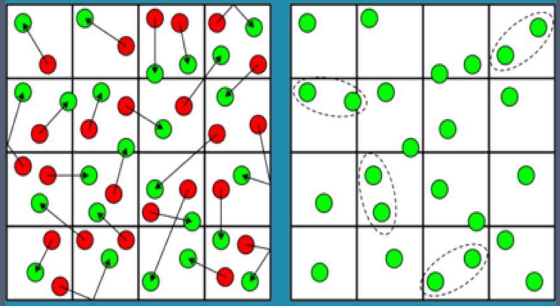
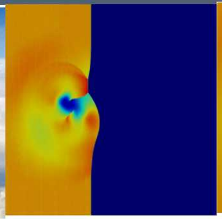
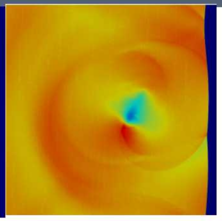
Sandia National Laboratories

SAND2019-11314C

DSMC Simulations of Compressible Turbulence







- *PRESENTED BY:*

M. A. Gallis, N. P. Bitter, J. R. Torczynski

U.S. DEPARTMENT OF ENERGY NNSA

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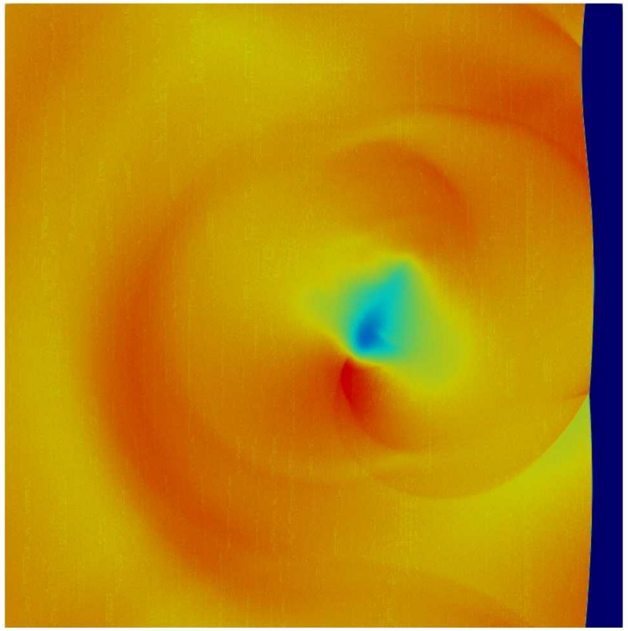
Examples of Compressible Turbulence

Interstellar Turbulence



Shock/Turbulence Interaction
Shocks/Shocklets interacting with acoustic waves

Supersonic Combustion
Heat release due to exothermic reactions

Compressible Turbulence

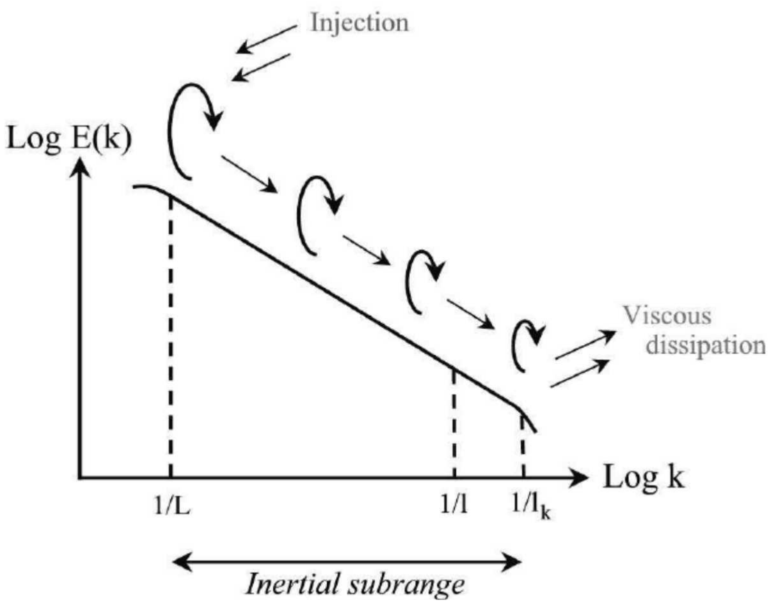
Compressible energy cascade is more complicated than incompressible

- In compressible turbulence, there are complex non-linear interactions of vortices, acoustic waves, and shock waves, leading to strong couplings between the velocity fields and the 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 non-equilibrium play a role in the baroclinic creation of turbulence.

- Both these classes of physical phenomena are observed 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.

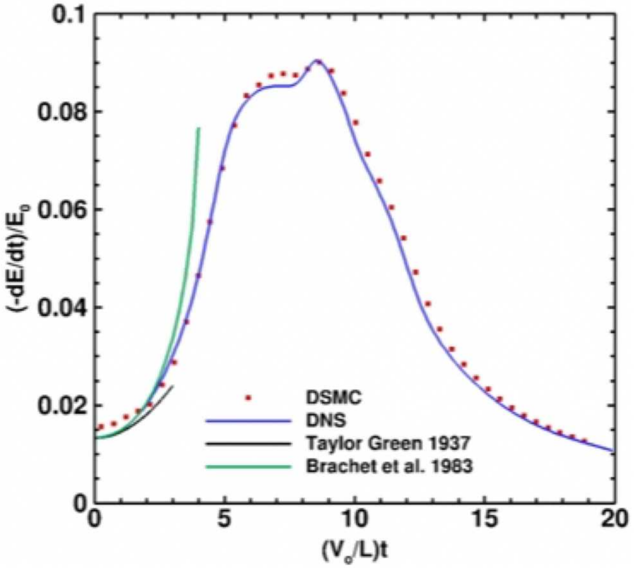
Taylor Green Flow

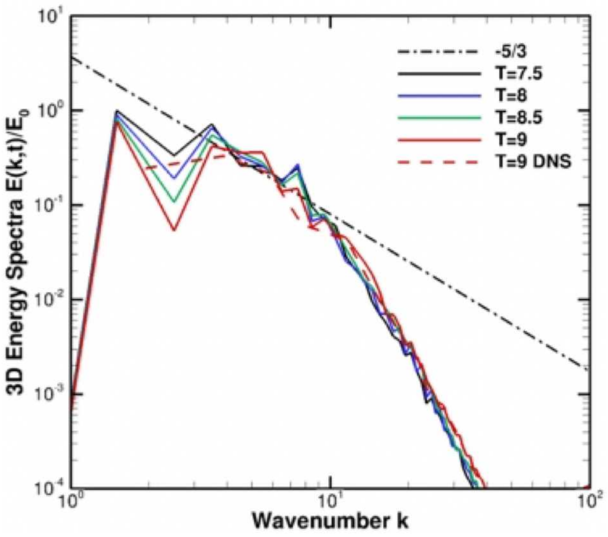
Taylor-Green (TG) vortex flow is a generic turbulent flow

- 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





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

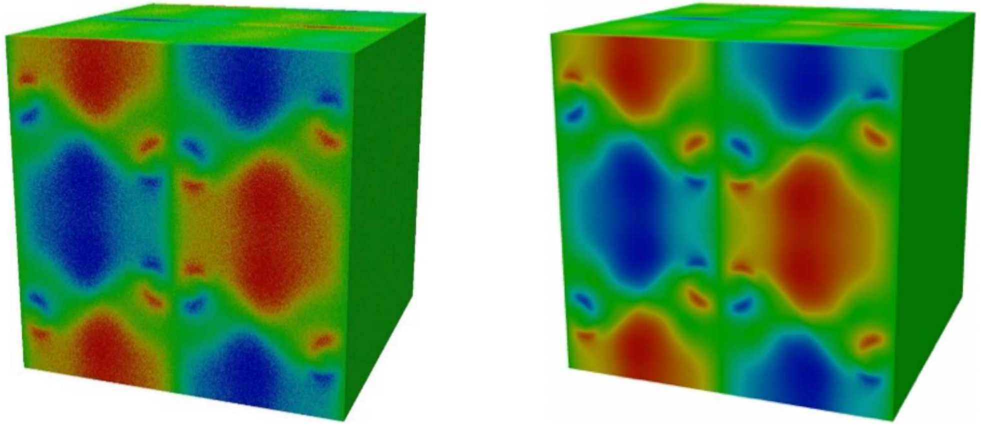
Gas parameters

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

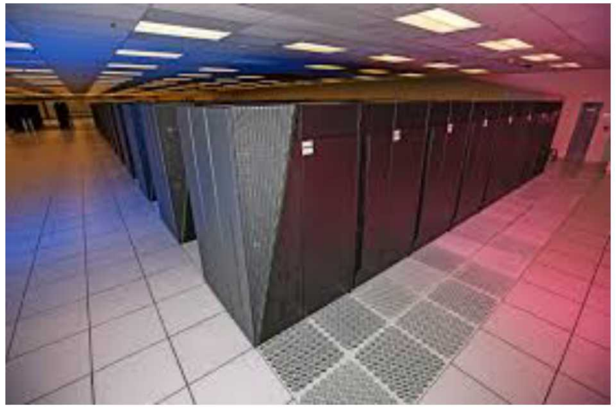
Simulation Parameters

Simulations performed on LLNL/Sequoia

- 32,768 nodes (×16 cores, ×2 threads), 30 hrs.



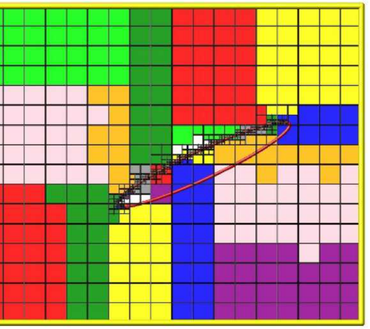
Taylor-Green flow from DNS and DSMC simulations.

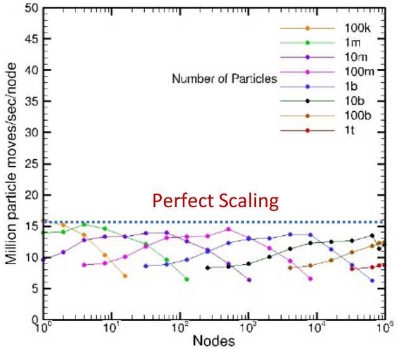


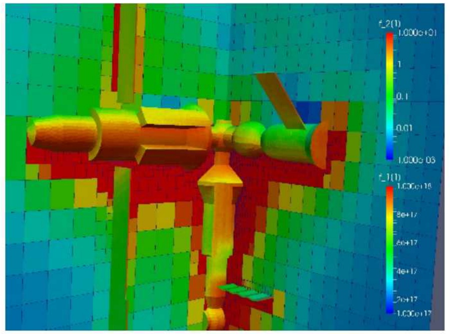
This is SPARTA

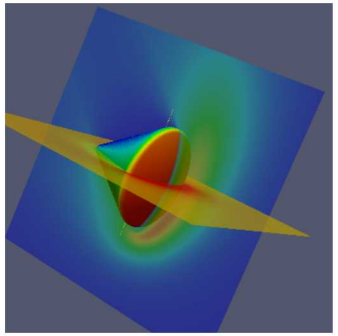
SPARTA = Stochastic PArallel Rarefied-gas Time-accurate Analyzer

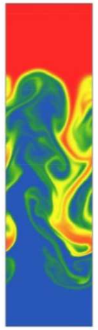
- 1D, 2D, 2D-Axisymmetric or 3D; Serial or Parallel.
- Cartesian, hierarchical grid.
  - Octree (up to 16 levels in 64-bit cell ID).
  - Load balancing, automatic grid adaptation, *in situ* visualization.
- Next-gen performance portability through Kokkos Abstractions.
  - Sequoia (1.57 million cores).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

