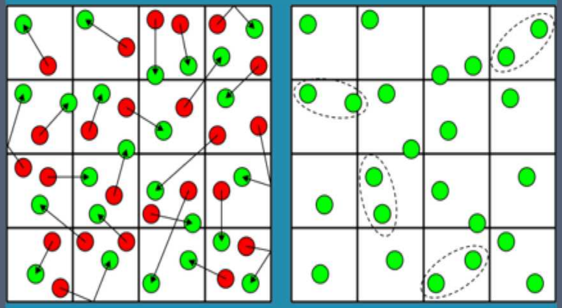
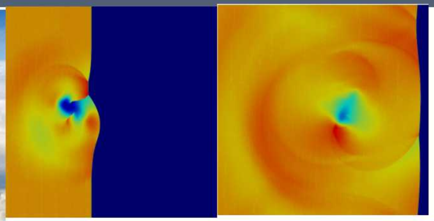
Sandia National Laboratories

SAND2020-0072C

DSMC Simulations of Compressible Turbulence





- *PRESENTED BY:*

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U.S. DEPARTMENT OF ENERGY NNSA

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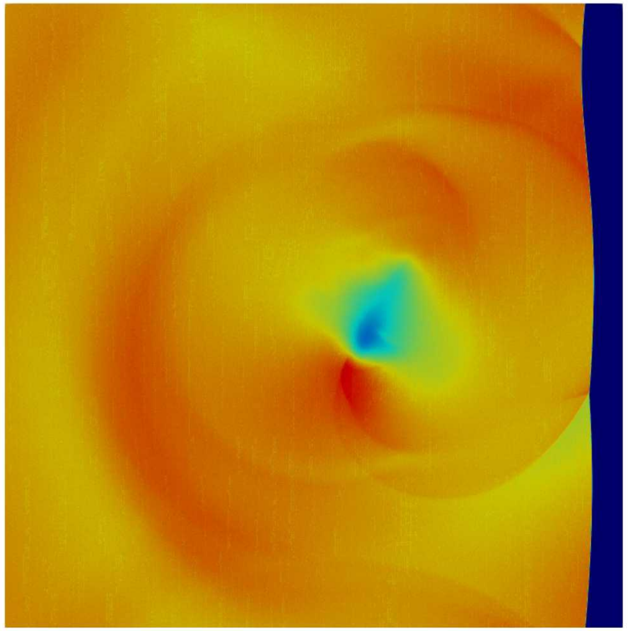
Examples of Compressible Turbulence

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

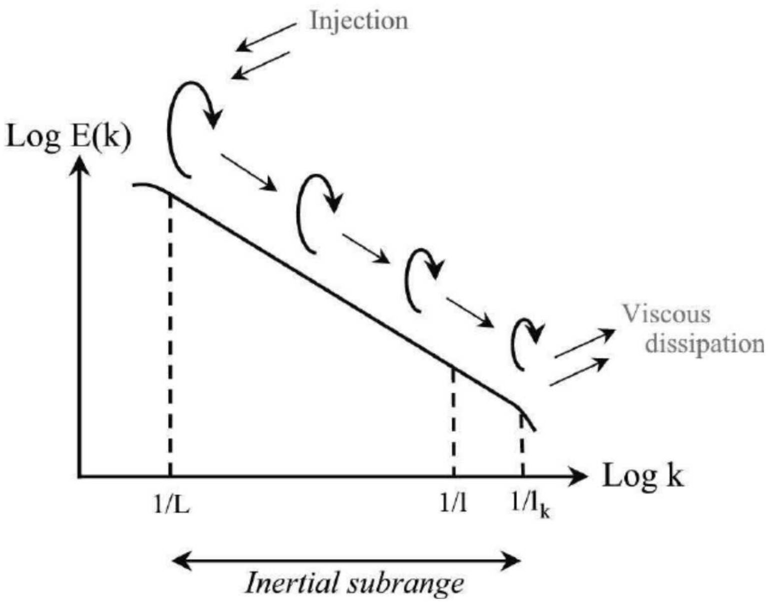


Shock/Turbulence Interaction
Shocks/Shocklets interacting with acoustic waves

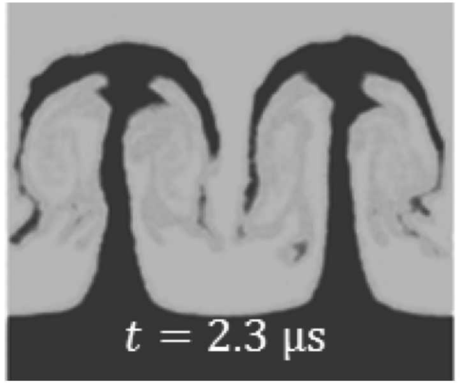
Supersonic Combustion
Heat release due to exothermic reactions

Compressible Turbulence

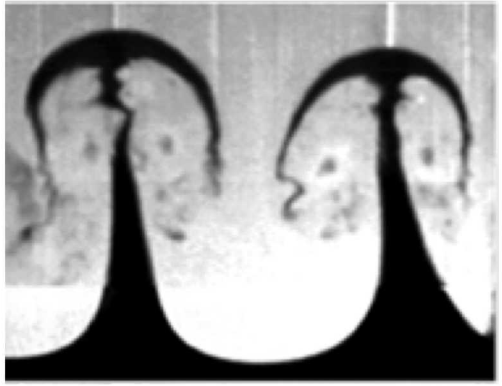
- Kinetic energy is generated at large scales, transferred gradually to smaller scales, and dissipated finally by viscosity at small scales close to the Kolmogorov length scale.
- Since the dissipation scale decreases with viscosity, could this scale become so small that the hydrodynamic description breaks down? (Frisch 1990)
- Such phenomena have been ruled out in Kolmogorov's theory (valid for small Mach numbers only)
- In compressible turbulence, complex nonlinear interactions of vortices, acoustic waves, and shock waves (baroclinic creation of vorticity) lead to strong couplings between the velocity fields and the thermodynamic fields.



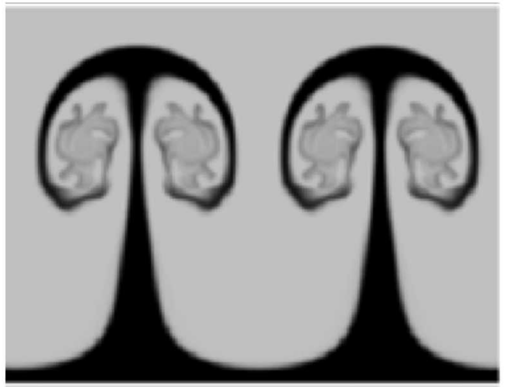
Baroclinic Creation of Vorticity



DSMC



Experiment (Morgan et al., JFM, 2012)

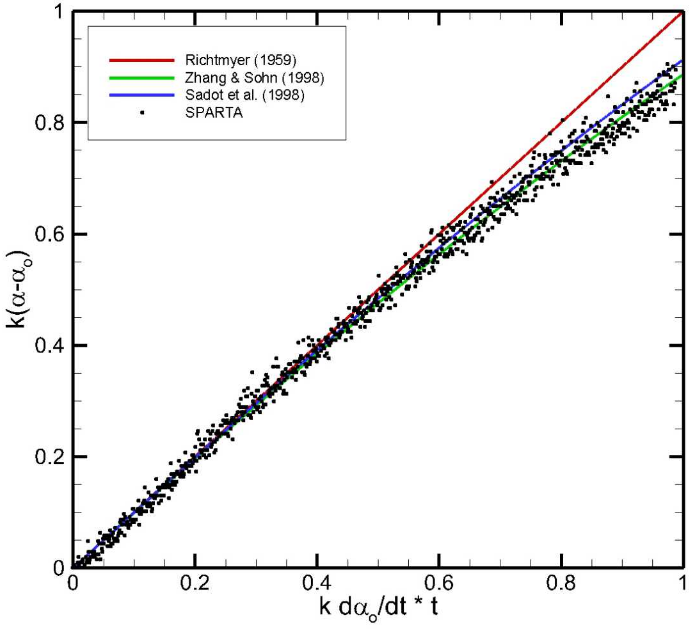


Navier-Stokes

The concentrated vorticity causes the interface to develop into mushroom-like shapes with spirals of the light gas circling the centers of vorticity.

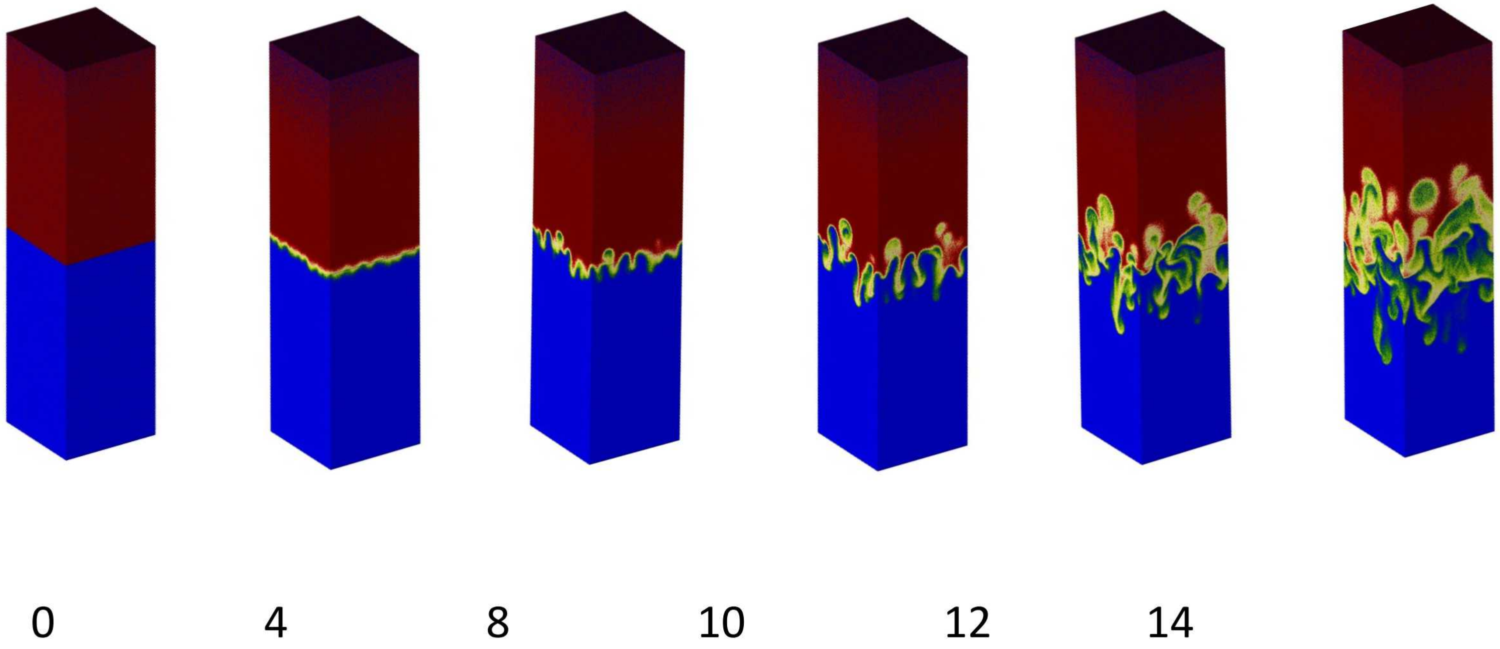
The spirals break, and strong mixing appears, while the stems of the mushroom get thinner.

Finally, the shaded vortices interact with the stems of the mushrooms.



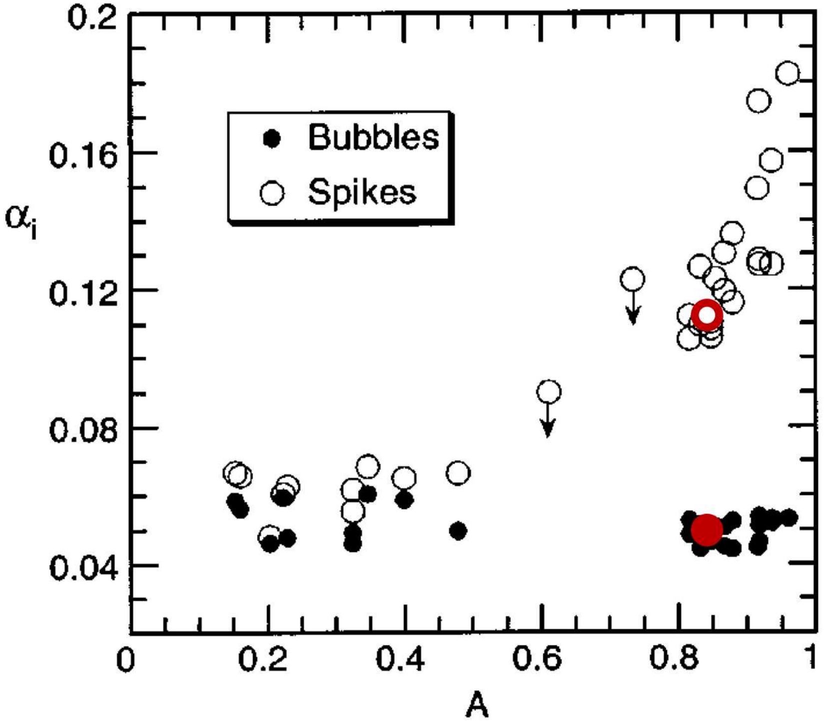
Nondimensional amplitude for an initially small perturbation compared to theoretical/empirical models (Gallis et al., Physics of Fluids 2015)

Rayleigh-Taylor Instability from a Flat Interface



Vorticity created due to density gradients

Rayligh-Taylor Instability (Ar/He) (Gallis et al., PR Fluids, 2016)



Dimonte & Schneider, Phys. Fluids (2000)
DSMC predictions in red.

Kolmogorov Scale and Mean Free Path

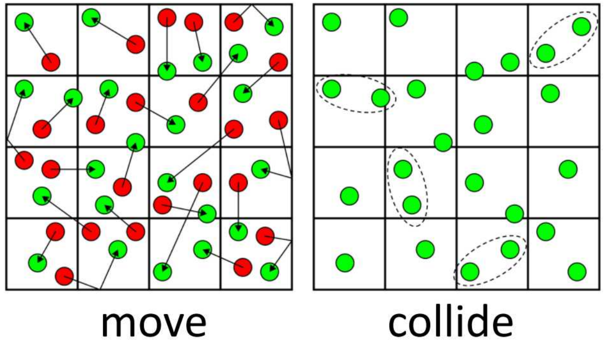
For a **gas** flow with a turbulent Mach number *M* and a turbulent Reynolds number ***Re*** the ratio of the Kolmogorov length scale η to the mean free path λ scales as:

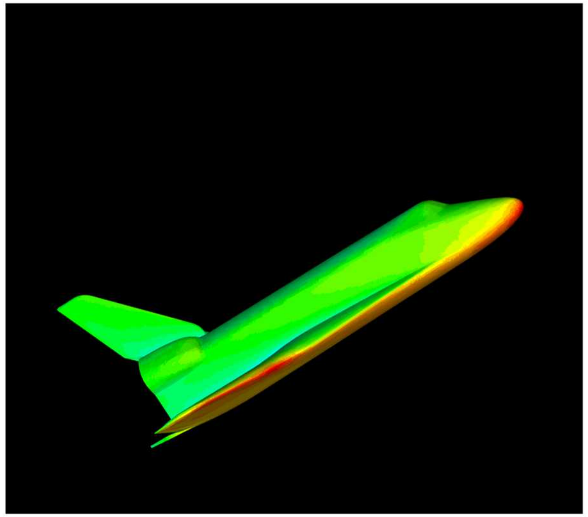
$$\frac{\eta}{\lambda} = \mathrm{Re}^{1/4} / M$$

- For Re = 1,000 and Ma = 1.0, this ratio is only 5
  - Smallest scale of turbulence (Kolmogorov scale) becomes comparable to the smallest scale of motion (mean free path)
  - At Kolmogorov scale, **medium is no longer continuum**
- Can molecular transport be represented by transport coefficients?
  - The question of whether turbulent energy dissipation is related to molecular dissipation has been repeatedly posed: von Neumann (1950), Tennekes and Lumley (1972), Frisch (1990)
- Hydrodynamic equations can be derived from kinetic theory by omitting molecular-level effects, considered physically unimportant.

Direct Simulation Monte Carlo (DSMC)

- DSMC was initially developed for rarefied hypersonic flow
  - Molecular gas dynamics (MGD), not CFD
- **Includes physics usually omitted from CFD**
  - **Thermal and chemical non-equilibrium**
  - **Stress and heat-flux tensor anisotropy**
  - **Thermal fluctuations**
- Shown to simulate gas flows very accurately
  - Proved to solve Boltzmann equation
  - Reproduces Chapman-Enskog velocity distribution
- Computational and algorithmic advances are now bringing hydrodynamic flows within reach:
  - Instabilities
  - Turbulence



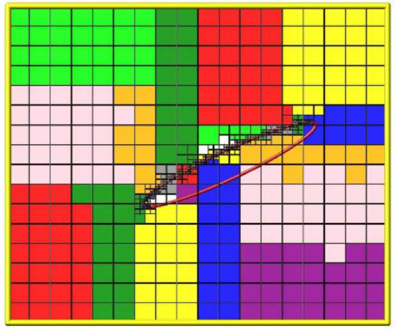


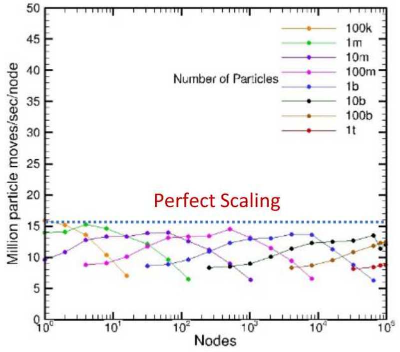
Could DSMC provide some insight into open questions of turbulence?

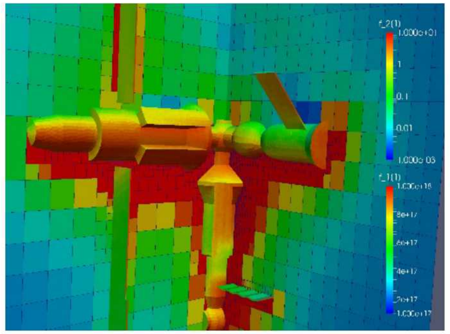
SPARTA: Sandia’s Exascale DSMC Code

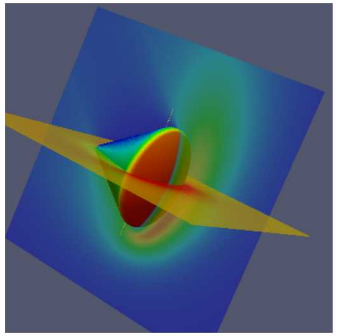
SPARTA = Stochastic PArallel Rarefied-gas Time-accurate Analyzer

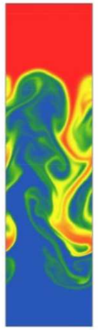
- 1D, 2D, 2D-axisymmetric or 3D; serial or parallel.
- Cartesian, hierarchical grid.
  - Octree (up to 16 levels in 64-bit cell ID).
  - Load balancing, automatic grid adaptation, *in situ* visualization.
- Next-gen performance portability through Kokkos Abstractions.
  - Sequoia (1.57 million cores).
  - 100% Trinity utilization (heterogenous run).
  - 100% Sierra (GPUs).
- Open source.
  - 3000+ downloads, 100+ users worldwide.
  - Collaborators: ORNL, LANL, ANL, LBNL, NASA, ESA, Academia.

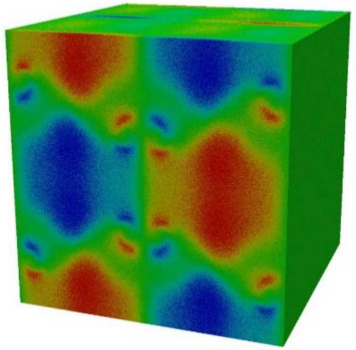


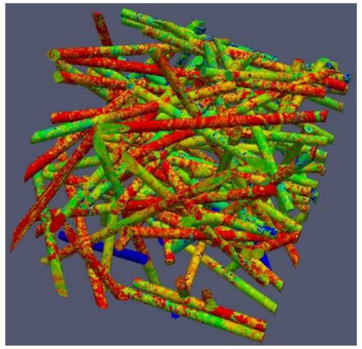






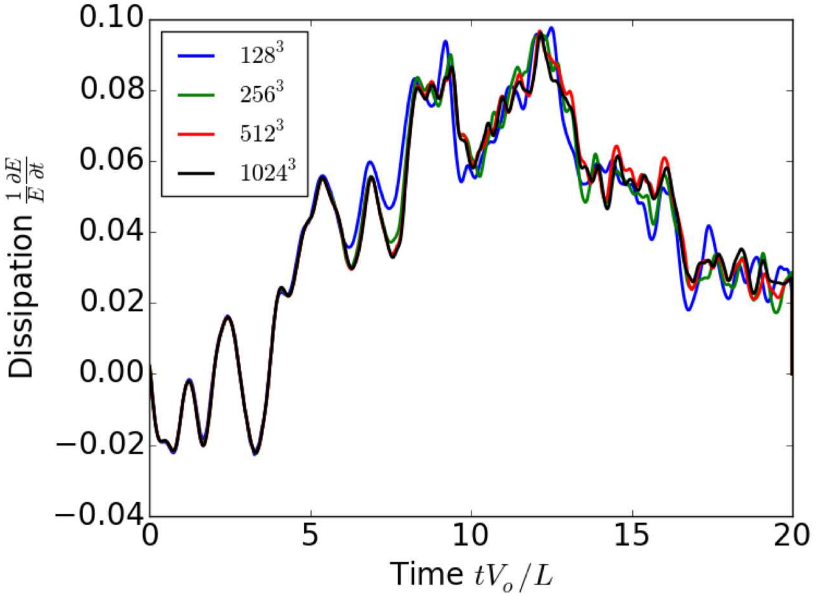




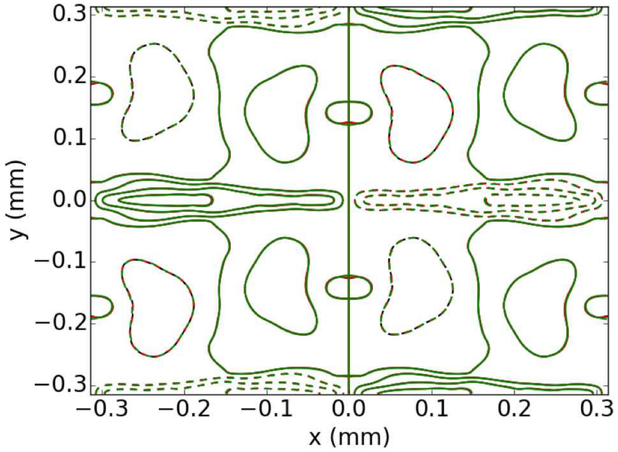


Direct Numerical Simulations

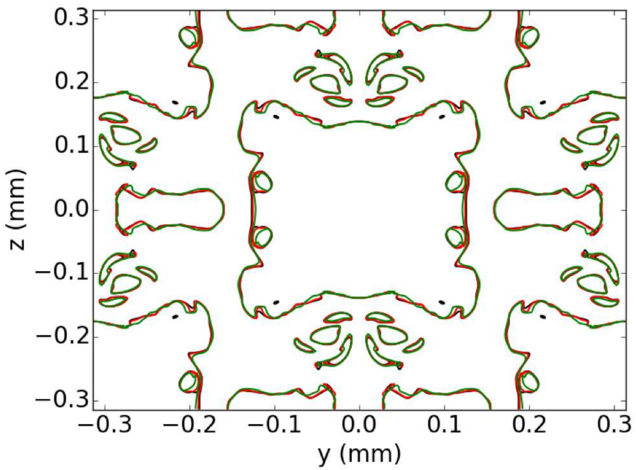
- DNS performed using two compressible finite volume codes:
    - US3D, University of MN
    - SPARC (Sandia Parallel Aerodynamics & Reentry Code)
- Blended flux scheme for high accuracy and stability:
    - Dissipative modified Steger-Warming scheme near shocklets
    - 6th order, low-dissipation, central scheme in smooth regions
    - Switch between schemes based on gradients in Mach number
- 4th order RK time advancement with CFL of 0.5
- Simulations are reasonably well converged on a 1024^3 mesh
    - Convergence is excellent up to about t=10
    - Slight differences are seen after t=10 due to strong nonlinearity



