

Dynamics of Non-Equilibrium Variables:
Multiscale-multiphysics applications of fluctuating hydrodynamics
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Fluctuating Hydrodynamics and Turbulence

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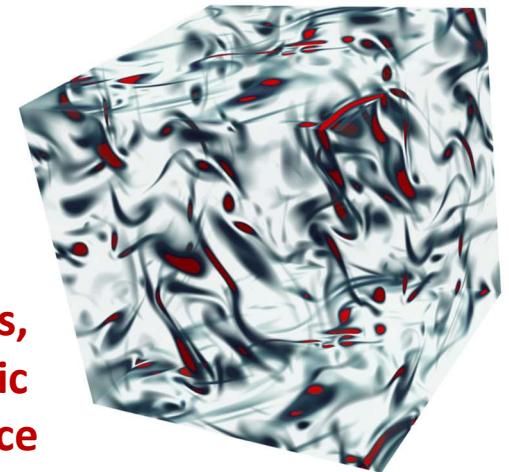
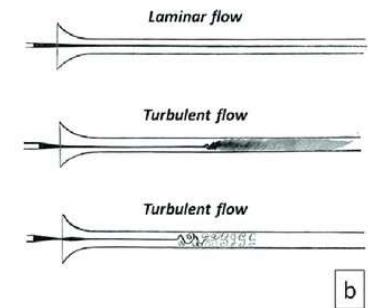
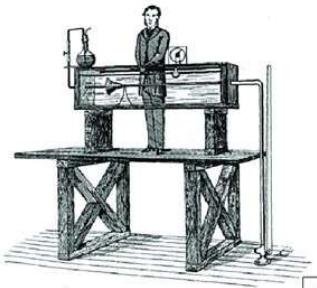
Supercomputing Platforms (~20,000 GPU-hours):

NERSC, Berkeley Lab (Perlmutter)

OLCF, Oak Ridge National Lab (Frontier)

Turbulence in Fluids

"Turbulence is the most important unsolved problem of classical physics."
Feynman Lectures (1964)



Homogenous,
isotropic
turbulence

Turbulence Terminology

Reynolds number

$$\text{Re} = \frac{\rho u L}{\eta}$$

ρ – density, η – viscosity
 u, L – characteristic velocity, length scale

Taylor microscale, l_λ , is length scale at which viscosity starts to affect the dynamics of turbulent eddies in the flow. Marks the start of the “near dissipation range.”

Taylor-Reynolds number, Re_λ , takes $L = l_\lambda$ and $u = \sqrt{|\nu^2|}$ (r.m.s. speed in eddies). Fully developed turbulence for $\text{Re}_\lambda \gtrsim 100$.

Kolmogorov microscale, l_η is length scale at which viscosity dominates and turbulent energy is dissipated into thermal energy.
Marks the start of the “far dissipation range.”

Compressible Navier-Stokes Equations with Forcing

Compressible Navier-Stokes equations

continuity

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0$$

momentum

$$\frac{\partial}{\partial t}(\rho \mathbf{v}) + \nabla \cdot (\rho \mathbf{v} \otimes \mathbf{v} + p \mathbf{I} + \boldsymbol{\Pi}) + \cancel{\rho \mathbf{a}_T} = 0$$

long-wavelength
turbulent forcing

External forcing imposed
at length scales above l_F ,
which marks the start of
the “inertial sub-range.”

$\boldsymbol{\Pi}$ – Stress tensor

energy

$$\frac{\partial}{\partial t}(\rho E) + \nabla \cdot (\mathbf{v}(\rho E + p) + \mathbf{Q} + \boldsymbol{\Pi} \cdot \mathbf{v}) + [\rho \mathbf{a}_T \cdot \mathbf{v} - \cancel{\langle \rho \mathbf{a}_T \cdot \mathbf{v} \rangle}] = 0$$

energy “thermostat”

