High-Resolution Simulations of Turbulence: 
intermittency, mixing, and dispersion

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The meaning of “High-Resolution”

**Size of computation** ($\sim N^3$ grid, for isotropic turbulence):
- 128$^3$ in 1980’s; 512$^3$ in 1990’s; 2048$^3$ in 2000’s

**Using state-of-the-art cyberinfrastructure:**
- Thousands (or tens of thousands) of processors
- Petascale computing power to come by 2010...

**Are the smallest scales resolved sufficiently well?**
- (The answer depends..)
Direct Numerical Simulation (DNS)

- 3-D incompressible Navier-Stokes equations for conservation of mass and momentum:

\[
\frac{\partial u_i}{\partial x_i} = 0 \\
\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_j \partial x_j}
\]

(And chemical species or heat)

- For fundamental understanding (canonical flows)

- For model development (share the data)
DNS: scales and requirements

To resolve full range of scales in space and time:
- size of domain $L_0 > L$ (largest length scale)
- grid spacing $\Delta x \lesssim \eta$ (Kolmogorov length scale)
- length of simulation $T \gg T_E$ (large-eddy time scale)
- time step $\Delta t < \tau_\eta$ (Kolmogorov time scale), further subjected to numerical stability constraints

Basic estimates for DNS at high Reynolds number:

$$N^3 \sim (L/\eta)^3 \sim Re^{9/4} \quad \text{and} \quad T_E/\tau_\eta \sim Re^{1/2}$$

- Fourier pseudo-spectral in space (FFTs), 2nd order in time
Historical Evolution of Computers and DNS

Adapted from NRC Report
Figure originally by K.R. Sreenivasan (1999)

- DNS now gives Reynolds no. comparable to or higher than in many laboratory experiments
- And can offer more (tremendous detail, quantities difficult to measure)
Some Questions and Issues

- **Intermittency at the Small Scales:**
  - Do dissipation and enstrophy scale the same at high $Re$?
  - Resolution effects on higher-order moments

- **Mixing of passive scalars:**
  - Do deviations from local isotropy persist at high $Re$?
  - Schmidt number ($Sc = \nu / D$) effects, over a wide range

- **Dispersion in a Lagrangian frame:**
  - How can we incorporate intermittency in stochastic modeling intended for high Reynolds numbers?
  - Statistics conditioned on local relative motion
Our work on High-resolution DNS

- **Stationary, isotropic turbulence:**
  - idealized geometry, with numerical forcing
  - yet justified by at least approximate small-scale universality (Kolmogorov 1941)

- Three $2048^3$ simulations using large CPU allocations at:
  - NERSC facility at Lawrence Berkeley (DOE: INCITE)
  - San Diego Supercomputer Center (NSF)
  - Pittsburgh Supercomputing Center (NSF)

- Code development and benchmarking for future $4096^3$
  (IBM BGW, 32k processors)
Intermittency at the Small Scales

- Intense fluctuations localized in space and time
  (topology of such regions in space is of interest)

- Structure functions and scaling exponents
  at viscous and inertial scales

- **Non-Gaussian statistics**: higher-order moments and
  far tails of PDF (subject to resolution and sampling)

- Statistics of local box averages (Kolmogorov 1962) and
  multifractal properties
Dissipation and enstrophy

- Second-order invariants of strain-rate and rotation-rate

\[ \epsilon = 2\nu s_{ij}s_{ij} \text{ vs. } \zeta = \omega_i\omega_i \]

- Fluctuations of \( \epsilon \) are responsible for:
  - anomalous scaling of velocity structure functions
  - intermittency corrections to inertial-range spectrum

- Most data sources show enstrophy to be more intermittent
  - but theories suggest same scaling in high-\( Re \) limit
Effects of Resolution

Most simulations in literature aim at high $Re$ (large $L/\eta$)
- usual criterion is $k_{max}\eta = 1.5$ which gives $\Delta x/\eta \approx 2$
- analytic behavior $r^m$ (at small $r$) often not well achieved in structure functions of higher order $m$

Under-resolution tends to miss extreme, localized events:
- does underestimation of high-order moments affect conclusion on “same scaling at high $Re$” for $\epsilon$ and $\zeta$?