Contours of u, t=9



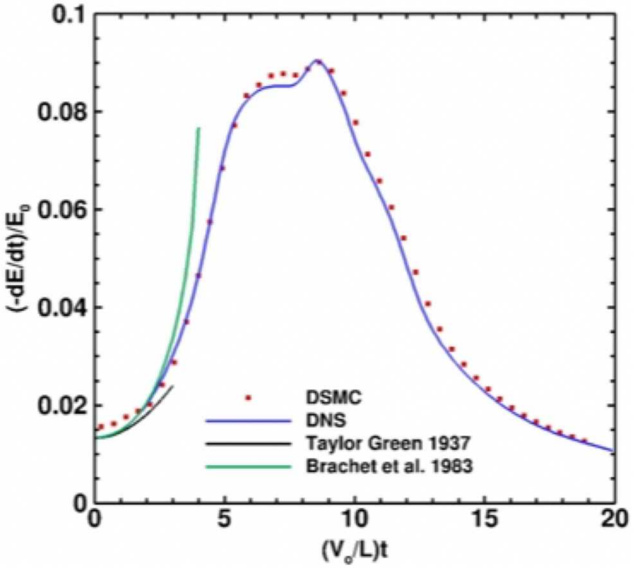
Contours of u, t=9

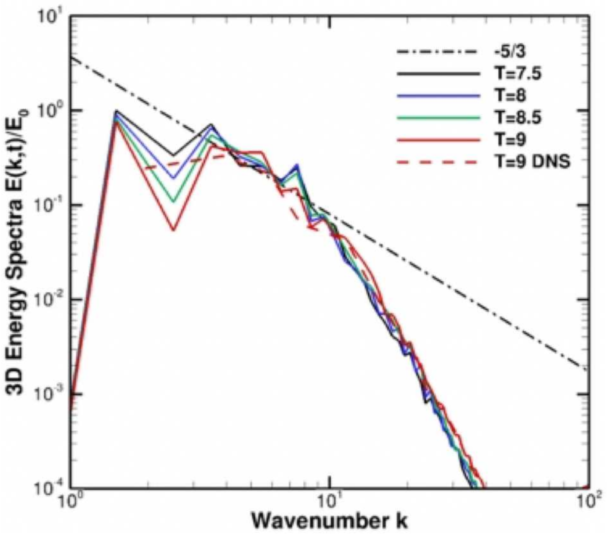


Taylor Green Flow at the Molecular Level

Taylor-Green (TG) vortex flow is a generic turbulent flow
- Incompressible TG flow is 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 buildup of a fully turbulent dissipative spectrum
- Late-time flow exhibits basic features of isotropic, homogeneous turbulence





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

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 = 0.01-0.25 ns, near-neighbor collisions
- Molecules/cell = 45, total molecules = 0.36 trillion

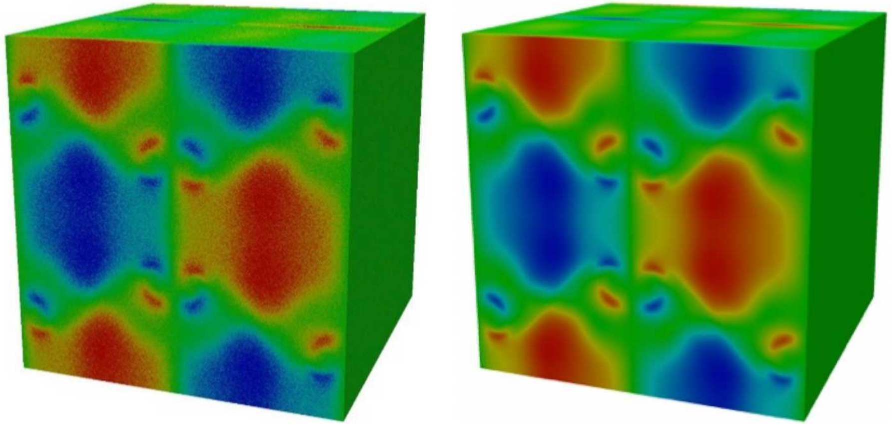
Gas parameters

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

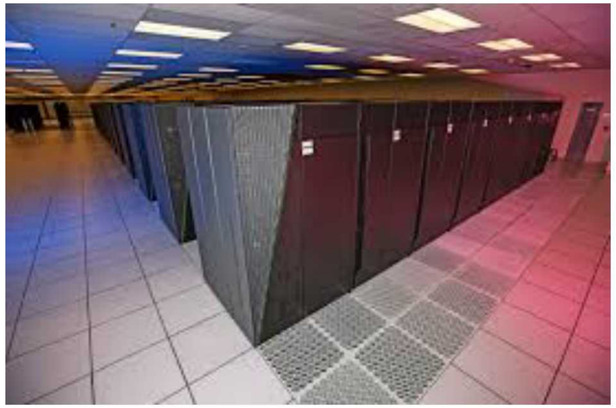
Simulation Parameters

Simulations performed on LLNL/Sequoia

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



Taylor-Green flow from DNS and DSMC simulations.

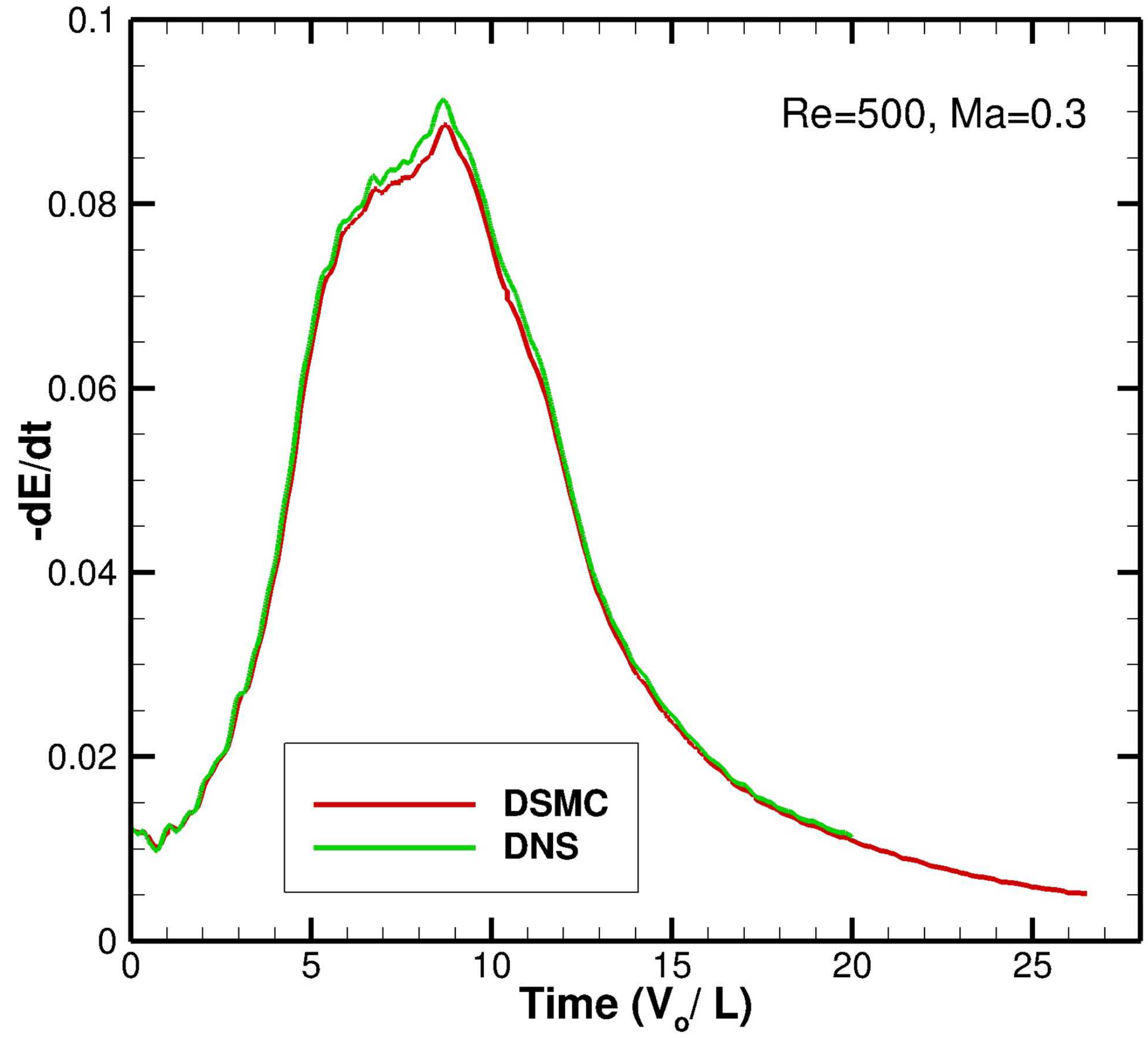


Low-Re, High-Ma Turbulent Flows

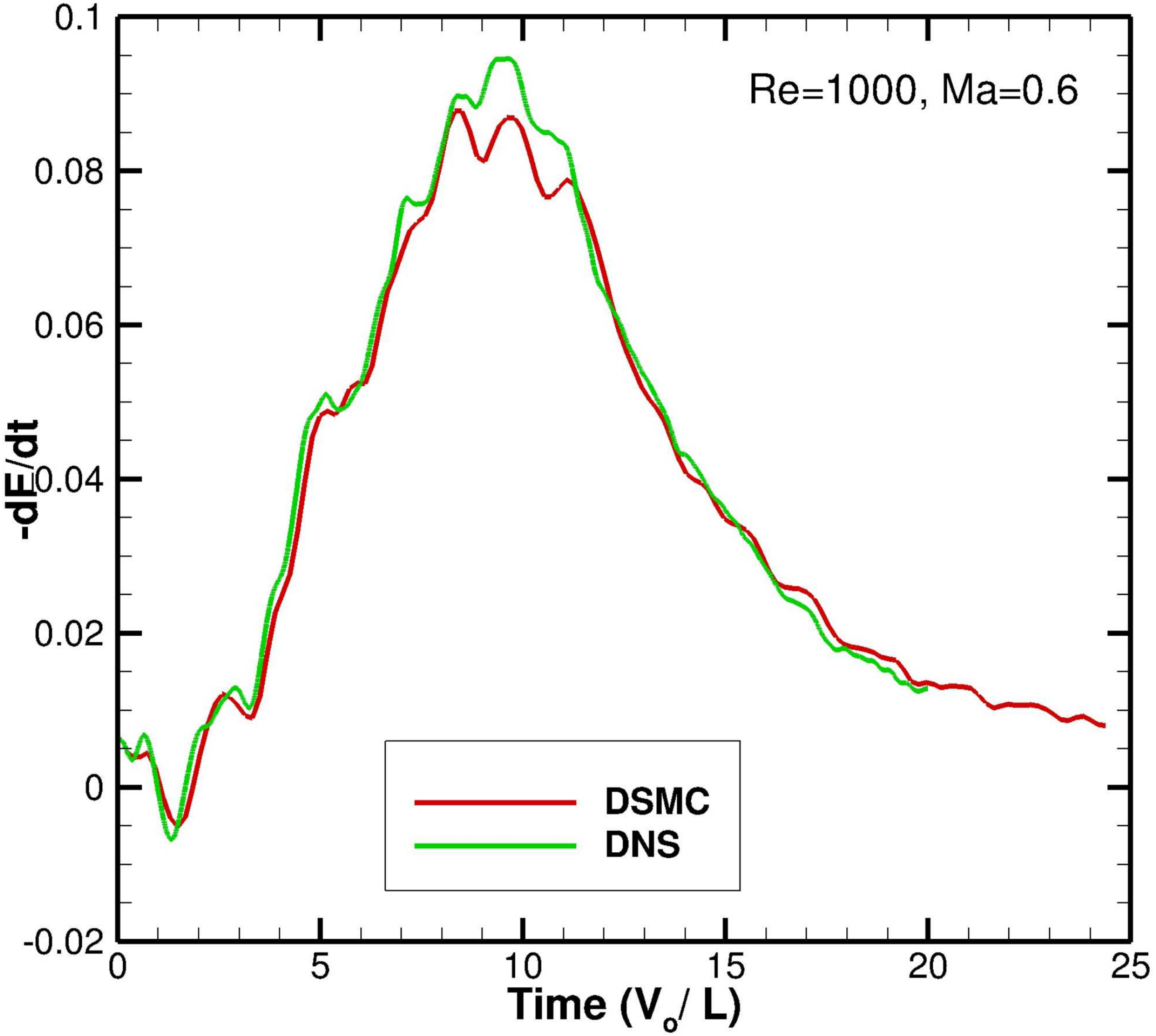
Re	Mach	η/λ	Kn
500	0.3	15.8	1.25×10^{-4}
1000	0.6	9.4	1.25×10^{-4}
1500	0.9	6.9	1.25×10^{-4}
2000	1.2	5.6	1.25×10^{-4}

- Here, Kn was kept constant, and Re was increased by increasing Ma.
- System Kn number places the flow fields well into the continuum regime.
- However, η/λ ratio suggests that **non-equilibrium effects including non-equilibrium transport and thermal fluctuations** may be important.

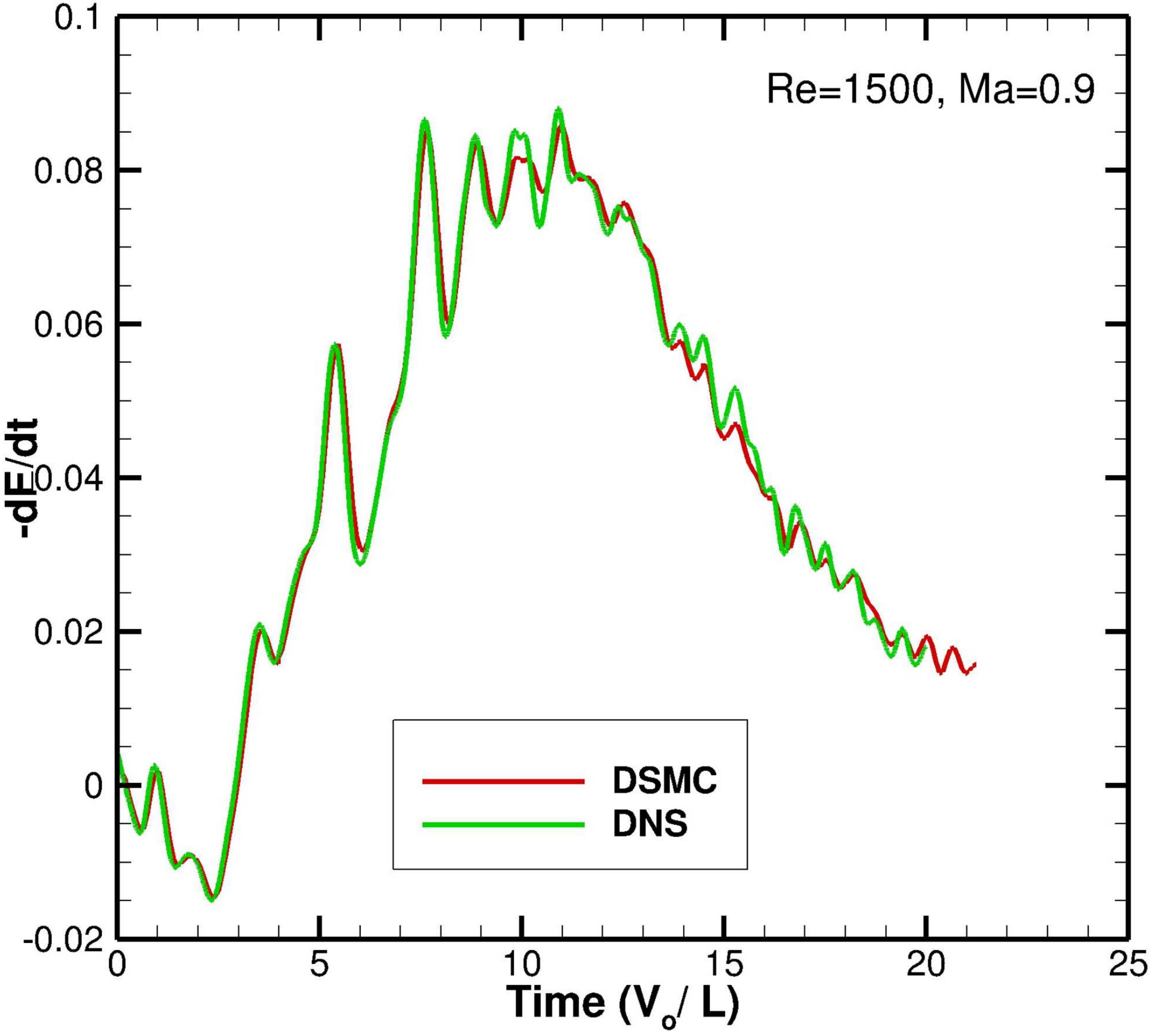
TG Energy Dissipation: Ma = 0.3, Re = 500



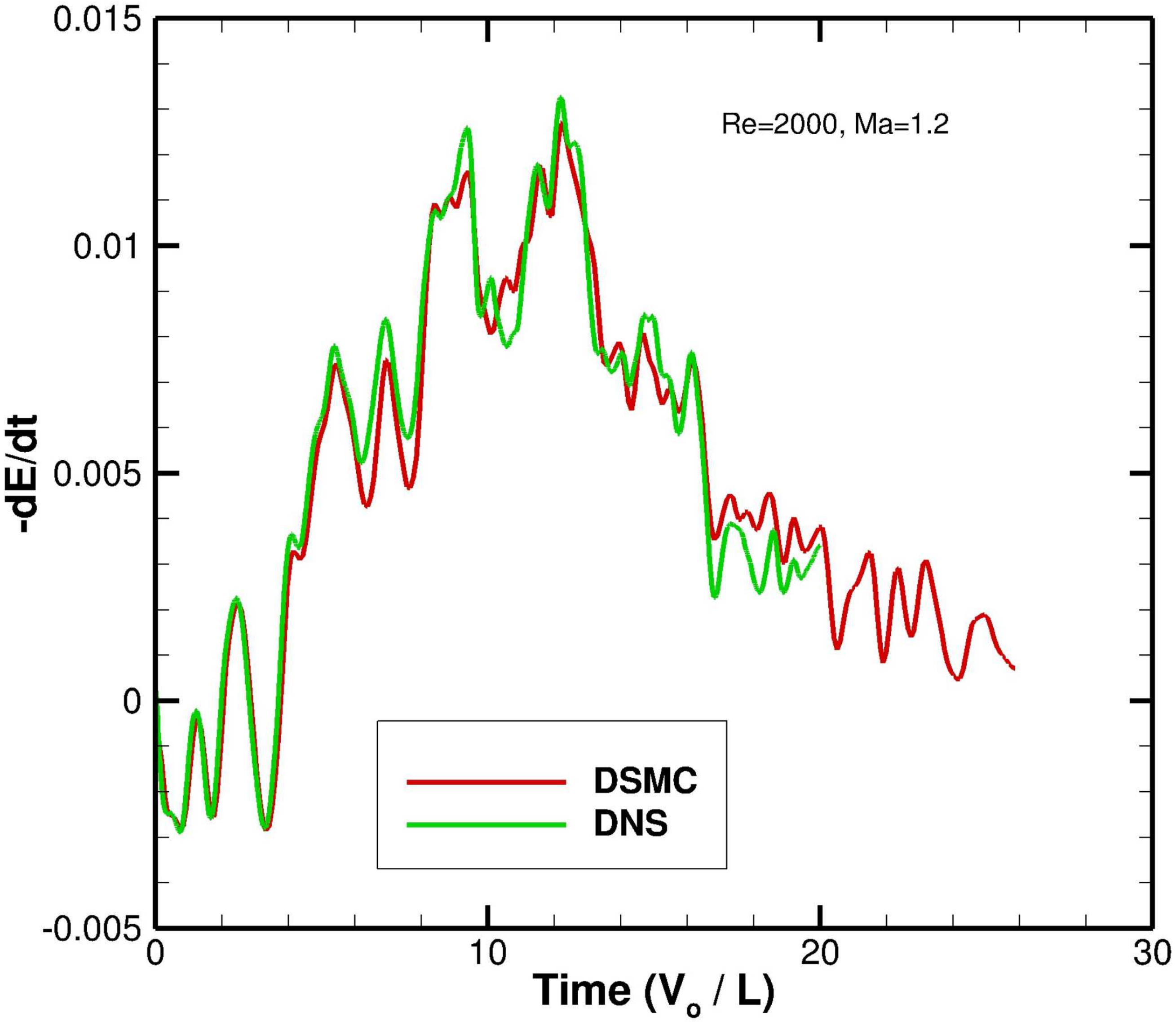
TG Energy Dissipation: Ma = 0.6, Re = 1000



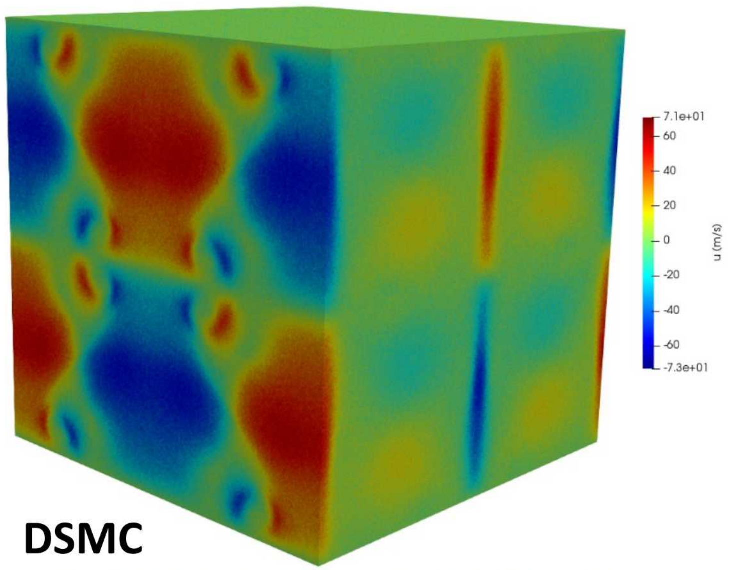
TG Energy Dissipation: Ma = 0.9, Re = 1500



