Fluid **Turbulence** and Mixing at High Reynolds Number

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- NERSC (INCITE computer time and consultant support)
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- Collaborators: K.R. Sreenivasan (Univ. Maryland, & Director, ICTP, Italy)
  R.O. Fox (Iowa State Univ. + DoE Ames Lab)

Fluid Mechanics and Turbulence

- We are all surrounded by fluids, and depend on them (air, water, etc) for survival. Some examples are:
  - engineering: airplanes, engines, pipelines
  - nature and environment: atmosphere, oceans, rivers
  - chemistry and biology: combustion, human body

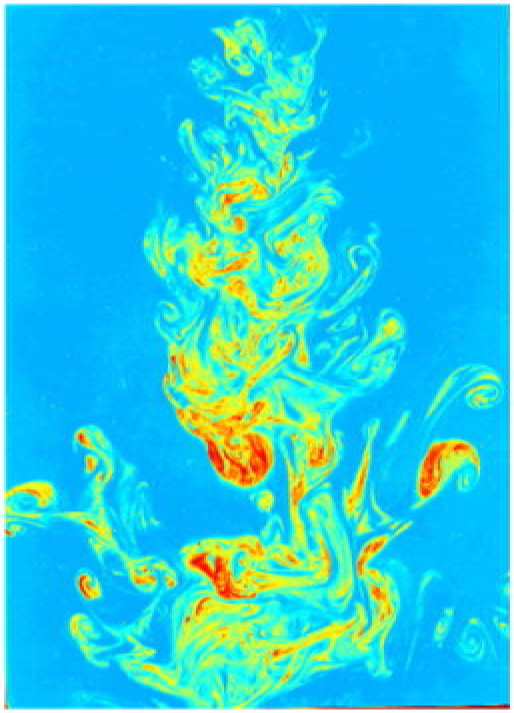
- Flow parameters can vary considerably:
  - low to high flow speeds (U)
  - small to large body dimensions (L)
  - fluids of different viscosities (ν)

- Reynolds 1883: flow becomes disorderly (turbulent) if **Reynolds number** ($Re \equiv UL/\nu$) exceeds some critical value

Examples

Space shuttle

Grid turbulence
in a wind-tunnel



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Turbulence: nature and complexity

- **Disorderly** fluctuations in time and three-dimensional space
- Most applications are at high Reynolds number
  - highly nonlinear, **wide range of scales**
  - energy transferred from large scales to small scales
- Agent of **efficient mixing** and dispersion
  - transport of heat or contaminants/substances
- As a field of scientific inquiry:
  - very difficult, many fundamental issues unresolved
  - require a combination of theory, experiment and computation

Turbulence: importance and applications

- astrophysics: plasma turbulence
- oceanography: stratified turbulence, marine ecology
- meteorology: weather prediction, hurricanes
- aeronautics: wing surface, clear air turbulence
- environment: air quality, rivers, and lakes
- combustion: reacting flow, turbulent mixing
- plus in many interdisciplinary problems…

In all cases, the complexities of turbulence limit our ability to predict natural phenomena and to design improved engineering devices

Some Quotes and References

- Often said (Feymann): “**last unsolved problem in physics**”

- Lumley & Yaglom: *Flow, Turbulence & Combustion* 2001:
“**A century of turbulence**”

  “...has suggested that this title is likely to make trouble, since it may be misinterpreted in databases as referring to politics.”

- *Columbia Electronic Encyclopedia*, 2004:

  - …“state of violent or agitated behavior in a fluid”
  - …“long thwarted attempts to fully understand it”
  - …“**advent of supercomputers** has enabled advances in… design of better airplane wings and artificial heart valves”

The basic equations

- Navier-Stokes: conservation of mass and momentum

$$\nabla \cdot \vec{u} = 0$$

$$\frac{\partial \vec{u}}{\partial t} + \vec{u} \cdot \nabla \vec{u} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \vec{u}$$

unsteadiness, nonlinear advection, pressure gradient, viscous forces

- Statistical averaging leads to more unknowns than equations, and the need for modeling, especially in engineering calculations

Let’s compute the (instantaneous) flow according to the exact N-S equations without modeling, then extract statistics

Direct Numerical Simulations (DNS): the promise

- **Tremendous detail** available from simulation resolving all the scales, including quantities difficult to measure in experiments:

  - ALL components of velocity gradients and scalar gradients

  - interaction between different scales (via Fourier decomposition)

  - statistics following the motion of infinitesimal fluid elements

  - ...with relative ease in selecting parameters

- Moin & Mahesh (Annu. Rev. Fluid Mech. 1998): A powerful tool for research: physical understanding and model testing/development

More on DNS: the requirements

- **Full range of scales in space and time**
  - size of domain $L_0 > L$ (largest length scale in the flow)
  - grid spacing $\Delta x \sim \eta$ (smallest, Kolmogorov length scale)
  - time step $\Delta t < \tau_\eta$ (shortest, Kolmogorov time scale)
  - length of simulation $T > T_E$ (large-eddy turnover time)

- CPU cost subject further to:
  - numerical stability restrictions on time-step size
    (2048^3 simulation: as many as 8,000 time steps per T_E)
  - scalability performance of **parallel computer codes**

High Reynolds Number DNS

- Why is simulating high Reynolds number important?
  - *Re* is high in most applications
  - many theories are based on a clear separation of scales

- The cost of achieving high *Re*:

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

- Overall CPU costs increase almost as N^4

A Grand Challenge problem in computational science

High-*Re* DNS: state-of-the-art

- Isotropic turbulence: simplest turbulent flow, suitable for study of small scales, which are approximately universal at high *Re*

- 4096^3 on the *Earth Simulator* in Japan:
  - Kaneda *et. al* (Phys. Fluids 2003): at Taylor-scaled Reynolds number ($R_\lambda \propto Re^{1/2}$) approx. 1,200, presented at SC'02
  - 16 Teraflops sustained on 40-Teraflop machine
  - velocity field only, for 2 large-eddy time scales

- Largest simulation (ours) in the US: 2048^3, R_λ ~ 600 - 700
  - At NERSC: mixing passive scalars in turbulence
  - aiming for longer simulation for better statistics

Basic scaling issues: Kolmogorov 1941

Notion of **scale similarity** at high Reynolds number

- **First hypothesis**, for small scales (size ~ $\eta \equiv (\nu^3/\langle\epsilon\rangle)^{1/4}$)

  - "locally isotropic" and universal, independent of details of large scales; determined only by viscosity (ν) and dissipation rate ($\langle\epsilon\rangle$)

$$\langle\epsilon\rangle \equiv 2\nu\langle s_{ij}s_{ij}\rangle \ ; \qquad \mathbf{S} \equiv [(\nabla\vec{u}) + (\nabla\vec{u})^T]/2$$

- **Second hypothesis**, for "inertial range" ($\eta \ll r \ll L$)

  - statistics depend only on $\langle\epsilon\rangle$ (rate of energy transfer from large to small scales), requires yet higher Reynolds no.