\mathbf{Q} – Heat flux

Optional: assume incompressibility and uniform isothermal conditions

Standard Picture of Turbulence: Energy Spectrum

inertial sub-range

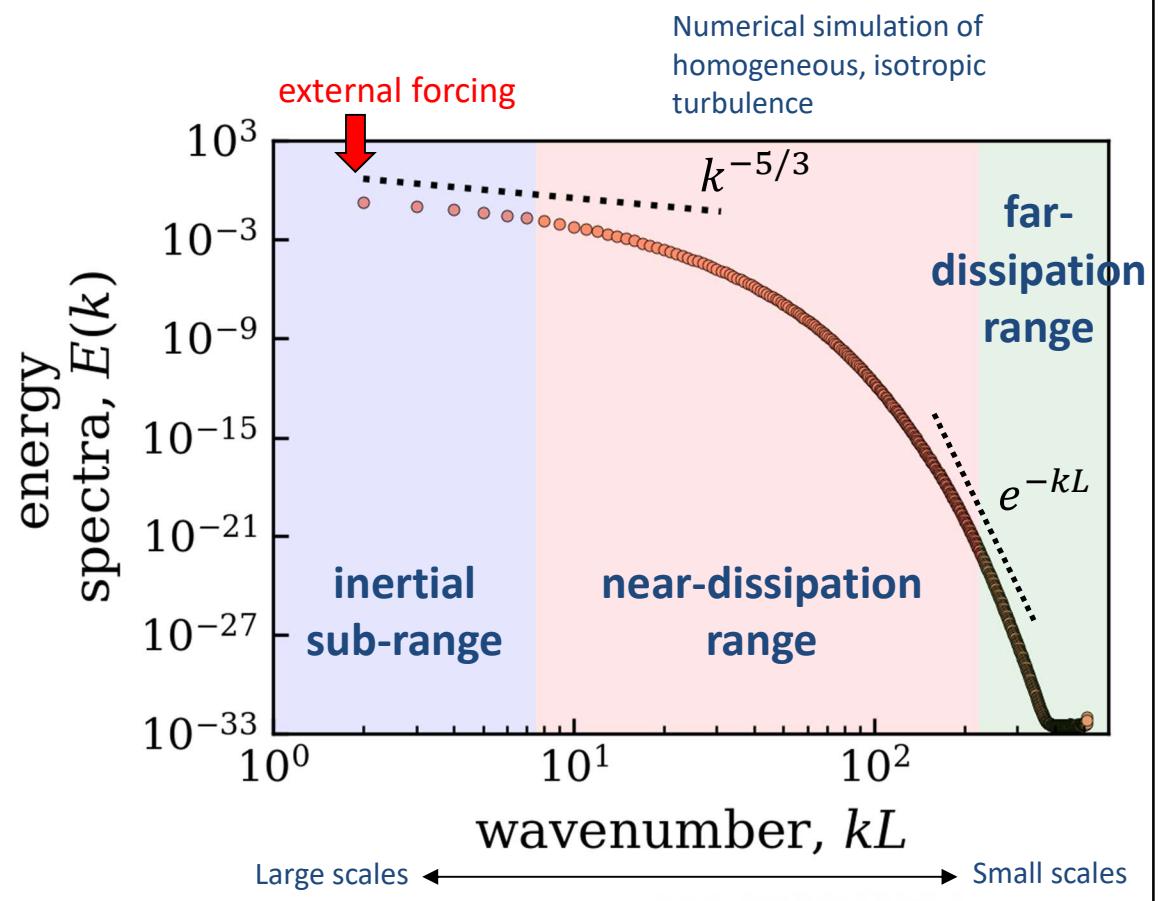
- inviscid energy cascades from large to small eddies
- $k^{-5/3}$ Kolmogorov scaling

near-dissipation range

- viscous effects start appearing
- intermittency starts growing

far-dissipation range

- viscous dissipation dominates
- strong intermittency



Thermal Fluctuations and Turbulence: Standard View

At standard conditions there are $N \approx 10^4$ air molecules per cubic mean free path so von Neumann (1949) argued that thermal fluctuations becomes relevant in turbulent flows only for length scales of order the mean free path.

