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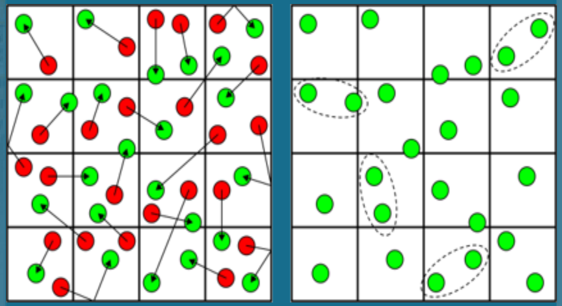
Exploring near-continuum turbulent compressible flow in the Taylor-Green vortex



BY:

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U.S. DEPARTMENT OF ENERGY NNSA

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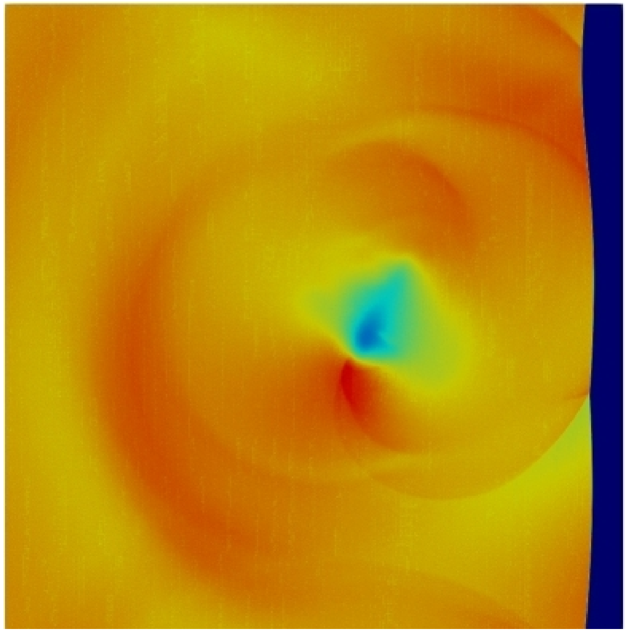
Examples of Compressible Turbulence

Interstellar/Intergalactic Turbulence
Creates fluctuations & redistributes angular momentum leading to star formation



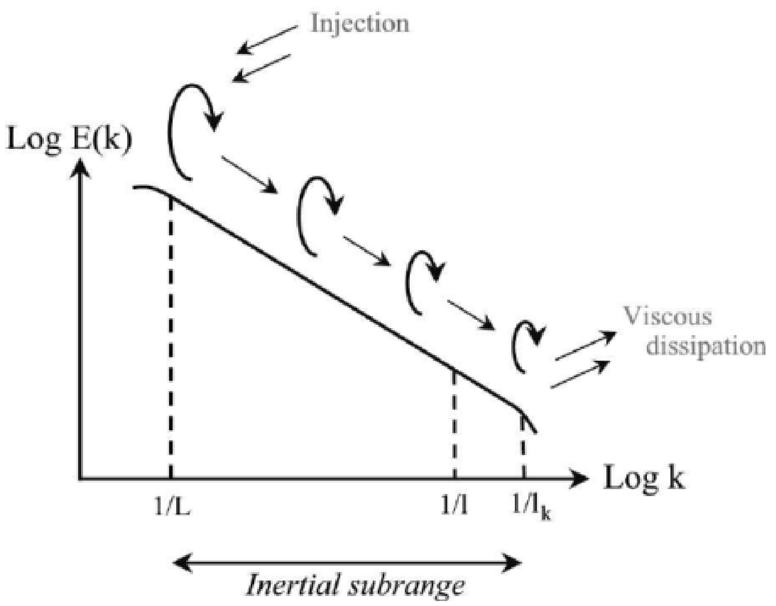
Shock/Turbulence Interaction
Shocks/shocklets interacting with acoustic waves

Supersonic Combustion
Heat release due to exothermic reactions

Compressible Turbulence

Compressible energy cascade is more complicated than incompressible

- In compressible turbulence, complex nonlinear interactions of vortices, acoustic waves, and shock waves lead to strong couplings between velocity and thermodynamic fields.
- The interaction between shock waves and rotating vortices baroclinically creates new vortices, which are amplified by compression and considerably increase the net vorticity.
- Thermal fluctuations and translational nonequilibrium play a role in the baroclinic creation of turbulence.
- These physical phenomena occur at the molecular level (mean-free-path level) and typically are not included in the Navier-Stokes equations.



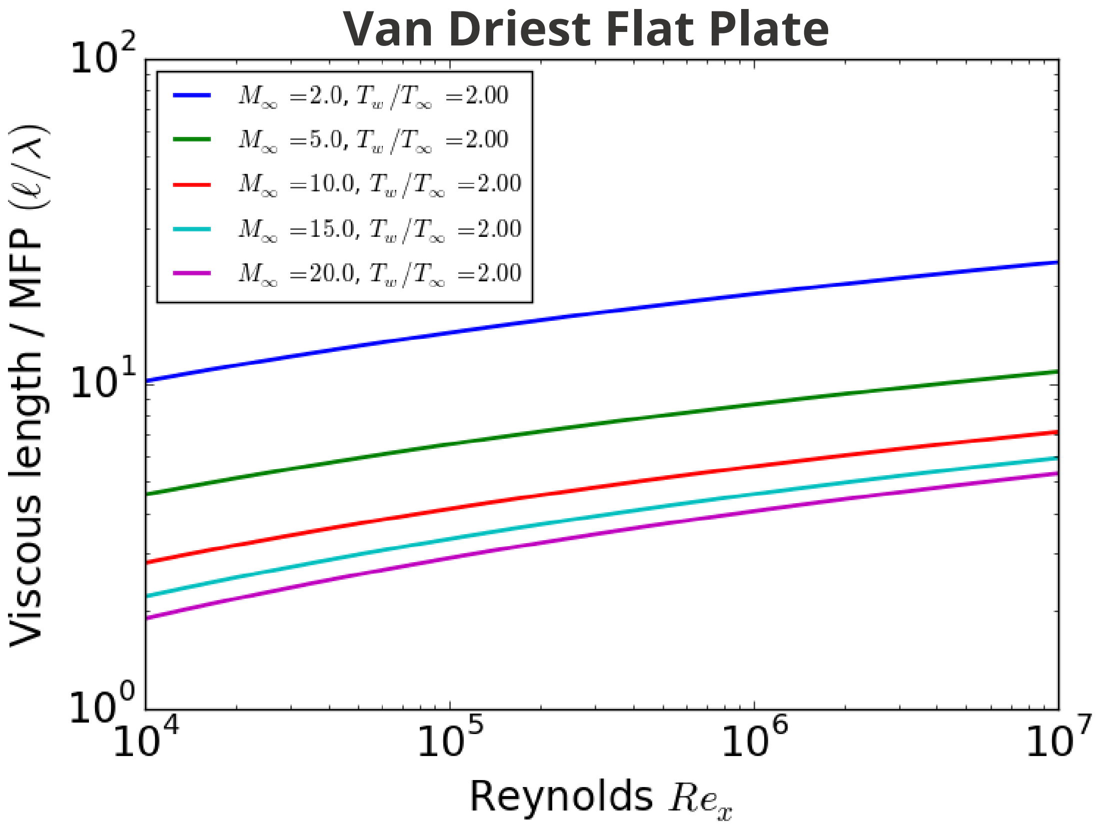
Turbulent energy cascade:
Kinetic energy is generated at large scales, transferred gradually to smaller scales, and dissipated finally by viscosity at small scales close to the Kolmogorov length scale.

