Molecular-Level Simulations of the Turbulent Taylor-Green Flow
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The Direct Simulation Monte Carlo (DSMC) method, a statistical, molecular-level 
technique that provides accurate solutions to the Boltzmann equation, is applied 
to the turbulent Taylor-Green vortex flow. The goal of this work is to investigate 
whether DSMC can accurately simulate energy decay in a turbulent flow. If so, 
then simulating turbulent flows at the molecular level can provide new insights be- 
cause the energy decay can be examined in detail from molecular to macroscopic 
length scales, thereby directly linking molecular relaxation processes to macroscopic 
transport processes. The DSMC simulations are performed on half a million cores 
of Sequoia, the 17 P
op platform at Lawrence Livermore National Laboratory, and 
the kinetic-energy dissipation rate and the energy spectrum are computed directly 
from the molecular velocities. The DSMC simulations are found to reproduce the 
Kolmogorov -5/3 law and to agree with corresponding Navier-Stokes simulations 
obtained using a spectral method. Sandia National Laboratories is a multimission 
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