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Hydrodynamic energy flux in many-particle system

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In our everyday lives, turbulent processes are almost omnipresent, from the swirling of coffee to the behavior of air and the formation of the universe, all of which involve turbulent flows [1]. One of the primary reasons this problem is challenging is that it encompasses a vast range of scales, from the largest motion scales (energy-containing eddies) to the smallest scales (Kolmogorov scales), where viscous dissipation takes place. Capturing the interactions across these scales requires immense computational resources and sophisticated modeling techniques.

Although researchers have extensively studied hydrodynamic turbulence through various numerical approximations of the Navier-Stokes equations. However, at the molecular level, turbulent processes display intriguing properties such as thermalization, which are not captured by the Navier-Stokes equations due to their continuum approximation.

Molecular dynamics (MD) simulations provide an alternative approach to studying turbulent flows' microscopic and macroscopic features. It solves Newton's equation of motion for each particle and gives us the position and velocities of individual particles at desired times, hence capturing the physics at the particle level. As it inherently captures the effect of thermal fluctuations on the macroscopic dynamics of the flow, it is suitable for studying the turbulent velocity fluctuations at the particle level.

This talk will focus on thermalization in Lenard-Jones gas using two-dimensional Molecular Dynamics simulations. We studied the evolution of large-scale vortex in a noisy environment, as shown in Fig 1(a). The flow is similar to that of hydrodynamic flow. The energy in the form of coherent vortices gets converted into the thermal energy following an energy scaling of $E(k) \propto k^{-3}$, where k is the wavenumber associated with the system. This scaling is consistent with the two-dimensional decaying turbulence theory, as Kraichanin predicted.

We also found the thermalized scale, $E(k) \propto k$ where the energy of the modes is found to be in equilibrium. The same scale has also been observed in two-dimensional Euler turbulence, which lacks viscosity. With time, all the energy available in the form of coherent modes gets converted to thermal energy, resulting in the thermalization of the system where the energy scaling is found to be $E(k) \propto k$ across all the wavenumbers [2].

References

[1] Frish.U.(1995). *Turbulence, the legacy of A.N Kolmogorov,* Cambridge University Press
[2] Thermalization in Lennard Jones gas, **arXiv:2311.06713**

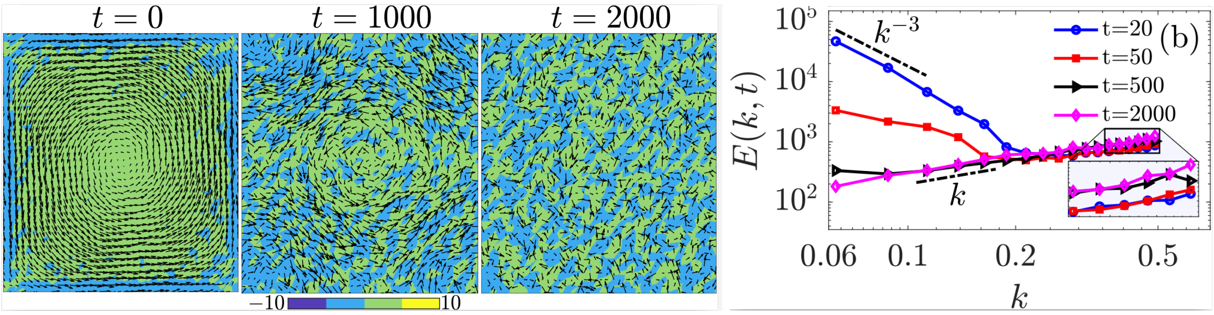

Figure 1: (L) velocity and vorticity field profiles represented by arrows and colors in our MD simulation. (R) The energy spectrum follows Kraichnain's theory at early time scales and thermalization scale at later times.