Turbulence, Turbulent Mixing and GPU-Accelerated Computing on TITAN

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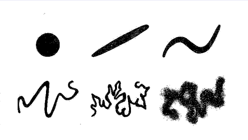
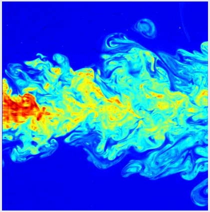
Part 1: The Science



OLCF Users Meeting, Oak Ridge, May 15, 2018

The Nature of Turbulence

Disorderly fluctuations in time and three-dimensional space
— multi-scale, nonlinear, stochastic; interdisciplinary
— crucial agent of transport, mixing and dispersion



(Sources: Wikipedia and Google search)

R. Feynman: "The Last Unsolved Problem of Classical Physics"

Also a Grand Challenge problem for high-performance computing

Introduction: Turbulent Mixing

Mixing: inter-mingling of entities of different properties in a fluid flow, with reduction of non-uniformity

- Between different chemical species, clean vs polluted air
- Between warm and cold fluids, fresh and salty water
- May or may not affect the fluid motion itself
- If not, called a "*passive scalar*" in fluid dynamics

Enhanced by turbulence, which carries "contaminants" around with fluid elements in disorderly motion

- Large local gradients may form, subsequently smoothed out ("dissipated") by molecular diffusion acting at the small scales
- Overall results depend on intensity of turbulence, and magnitude of molecular diffusivity versus kinematic viscosity of the fluid

Some Examples of Tea-Cup Turbulence

- Very common occurrences in our daily lives
- Just as important in industry (jet engines, automobiles) and environment (pollutants, cloud physics, river sediment)

Evolution Equation for Passive Scalars

Advection-diffusion equation for scalar fluctuations in the presence of a uniform mean gradient:

$$\partial\theta + \mathbf{u}\cdot\nabla\theta = -\mathbf{u}\cdot\nabla\langle\Theta\rangle + D\nabla^2\theta$$

(fluctuating) velocity field governed by Navier-Stokes equations for conservation of mass and momentum:

$$\begin{aligned} \nabla\cdot\mathbf{u} &= 0 \\ \partial\mathbf{u}/\partial t + \mathbf{u}\cdot\nabla\mathbf{u} &= -\nabla(p/\rho) + \nu\nabla^2\mathbf{u} + \mathbf{f} \end{aligned}$$

- Simplified geometry, amenable to pseudo-spectral methods
- Numerical forcing to maintain statistical stationarity in time

Resolution Requirements in DNS

Range of scales increases with the Reynolds number:

- Domain size should be larger than largest scale (L)
- Grid spacing should be comparable to smallest scale (η)
- Number of grid points scale as $(L/\eta)^3 \propto {R_\lambda}^{9/2}$ where R_λ is Taylor-scale Reynolds number (based on intermediate scales)
- More expensive if higher Reynolds number or better resolution is needed or required (e.g. for study of intermittency)

Some notable references in the field:

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

The Schmidt Number ($Sc = \nu / D$)

Varies widely among different applications:

- $\lesssim 1$ for most gases, including temperature fluctuations in air
  - easiest to measure in laboratory, relevant to combustion
- $\ll 1$ in liquid metals (high thermal conductivity and diffusivity)
  - experiments are difficult, very little data
- $\gg 1$ most liquids: 7 for heat in water, 700 for salinity in ocean
  - scales as small as $\eta_B = \eta Sc^{-1/2}$ (Batchelor JFM 1959)
  - a challenge for both measurement and computation

Algorithmic requirements can depend strongly on Sc

- $Sc \ll 1$: needs very small time steps, large domains
- $Sc \gg 1$: needs very small grid spacings

Strategy towards High Schmidt number

Ideally, we want both high *Re* and high *Sc*

- Every halving of Δx, with a factor of $2^4 = 16$X increase in CPU requirements enables at most 4X increase in *Sc*
- Yeung *et al.* (2004): $Sc = 1024$, 512^3, but at $R_\lambda \sim 8$
- Donzis & Yeung (2010): $Sc = 64$, at $R_\lambda \sim 38$
- Add scalar to 8192^3 DNS (Yeung *et al.* PNAS 2015)??

