SAND2022-8368C

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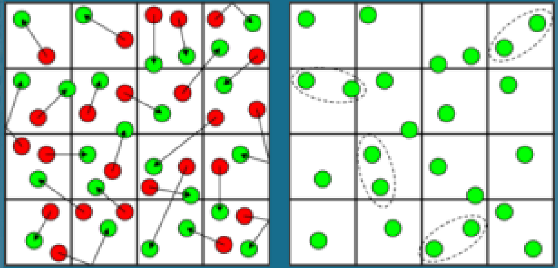
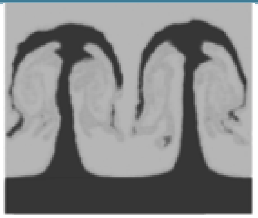
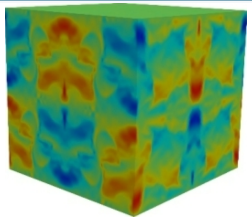
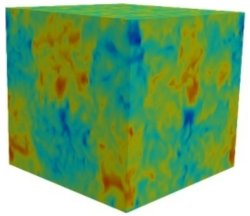
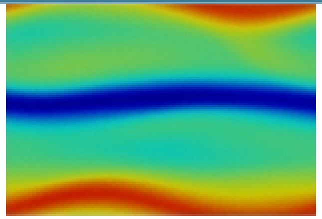
The Navier-Stokes Equations Do Not Describe the Smallest Scales of Turbulence











Ryan M. McMullen, John R. Torczynski, Michael A. Gallis
Engineering Sciences Center, Sandia National Laboratories, Albuquerque, New Mexico

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U.S. DEPARTMENT OF ENERGY NNSA National Nuclear Security Administration

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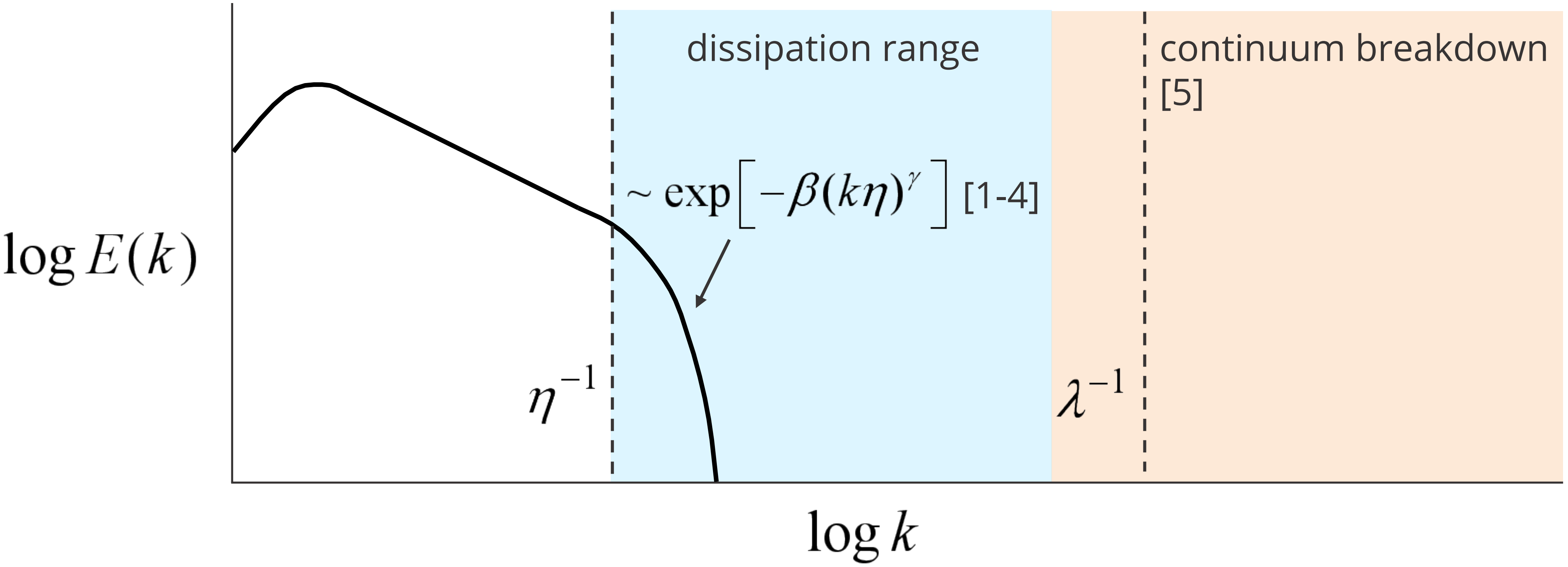
The turbulent energy spectrum according to Navier-Stokes



[1] Chen et al., Phys. Rev. Lett. (1993)
[2] Sirovich et al., Phys. Rev. Lett. (1994)
[3] Khurshid et al., Phys. Rev. Fluids (2018)
[4] Buaria & Sreenivasan, Phys. Rev. Fluids (2020)
[5] Bird, Clarendon Press (1994)

What about thermal fluctuations?

All finite systems exhibit random molecular fluctuations

Center-of-mass velocity u_{th} in volume l^3 :

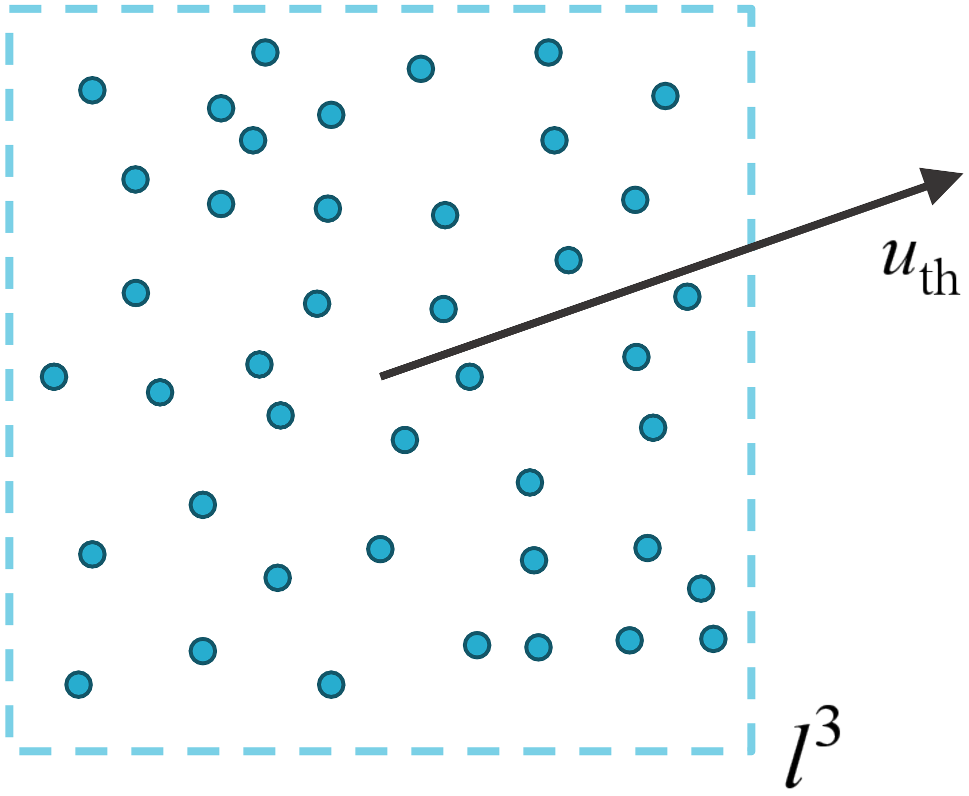
$$\langle u_{\text{th}} \rangle = 0, \quad \langle u_{\text{th}}^2 \rangle \sim \frac{k_B T}{\rho l^3}$$

