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

Allocation: NSF PRAC/3,870 Knh
PI: Sarma L. Rani[1]
Collaborator: Rohit Dhariwal[1]

[1]University of Alabama in Huntsville

EXECUTIVE SUMMARY

The overall objective of our research is to investigate the role of turbulence in driving the relative velocities and positions of inertial particles in isotropic turbulence. During the second year of this PRAC grant, we investigated the relative motion of high-inertia particle pairs in isotropic turbulence. We performed direct numerical simulations (DNS), as well as Langevin simulations (LS) based on a probability density function (PDF) kinetic model for pair relative motion. We developed a stochastic theory that involved deriving closures in the limit of high Stokes numbers for the diffusivity tensor in the PDF equation for particle pairs. Quantitative analysis of the stochastic theory was performed through a comparison of the particle pair statistics obtained using LS with those from DNS. The high-performance computing (HPC) resources of the Blue Waters system were invaluable and indispensable in performing the DNS and LS runs needed to validate the stochastic theory.

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) 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 time scale 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, the current study has two main objectives. First, we perform a quantitative analysis of the three forms of the diffusivity derived in [1]. The second objective is to compute the relative motion statistics of particle pairs using both DNS and LS, and compare the corresponding results.

METHODS & CODES

DNS of forced isotropic turbulence were performed 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 is 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, a pseudospectral approach is adopted wherein the nonlinear terms are first computed in physical space and then transformed into the spectral space. The P3DFFT library [2] is used to carry out the transforms between physical and spectral spaces.

RESULTS & IMPACT

The RDF is a well-established measure of particle clustering. In fig. 1, the RDF is presented as a function of St_η at four separations r/η = 6, 12, 18, and 24 (η is the Kolmogorov length scale). The results from LS are compared with the data from the DNS performed in the current study, the Février, et al. [3] DNS, and also with the results from the Zaichik and Alipchenkov [4] theory. The Février, et al. [3] data were for Re_λ = 69, while the current DNS data are for Re_λ = 76. There is excellent agreement between the LS RDF and the two sets of DNS RDFs at all four separations, particularly for St_η > 10. The Zaichik and Alipchenkov [4] theory significantly overpredicts the RDFs for high Stokes numbers at all separations. The current DNS study, as well as the stochastic theory, provided the basis for the first-ever investigation of the validity of the Zaichik and Alipchenkov [4] theory in the high-Stokes-number limit.

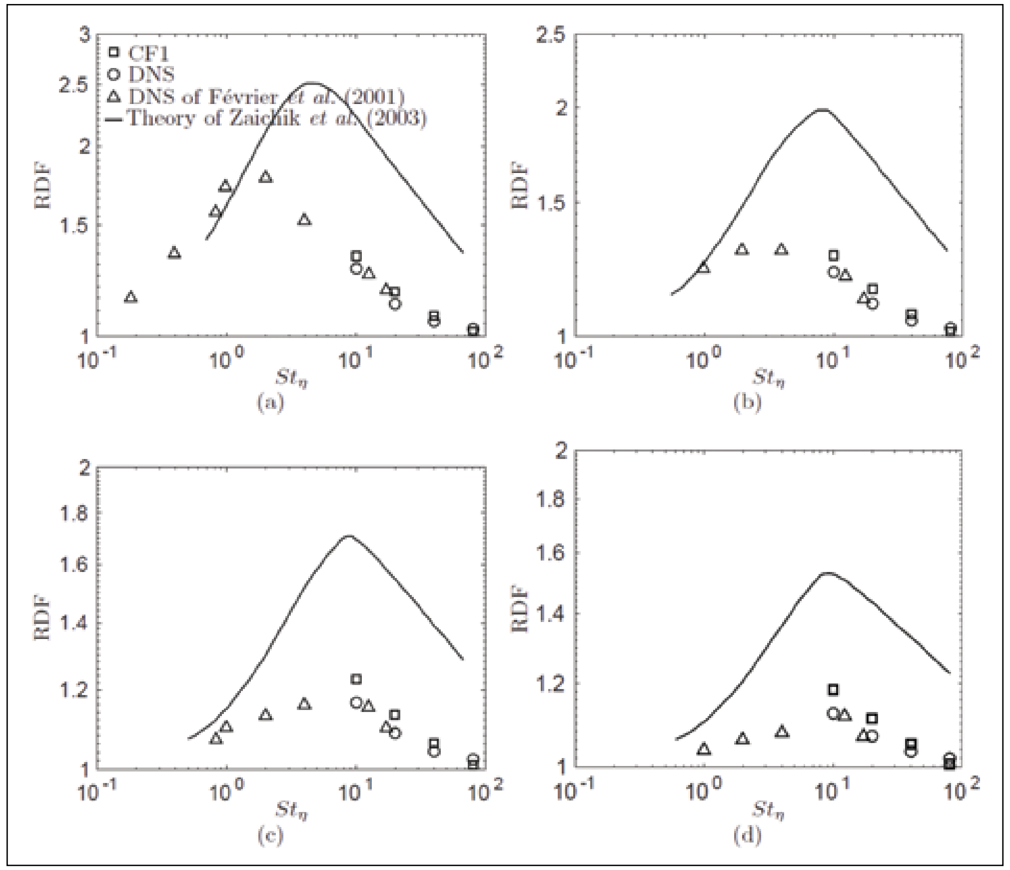

Figure 1: Radial distribution function as a function of St_η. (a) r/η = 6, (b) r/η = 18. Squares and circles represent CF1 (current stochastic theory) and current DNS at Re_λ = 76; triangles represent DNS at Re_λ = 69 from [3]. Solid line represents data from [4] for Re_λ = 69.

WHY BLUE WATERS

Direct numerical simulation is 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 very 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 micro-scale Reynolds number $Re_\lambda \sim 600$ with grid sizes ~ 2048^3. This will require running our code on tens of thousands of cores. Also, each DNS run is expected to generate several terabytes of data. Due to these central processing unit time and storage requirements, the Blue Waters supercomputer is the ideal platform to achieve our objective. It would be relevant to mention that during the last year, 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 the Blue Waters access, where we ran the code on 625 nodes using 20,000 cores.

PUBLICATIONS AND 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. *69th Annual Meeting of the Division of Fluid Dynamics* (American Physical Society, Portland, Ore., November 20–22, 2016).

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. *69th Annual Meeting of the Division of Fluid Dynamics* (American Physical Society, Portland, Ore., November 20–22, 2016).