Get the best bargain that we can

- Insist on velocity field with inertial range characteristics
- A Schmidt number comparable to that for salinity in the ocean
- Develop the best algorithm on the best machine available: INCITE 2017 Award on Titan (Used over 100 M core hours)

Project Goals Pursued in INCITE 2017

Algorithm for disparate resolution requirements at high Sc

- Velocity on a coarser grid, scalar on a finer grid
- Scalar field by compact finite difference (less communication)
- Dual communicator, scalar computed primarily on GPU

Simulation I: Very High Sc, moderate Reynolds number

- 8192^3 scalar field, $Sc = 512$; 1024^3 velocity field, $R_\lambda = 140$
- Want to establish asymptotic high Sc behaviors definitively

Simulation II: High Sc, High Reynolds number

- 8192^3 scalar field, $Sc = 8 - 16$; 2048^3 velocity field, $R_\lambda = 390$
- Intermittency of scalar and energy dissipation rates

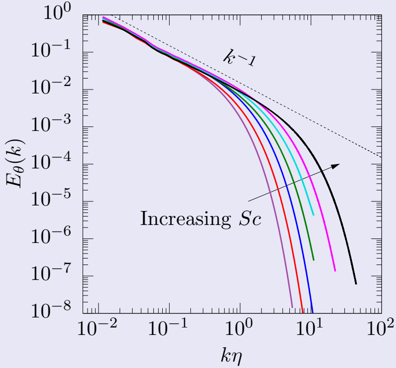
Passive Scalars: Some Physical Questions

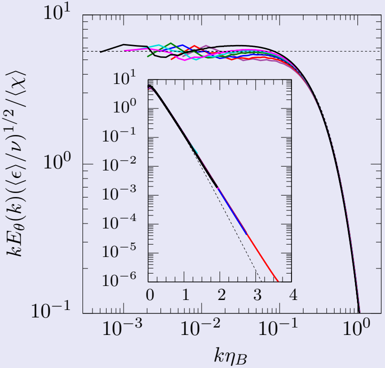
Note $d\langle\theta^2\rangle/dt = -2\langle\mathbf{u}\theta\rangle\cdot\nabla\langle\Theta\rangle - \langle\chi\rangle$ where $\langle\chi\rangle = 2D\langle\nabla\theta\cdot\nabla\theta\rangle$ is the mean scalar dissipation rate

- How are scalar fluctuations distributed among different scales?
  - $Sc \gg 1$, in viscous-convective range: $1/\eta \ll k \ll 1/\eta_B$
- Theory of "local isotropy" in turbulence:
  - Do scalar gradients lose preferential orientation as $Sc \to \infty$?
- Scalar dissipation fluctuations and intermittency
  - How do "extreme events" of χ scale with Sc, and compare with those of energy dissipation, at high Reynolds no.?

Batchelor Scaling of the Spectrum

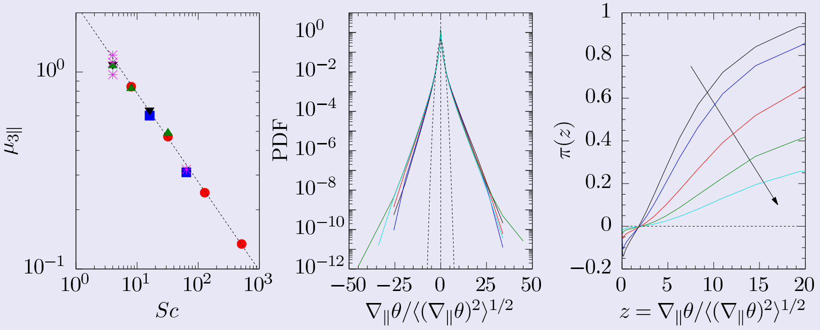
- Batchelor (JFM 1959) predicted $E_\theta(k) = C_B \langle\chi\rangle(\nu/\langle\epsilon\rangle)^{1/2}k^{-1}$ in V-C range where $k\eta \gg 1$ and $k\eta_B \ll 1$. A formula by Kraichnan (1968) also predicts behavior at $k\eta_B > 1$ well
- Batchelor suggested $C_B = 2$, but most simulations give $5 \sim 6$





Local isotropy

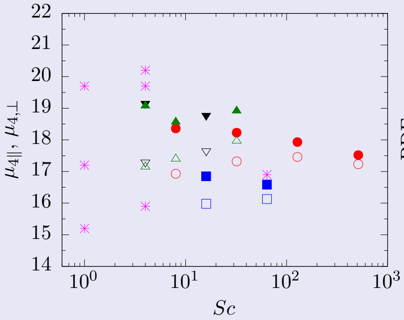
- The idea that small scales "should" be isotropic even if the large scales are not — less valid for scalars than velocity field...
- Skewness of $\nabla\phi$ in direction of mean gradient:
  - a definite decrease beyond $Sc = 4$: roughly $Sc^{-0.5}$.
- Asymmetry in PDF: $\pi(z) \equiv (p(z) - p(-z))/(p(z) + p(-z))$



