DIRECT NUMERICAL SIMULATIONS OF THE RELATIVE MOTION OF HIGH-INERTIA PARTICLES IN ISOTROPIC TURBULENCE

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EXECUTIVE SUMMARY

The overall goal of our research is to investigate the role of turbulence in driving the relative velocities and relative positions of inertial particles in isotropic turbulence. During the second year of the PRAC grant, we hypothesized that the deterministic forcing used in the Direct Numerical Simulations (DNS) to achieve stationarity had the effect of artificially increasing the temporal coherence of eddies as the Reynolds number increased. This artifact, we surmised, would lead to higher Eulerian two-time correlations, and, thereby, diffusivities, particularly at large separations. In the third year, we investigated the effects of forcing on the Eulerian two-time correlations of fluid relative velocities in DNS of isotropic turbulence. Accordingly, we performed DNS of homogeneous, isotropic turbulence containing disperse but fixed particles for two grid sizes—128^3 and 512^3—while employing two forcing schemes, one deterministic and the other stochastic. The high-performance computing resources of the Blue Waters system were indispensable in performing the DNS runs needed to validate the hypothesis.

RESEARCH CHALLENGE

Turbulence-driven relative motion of high-inertia particles is relevant in astrophysical scenarios such as the interstellar medium, protoplanetary disks, and the atmospheres of planets and dwarf stars. Specifically, the "sticking" of dust particles in protoplanetary disks is believed to be the mechanism for planetesimal formation. An intriguing question that astrophysicists are investigating concerns the effects of turbulence on the dispersion, sedimentation, collisional coalescence, and fragmentation of dust grains. The viscous relaxation times, τ_v, of these particles are significantly large, with estimated $St_\eta \sim 10–100$, where $St_\eta = \tau_v/\tau_\eta$ is the Stokes number based on the Kolmogorov time scale τ_η.

The two principal quantities describing the relative motion of inertial particles in a turbulent flow are: (1) radial distribution function (RDF), which is a measure of the spatial clustering of particles; and (2) probability density function (PDF) of pair relative velocities, which is a key input to the particle-pair encounter rate. The RDF and the relative velocity PDF are both key inputs to the particle collision kernel, and depend sensitively on the Stokes number St_η.

Recently, we developed a stochastic theory for the relative velocities and positions of high-inertia pairs in forced isotropic turbulence [1]. The theory involved deriving a closure for the diffusivity tensor characterizing the relative-velocity-space diffusion current in the PDF kinetic equation of particle-pair separation and relative velocity. Since we had considered the $St_l >> 1$ limit, the pair PDF equation is of the Fokker–Planck form (St_l is the Stokes number based on the integral timescale of turbulence). Using the diffusivity formulation, one can perform Langevin simulations of pair relative velocities and positions, which is equivalent to simulating the Fokker–Planck equation.

In this context, we surmised that the forcing artificially increased the temporal coherence of the large-scale eddies, particularly as Re_λ was increased. The increased coherence led to higher magnitudes of the two-time correlations of fluid relative velocities (and thereby diffusivities) at separations that scaled with the integral length scale. The third-year study was motivated by the desire to quantitatively investigate the above hypothesis. Accordingly, we performed direct numerical simulations of forced isotropic turbulence laden with disperse but fixed particles. Two types of forcing were used to achieve statistical stationarity in the DNS runs.

METHODS & CODES

We performed DNS of forced isotropic turbulence using a discrete Fourier-expansion-based pseudospectral method. Simulations were performed over a cubic domain of length 2π discretized using N^3 grid points, with periodic boundary conditions in all three directions. The fluid velocity was advanced in time by solving the Navier–Stokes equations in rotational form as well as the continuity equation for an incompressible fluid. Direct evaluation of the nonlinear convective terms in the Navier–Stokes equations is extremely computationally intensive. Hence, we adopted a pseudospectral approach wherein the nonlinear terms were first computed in physical space and then transformed into the spectral space. We used the P3DFFT library [2] to carry out the transforms between physical and spectral spaces.

RESULTS & IMPACT

In Fig. 1, we present the longitudinal component of the Eulerian two-time correlation of fluid relative velocities, i.e., $\langle \Delta u(r,x,0)\ \Delta u(r,x,\tau)\rangle_{||}$, as a function of dimensionless time separation $\tau^* = \tau u_{rms}/L$ for $Re_\lambda = 210$. We compared the correlations obtained from the DF and SF1–SF5 simulations compared at four dimensionless separations, r/L = 0.56, 1.12, 2.24 and 3.36, where L is the integral length scale and u_{rms} is the RMS fluctuating velocity. It is clear that at all four separations, the DF longitudinal correlation is higher than the SF1–SF5 correlations (except at small τ^*). At the three separations greater than L, we see that the DF correlation is significantly greater than the SF correlations.