TG Energy Dissipation: Ma = 1.2, Re = 2000



TG: Ma = 0.3, T = 8.7



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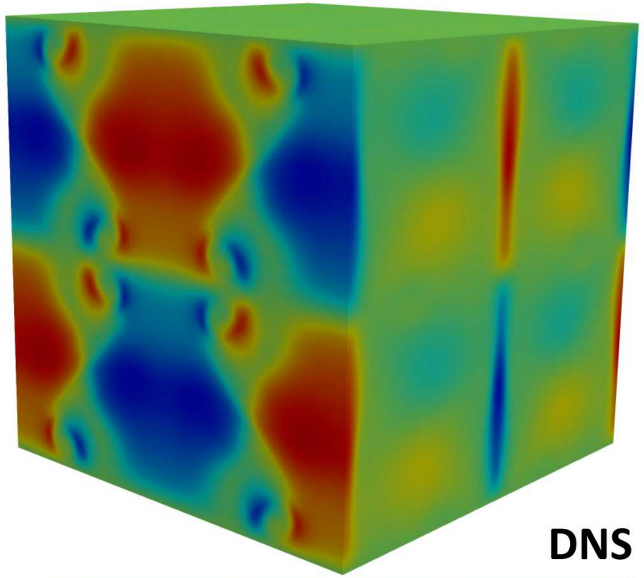
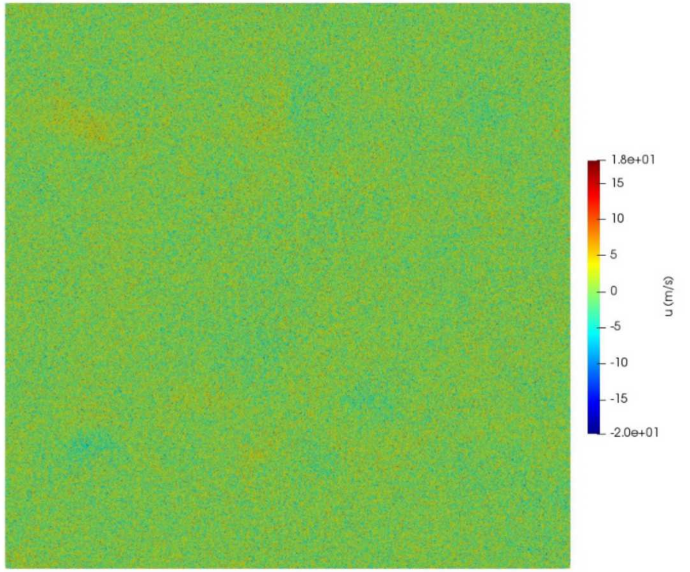
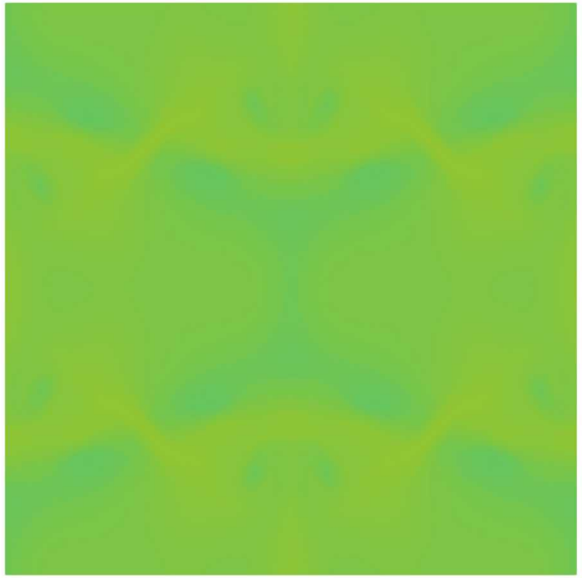
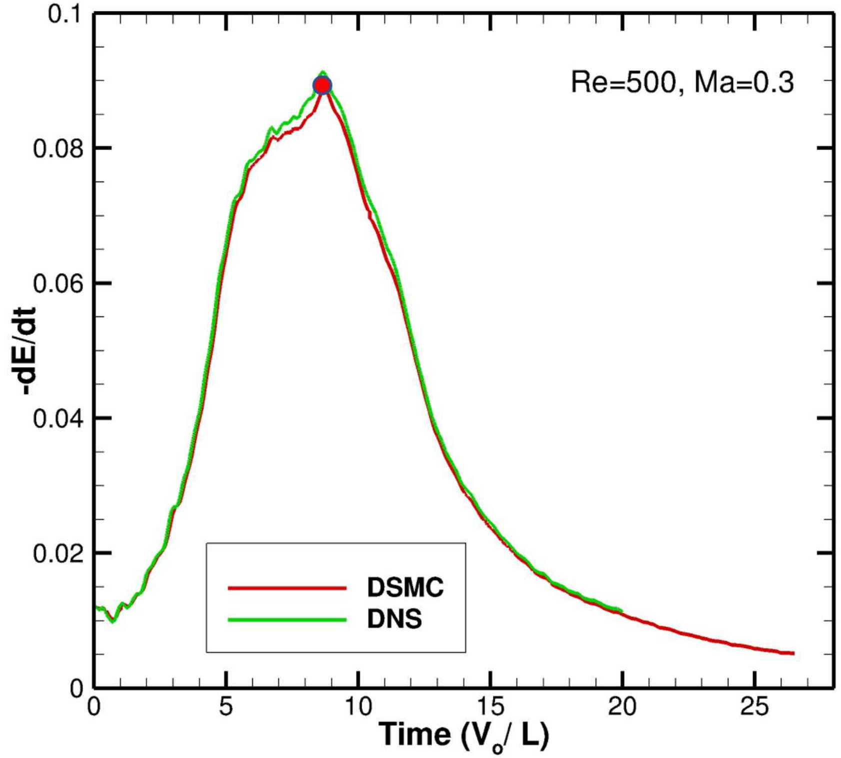


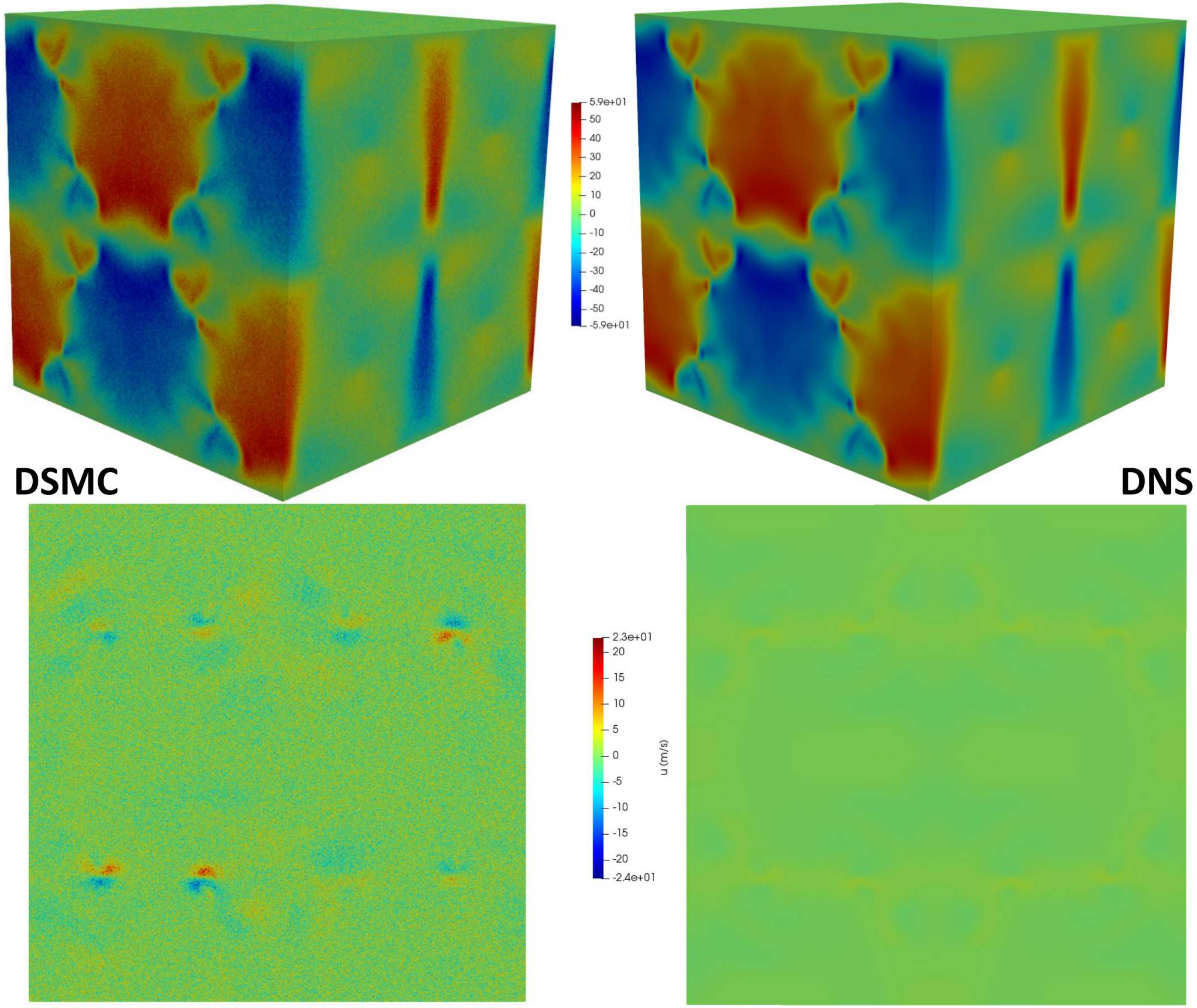
DNS

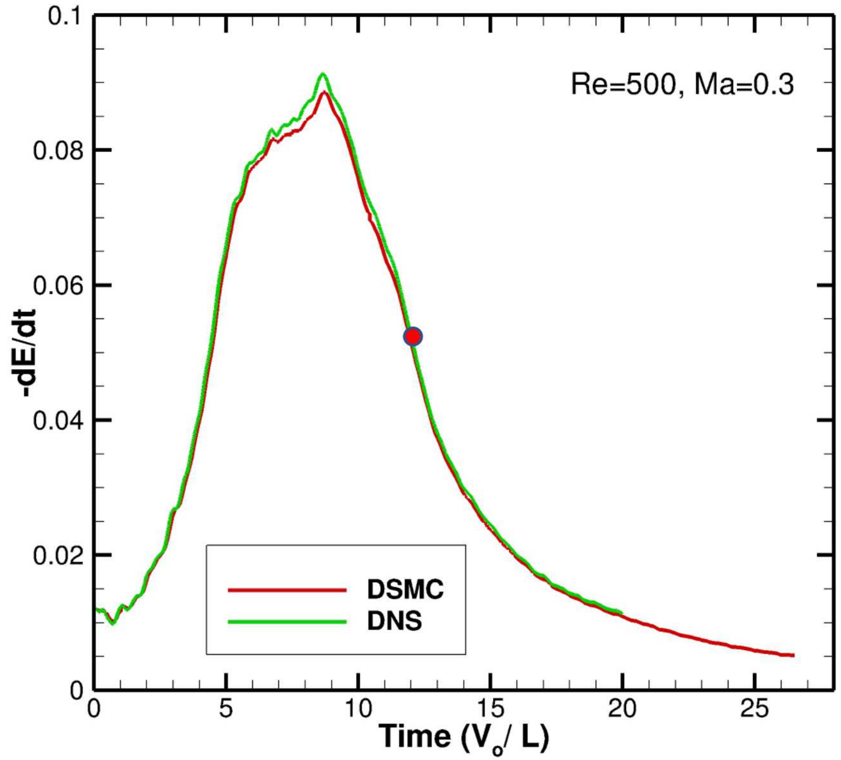




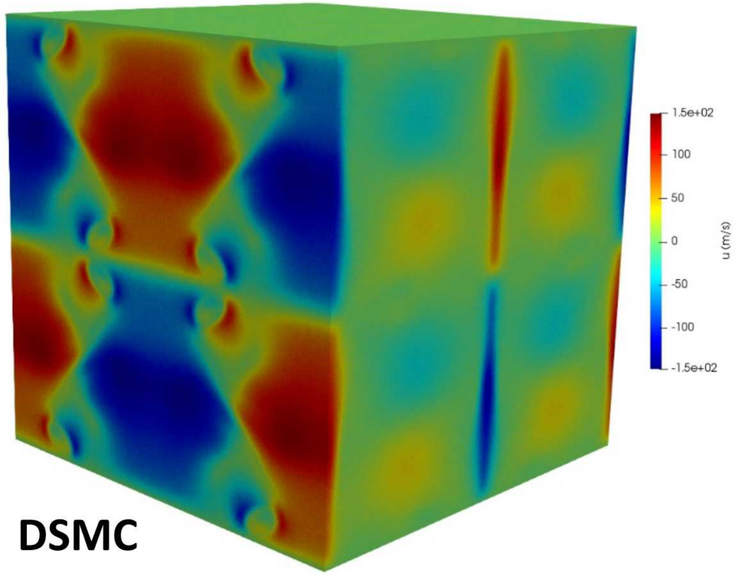


TG: Ma = 0.3, T = 12.01





TG: Ma = 0.6, T = 8.45



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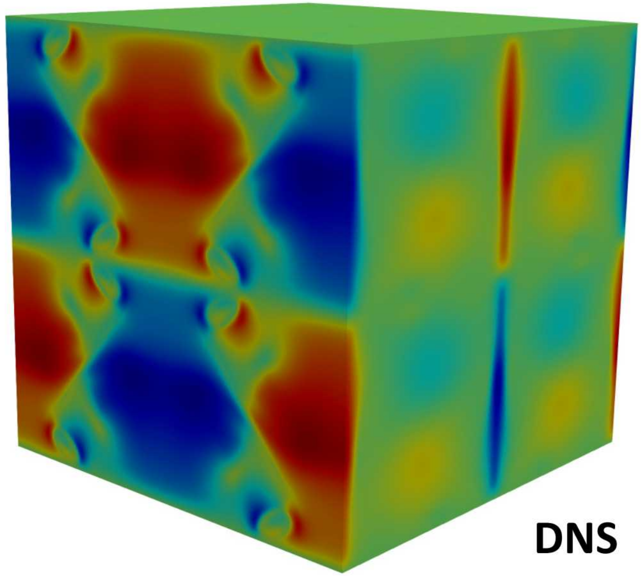

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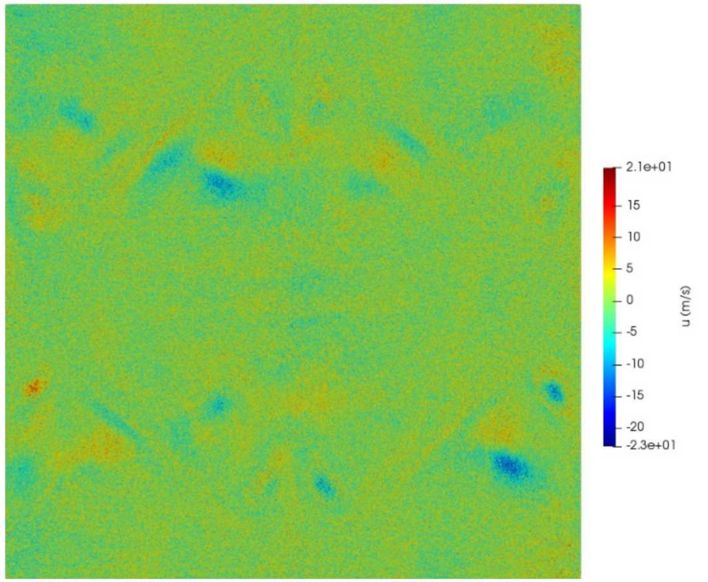
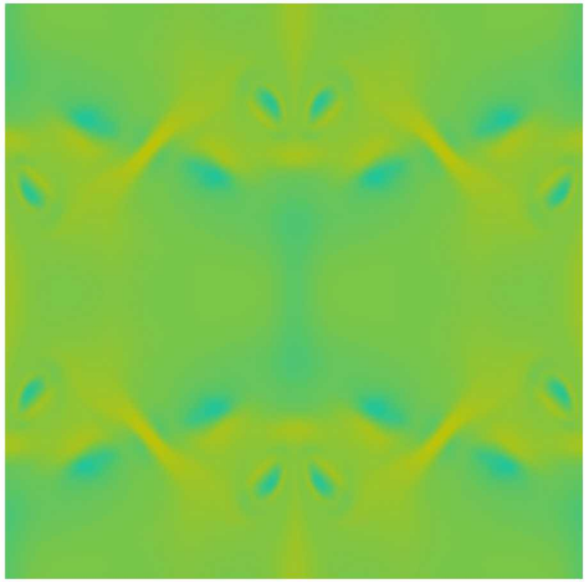
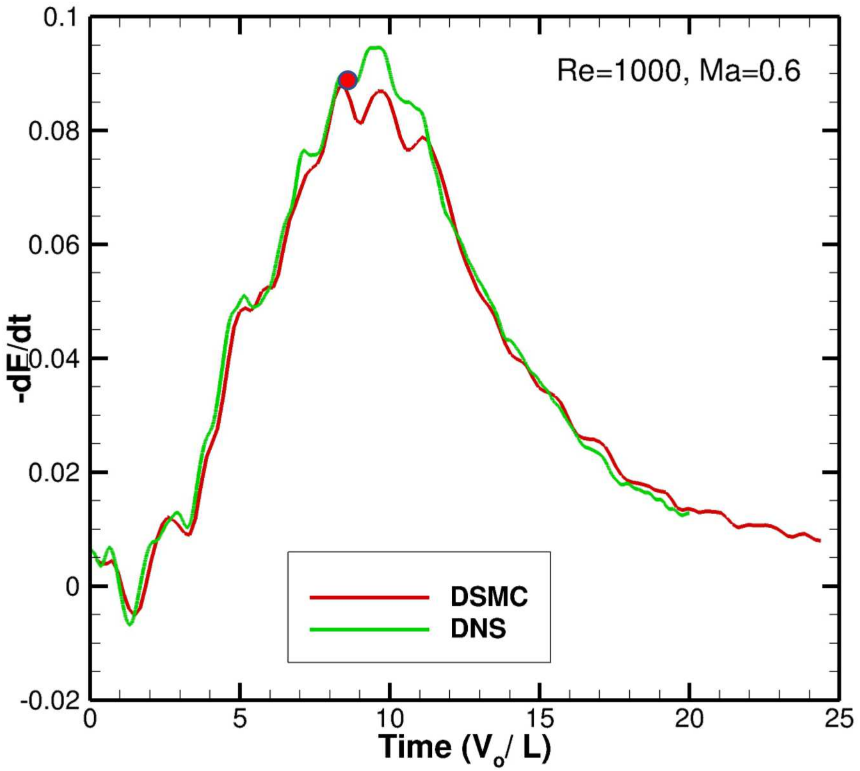
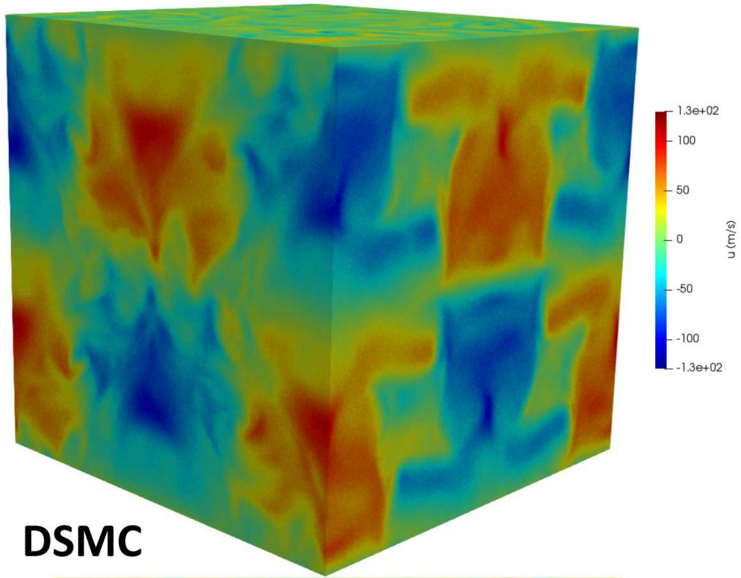






TG: Ma = 0.6, T = 18.47



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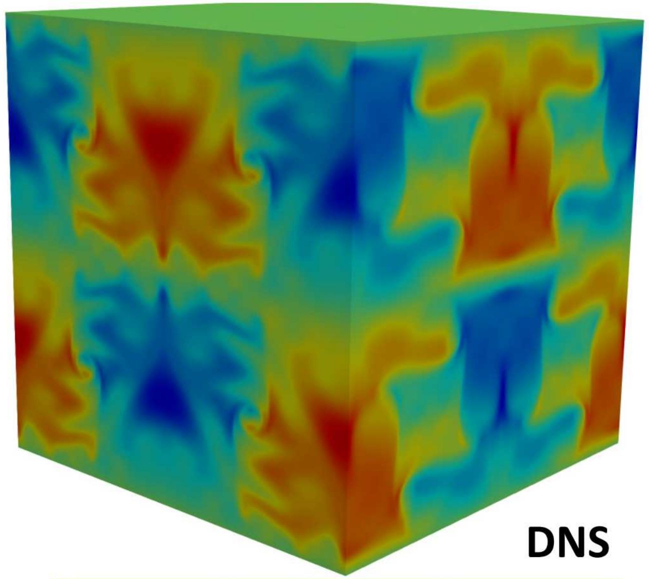

