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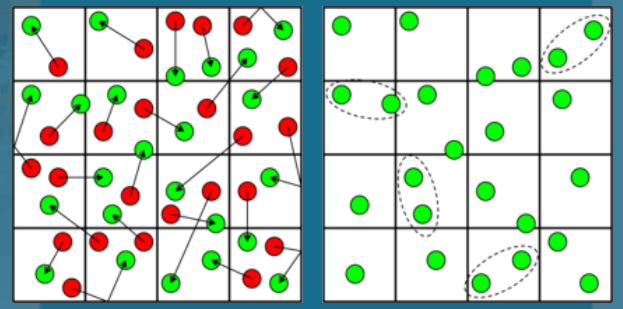
Noncontinuum Effects at the Smallest Scales of Turbulence



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32nd International Symposium on Rarefied Gas Dynamics
Seoul, South Korea, July 4-8, 2022

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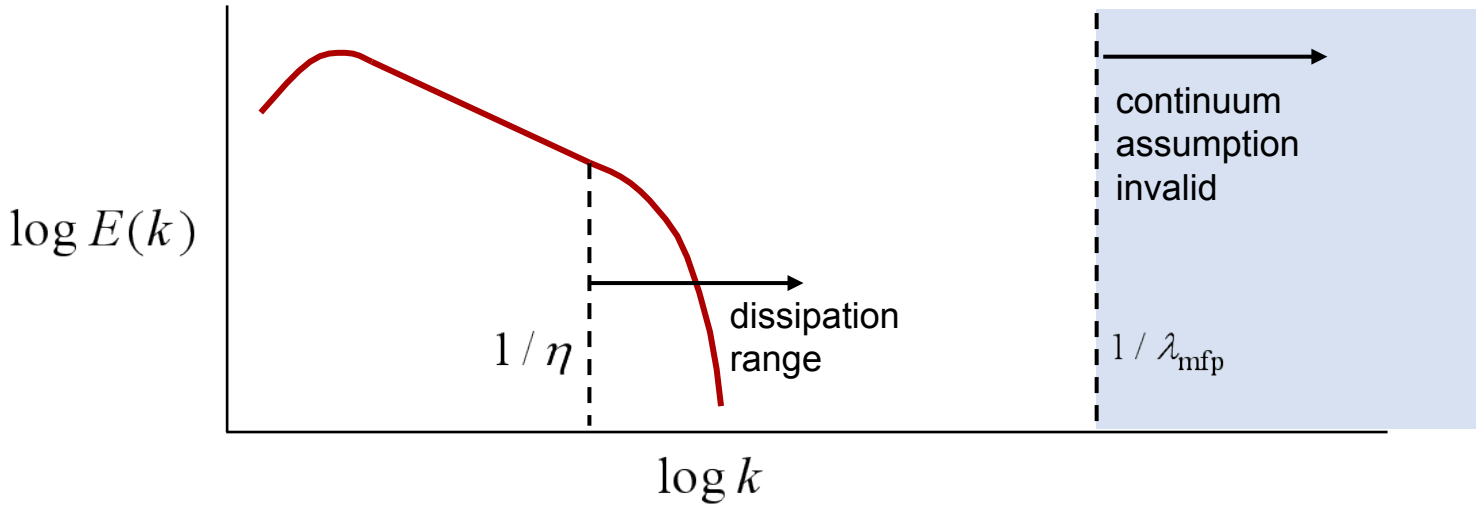
Classical Understanding of Turbulence

- Fully turbulent flows consist of a wide range of scales that are categorized (somewhat arbitrarily) as ranging from large to small.
- Large scales are about the size of the flow and contain most of the energy.
- Small scales are responsible for most of the energy dissipation (dissipation range).



Energy Cascade

Are the Microscopic and Macroscopic Levels of Turbulence Decoupled?

- In the study of turbulence, the Navier-Stokes (NS) equations are usually regarded as the fundamental mathematical equations.
- When the Knudsen number is large and rarefaction effects are therefore important, the Boltzmann equation is used to describe rarefied gas dynamics.
- **Usually** rarefaction effects are absent in turbulence and turbulence is absent in rarefied flow because the Knudsen number is inversely proportional to the Reynolds number.
- Betchov (1957 JFM and 1960 RGD-2) and more recently Eyink (2021) suggested that thermal fluctuations (absent in the NS equations) can terminate the cascade at scales that are much larger than the mean free path.
- The small scales of turbulence are not experimentally accessible.
- However, these length scales are accessible to molecular simulations.

Simulating turbulence at the molecular level
Can we learn something?

Are the hydrodynamic and molecular length and time scales too far apart?

For a **gas** flow with a turbulent Mach number Ma and a turbulent Reynolds number Re, the ratio of the Kolmogorov length scale to the mean free path scales as:

$$Re^{1/4}/Ma$$

The ratio of the Kolmogorov time scale to the mean collision time scales as:

$$Re^{1/2}/Ma^2$$

Thus, for Re = 10,000 and Ma = 1, these ratios are only O(10) and O(100)

New length scales may be introduced

- Gas-surface interactions (velocity slip, temperature jump)
- Shock-turbulence interactions (shock thickness, O(10) mean free paths)
- Chemical reactions in turbulent flow (non-equilibrium energy transfer)

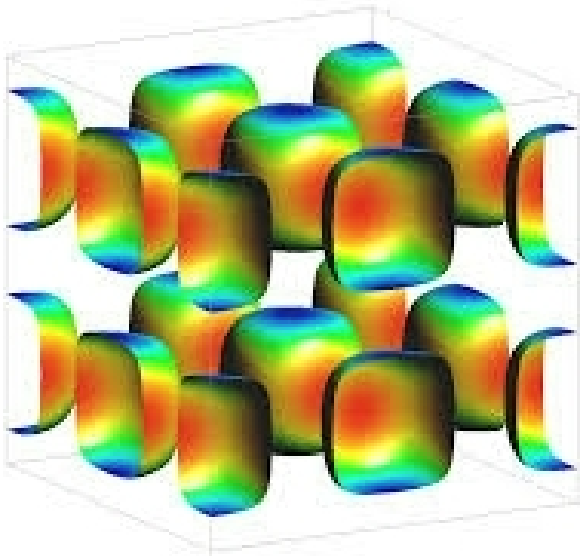
Taylor-Green Vortex Flow

Taylor-Green (TG) vortex flow is a generic turbulent flow

- Often used in validation of codes and evaluation of subgrid scale models
- Initial condition contains only a single length scale (single wave number)

Turbulent energy cascade can be observed numerically in TG flow

- Flow undergoes a rapid build-up of a fully turbulent spectrum
- Late-time flow exhibits basic features of homogeneous isotropic turbulence



Initial vorticity isosurface

$$u = V_0 \sin[x/L]\cos[y/L]\cos[z/L]$$

$$v = -V_0 \cos[x/L]\sin[y/L]\cos[z/L]$$

$$w = 0$$

$$p = p_0 + \left(\rho_0 V_0^2/16\right)\left(\cos[2x/L] + \cos[2y/L]\right)\left(2 + \cos[2z/L]\right)$$

$$-\pi L \le \{x, y, z\} \le \pi L$$

$$E = \int \frac{1}{2}\rho\left(u^2 + v^2 + w^2\right)dV = \text{turbulent kinetic energy}$$

