SAND2023-00095C

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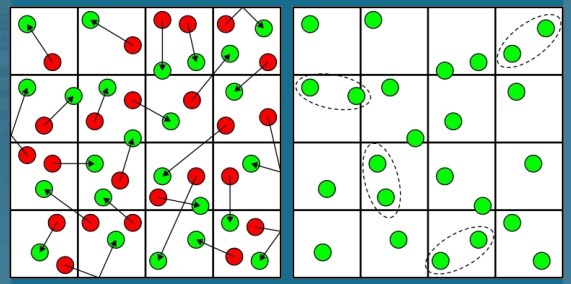
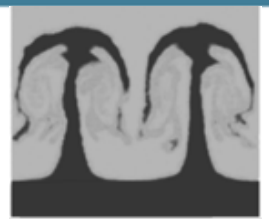
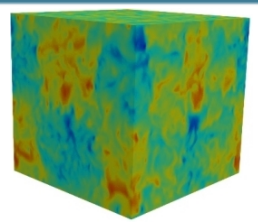
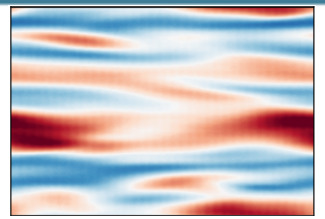
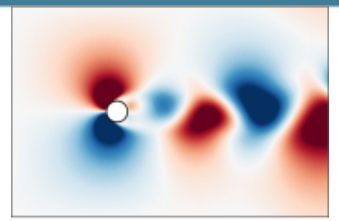
Molecular-level simulations of turbulence via the direct simulation Monte Carlo method











Ryan M. McMullen, John R. Torczynski, and Michael A. Gallis

American Physical Society 2023 March Meeting

Las Vegas, Nevada USA

March 7, 2023

Talk F60.010

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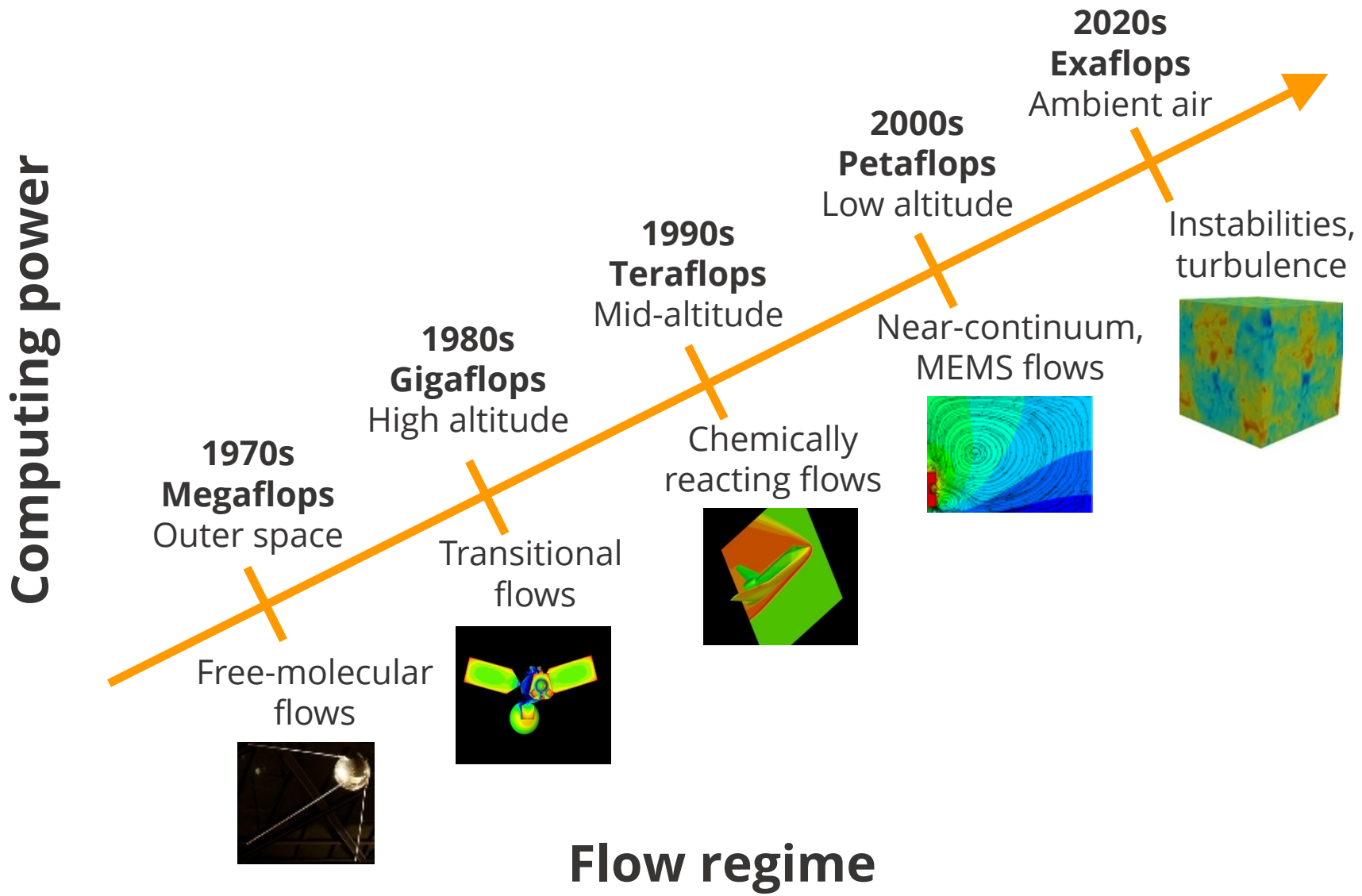
Molecular gas dynamics: from free-molecular flow to turbulence in 50 years



Direct simulation Monte Carlo (DSMC)

DSMC is the dominant method for MGD [1]

No PDEs solved - tracks very large numbers (~10^{12}) of particles, each representing many actual molecules

- Move ballistically, collide & reflect stochastically
- Flow quantities from averages over molecules in each cell

Inherently includes physics usually not in traditional CFD

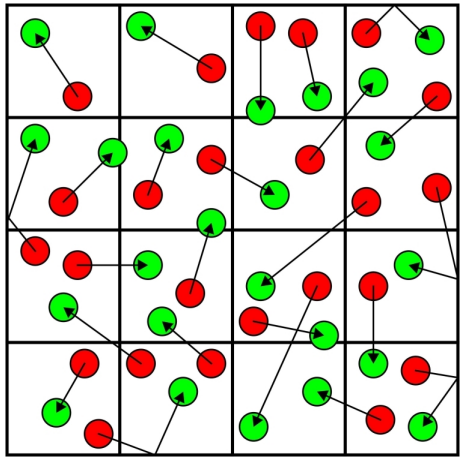
- Thermal and chemical nonequilibrium
- Pressure and heat-flux tensor anisotropy
- Thermal fluctuations

Simulates gas flows very accurately

- Solutions converge to solutions of the Boltzmann Equation [2]
- Reproduces Chapman-Enskog distribution [3]

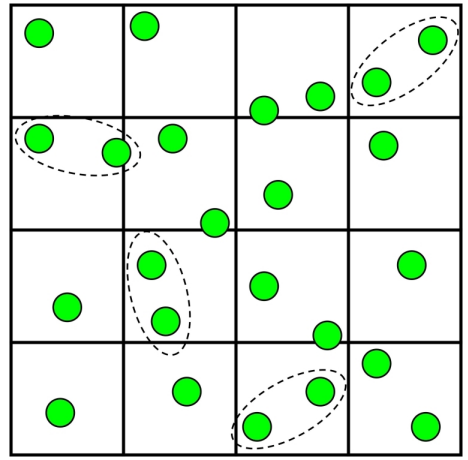
Computational and algorithmic advances have brought turbulent flows within reach of DSMC!

move



$$\frac{d\mathbf{x}_i}{dt} = \mathbf{v}_i$$

collide



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

What can we learn from molecular-level simulations of turbulence?