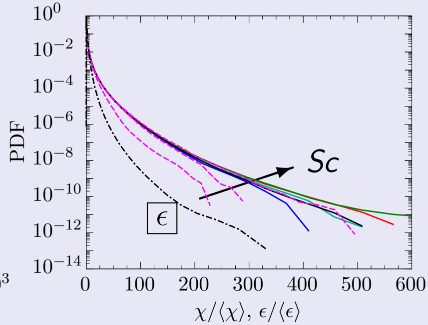
Saturation of Intermittency

- Flatness factor of scalar gradients which are highly non-Gaussian
- Likelihood of samples of very large $\chi/\langle\chi\rangle$ (hundreds, or higher)
- Finite resolution can underestimate large gradients

Various Reynolds nos. and resolutions



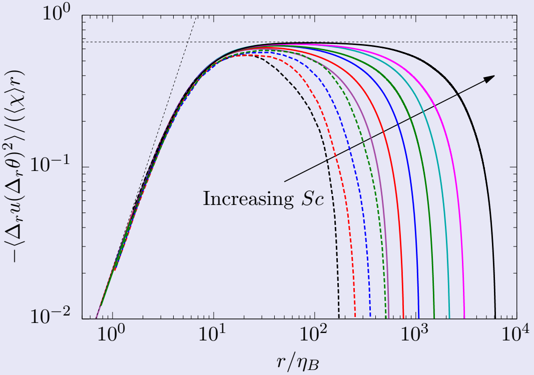
$R_\lambda \sim 140$



Spatial structure: Yaglom's relation

- For velocity, an "exact" K41 result is $\langle(\Delta_r u)^3\rangle = -\frac{4}{5}\langle\epsilon\rangle r$.
- For scalars, Yaglom (1949) predicted, for intermediate r

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



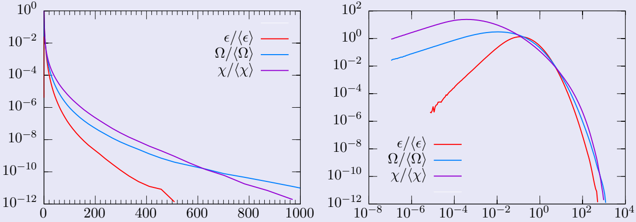
About "Extreme Events"

- In turbulence, probability distribution of velocity and scalar fluctuations taken at a point are usually close Gaussian
- But gradients in space are non-Gaussian, with localized fluctuations of high intensity (spottiness in space)
- Quadratic measures of such gradients are important:
  - $\epsilon \equiv 2\nu s_{ij}s_{ij}$: energy dissipation rate (strain rates)
  - $\Omega \equiv \nu\omega_i\omega_i$: enstrophy (vorticity squared)
  - $\chi \equiv 2D(\partial\theta/\partial x_i)(\partial\theta/\partial x_i)$: scalar dissipation rate

  Changes in shape and orientation of fluid elements, and occurrence of large gradients (v. important in combustion)
- Properties of ϵ taken pointwise or averaged over selected scale sizes are crucial in intermittency theory

"Extreme Events" for Scalar Dissipation

PDFs of normalized energy dissipation, enstrophy, and scalar dissipation at $Sc = 8$ (8192^3), R_λ 390 [D. Buaria]



- Extreme events of amplitude of order 1000 times the mean
- Value of $Sc = 8$ chosen conservatively for accuracy — results may not change much if Sc increased further.
- Cross-over between PDFs of Ω and χ to be investigated

Science Results: Summary and Further Questions

DNS of High Sc mixing up to $Sc = 512$, at $R_\lambda \sim 140$

- Viscous-convective scaling (between η and $\eta_B = \eta/\sqrt{Sc}$)
- Reduction of anisotropy in the $Sc \gg 1$ limit
- Saturation of intermittency in small scales as Sc increases

Evidence of extreme events in scalar dissipation rate

Further questions and extensions

- More analyses: e.g to explain skewness of scalar gradients varying as $Sc^{-1/2}$, and to obtain statistics of locally averaged χ
- INCITE 2018 project on Titan:
  - Differential diffusion between $Sc = 4$ and 512
  - Active scalars in oceanic context: density of seawater depends on both temperature ($Sc = 7$) and salinity ($Sc = 700$)

Some Publications

- Gotoh, T. & PKY (2013) "Passive scalar transport: a computational perspective". in *Ten Chapters in Turbulence*, Cambridge University Press, UK.
- † Clay, M.P., Buaria, D., PKY & Gotoh, T. (2018) GPU acceleration of a petascale application for turbulent mixing at high Schmidt number using OpenMP 4.5.
  Comput. Phys. Commun., **228**, 100-114.
- Donzis, D.A., Sreenivasan, K.R. & PKY (2010) The Batchelor spectrum for mixing of passive scalars in isotropic turbulence.
  Flow, Turb. & Combust., **85**, 549-566.
- PKY, Zhai, X.M & Sreenivasan, K.R. (2015). Extreme events in computational turbulence. *PNAS*, **112**, 12633-12638.

†: INCITE publication