Compare to kinetic energy in Kolmogorov-scale eddy [1]

$$\theta_\eta \equiv \frac{k_B T}{\rho u_\eta^2 \eta^3} \sim 10^{-9} - 10^{-6}$$

But $E(k)$ decays exponentially fast for $k\eta > 1$…

Thermal fluctuations may dominate dissipation range, even when $k << \lambda^{-1}$ [1,2]



[1] Eyink et al., Phys. Rev. E (2022)
[2] Betchov, J. Fluid Mech. (1957)

Molecular-level simulations of turbulence

Dissipation range is extremely difficult to measure experimentally

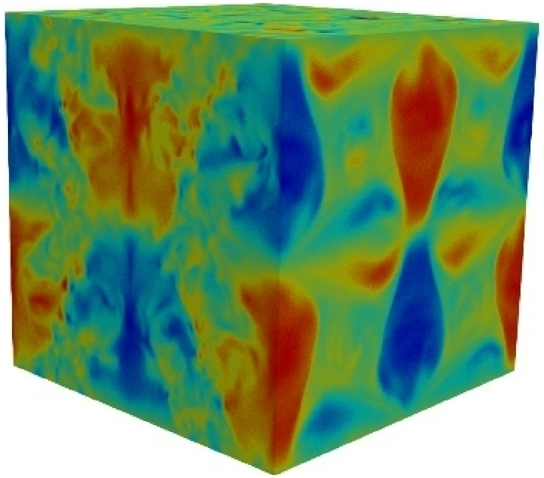
But can investigate with molecular-level simulations

Simulate Taylor-Green (TG) vortex flow [1] using DSMC

- Re = $\rho_0 V L/\mu_0$ = 500, 1000, 1500
- Ma = V/a_0 = 0.3, 0.6, 0.9
- Kn = λ/L = 9.7 x 10^{-4}

Compare with compressible Navier-Stokes (NS) simulations

- Use Sandia's finite-volume code SPARC [2]



[1] Taylor & Green, Proc. R. Soc. Lond. A (1937)
[2] Howard et al., 23rd AIAA CFD (2017)

Direct simulation Monte Carlo (DSMC)

No PDEs solved – tracks very large numbers (~10^{12}) of computational "molecules"

- Each represents $F \gg 1$ actual molecules
- Move ballistically, collide & reflect stochastically
- Flow quantities from averages over molecules in each cell

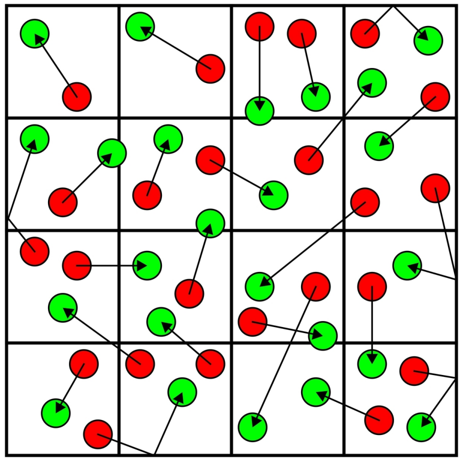
Inherently includes physics usually not in NS

- Thermal and chemical nonequilibrium
- Pressure and heat-flux tensor anisotropy
- Thermal fluctuations

Simulates gas flows very accurately

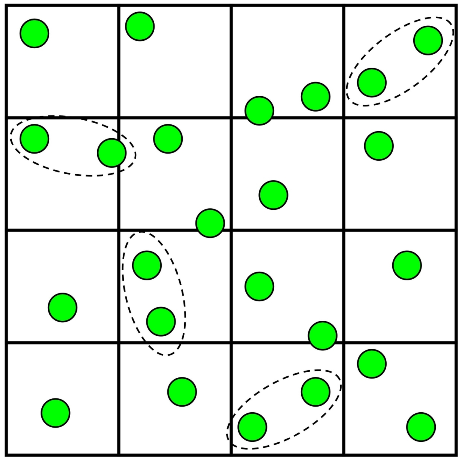
- Converges to solutions of the Boltzmann Equation [1]
- Reproduces Chapman-Enskog distribution [2]

move



$$\frac{\mathrm{d}\mathbf{x}_i}{\mathrm{d}t} = \mathbf{v}_i$$

collide



$$\frac{\mathrm{d}(m_i \mathbf{v}_i)}{\mathrm{d}t} = \mathbf{F}(\mathbf{x}_i) + \mathbf{C}(\mathbf{v}_i)$$

[1] Wagner, J. Stat. Phys. (1992)
[2] Gallis et al., Phys. Rev. E (2004)

SPARTA: An exascale DSMC code

SPARTA: Stochastic PArallel Rarefied-gas Time-accurate Analyzer

Implementation is similar to Molecular Dynamics (MD)

- Single-processor to massively-parallel platforms
- Load balancing, in-situ visualization, on-the-fly FFTs, adaptive grid

Extremely complicated geometries can be treated

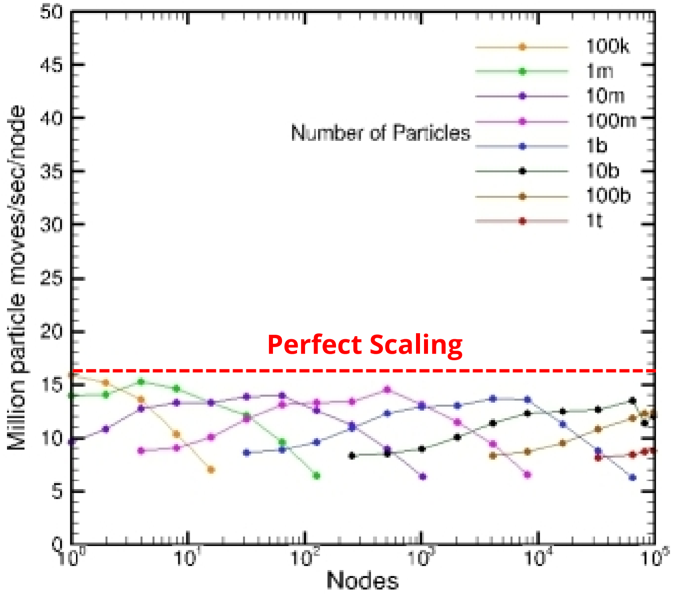
- Domain can be 2D, axisymmetric, 3D
- Gas molecules use hierarchical Cartesian "ijk" grid
- Body surfaces represented by triangular elements which cut gas grid cells

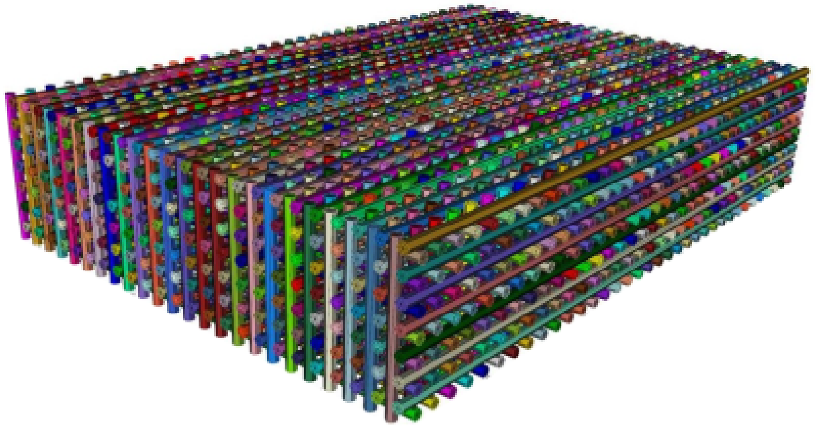
Developed with next-generation architectures in mind

- Write application kernels only once
- Efficient on many platforms: GPU, manycore, heterogeneous, ...