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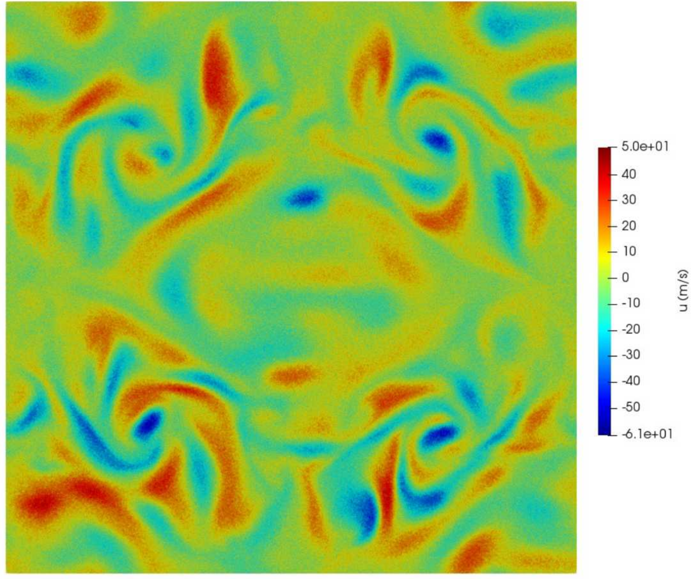
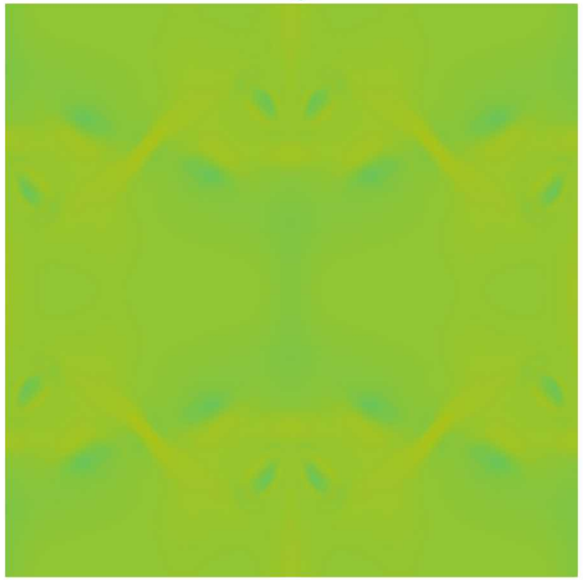
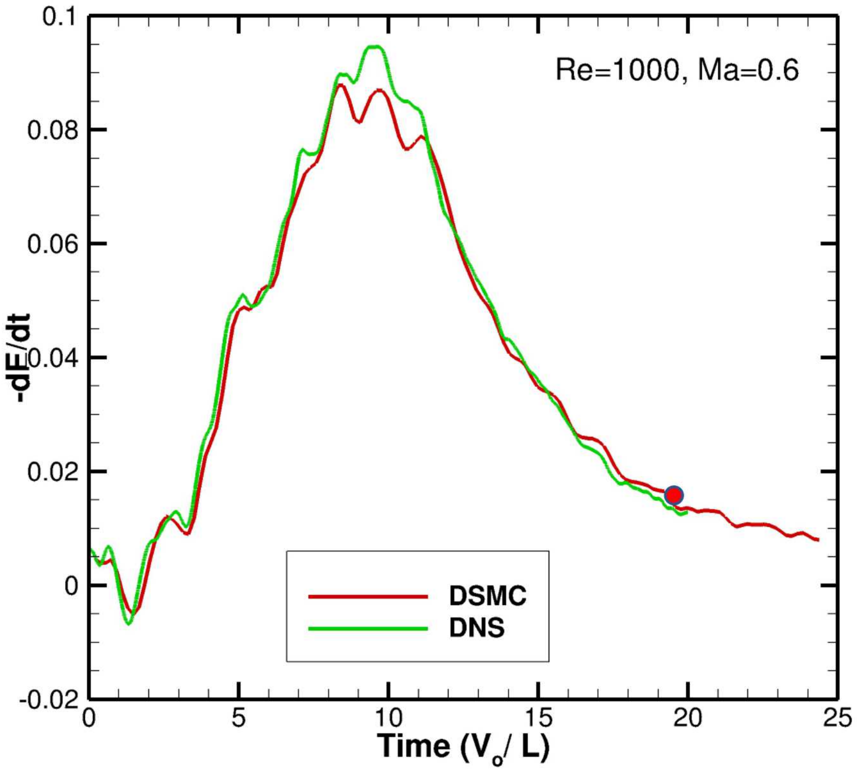
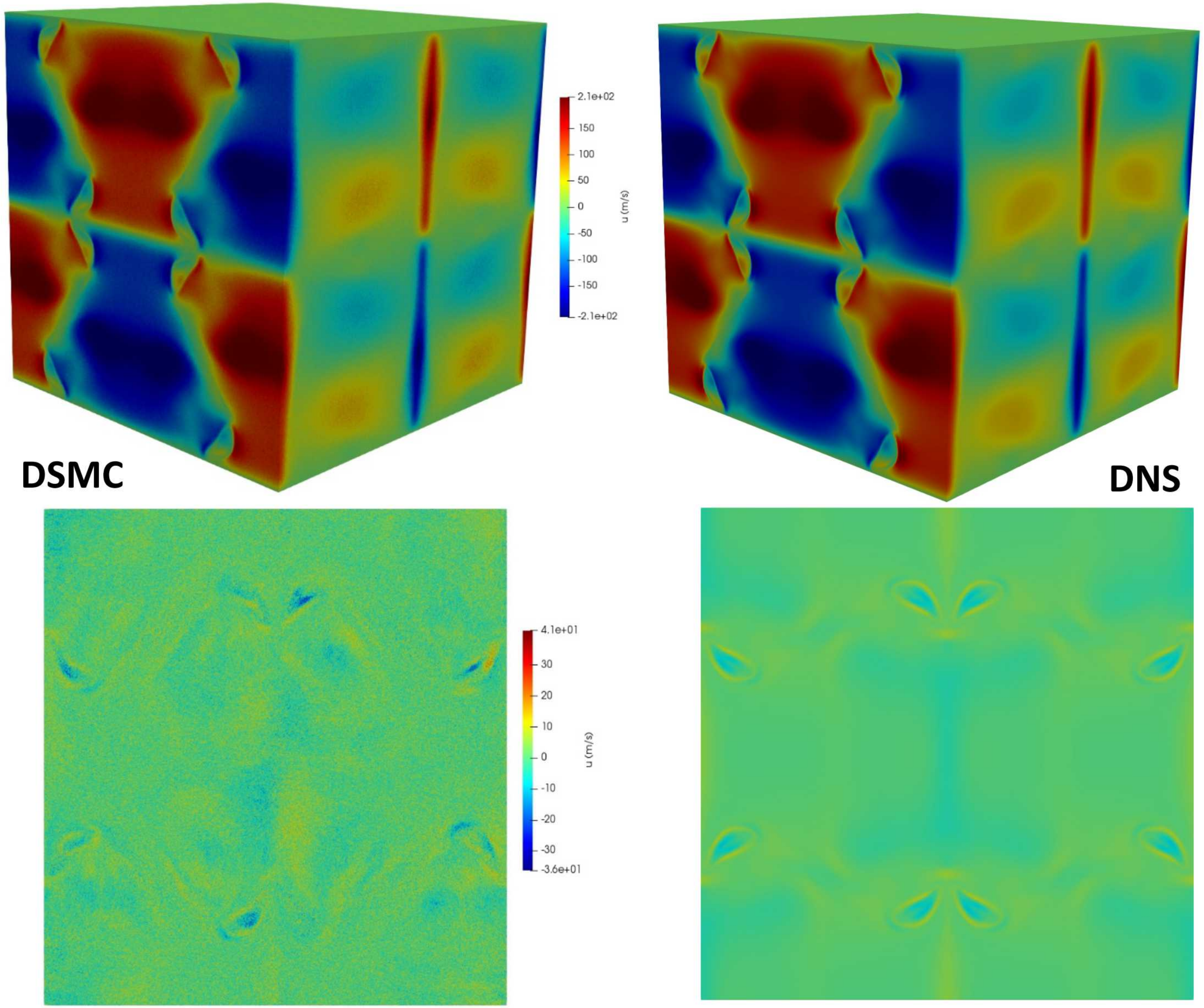
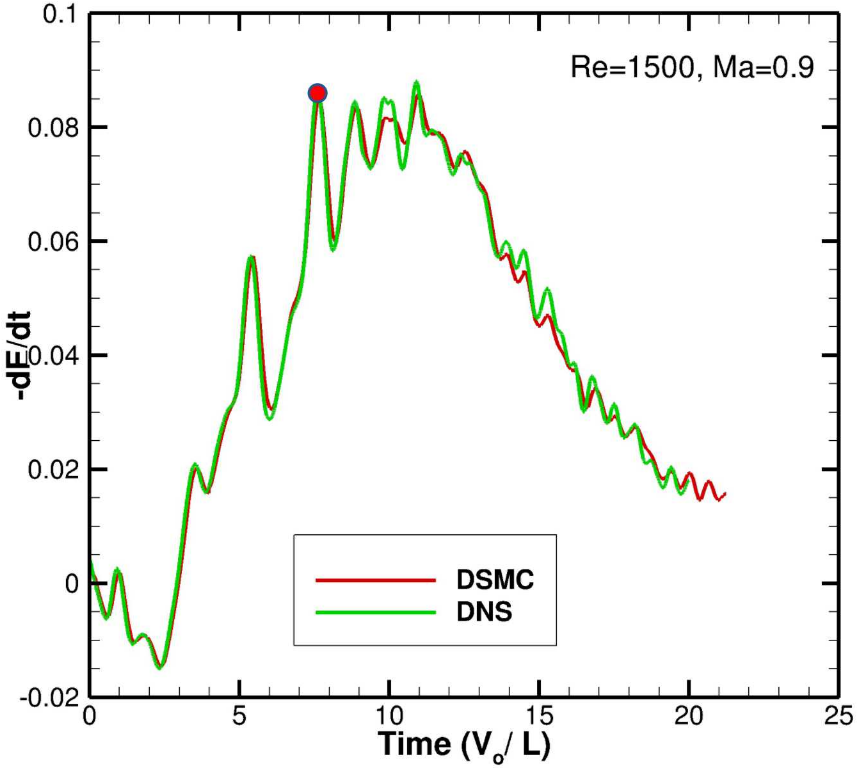




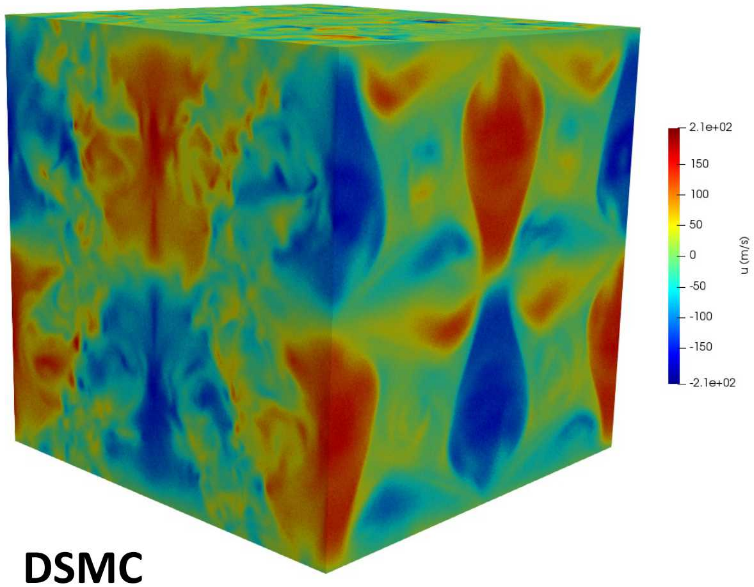


TG: Ma = 0.9, T = 7.63


2.1e+02
150
100
50
0
-50
-100
-150
-2.1e+02
u (m/s)
DSMC
DNS
4.1e+01
30
20
10
0
-10
-20
-30
-3.6e+01
u (m/s)


Re=1500, Ma=0.9
-dE/dt
Time (V$_o$/ L)
0.1
0.08
0.06
0.04
0.02
0
-0.02
0
5
10
15
20
25
DSMC
DNS

TG: Ma = 0.9, T = 14.77



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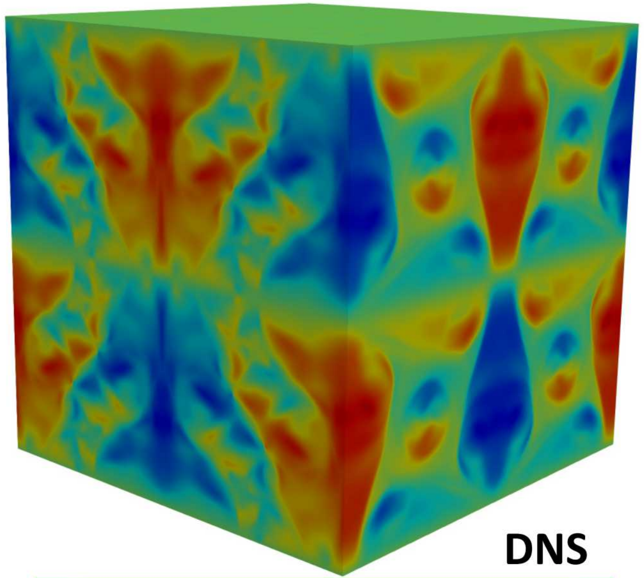

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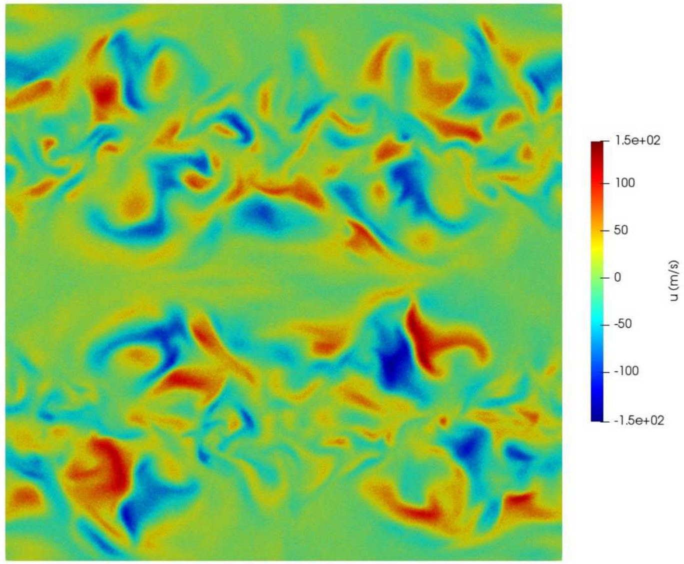
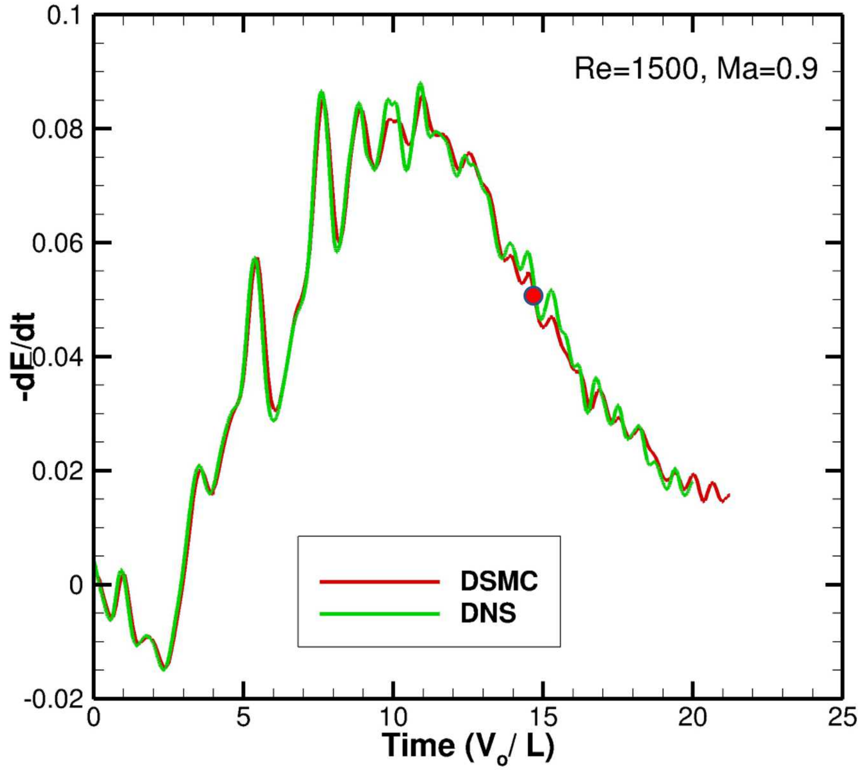
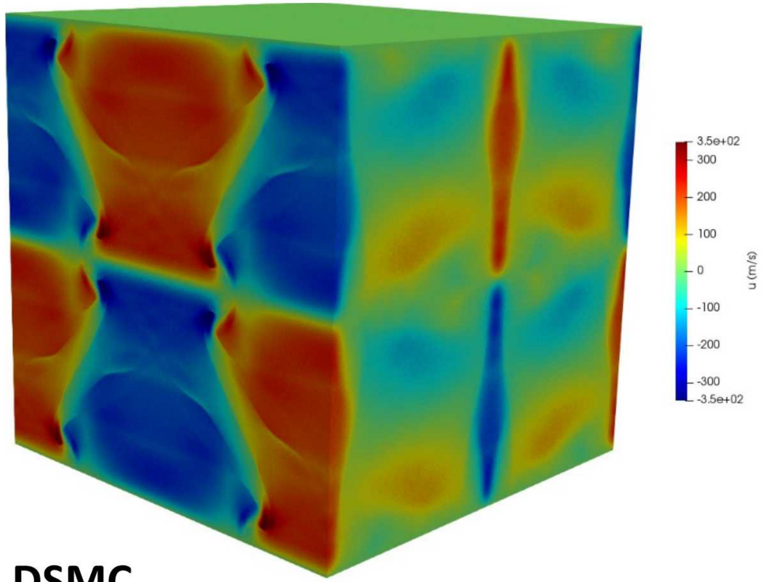
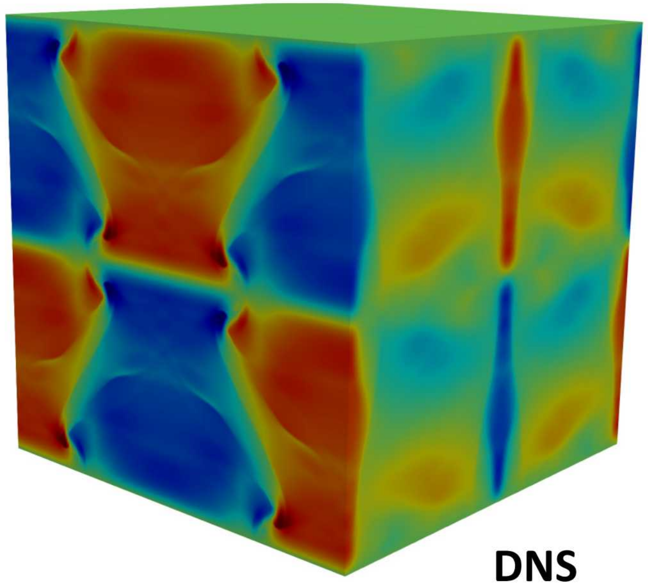