Simulation Overview: Velocity Field

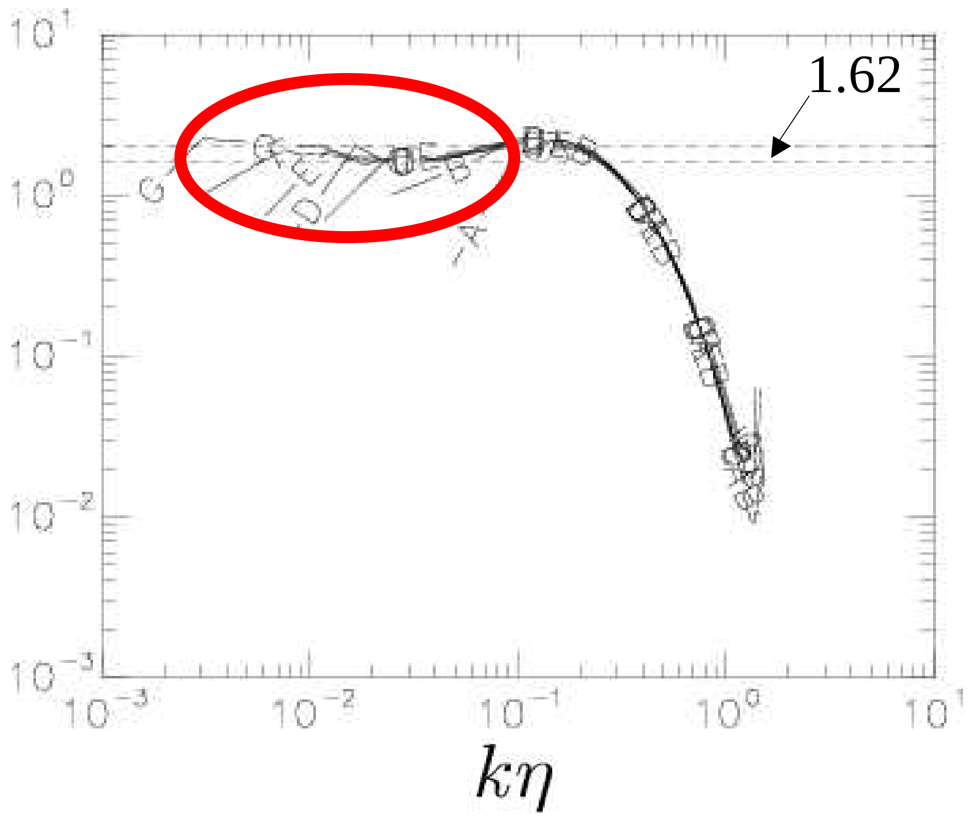
- Numerical scheme:
  - energy input by forcing at the large scales, for stationarity
  - Fourier pseudo-spectral in space: Fast Fourier Transforms with number of operations scaling as $N^3\log_2 N$
  - periodic in 3D (OK if focus on the small scales)
  - second order Runge-Kutta in time

- Our database:
  - Taylor-scale Reynolds numbers from 38 to 700
  - grid resolution 64^3 to 2048^3, $\Delta x/\eta \approx 2$ in most cases

Inertial Range: Energy Spectrum

- K41: $E(k) = C_K \langle \epsilon \rangle^{2/3} k^{-5/3}$ where C_K is Kolmogorov constant

A to G: R_λ 38 (64^3) to R_λ 700 (2048^3)



- Universality at high wavenumbers.
- Consistent with DNS at even higher *Re* (Kaneda *et. al* 2003) and experiments (Sreenivasan 1995).
- Intermittency correction due to fluctuations of ϵ : *E(k)* drops slightly faster than $k^{-5/3}$

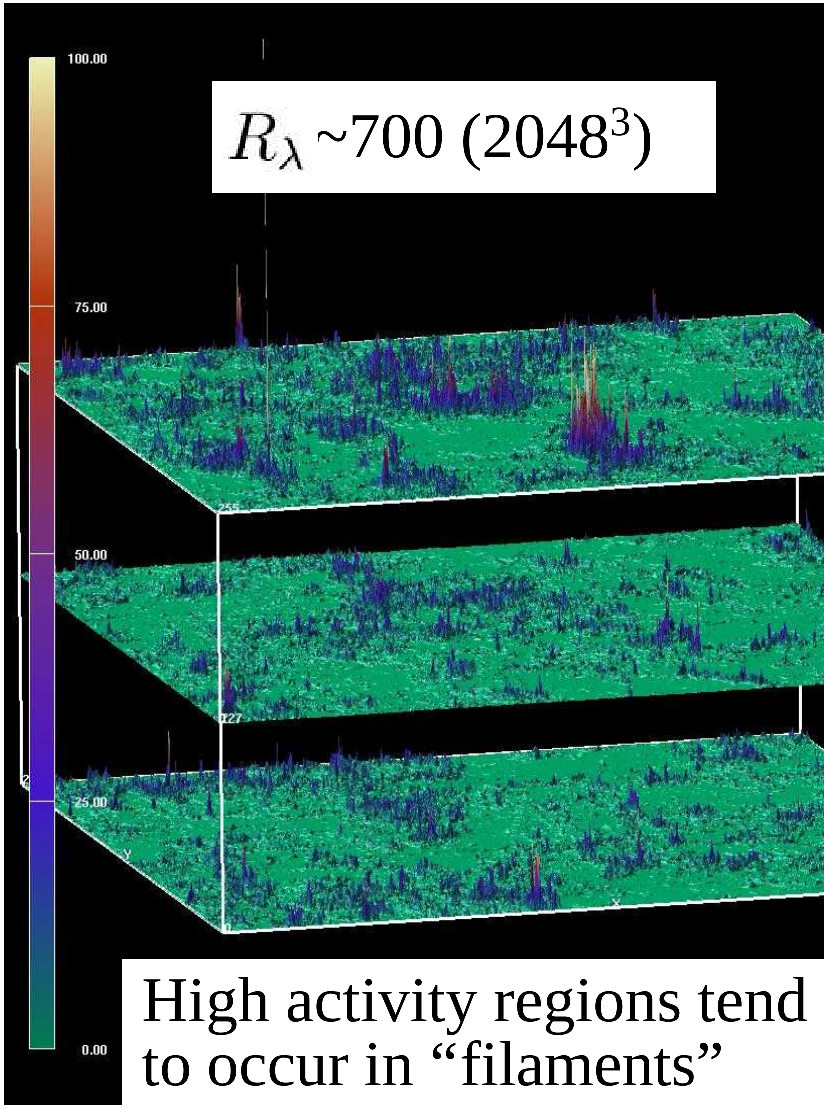
Intermittency at the Small Scales

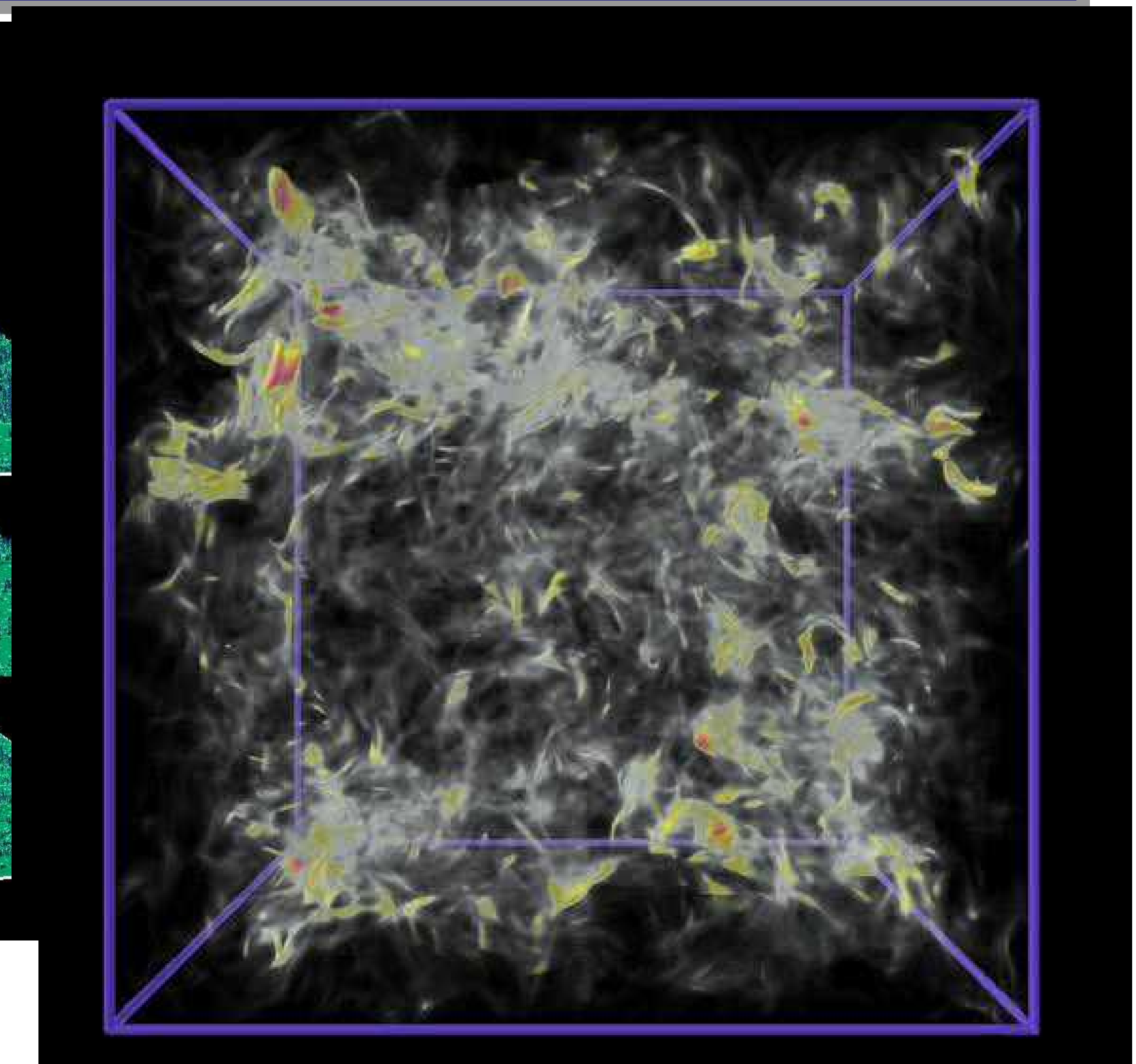
Intermittency: **localized, short-lived bursts of intense activity**