[1] Bird, Clarendon Press (1994)
[2] Wagner, J. Stat. Phys. (1992)
[3] 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

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

Developed with next-generation architectures in mind

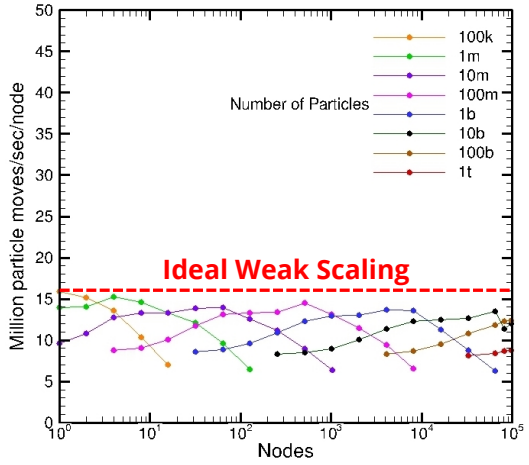
- Write application kernels only once
- Efficient on many platforms: GPU, manycore, heterogeneous, …

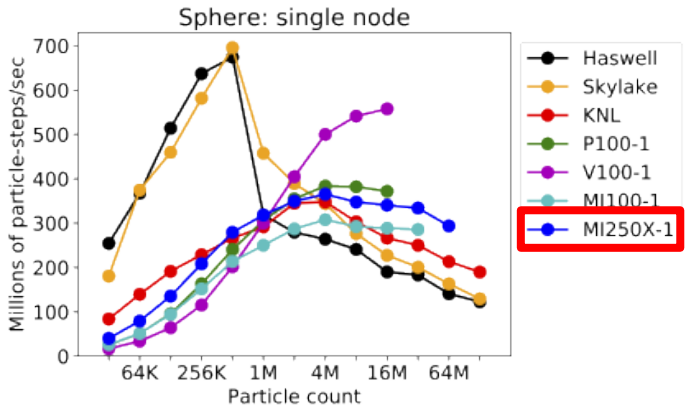
Complex geometries are easily treated

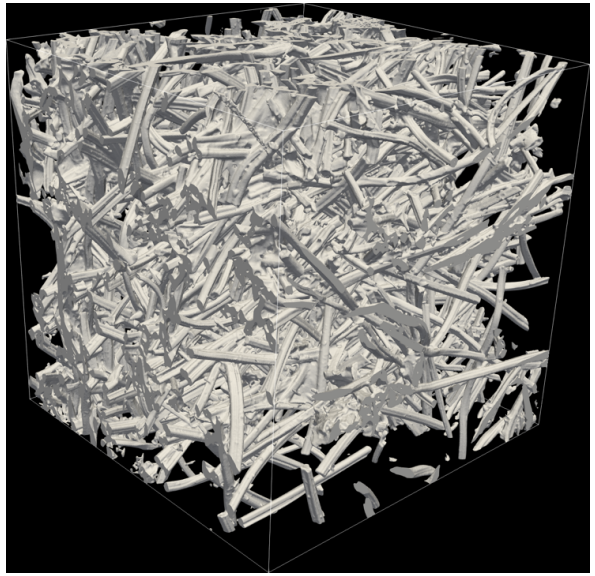
- Domain can be 2D, axisymmetric, 3D
- Gas molecules use hierarchical Cartesian “ijk” grid
- Body surfaces represented by triangular elements which cut gas grid cells