Yakhot & Sreenivasan (2005) suggests a need for smaller $\Delta x/\eta$ (or higher $k_{max}\eta$) than in usual practice
Dissipation vs Enstrophy: Effect of Reynolds no.

- Same mean value, but larger higher moments for enstrophy

- **Tails of the PDFs:**
  - stretched-exponential fit, e.g.
  
  \[
  f_\epsilon \sim \exp[-\alpha (\epsilon/\langle \epsilon \rangle)^\beta]
  \]

  - better than log-normal theory

- **Stretched-exponential parameters** versus Reynolds number: is there an asymptotic trend?

PDFs of $\epsilon/\langle \epsilon \rangle$ and $\zeta/\langle \zeta \rangle$

$R_\lambda \sim 140 \ (256^3)$ and $700 \ (2048^3)$

\[
\begin{align*}
\epsilon/\langle \epsilon \rangle, \text{ etc.}
\end{align*}
\]
Dissipation vs Enstrophy: Moments and Resolution

Three simulations at $R_{\lambda} 140$, on $256^3$, $512^3$ and $2048^3$ ($k_{max} \eta \sim 1.5, 3, 12$)

Higher-order moments are underestimated at $k_{max} \eta \sim 1.5$, but $k_{max} \eta \sim 3$ ($\Delta x \approx \eta$) seems to be sufficient up to order 4.

Ratios of moments of $\epsilon$ and $\zeta$ show less sensitivity
Mixing of Passive Scalars

Schmidt number, $Sc \equiv \nu/D$ of “scalar” varies:
- 0.7 for heat in air, $O(1)$ for gaseous flames
- 7 for heat and salinity in water, $O(10^3)$ in some liquids

Weakly diffusive regime ($Sc \gg 1$) is more difficult:
- fluctuations arise at smaller scales than velocity field
- resolve Batchelor scale $\eta_B = \eta S c^{-1/2}$, at expense of $Re$

Some engineering literature use the Peclet no. $Pe = Re Sc$, but effects of increasing Reynolds no. and increasing Schmidt no. are different
Inertial-convective range at high Reynolds no. 2048³, at $R_\lambda \sim 700$ (higher than needed for velocity field)

$$E_\phi(k) = C_{OC} \langle \chi \rangle \langle \epsilon \rangle^{-1/3} k^{-5/3}$$

$$\langle \Delta_r u (\Delta_r \phi)^2 \rangle = -(2/3) \langle \chi \rangle r$$

Clear demonstration of both Obukhov-Corrsin scaling and Yaglom relation, better than in the past, and consistent with experiment
Scalar Gradients: Local Anisotropy

Component along mean gradient has positive skewness factor

Increasing $R_\lambda$ at $Sc \lesssim 1$

![Graph 1](image1)

Increasing $Sc$ at Low $R_\lambda$

![Graph 2](image2)

- **High $Re$**: local anisotropy is sustained (contrast to velocity)
- **High $Sc$**: return to local isotropy (beyond threshold depending on $Re$)
Scalar Gradients: Intermittency

PDF of component along mean gradient

Increasing $R_\lambda$ at $Sc = 1$

Increasing $Sc$ at $R_\lambda \sim 140$

$\nabla_\parallel \phi / \langle (\nabla_\parallel \phi)^2 \rangle^{1/2}$

- **High $Re$:** increasing intermittency (more than velocity field)
- **High $Sc$:** saturation of intermittency occurs beyond $Sc = O(4)$
Energy and Scalar Dissipation Rates

\[ \varepsilon = 2\nu s_{ij}s_{ij} \quad R_\lambda \approx 700 (2048^3) \quad \chi = 2D(\partial\phi/\partial x_i)^2 \]

Scalar dissipation has higher peaks, and is more intermittent
3D visualization

Energy dissipation ($\varepsilon$) \[ R_\lambda \sim 160 \ (256^3) \] Scalar dissipation ($\chi$)