Moser (2006) derived this ratio of Kolmogorov length scale, l_η , to mean free path, l_{mfp} ,

$$\frac{l_\eta}{l_{\text{mfp}}} \approx \frac{1}{4} \frac{\sqrt{\text{Re}_\lambda}}{\text{Ma}}$$

Ma – Mach number

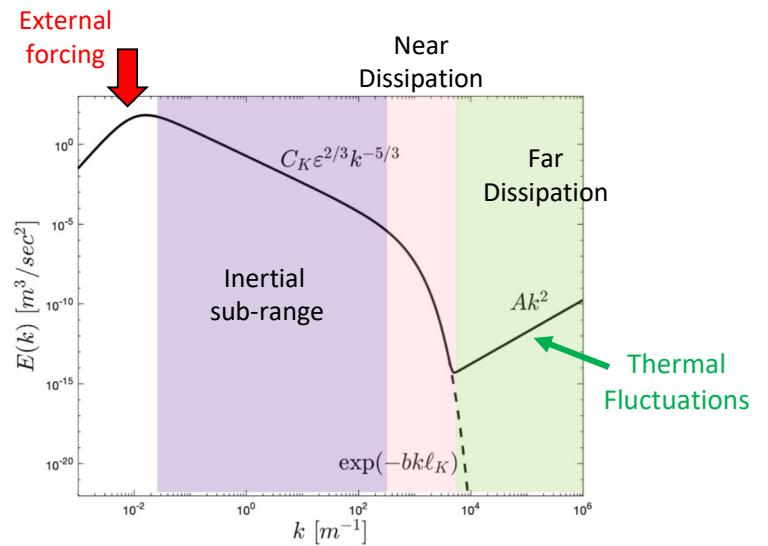
For typical subsonic turbulence, $l_\eta \approx 10 l_{\text{mfp}} - 100 l_{\text{mfp}}$, so thermal fluctuations were only expected to be noticeable *deep* into the far dissipation range.

Thermal Fluctuations and Turbulence: Dissenting Opinion

Betchov (1957) had a dissenting opinion and argued that thermal fluctuations would be noticeable in turbulent flows at scales larger than a mean free path.

Bandak et al. (2022) estimated the length scale at which the exponentially decaying energy density of turbulence would equal the energy density of thermal fluctuations.

By their estimates the thermal fluctuation spectrum, which goes as k^2 , dominates somewhere close to the border between the near and far dissipation regions.



Bandak et al., PRE, 2022

So what? Who cares?

In laboratory experiments, the Taylor microscale is $l_\lambda \approx 1 - 10$ mm and the Kolmogorov microscale is $l_\eta \approx 1 - 10$ μm .

The current generation of turbulence experiments cannot resolve the Kolmogorov microscale but the next generation is being designed to see it.

There are *many* theories and simulations for the far dissipation regime but they are all based on the deterministic Navier-Stokes equations.

But if thermal fluctuations dominate turbulence in the far dissipation regime then what's the point of those experiments, theories, and simulations?

Compressible Fluctuating Hydrodynamics

Stochastic Navier-Stokes equations, as formulated by Landau and Lifshitz.

continuity

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0$$

momentum

$$\frac{\partial}{\partial t} (\rho \mathbf{v}) + \nabla \cdot (\rho \mathbf{v} \otimes \mathbf{v} + p \mathbf{I} + (\Pi + \tilde{\Pi})) + \rho \mathbf{a}_T = 0$$

energy

$$\frac{\partial}{\partial t} (\rho E) + \nabla \cdot (\mathbf{v} (\rho E + p) + (\mathbf{Q} + \tilde{\mathbf{Q}}) + (\Pi + \tilde{\Pi}) \cdot \mathbf{v}) + [\rho \mathbf{a}_T \cdot \mathbf{v} - \langle \rho \mathbf{a}_T \cdot \mathbf{v} \rangle] = 0$$

Add a Langevin-type white-noise **stochastic flux** to Navier-Stokes eqns., while satisfying **fluctuation-dissipation balance**

stress tensor
heat flux
stress tensor

Dissipative and Stochastic Fluxes

dissipative stress tensor (deterministic)

$$\Pi_{ij} = -\eta \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \delta_{ij} \left[\left(\lambda - \frac{2}{3}\eta \right) \nabla \cdot \vec{v} \right]$$