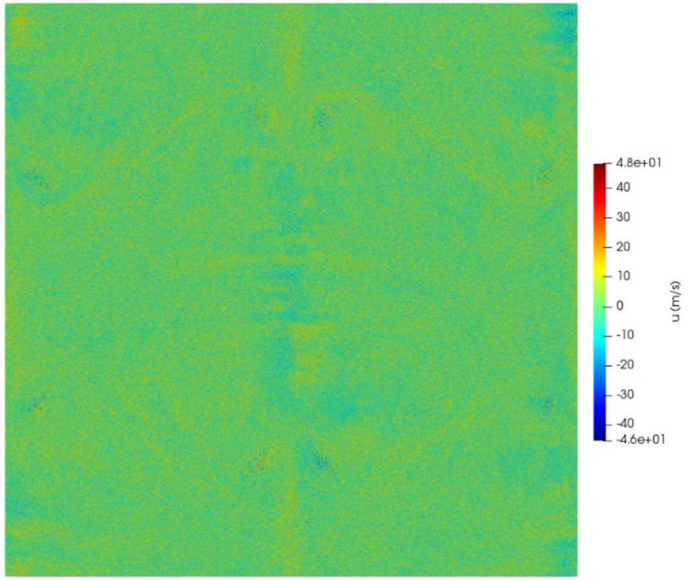
TG: Ma = 1.2, T = 6.87

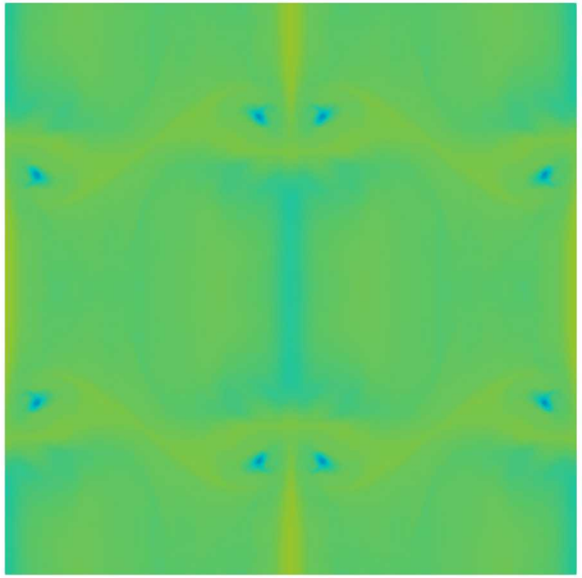


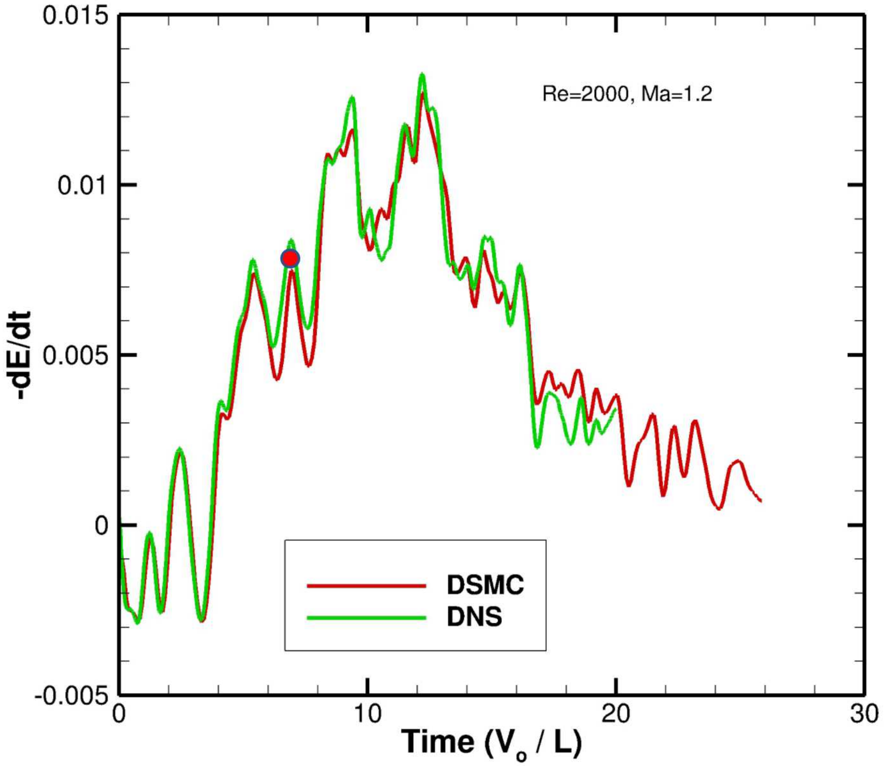


DSMC

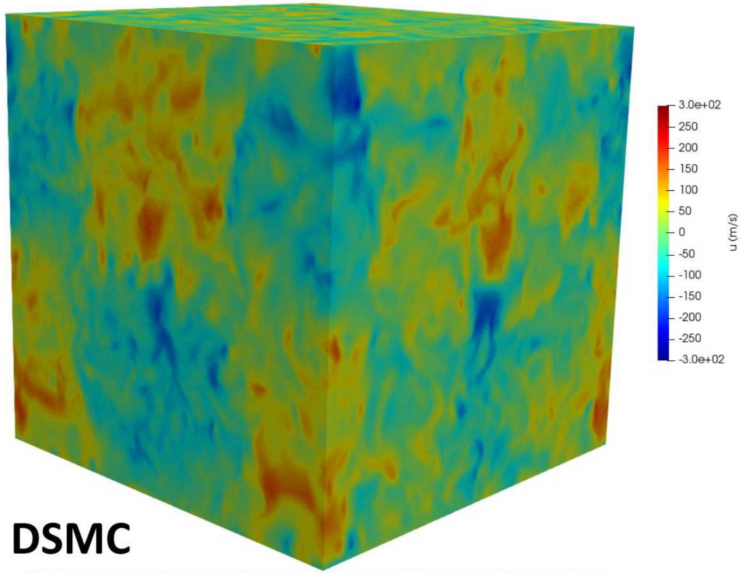
DNS



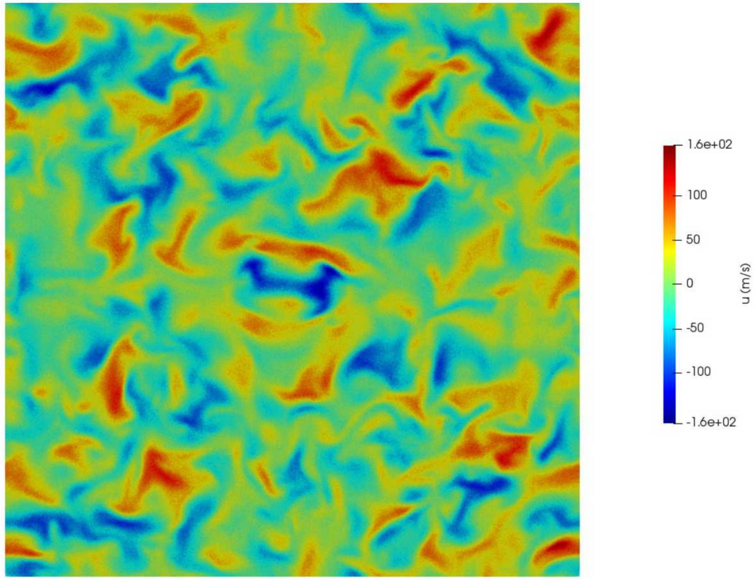


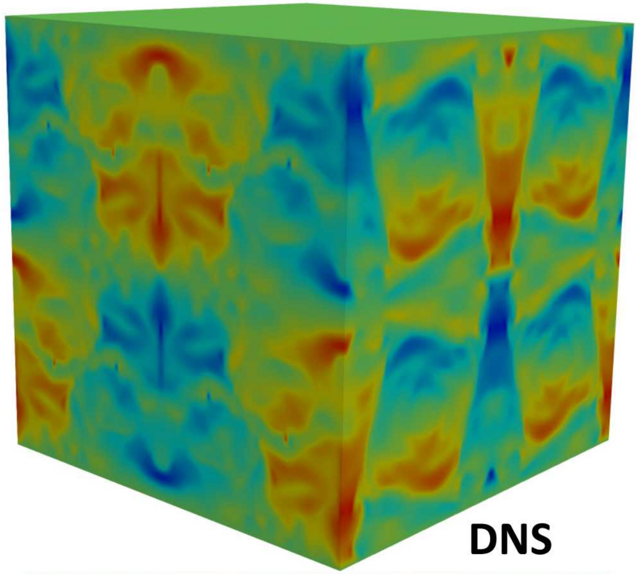


TG: Ma = 1.2, T = 18.56

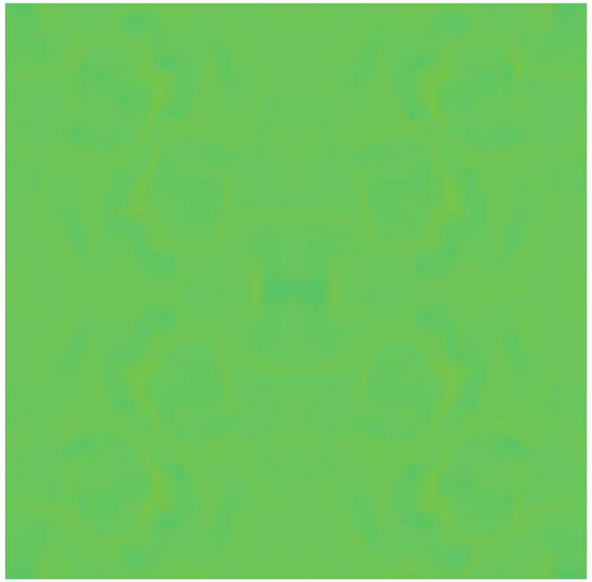


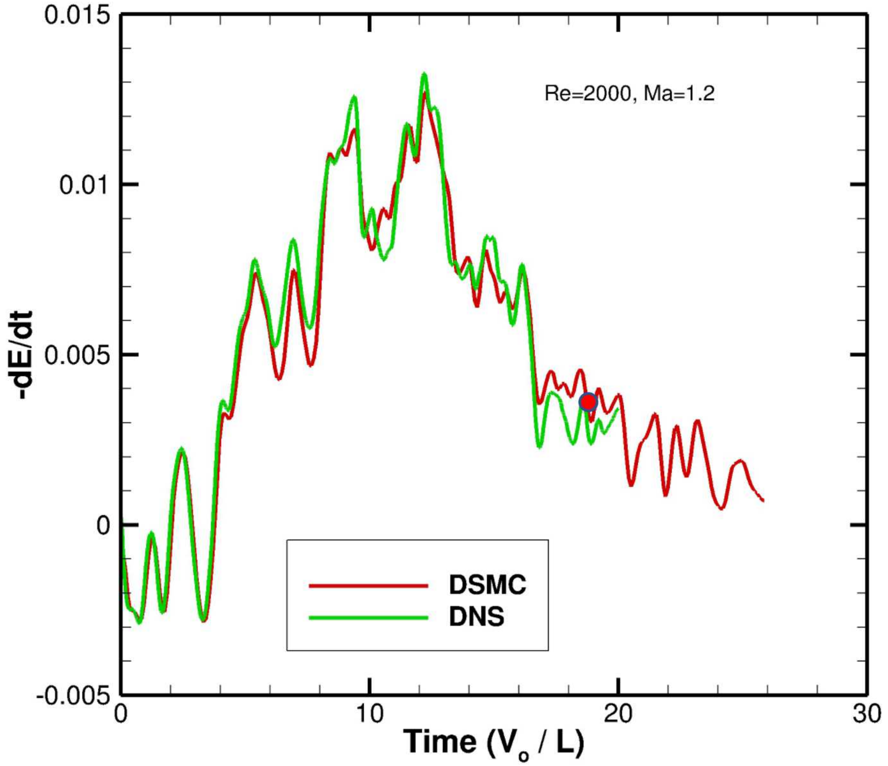
DSMC





DNS





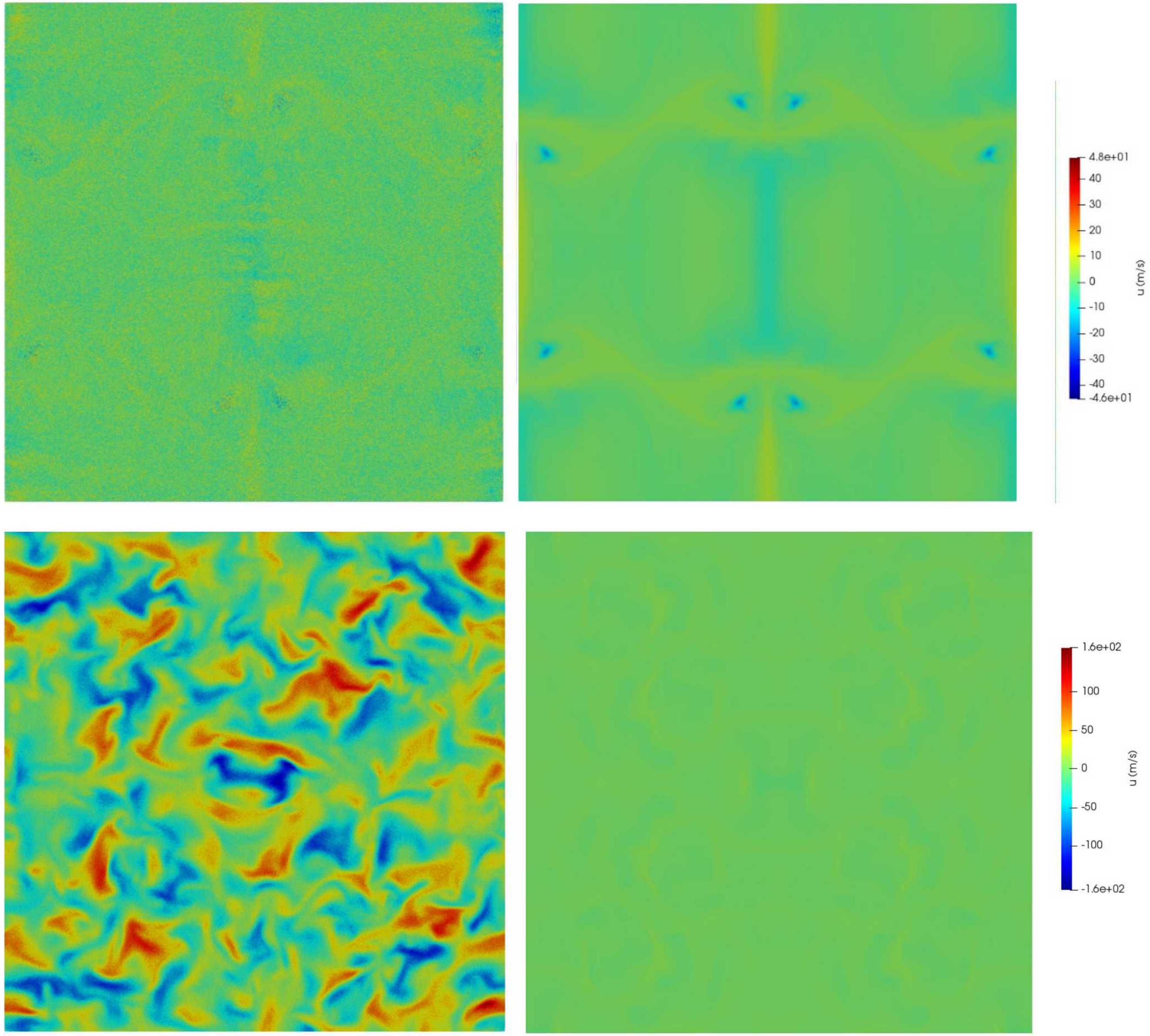
What is the nature of the fluctuations?

DSMC and DNS are in agreement for:

- All times at low Mach numbers
  incompressible flow
- Early times at high Mach numbers
  laminar part of the evolution

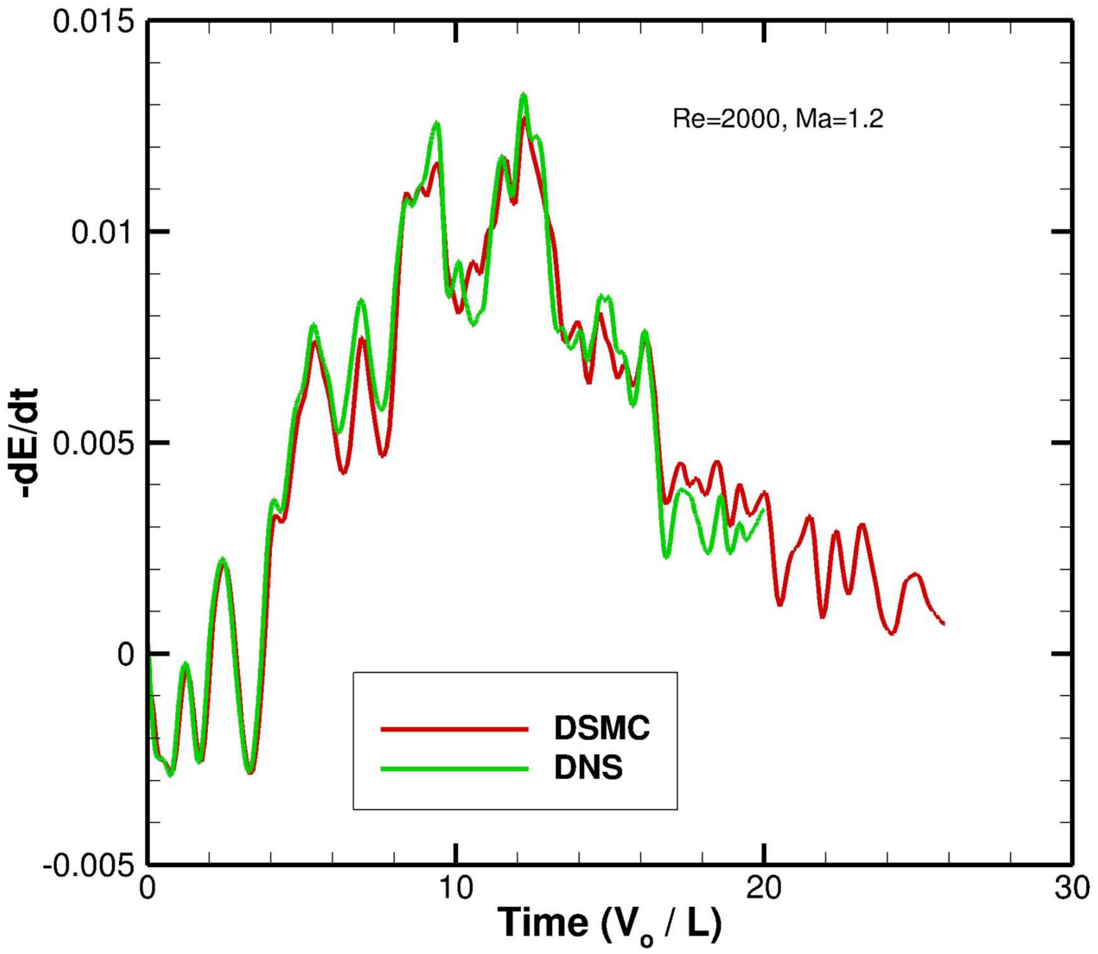
- Fluctuations appear past the maximum dissipation point at high Mach numbers.
  Shocklets appear, strong compression

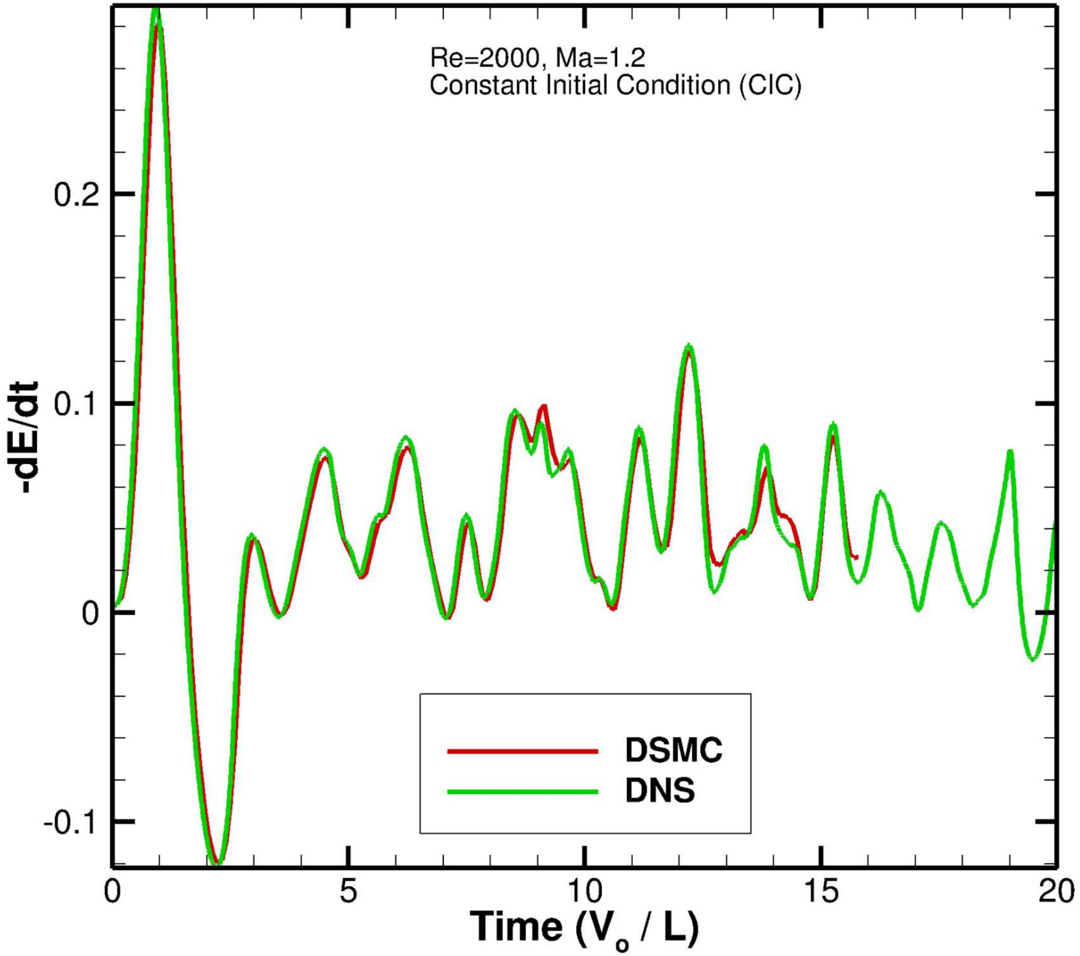
The interaction between shock waves/strong compression and rotating vortices/thermal fluctuations baroclinically creates new vortices.



TG Energy Dissipation: Ma = 1.2, Re = 2000

Variable vs Constant Density Initial Condition

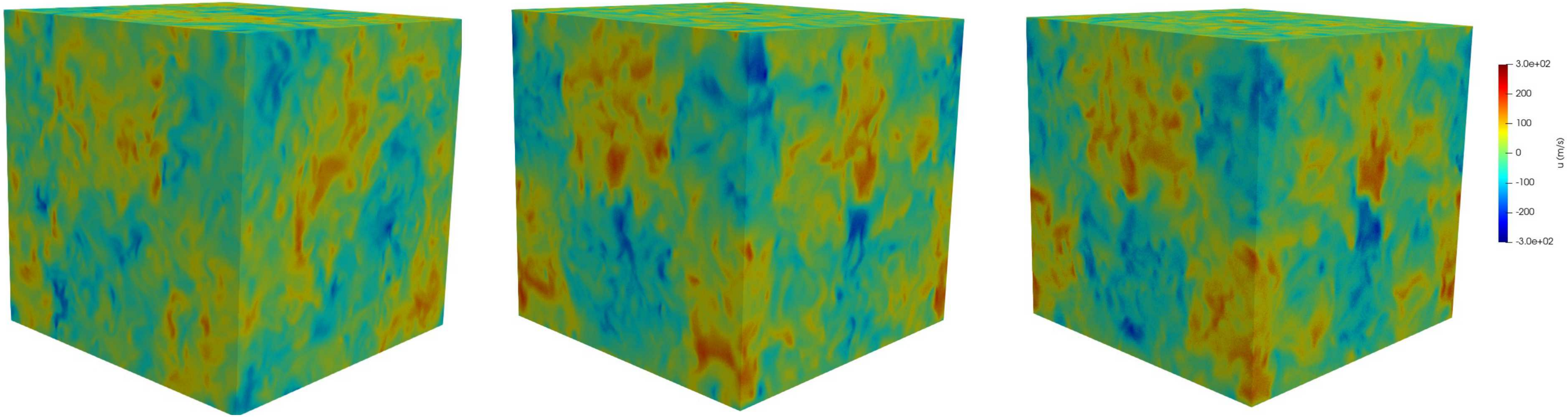




Constant density initial condition is known to produce laminar flow.

For laminar flow the agreement between DSMC and DNS is much better.

What is the nature of the fluctuations?



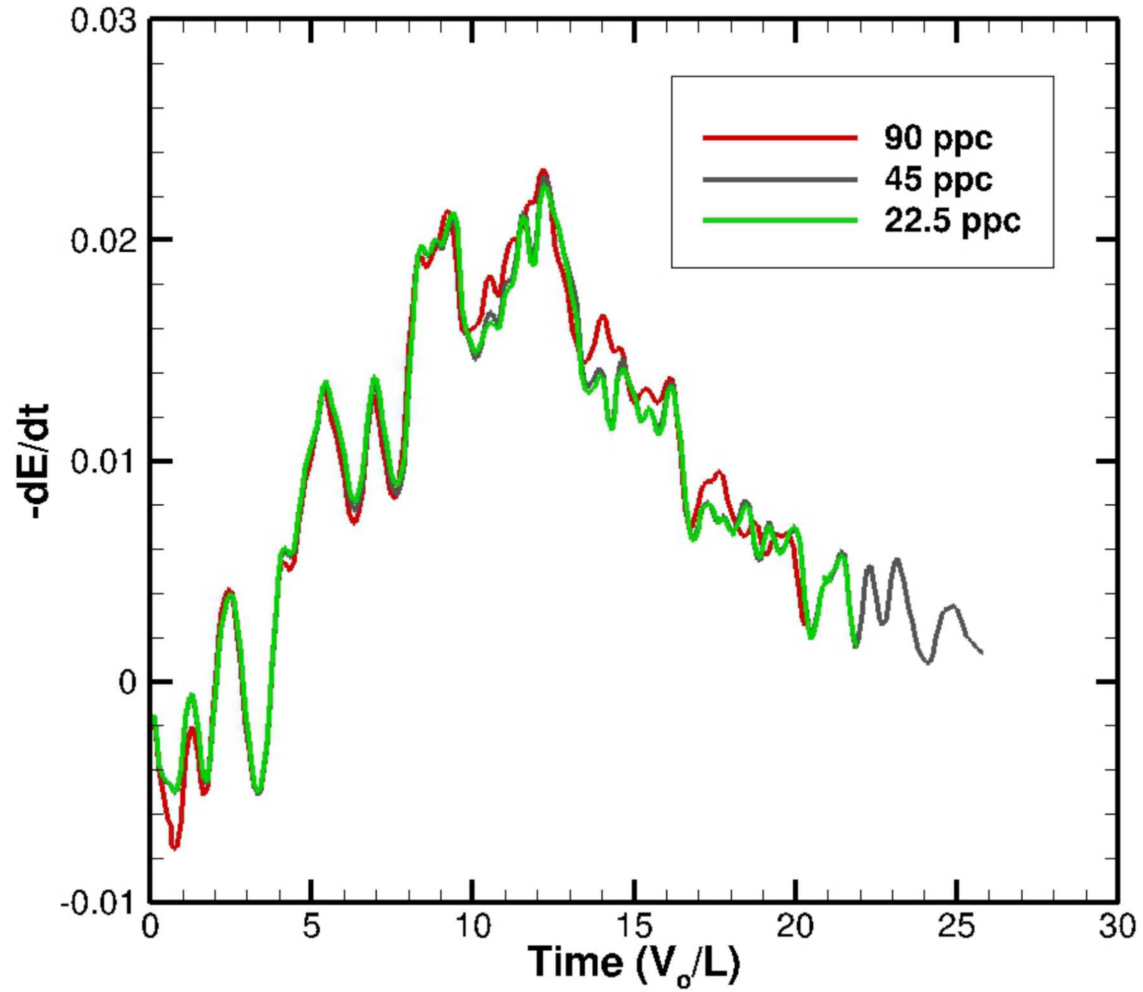
Simulators per cell

90 45 22.5

The simulations were repeated using different numbers of simulators per cell (simulation ratio) and showed similar levels (amplitude) of fluctuations.