Taylor-Green Simulation Conditions

Numerical parameters

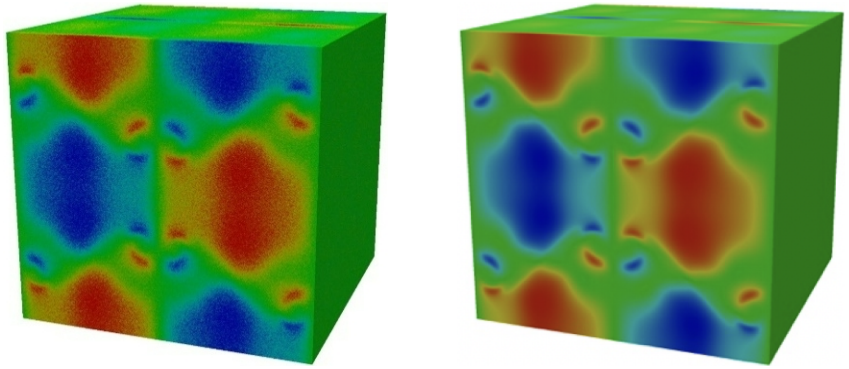
- Cubical domain, triply periodic boundaries
- Side length = $2\pi L$, L = 0.0001 m
- Total cells 2000^3 = 8 billion
- Time step = 0.01-0.25 ns, near-neighbor collisions
- Molecule Simulators = 0.36 trillion
- Simulation ratio = 16,154
- Time averaging window 10,000 timesteps
- Re = 500, 1000, 1500

Gas parameters

- Molecular mass = 66.3×10^{-27} kg, monatomic
- Temperature = 273.15 K, viscosity = 2.985×10^{-5} Pa·s
- Molecular model = HS

Simulation Parameters

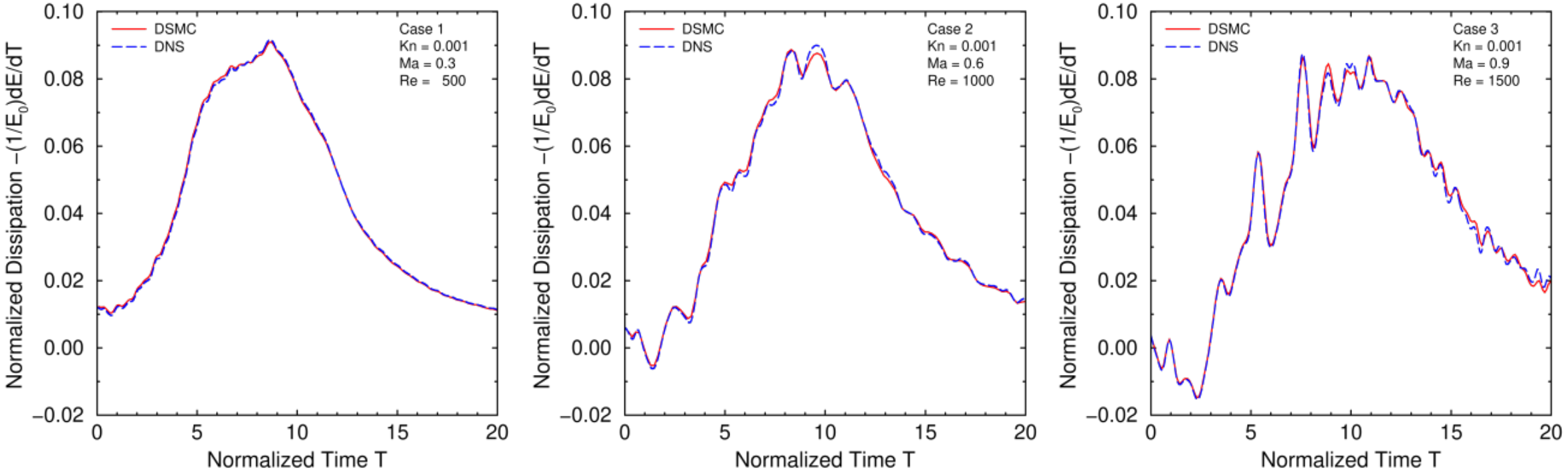
Simulations performed on LLNL/Sierra



DSMC DNS

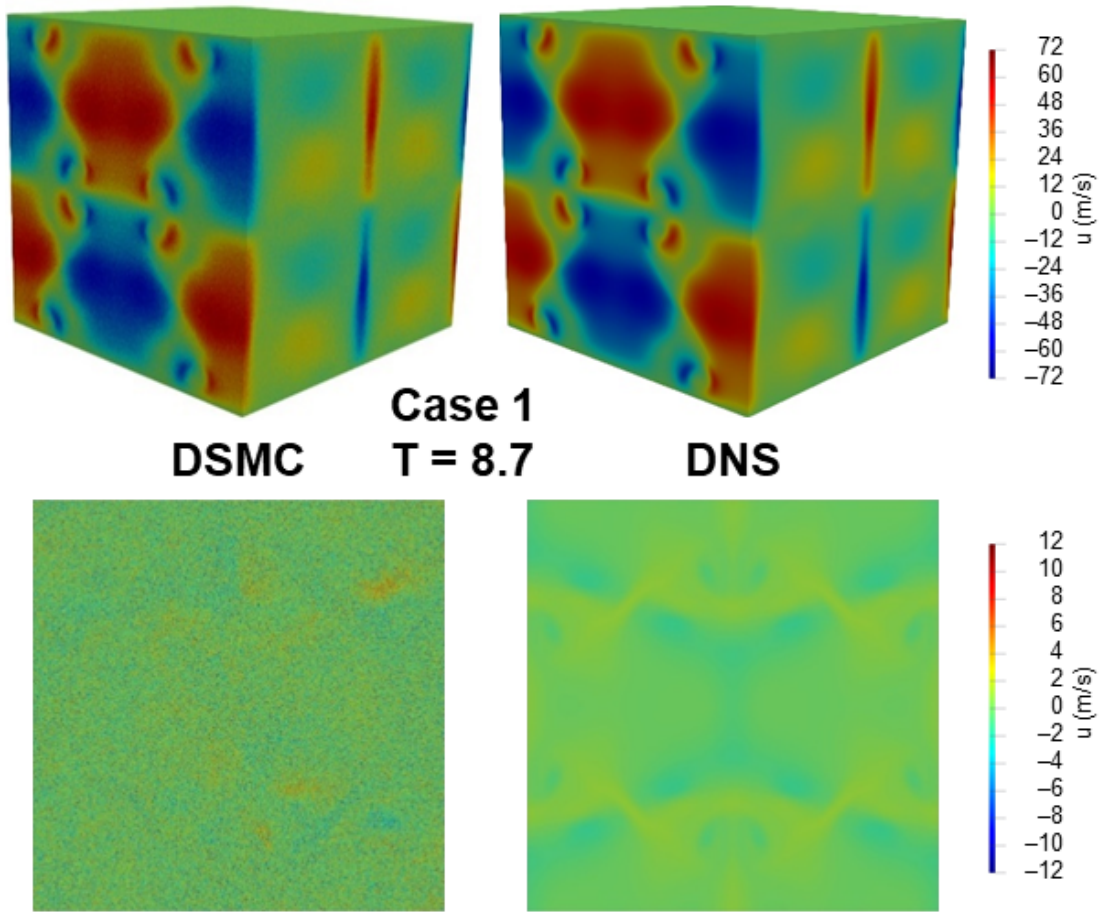
Taylor-Green flow from simulations.