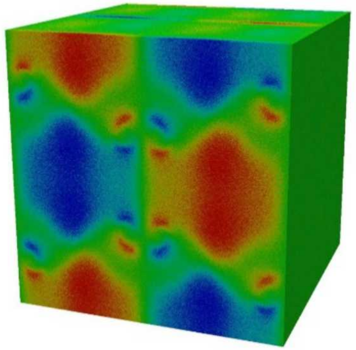


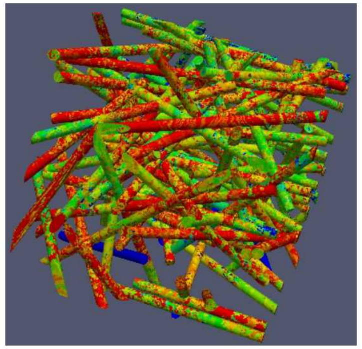




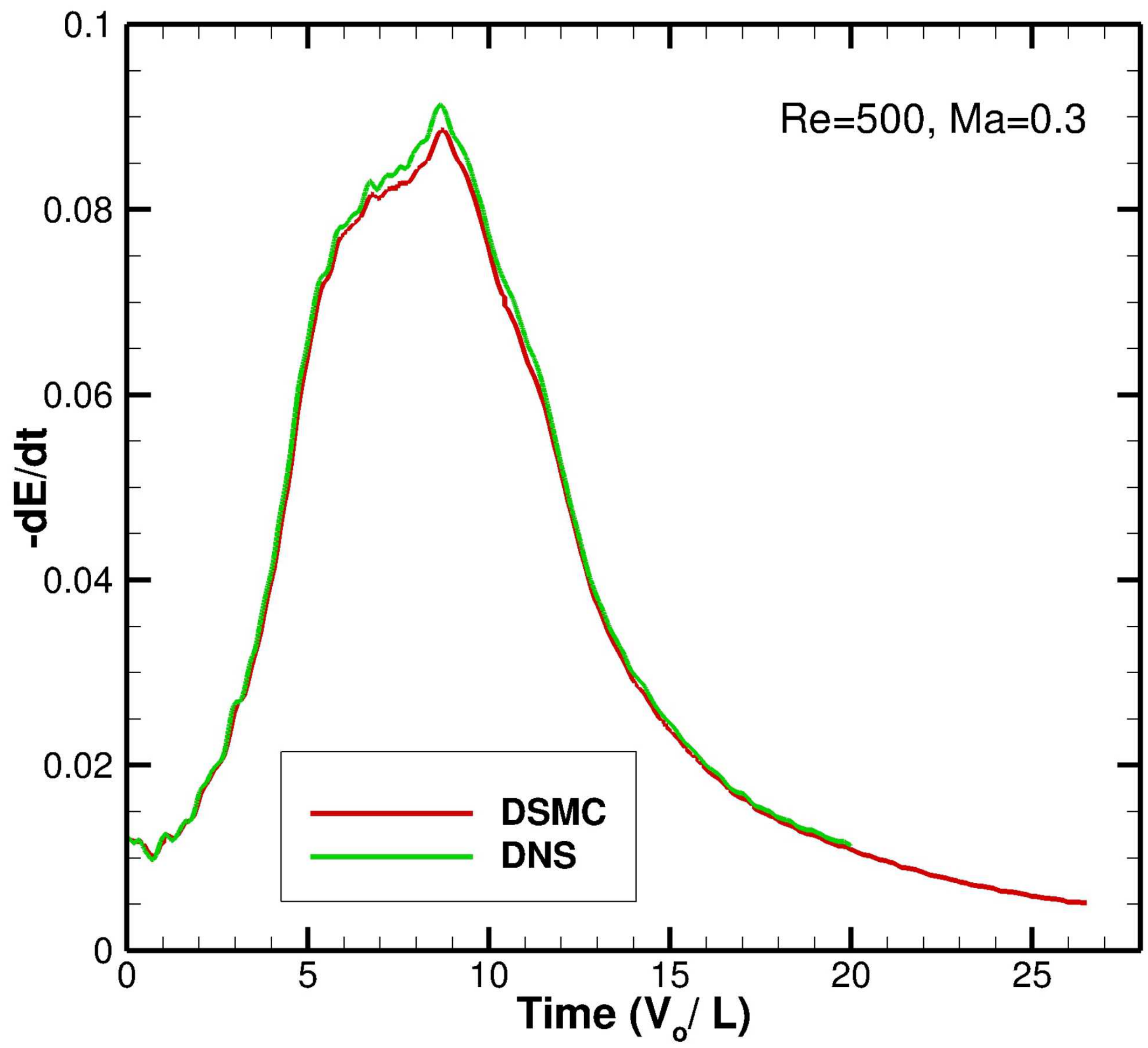




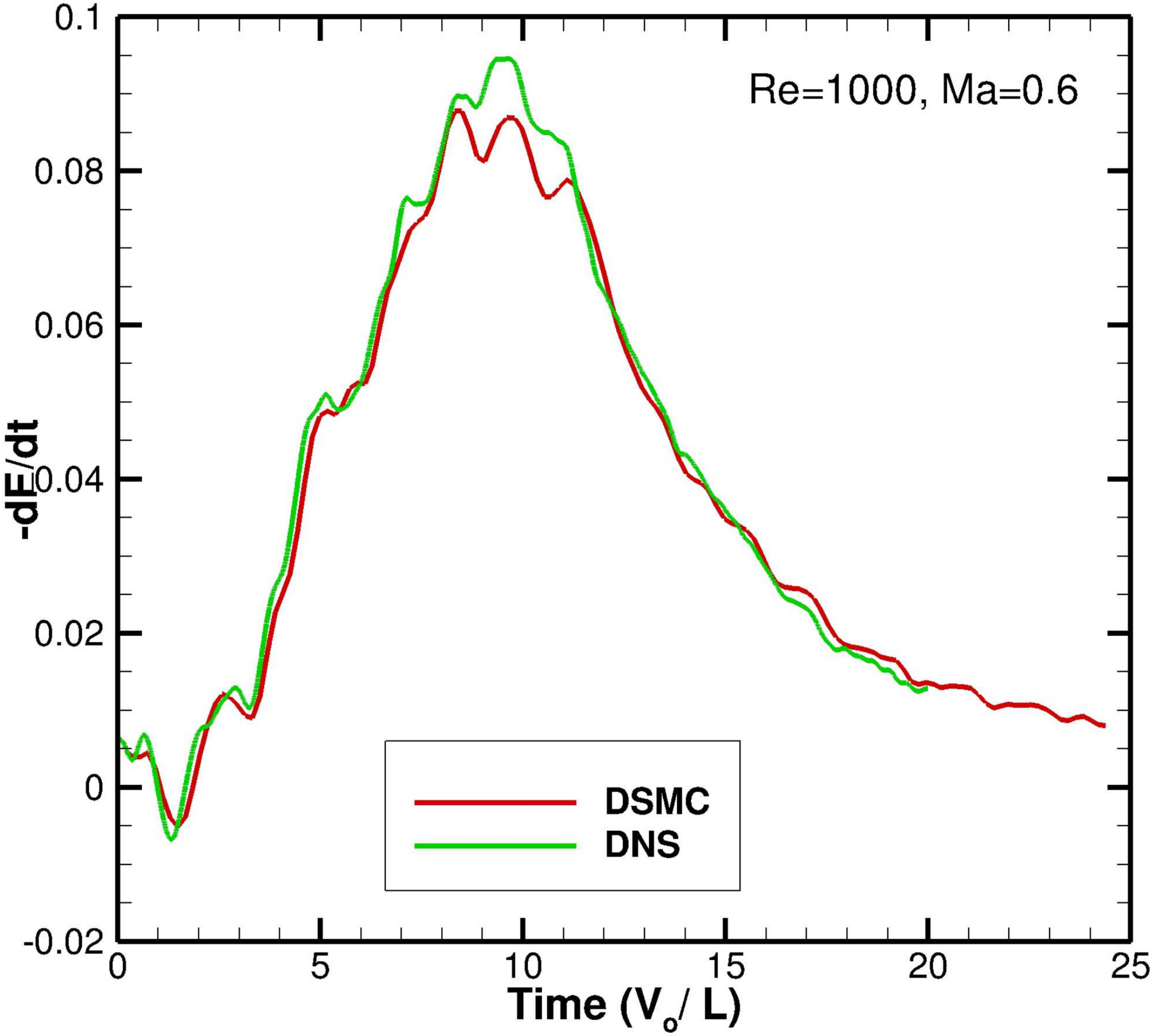




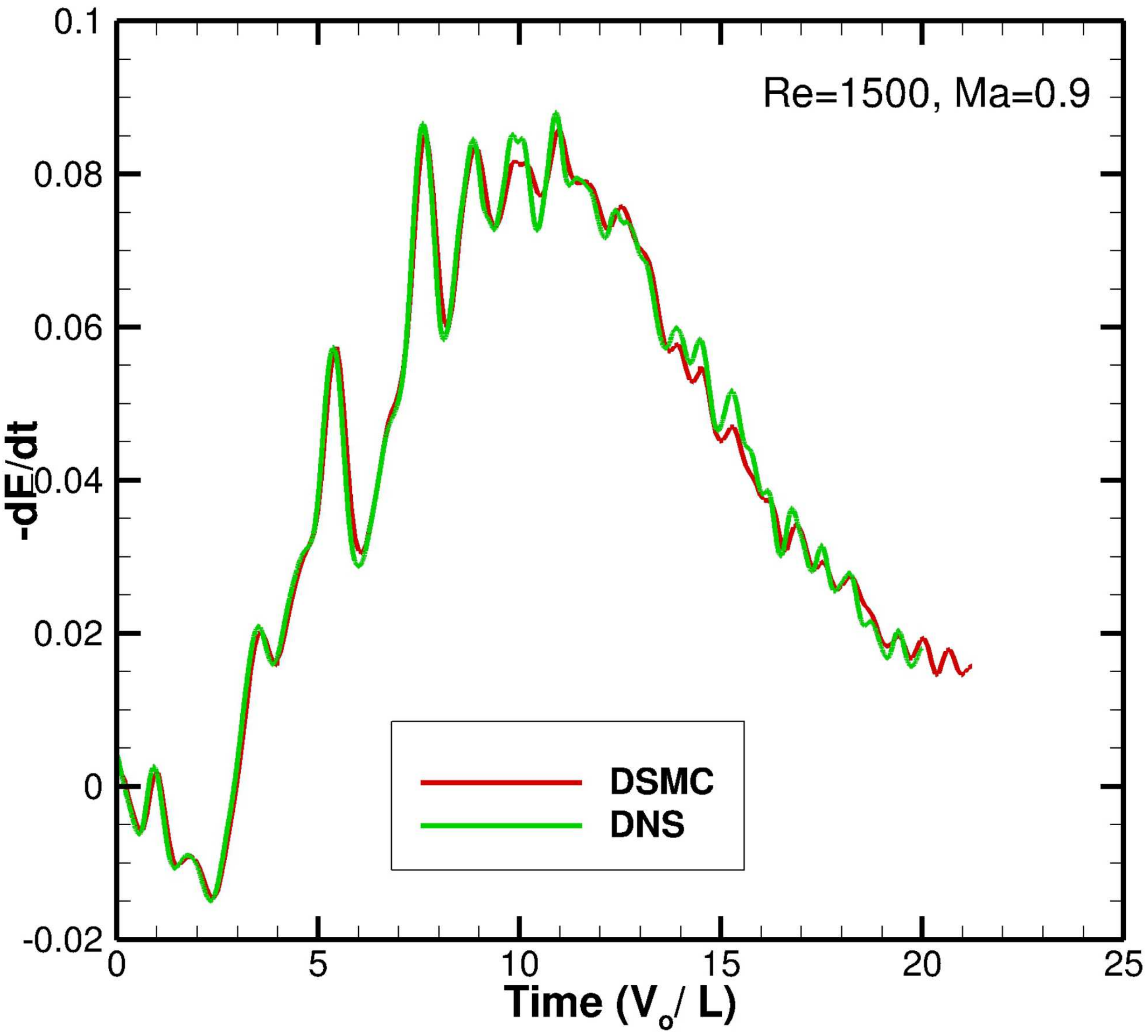
TG Ma=0.3, Energy Dissipation



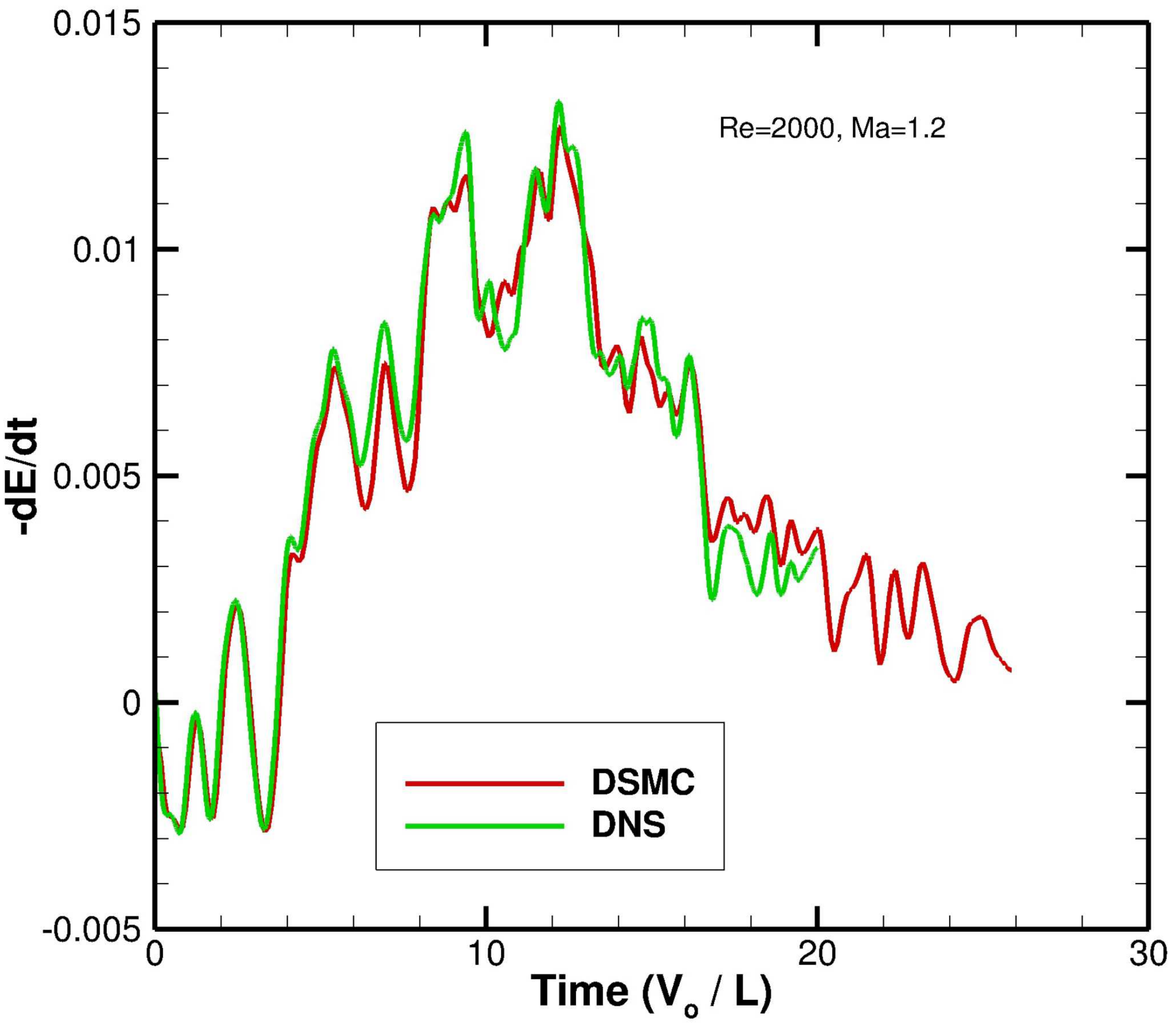
TG Ma=0.6, Energy Dissipation



TG Ma=0.9, Energy Dissipation

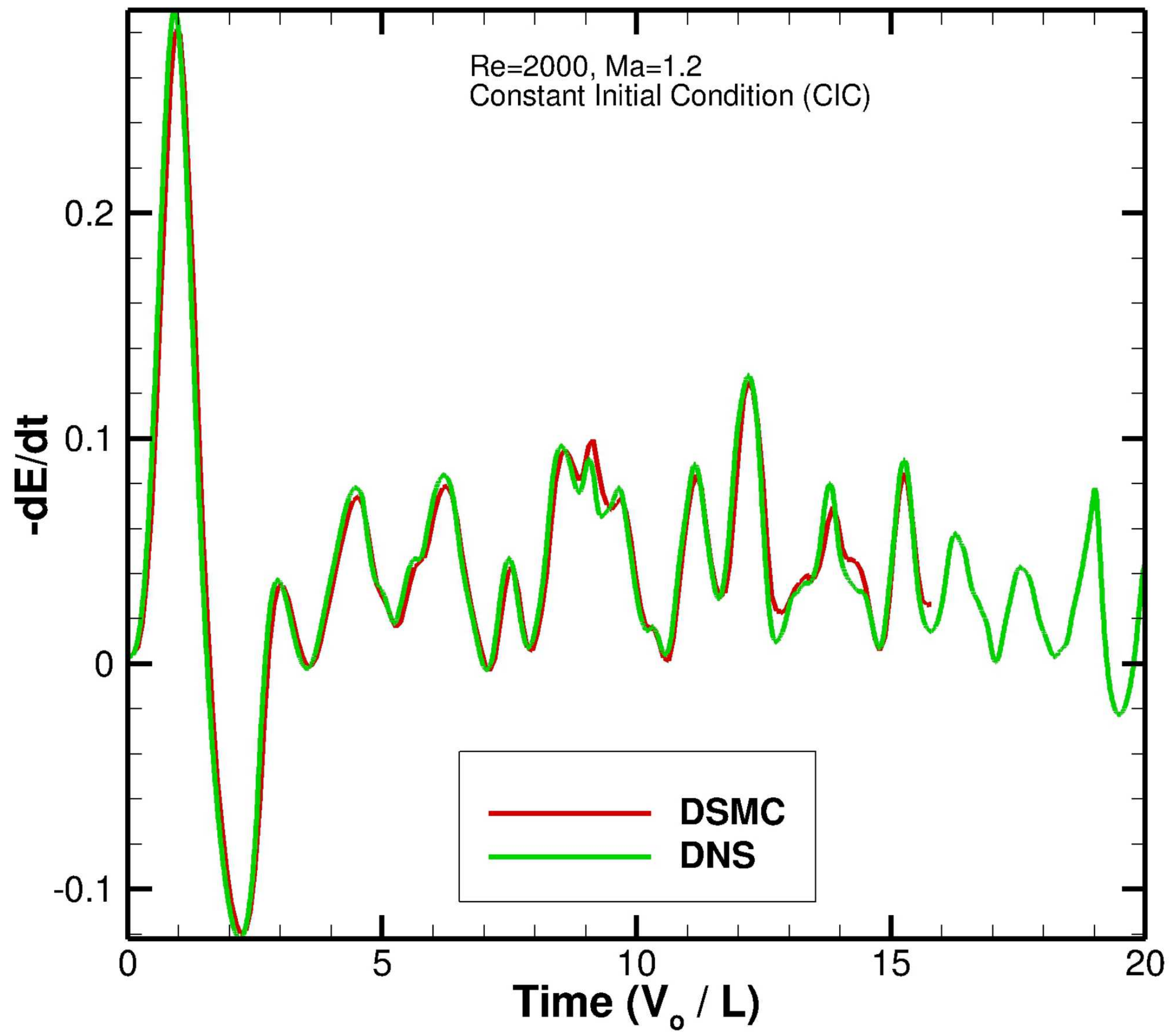


TG Ma=1.2, Energy Dissipation

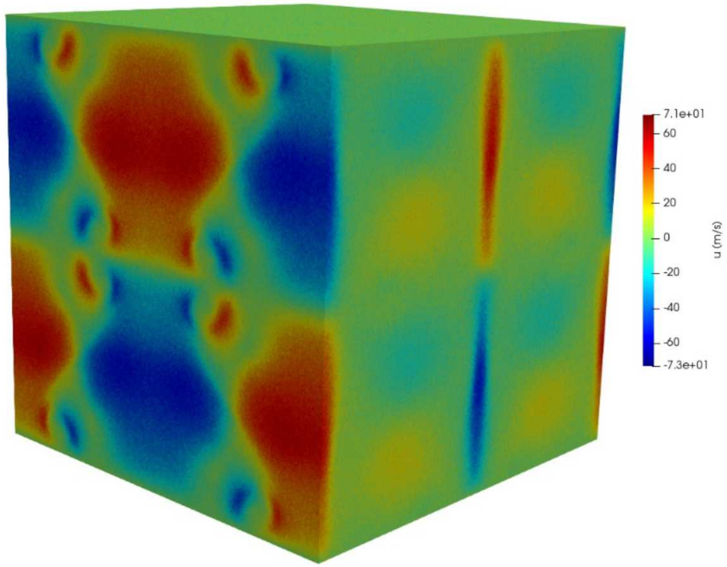


TG, Ma=1.2, Energy Dissipation