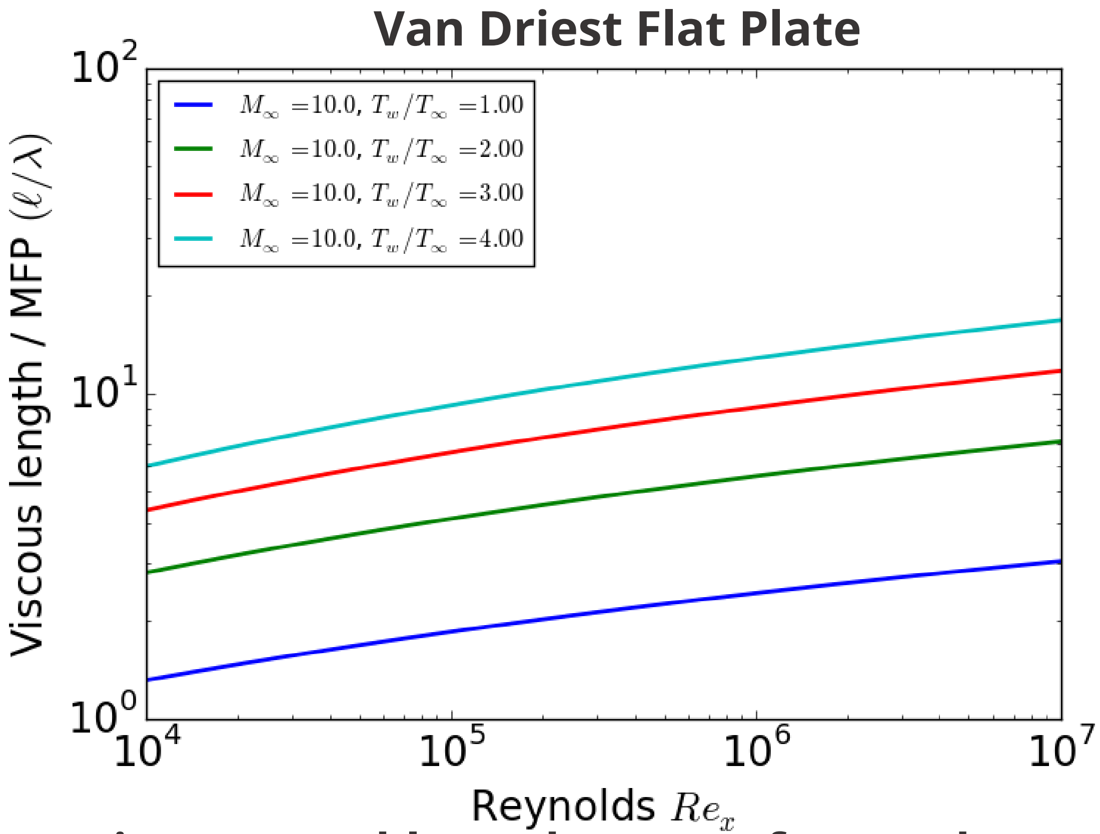
Viscous Length Scale & Mean Free Path

Approximate scaling:

$$\frac{\ell}{\lambda} \approx \frac{2}{M\sqrt{\gamma \pi C_f}}$$

Ref	Flow	$\ell = u_\tau/\nu$ (μm)	λ (μm)	ℓ/λ
Martin 2007	Mach 6, flat plate, flight	53	7.7	6.9
Duan 2016	Mach 6, wind tunnel	52	10	5.2
Duan 2011	Mach 21, wedge, flight	12	3.5	3.3





Viscous length scale associated with turbulence is comparable to the mean free path, suggesting molecular effects could come into play

Motivation

- Navier-Stokes equations assume the continuum hypothesis
- Shocks in compressible turbulence violate the continuum hypothesis
- Viscous length scale is comparable to the mean free path
- Noncontinuum molecular phenomena may be relevant when turbulent scales become comparable to the molecular level scales
- Under such conditions, the turbulent energy cascade may no longer be described by the overall energy dissipation rate and kinematic viscosity
- This dependence of the turbulent energy cascade on small-scale motions motivates our study

Question

"How does noncontinuum turbulent flow differ from continuum turbulent flow?"

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

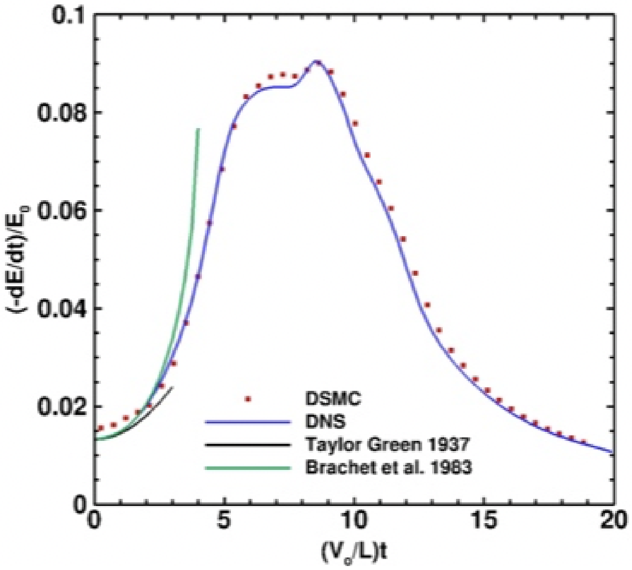
Taylor Green Flow at the Molecular Level

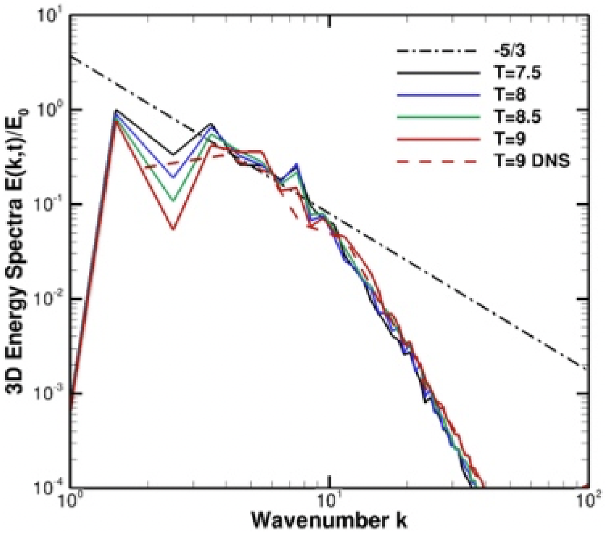
Taylor-Green (TG) vortex flow is a canonical turbulent flow

- Incompressible TG flow is used to validate codes and assess subgrid-scale models
- Initial condition contains only a single length scale (single wave number)

Turbulent energy cascade can be observed numerically in TG flow

- Early-time flow exhibits a rapid buildup of a fully turbulent dissipative spectrum
- Late-time flow exhibits the basic features of isotropic, homogeneous turbulence





Incompressible turbulent TG flow has been successfully simulated at the molecular level.

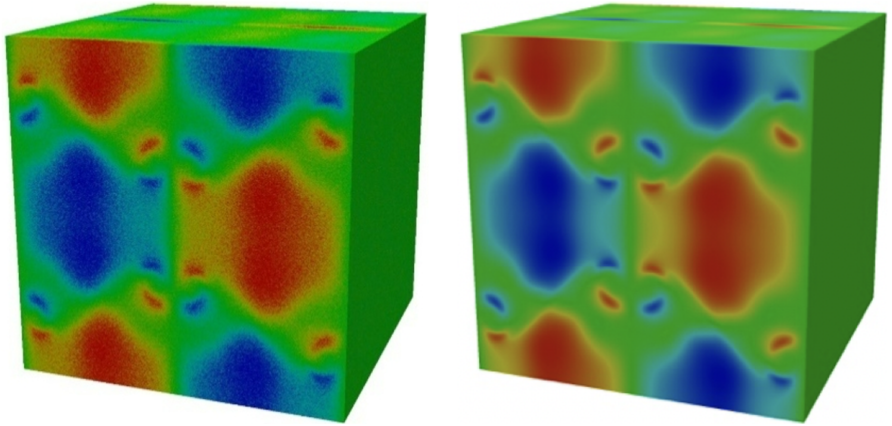
Gallis et al., Molecular-Level Simulations of Turbulence and Its Decay, Phys. Rev. Lett. 118, 064501 (2017).

Taylor-Green Simulation Conditions

Mach Numbers: 0.3, 0.6, 0.9, 1.2

Numerical parameters

- Cubical domain, triply periodic boundaries
- Side length = $2\pi L$, L = 0.0001 m, cells/side = 2000
- Cell size = 314 nm, total cells 2000^3 = 8 billion
- Time step = 2.5-10 ps, near-neighbor collisions
- Molecules/cell = 45, total molecules = 0.36 trillion



Taylor-Green flow from DNS and DSMC simulations.

Gas parameters

- Molecular mass = 66.3×10^{-27} kg, monatomic
- Temperature = 273.15 K, viscosity = 2.8709×10^{-5} Pa·s
- Molecular model = Variable Soft Sphere (VSS)
- Classic Taylor-Green initial conditions with constant temperature.