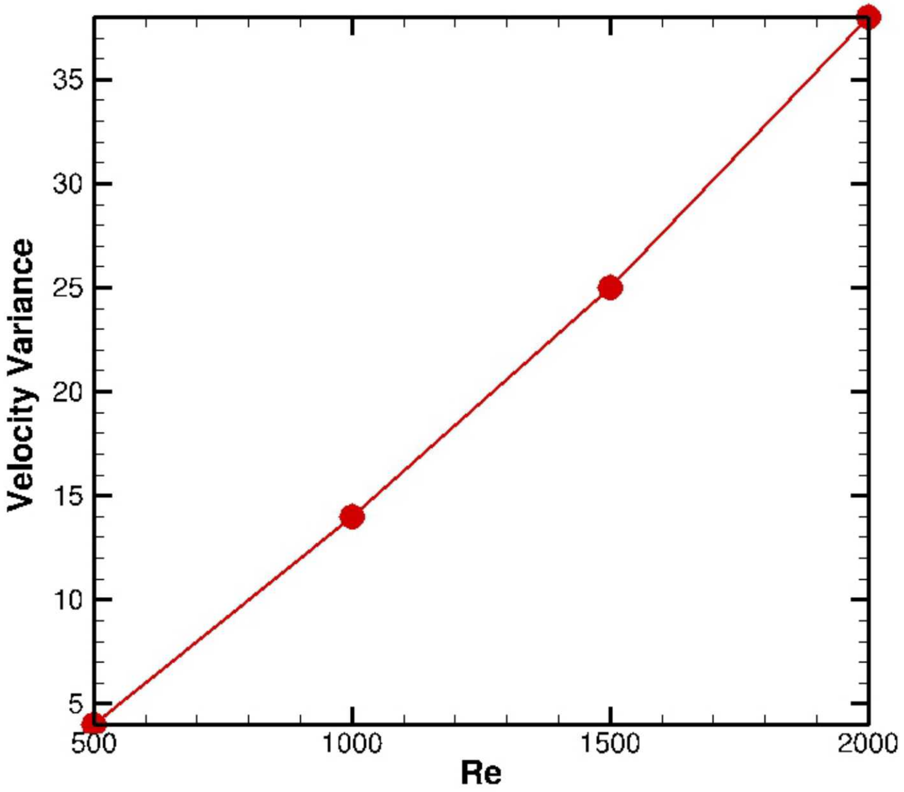
The nature of the fluctuations does not appear to be influenced by the simulation parameters.

Energy Dissipation Versus Simulation Ratio



Simulation ratio weakly influences dissipation rates.

Fluctuations as Function of Re-Ma



u-velocity fluctuations on the y-z plane are a function of the Re-Ma number.

- The level of numerical uncertainty (noise) in all four simulations was the same.
- **The intensity of thermal fluctuations is proportional to the compressibility of the gas (De Zarate, 2006).**
- **For high Mach numbers, thermal fluctuations are amplified due to baroclinic creation of vorticity.**

Low-Re, High-Ma Turbulent Flows

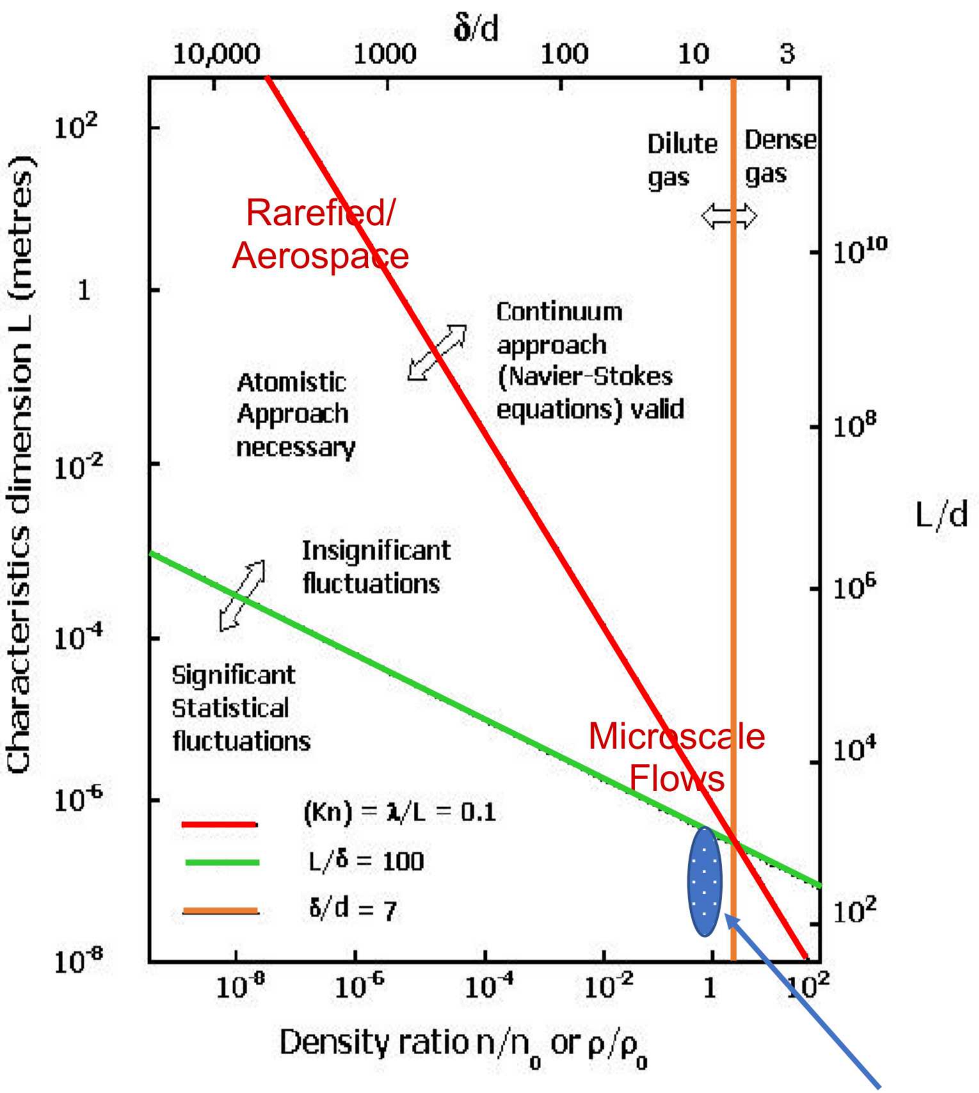
Re	Mach	η/λ	Kn	Molecules/η^3
500	0.3	15.8	$1.25\text{x}10^{-4}$	$3.2\ 10^7$
1000	0.6	9.4	$1.25\text{x}10^{-4}$	$6.6\ 10^6$
1500	0.9	6.9	$1.25\text{x}10^{-4}$	$2.7\ 10^6$
2000	1.2	5.6	$1.25\text{x}10^{-4}$	$1.4\ 10^6$

For atmospheric density, the number of real molecules in a volume η^3 can be small enough so that molecular fluctuations cannot be ignored.

Molecular vs Continuum

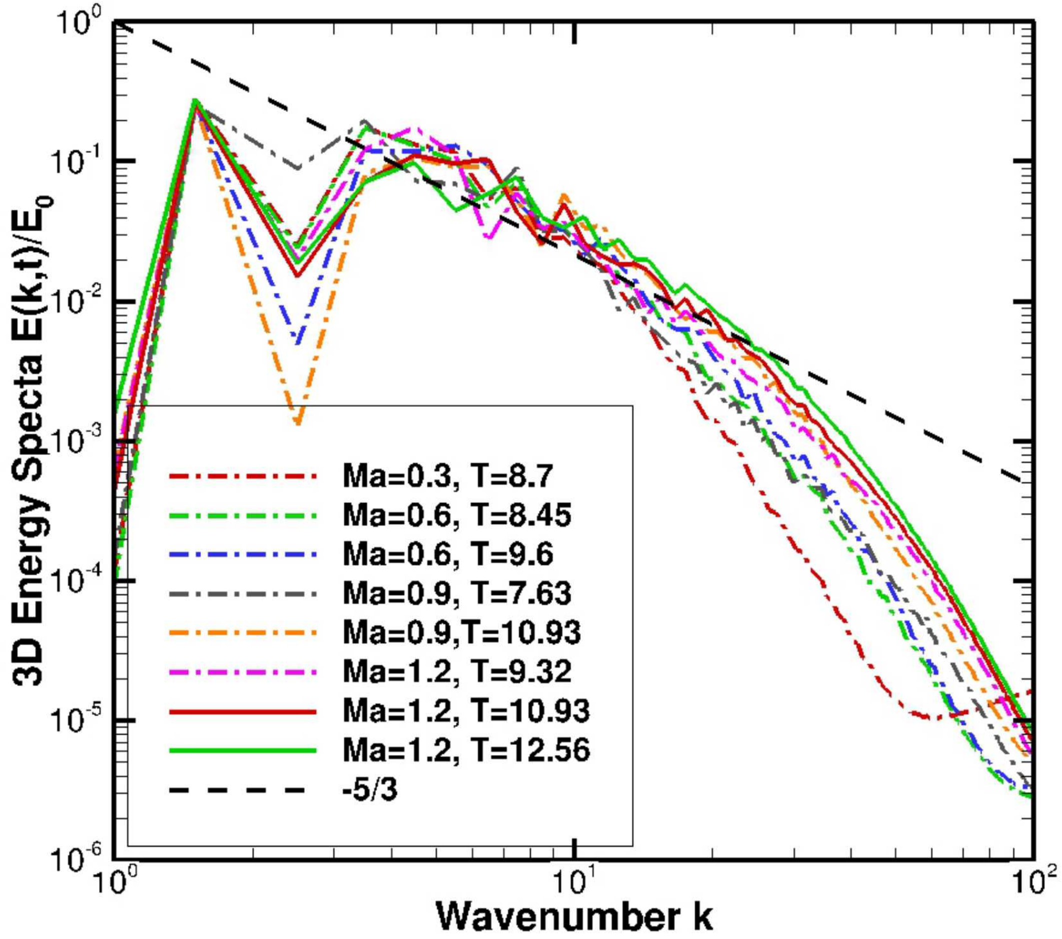
Re	Mach	η/λ	Molecules/η^3
500	0.3	15.8	$3.2\ 10^7$
1000	0.6	9.4	$6.6\ 10^6$
1500	0.9	6.9	$2.7\ 10^6$
2000	1.2	5.6	$1.4\ 10^6$

Equilibrium fluctuations are noticeable when the number of molecules in the Kolmogorov microscale < 10^7 .

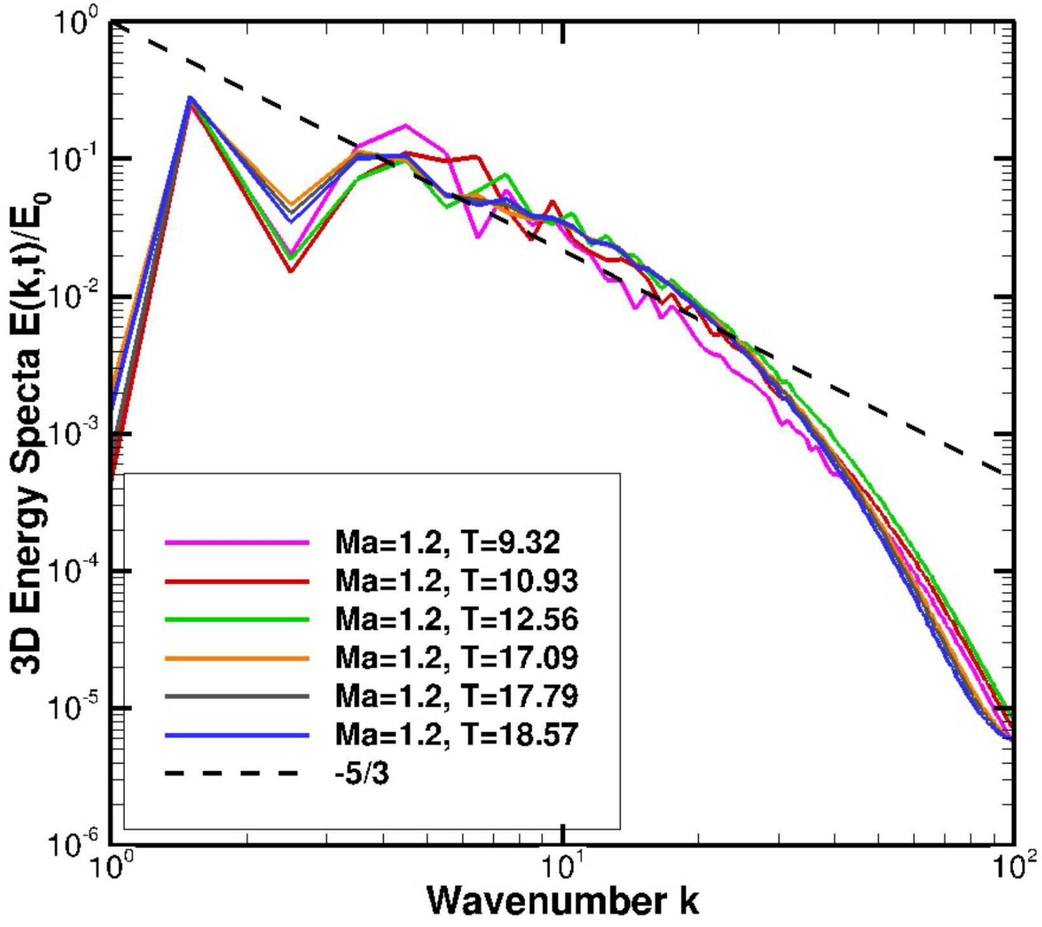


We are here

Energy Spectra

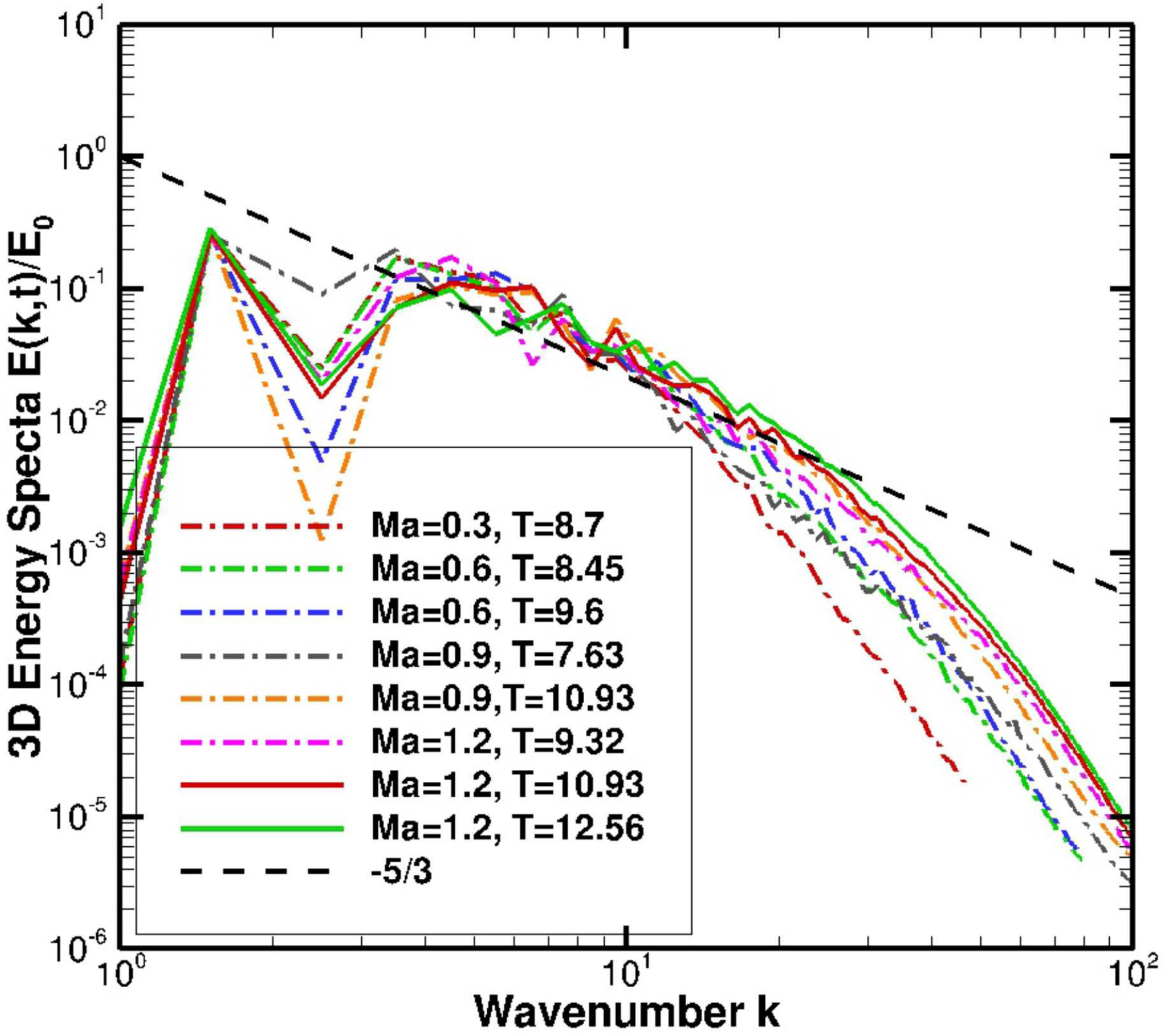


Spectra for all Mach numbers near the maximum dissipation point.

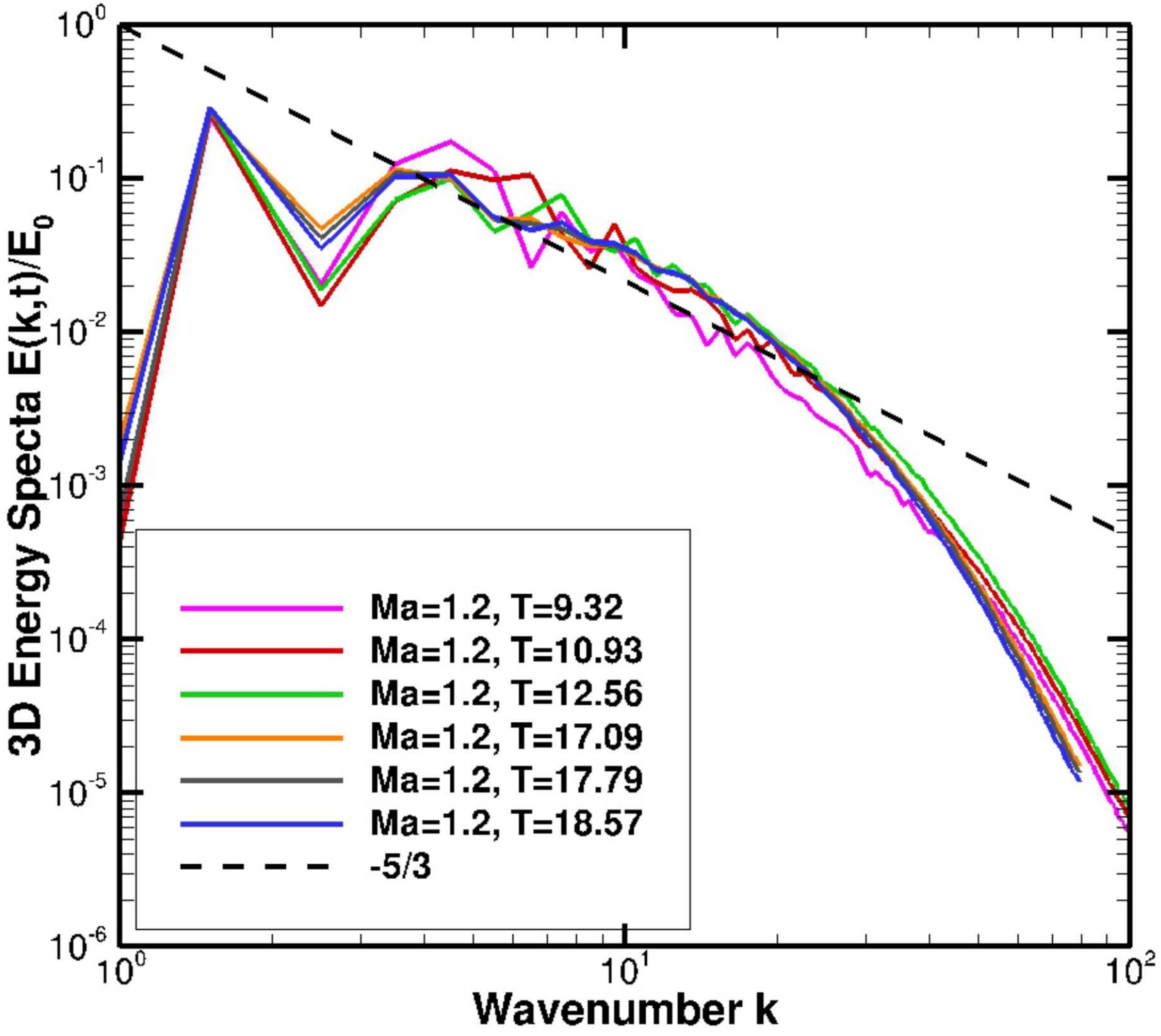


Spectra for Ma = 1.2 at multiple times

Energy Spectra



Spectra for all Mach numbers near the maximum dissipation point.