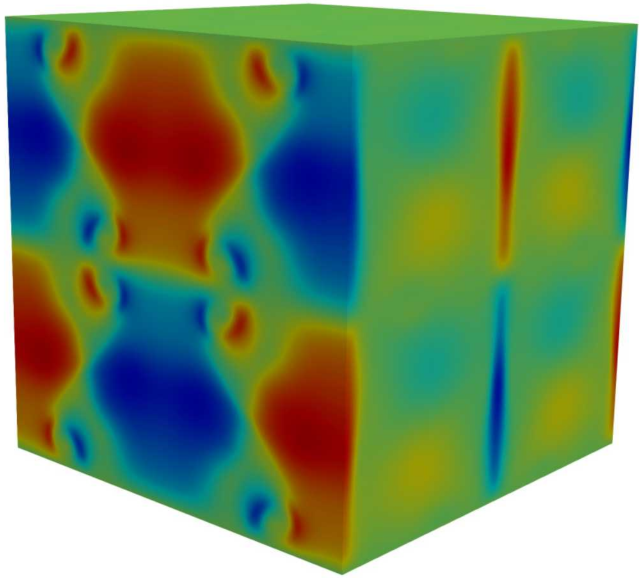
Constant Density Initial Condition

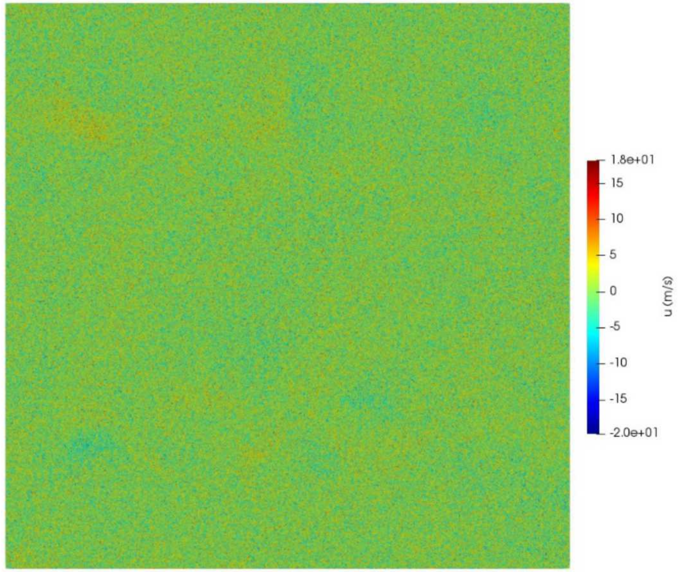


TG Ma=0.3,T=8.7

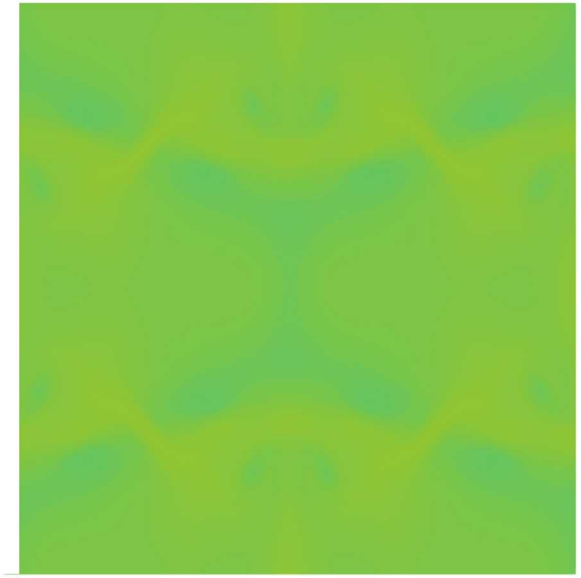


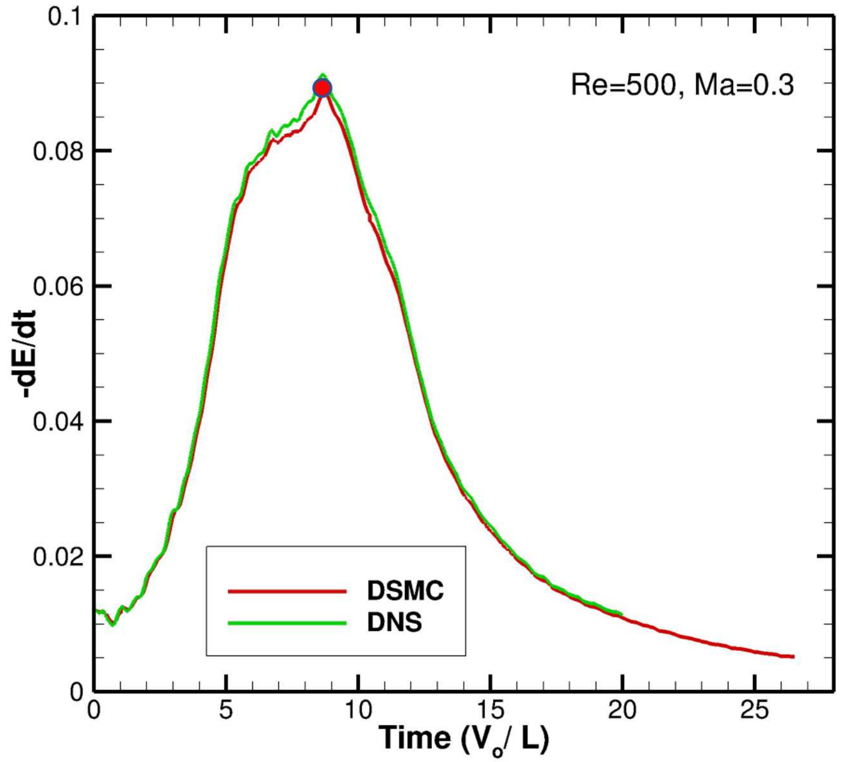
7.1e+01
60
40
20
0
-20
-40
-60
-7.3e+01
u (m/s)





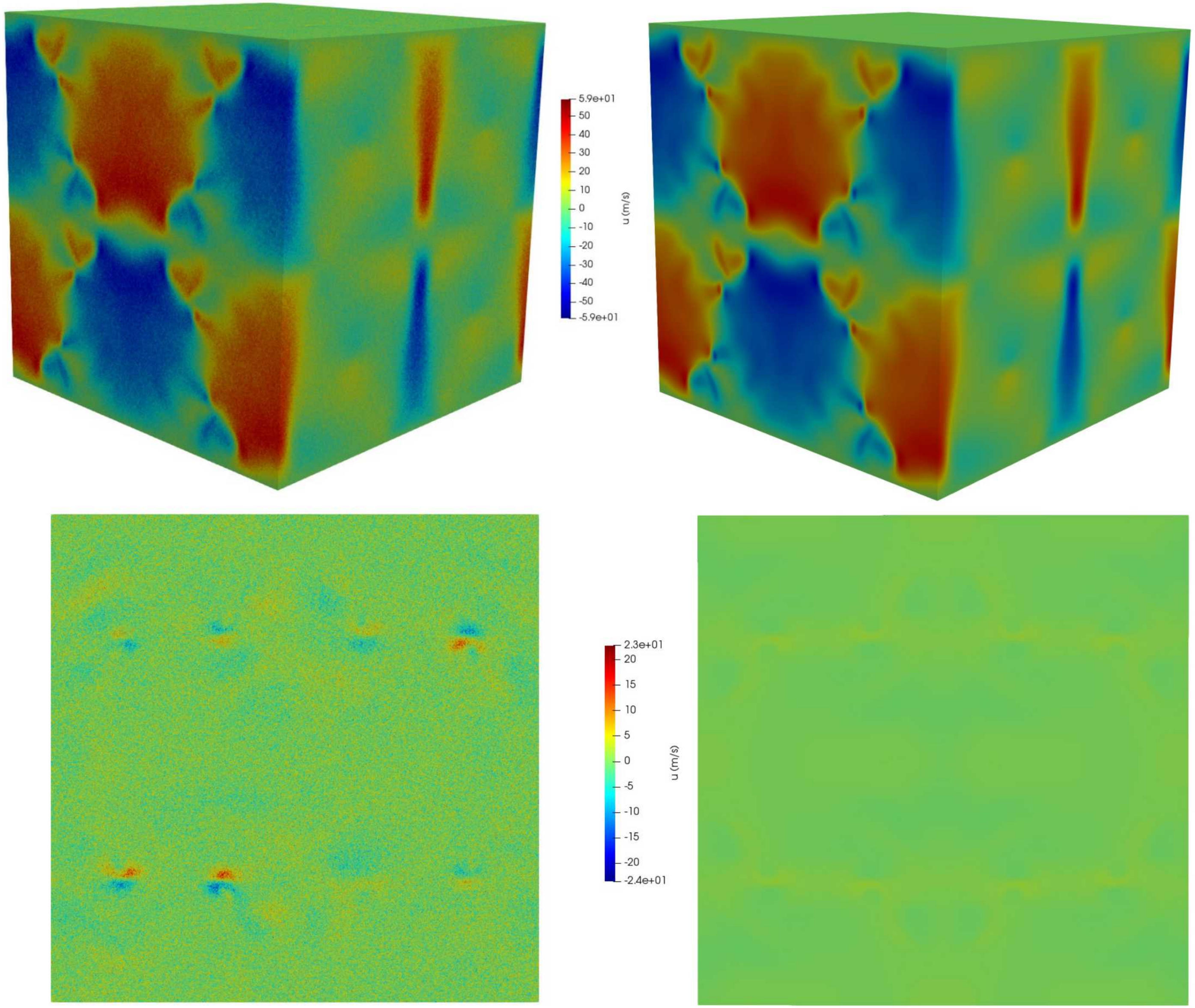
1.8e+01
15
10
5
0
-5
-10
-15
-2.0e+01
u (m/s)

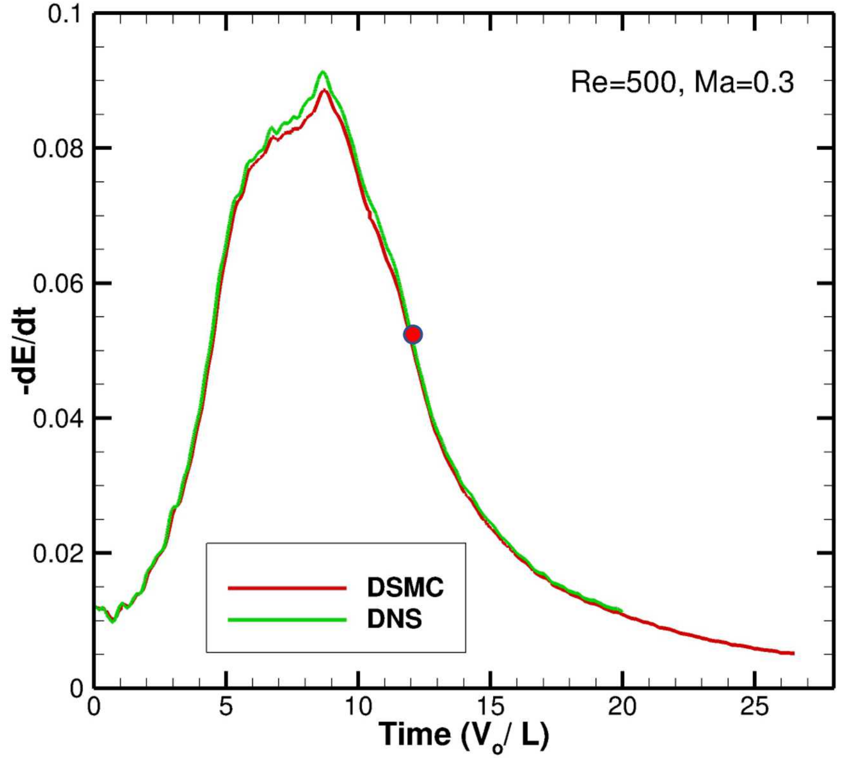




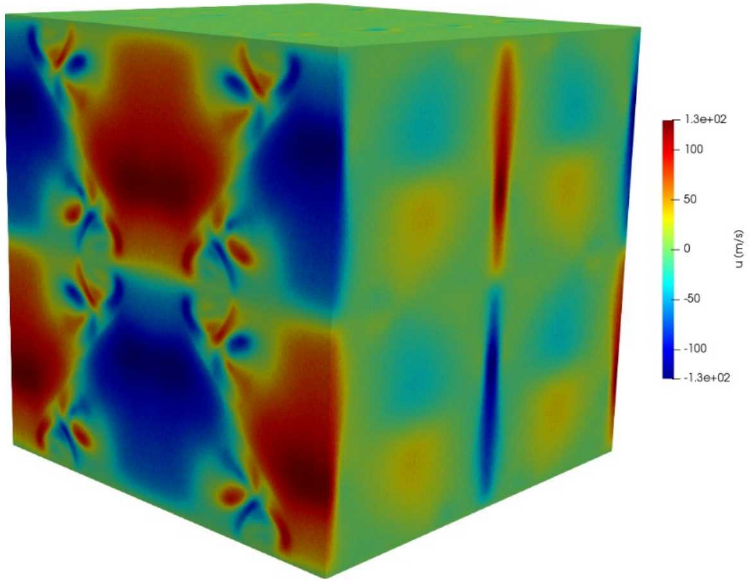
Re=500, Ma=0.3
DSMC
DNS
-dE/dt
Time (V$_o$/ L)
0
0.02
0.04
0.06
0.08
0.1
0
5
10
15
20
25