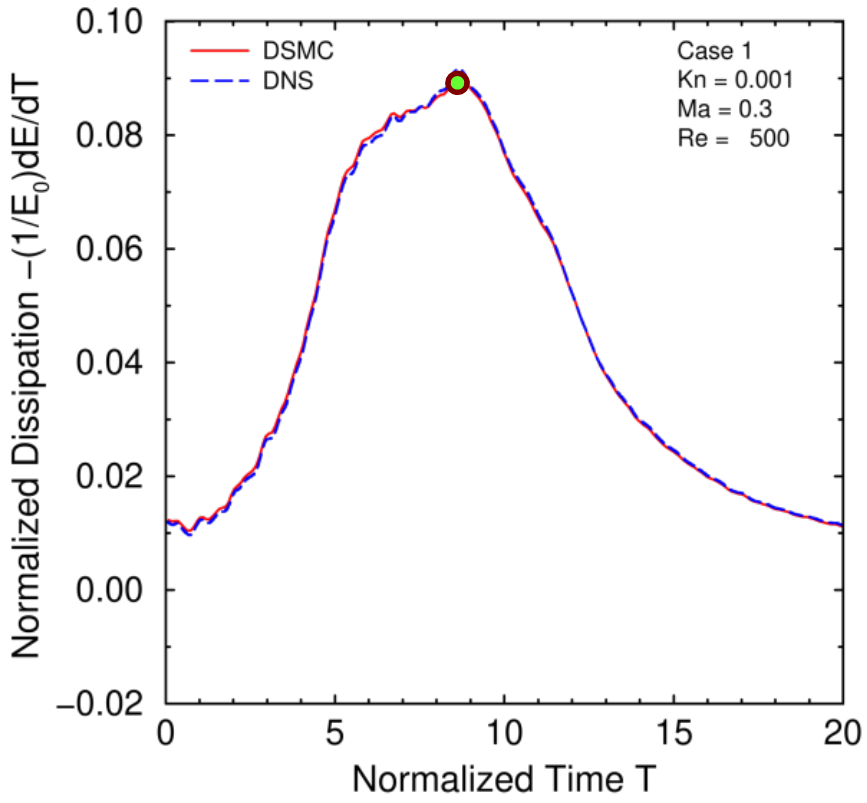
TG Energy Dissipation



Energy dissipation reveals the fine details of the energy cascade.
DSMC and DNS produce the same evolution of the initial conditions to the turbulent state.