Simulation Parameters

Simulations performed on LLNL/Sequoia

- 32,768 nodes (×16 cores/node, ×4 threads/core), 30 hrs.

Low-Re, High-Ma Turbulent Flows

Re	Mach	η/λ	Kn
500	0.3	15.8	0.001
1000	0.6	9.4	0.001
1500	0.9	6.9	0.001
2000	1.2	5.6	0.001

- Here, Kn is kept constant, and Re is increased by increasing Ma.
- System Knudsen number places the flow in the **continuum regime**.
- However, η/λ ratio suggests that **non-equilibrium effects including non-equilibrium transport** and **thermal fluctuations** may be important.
  - η is the Kolmogorov length scale
  - λ is the molecular mean free path

Simulations

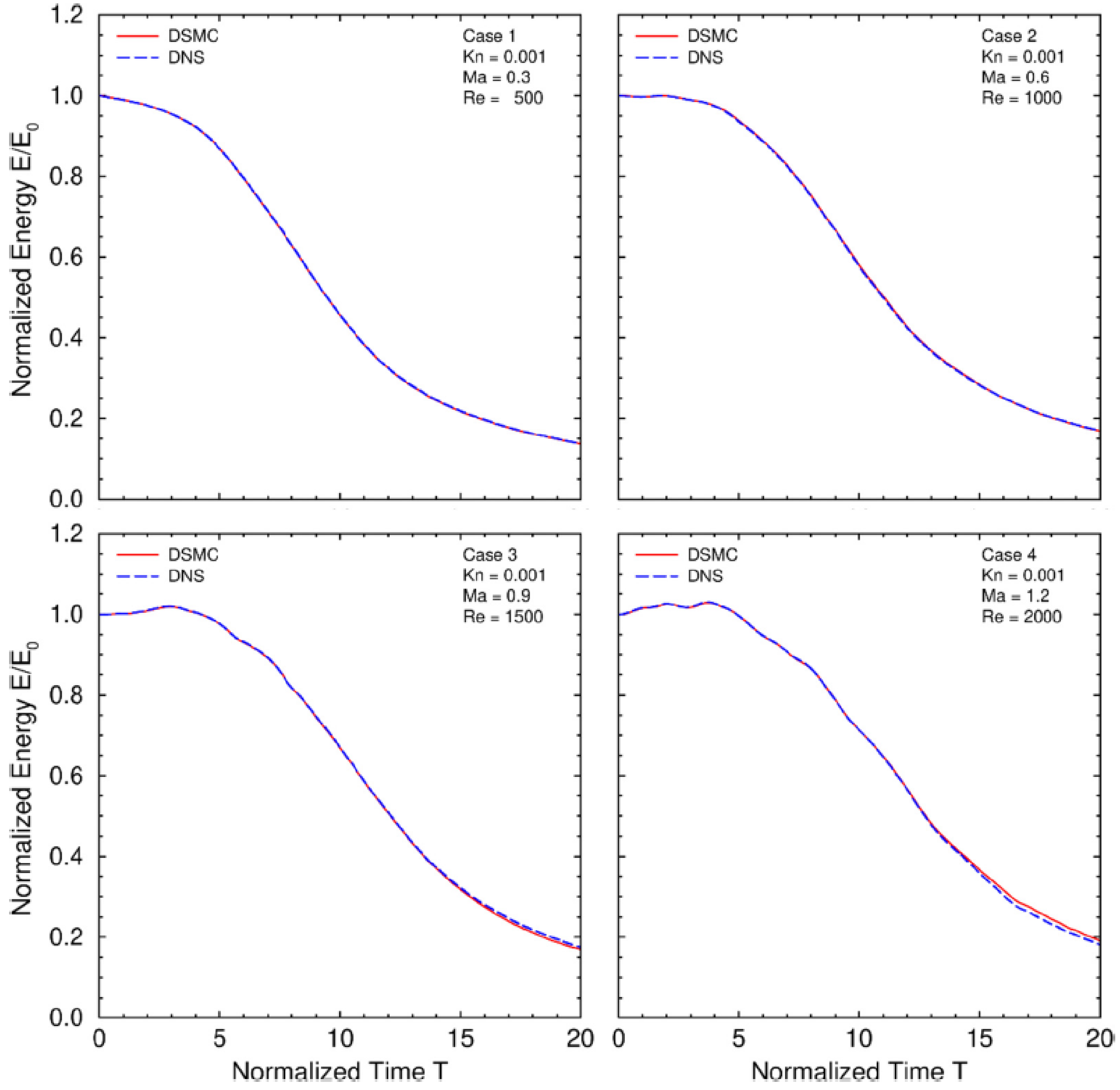
Molecular Gas Dynamics

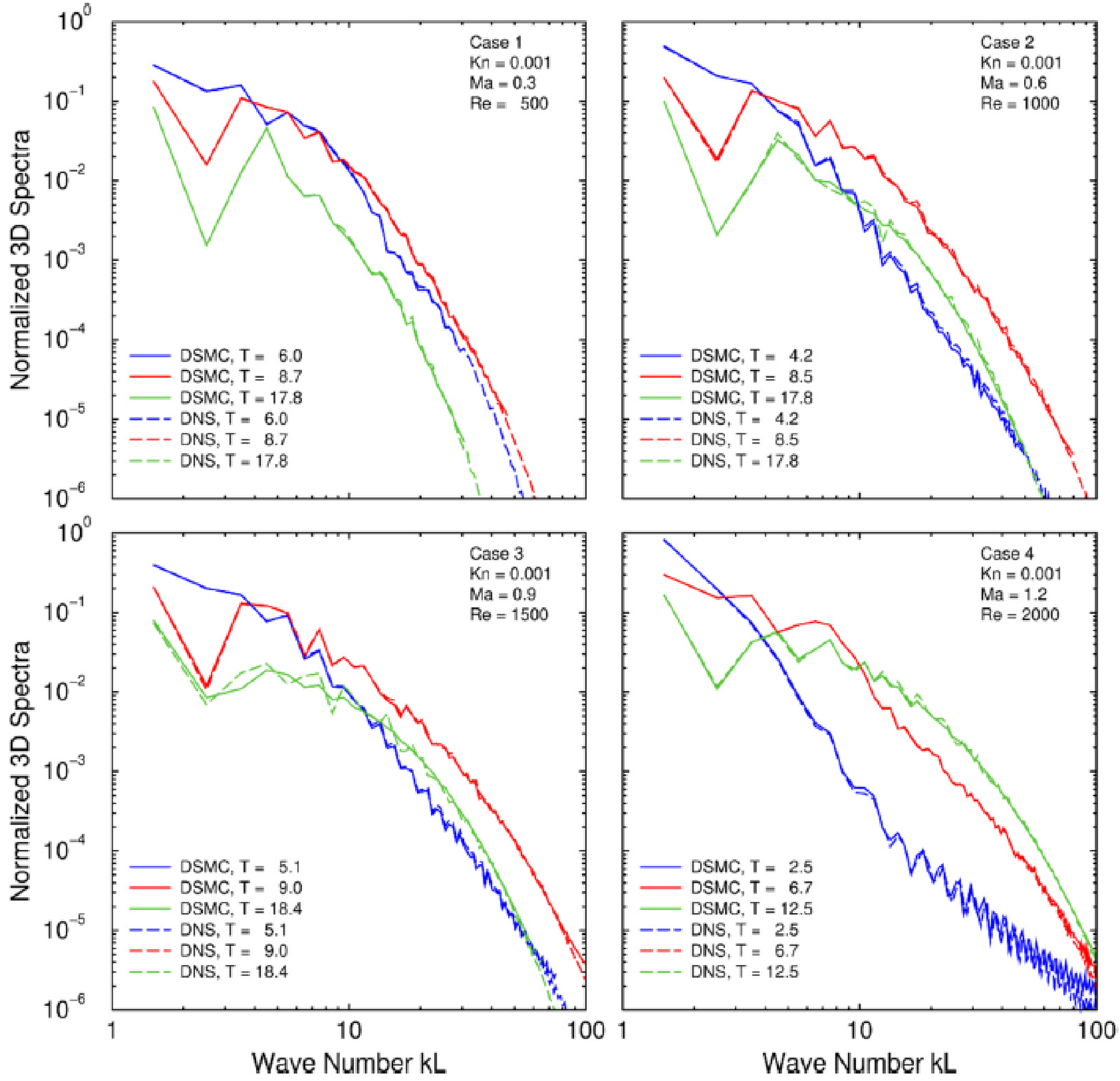
- Direct Simulation Monte Carlo (DSMC)
  - Initially developed for rarefied hypersonic flow
- Includes physics usually omitted from CFD
  - Thermal & chemical nonequilibrium
  - Stress and heat-flux tensor anisotropy
  - Thermal fluctuations
- SPARTA (**S**tochastic **PA**rallel **R**arefied-gas **T**ime-accurate **A**nalyzer)
  - Open source code available at sparta.sandia.gov