- Significant probability of large deviation from the mean
- **Fluctuations of the energy dissipation rate**
  - intense local straining can cause local flame extinction
  - important in relative dispersion and stochastic modeling
  - subject of "intermittency models" for refinements of K41
- Increases with Reynolds number
- Visualization of 3D fields possible, thanks to NERSC Staff

Intermittency: energy dissipation rate

R_λ ~700 (2048^3)

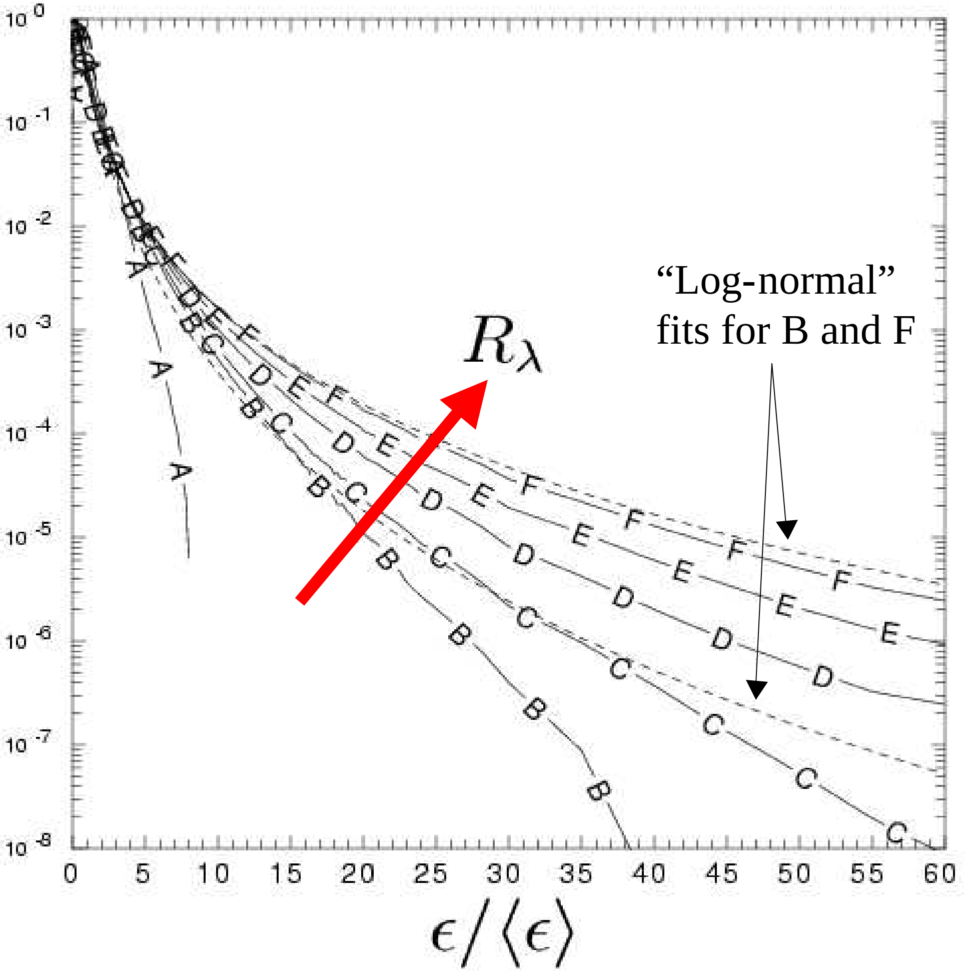




High activity regions tend to occur in “filaments”

PDF and Statistics of the Energy Dissipation

A to F: R_λ 8 (128^3) to R_λ 700 (2048^3)



- Wider “tails” at higher *Re*
- log(ϵ) often modeled as having a normal (Gaussian) distribution
- Multifractal description uses probability distribution of local averages of ϵ in box of size *r*

Passive Scalars

Diffusive contaminant/material that does not affect the flow
e.g. small temperature differences, low species concentrations

- Scalar fluctuation field $\phi(\vec{x}, t)$ evolves by

$$\frac{\partial \phi}{\partial t} + \vec{u} \cdot \nabla \phi = -\vec{u} \cdot \nabla \Phi + D \nabla^2 \phi$$

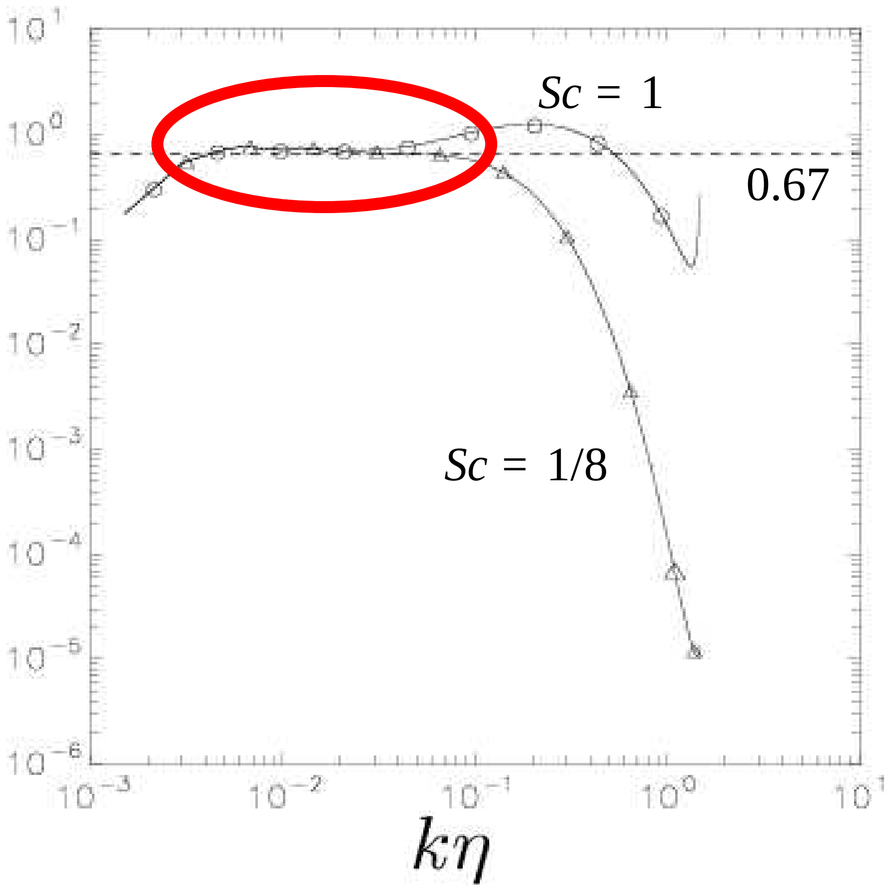
  - **production** due to velocity acting on mean scalar gradient
  - advective **transport** breaks large blobs into smaller scales
  - molecular diffusivity causes **dissipation** at small scales

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

Scalar Spectrum: Inertial-Convective Range

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

R_λ ~700 (2048^3)



- Intermediate wavenumbers for *Sc*=*O*(1) or less: extension to K41 by Obukhov 1949 and Corrsin 1951

- This may be the clearest demonstration of O-C scaling ever obtained, at least in DNS

- Value of C_{OC} agrees with experiments (Sreenivasan 1996)

