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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 because 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 Pflop 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 laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

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