Direct Numerical Simulations

- SPARC (**S**andia **P**arallel **A**erodynamics & **R**eentry **C**ode)
  - Compressible finite volume code
- Blended flux scheme for high accuracy and stability
  - 6th -order, low-dissipation, central-scheme in smooth regions
  - Dissipative modified Steger-Warming scheme near shocklets
  - Switch between schemes based on gradients in Mach number
- 4th order RK time advancement with CFL of 0.5

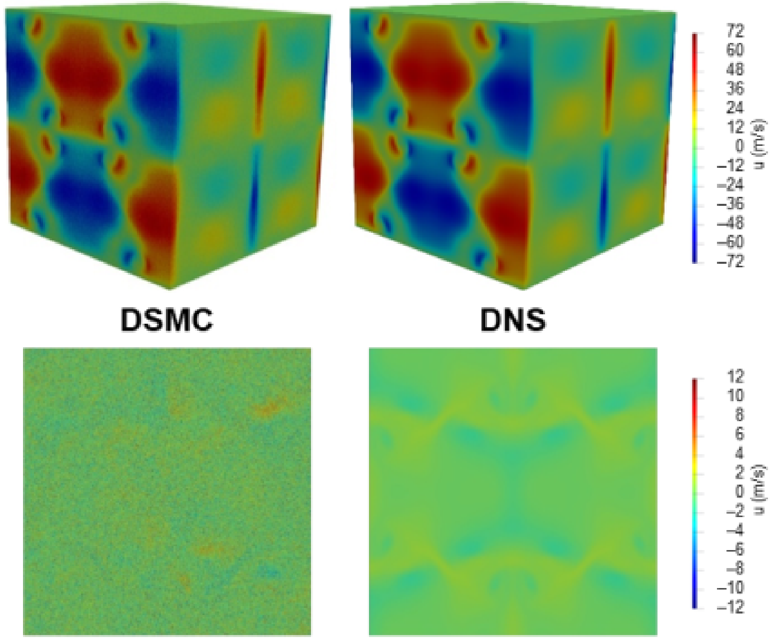
Kinetic Energy & Energy Spectra

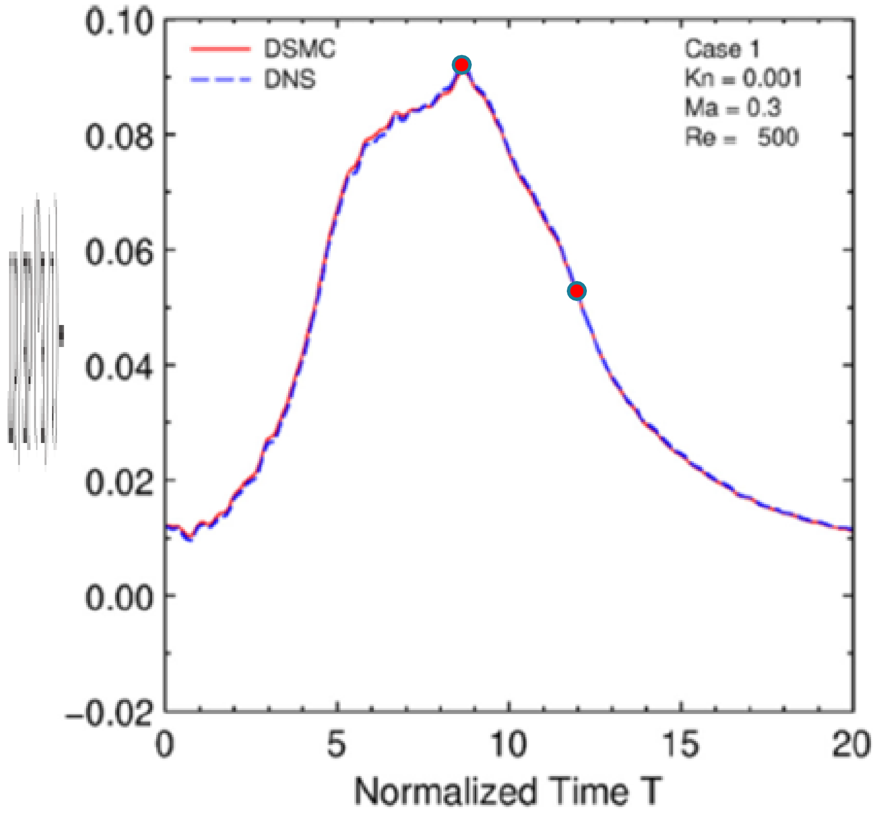




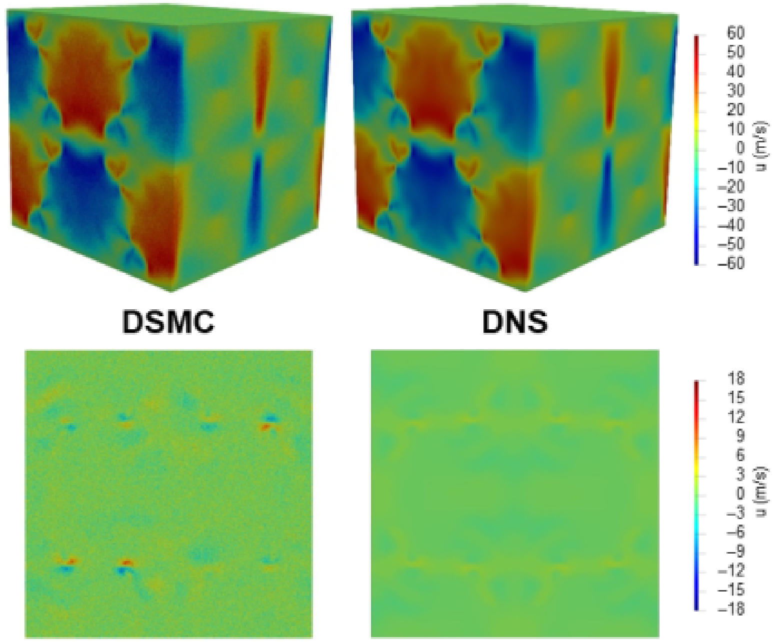
TG: Ma = 0.3, Re = 500

$T = 8.7$



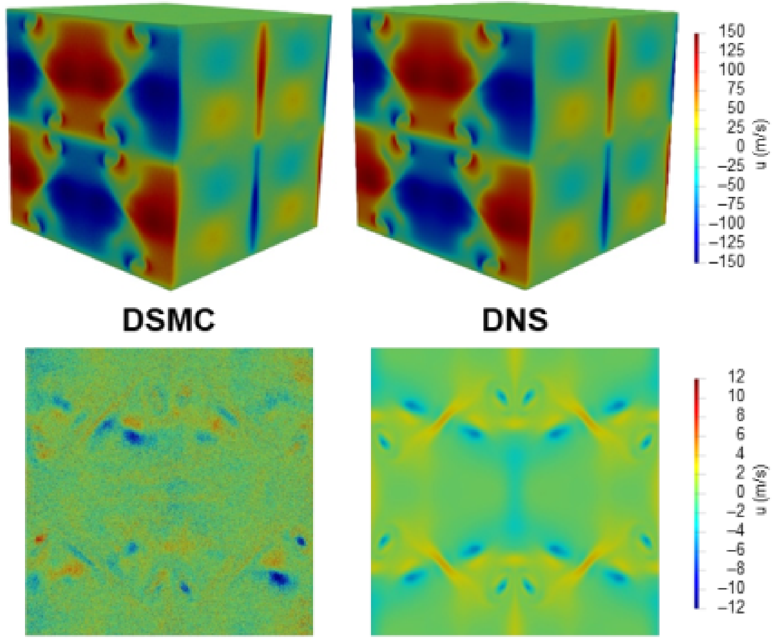


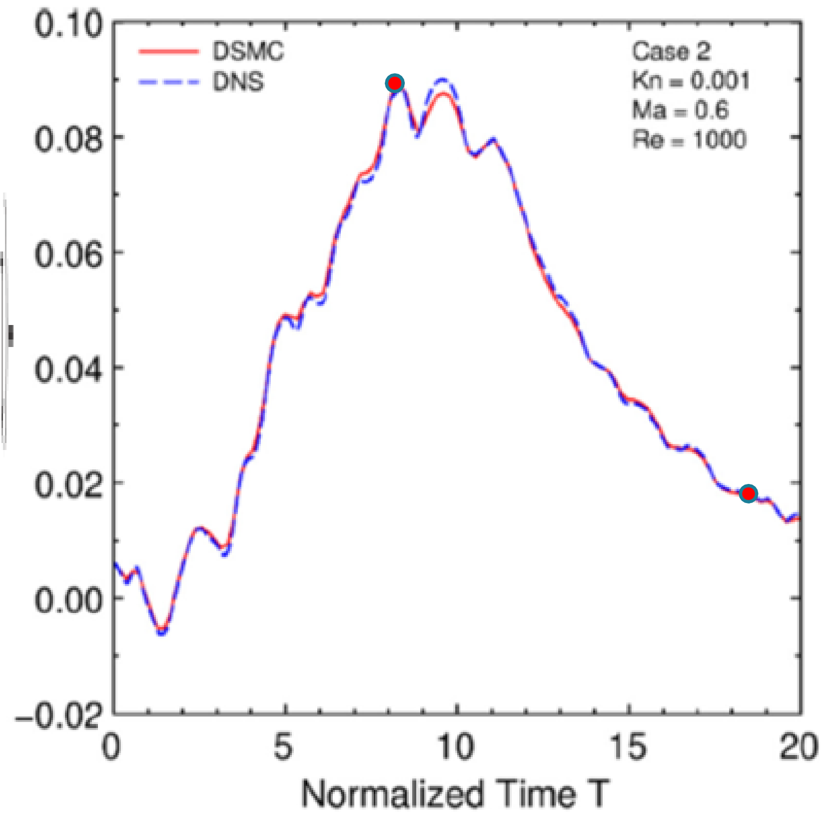
