubes each identified with at least one extreme event:
    - how long do they last (by some criterion)?
- Focus on one specific event, observe via visualization the processes of production/growth, transport, eventual dissipation
- Individual terms in instantaneous enstrophy budget equation:

$$\frac{\partial\Omega}{\partial t} = -\frac{\partial u_j\Omega}{\partial x_j} + \nu\frac{\partial^2\Omega}{\partial x_j\partial x_j} + 2\omega_i\omega_j s_{ij} - 2\nu\frac{\partial\omega_i}{\partial x_j}\frac{\partial\omega_i}{\partial x_j}$$

Temporal Evolution: Time Traces

Each pair of lines (solid for ϵ, dashed for Ω) represent time history of one extreme event

- Phases of generation, sustenance, decay
- Lifetime above threshold 1000: approx 5 $\tau_\eta = (\nu/\langle\epsilon\rangle)^{1/2}$
- All extreme events remain above 50 for approx 30 τ_η



Life History of Extreme Event(s) [Video]

What is new, is it robust

- In all (> 30) 8192^3 snapshots examined, peak ϵ and Ω are over 10^4 times the mean, within one grid spacing apart
— extreme events in both scale together, occur together
- In contrast to classical notions, extreme events in enstrophy (vorticity) not worm-like, but "chunky" in appearance
— vs more filament-like at lower R_λ or lower thresholds
- Effects of resolution, statistical sampling, and machine precision?
  - improved resolution captures extreme events better
  - fast-changing events: more frequent sampling helpful
  - differences between single vs double precision appear minimal

— Manuscript to be submitted to *Proc. Nat. Acad. Sci.* —

Implications of This Work (So Far)

- A new body of fundamental data unsurpassed in accuracy and detail for high Reynolds number turbulence
  - conventional descriptions of organized vortical motions should be revisited, to account for extreme events
  - long simulations vs. shorter simulations with frequent sampling
- New knowledge of extreme dissipation rate fluctuations will enable advances in theories of fine-scale intermittency
  - e.g. in turbulent combustion and pollutant dispersion, which are both problems of wide societal impact
- Experience in facing challenges in Petascale computing + data

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, on BW:
  - very large resource allocation on multi-Pflop machine
  - dedicated and expert staff assistance (even late nights!)
  - generous storage capacity (now 0.5 PB, will need yet more)

Plans: Lagrangian Intermittency and Dispersion

- Lagrangian viewpoint following infinitesimal fluid elements
  - dispersion of pollutants, cloud/vapor droplets, particulates, etc
  - difficult to measure; easier in DNS (Yeung, ARFM 2002)
- Acceleration of "fluid particle" depends heavily on local velocity gradients: effects of high strain rate vs rotation rate
- Backward tracking: find out whether the pollutants came from.
  - relative motion of 2,3,4 particles at some given distance apart
  - as a major postprocessing task, since N-S irreversible in time
- Current status: making progress on improving scalability of particle tracking applied to $O(10^8)$ particles

Plans: Turbulent Mixing and Molecular Diffusivity

- Fluctuations of temperature, species concentration, and other properties transported by the turbulent flow
    - simple demo: stirring in a cup (uniformity comes quickly)
    - small-scale phenomenon, big impact in industrial processes
- Coupling between turbulent transport and molecular diffusion:
    - Schmidt number $Sc \equiv \nu/D$: $O(0.01)$ for liquid metals, $O(1)$ for most gases, $O(1000)$ in some liquids
    - may require smaller Δt (if $Sc \ll 1$) or smaller Δx (if $Sc \gg 1$)
- Consider coupling with density stratification (in environment), intermittency of scalar dissipation rate (in combustion), etc.

Concluding Remarks

- A large PRAC allocation of Blue Waters resources has made possible a half-trillion-points numerical simulation of turbulence at high Reynolds number and good scale resolution
- New physical insights obtained in studies of extreme events associated with fine-scale intermittency
- Next target: understand turbulent mixing and dispersion via forward and backward tracking at high Reynolds nuumber
- Long-term: flows with more complex physics, such as anisotropy due to Coriolis and electromagnetic forces