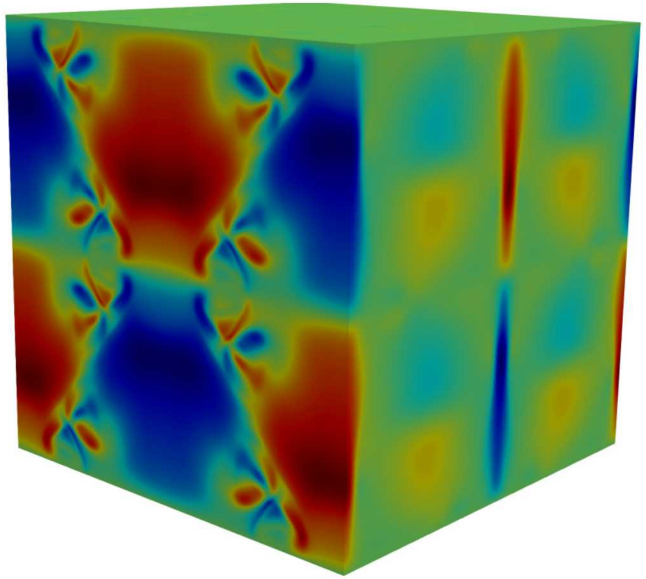
TG Ma=0.3, T=12.01

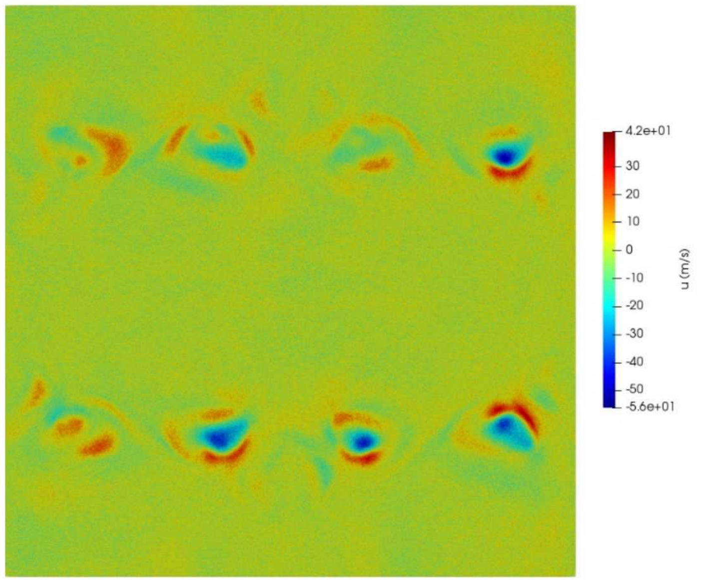


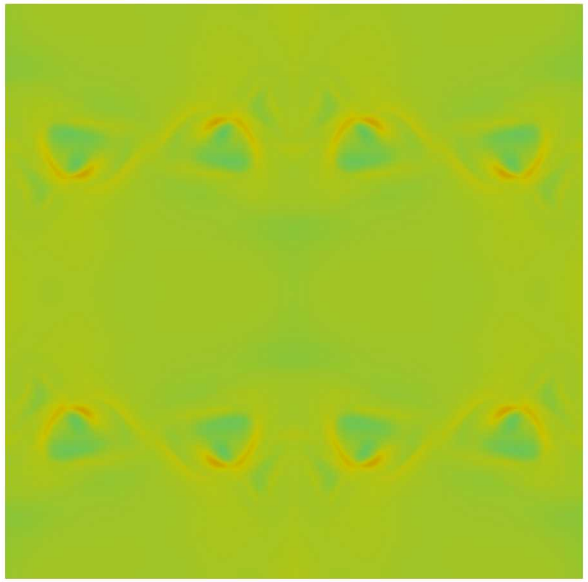


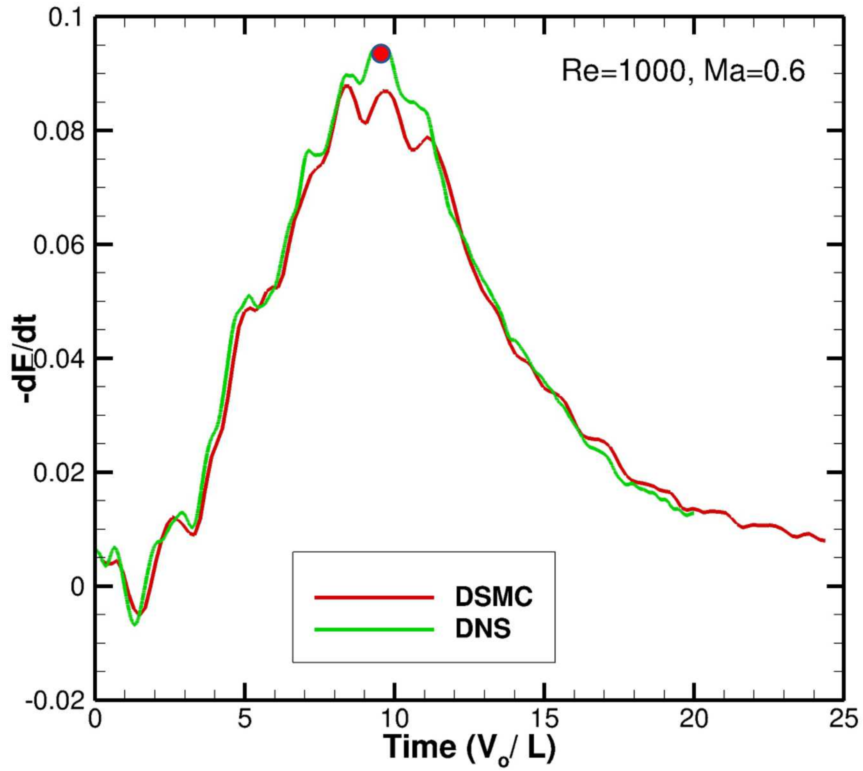
TG Ma=0.6, T=9.60


1.3e+02
100
50
0
-50
-100
-1.3e+02
u (m/s)

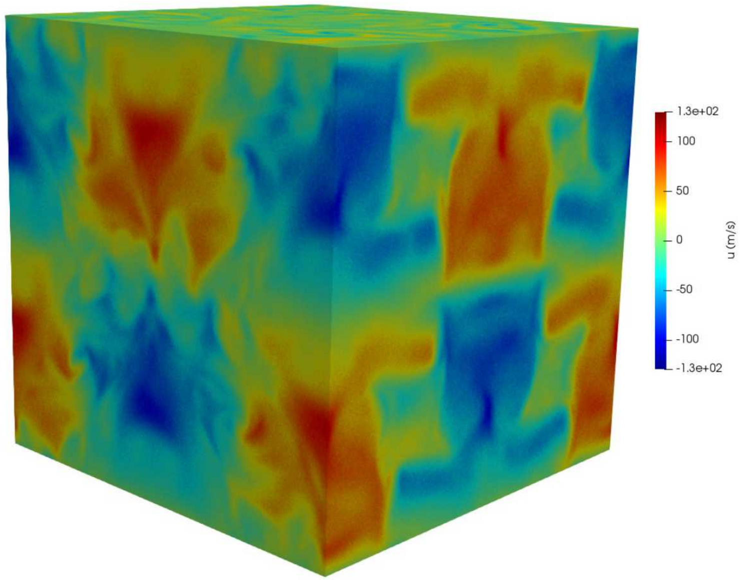


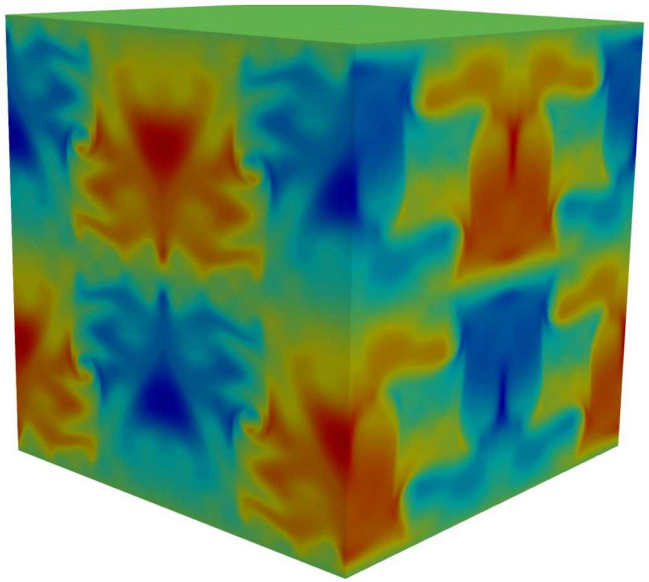

4.2e+01
30
20
10
0
-10
-20
-30
-40
-50
-5.6e+01
u (m/s)

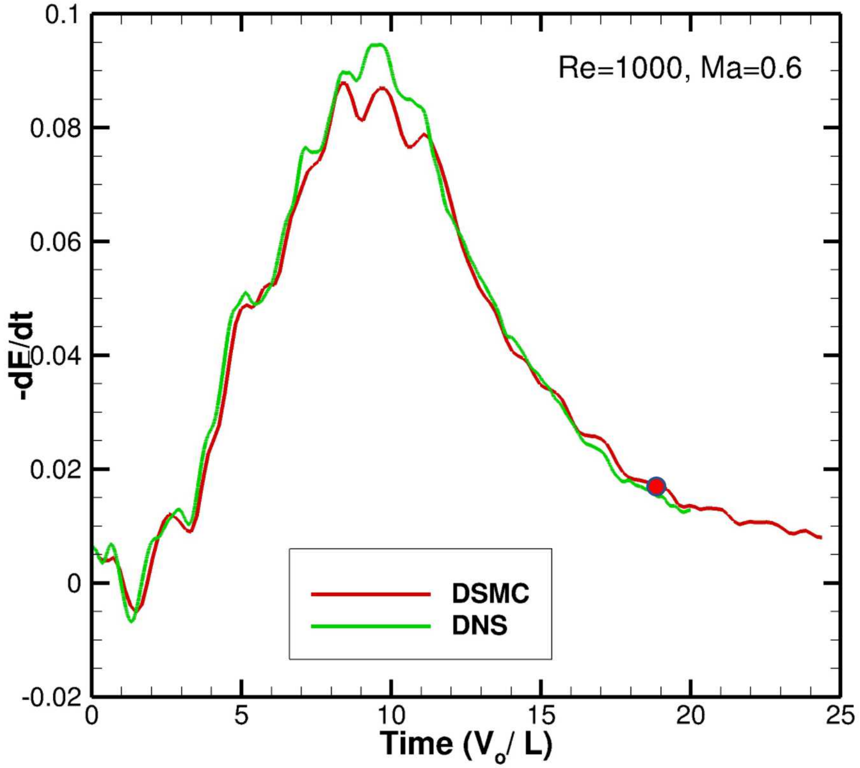


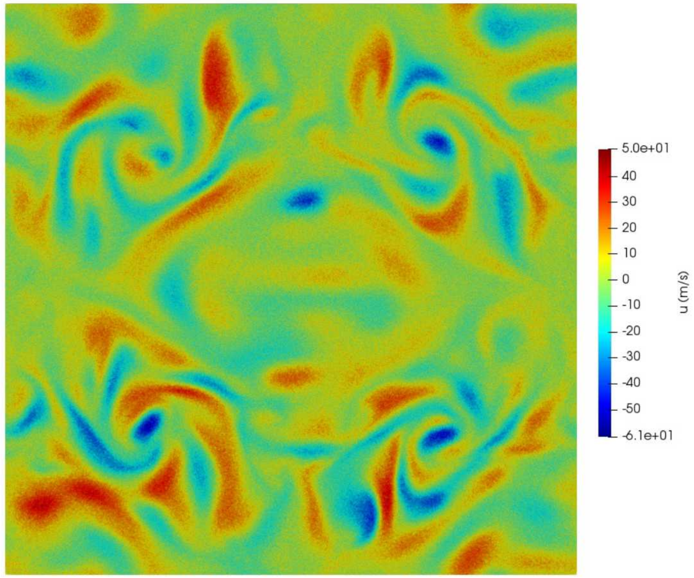

Re=1000, Ma=0.6
DSMC
DNS
-dE/dt
Time (V_o/ L)
0.1
0.08
0.06
0.04
0.02
0
-0.02
0
5
10
15
20
25