η - shear viscosity
 λ - bulk viscosity

fluctuating stress tensor (stochastic) [Español, *Physica A* (1998)]

$$\tilde{\Pi}(\mathbf{r}, t) = \sqrt{2k_B T \eta} \tilde{\mathcal{Z}}^{\Pi} + \left(\pm \sqrt{\frac{k_B \lambda T}{3}} - \frac{\sqrt{2k_B \eta T}}{3} \right) \text{Tr}(\tilde{\mathcal{Z}}^{\Pi}) \mathbb{I}$$
$$\tilde{\mathcal{Z}}_{3 \times 3}^{\Pi} = \frac{\mathcal{Z}_{3 \times 3} + \mathcal{Z}_{3 \times 3}^T}{\sqrt{2}}$$

dissipative heat flux (deterministic)

$$\vec{Q} = -\kappa \nabla T$$

κ – thermal diffusivity

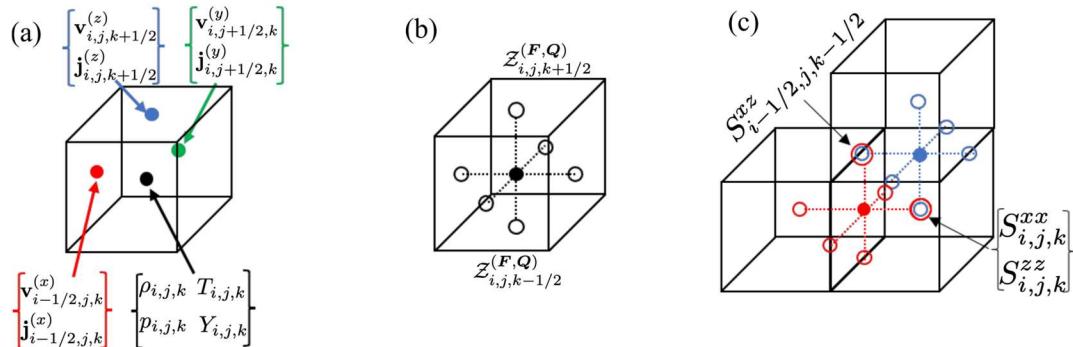
fluctuating heat flux (stochastic)

$$\tilde{\vec{Q}} = \sqrt{2\kappa k_B T^2} \mathcal{Z}^Q$$

Finite-Volume Numerical Scheme

During Aleks Donev's post-doc at Berkeley Lab we developed several efficient, accurate numerical schemes for fluctuating hydrodynamic equations. We've been refining these stochastic PDE schemes for over a decade.