Scalar Field at the Small Scales

- **Departure from local isotropy** (in response to mean gradient)

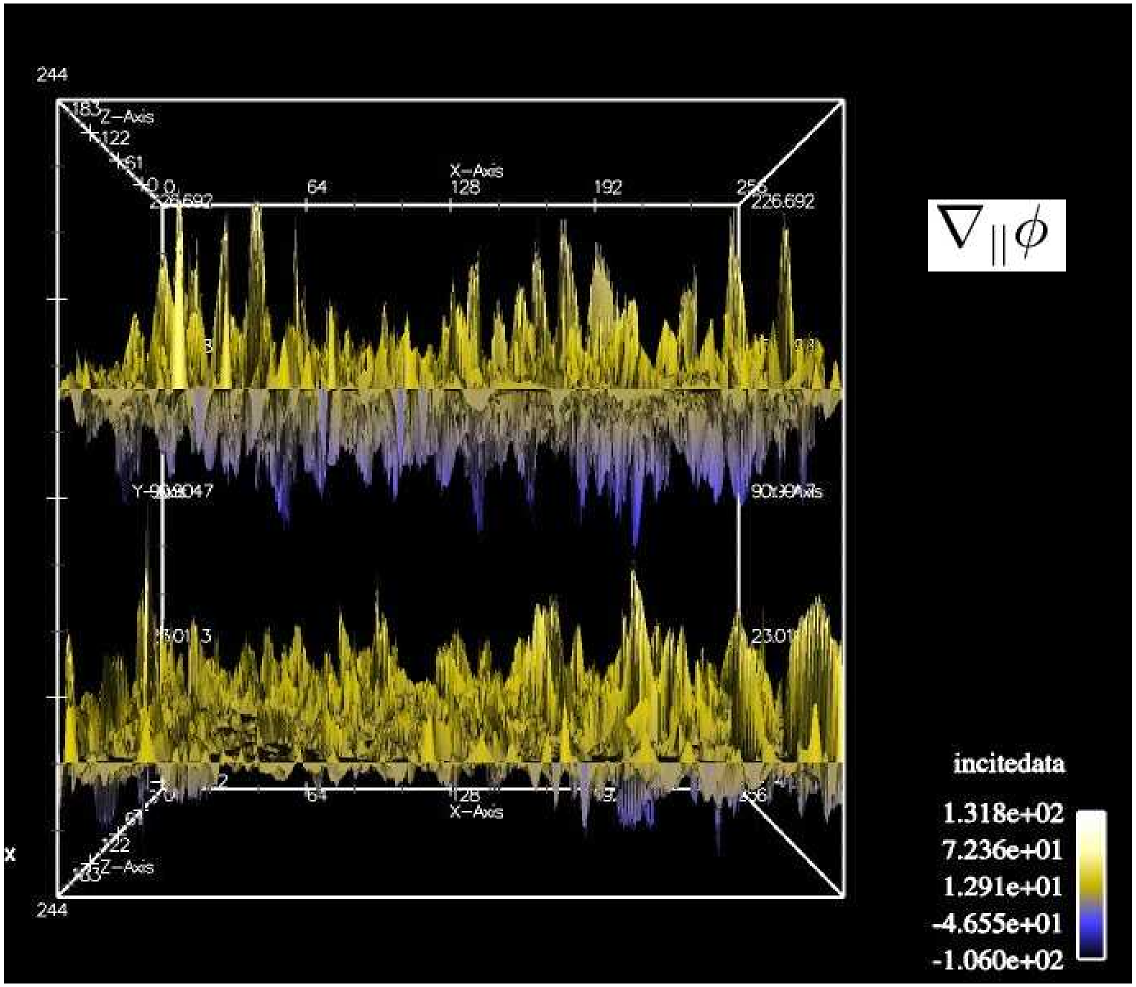
  - $\nabla_{||}\phi$ has a skewed probability distribution, sustained at high Reynolds number

- **More intermittent than the velocity field**:

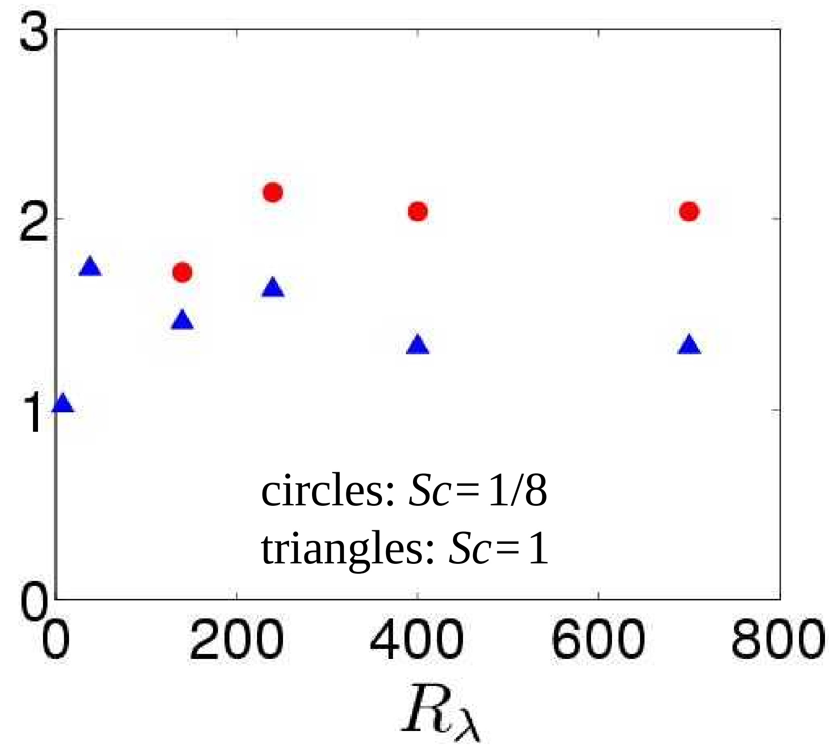
  - scalar dissipation rate $\chi \equiv 2D\nabla\phi \cdot \nabla\phi$, vs. energy dissipation

- Effect of Schmidt number (especially for *Sc* > 1) is different from that of Reynolds number