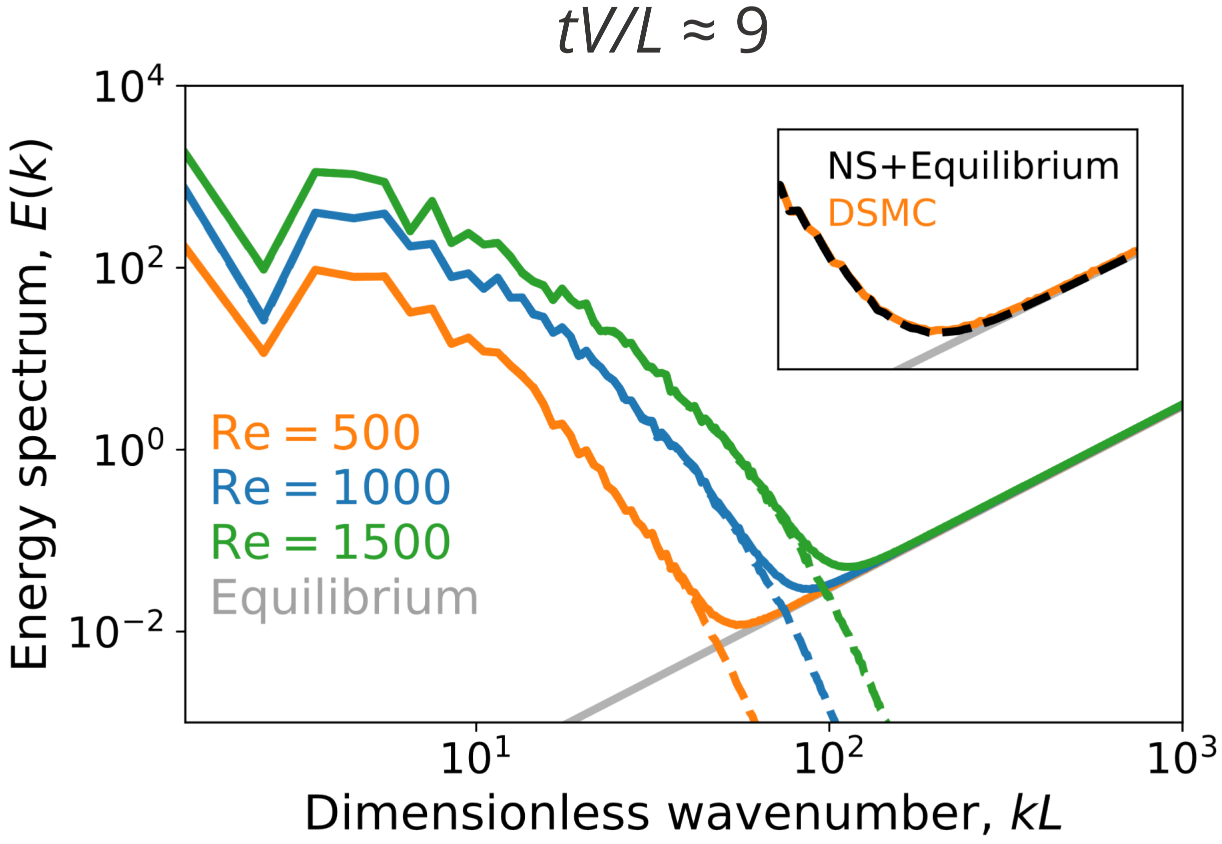
Open-source code available: http://sparta.sandia.gov

- 10,000+ downloads, 100+ verified users worldwide
- Collaborators: ORNL, LANL, ANL, LBNL, NASA, Purdue, UIUC, ESA





DSMC and NS spectra comparison



Equilibrium spectrum: $E(k) = F\frac{3k_BT}{4\pi^2\rho}k^2$

Excellent agreement for low k

DSMC spectra show large-k departure from NS due to thermal fluctuations

NS equations are inaccurate for $k > k_c$

Fluctuation variance overestimated in DSMC when $F > 1$

- These simulations use $F = 16{,}154$
- Want to determine the k_c that would be observed in a physical gas

Equilibrium DSMC spectra

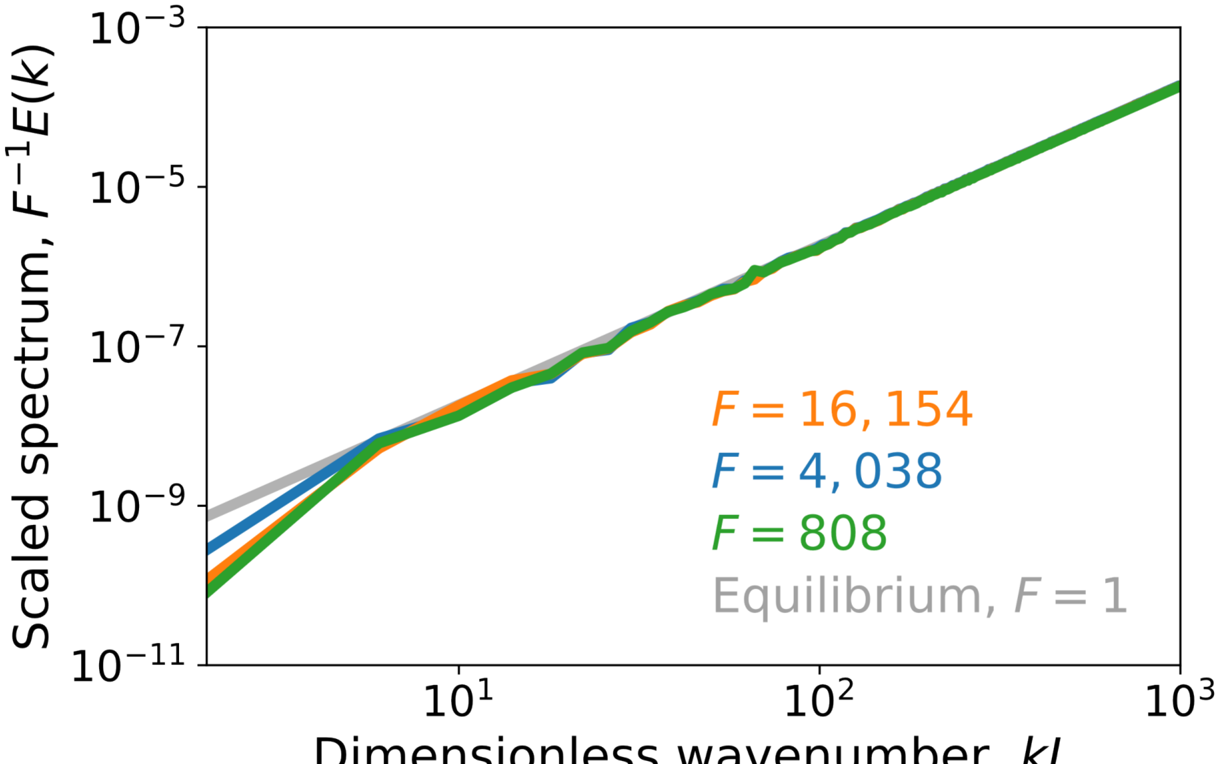
Equilibrium spectrum:

$$E(k) = F\frac{3k_B T}{4\pi^2 \rho}k^2$$

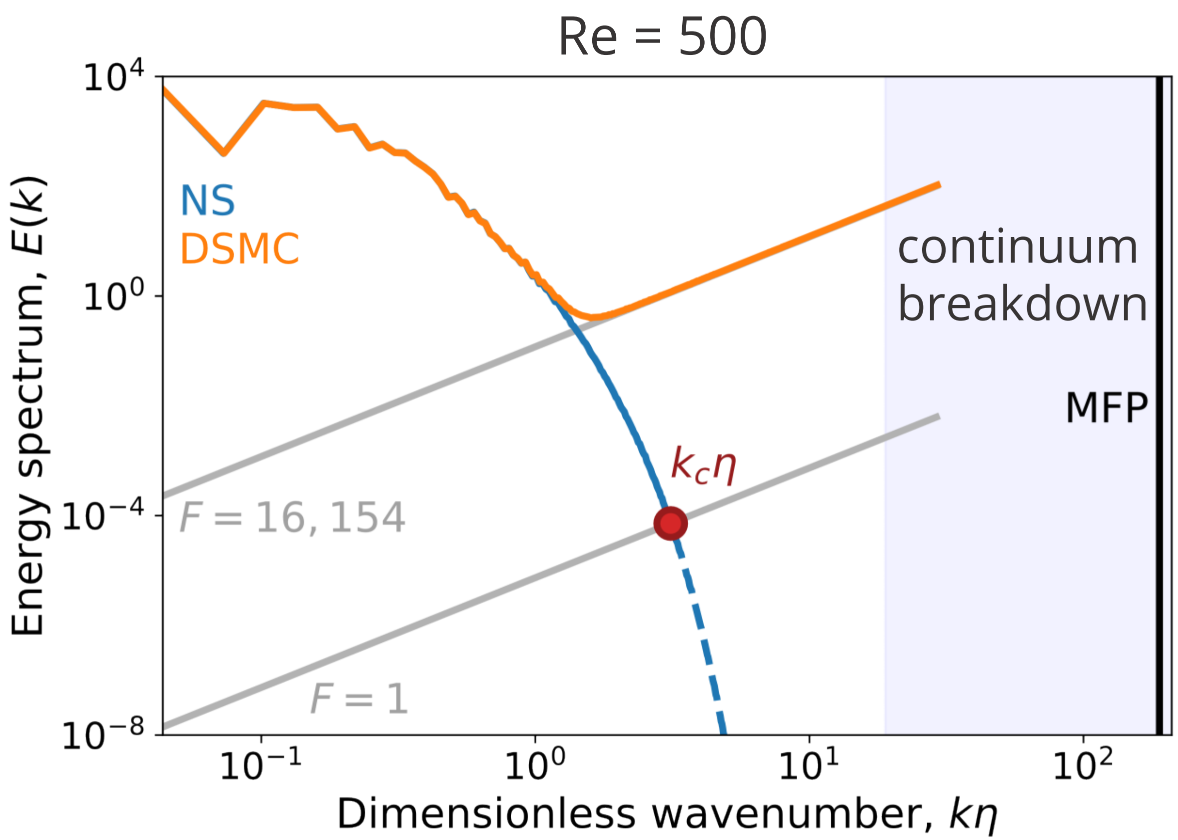
DSMC spectra obey simulation ratio scaling

F = 1 corresponds to physical gas

- Use this to determine k_c



Crossover wavenumber



$$k_c \eta \approx 3.1$$

Thermal fluctuations dominate almost the entire dissipation range

- Similar for other Re
- Agrees with fluctuating hydrodynamics predictions for liquids [1]

$$l_c / \lambda \approx 61$$

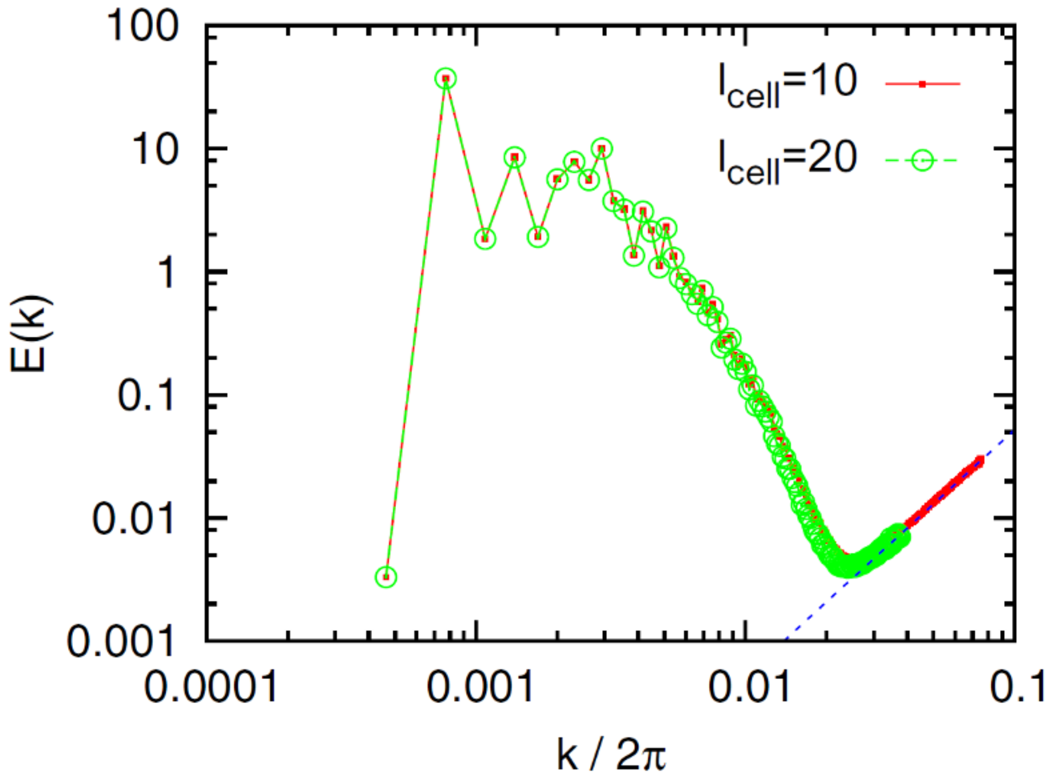
Crossover scale is in a regime where NS equations widely believed to be valid [2]

[1] Bell et al., J. Fluid Mech. (2022)
[2] Bird, Clarendon Press (1994)