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

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

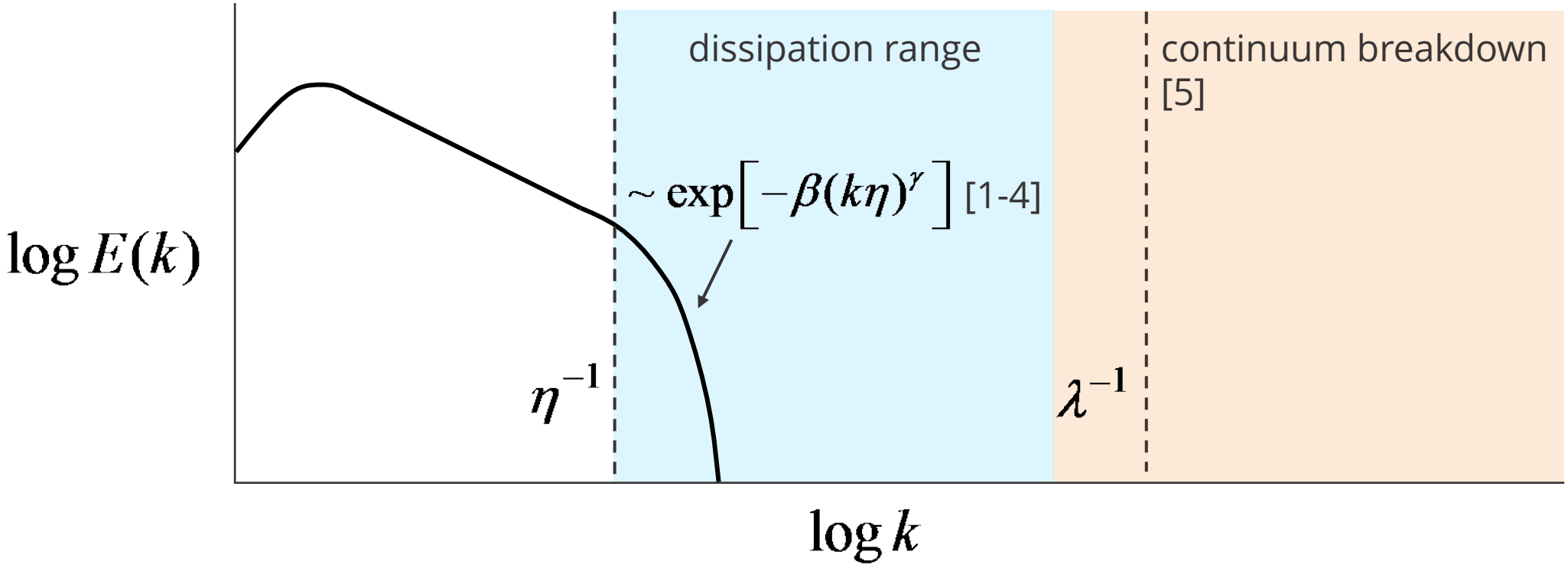






FiberForm™

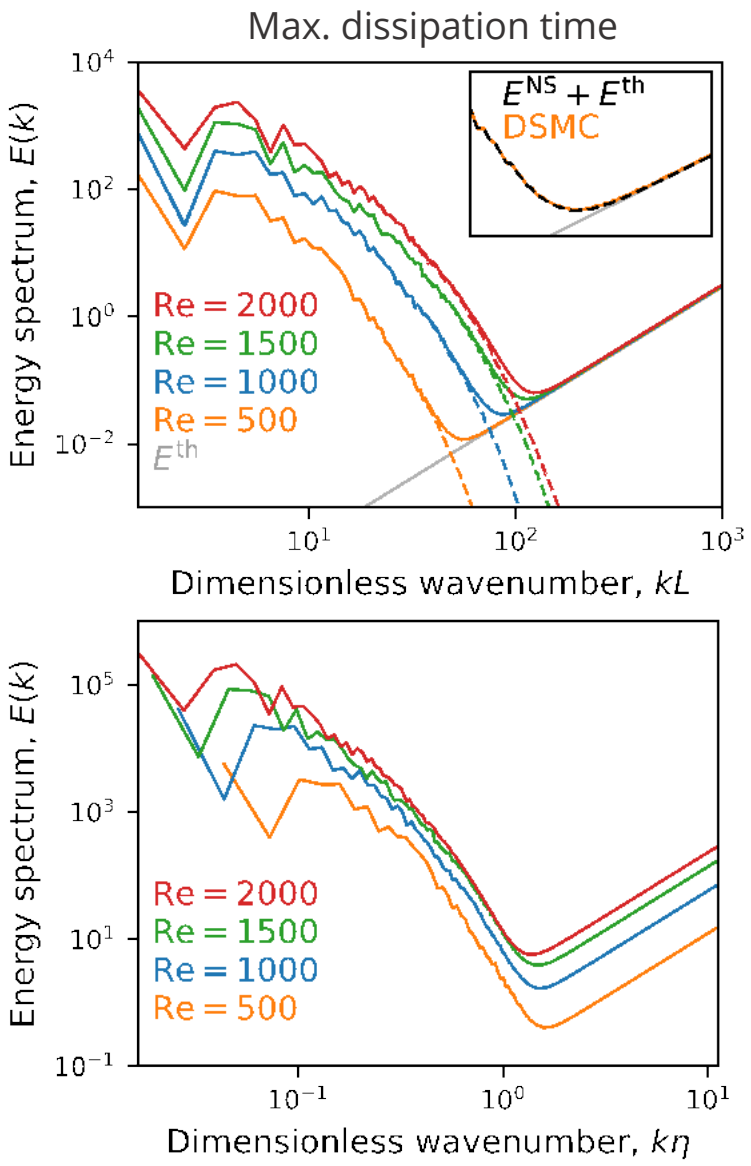
The turbulent energy spectrum according to Navier-Stokes



This picture neglects thermal fluctuations.

[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)

Thermal fluctuations dominate the dissipation range



Order-of-magnitude estimates

Compare thermal fluctuation energy to 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 $k\eta > 1$ and $E^{th}(k) \sim k^2$ …

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

DSMC results

Excellent agreement between NS and DSMC for low k

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

NS equations are inaccurate for $k > k_c$:

$$k_c \eta = O(1)$$

$$l_c / \lambda_{mfp} \; ? \; 1$$

Agrees with fluctuating hydrodynamics simulations for liquids [3]

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

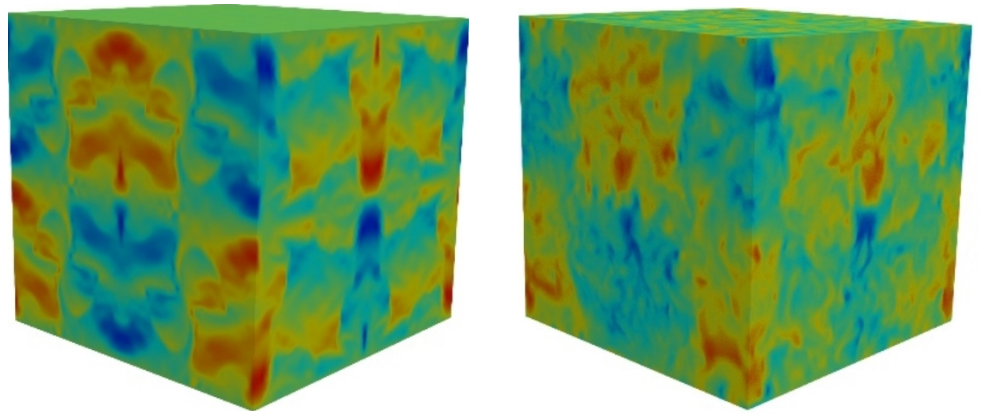
Thermal-fluctuation effects on larger scales

No observed effects on global or large-scale statistics

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

Implications for predictability of turbulence?

- 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"



NS DSMC

[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 Poincaré (2003)
[8] Eyink & Bandak, Phys. Rev. Res. (2020)
[9] Thalabard et al., Comms. Phys. (2020)

Turbulent flow over TPS materials

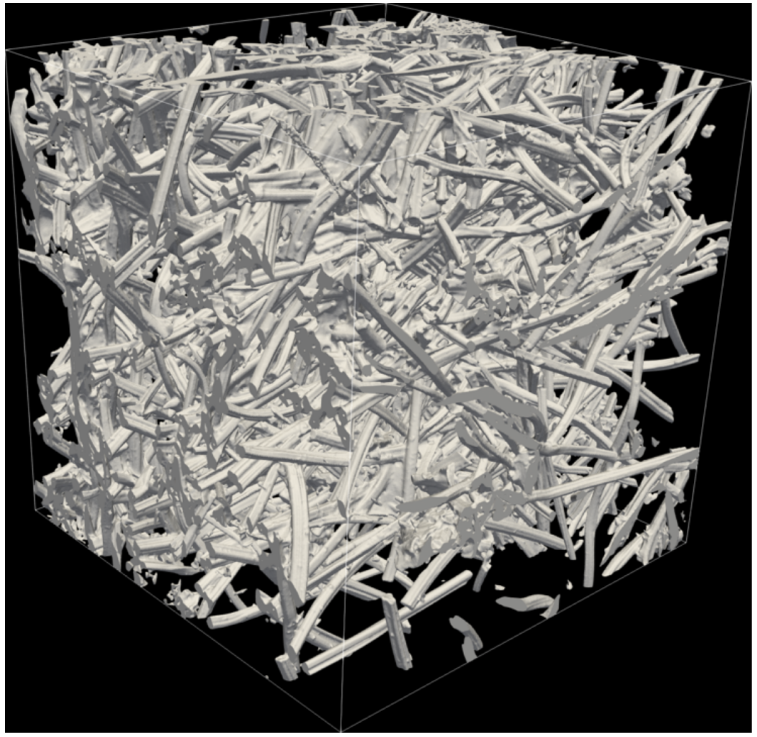
Thermal-protection-system (TPS) materials on reentry vehicles ablate and become:

- Rough
- Permeable

→ Affects loading and may compromise vehicle performance

Length scales ~ mean free path (MFP)

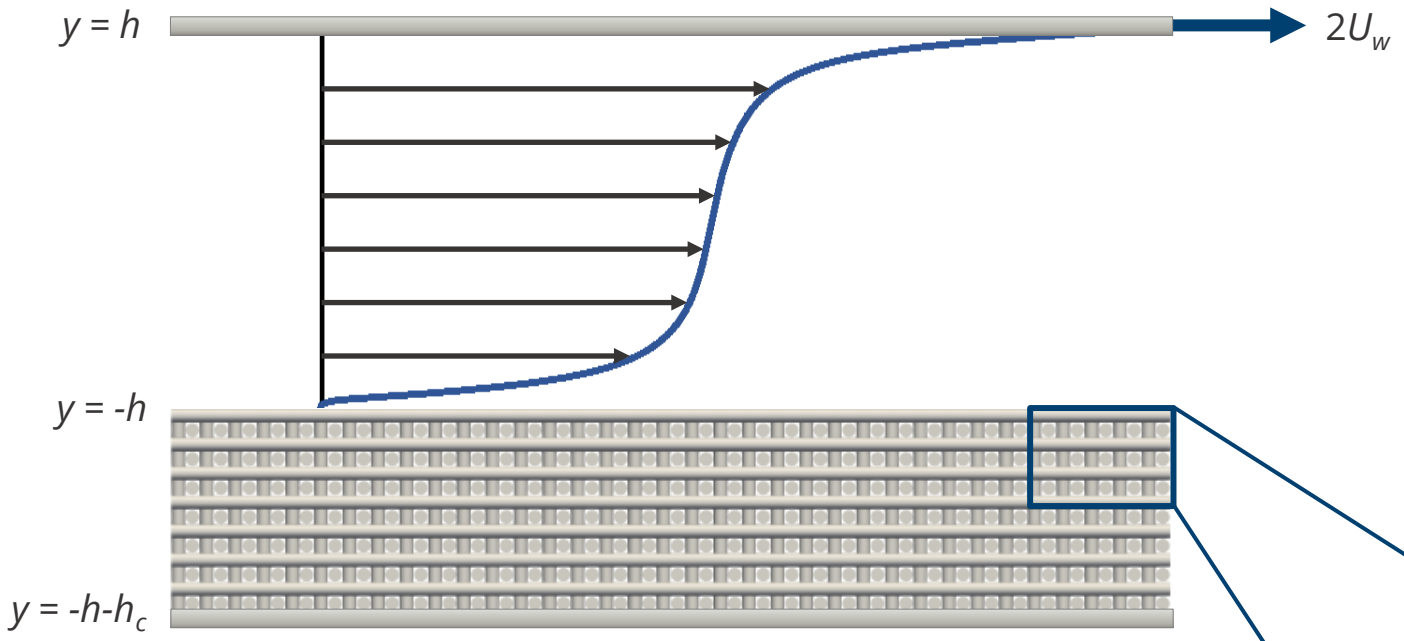
→ Noncontinuum effects may be significant