TG Ma=0.3, T=8.7

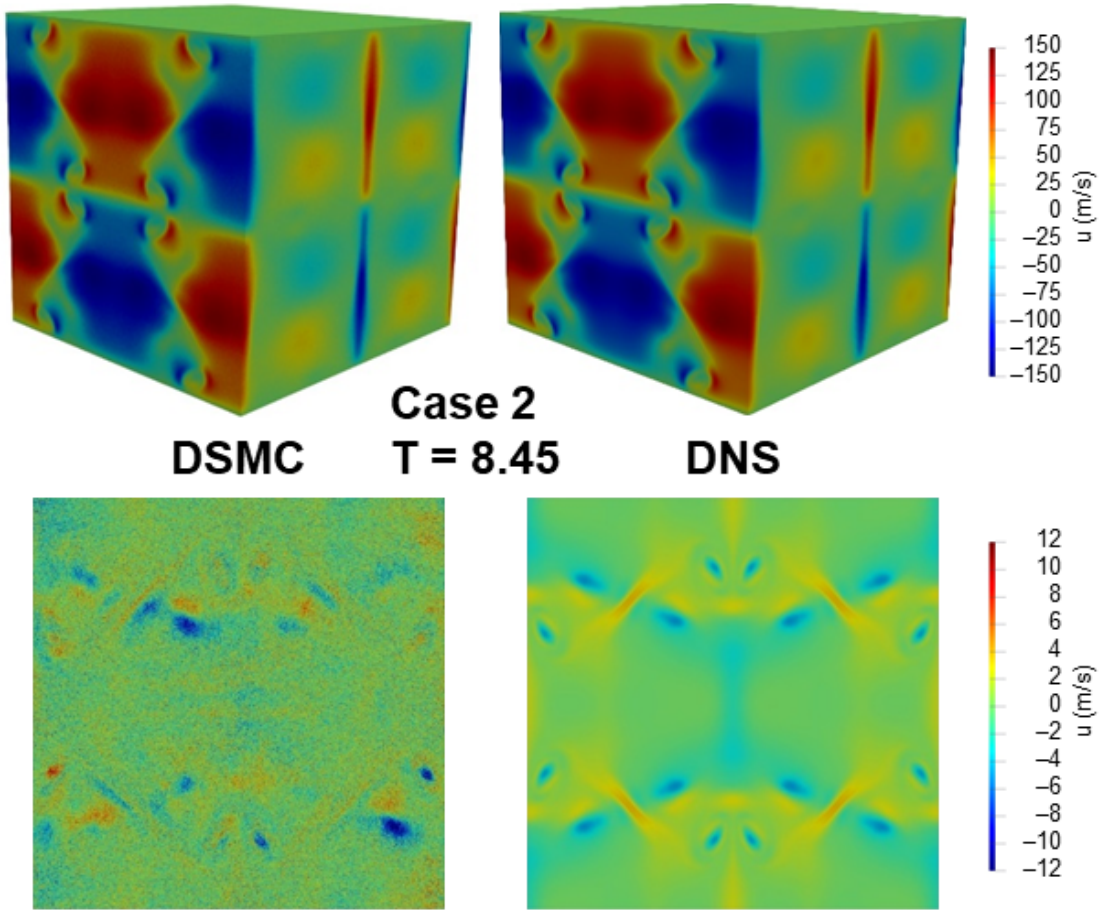


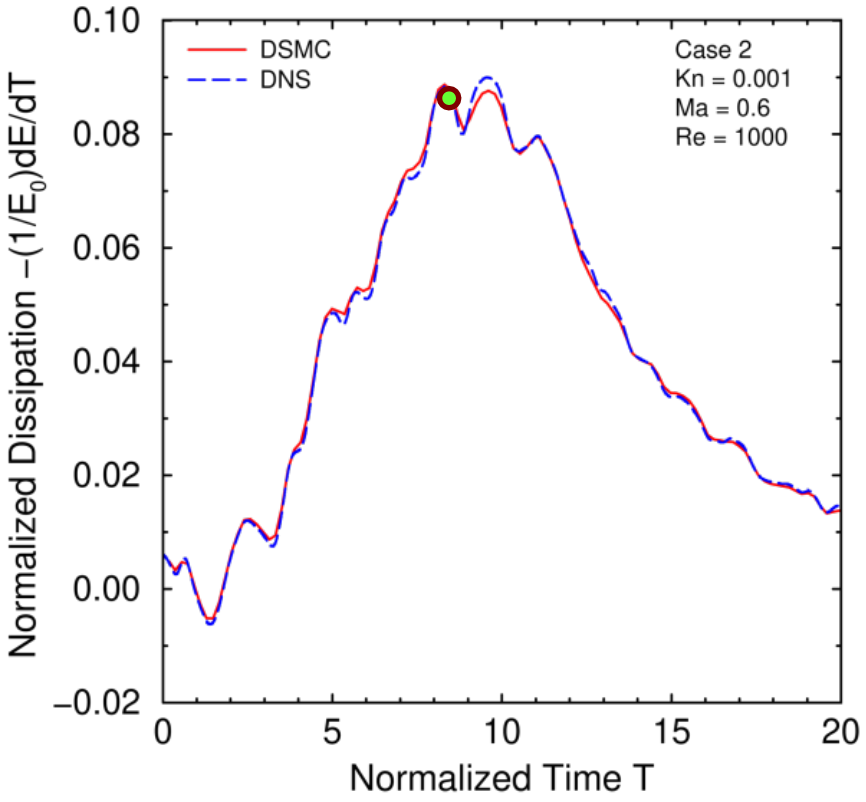


Flow fields have been averaged over 10,000 moves

DSMC and DNS agree up to the point of maximum dissipation

TG Ma=0.6, T=8.45

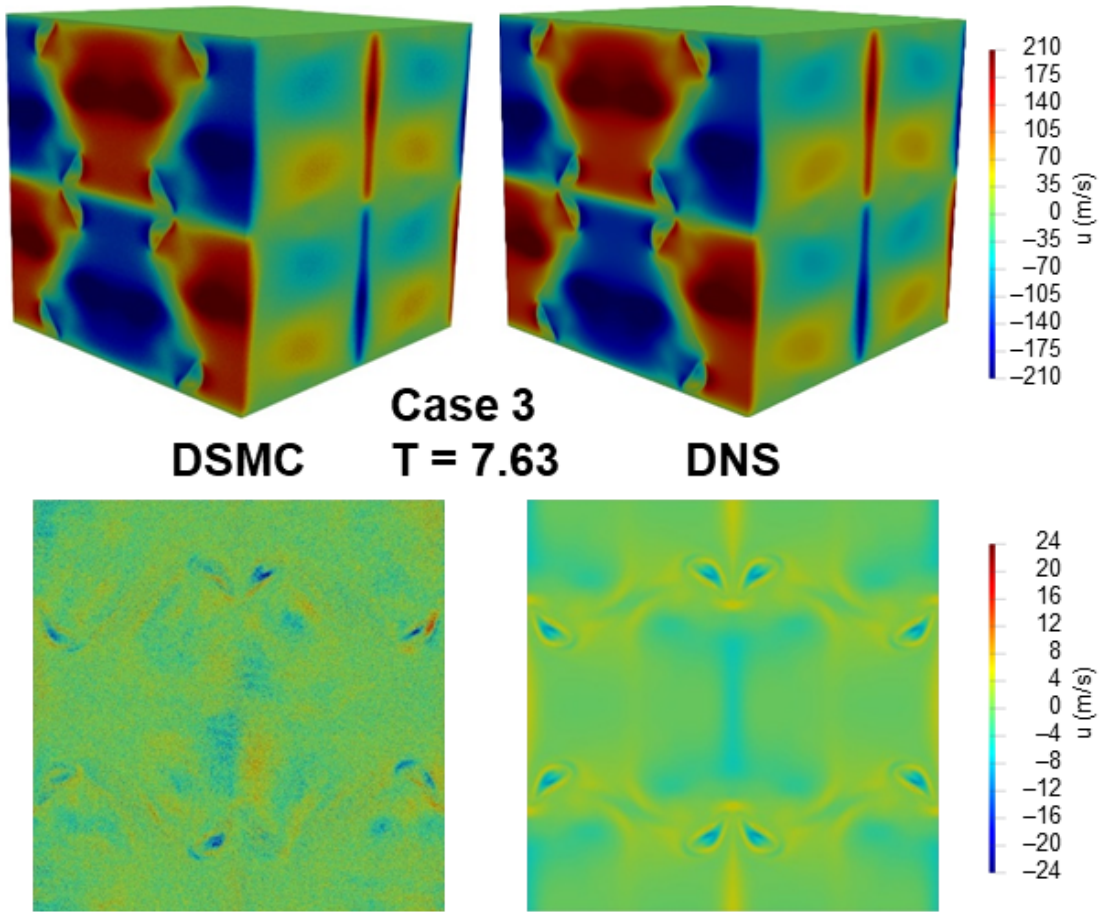


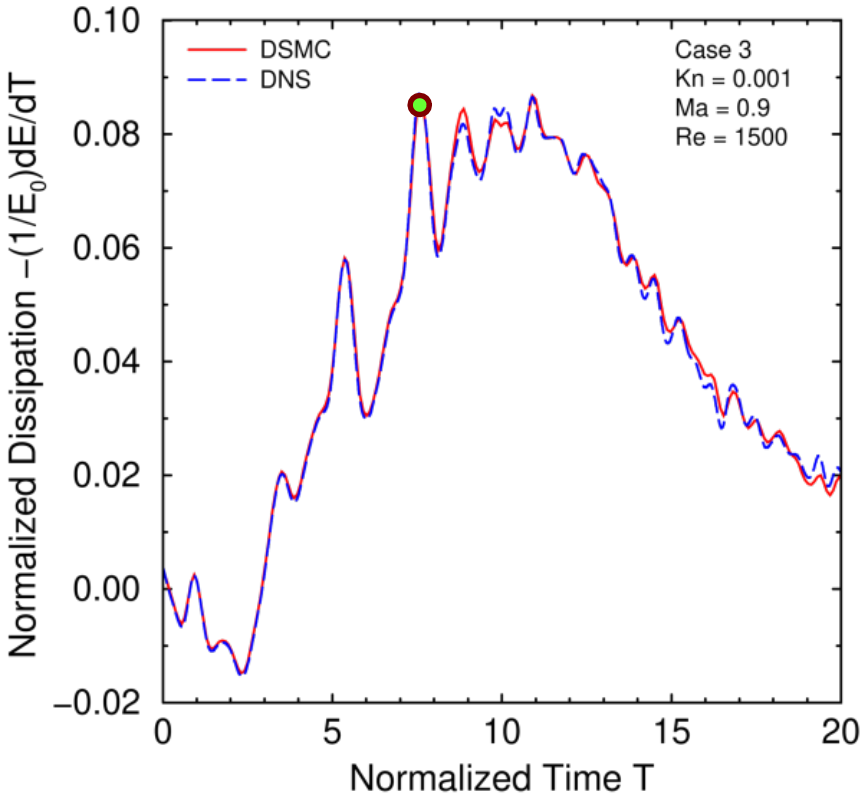


Flow fields have been averaged over 10,000 moves

DSMC and DNS agree up to the point of maximum dissipation

TG Ma=0.9, T=7.63

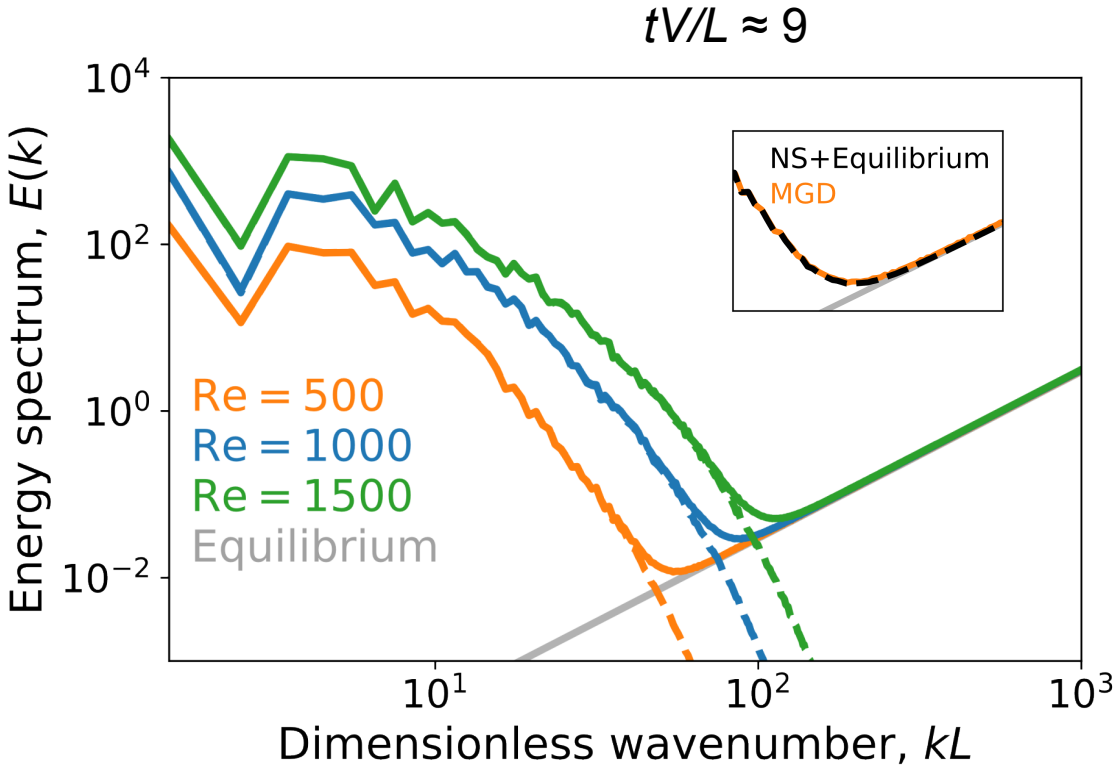




