Resolution Effects and Local Averaging in Turbulence Simulations up to 4 Trillion Grid Points

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Turbulence? Since the days of Leonardo da Vinci

(A Picture is Worth A Thousand Words)
Disorderly fluctuations over a wide range of scales

- Pervasive in many branches of science and engineering
- Reynolds number: a measure of the range of scales
- Numerical simulation often best source for detailed information

A Grand Challenge problem in computing

- Flow is 3D: domain decomposition, and communication-intensive
- Every step-up in problem size: 8X in number of grid points

Some notable references in the field:

- Kaneda et al. PoF 2003: $4096^3$, on Earth Simulator
- Yeung, Zhai & Sreenivasan PNAS 2015: $8192^3$, on Blue Waters
- Ishihara et al. PRF 2016: $12288^3$, on K Computer
Some Fundamental Questions

- Intermittency at high Reynolds number
  - How large/extreme fluctuations can be, and how likely?
  - How high a Reynolds number is high enough? For what purpose?
  - In both space and time

- Turbulent mixing and dispersion
  - How do things far apart come together? Or spread around?
  - Does molecular diffusivity matter, and to what extent?

- Turbulence in broader contexts, both natural and man-made:
  - Combustion: how does mixing interact with the chemistry?
  - The oceans: how are heat and salinity coupled to the flow?
  - etc., etc.

Some understanding of these questions is necessary in the design of improved engineering devices and responses to natural disasters, say.
Forced isotropic turbulence, $R_\lambda$ up to 1300; various resolutions

- Largest production run at $8192^3$, using 262,144 parallel processes
- Some shorter (yet arduous) runs at $12288^3$ and $16384^3$ (4 trillion)
- Hundreds of millions of core hours, 2.5 PB Nearline storage

Topics and Publications (to date):

- Extreme events (Y, Zhai & Sreenivasan PNAS 2015)
- Velocity increments and similarity (Iyer, S & Y, PRE 2015, 2017)
- Nested OpenMP for low-diffusivity mixing (Clay, et al. CPC 2017)
- Highly scalable particle tracking (Buaria & Y, CPC 2017)
- Resolution and extreme events (Y, S & Pope, PRF 2018)
Sources of errors and uncertainties in DNS:

- Resolution in space: requires $\Delta x/\eta \leq 1$?
- Resolution in time: is Courant number $< 1$ small enough?
- Aliasing errors due to nonlinear terms in Navier-Stokes equations
- Statistical: average over independent trials when possible

Can a simulation at higher resolution resolve any doubts?

- Higher moments, extreme fluctuations inherently more sensitive
- An expensive proposition, may have to be short
- Small scales most sensitive, but they have short time scales — hence shorter test runs may well suffice
Spatial Resolution in Pseudo-Spectral DNS

\[ k_{\text{max}} = \sqrt{2}N/3; \quad \Delta x/\eta \approx 2.96/(k_{\text{max}}\eta) \]

- \( k_{\text{max}}\eta \approx 1.5 \) may be fine for low-order velocity statistics

- But better resolution needed for small-scale statistics, especially at high Reynolds numbers (Yakhot & Sreenivasan 2005)

- Refine the grid, run again at same \( Re \), and compare (e.g. acceleration statistics, Yeung \textit{et al.} PoF 2006)

- For a given snapshot, what features may be less reliable?
  - Take best-resolved velocity field, truncate at some wavenumber \( k_c \). Compute various statistics again, compare, and repeat
  - Large differences would indicate insufficient accuracy
  - A post-processing task, not a large new simulation — but, no information on global error after N-S time evolution
Temporal Resolution

- Courant number constraint for numerical stability:

\[
C = \left[ \frac{|u| \Delta t}{\Delta x} + \frac{|v| \Delta t}{\Delta y} + \frac{|w| \Delta t}{\Delta z} \right]_{\max} \sim \alpha \frac{u' \Delta t}{\Delta x}
\]

- Classical scaling and our experience in the simulations (take \(\alpha = 12\))

\[
\Delta t/\tau_\eta \approx (C/12)(15)^{1/4}(\Delta x/\eta) \ R_\lambda^{-1/2}
\]

- \(\Delta t/\tau_\eta\) often well under 1%: much less than \(\Delta x/\eta\) (which is \(O(1)\))

- But there are time scales smaller than \(\tau_\eta\) in the simulations
  - \(\eta/u'\): advection of small scales by large scales (Tennekes 1975)
  - \(\Delta x/u'\): advection over 1 grid spacing (re: Courant number)

- Short tests (approx 10 \(\tau_\eta\), say) at \(C = 0.6, 0.3, 0.15\) can help.
  - three spatial resolutions; \(R_\lambda\) 390, 650 (easier than for \(R_\lambda\) 1300 ...)

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Resolution and Local Averaging
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\[ \epsilon \equiv 2\nu s_{ij} s_{ij} ; \quad \Omega \equiv \omega_i \omega_i \]

- Quadratic measures of local rates of strain and rotation of fluid elements subjected to disorder in turbulence
  - symmetric and anti-symmetric parts of velocity gradient tensor
- High strain rate: dispersion, breakup of flame surfaces
- High rotation rate: vortex filaments, preferential concentrations
- Fluctuations of \( \epsilon \) vital in theories of intermittency (Kolmogorov 1962)
  - properties of local averages over 3D region of linear size \( r \), with \( r \) varied through dissipative and inertial ranges
  - larger fluctuations expected at higher Reynolds numbers
- Homogeneous turbulence: \( \langle \epsilon \rangle = \nu \langle \Omega \rangle \), but higher moments differ
Dissipation and Enstrophy: PDFs and Spatial Filtering