Molecular-dynamics simulations

Komatsu et al. [1] observed thermal fluctuations in MD simulations of TG flow

- Crossover at $k\eta \approx 1$
- But $\eta \approx 7$ molecular diameters ($\sim \lambda$)
  - $\theta_\eta \approx 0.5$
  - Present DSMC: $\theta_\eta \sim 10^{-6}$
- Concluded observable only due to microscopic system size



[1] Komatsu et al., Int. J. Mod. Phys. C (2014)

Thermal-fluctuation effects on other statistics

Equilibrium spectrum for $k > k_c$ suggests simple model for velocity

$$u_i = u_i^{\mathrm{NS}} + u_i^{\mathrm{th}},$$

$$u_i^{\mathrm{th}} \sim \mathrm{N}\left(0, Fk_BT / \rho l^3\right)$$

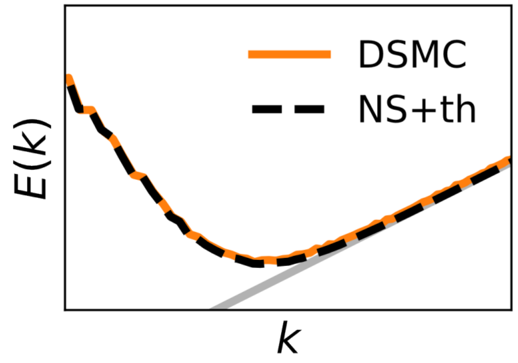
Use to look at other statistics, e.g. longitudinal structure functions

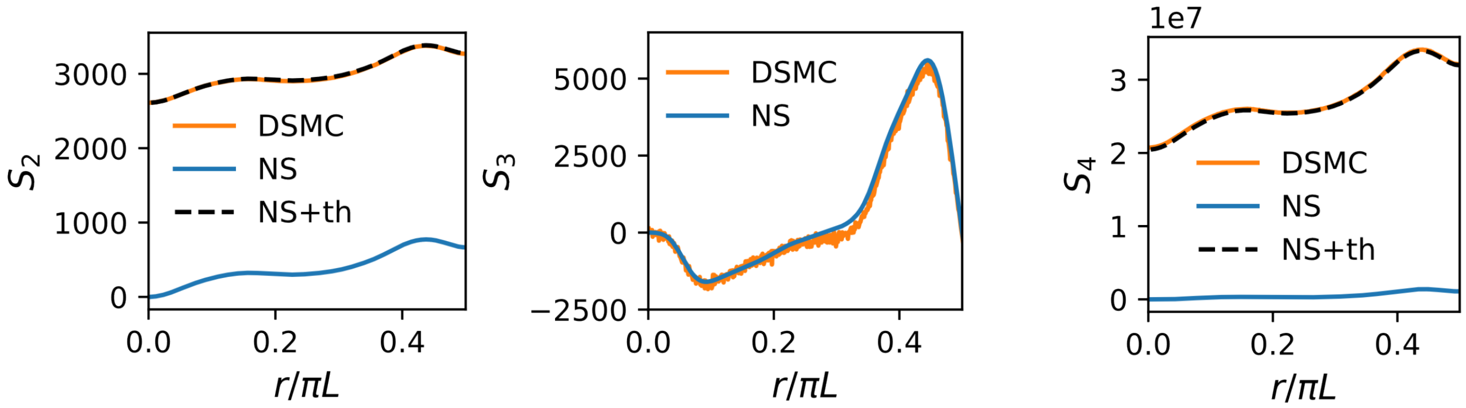
$$S_n(r) = \langle [u(x+r) - u(x)]^n \rangle$$

$$S_2(r) = S_2^{\mathrm{NS}}(r) + 2\frac{Fk_BT}{\rho l^3},$$

$$S_3(r) = S_3^{\mathrm{NS}}(r),$$

$$S_4(r) = S_4^{\mathrm{NS}}(r) + 12\frac{Fk_BT}{\rho l^3}S_2^{\mathrm{NS}}(r) + 12\left(\frac{Fk_BT}{\rho l^3}\right)^2$$





Structure function predictions for $F = 1$

Separate into NS and thermal correction:

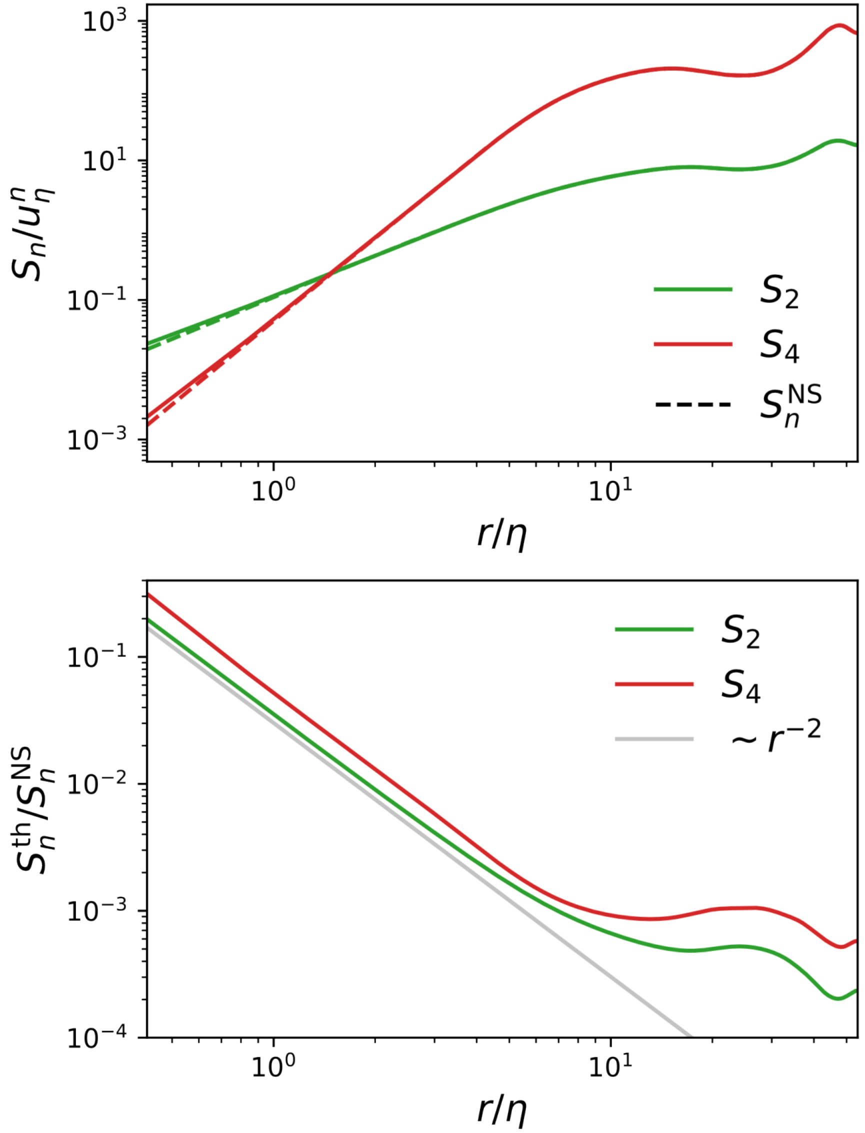
$$S_2(r) = S_2^{\mathrm{NS}}(r) + \underbrace{2\frac{k_B T}{\rho l^3}}_{S_2^{\mathrm{th}}}$$

$$S_4(r) = S_4^{\mathrm{NS}}(r) + \underbrace{12\frac{k_B T}{\rho l^3} S_2^{\mathrm{NS}}(r) + 12\left(\frac{k_B T}{\rho l^3}\right)^2}_{S_4^{\mathrm{th}}}$$