Flow fields have been averaged over 10,000 moves

DSMC and DNS agree up to the point of maximum dissipation

DSMC and DNS Spectra Comparison



Excellent agreement for low *k*.

DSMC shows large-*k* departure from NS spectrum due to thermal fluctuations.

NS equations are inaccurate for $k > k_c$.

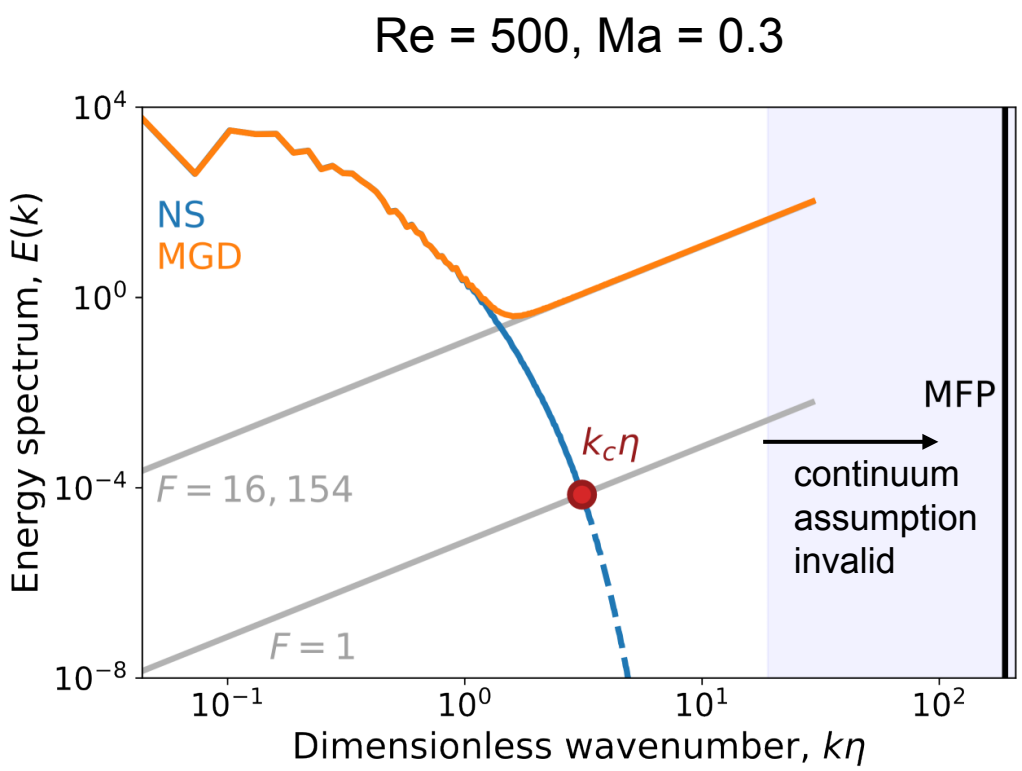
Fluctuation variance overestimated in DSMC when $F > 1$.

- These simulations use $F = 16{,}154$

Want to determine the k_c that would be observed in a physical gas.