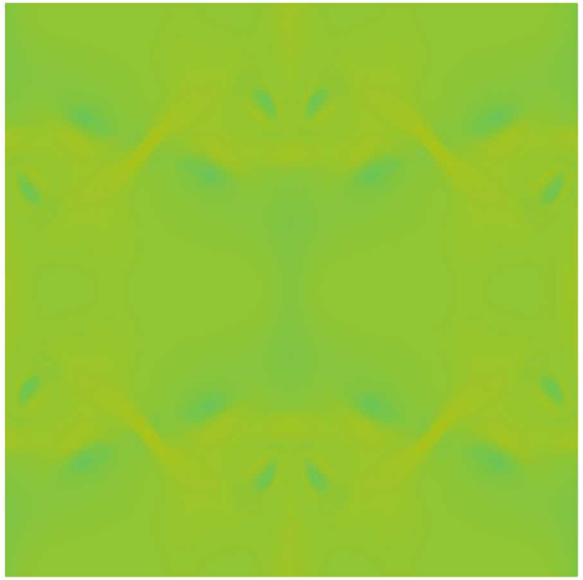
TG Ma=0.6, T=18.47



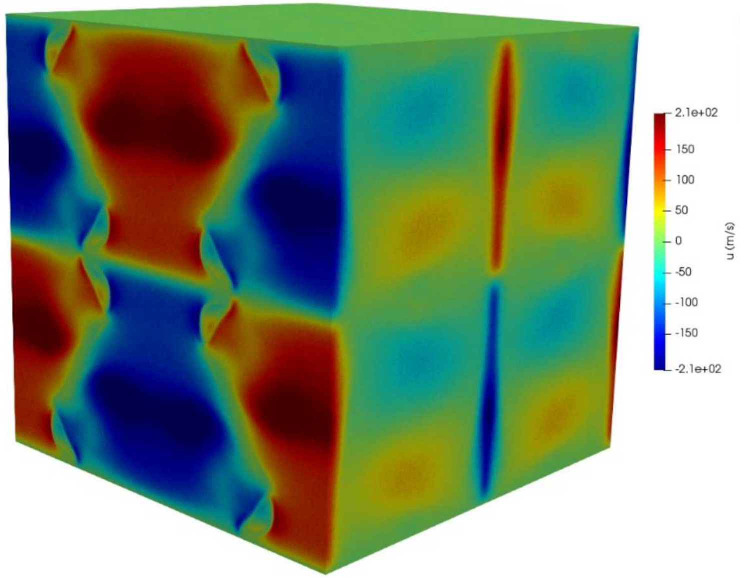


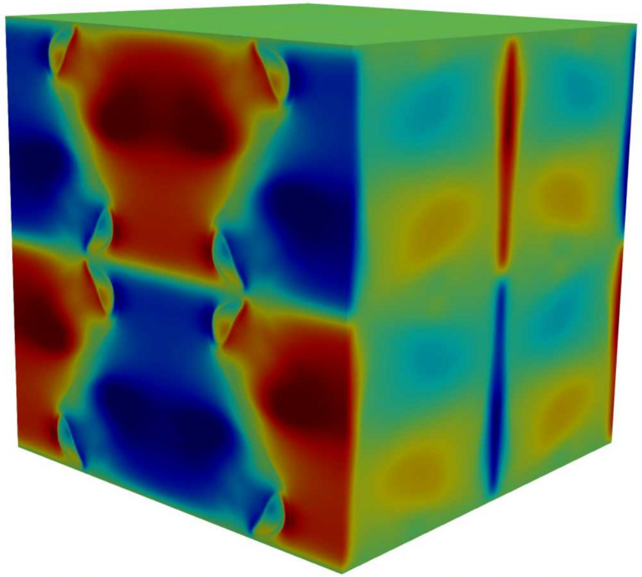


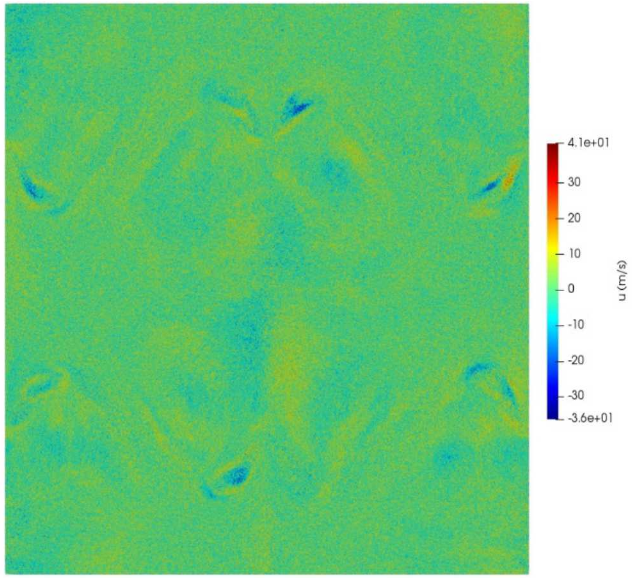


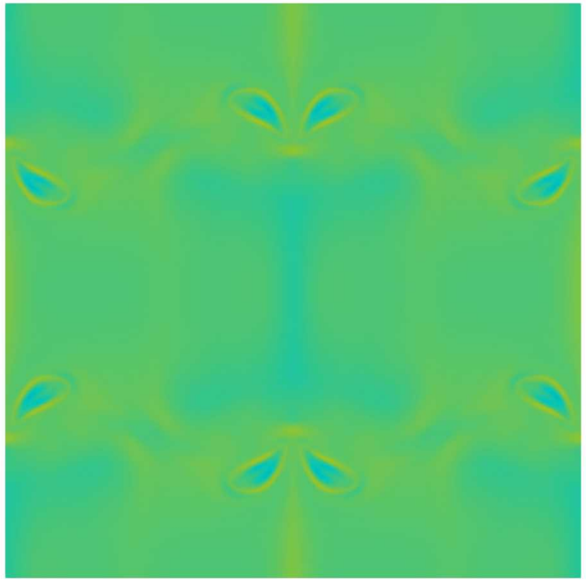


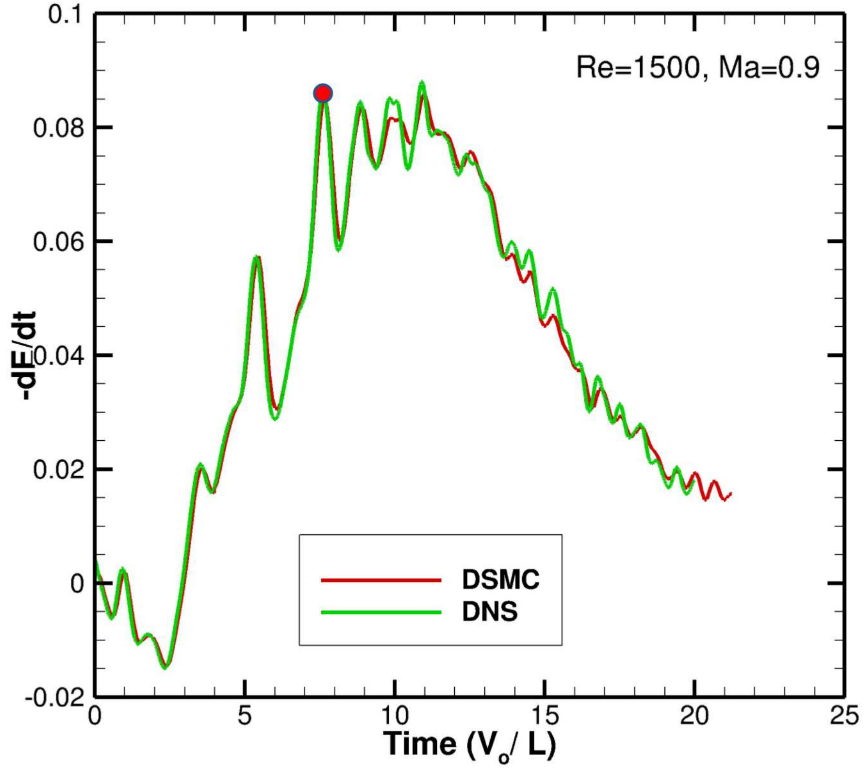
TG Ma=0.9,T=7.63


2.1e+02
150
100
50
0
-50
-100
-150
-2.1e+02
u (m/s)

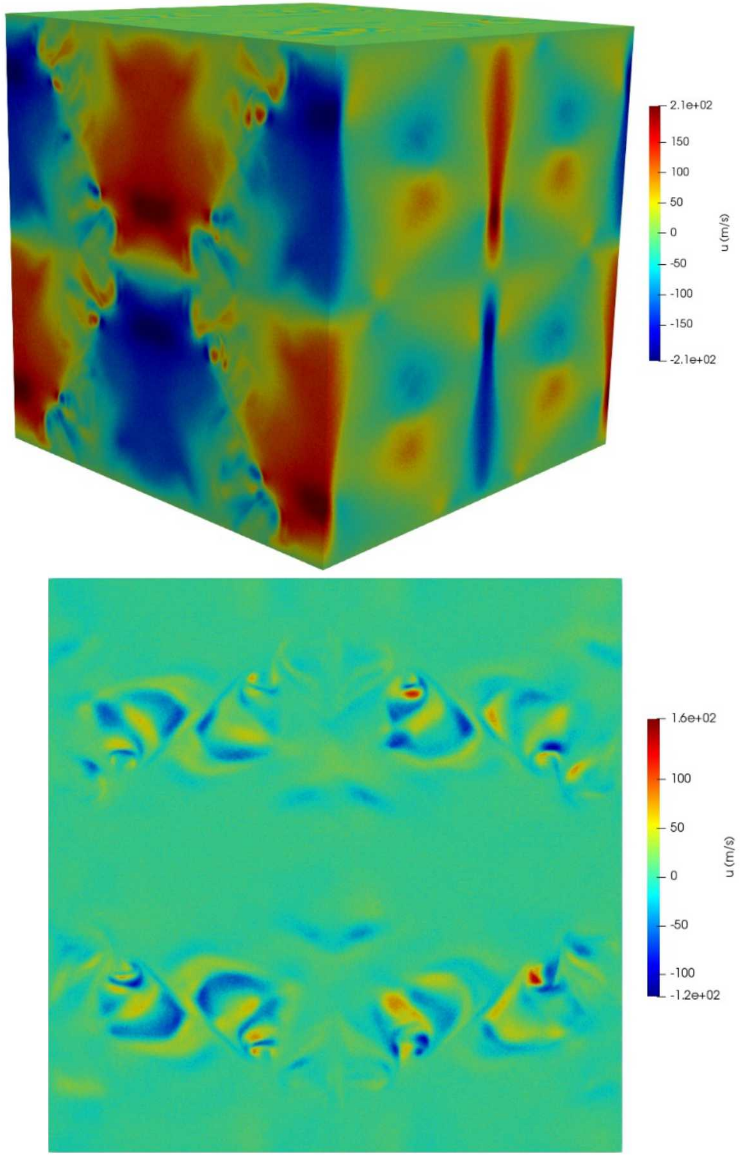


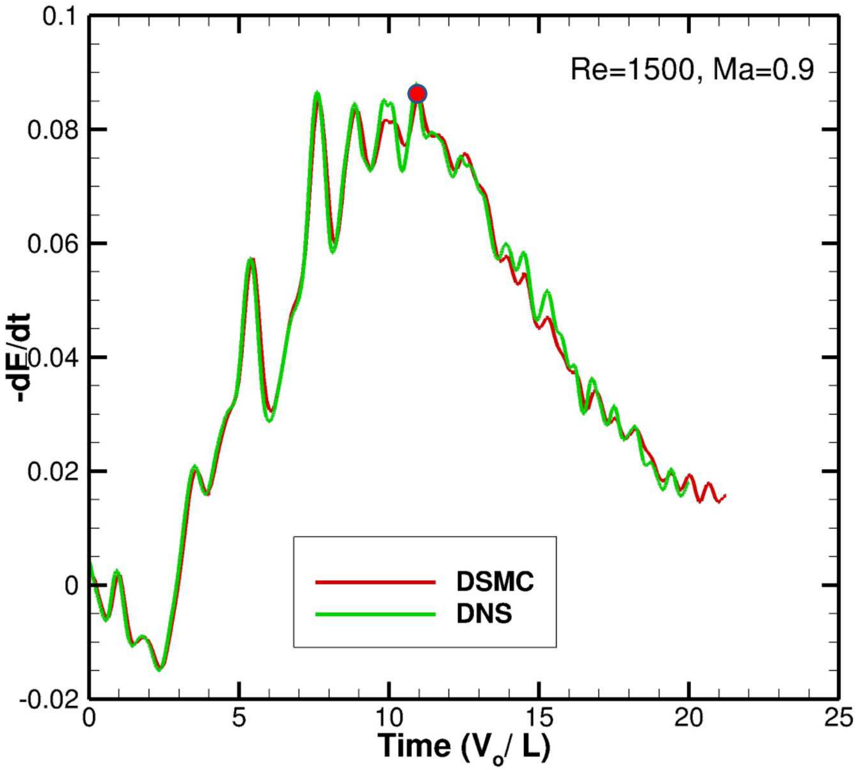

4.1e+01
30
20
10
0
-10
-20
-30
-3.6e+01
u (m/s)



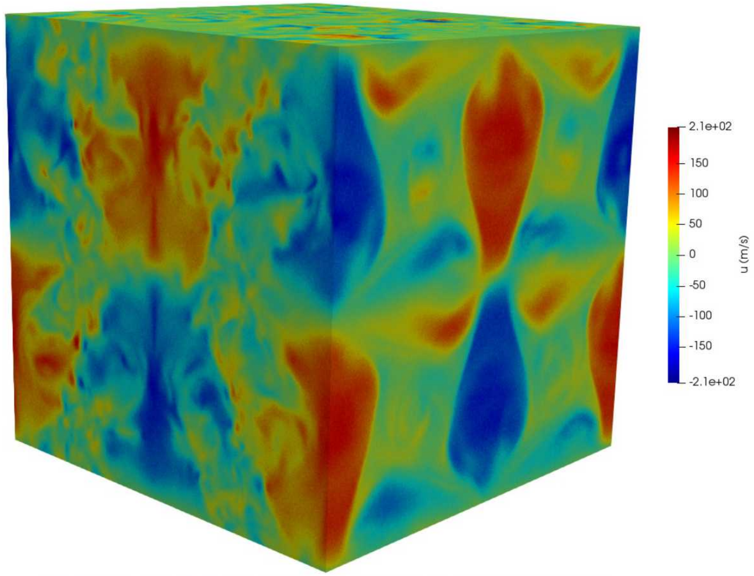

Re=1500, Ma=0.9
DSMC
DNS
-dE/dt
Time (V$_o$/ L)
0.1
0.08
0.06
0.04
0.02
0
-0.02
0
5
10
15
20
25