High activity topology: filaments ($\varepsilon$) and sheet-like structures ($\chi$)
Dispersion: Lagrangian viewpoint

- Lagrangian frame: observer moving with the fluid
- Pollutant “cloud”: position, linear size, surface area, volume via motions of fluid particles singly and up to four
- DNS gives full instantaneous velocity field, hence can provide much more comprehensive data than experiment
- Inertial-range similarity more difficult than for Eulerian statistics, because range of time scales increase more slowly
- Reynolds number dependence is very important for use of data in stochastic modeling
Statistics of the Acceleration

\[ a_0 = \frac{1}{3} \frac{\langle a_i a_i \rangle}{\langle \epsilon \rangle^{3/2} \nu^{-1/2}} \]

- \( \frac{d\mathbf{u}^+}{dt} \) (Lagrangian) force/mass (Eulerian)
- Modeling: model the acceleration, recover velocity and position by integration
- Variance \( \langle a^2 \rangle \) departs from Kolmogorov universality
- Highly intermittent, closely related to local relative motion (strain or rotation)

From Sawford et al. Phys. Fluids 2003
Solid: our data+Gotoh. Open: experiments.
Lagrangian conditional statistics

Conditional velocity autocorrelation

\[ \rho(\tau; u|Z) \equiv \frac{\langle u^+(t)u^+(t+\tau)|Z^+(t) = Z \rangle}{\langle u^2|Z \rangle} \]

- In regions of large velocity gradients:
  - \( u^+ \) decorrelates faster, while \( |a^+| \) gets large

- Statistics conditioned on local “pseudo-dissipation”
  \[ \varphi = \nu (\partial u_i / \partial x_j)^2 \]
  - captures both strain and rotation
  - \( \ln \varphi \) is almost a Gaussian process
  - conditional acceleration is less intermittent
Flow structure: conditioning on enstrophy

- Analyses in local axes $\parallel$ and $\perp$ to vorticity vector suggest behavior for large $\zeta$ at low $R_\lambda$ is an indication of “vortex-trapping” effects.
- **High $R_\lambda$:** effect is weak because of rapid changes in vorticity vector orientation.
Algorithms and Data Structure

Slabs ("1-D decomposition")

- MPI_ALLTOALL communication for transposes
- No. of processors must be integer factor of $N$

Pencils ("2-D decomposition")

- More communication calls, but among fewer processors
- Scales better for larger problems; necessary for $4096^3$
Performance Measures

IBM SP Power 4 at SDSC and Blue-Gene W at IBM Watson

<table>
<thead>
<tr>
<th>Machine</th>
<th>SP4 (1D)</th>
<th>BGW (2D)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Problem size</td>
<td>$2048^3$</td>
<td>$4096^3$</td>
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<tr>
<td>No. of procs.</td>
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<td>2048</td>
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<td>CPU/step/proc</td>
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<tr>
<td>Mflop/s/proc</td>
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<td>490</td>
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<tr>
<td>Aggreg. Tflop/s</td>
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<td>1.0</td>
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<tr>
<td>Mem/proc(Mb)</td>
<td>233</td>
<td>1410</td>
</tr>
</tbody>
</table>

- Perfect scaling would be $\text{CPU} \propto N^3 \ln_2 N/\text{PROCS}$
- **Weak scaling (vary $N$):** excellent, $> 100\%$ in some cases
- **Strong scaling (vary PROCS):** very good, 86$\%$ between 16 and 32 K procs for $4096^3$
Outlook: our database

Large database achieved for:
- highest $Re$ for passive scalars and Lagrangian statistics
- highest $Sc$ for scalars at low/moderate $Re$

Potential for many fields of study:
- reacting flows: intermittency, differential diffusion
- droplet dynamics, zooplankton behavior
- subgrid modeling, wavelet analyses, cosmology ...

Maintain the data, and share with the community
Outlook: future computations

- $4096^3$ and higher: towards Petascale computing
- Simulations to resolve small scales better
- Simulations to sample large scales better
- Active scalars: reacting flow, thermal stratification
- Lagrangian statistics in more complex flows:
  - homogeneous shear, fully-developed channel