Scalar Gradients: Local Anisotropy

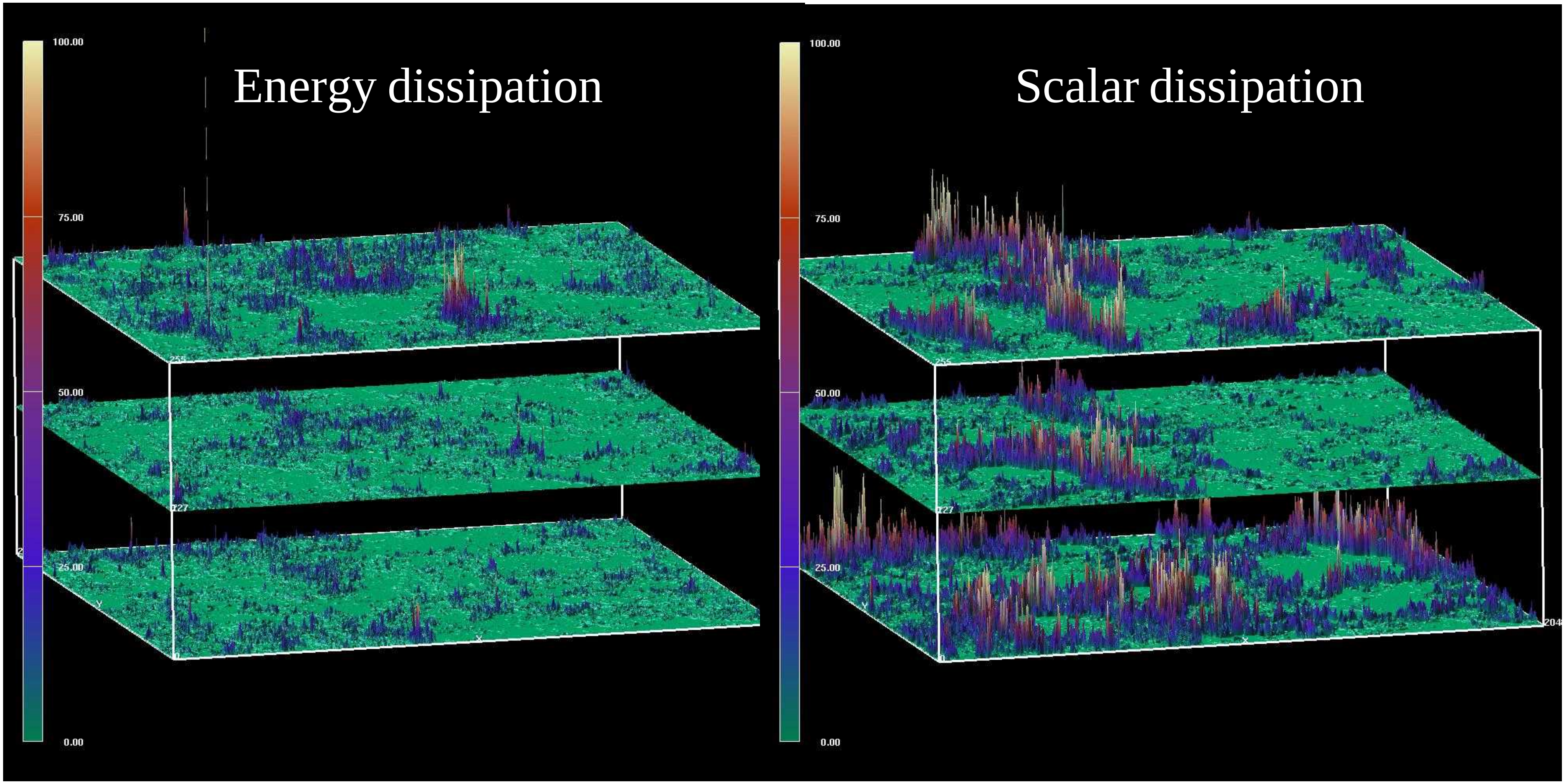


- Zero mean value, but positive samples more likely
- Odd-order moments, e.g. skewness factor of $\nabla_{||}\phi$



Energy dissipation and scalar dissipation

R_λ ~700 (2048^3)



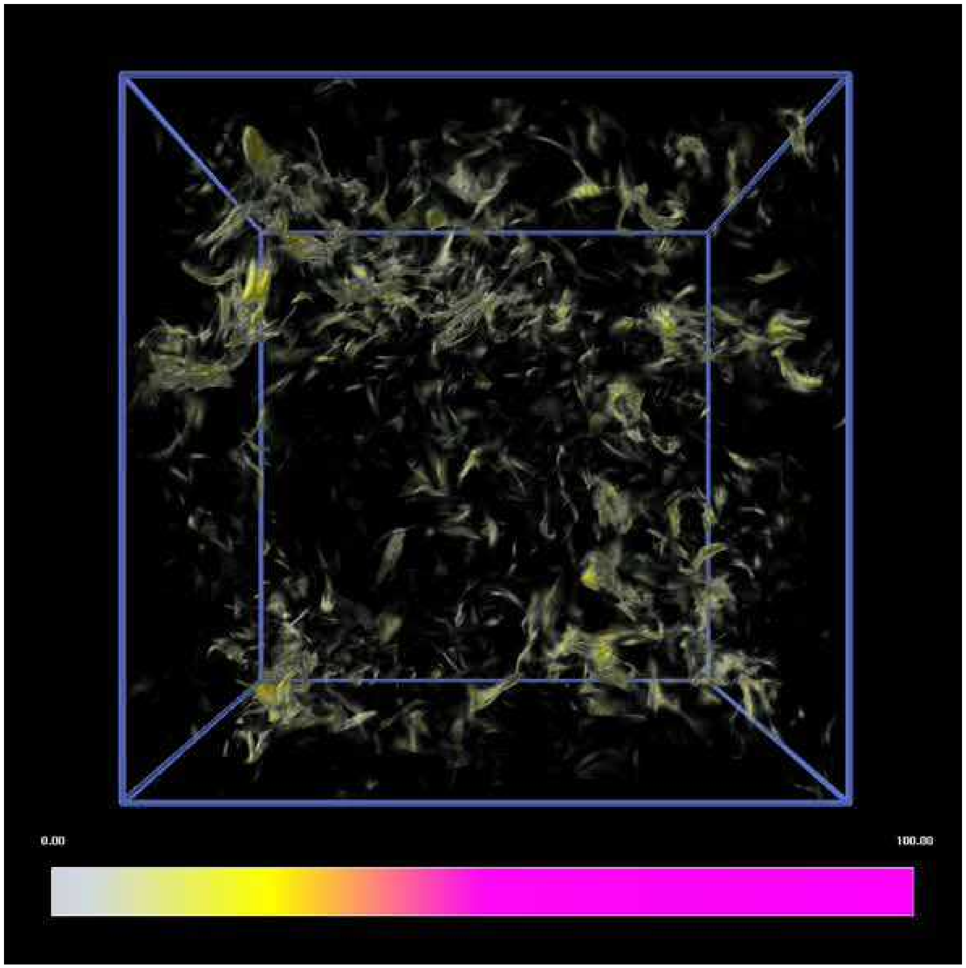
Scalar dissipation shows higher peaks

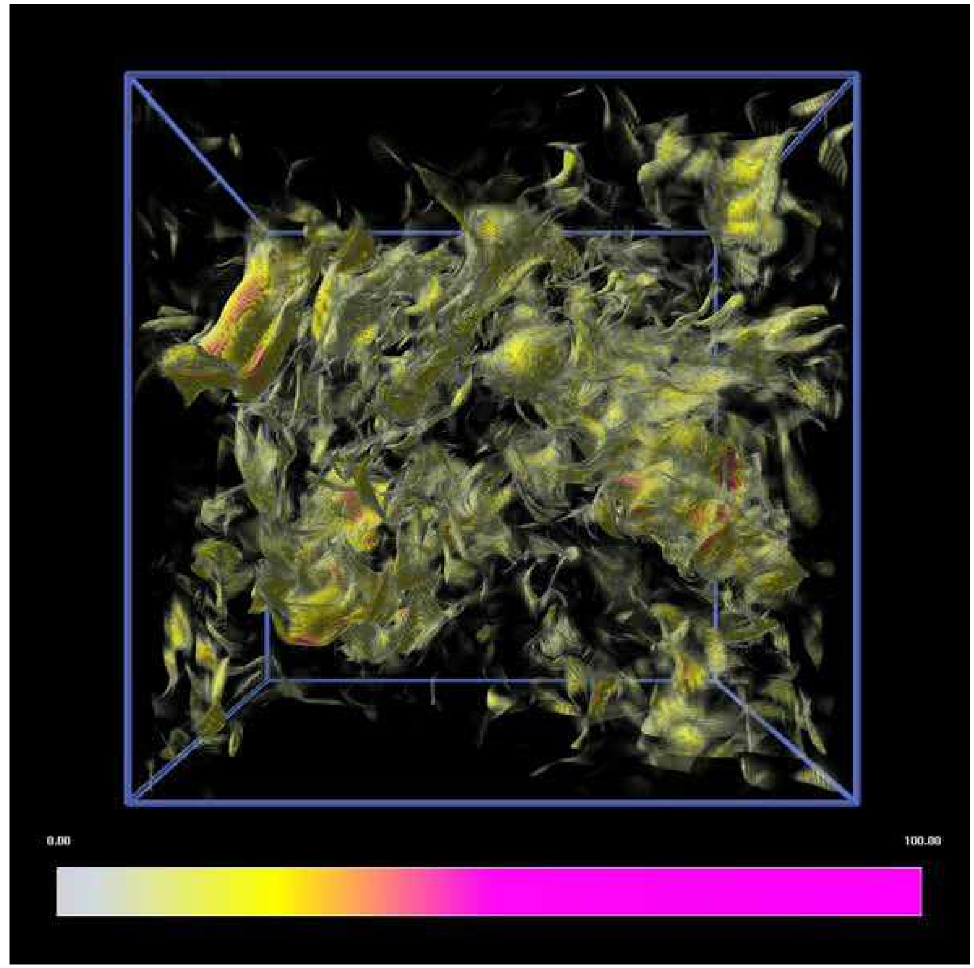
Energy dissipation and scalar dissipation

R_λ ~160 (256^3)

Energy dissipation (ϵ)

Scalar dissipation (χ)