$T = 12.1$



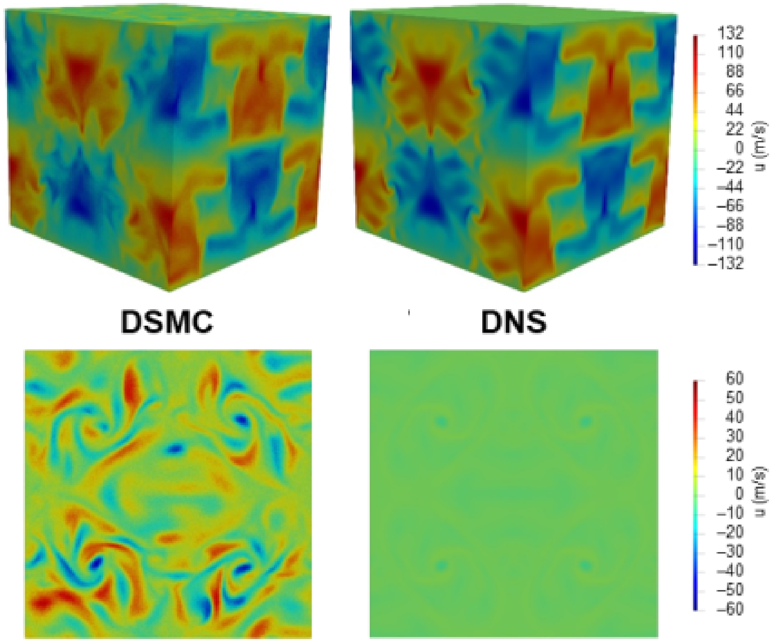
TG: Ma = 0.6, Re = 1000

$T = 8.45$



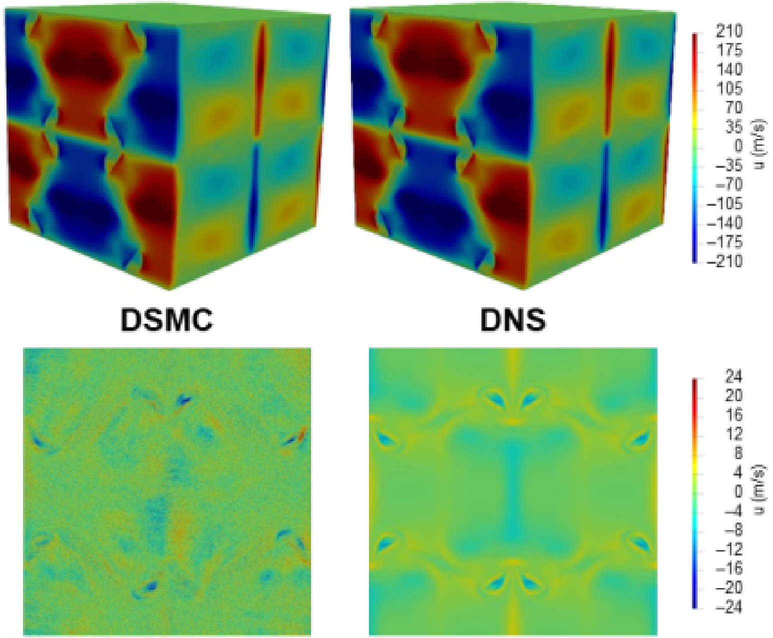


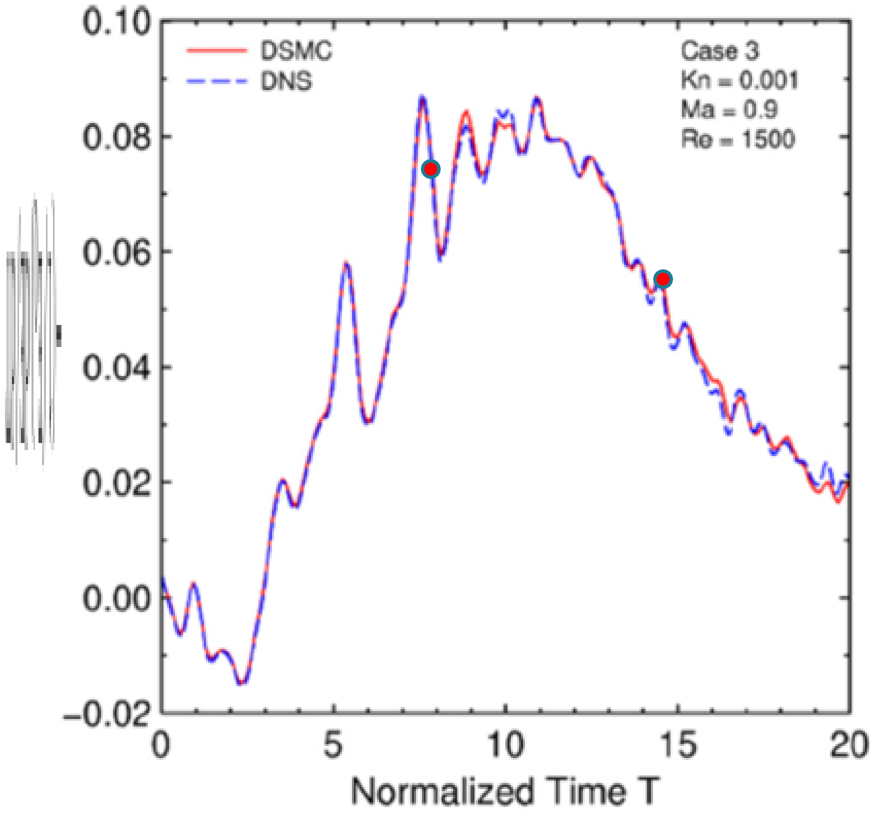
$T = 18.47$



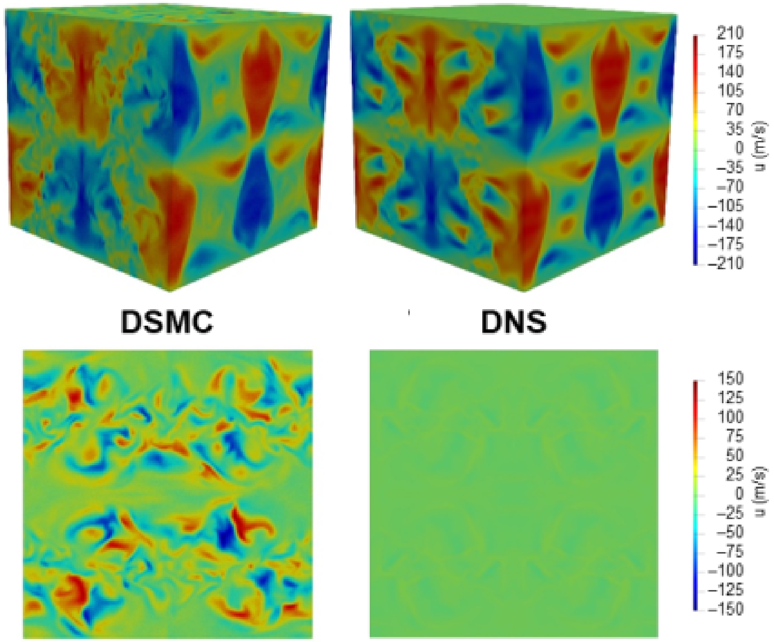
TG: Ma = 0.9, Re = 1500

$T = 7.63$

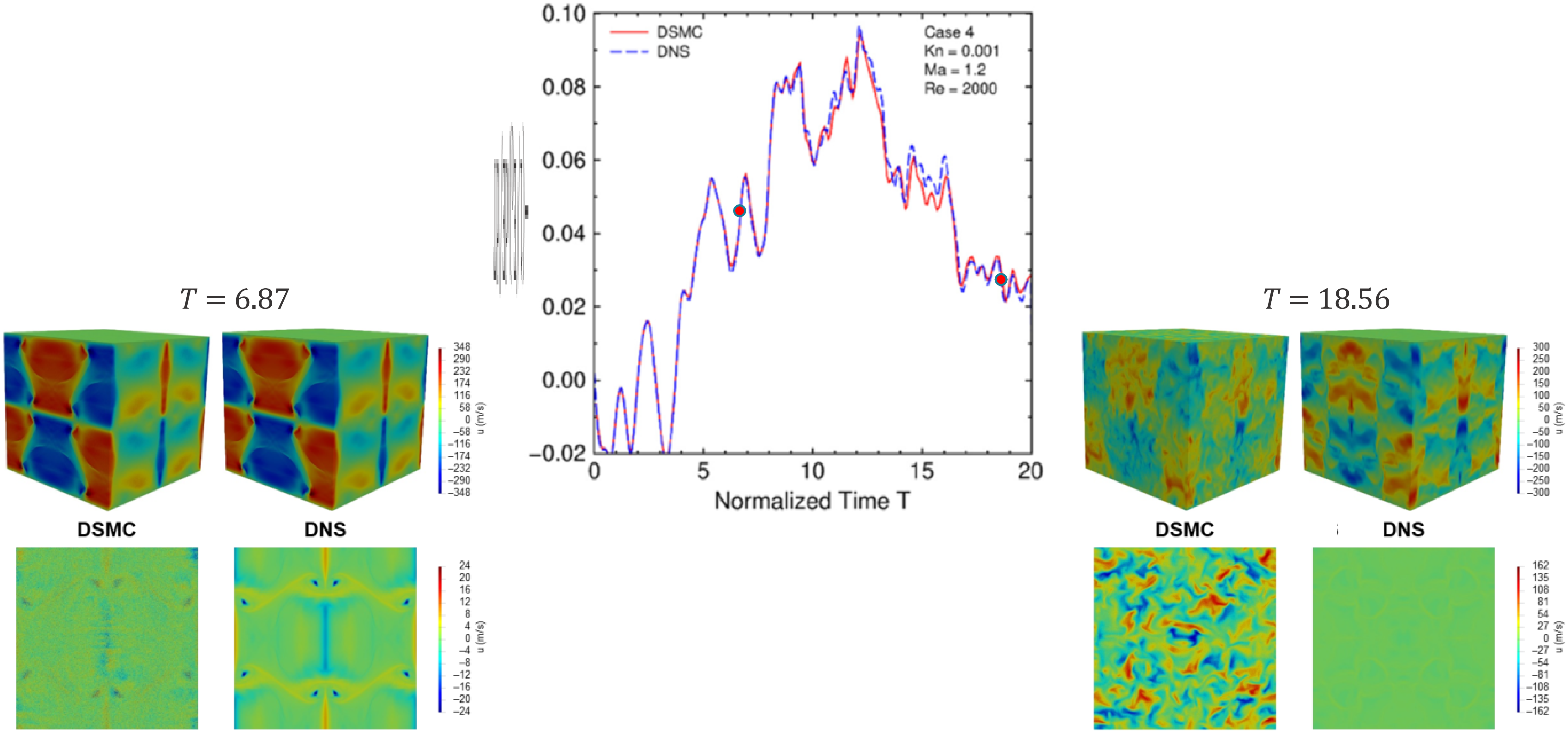




$T = 14.77$