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

Crossover Wavenumber



$$k_c\eta \approx 3.1$$

Thermal fluctuations dominate almost the entire dissipation range

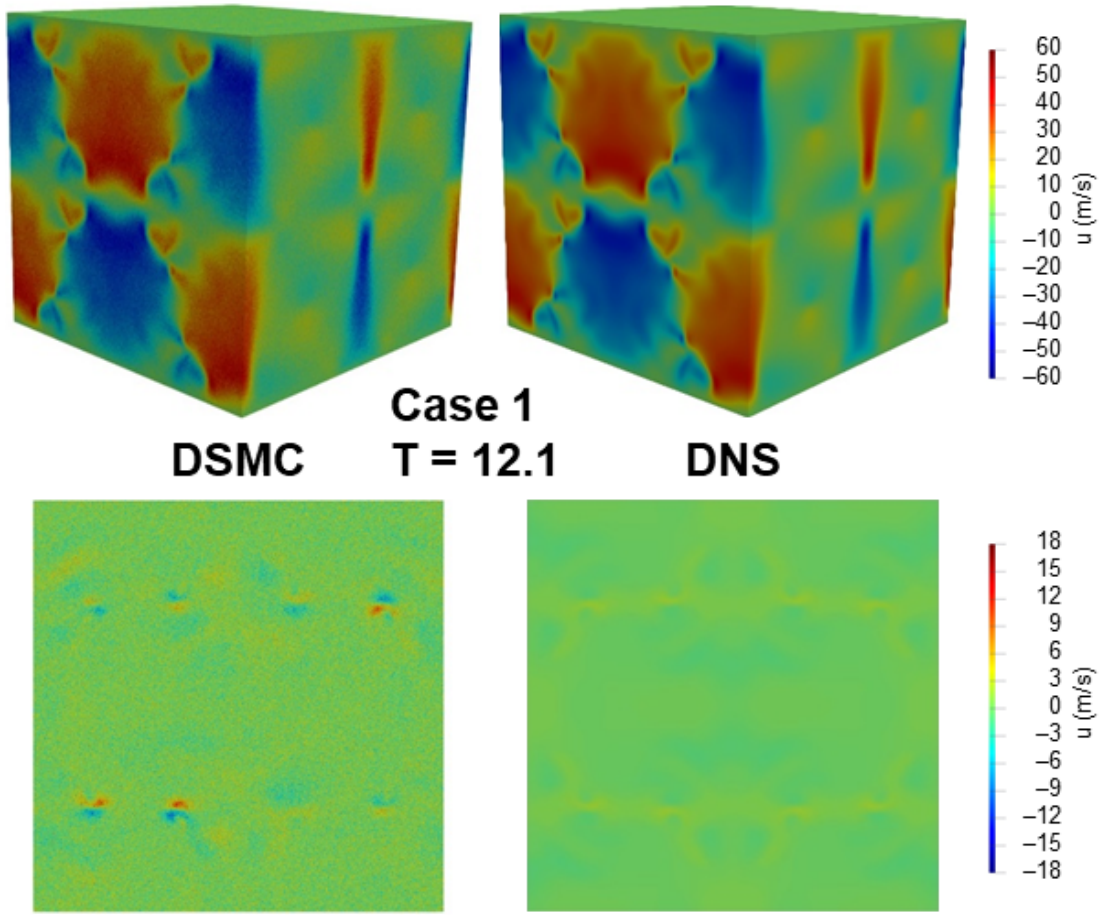
- Similar for other Re

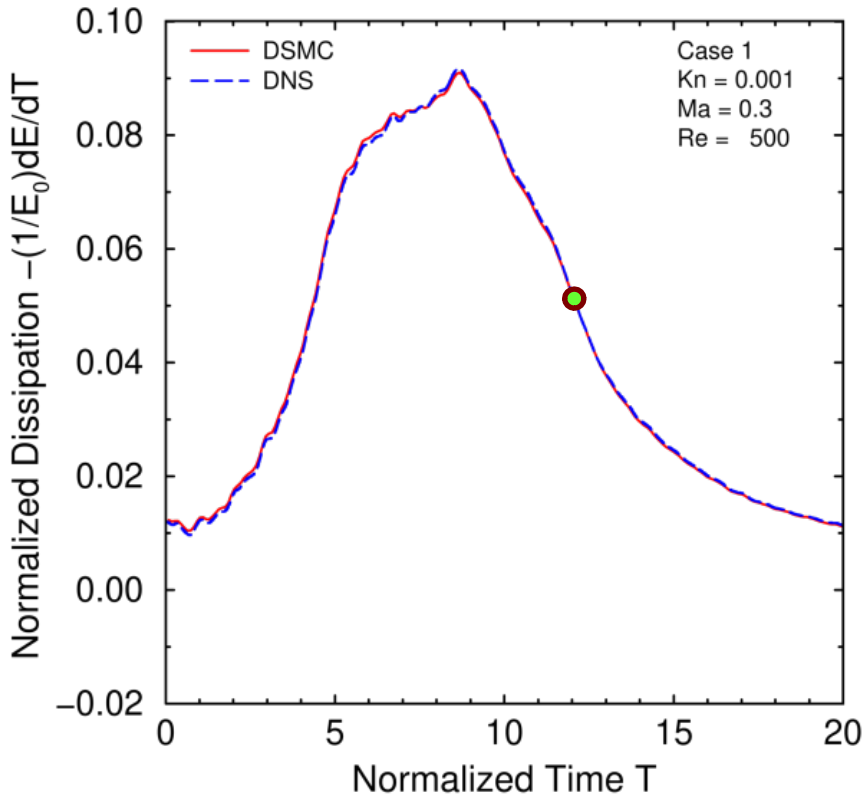
$$l_c / \lambda_{\mathrm{mfp}} \approx 61$$

Crossover scale is much larger than the Mean Free Path (MFP) – in a regime where NS equations widely believed to be valid.

Agrees with previous estimates (Betchov, 1957, Eyink *et al.* 2021) and with recent simulations using the fluctuating NS equations (Bell *et al.* 2022)