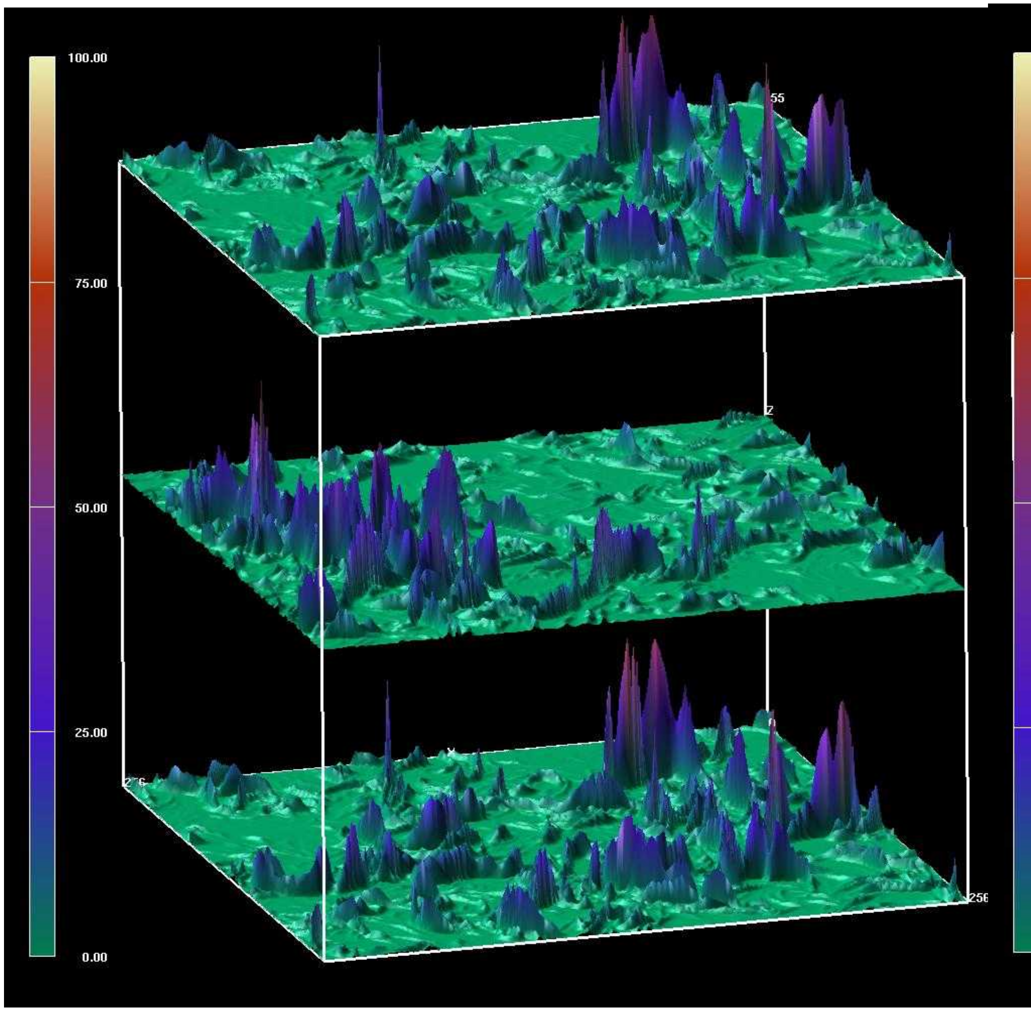




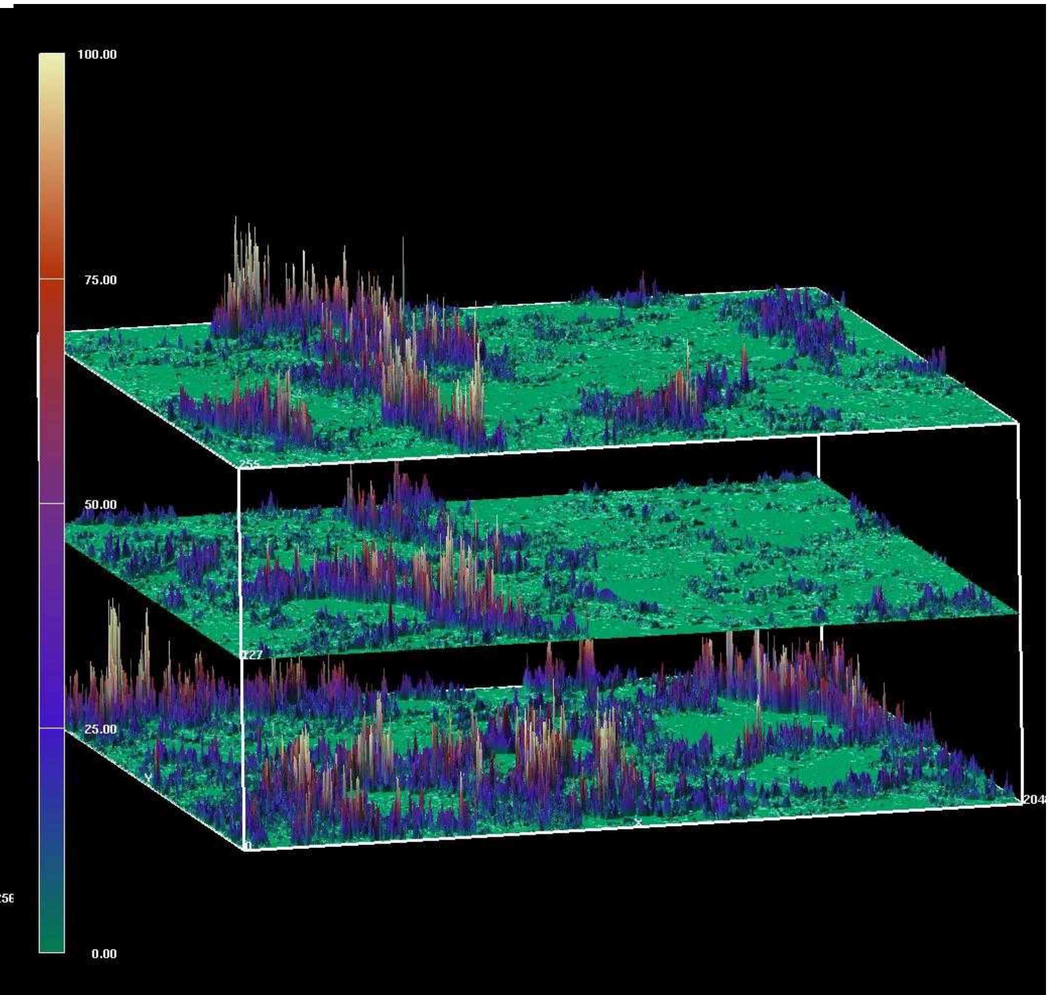
High activity topology: filaments (ϵ) and sheet-like structures (χ)