FiberForm™

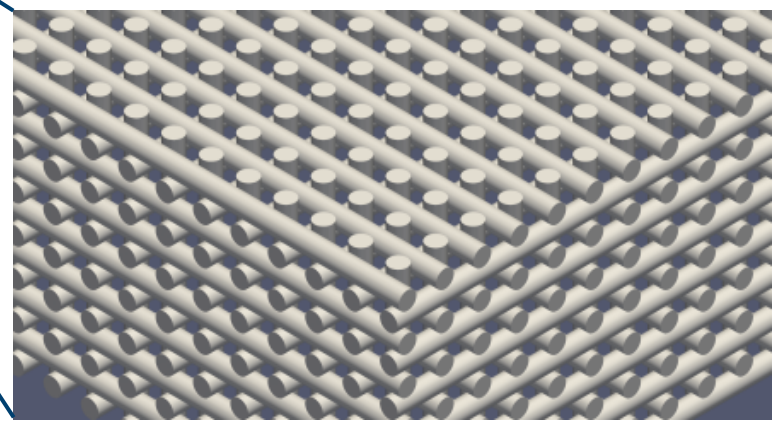
Simulate compressible turbulent flow over MFP-scale permeable wall with DSMC

Permeable-wall minimal Couette flow [1]



$h = 5 \times 10^{-4}$ m
$h_c = 5.5 \times 10^{-4}$ m
$L_x = 1.75\pi h$
$L_y = 2h+h_c$
$L_z = 1.2\pi h$

$R_c = 1.87 \times 10^{-5}$ m
$s = 0.1R_c$
$\varepsilon = 0.47$



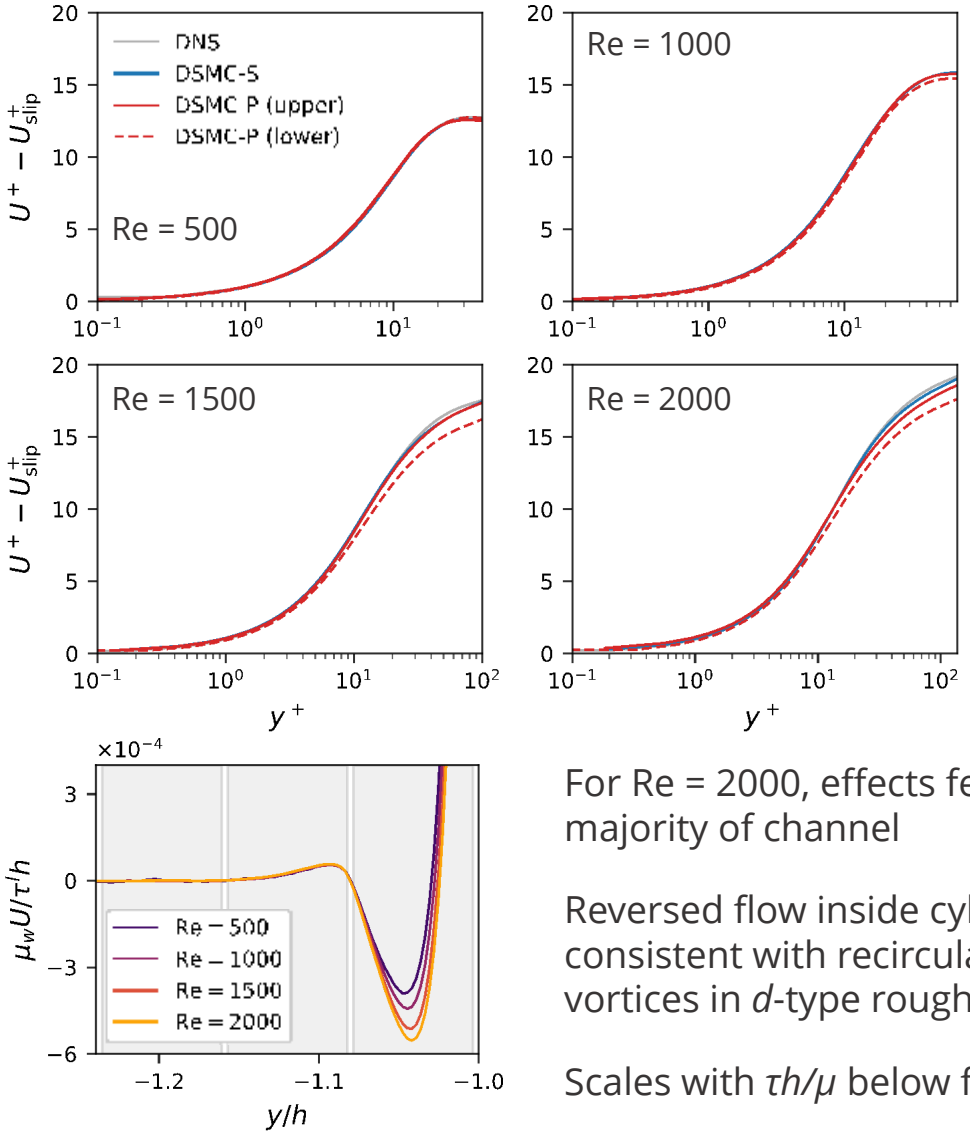
Re_h	Ma	Re_τ	Kn_h	Kn_s	$Kn_\tau = \lambda^+$
500	0.3	40	9.7×10^{-4}	0.26	0.04
1000	0.6	67		0.25	0.06
1500	0.9	100		0.23	0.09
2000	1.2	136		0.21	0.11

$Re_h = \rho_b U_w h/\mu_w$ $\quad$ $Ma = U_w/a_w$ $\quad$ $Kn_h = \lambda/h$

[1] Hamilton et al., J. Fluid Mech. (1995)