staggered grid finite-volume discretization

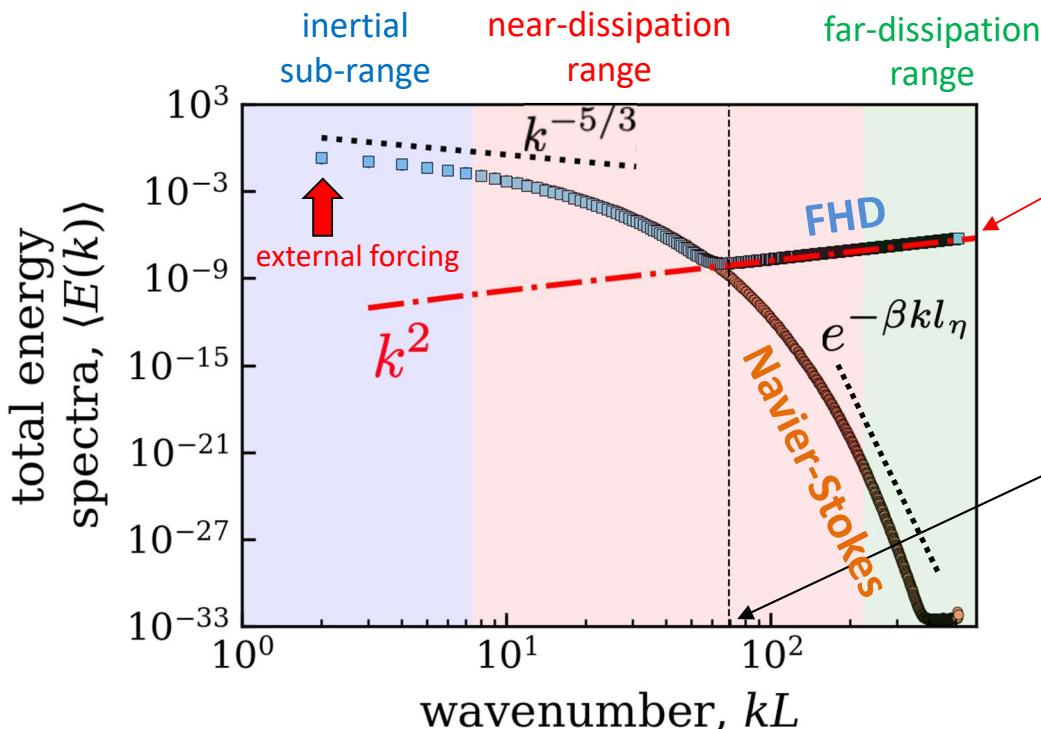


optimized 3-stage Runge-Kutta explicit integration

cell-centered (scalars):
density, energy, temperature
face-centered (vectors):
velocity and heat fluxes
edge- and cell-centered (tensors):
stress tensor

Srivastava et al., *Staggered scheme for the compressible fluctuating hydrodynamics of multispecies fluid mixtures*, Phys. Rev. E, 107 (2023)

Fluctuating Hydrodynamics of Turbulence: Energy Spectrum



Aleks' comment

$Re_\lambda = 52$

$Ma = 0.2$

thermal spectra (equipartition)

$$E_{\text{th}}(k) = \frac{3k_B \langle T \rangle}{2\langle \rho \rangle} 4\pi k^2$$

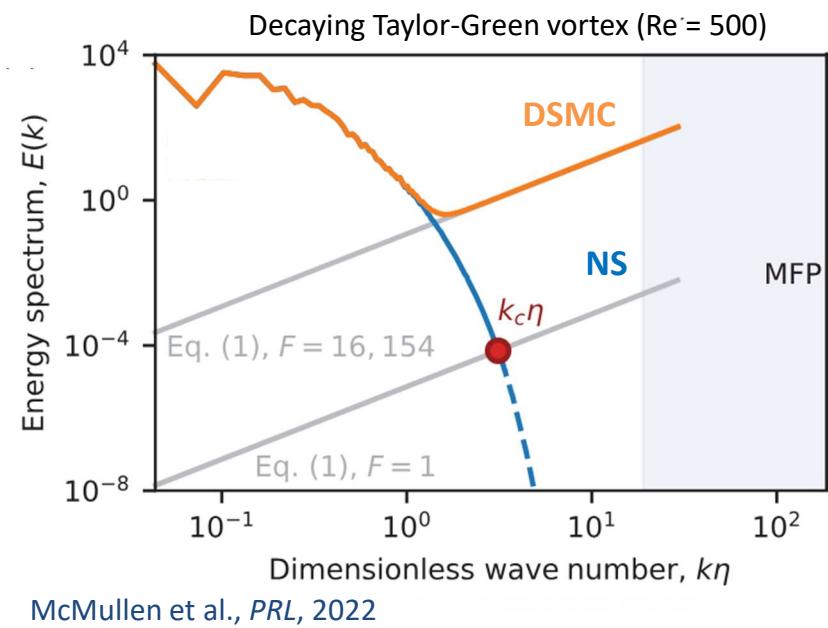
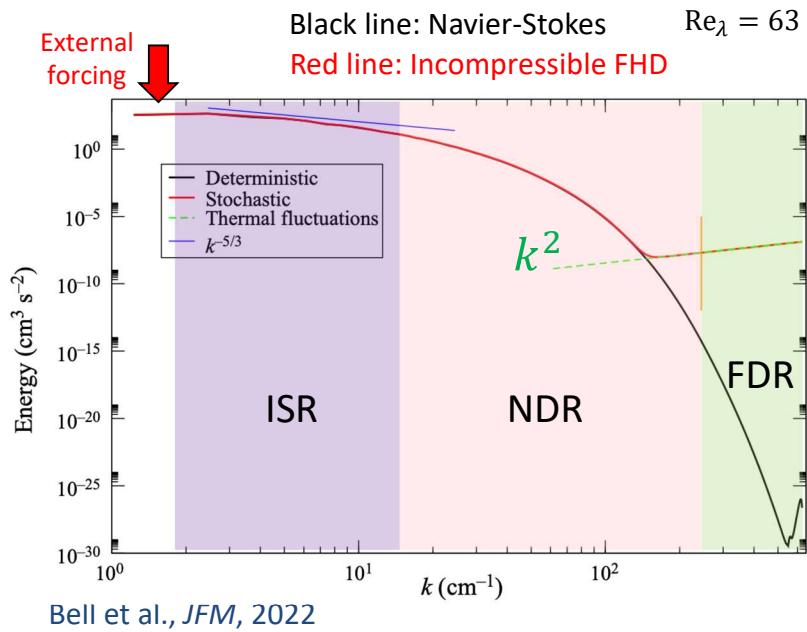
thermal crossover length