Scalar dissipation rate: *Re* effect

$R_\lambda \sim 160\ (256^3)$

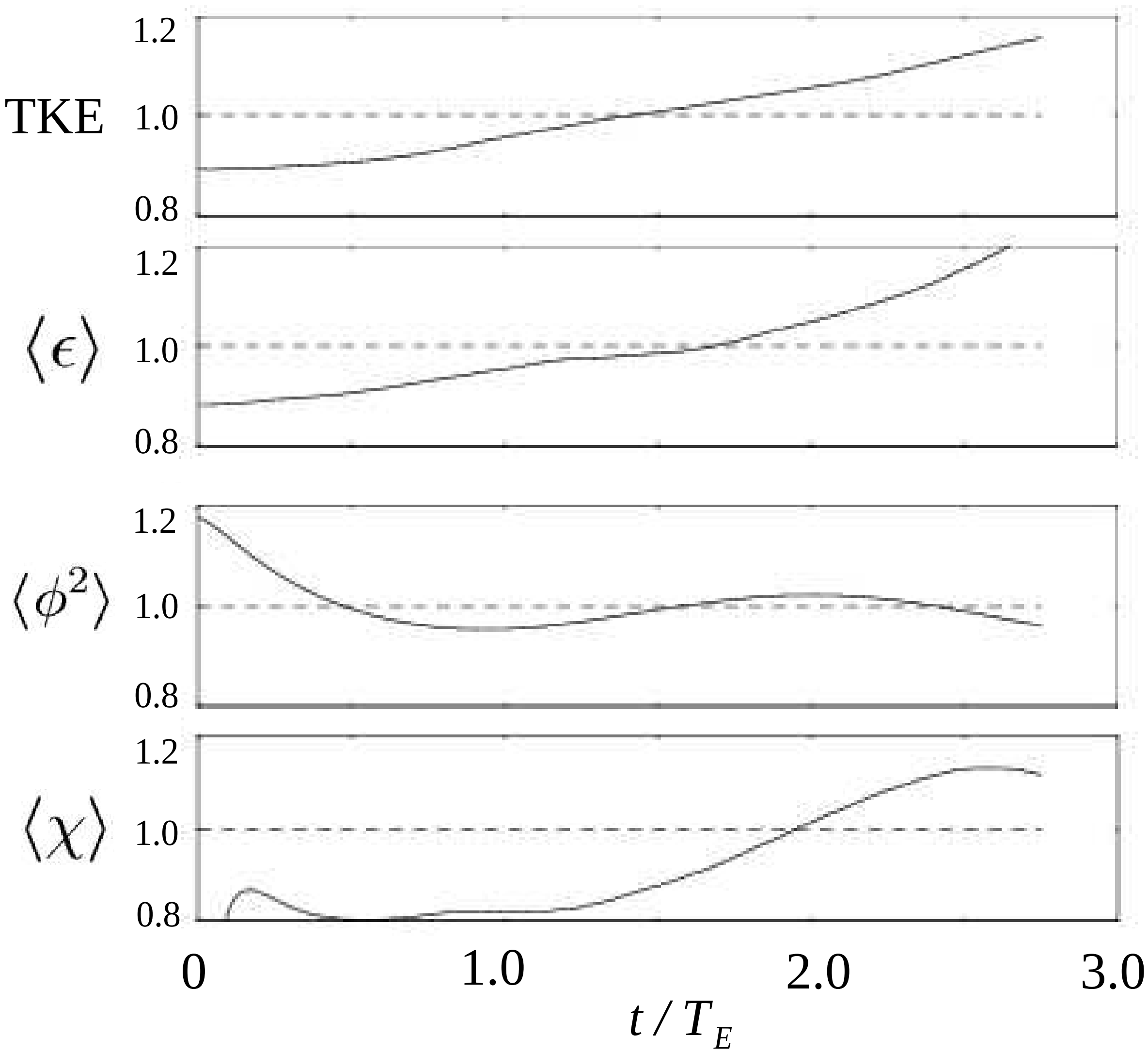


$R_\lambda \sim 700\ (2048^3)$



Peaks more intense and localized at higher Reynolds number

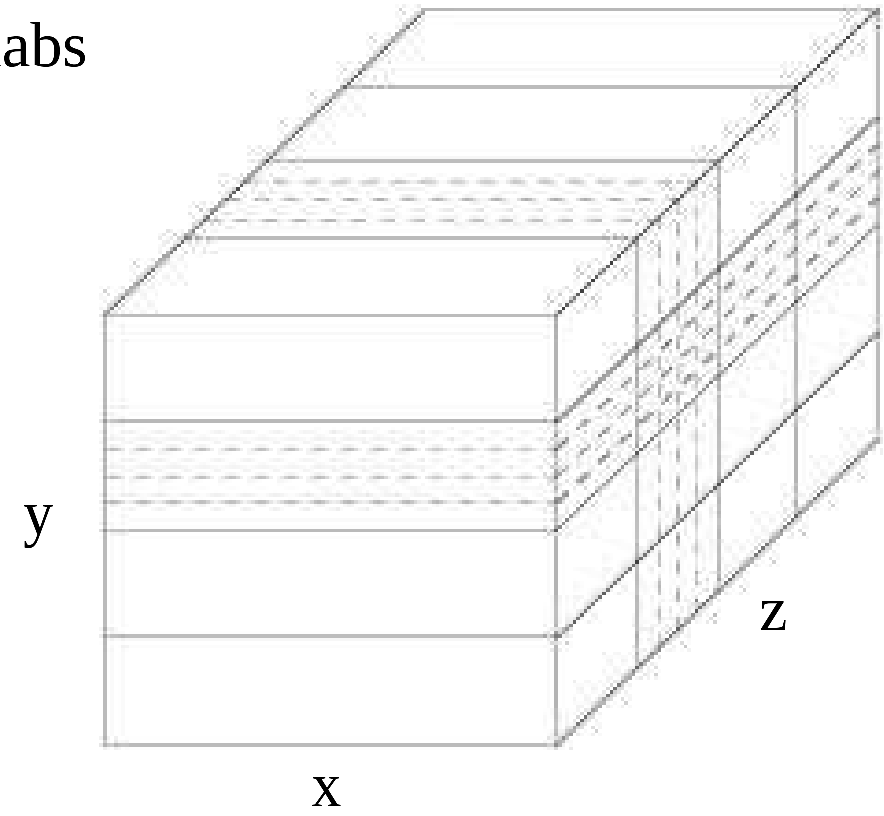
A Matter of Statistics



- Turbulence statistics have a natural variability in time
- Some quantities are more sensitive: e.g. fewer samples of large scales in a finite domain
- Accurate sampling is important: e.g. at least 5 T_E; **needs longer run** for high-quality results

Parallel Algorithm and Data Structure

- Distributed memory, equal-sized slabs
- IBM-optimized ESSL library for FFT calls
- MPI_ALLTOALL communication used to swap between *x*-*y* and *x*-*z* slabs
- **Various improvements suggested by consultants**



Performance on Seaborg

Problem size	1024	2048
No. processors	256	2048
CPU/step/proc	63 secs	84 secs
Performance per-proc.	178 Mflop/s	135 Mflop/s
Aggregate	182 Gflop/s	247 Gflop/s
Per-proc peak memory	282 MB	565 MB
Size of restart dataset	20 GB	160 GB

- Approx. 70% scalability, better if use 15 procs of 16-proc node (suggestion by David Skinner, NERSC)
- Bottleneck is in **all-to-all communication**
- Essentially perfect load balance across all processors

Summary of Accomplishments (at NERSC)

- Turbulent **mixing at highest *Re*** (R_λ ~ 600-700) in DNS, 2048^3

  - clear attainment of inertial-convective range

  - sustained departures from local isotropy of scalars

  - scalar dissipation highly intermittent, with sheet-like structure

- **Huge database** (including past data) to analyze, e.g.

  - multifractal properties, conditional statistics in modeling

  - differential diffusion of multiple scalars with different molecular diffusivities (inefficient combustion, undesirable by-products)

→ Progress towards DNS of Turbulent Reacting Flows…

Turbulent Reactive Flow: phenomena and challenges

- Often associated with combustion, but also arises in atmospheric aerosols, nanomaterial synthesis, etc