Significant deviations (~ 5%) at $r = \eta$

- Grow like r^{-2}
- Thermal fluctuations dominate for separations smaller than

$$\frac{r^*}{\eta} \sim \theta_\eta^{1/2}\left(\frac{l}{\eta}\right)^{-3/2}$$



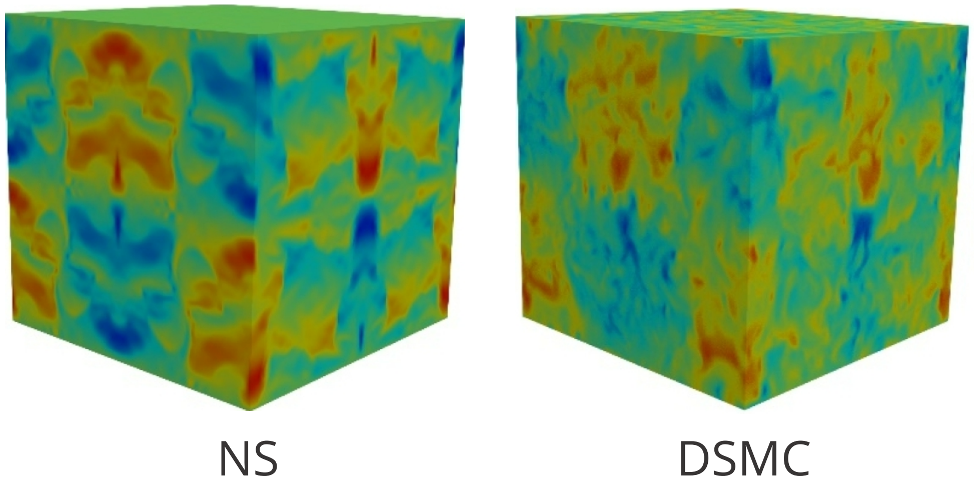
Thermal-fluctuation effects on larger scales

No observed effects on global or large-scale statistics

However, they do influence realizations of larger scales [1,2]

Implications for predictability?

- Maximal Lyapunov exponent? [1,3,4]
  - $\delta(t) \sim \exp(\mathrm{Re}^{\beta}\, t)$
- Superfast amplification? [5]
  - $\delta(t) \sim \exp(C\, \mathrm{Re}^{1/2}\, t^{1/2} + C_1 t)$
- Spontaneous stochasticity? [6-9]
  - "Intrinsic randomness"



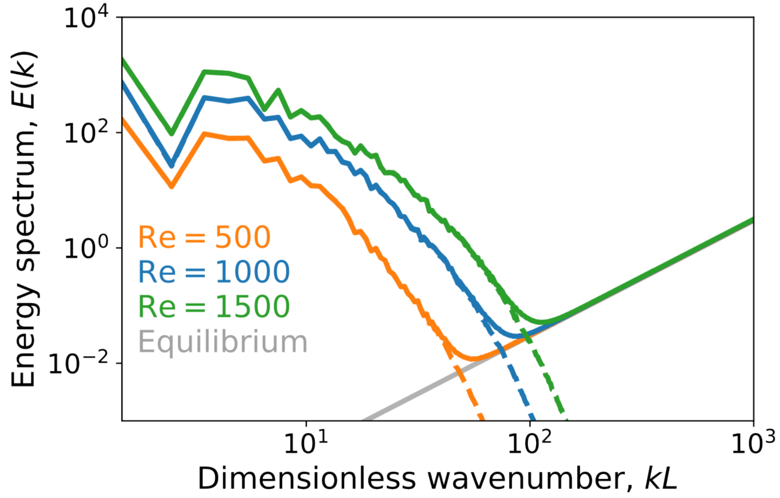
[1] Ruelle, Phys. Lett. A (1979)
[2] Gallis et al. Phys. Rev. Fluids (2021)
[3] Boffetta & Musacchio, Phys. Rev. Lett. (2017)
[4] Berera & Ho, Phys. Rev. Lett. (2018)
[5] Li et al., J. Fluid Mech. (2020)
[6] Lorenz, Tellus (1969)
[7] Kupiainen, Ann. Henri Poinaré (2003)
[8] Eyink & Bandak, Phys. Rev. Res. (2020)
[9] Thalabard et al., Comms. Phys. (2020)

Summary

R. M. McMullen, M. C. Krygier, J. R. Torczynski, and M. A. Gallis,
Phys. Rev. Lett. **128**, 114501 (2022).

DSMC shows that the Navier-Stokes equations are not accurate in the dissipation range for turbulence in gases

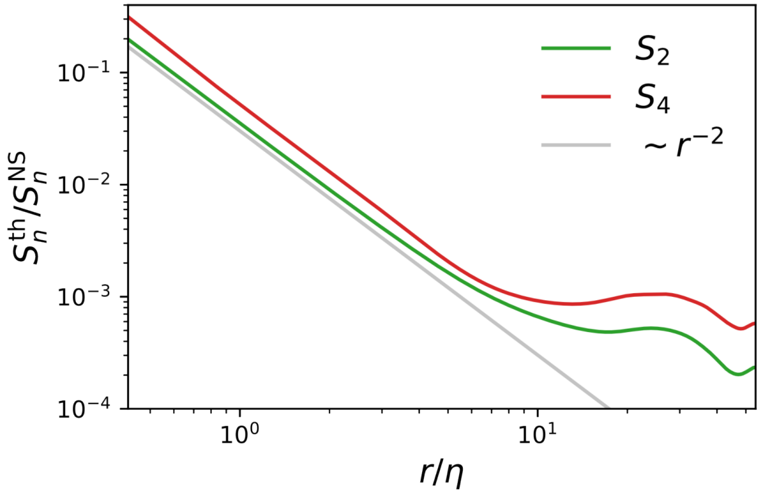
$$k_c \eta = O(1),$$
$$l_c / \lambda \; ? \; 1$$



Agrees with previous estimates [1,2] fluctuating hydrodynamics simulations of liquids [3], and microscopic MD simulations [4]

Simple model for velocity field reproduces DSMC structure functions

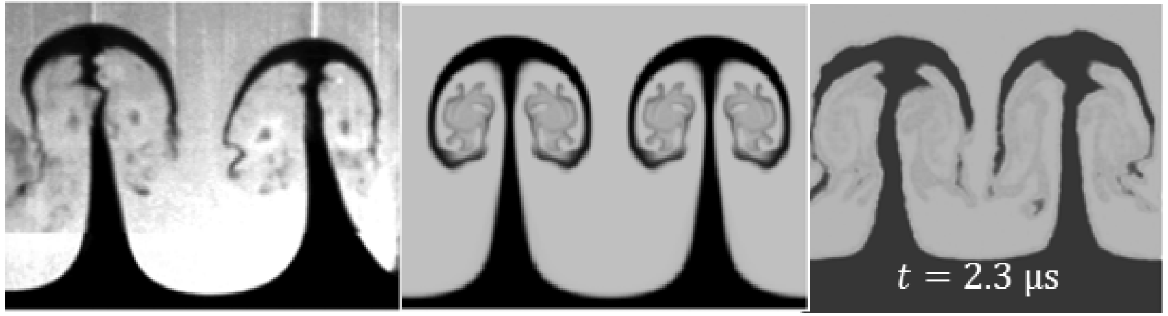
- Predicts significant modifications below Kolmogorov scale



What role do thermal fluctuations play in predictability?