$$u_\eta^2 l_\eta \exp(-\beta k_{\text{th}} l_\eta) \approx \frac{k_B \langle T \rangle}{\langle \rho \rangle} k_{\text{th}}^2$$

We find that thermal fluctuations dominate turbulence at length scales significantly **larger** than the Kolmogorov microscale.

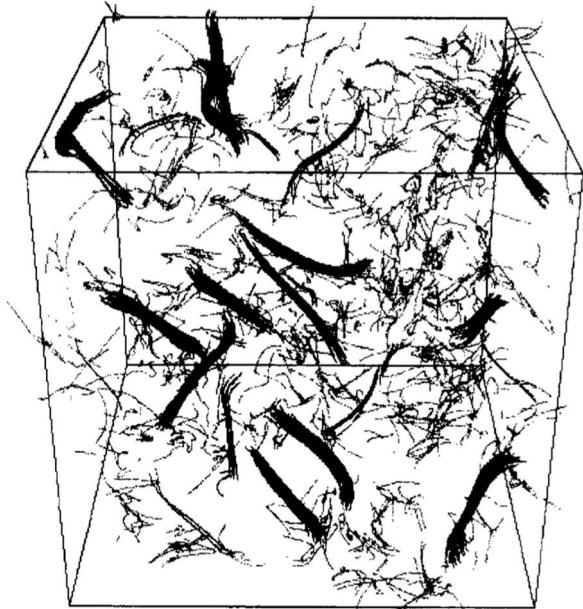
Independent Verifications of Energy Spectrum

Our turbulence simulations using incompressible fluctuating hydrodynamic and particle-based simulations (DSMC) by the Sandia group both indicate that the crossover where thermal fluctuations dominate turbulence lies within the Near Dissipation Regime (NDR).