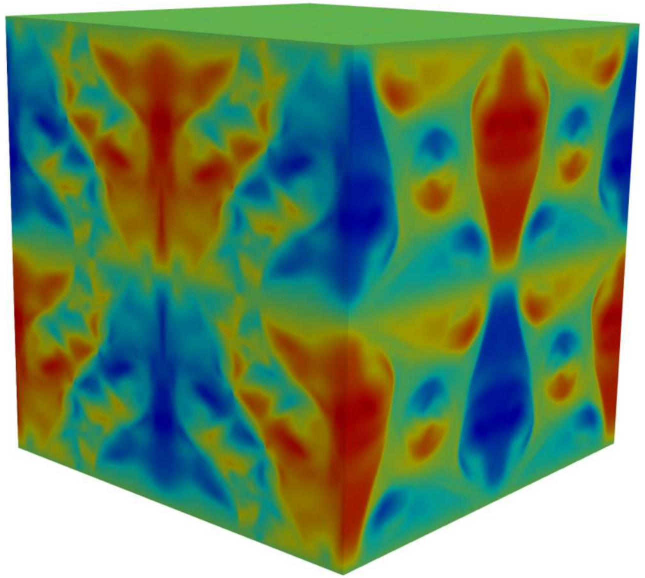
TG Ma=0.9, T=10.93

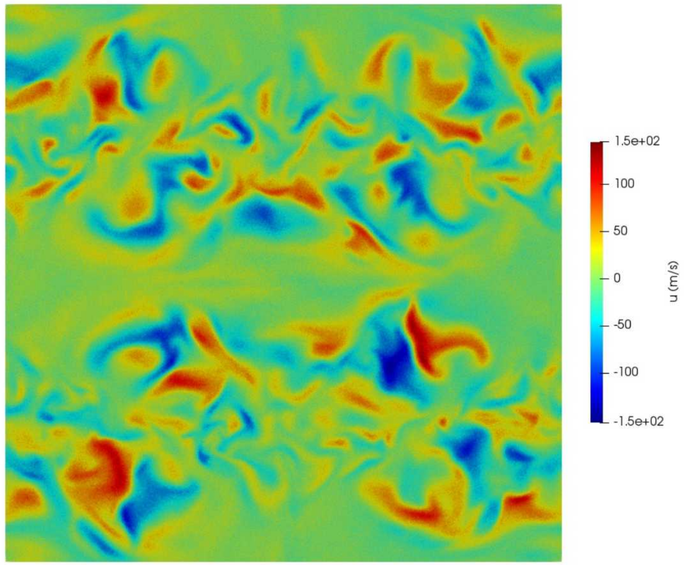


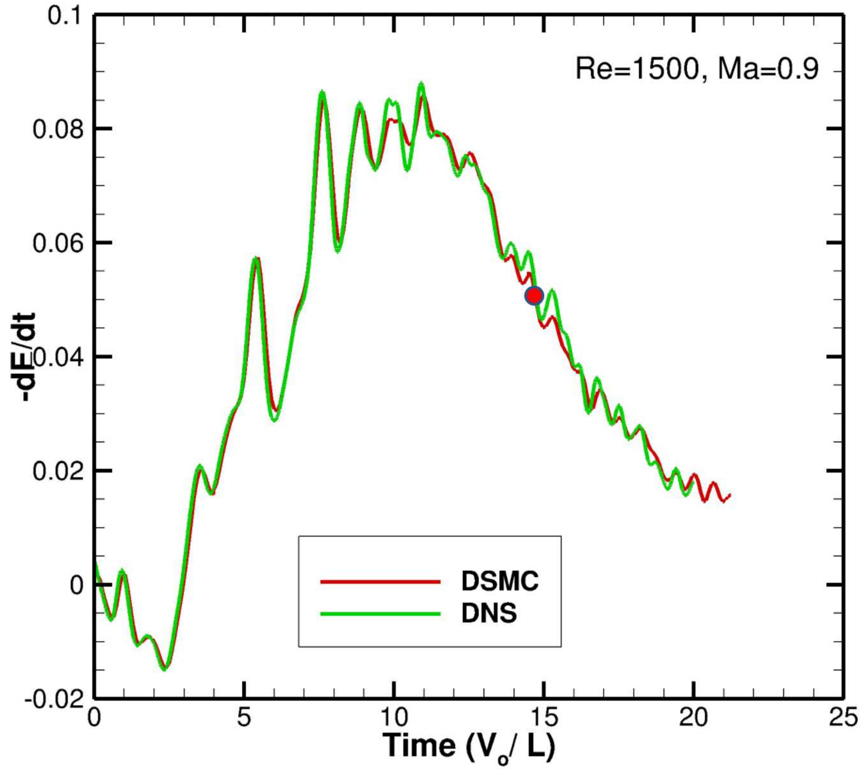


TG Ma=0.9, T=14.77

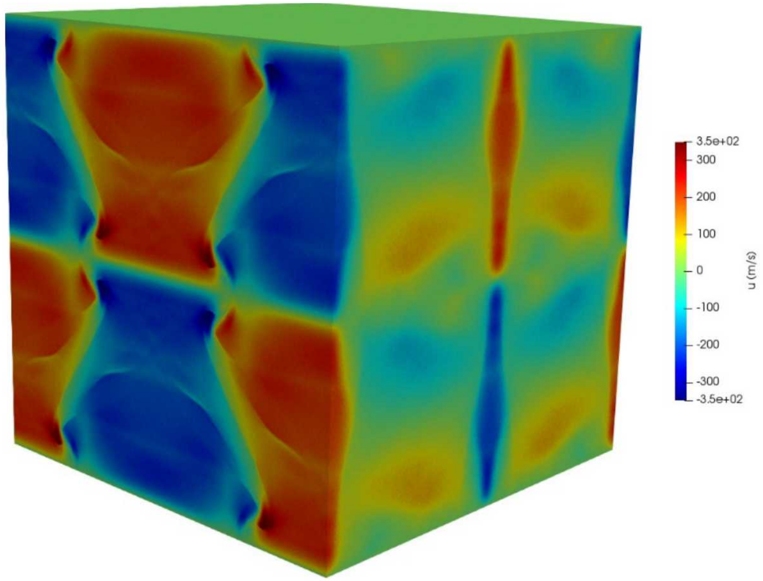




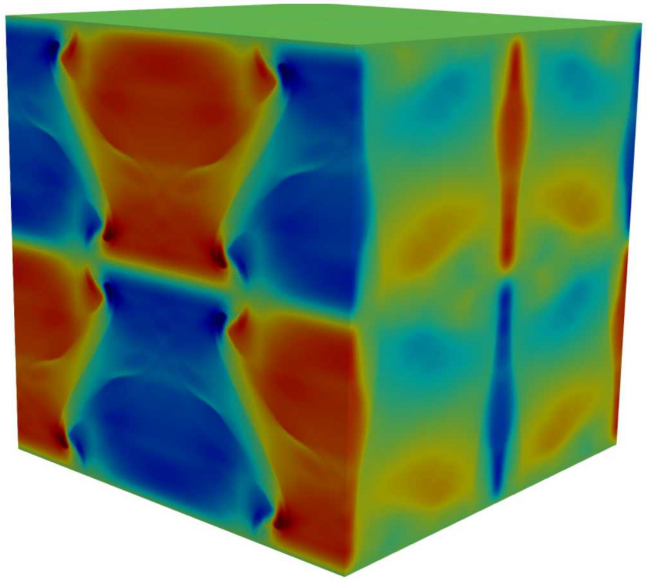


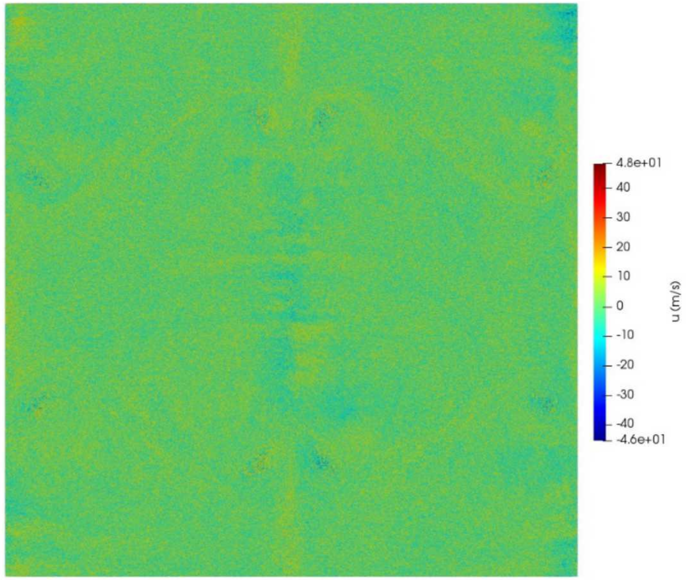


TG Ma=1.2, T=6.87

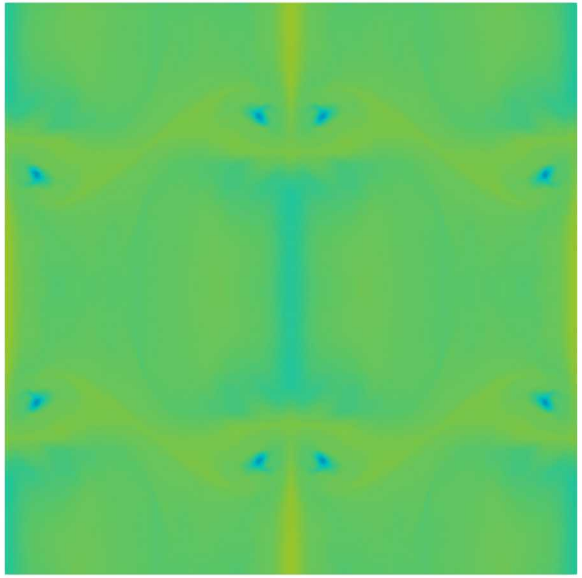


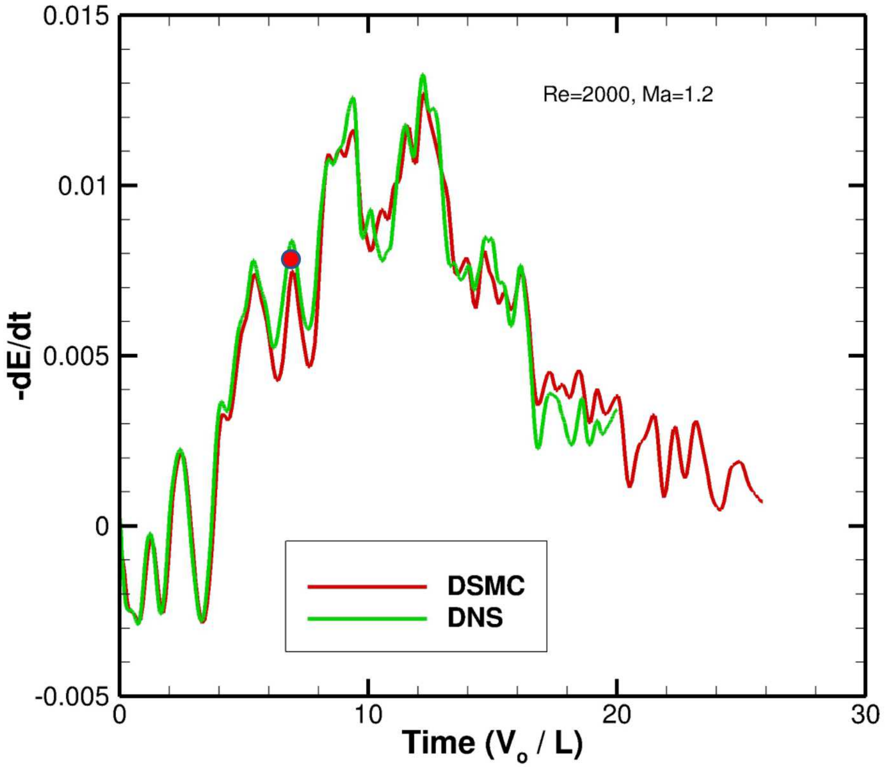
3.5e+02
300
200
100
0
-100
-200
-300
-3.5e+02
u (m/s)





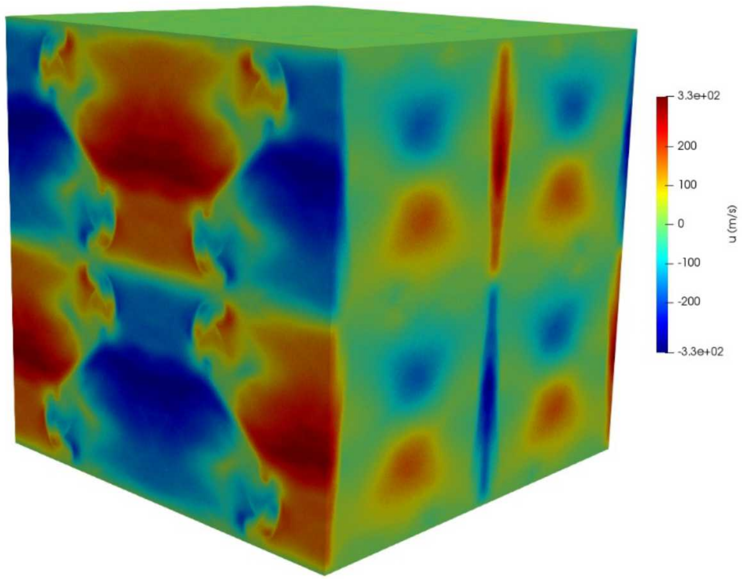
4.8e+01
40
30
20
10
0
-10
-20
-30
-40
-4.6e+01
u (m/s)

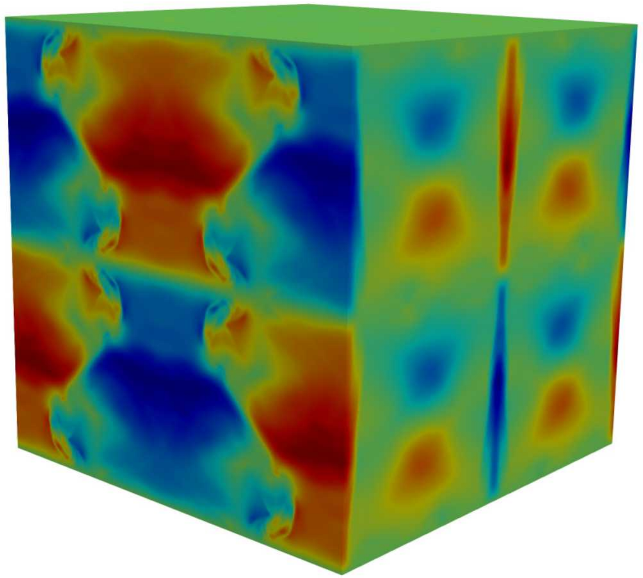


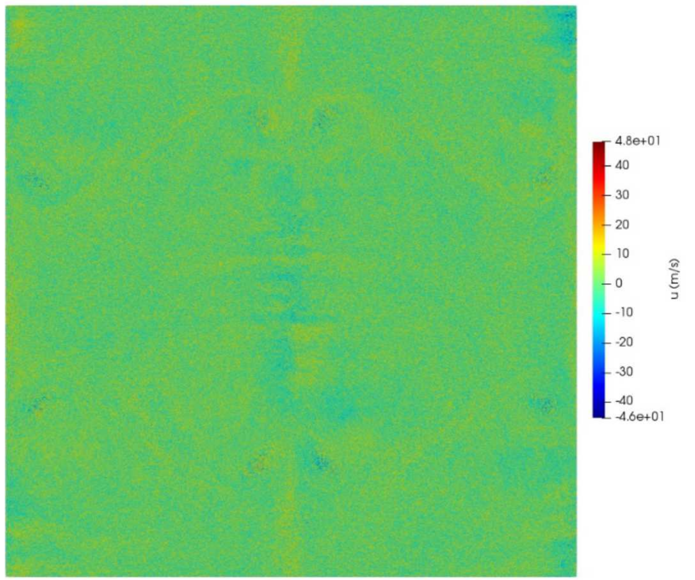


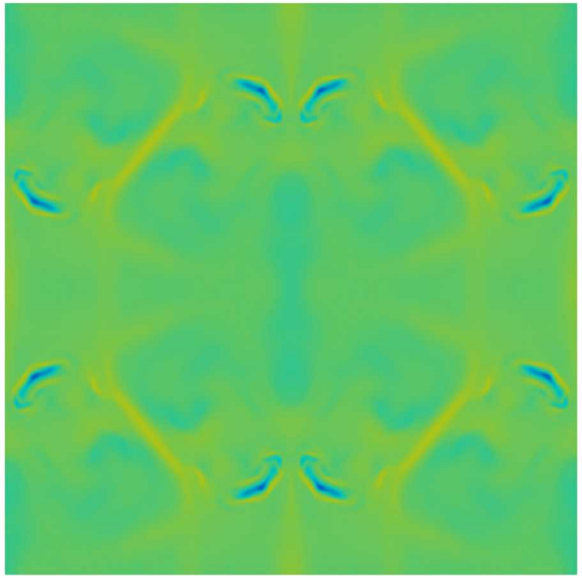
Re=2000, Ma=1.2
DSMC
DNS
-dE/dt
0.015
0.01
0.005
0
-0.005
0
10
20
30
Time (V_o / L)

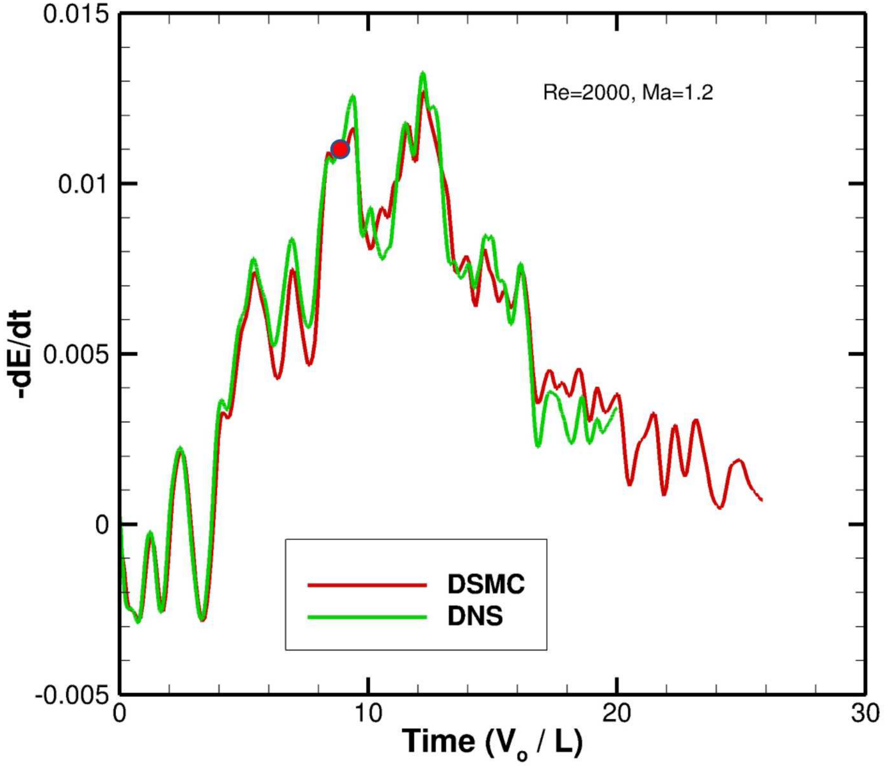
TG Ma=1.2, T=9.32


3.3e+02
200
100
0
-100
-200
-3.3e+02
u (m/s)