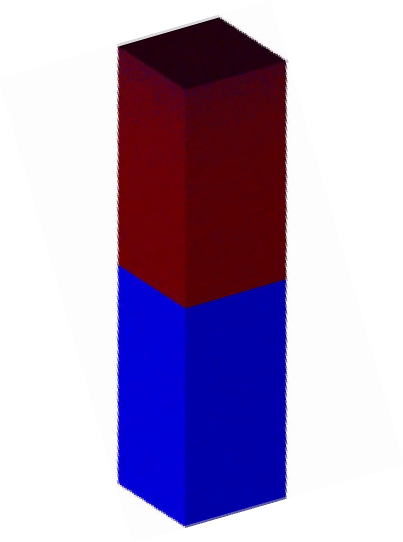
[1] Betchov, J. Fluid Mech. (1957)
[2] Eyink et al., Phys. Rev. E (2022)
[3] Bell et al., J. Fluid Mech (2022)
[4] Komatsu et al., Int. J. Mod. Phys. C (2014)

DSMC simulations of other near-continuum flows

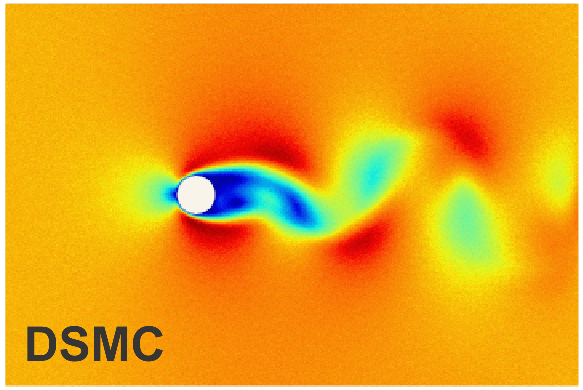


Experiment [1] CFD [1] DSMC

Richtmyer-Meshkov



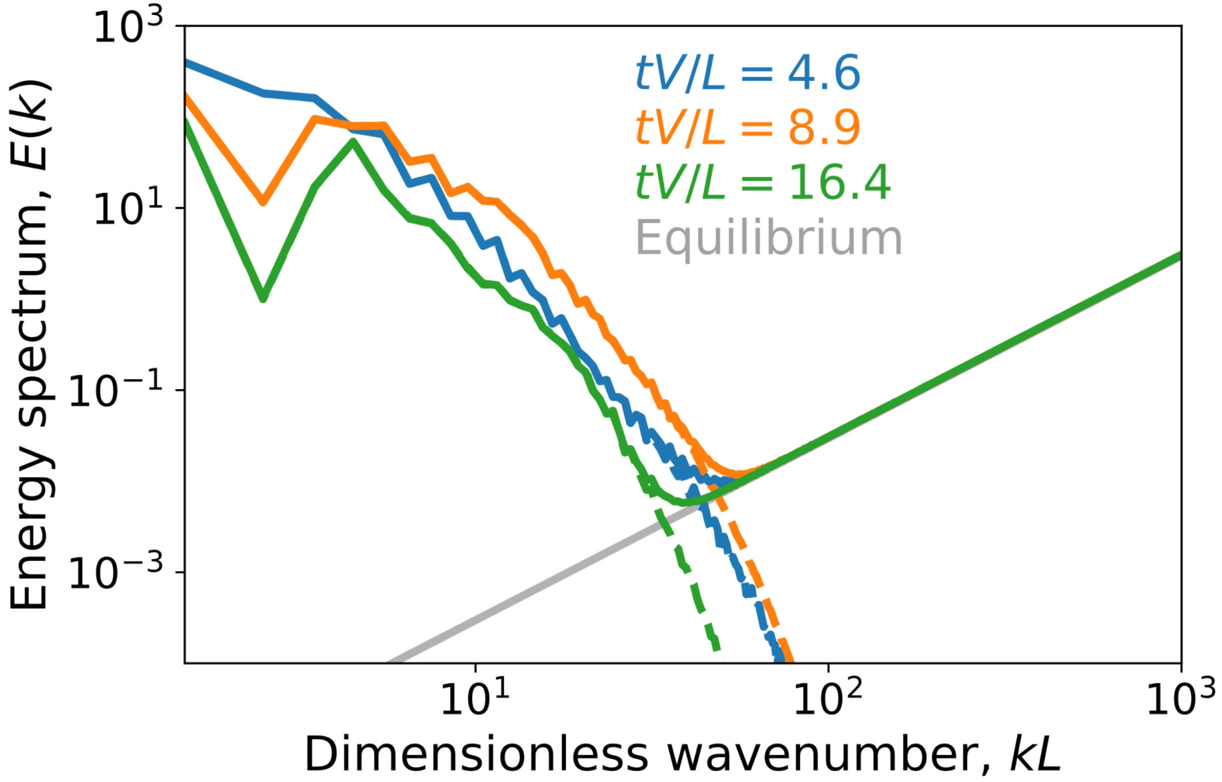
Rayleigh-Taylor



Vortex shedding with slip

[1] Morgan et al., J. Fluid Mech (2012)