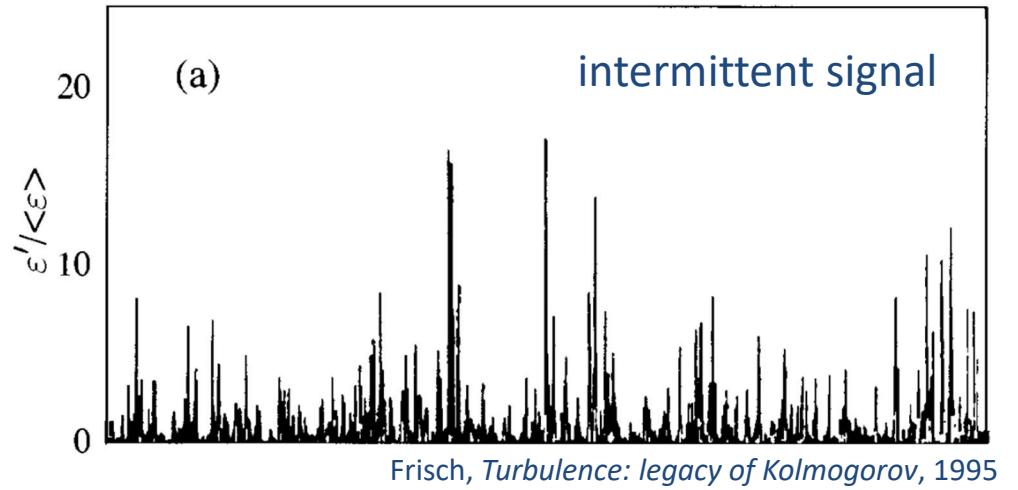


Standard Picture of Turbulence: Intermittency

intermittent vortex filaments



She et al., *Nature*, 1990

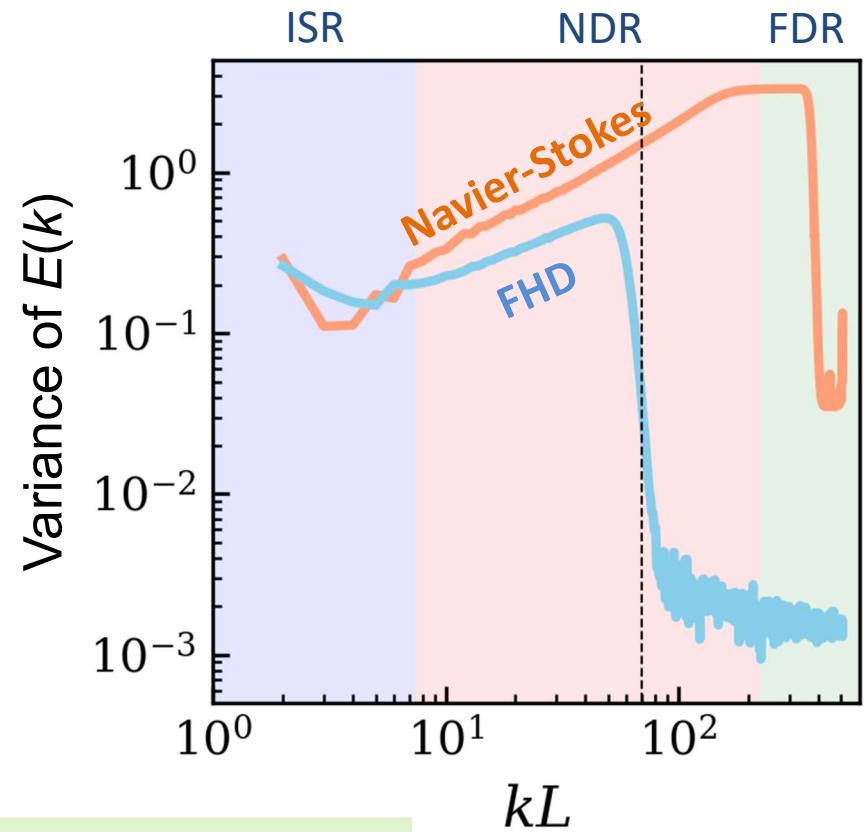
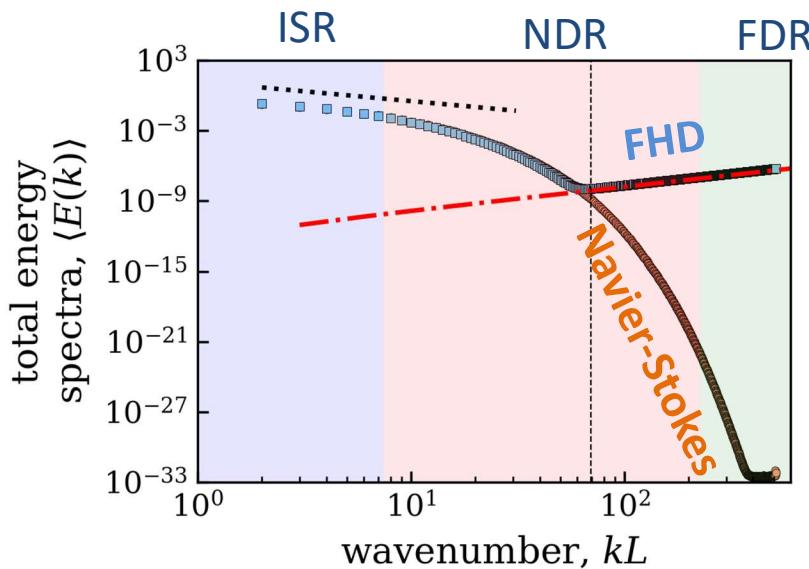