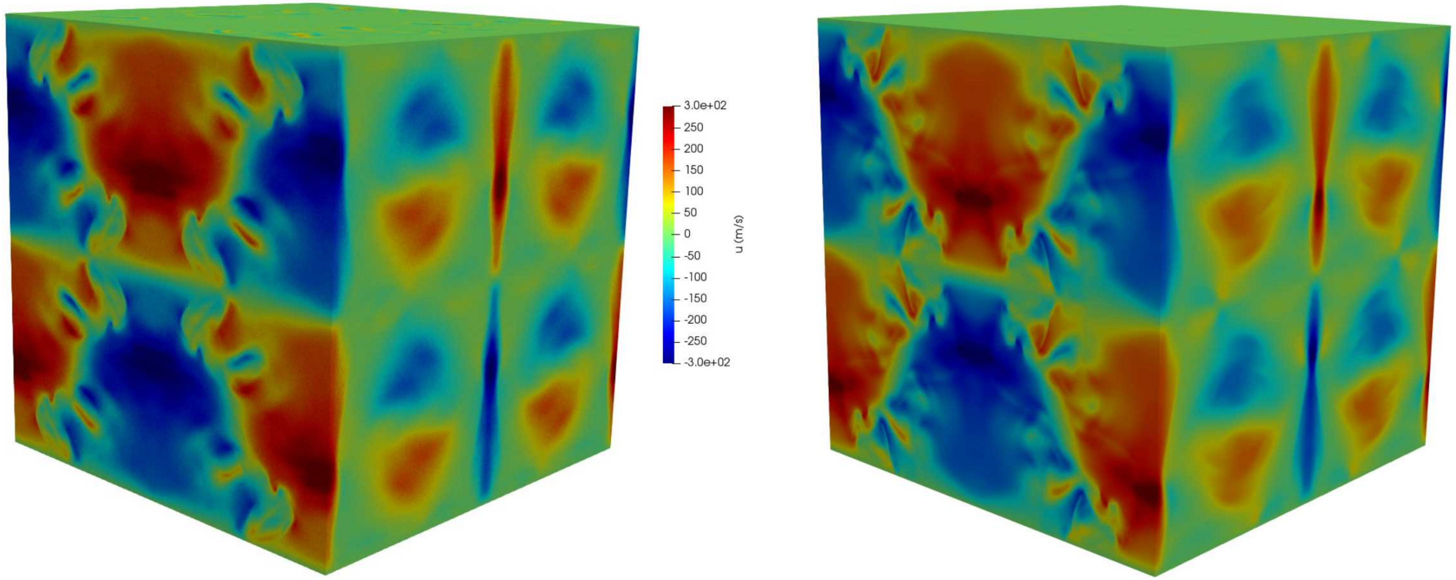


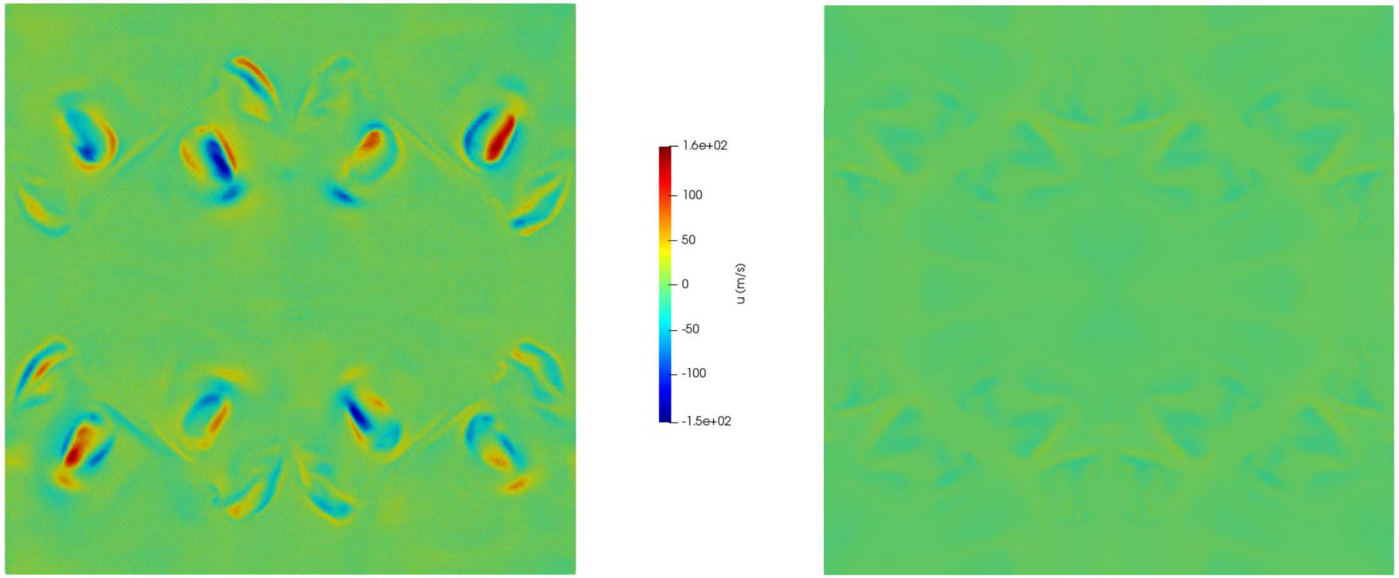

4.8e+01
40
30
20
10
0
-10
-20
-30
-40
-4.6e+01
u (m/s)

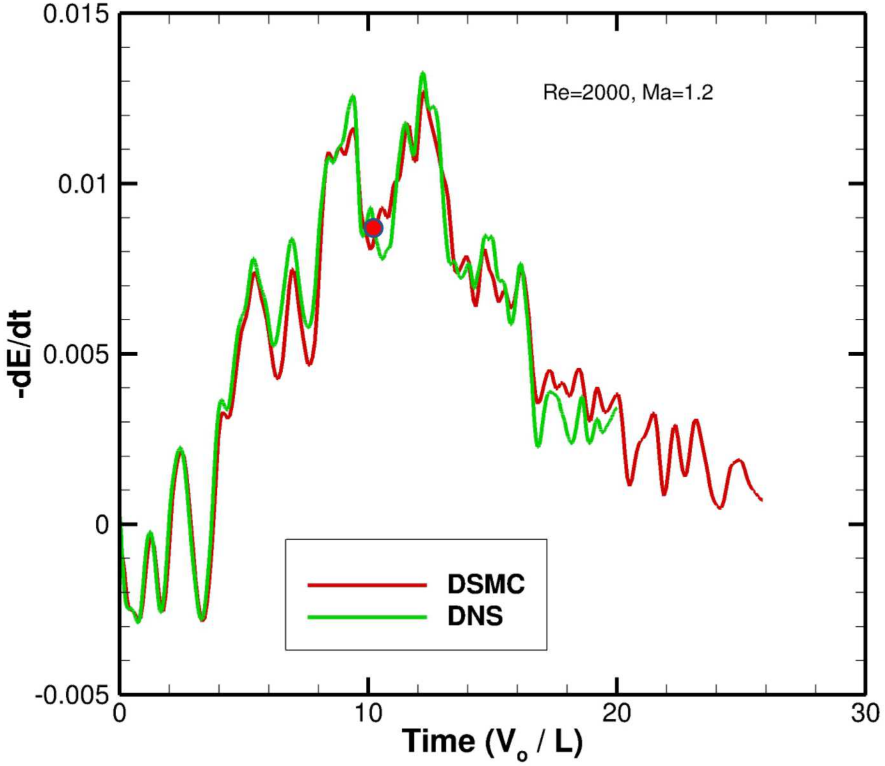



Re=2000, Ma=1.2
DSMC
DNS
-dE/dt
Time (V$_o$ / L)
0.015
0.01
0.005
0
-0.005
0
10
20
30