TG Ma=0.3, T=12.01

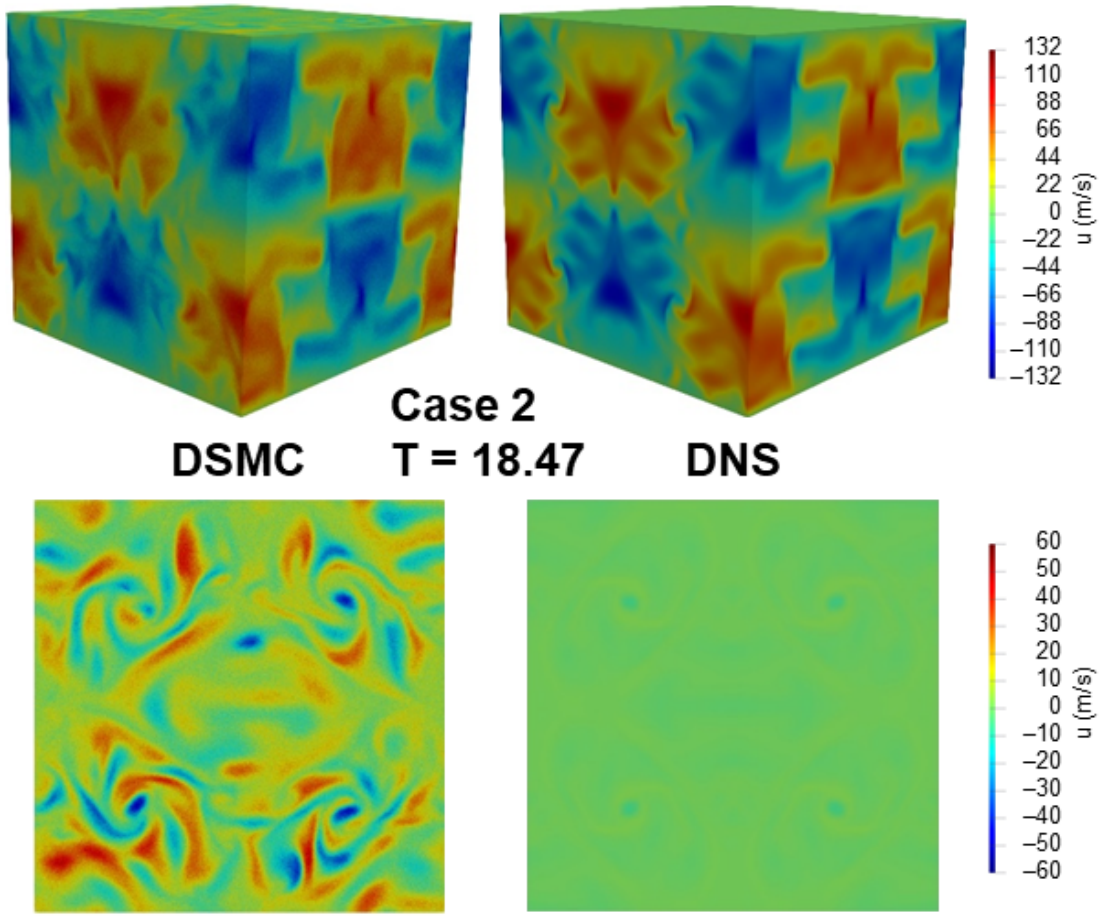


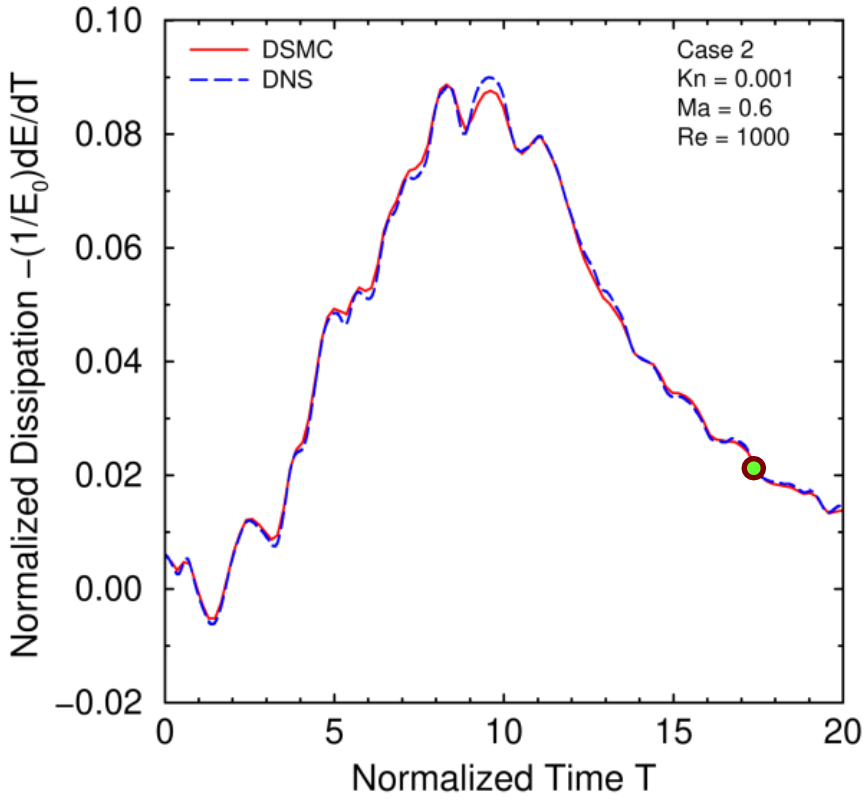


Thermal fluctuations break the symmetry

Flow fields have been averaged over 10,000 moves

TG Ma=0.6, T=18.47

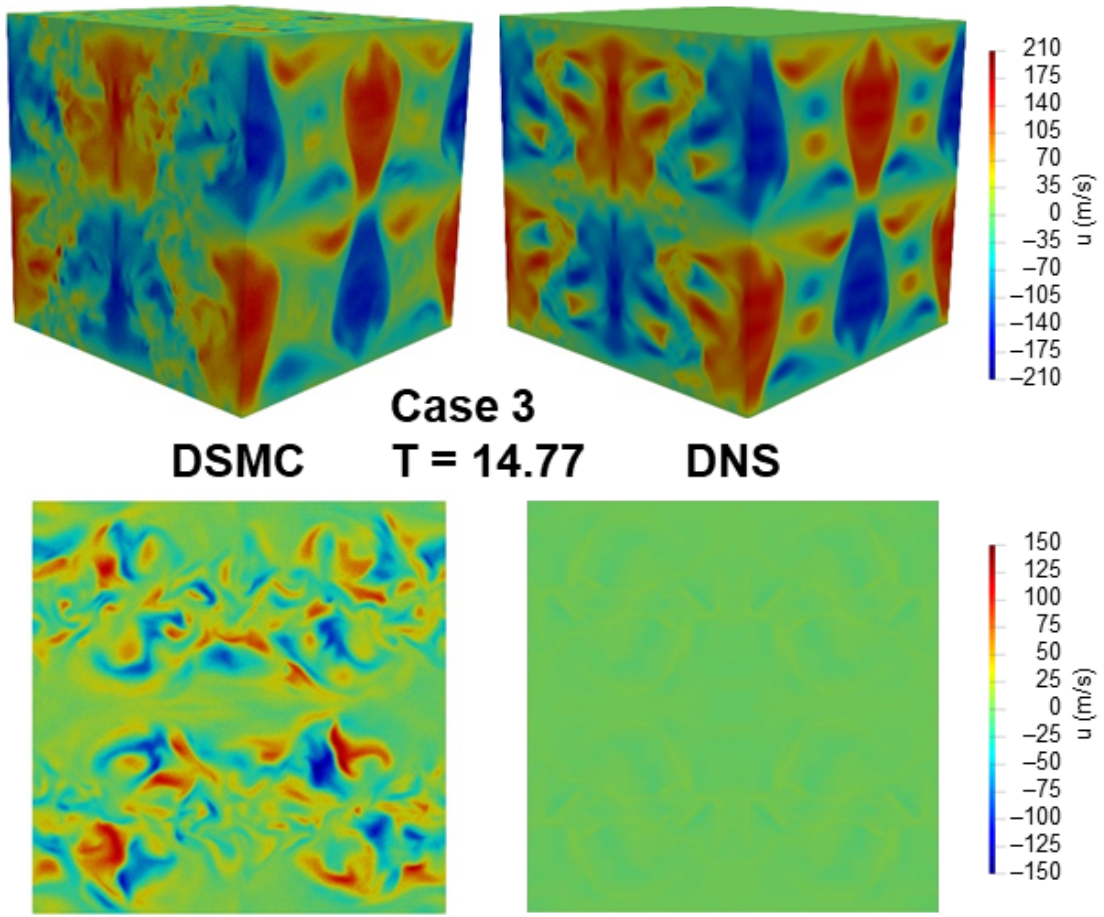


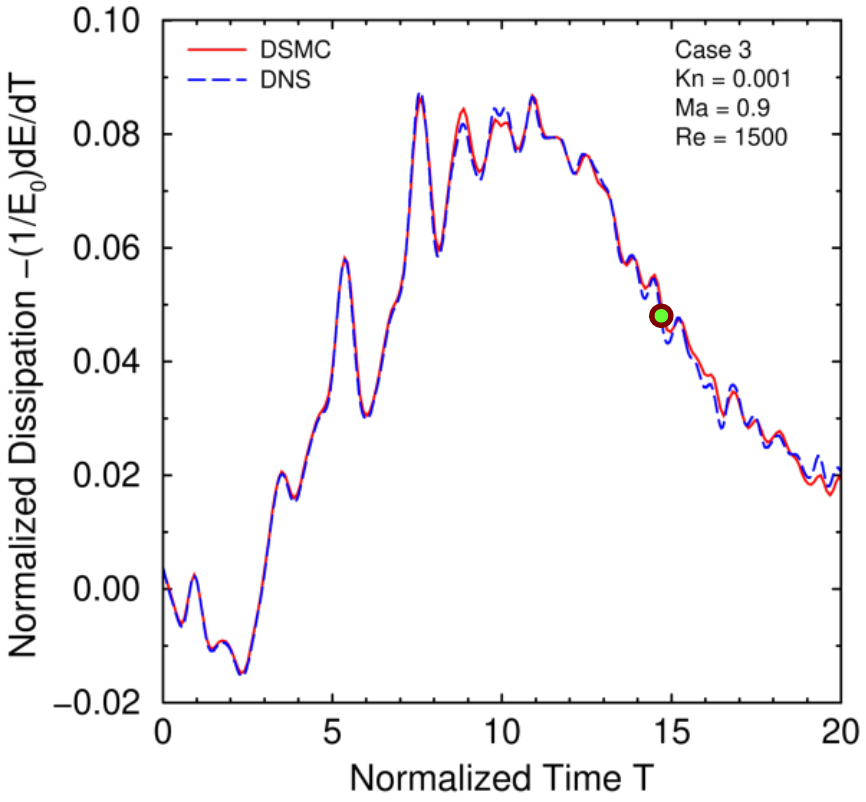


Thermal fluctuations break the symmetry

Flow fields have been averaged over 10,000 moves

TG Ma=0.9, T=14.77





Thermal fluctuations break the symmetry

Flow fields have been averaged over 10,000 moves

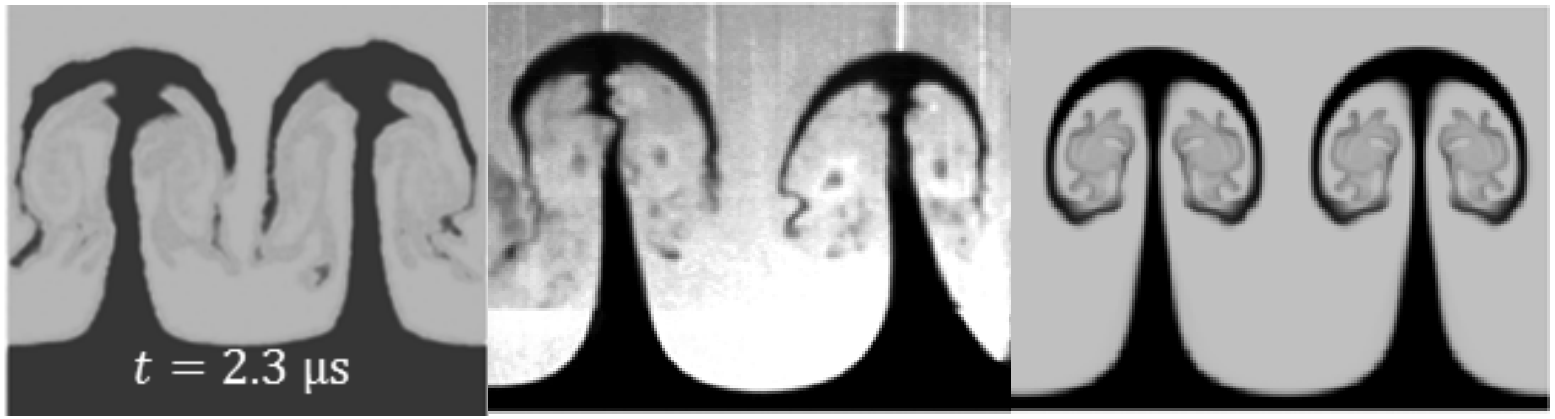
Spontaneous Stochasticity?

At early times, DSMC and DNS produce similar profiles. At later times, their profiles differ. Why?

Thermal fluctuations may cause unpredictability as they become amplified and introduce more structure to the flow field (Ruelle, 1979).

Similar to Spontaneous Stochasticity?