Frisch, *Turbulence: legacy of Kolmogorov*, 1995

turbulence intermittency

- highly non-Gaussian hydrodynamic fields
- localized bursts of extreme activity in a sea of largely quiet flow

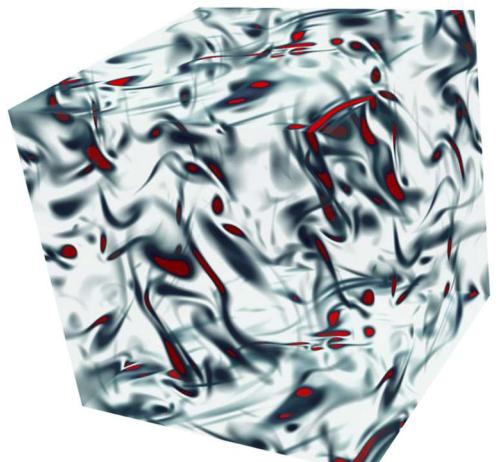
Reduced Temporal Intermittency in the Dissipation Range



Temporal fluctuations in the kinetic energy are substantially reduced across the NDR and FDR

Reduced Intermittency in the Dissipation Range: Vorticity

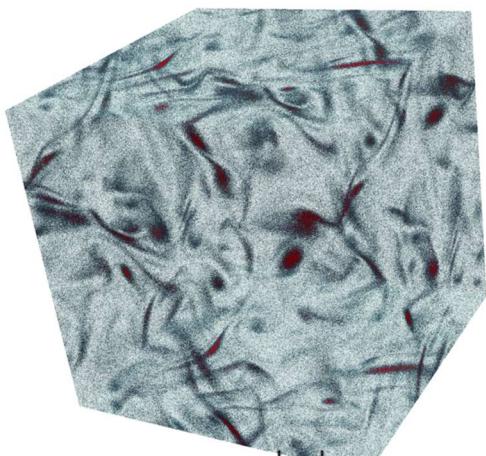
Navier-Stokes



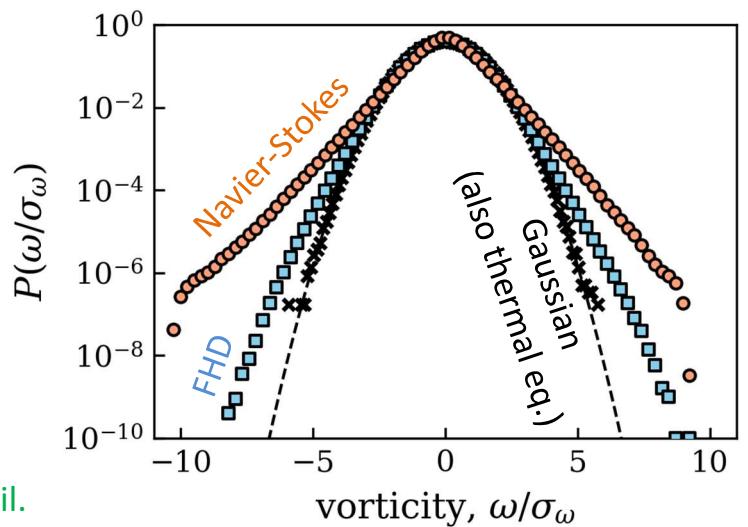
FHD (equil.)



FHD



local vorticity distribution



Sharp vorticity bursts homogenized by thermal fluctuations

0.2mm³ of nitrogen gas, discretized over 1024³ finite-volume grid
2048 AMD MI250X GPUs; 12 hours for 1ms of simulation

Concluding Remarks

- Molecular fluctuations fundamentally modify compressible turbulence at large and practically-relevant length scales \gg molecular mean free path
- Our results indicate that intermittency effects are substantially reduced across the entire dissipation range of turbulence
- Fluctuating hydrodynamics is a (perhaps the only) tractable numerical method to model these effects at such large length scales
- We have developed a robust numerical framework for modeling compressible FHD & turbulence

Thank you for staying for my talk!

<https://github.com/AMReX-FHD/FHDeX>

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