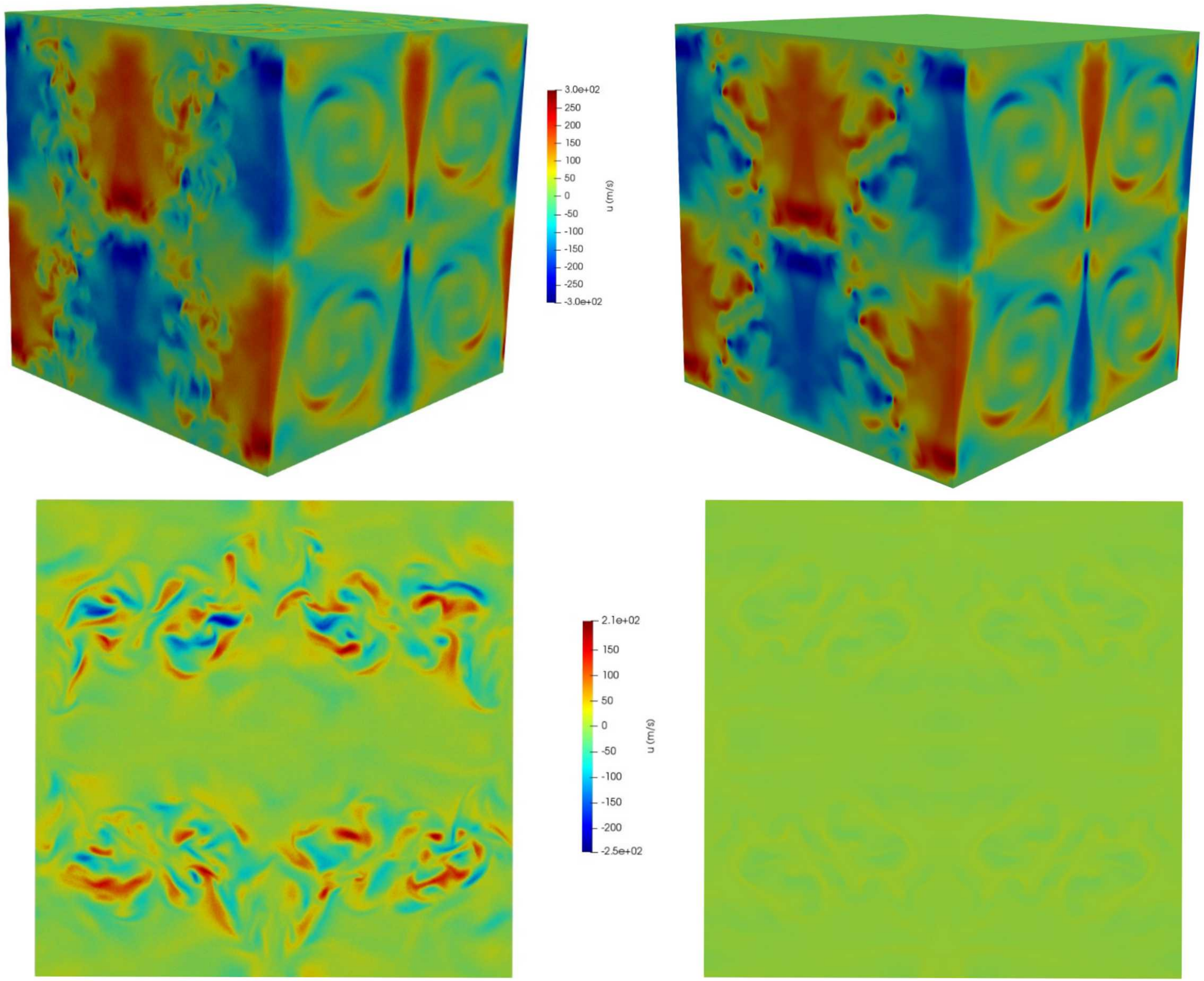
TG Ma=1.2, T=10.93

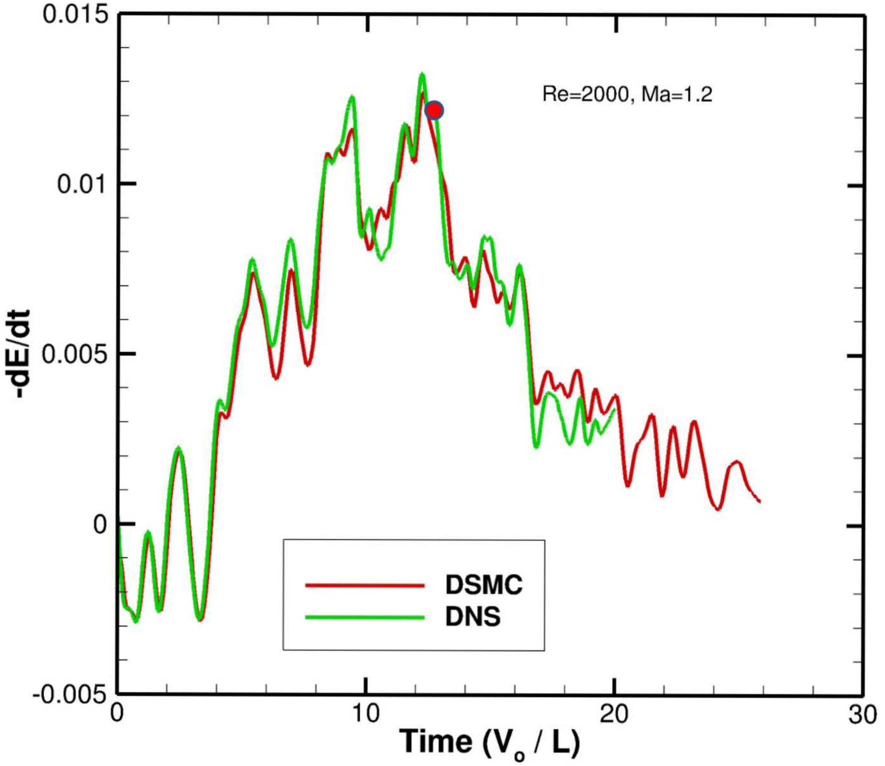




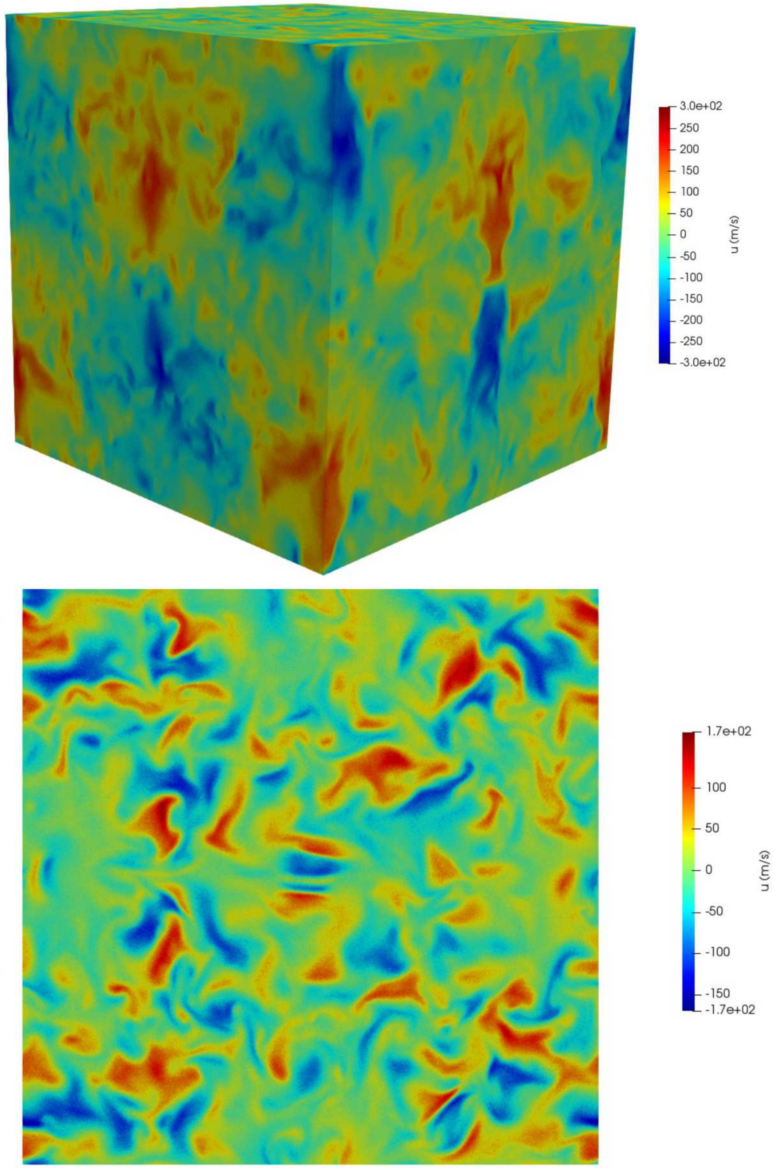


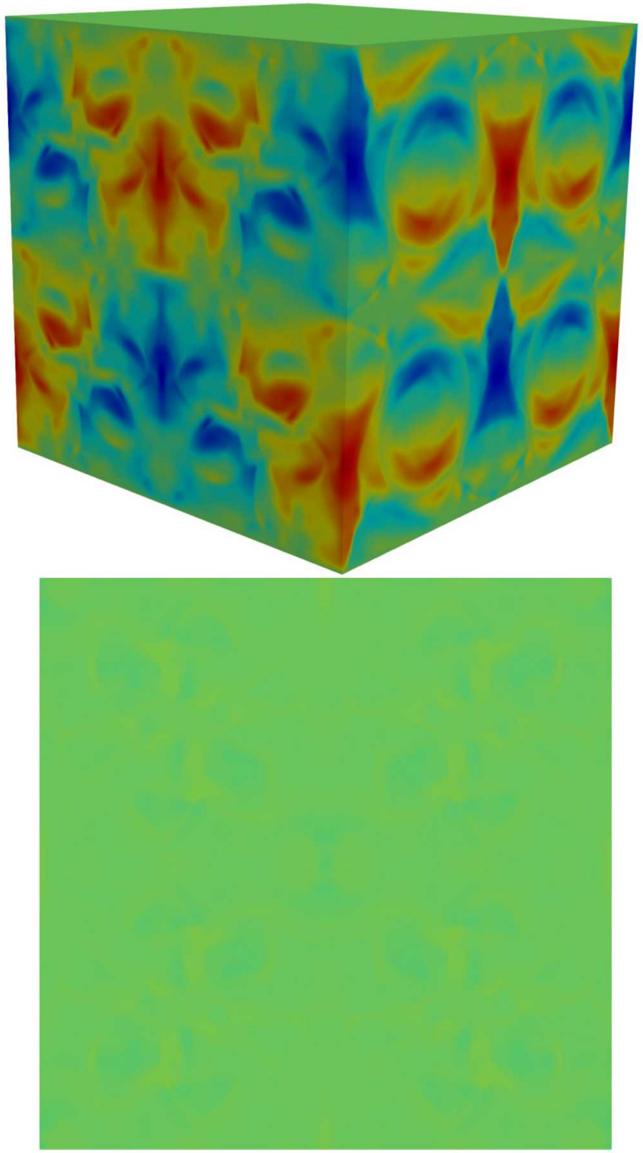
TG Ma=1.2, T=12.56

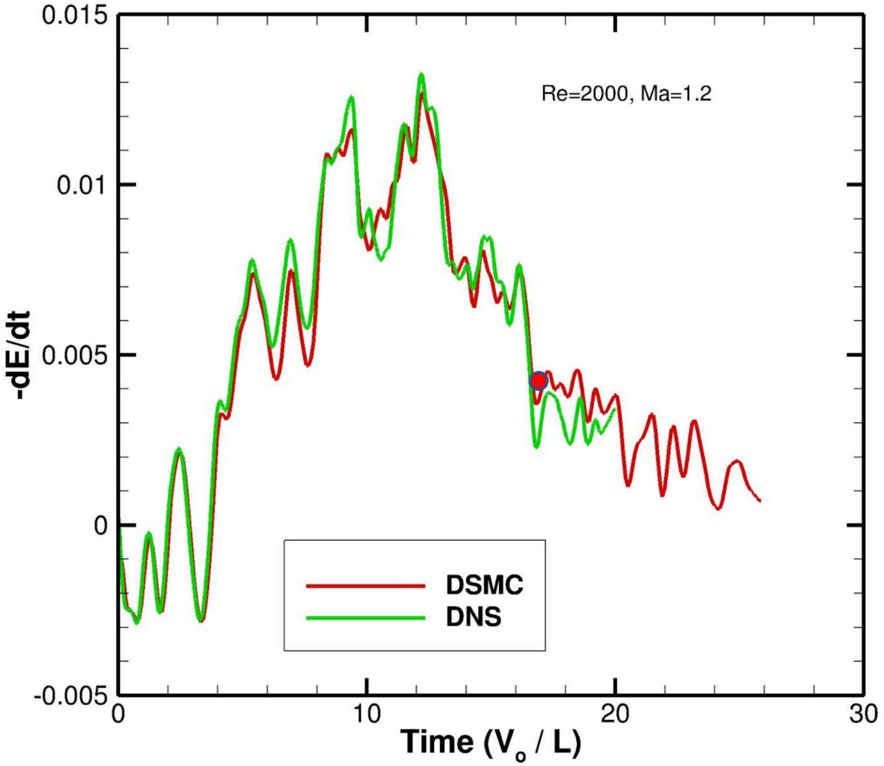




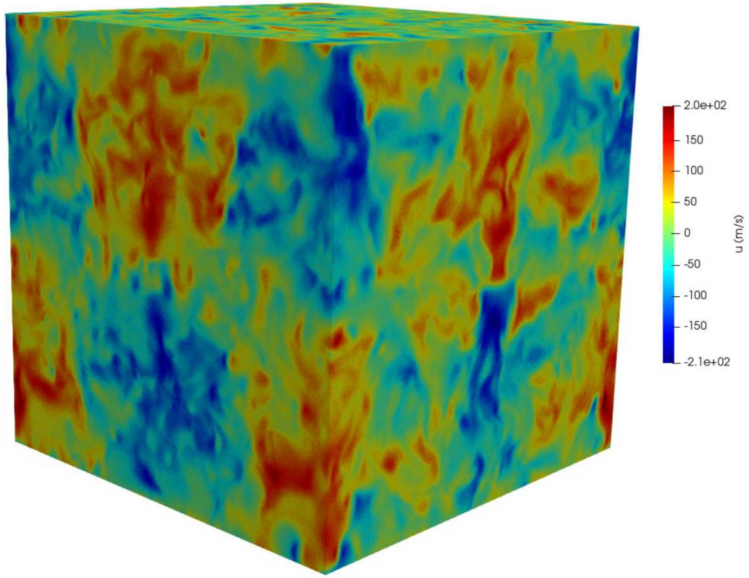
TG, Ma=1.2, T=17.09

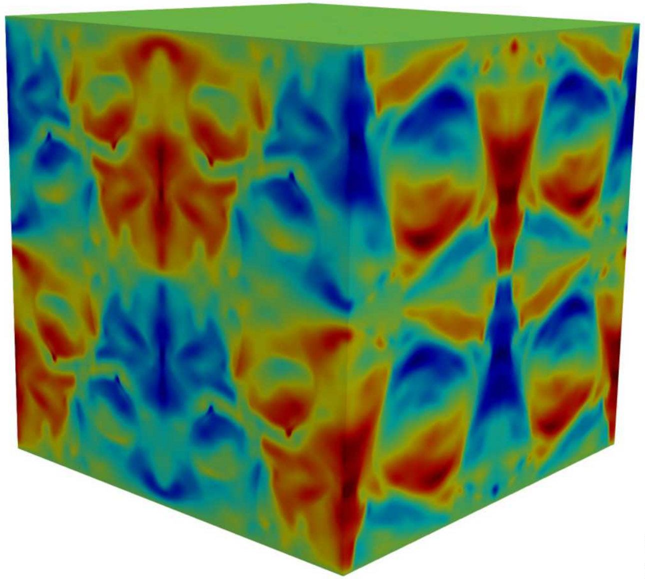


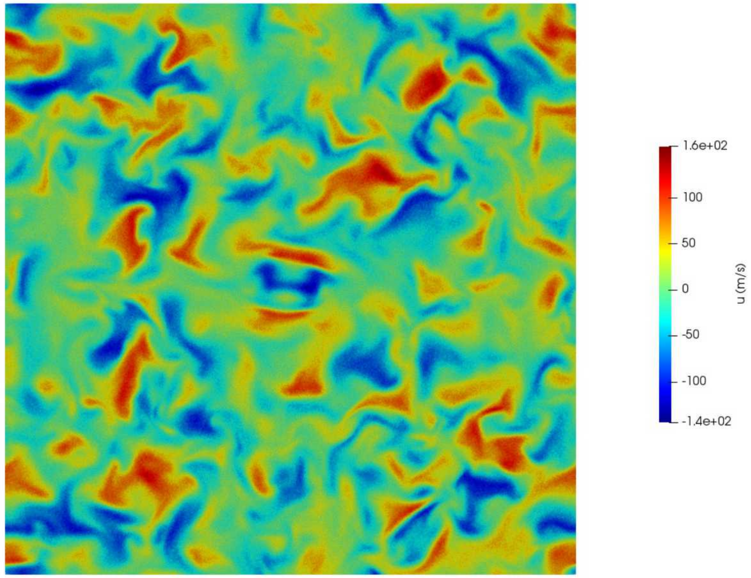


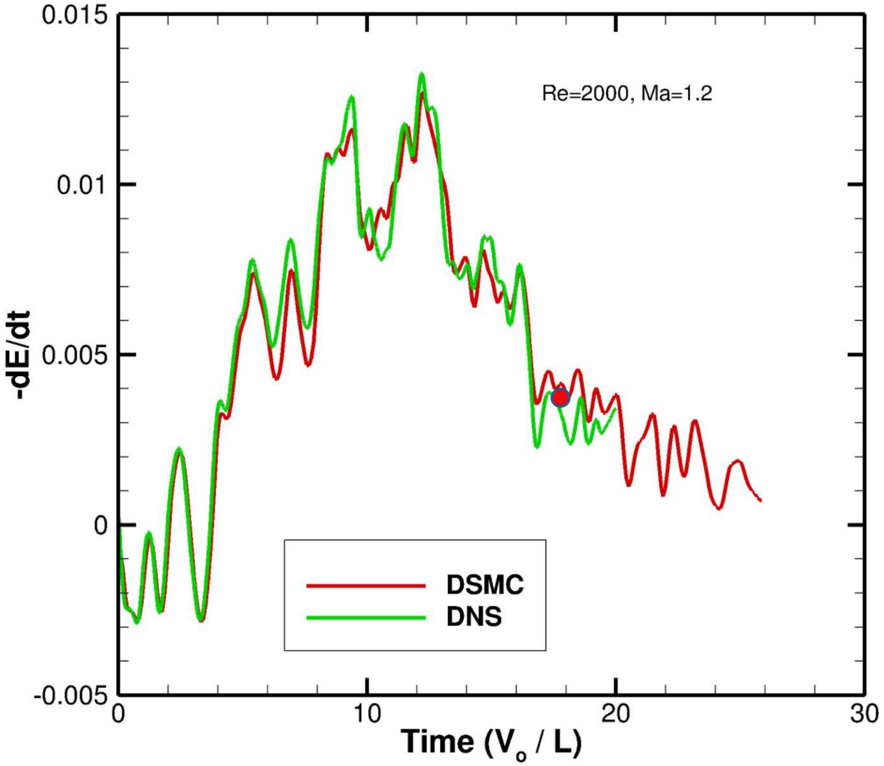


TG Ma=1.2, T=17.74

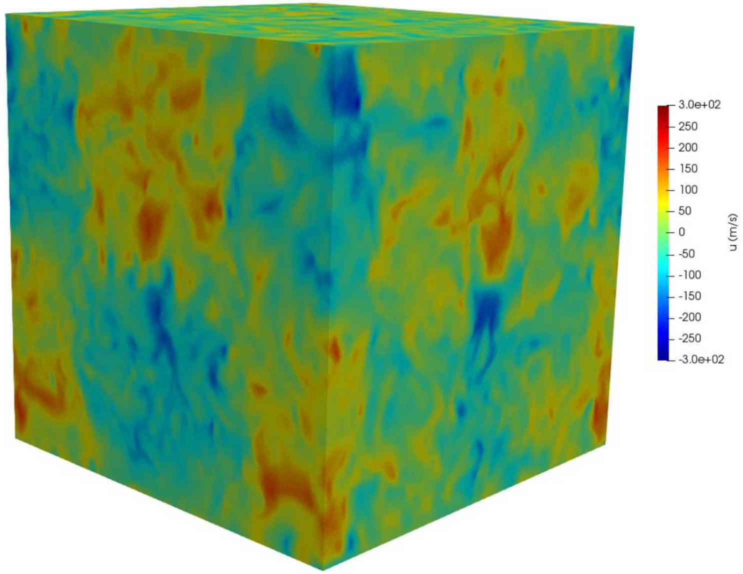


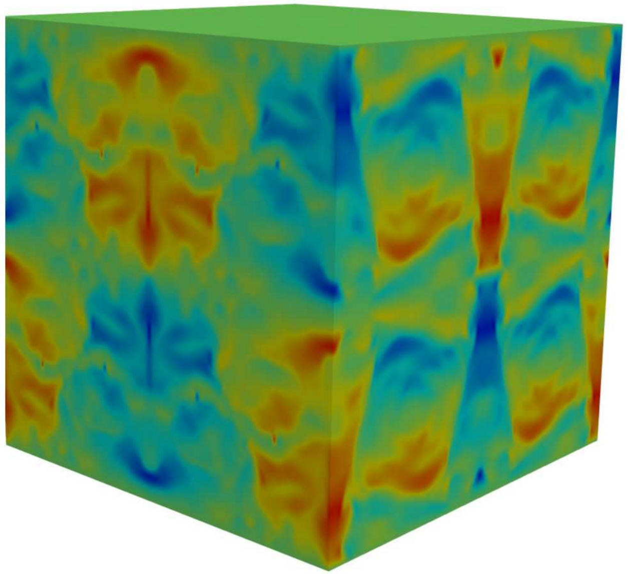


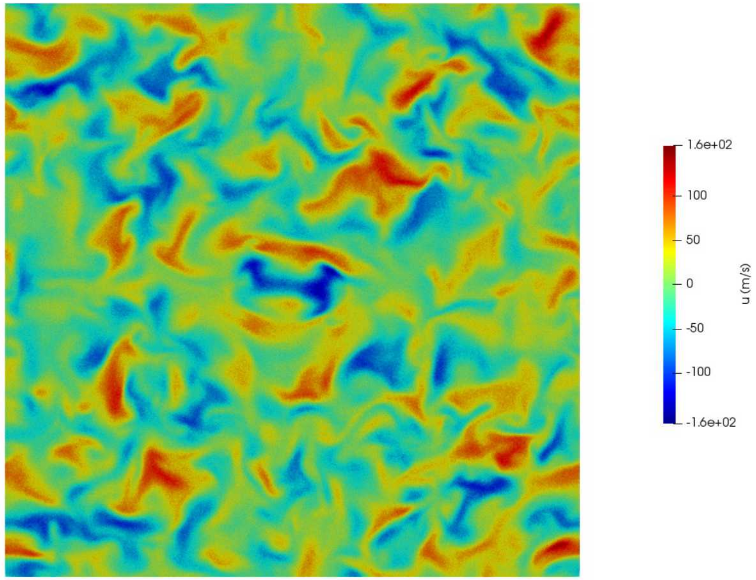


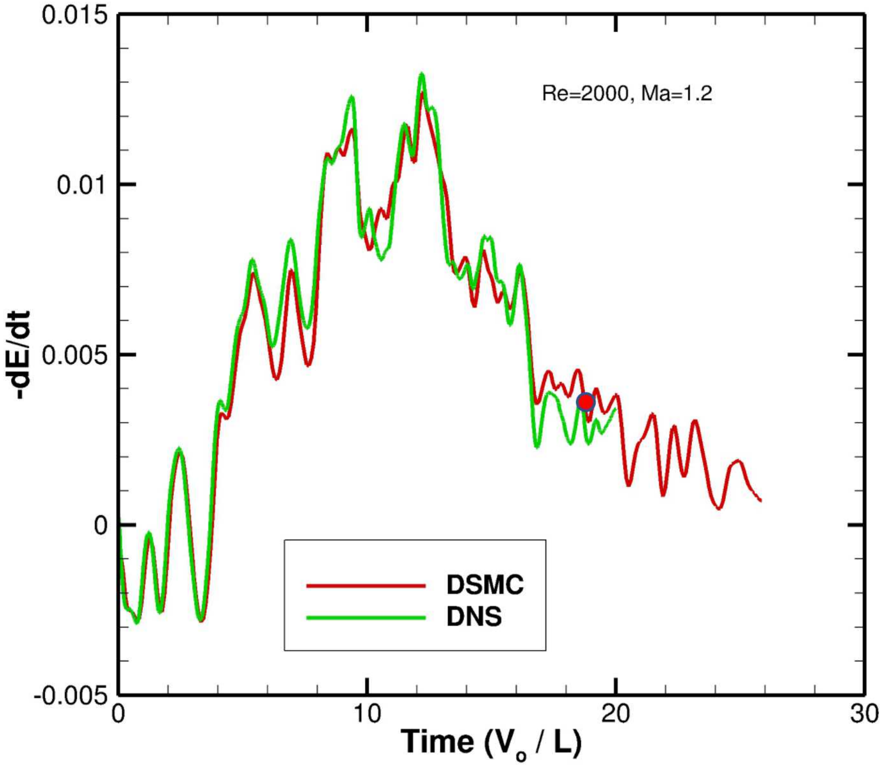


TG Ma=1.2, T=18.56



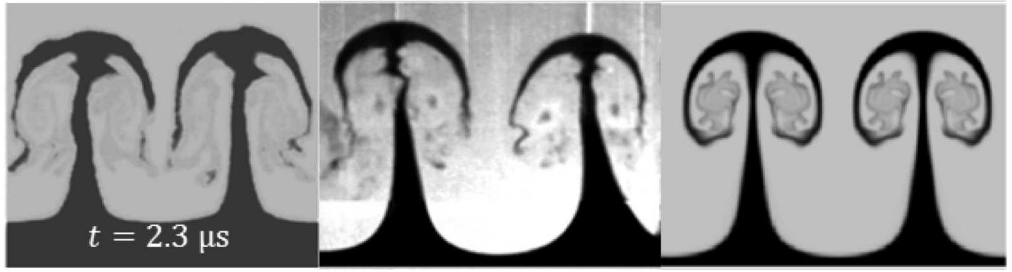






Conclusions

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



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

At low Mach numbers, DSMC and DNS produce the similar profiles.

At higher Mach numbers, shocks and shocklets in an apparently (?) baroclinic creation of vorticity introduce more structure to the DSMC flow field.

Spectral analysis of the velocity fields is necessary.