Permeability effects

Mean velocity profiles



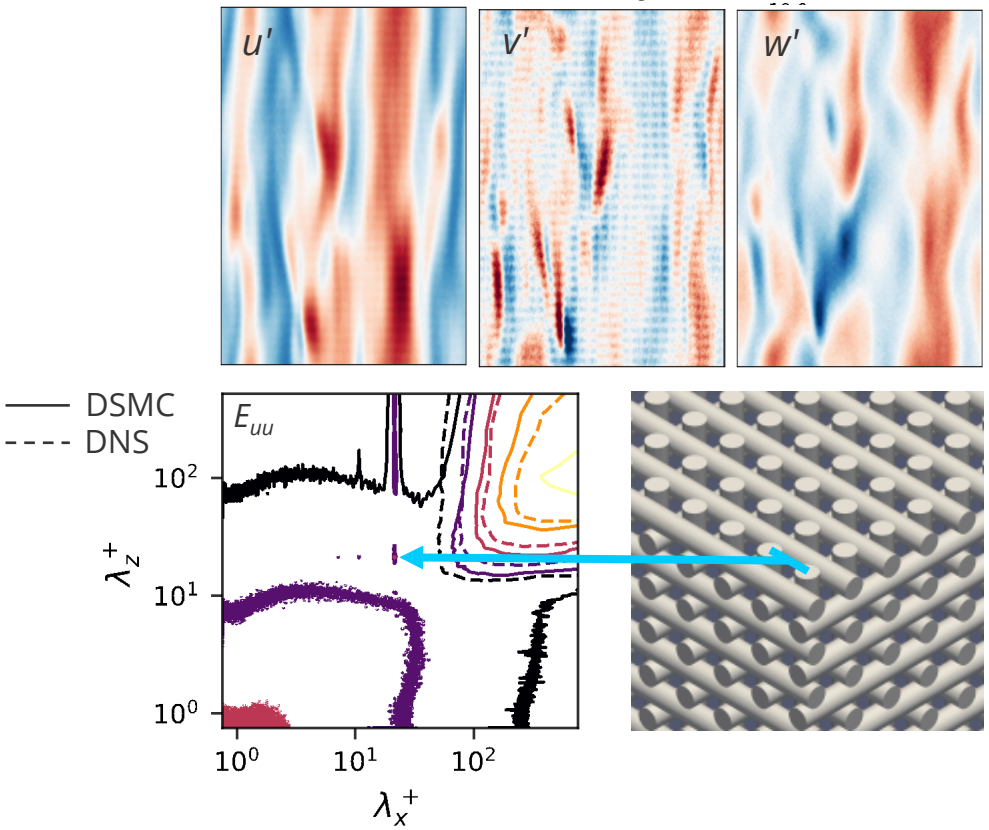
For Re = 2000, effects felt across majority of channel

Reversed flow inside cylinders consistent with recirculation vortices in *d*-type roughness [1,2]

Scales with $\tau h/\mu$ below first layer

Near-wall fluctuations

Re = 2000, $y^+ = 5$



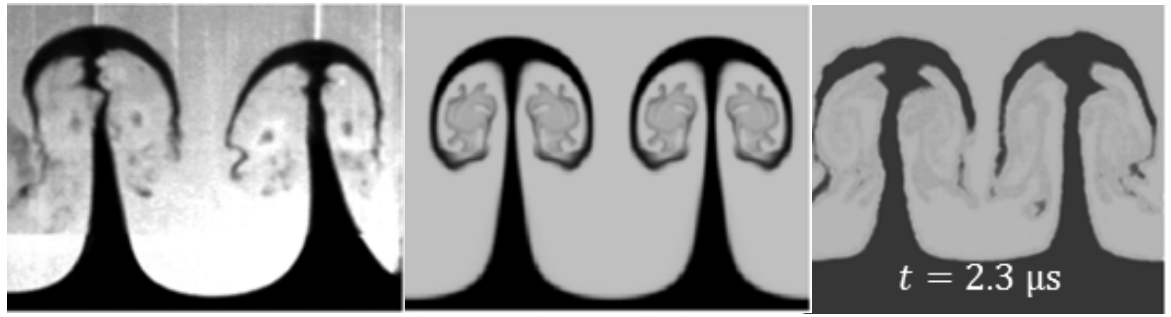
Cylinder structure modulates near-wall structures

Spanwise organization across entire channel span

Rarefaction increases permeability by 13% [3]

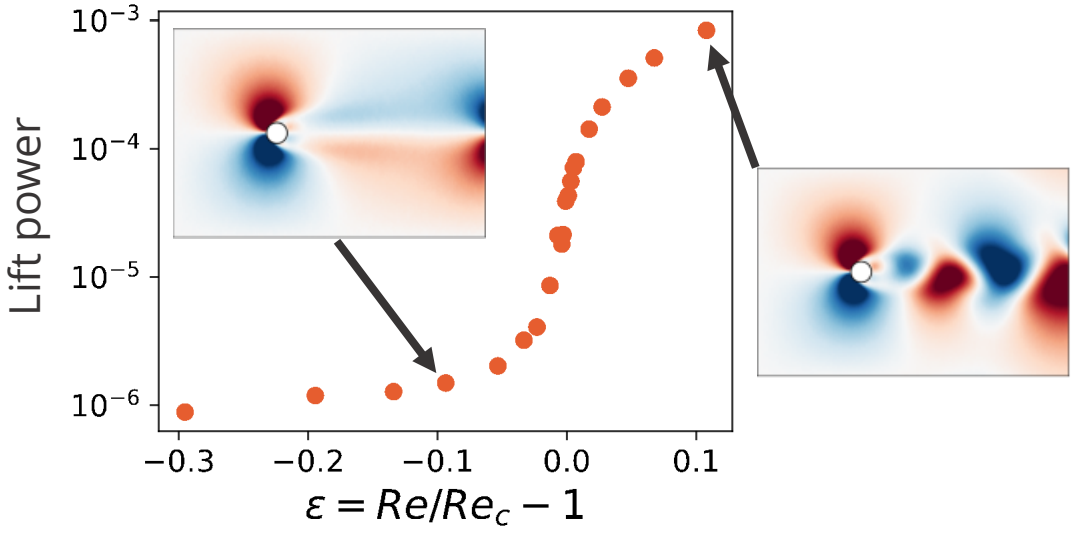
[1] Kuwata & Suga, J. Fluid Mech. (2017)
[2] Perry et al., J. Fluid Mech. (1969)
[3] Klinkenberg, Am. Petrol. Inst. (1941)

DSMC simulations of hydrodynamic instabilities

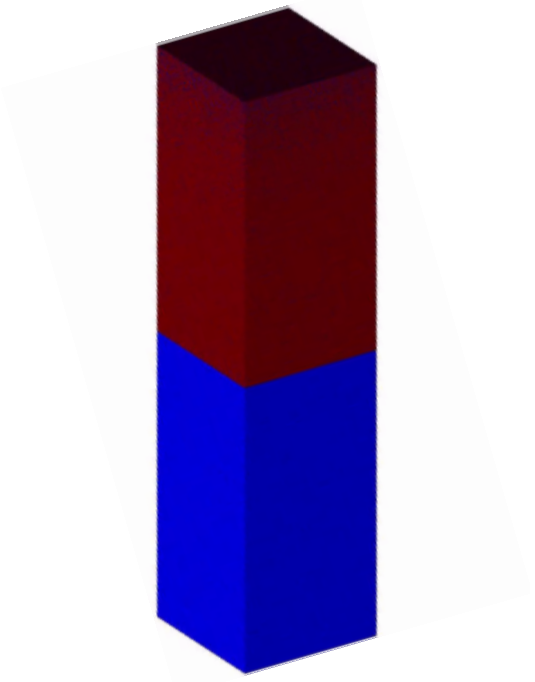


Experiment [1] CFD [1] DSMC

Richtmyer-Meshkov



Vortex shedding



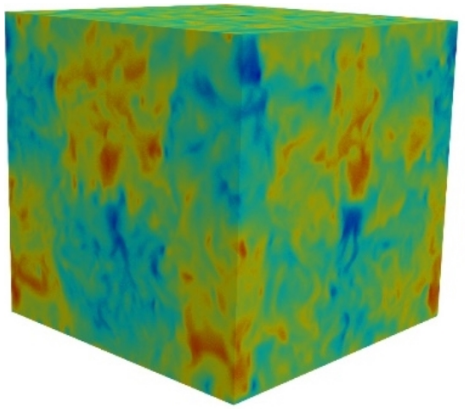
Rayleigh-Taylor

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

Summary

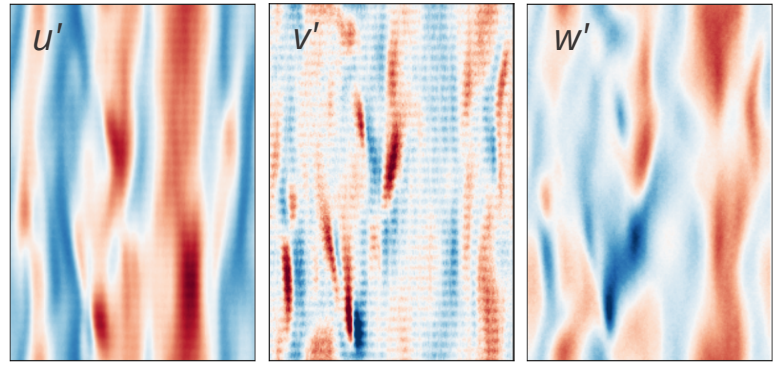
DSMC inherently includes physics absent from NS simulations of turbulent flows