Re = 500 spectra at different times

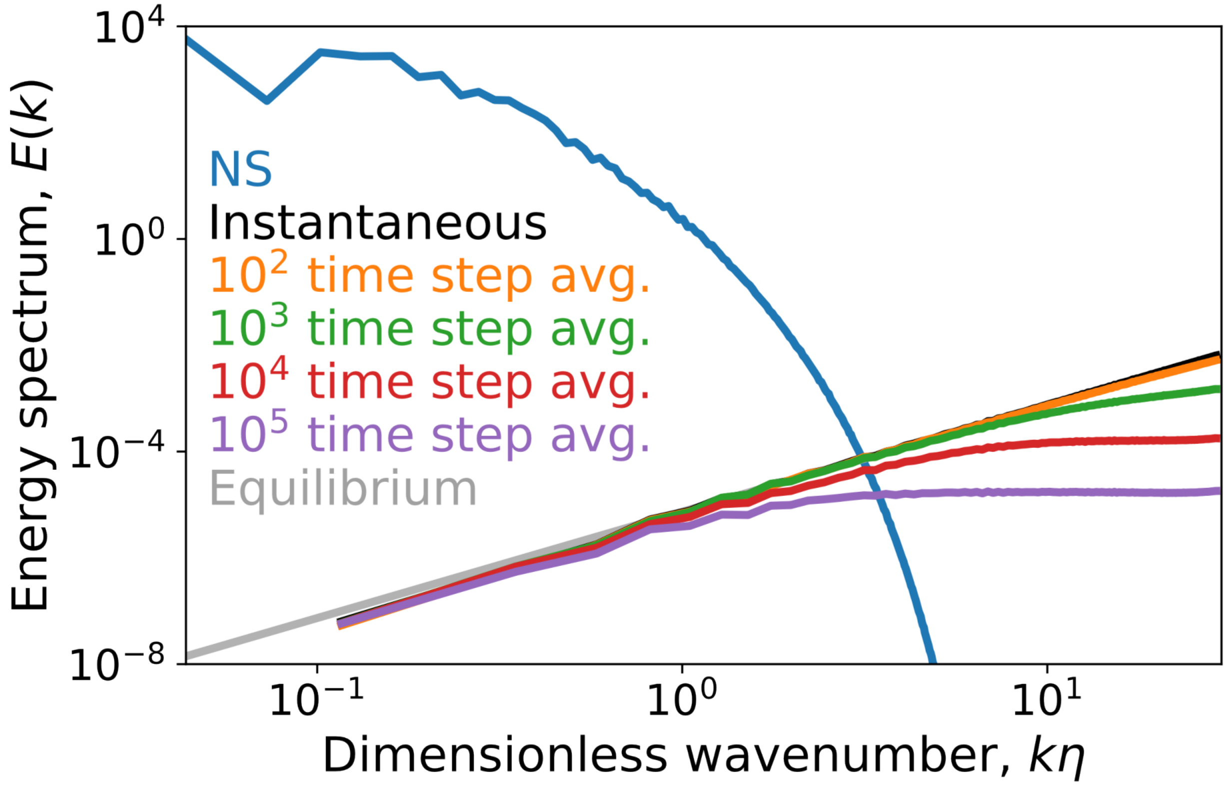


Time averaging

Averaging is common practice to reduce statistical noise in DSMC

Here, 10^5 timesteps corresponds to $\approx 0.5\tau_\eta$

Only changes crossover scale by ≈10%



Viscosity determination for DSMC

Cells are large, so transport is enhanced

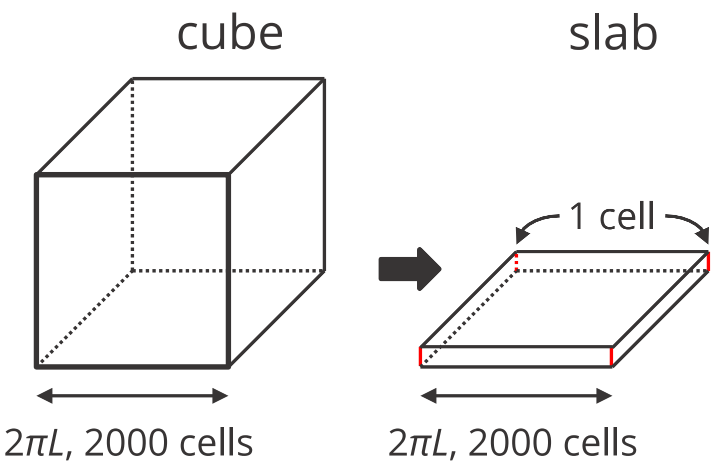
- Viscosity is 36% larger than molecular value
- Near-neighbor collisions reduce mean collision separation

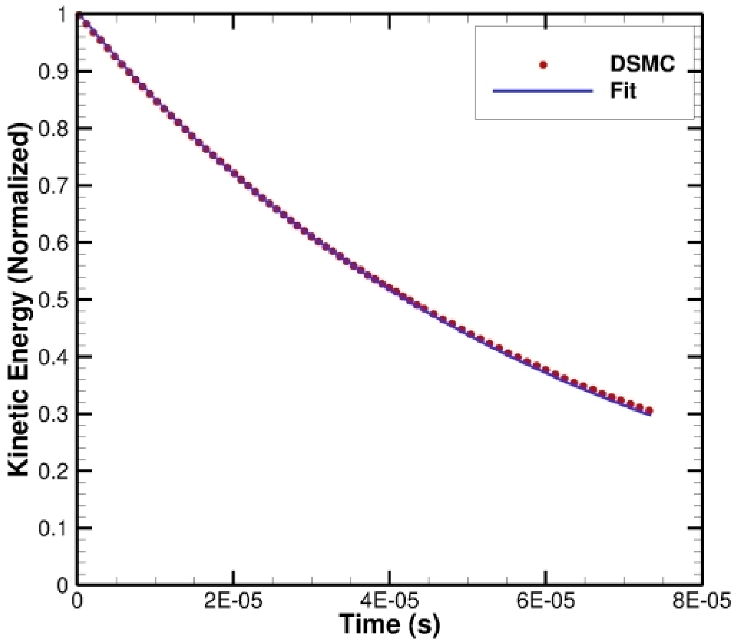
Simulate some other flow to find viscosity

- Use a similar but much easier flow
- 2D TG vortex energy decay:

$$E = E_0 \exp(-4\mu_{\text{eff}} t / \rho_0 L^2)$$

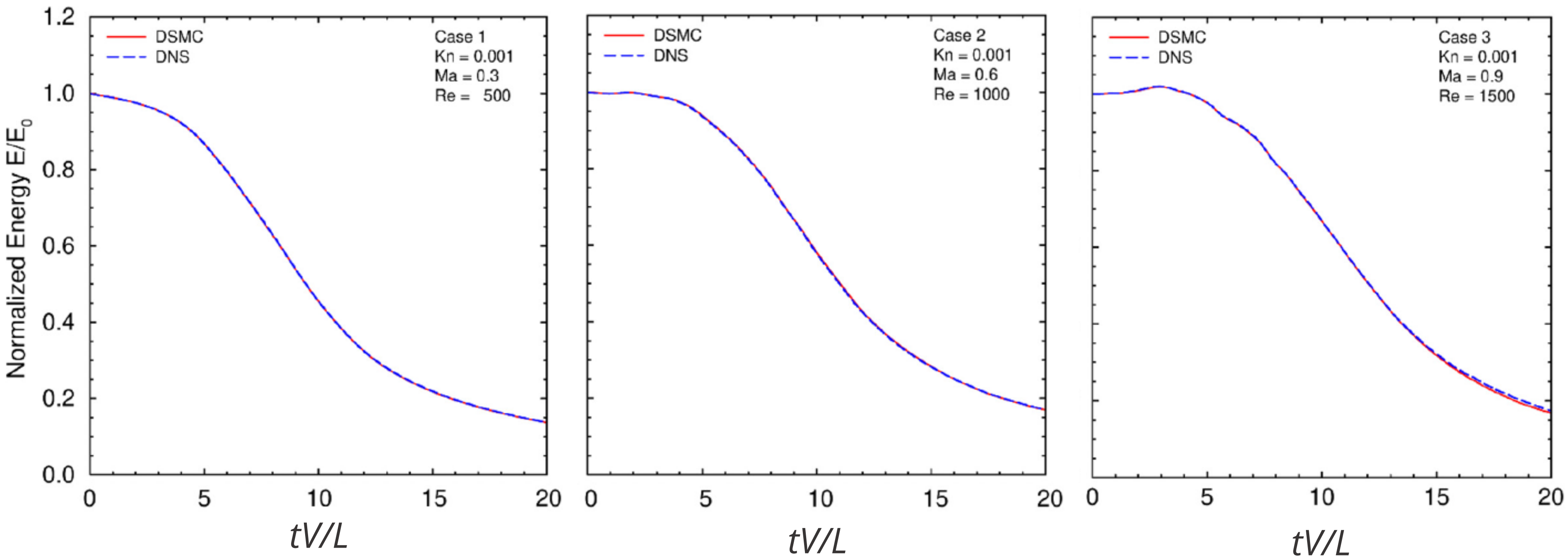
Use effective viscosity in NS simulations for comparison





Kinetic energy decay

Excellent agreement between MGD and NS! *



*DSMC data are time-averaged before computing energy