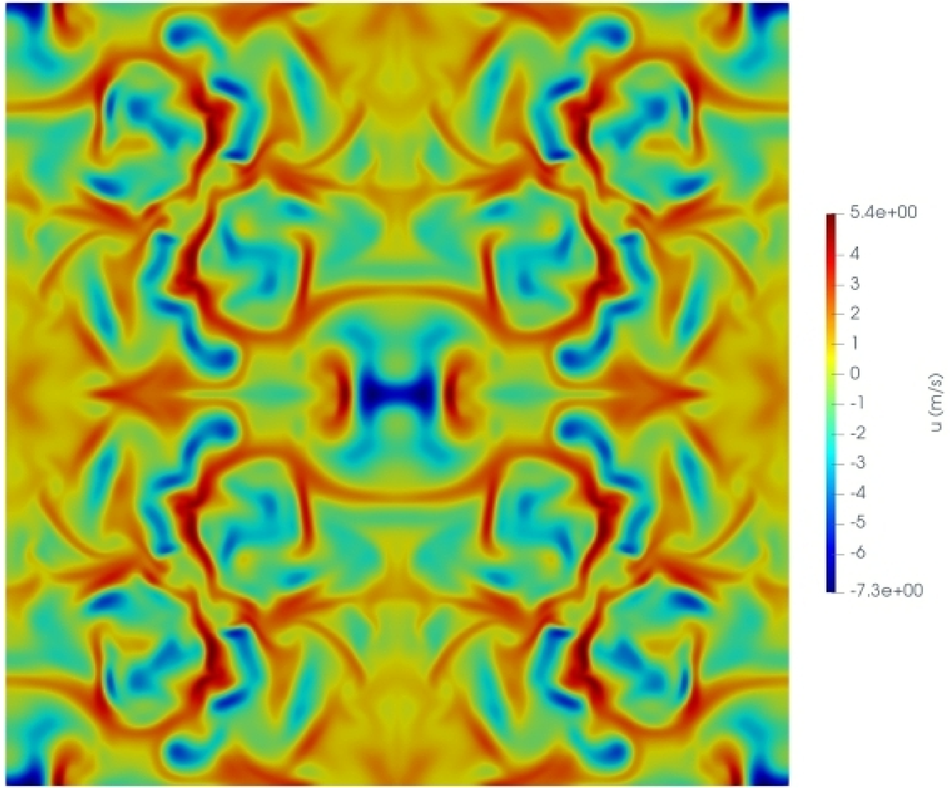


TG: Ma = 1.2, Re = 2000

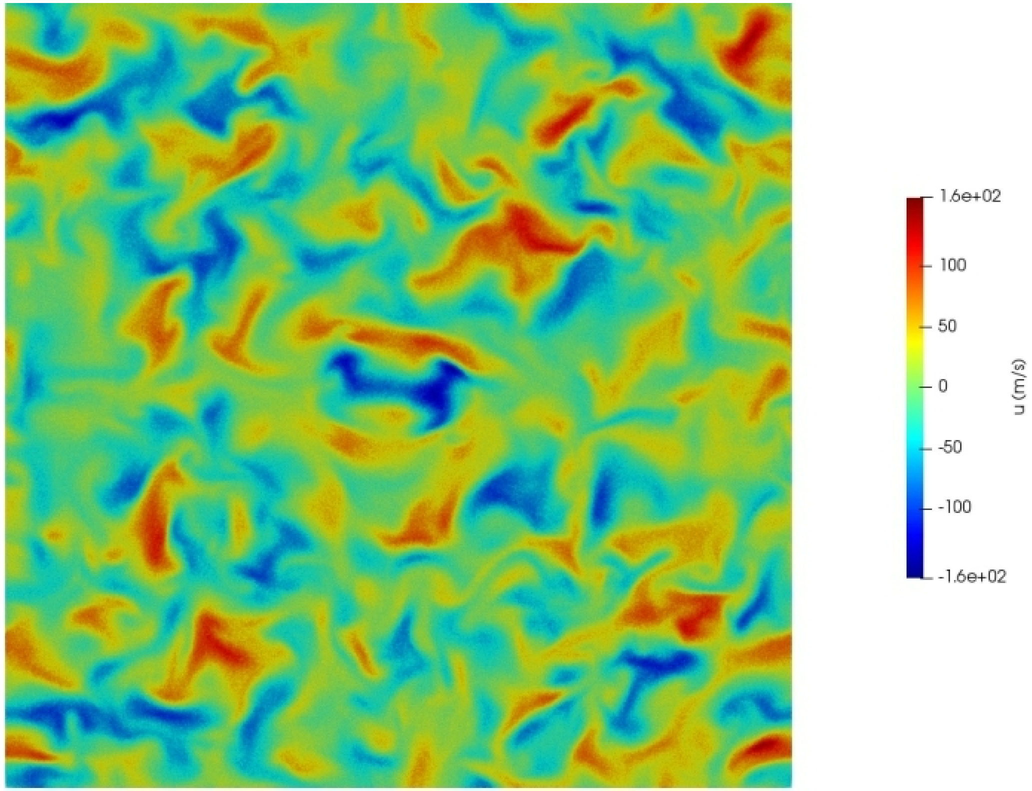


TG: Ma = 1.2, Re = 2000, t = 18.56

Y-Z plane u-velocity, auto-scaled



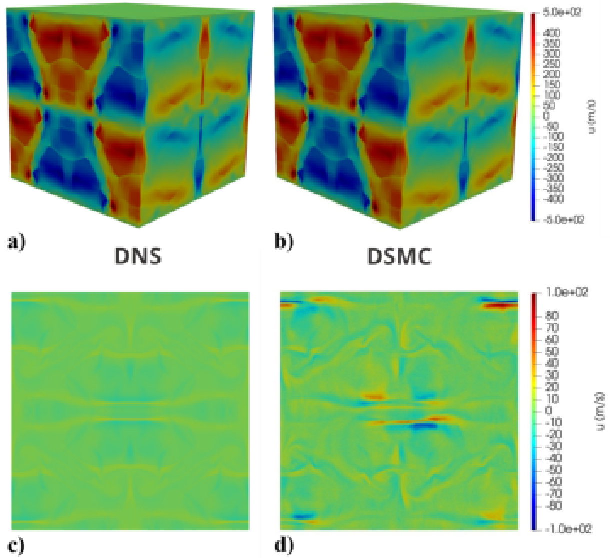
DNS



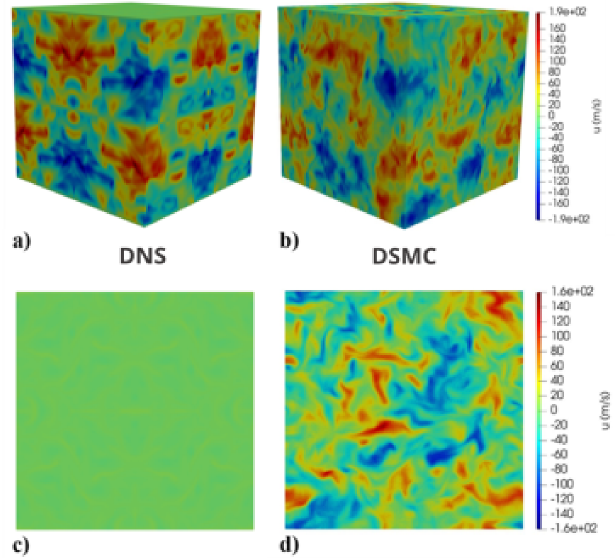
DSMC

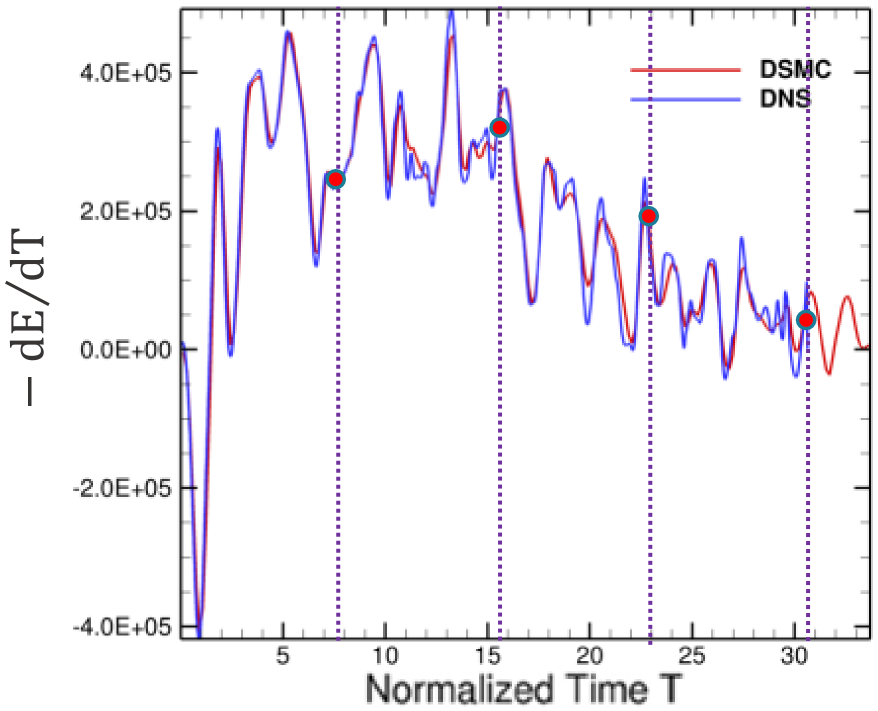
TG: Ma = 2.0, Re = 3316.7 (Polytropic)