- Thermal fluctuations dominate the dissipation range



DSMC is capable of simulating turbulent flow over complex MFP-scale geometries

- Enables wall-bounded turbulence simulations where noncontinuum and nonequilibrium effects are significant



For large scales, NS and DSMC agree surprisingly well, even for Knudsen numbers of $O(10^{-1})$

- Need better understanding of limits of NS equations for turbulent flows

Future directions and outlook

Dispersion and mixing

- Can easily track individual molecules [1]

Chemically reacting turbulence

- Fluctuation and nonequilibrium effects naturally included

Characterizing molecular-fluctuation effects on instabilities

- Transition in hypersonic environments [2,3]

Courtesy of NASA Ames

DSMC can be a valuable tool for studying instabilities and turbulence, especially in the exascale era!

[1] van de Water et al., Phys. Rev. Lett. (2022)
[2] Luchini, AIAA J. (2017)
[3] Fedorov and Tumin, AIAA J. (2017)

Effects of thermal fluctuations on turbulence

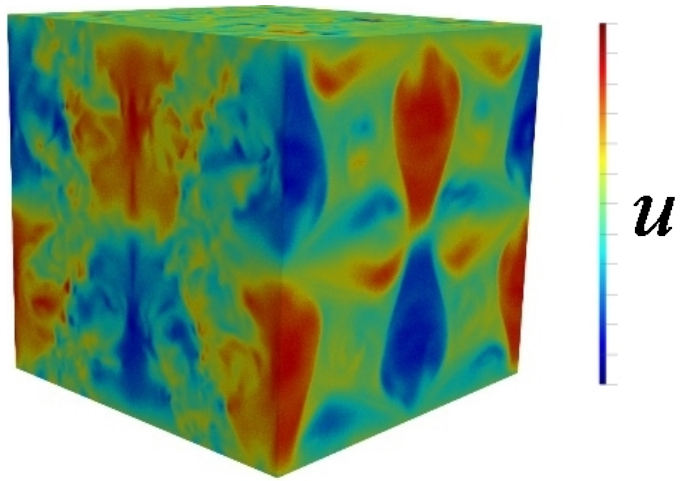
Order-of-magnitude estimates suggest that thermal fluctuations compete with turbulence at much larger scales than mean-free-path (MFP) considerations would suggest [1,2]

Extremely difficult to verify experimentally

Molecular gas dynamics (MGD) enables direct investigation of the effect of thermal fluctuations on turbulence

Simulate Taylor-Green vortex flow [3] using MGD and the compressible Navier-Stokes (NS) equations

- Re $= \rho_0 VL/\mu_0 = 500, 1000, 1500$
- Ma $= V/a_0 = 0.3, 0.6, 0.9$
- Kn $= \lambda/L = 9.7 \times 10^{-4}$
- NS simulations use Sandia-developed finite volume code SPARC [4]



[1] Betchov, J. Fluid Mech. (1957)

[2] Bandak et al., arXiv (2021); Eyink et al., Phys. Rev. E (2022)

[3] Taylor & Green, Proc. R. Soc. Lond. A (1937)

[4] Howard et al., 23rd AIAA CFD (2017)

Equilibrium MGD spectra

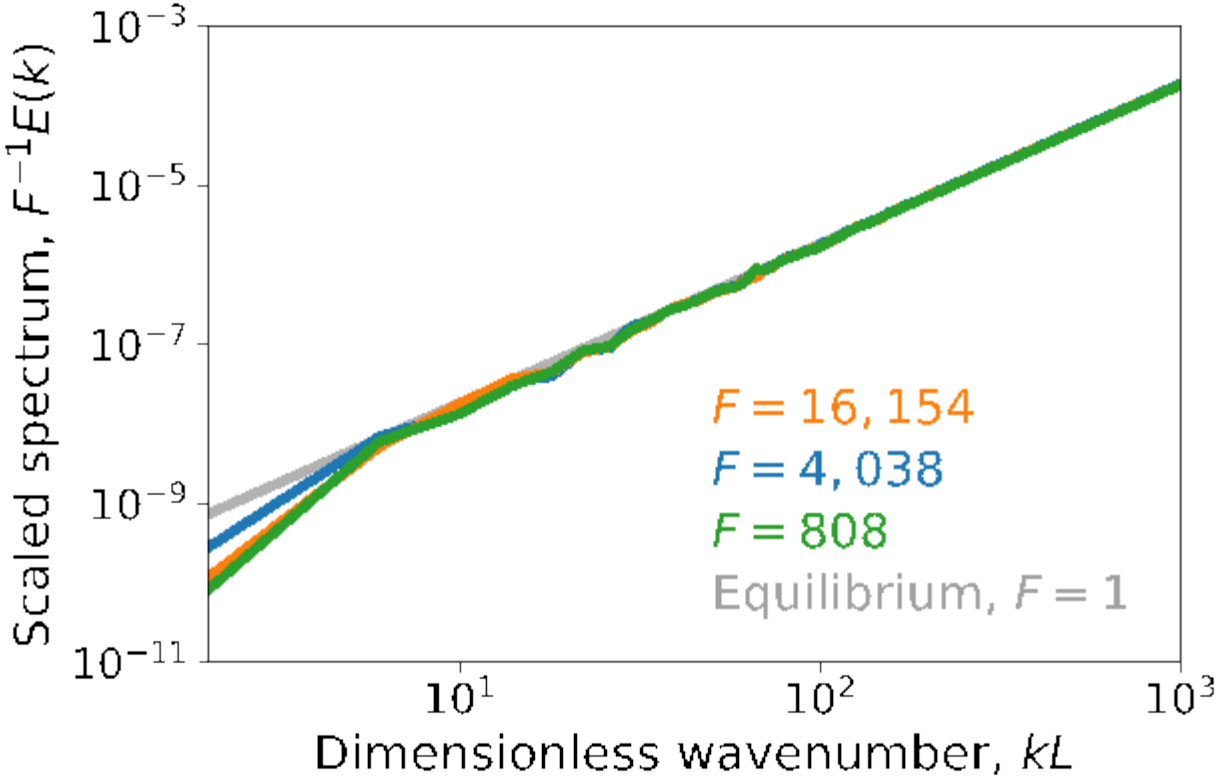
Equilibrium spectrum:

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

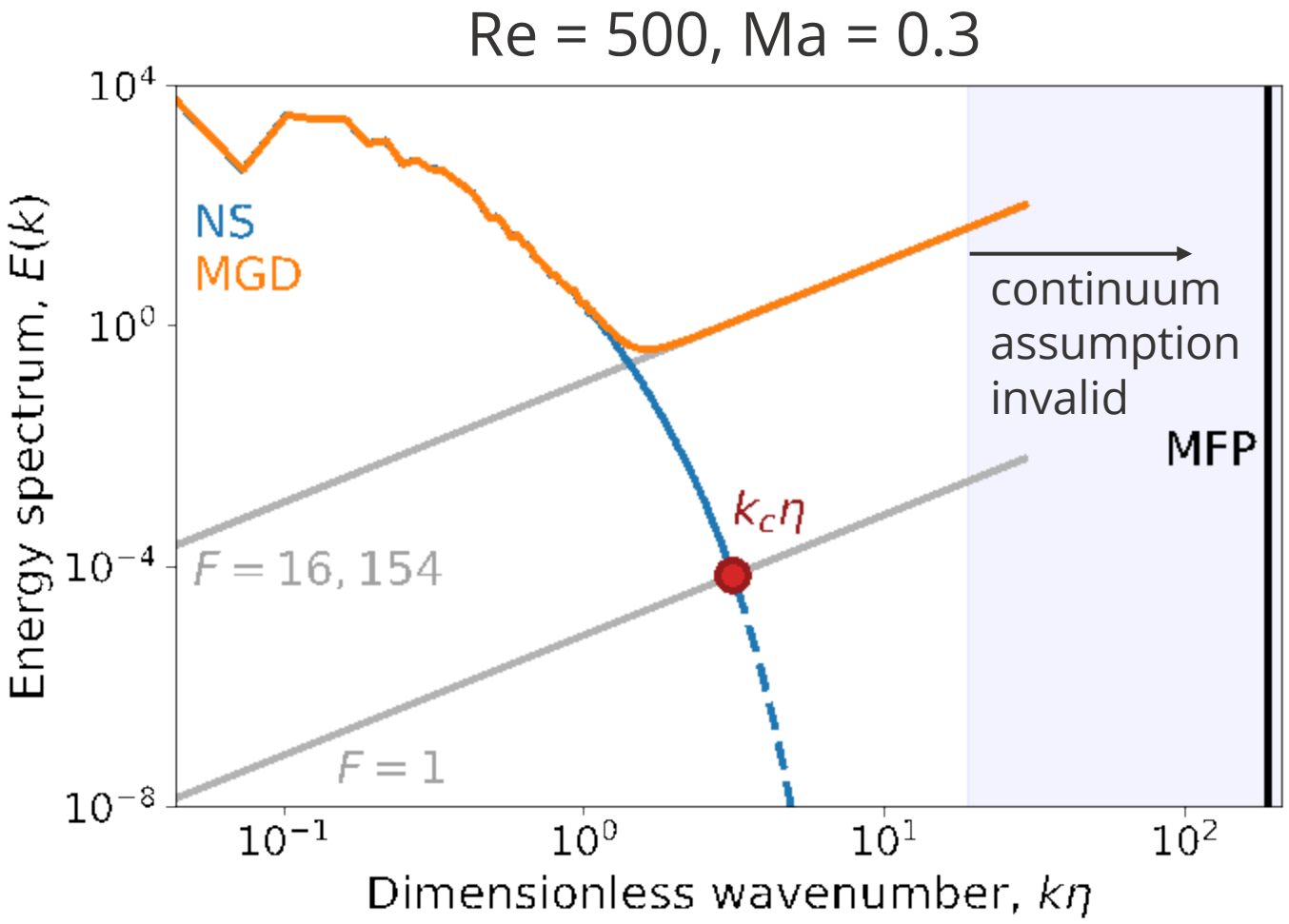
MGD spectra obey simulation ratio scaling

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

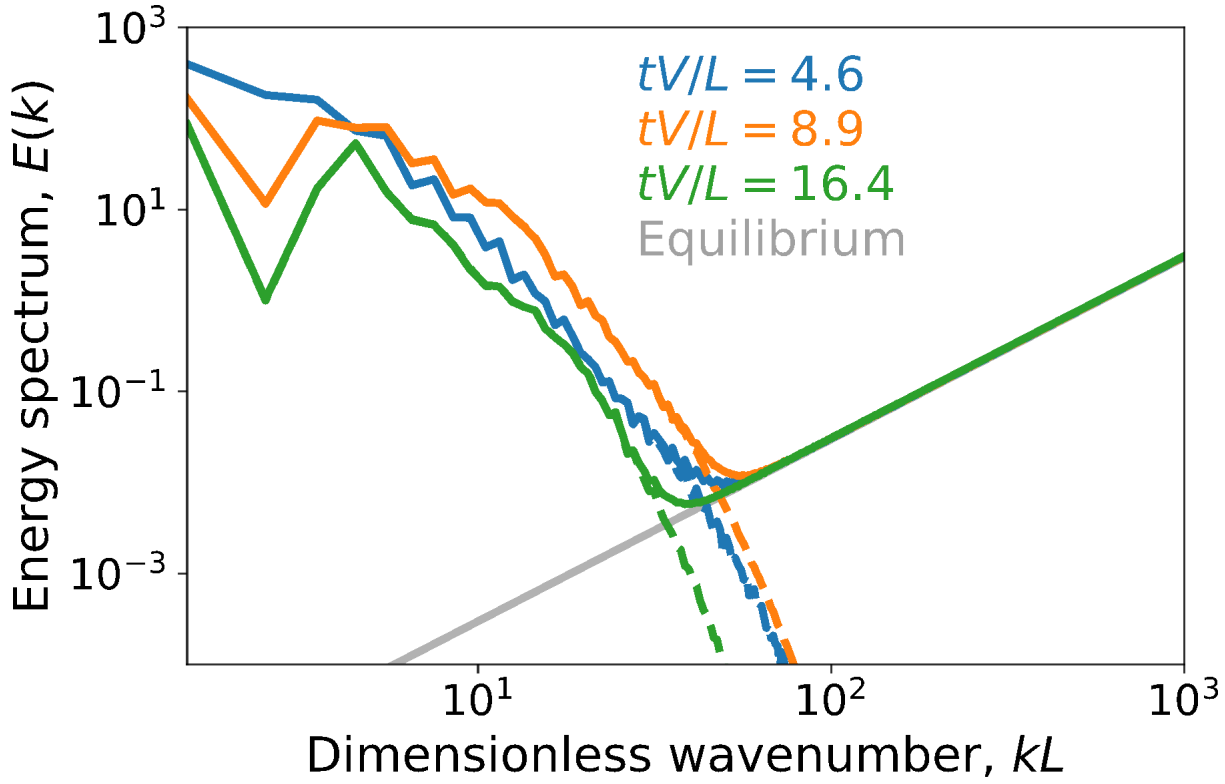
- Similar for other Re

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

Crossover scale is much larger than the MFP – in a regime where NS equations widely believed to be valid [1]

[1] Bird, Clarendon Press (1994)