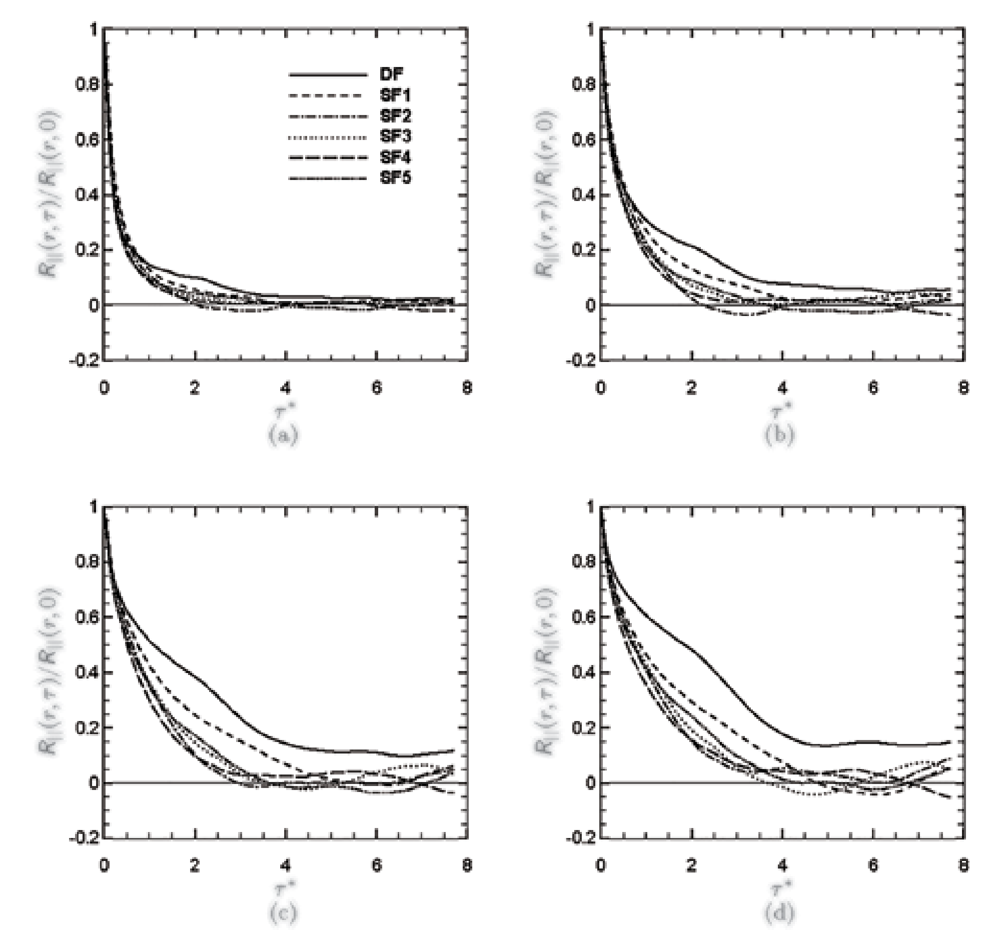

Figure 1: Longitudinal correlation $R_{||}(r,\tau)=\langle \Delta u(r,x,0)\ \ \Delta u(r,x,\tau)\rangle_{||}$ as a function of dimensionless time separation $\tau^* = \tau u_{rms}/L$ for $Re_\lambda = 210$ at four dimensionless separations: (a) r/L = 0.56, (b) r/L = 1.12, (c) r/L = 2.24, and (d) r/L = 3.36. DF stands for deterministic forcing and SF for stochastic forcing.

WHY BLUE WATERS

Direct Numerical Simulations are the most accurate numerical approach to resolve all the temporal and length scales in a turbulent flow. However, DNS of particle-laden turbulent flows are computationally intensive, since in DNS the cost of a simulation scales as Re3, where Re is the Reynolds number. The overall computational objective of this project is to simulate particle-laden isotropic turbulence at Taylor microscale Reynolds number $Re_\lambda \sim 600$ with grid sizes ~ $2{,}048^3$. This requires running our code on tens of thousands of cores. Also, each DNS run generates several terabytes of data. Due to these CPU time and storage requirements, the Blue Waters supercomputer is the ideal platform to achieve our objective. Further, Blue Waters proved to be an invaluable resource in computing key inputs to our stochastic theory. For instance, the theory requires as an input the two-time Eulerian correlations of fluid relative velocities seen by particle pairs. Evaluation of the two-time correlation for nearly half a trillion pairs is a highly computationally intensive process. We were only able to compute this quantity because of access to Blue Waters, where we ran the code on 20,000 cores.

PUBLICATIONS & DATA SETS

Dhariwal, R., S.L. Rani, and D.L. Koch, Stochastic Theory and Direct Numerical Simulations of the Relative Motion of High-Inertia Particle Pairs in Isotropic Turbulence. *Journal of Fluid Mechanics*, 813 (2017), pp. 205–249.

Dhariwal, R., S.L. Rani, and D.L. Koch, Effects of Deterministic and Stochastic Forcing Schemes on Inertial Particle Statistics in DNS of Isotropic Turbulence. *American Physical Society 69th Annual Meeting of the Division of Fluid Dynamics* (November 20–22, 2016, Portland, Ore.).

Rani, S.L., R. Dhariwal, and D.L. Koch, Comparison of Stochastic Theory and DNS for the Relative Motion of High-Inertia Particle Pairs in Isotropic Turbulence. *American Physical Society 69th Annual Meeting of the Division of Fluid Dynamics* (November 20–22, 2016, Portland, Ore.).