- Enstrophy is more intermittent. But dissipation is more sensitive
- \( R_\lambda \) 650, \( k_{\text{max}} \eta = 2.8 \) \((4096^3)\); cutoff at \( k_c/k_{\text{max}} = 1, 0.75, 0.5 \)

Far (power-law like) tails due to high \( k \) modes, affected by aliasing

Better spatial resolution: similar issue, pushed to larger amplitudes
Resolution in time: Peak dissipation and enstrophy

\[ R_\lambda \sim 650, \ C = 0.6, 0.3, 0.15; \ \epsilon/\langle \epsilon \rangle \text{ and } \Omega/\langle \Omega \rangle \text{ vs. } t/\tau_\eta \]

- \[ k_{max} \eta \approx 1.3 \]
- \[ k_{max} \eta \approx 2.7 \]
- \[ k_{max} \eta \approx 5.4 \]

- \( C = 0.6 \) gives spuriously large peaks; 0.3 and 0.15 almost the same
- Sensitivity greater for \( \epsilon/\langle \epsilon \rangle \), consistent with effects of filtering
Resolution in space: Peak dissipation and enstrophy

\[ R_\lambda \sim 650, \ k_{\text{max}} \eta = 1.3, 2.7, 5.4; \ \epsilon/\langle \epsilon \rangle \ \text{and} \ \Omega/\langle \Omega \rangle \ \text{vs.} \ t/\tau_\eta \]

- At \( C = 0.6 \): impact of using higher \( k_{\text{max}} \eta \) is somewhat erratic
- \( C = 0.3 \) or lower: \( k_{\text{max}} \eta \) at 5.4 captures larger gradients
$C = 0.15, \ k_{max} \eta \approx 1.3 \ 2.7 \ 5.4$: Convergence apparently achieved

$R_\lambda \sim 390$

$R_\lambda \sim 650$

Tails stretch out further: as $R_\lambda$ increases, and $\Omega$ relative to $\epsilon$
Compare dissipation and enstrophy PDFs again

Best data at $C = 0.15$ (RK2), $k_{\text{max}} \eta \approx 5.4$: tails do not coincide, but the two PDFs have a strong similarity in shape ("stretched exponentials")

$$f_\epsilon (\epsilon/\langle \epsilon \rangle) \sim \exp[-b_\epsilon (\epsilon/\langle \epsilon \rangle)^{\gamma_\epsilon}]; \quad f_\Omega (\Omega/\langle \Omega \rangle) \sim \exp[-b_\Omega (\Omega/\langle \Omega \rangle)^{\gamma_\Omega}]$$

- Very good fit with $\gamma_\epsilon = \gamma_\Omega$ (dashed lines); $b_\epsilon > b_\Omega$
- Green dashed line is PDF of $2\epsilon/\langle \epsilon \rangle$
- Explanations may be possible using multi-fractal theory

$R_\lambda \sim 390$

$R_\lambda \sim 650$
\( R_\lambda \approx 1300: \) Need to go beyond \( 8192^3 \)

8192\(^3\), \( C = 0.6, \Delta x/\eta \approx 1.5 \)
(YZS, PNAS 2015)

12288\(^3\), \( C = 0.3, \Delta x/\eta \approx 1 \)
(D. Buaria, 95% holiday disc. on BW)

- Insufficient accuracy in time can lead to over-estimation of likelihood and intensity of extreme events (affected by aliasing errors)
- What about inertial range statistics, averaged over regions of linear size \( \eta \ll r \ll L \) (expecting some smoothing in space)?
Kolmogorov Refined Similarity (1962): replace $\langle \epsilon \rangle$ in inertial range formulas at scale size $r$ by a local volume average

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

3D averages are important, but 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, only recently available (Iyer 2014)

Inertial Range (intermediate scales):
- $\langle \epsilon_r^q \rangle / \langle \epsilon \rangle^q \propto (r/\eta)^{-\tau_q}$ for orders $q = 2, 4, 6\ldots$
- Find $\tau_q$: look for best fit of flat region for $\langle \epsilon_r^q \rangle / \langle \epsilon \rangle^q (r/\eta)^{\tau_q}$
- Exponents provide useful test of intermittency theories
Scaling Exponents

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

$q = 6$

$q = 4$

$q = 2$

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

A measure of rotation in fluid flow
- Line integral of velocity vector along a closed path $C$, equivalent to integral of vorticity ($\omega \equiv \nabla \times u$) around the enclosed area
  \[ \Gamma = \oint_C u \cdot ds = \iint_A \omega \cdot n \, dA \]
- Aerodynamics: circulation proportional to lift force
- Turbulence: spatial structure of vorticity field

What do we know about circulation in turbulence?
- Not so much — not a directly measurable quantity
- Theory — perhaps shape of closed path plays only a minor role?
- Vorticity is highly intermittent, but integration weakens this property
- DNS results show only very weak intermittency at intermediate scales (and a low sensitivity to numerical errors)
Concluding Remarks I: BW and Turbulence

An exciting journey, some eventful moments, but very rewarding:

- High-resolution simulations allowed us to address difficult questions
- Learned some lessons, but perhaps that is how science is done (?)
- A serious ramp-up in publication activity is under way
NSF infrastructure investments have had huge impact:

- Computational science as pursuit of scientific inquiry using computational methods and resources not imaginable before
- The meaning of “massive parallelism” changing over time, while researchers were challenged, and helped, to dream on ...
- Massive datasets, and gains in human resource development

As we look towards the “next Blue Waters”:

- Recent architectural trends demand a change in paradigm for many (turbulence or not), and willingness to take risks
- The need for computational resources knows no boundaries in regard to discipline, nor the fundamental or applied debate
- Greater support needed for data and software repositories, as well as algorithmic development (often involving much risk!)