$T = 7.66$

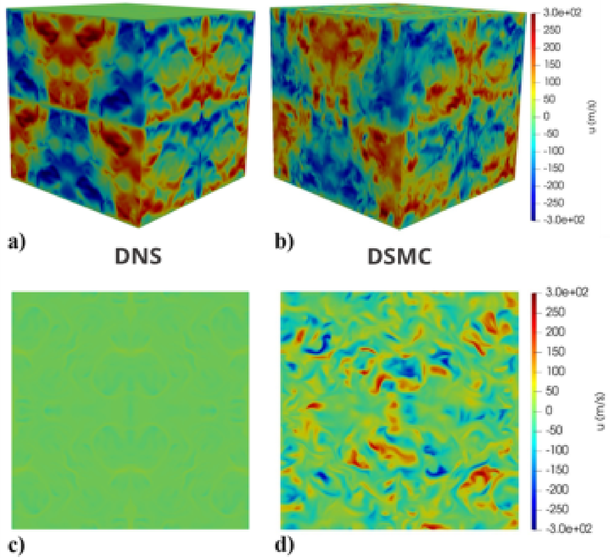


$T = 22.97$

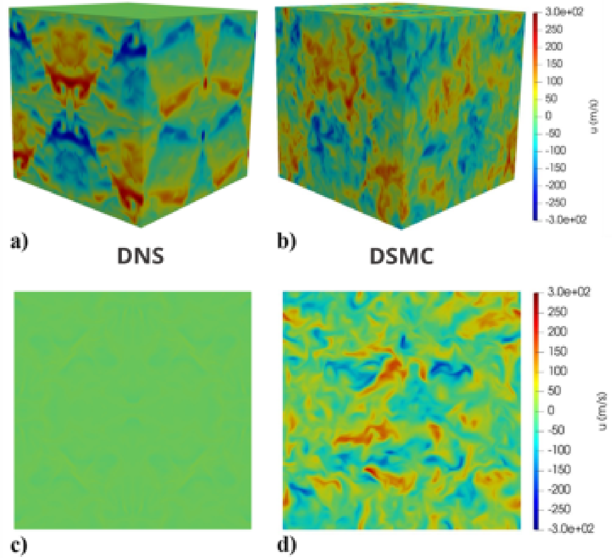




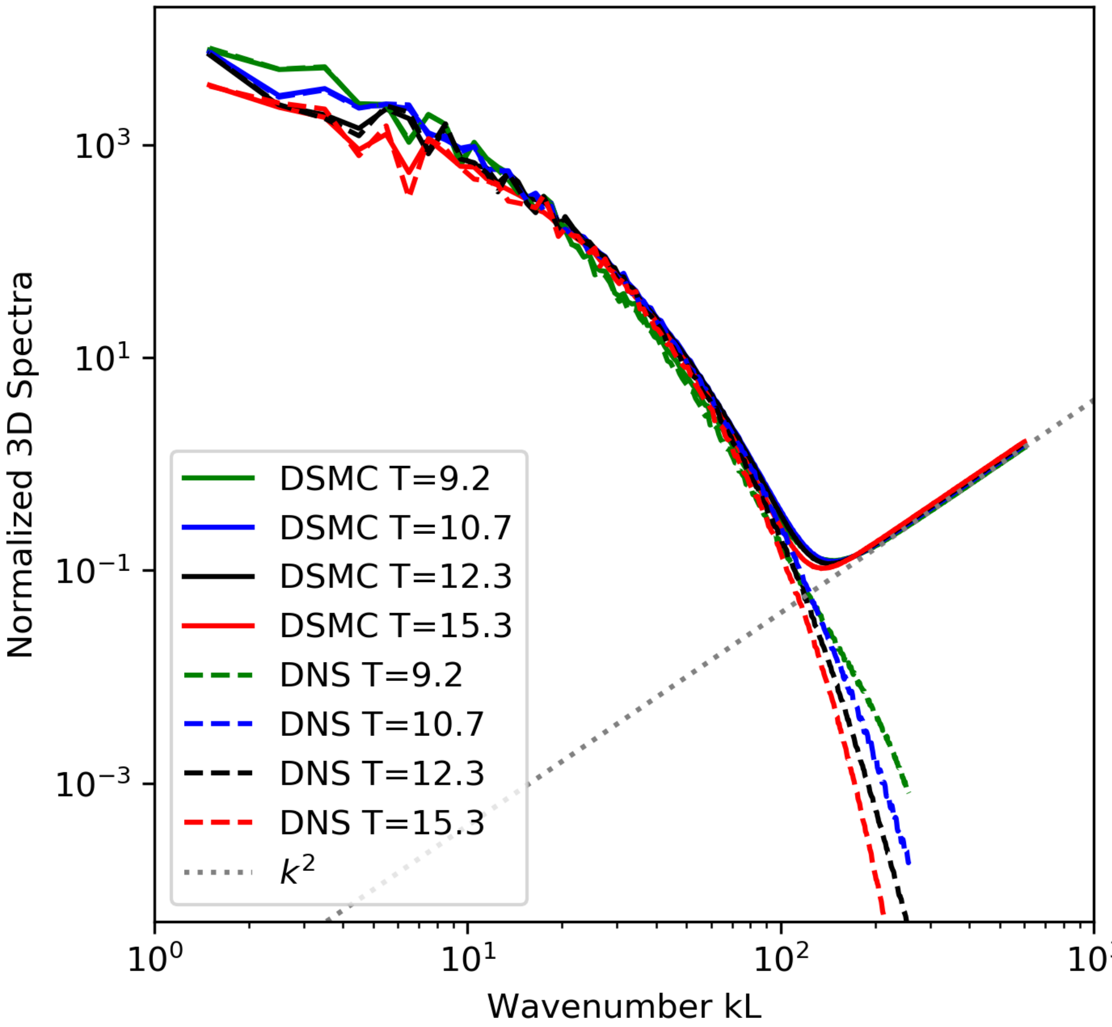
$T = 15.31$



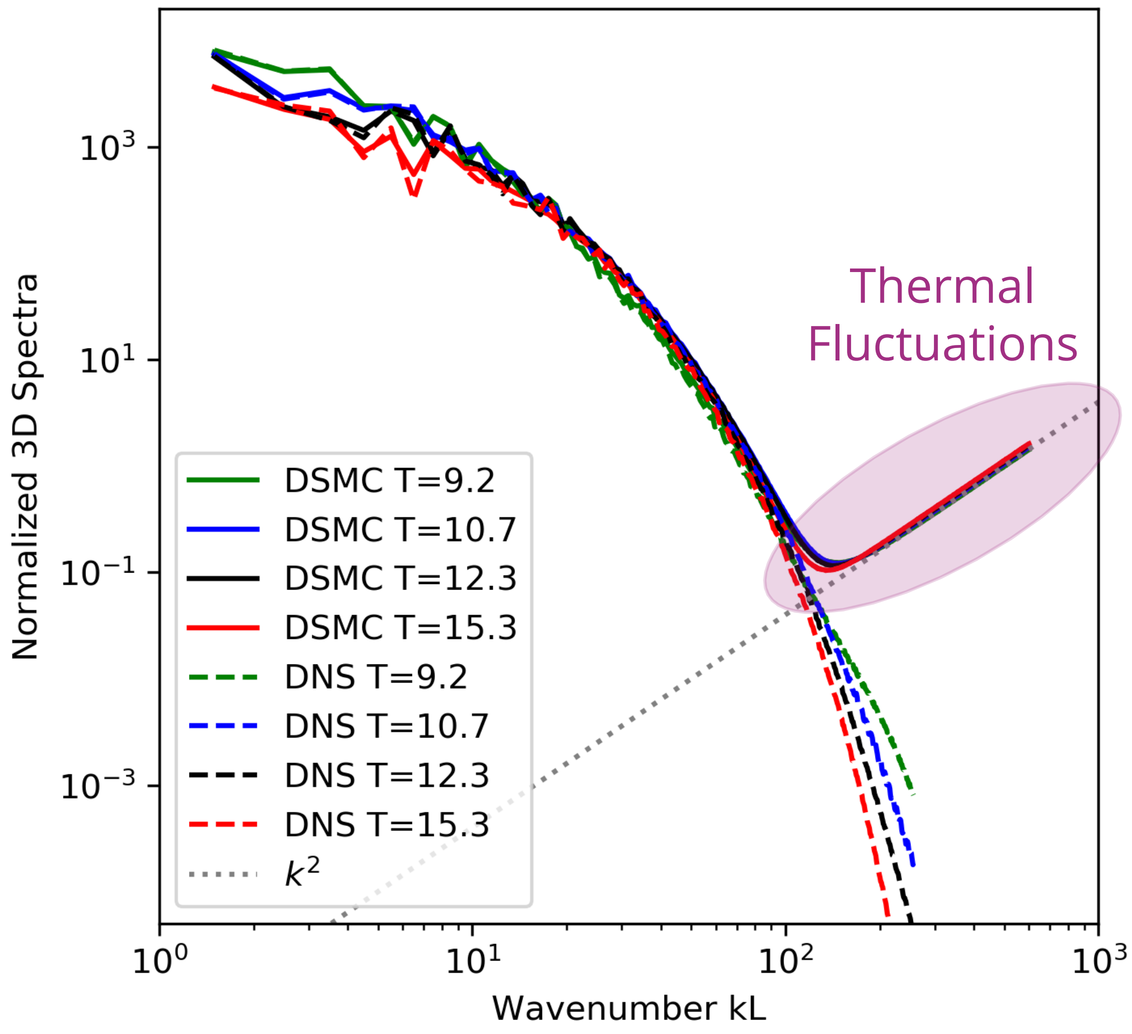
$T = 30.63$



TG Energy Spectra: Ma = 2.0, Re = 3317 (Polytropic)



TG Energy Spectra: Ma = 2.0, Re = 3317 (Polytropic)



Conclusions

- At low Mach & Reynolds numbers and early times, DSMC and DNS produce similar profiles (small wavenumbers, incompressible flow, or large η/λ).
- At higher Mach & Reynolds numbers and past maximum-dissipation-point times, DSMC breaks the symmetry of the initial condition while DNS preserves it.
- Differences are observed when the Kolmogorov scales are comparable to the mean free path, indicating molecular level effects are dynamically relevant.
- Translational nonequilibrium across shocklets could also play a role.
- Differences between molecular gas dynamics and Navier-Stokes equations are seen at conditions relevant to compressible turbulent boundary layers.

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