Re = 500 spectra at different times

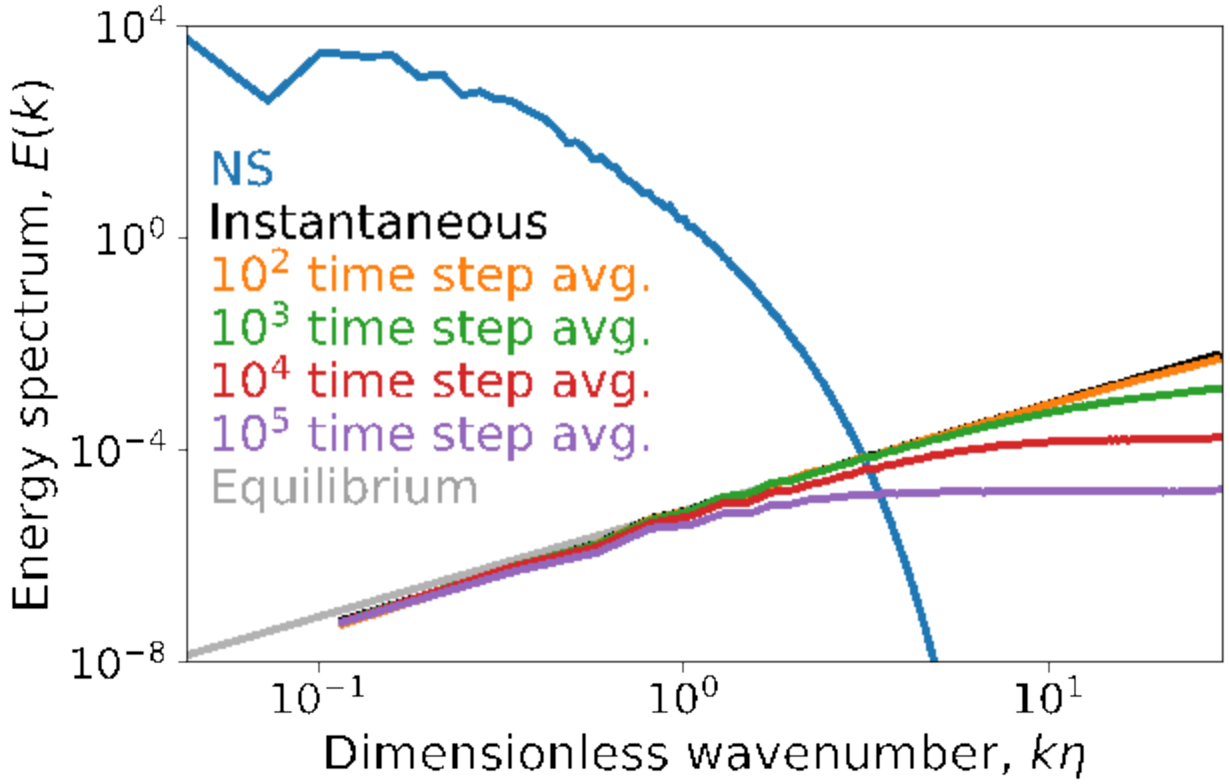


Time averaging

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

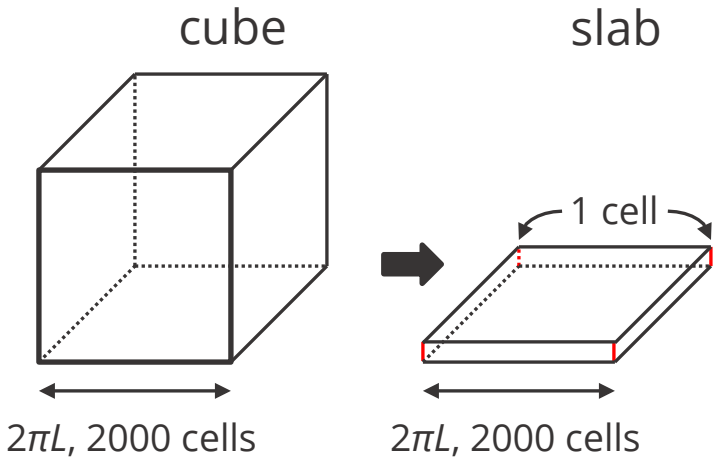
- Viscosity is 36% larger than molecular value
- Near-neighbor collisions reduce mean collision separation

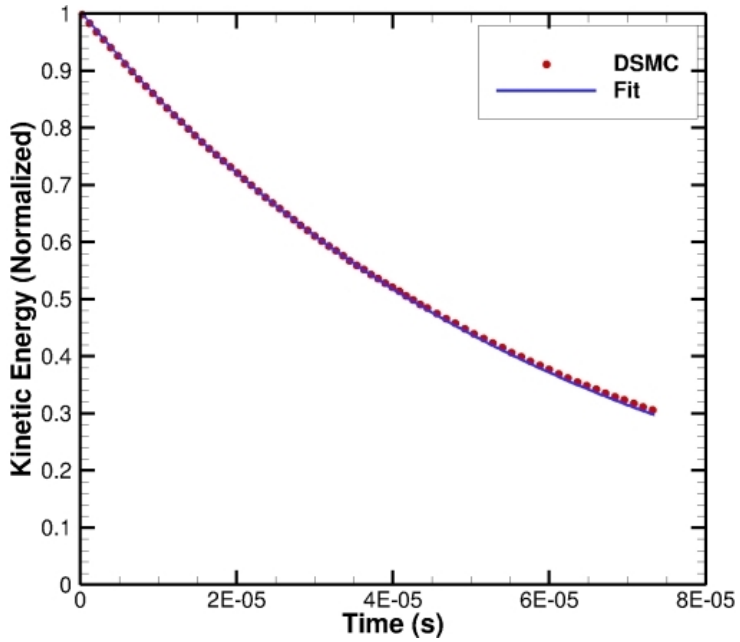
Simulate some other flow to find viscosity

- 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

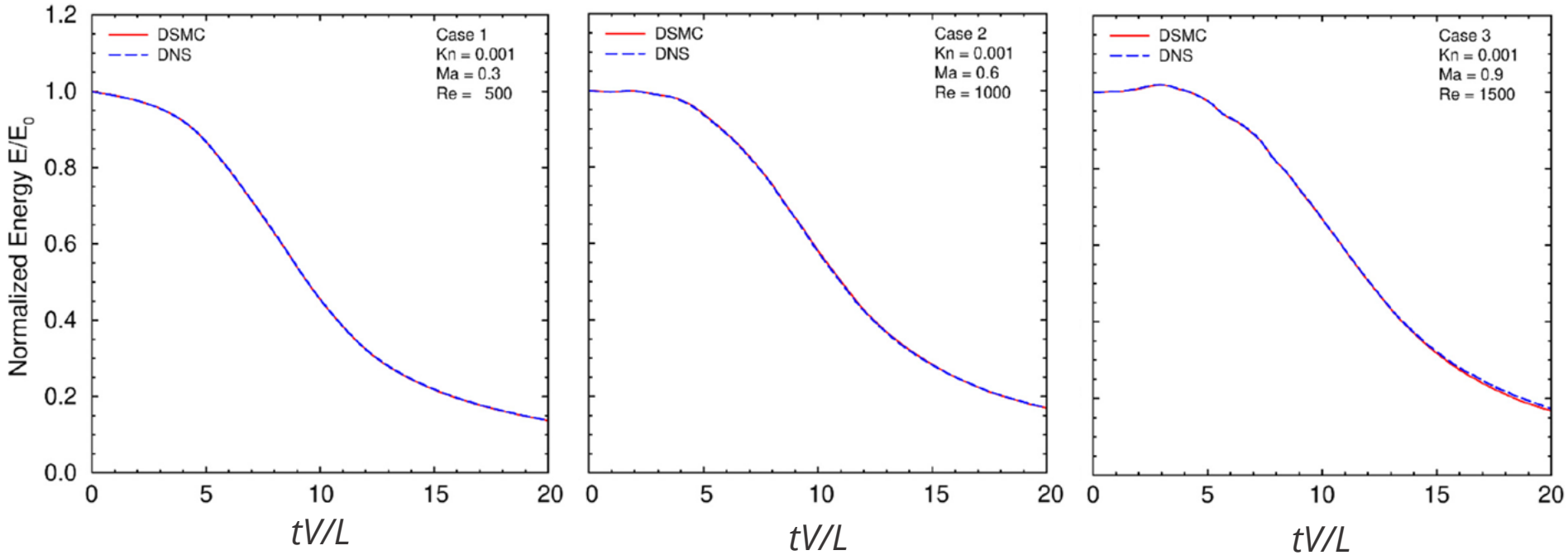




Kinetic energy decay

Excellent agreement between MGD and NS! *

- Scale-by-scale comparison?



*Here, DSMC data are time-averaged before computing flow quantities