Spectra for Ma = 1.2 for multiple times

Conclusions

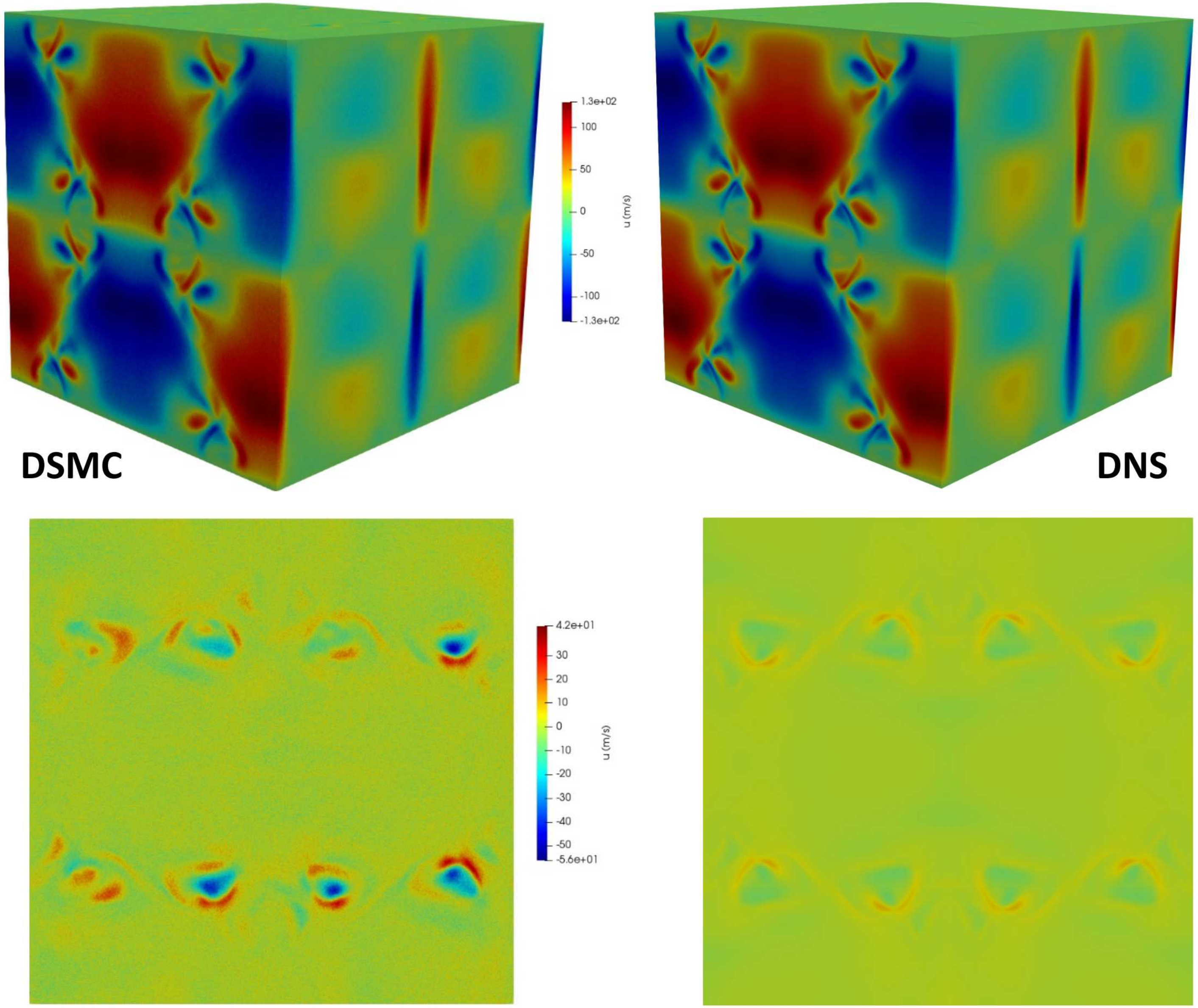
At low Mach numbers and early times, DSMC and DNS produce the similar profiles (laminar or incompressible flow).

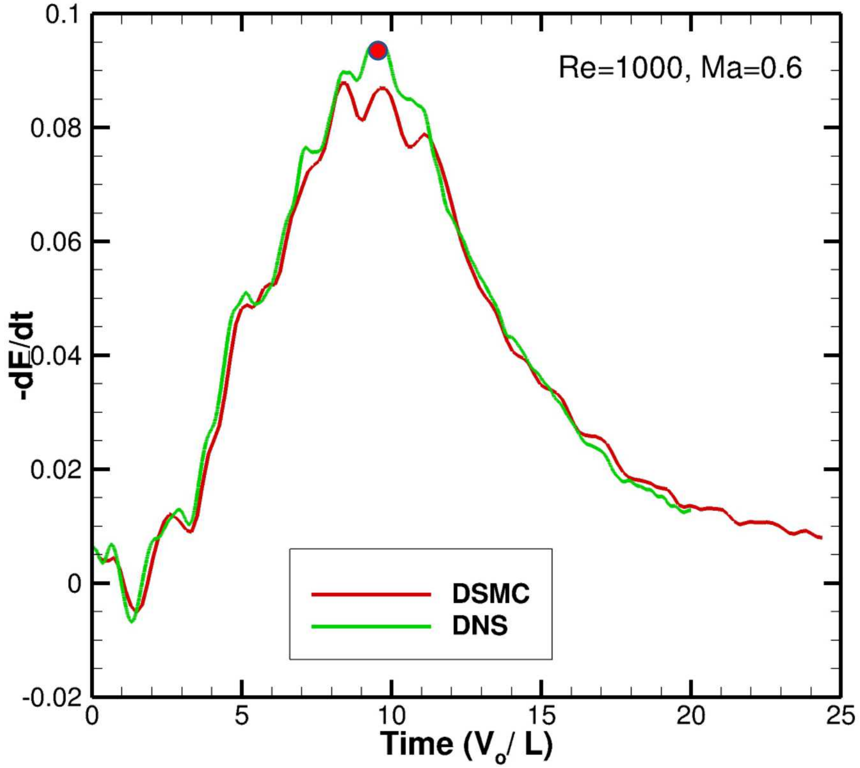
At higher Mach numbers and past maximum-dissipation-point times, instabilities of laminar compressible flow (RMI/RTI) rearrange the vorticity, increasing its spatial and temporal complexity and introducing more structure to the DSMC flow field.

This phenomenon appears only when Kolmogorov scales are comparable to the mean free path, where thermal fluctuations are important.

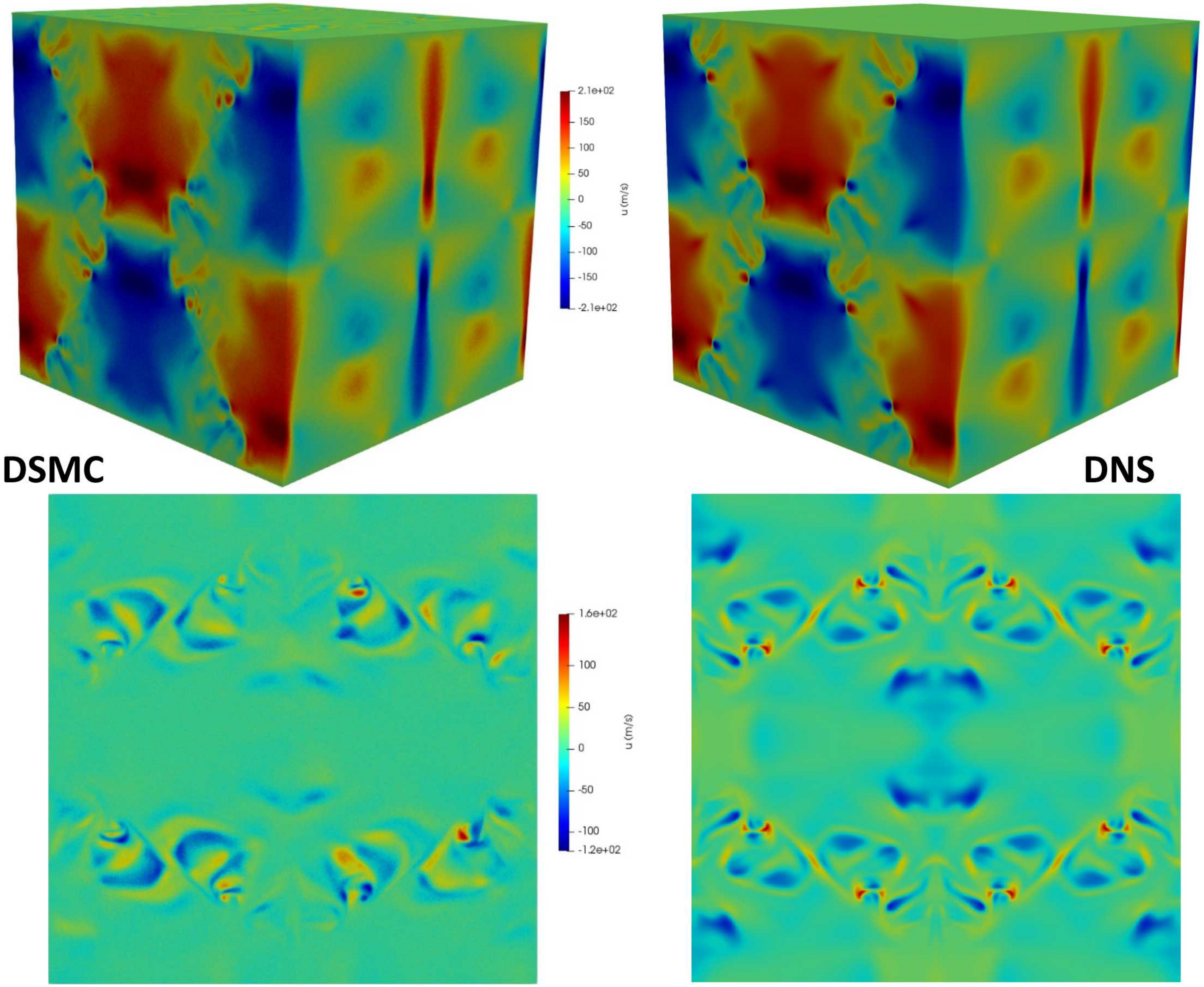
These finer-scale features and non-equilibrium transport do not appear to affect energy dissipation significantly.

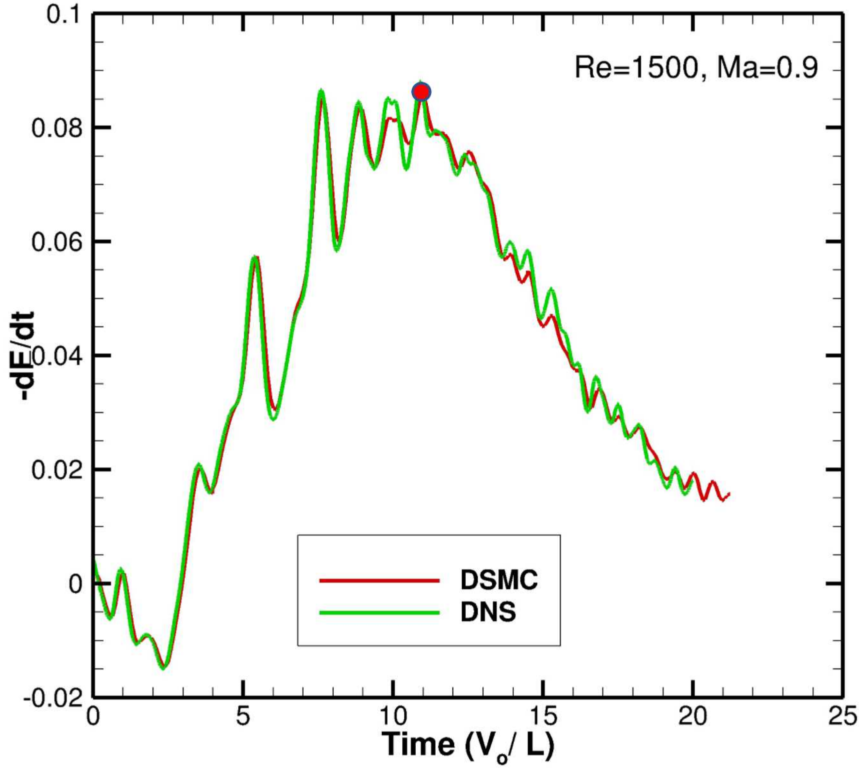
TG: Ma = 0.6, T = 9.60


1.3e+02
100
50
0
-50
-100
-1.3e+02
u (m/s)
DSMC
DNS
4.2e+01
30
20
10
0
-10
-20
-30
-40
-50
-5.6e+01
u (m/s)

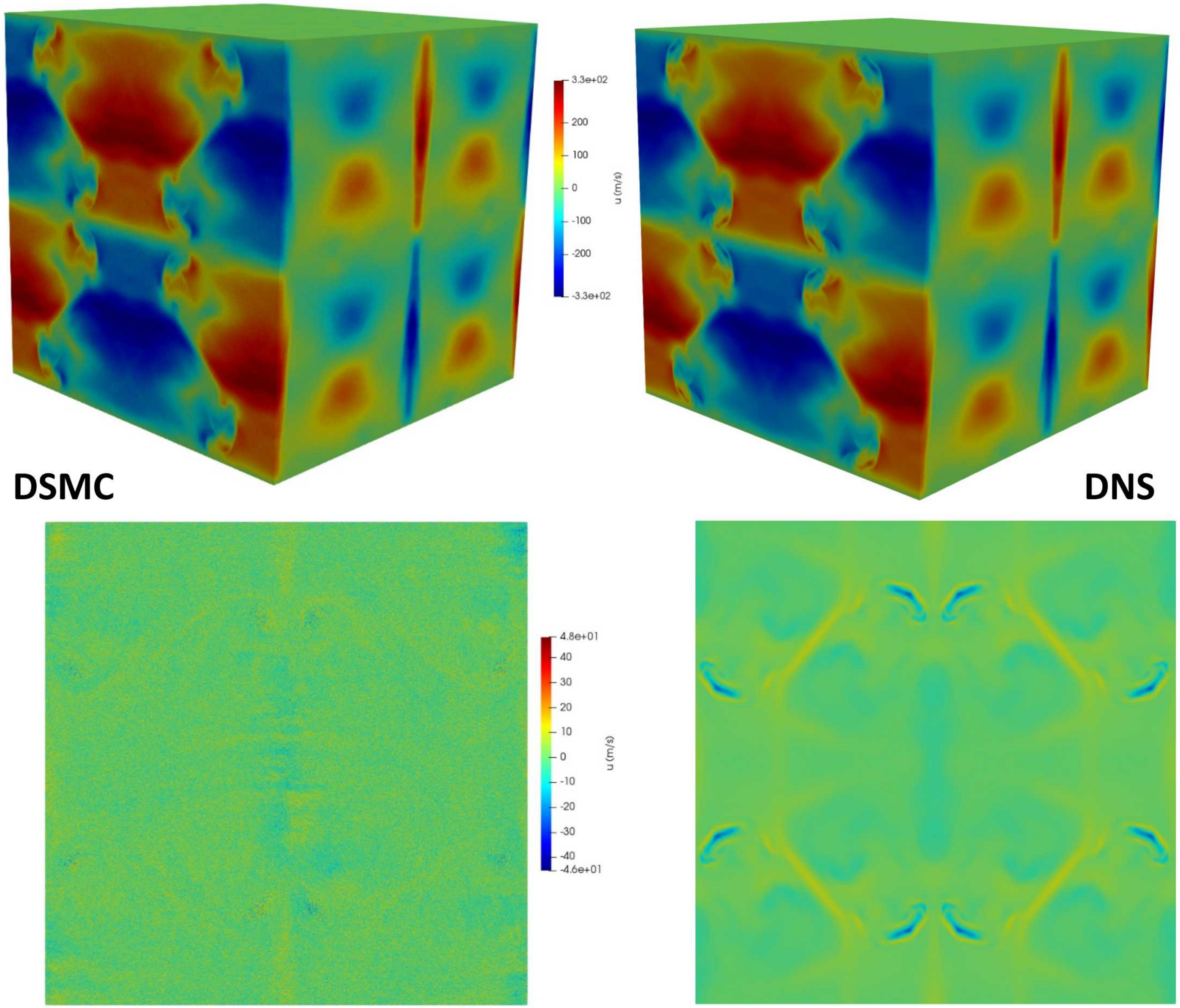

Re=1000, Ma=0.6
-dE/dt
0.1
0.08
0.06
0.04
0.02
0
-0.02
0
5
10
15
20
25
Time (V_o/ L)
DSMC
DNS

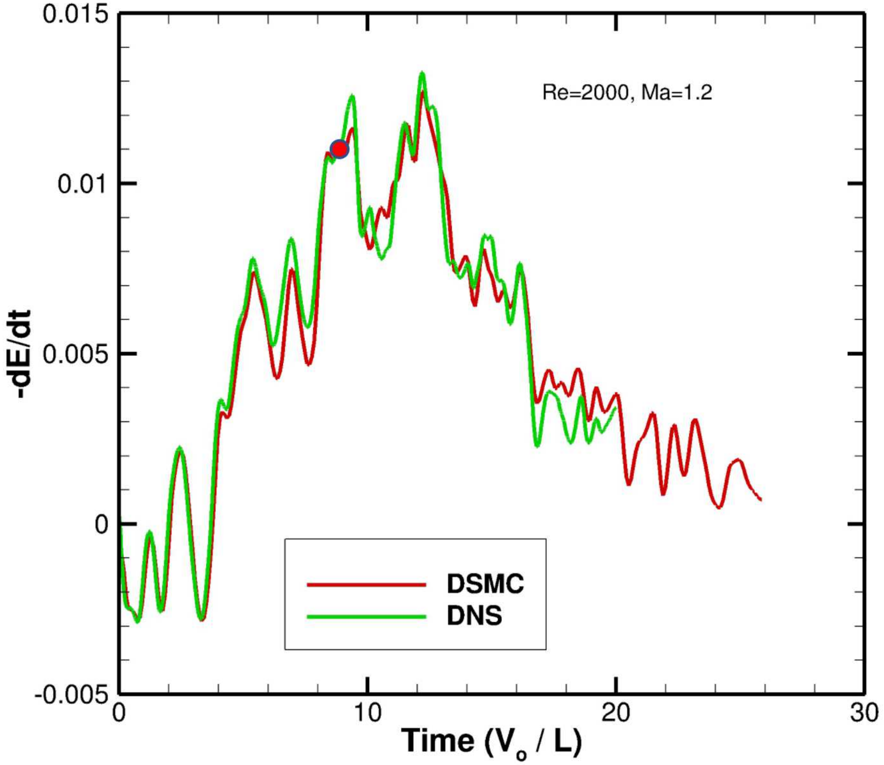
TG: Ma = 0.9, T = 10.93



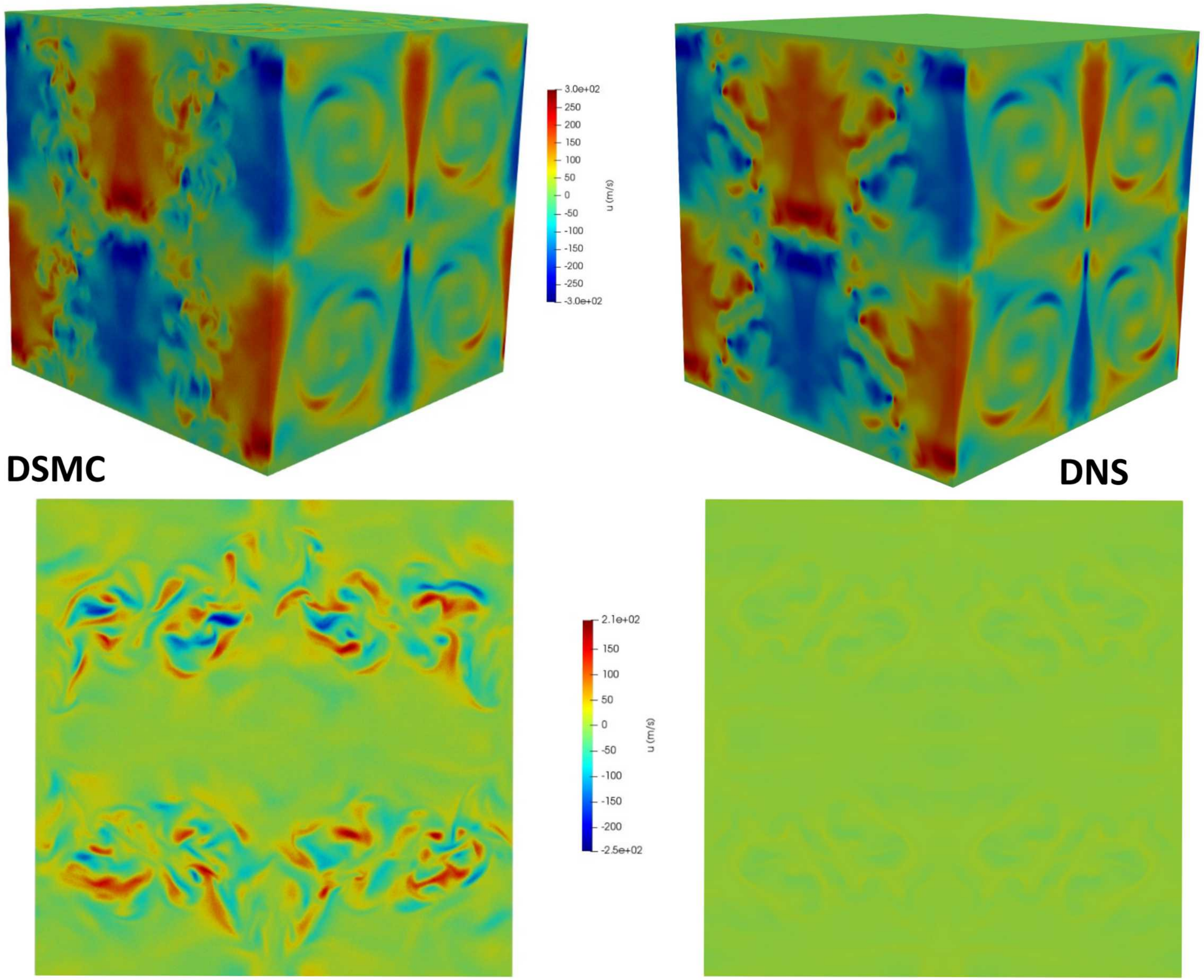


TG: Ma = 1.2, T = 9.32


3.3e+02
200
100
0
-100
-200
-3.3e+02
u (m/s)
DSMC
DNS
4.8e+01
40
30
20
10
0
-10
-20
-30
-40
-4.6e+01
u (m/s)

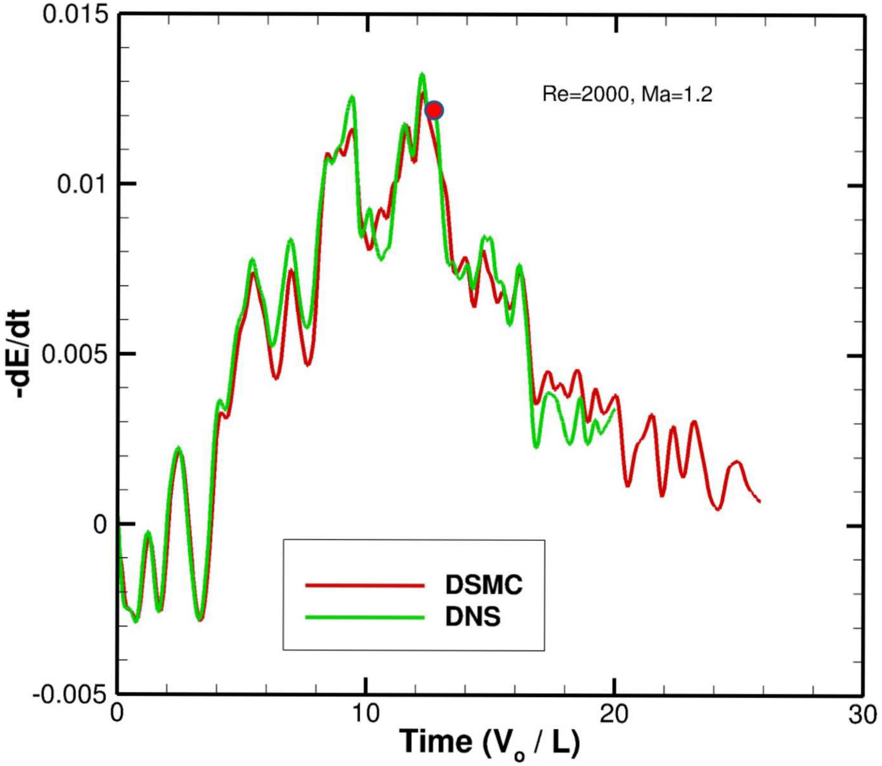

0.015
0.01
0.005
0
-0.005
-dE/dt
0
10
20
30
Time (V_o / L)
Re=2000, Ma=1.2
DSMC
DNS