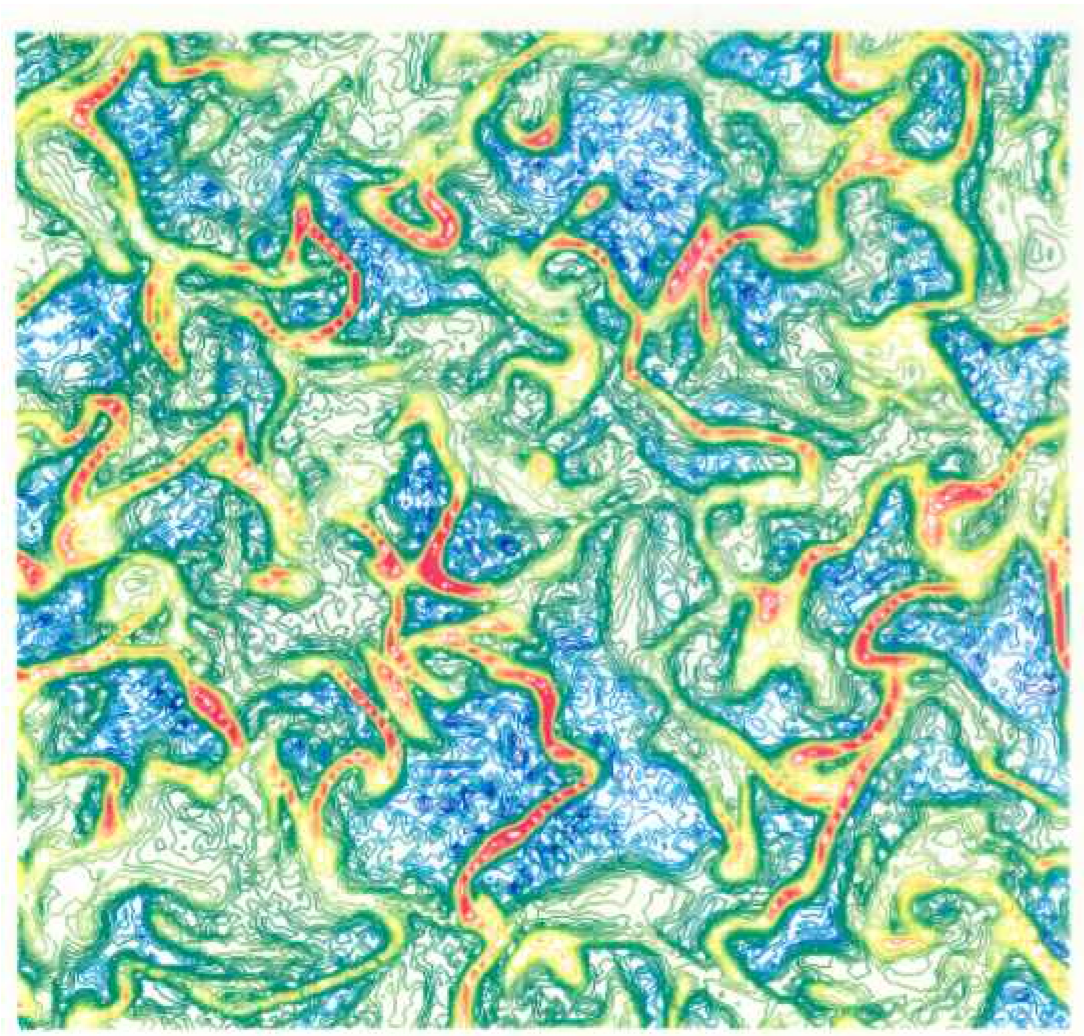
- Complex interactions between turbulence and chemistry
    - **premixed**: slow chemistry, propagation of a flame front
    - **non-premixed**: fast chemistry, controlled by rate of mixing
    - regime of finite-rate chemistry is the most difficult

- Damkohler no. (*Da*): turbulence to chemistry time scale ratios

- Highly nonlinear reaction schemes, e.g. k[A][B] (or worse…)

- **Non-equilibrium** phenomena e.g. local extinction, reignition strongly affected by small-scale intermittency (Bilger 2004, Sreenivasan 2004)

Example: contours of reaction rates



For single-step, first-order reaction: consider regions of high scalar dissipation, high reaction rate, and extinction.

Ref: *Computational Models for Turbulent Reacting Flows*, R.O. Fox, Cambridge Univ. Press, 2003.

Reacting Flow: DNS Formulation

- One-step reversible reaction (fuel, oxidant, products)

$$F + rO \rightleftarrows (1 + r)P$$

where *r* is stochiometric coefficient

- If all species have same diffusivities: can solve equations for

  - "mixture fraction" (a linear combination of the species concentrations), which behaves as a conserved scalar

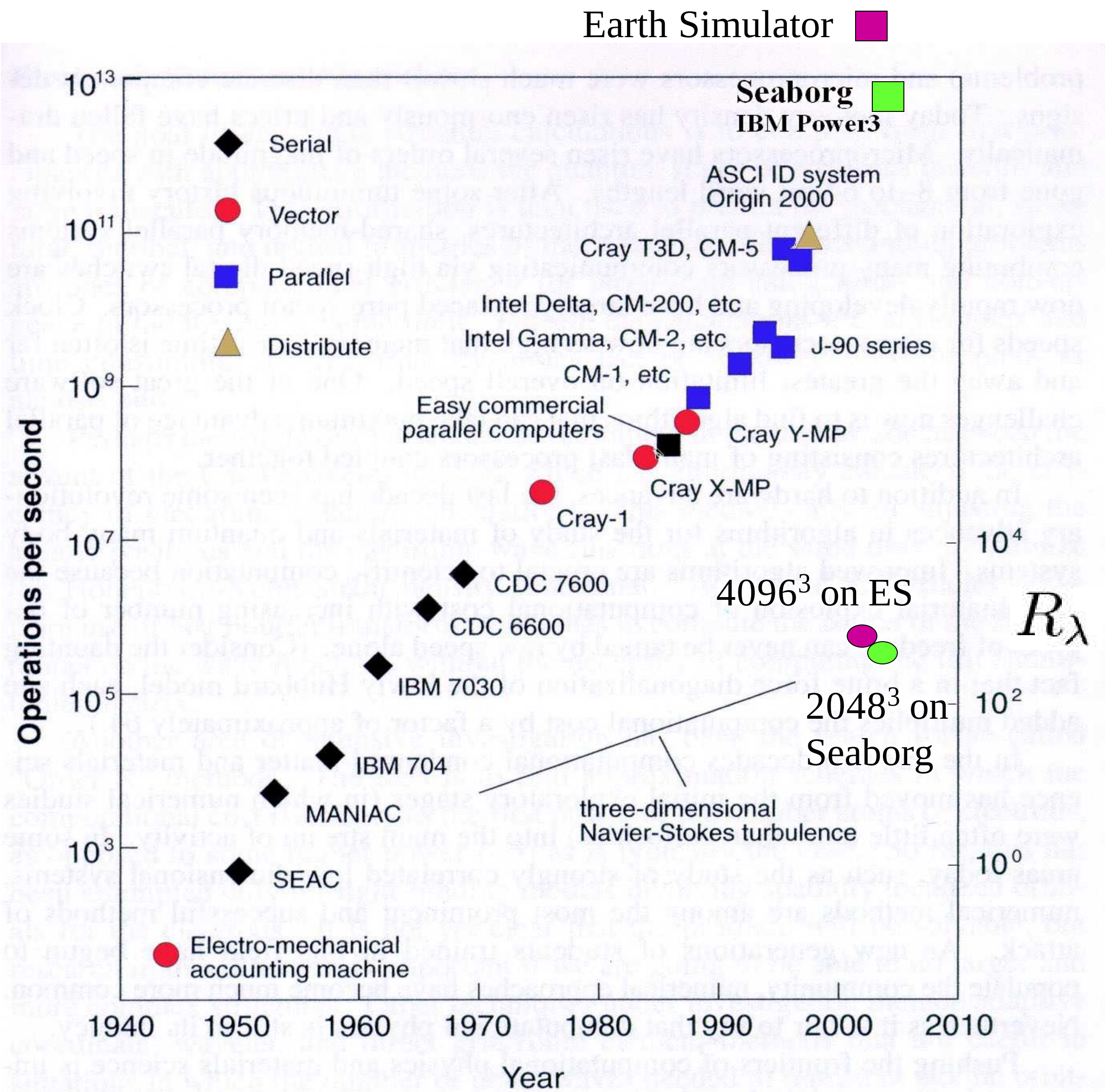
  - "progress variable" (e.g. product concentration), which may evolve from zero to equilibrium value

Reacting Flow: Future Goals

To move beyond basic studies by others who focused on decaying isotropic turbulence at low Reynolds number:

- systematic study at **different *Re*, *Sc* and *Da***.
- critical needs in novel **theory and model development**
  (e.g. behavior of scalar dissipation rate)
- differential diffusion, with emphasis on small scales

DNS and the Evolution of Computers



- Ref: NRC Report

“Condensed matter and materials physics; basic research for tomorrow’s technologies” (1999)

Figure originally by K.R. Sreenivasan.

- Reynolds number now comparable to or higher than in many laboratory experiments

The Last Word…

- Thanks to our **1.2M INCITE Award**, we now have:
  - largest production DNS (2048^3) done in the US
  - highest Reynolds number in DNS for turbulent mixing
- **The future** is bright:
  - US may be able to reclaim title of world's fastest supercomputer in 2005 or 2006 (benchmarking has started)
  - we are well positioned for the next Grand Challenge of reacting turbulence, at high Reynolds and a range of Damkohler numbers
  - many exciting collaborations ahead with other researchers