For systems with a sufficient amount of energy at the small scales, “formally deterministic fluid systems…are observationally indistinguishable from indeterministic systems” (E. N. Lorenz, 1969).



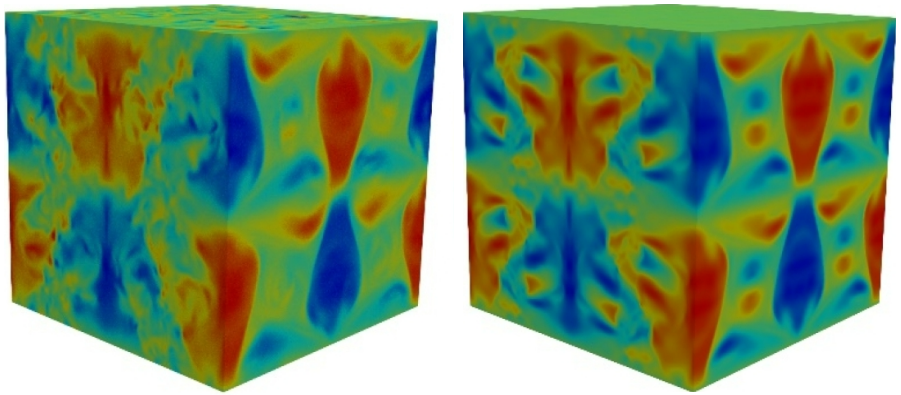
DSMC **Experiment** **Navier-Stokes**

Conclusions

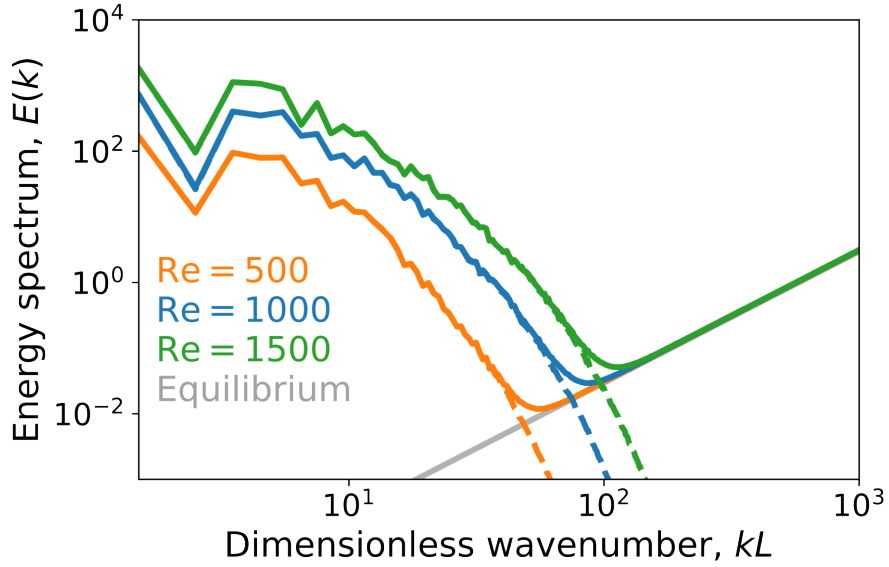
Nature is molecules, not equations, so simulations should be molecular as well.

Molecular-level DSMC simulations give the first direct evidence that the Navier-Stokes equations are not accurate in the dissipation range for turbulence in gases.

Thermal fluctuations break symmetries and thereby can allow flows to evolve along phase-space trajectories different from those predicted by the NS equations.



DSMC DNS



R. M. McMullen, M. C. Krygier, J. R. Torczynski, and M. A. Gallis, The Navier-Stokes equations do not describe the smallest scales of turbulence in gases, *PRL, 2022.*

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