TG: Ma = 1.2, T = 12.56

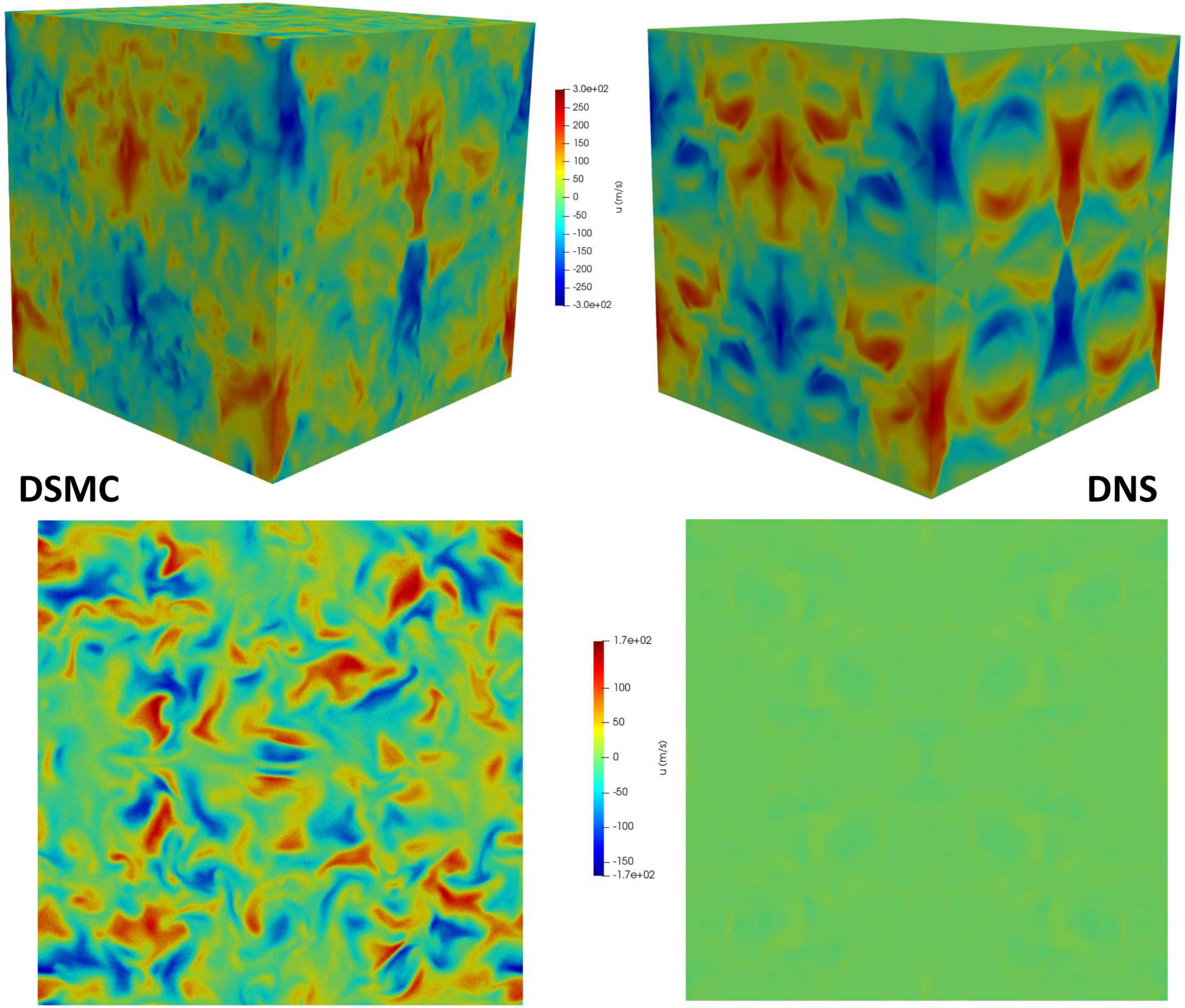


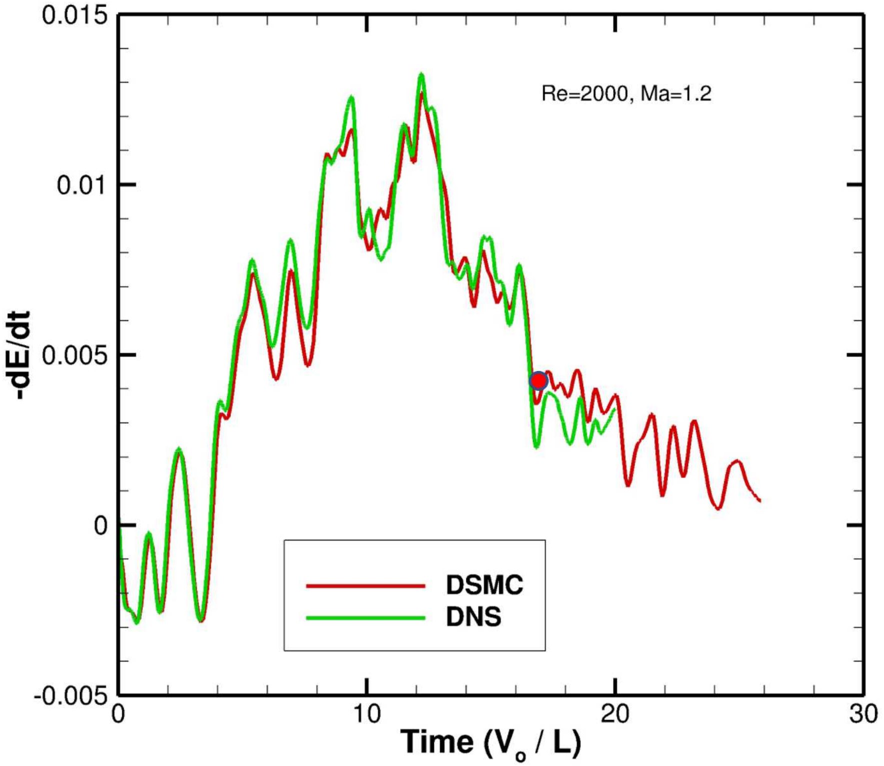
DSMC

DNS

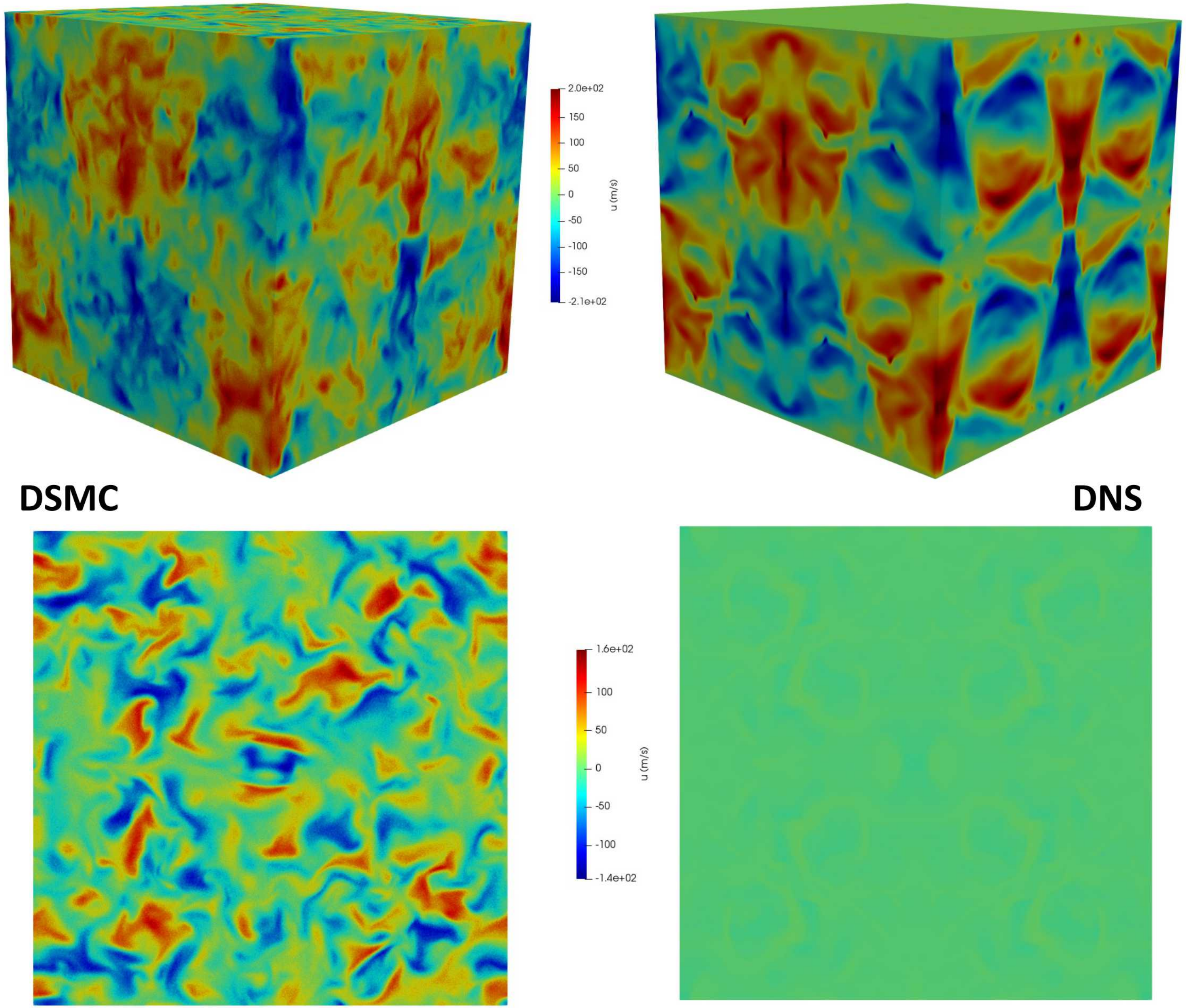


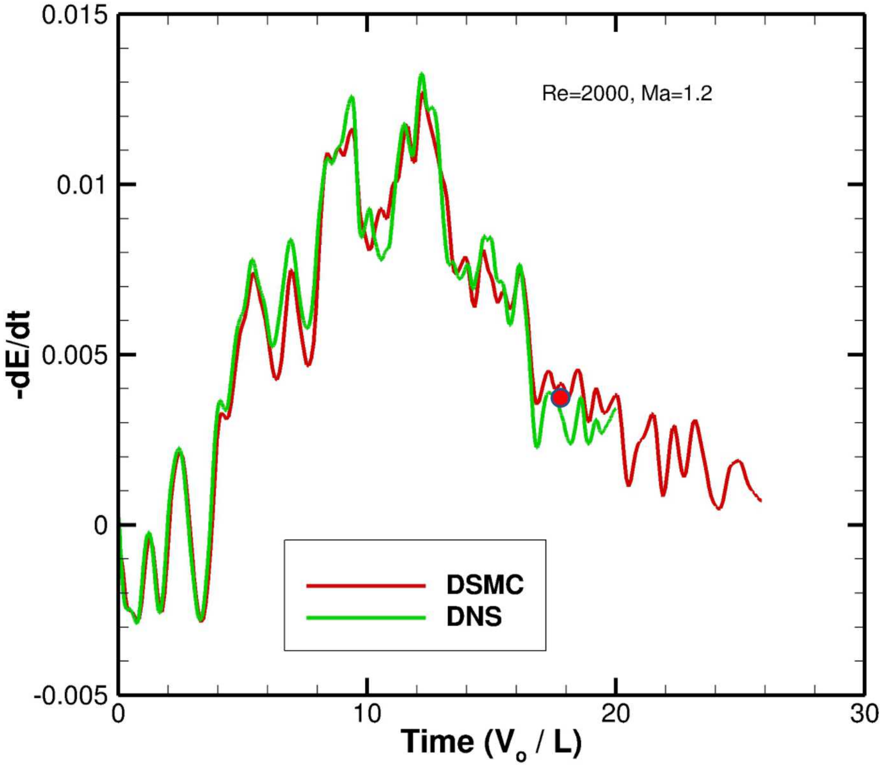
TG: Ma = 1.2, T = 17.09



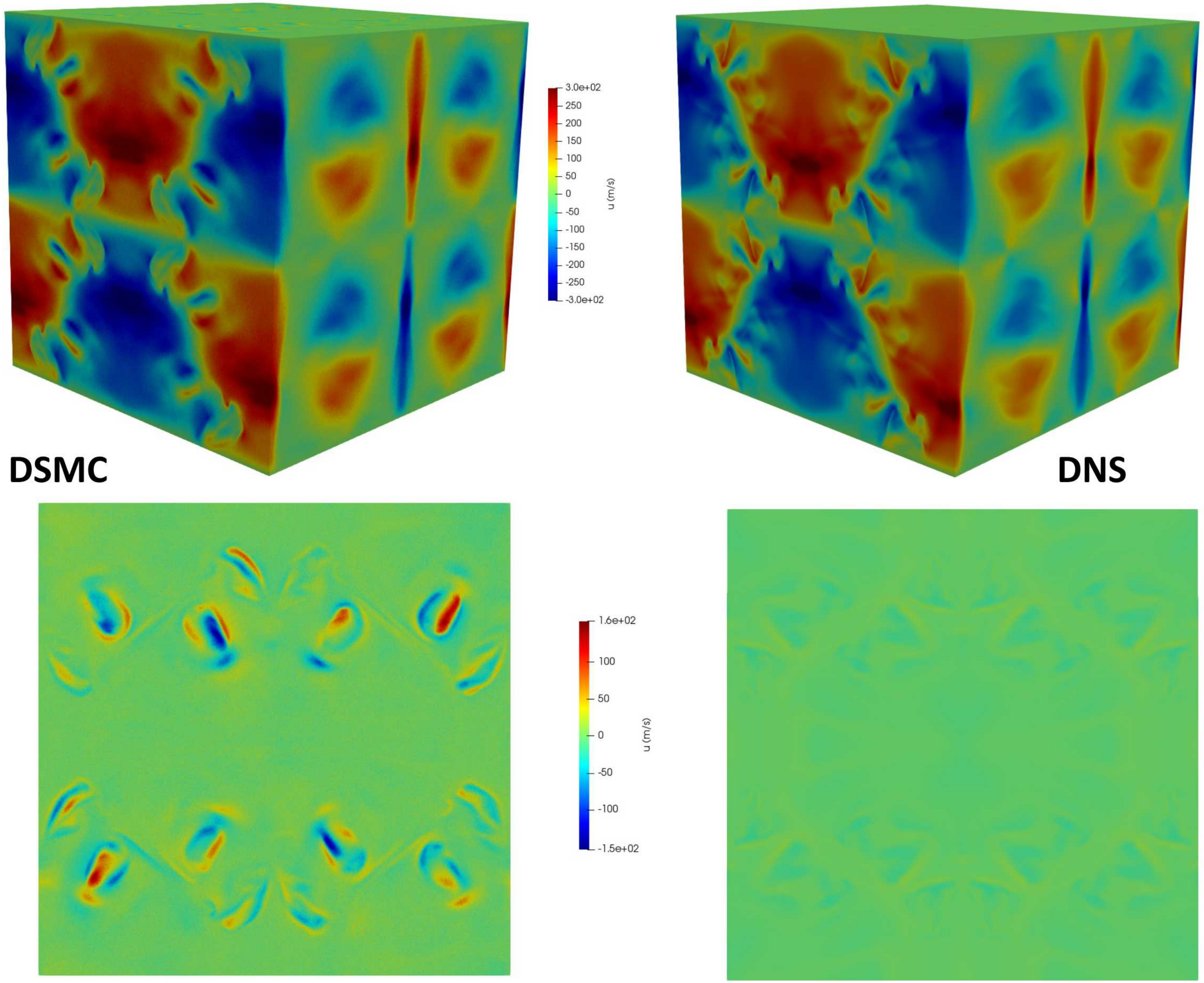


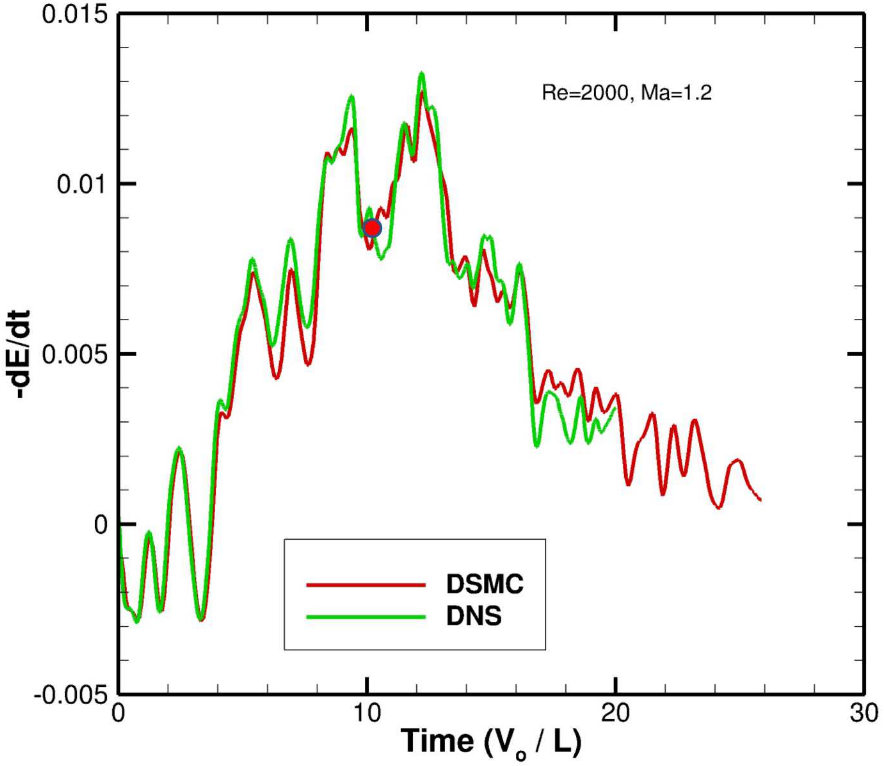
TG: Ma = 1.2, T = 17.74



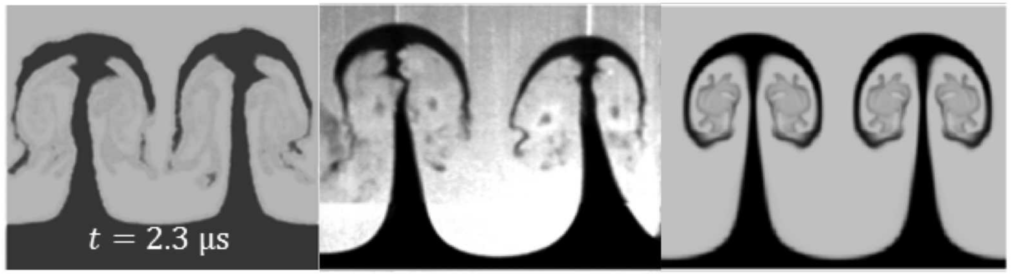


TG: Ma = 1.2, T = 10.93





Baroclinic Creation of Vorticity



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

DSMC includes thermal fluctuations, which can produce additional structure through baroclinic creation of vorticity.

Viscosity Determination

Cells are large, so transport is enhanced

- Near-neighbor collisions reduce MCS
- Viscosity is larger than molecular value

Simulate some other flow to find viscosity

- Use a similar but much easier flow

3D TG vortex energy decay is complicated

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

$$w = 0,\quad p = p_0 + \left(\rho_0 V_0^2/16\right)\left(\cos[2x/L] + \cos[2y/L]\right)\left(2 + \cos[2z/L]\right)$$

$$-\pi L \le \{x, y, z\} \le \pi L \text{ at } t = 0,\quad E = \text{turbulent energy cascade}$$

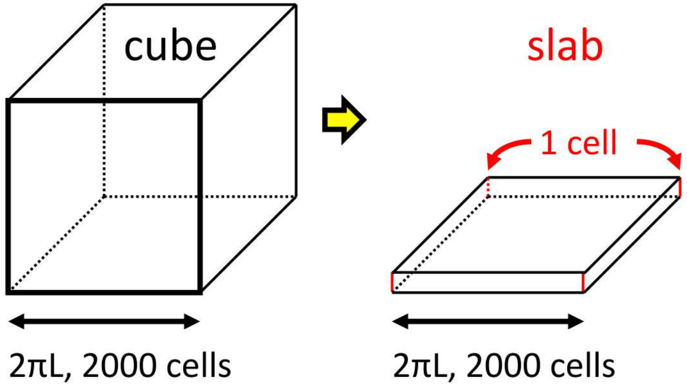
2D TG vortex energy decay is simple

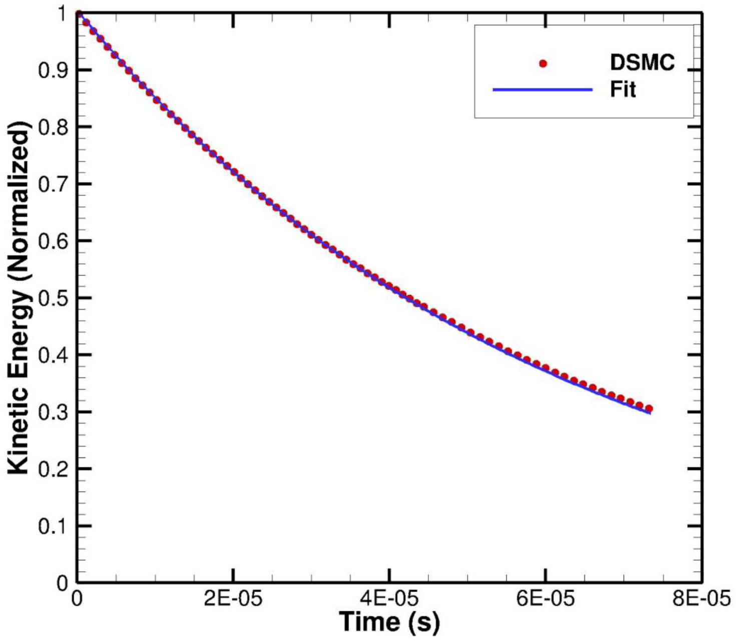
$$u = V_0 \sin[x/L]\cos[y/L],\quad v = -V_0 \cos[x/L]\sin[y/L]$$

$$w = 0,\quad p = p_0 + \left(\rho_0 V_0^2/4\right)\left(\cos[2x/L] + \cos[2y/L]\right)$$

$$-\pi L \le \{x, y\} \le \pi L \text{ and } z = 0 \text{ at } t = 0,$$

$$E = E_0 \exp\left[-4\mu_{\text{eff}} t/\rho_0 L^2\right],\quad E_0 = \rho_0 (\pi L)^2 \Delta z V_0^2$$





Perform DSMC simulations of 3D Taylor-Green Vortex at Re = 500