Massively parallel simulations of inertial particles in high-Reynolds-number turbulence

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Abstract: We present particle clustering and relative velocity statistics in high-Reynolds-number turbulence obtained from direct numerical simulation (DNS). Our DNS code uses two-dimensional domain decomposition for large-scale parallelization on thousands of processors and is capable of efficiently simulating inertial particle and passive scalar transport in isotropic turbulence and homogeneous turbulent shear flow. In addition to providing valuable physical insight, the DNS is used to improve experimental measurements of particle trajectories by our collaborators. From these particle statistics, we can compute the particle collision rate, and hence better predict the evolution of the droplet size distribution in particle-laden flows such as clouds.

Keywords: Computational Fluid Dynamics, Direct Numerical Simulation, Inertial Particles, Isotropic Turbulence, Homogeneous Turbulent Shear Flow.

1 Introduction

Despite their ubiquity in engineering and environmental phenomena, particle-laden turbulent flows are still poorly understood. For example, the rapid growth of the particle size distribution in clouds cannot be explained by standard microphysical models and is thought to be related to enhanced droplet collision rates induced by turbulence [1, 2, 3, 4]. Aerosols released from anthropogenic processes cluster in the atmosphere at rates determined by turbulence and modulate the global radiation from the sun. These aerosols are currently the greatest source of uncertainty in global climate models [5].

Much of the uncertainty regarding particle motion in turbulence is due to the huge separation of both spatial and temporal scales at Reynolds numbers R_λ characteristic of industrial and natural flows. This scale separation requires extensive computational resources which increase rapidly with R_λ. We address these computational requirements through our highly scalable DNS code for particle-laden turbulence, described in §2. Using this code, we calculate inertial particle clustering, relative velocity, and collision statistics, as discussed in §3.

2 Code Description

Our pseudospectral, DNS code implements two-dimensional ('pencil') domain decomposition for isotropic turbulence and homogeneous turbulent shear flow using the P3DFFT library [6]. This parallelization strategy allows us to perform a calculation of N^3 grid points on up to N^2 processors (using MPI) and to achieve high values of R_λ. Lagrangian fluid particles, inertial particles, and diffusive scalars can be introduced into the flow. Particle updates are parallelized using a novel exponential integrator scheme [7] and efficient ghost-cell communication.

This is the most general and efficient turbulence simulation code of its kind. We discuss code scaling, communication patterns, interpolation schemes, and time-integration techniques for large-scale parallelization on state-of-the-art computational platforms.

3 Simulations of particle-laden turbulence

Using DNS, we quantify inertial particle clustering (via the radial distribution function) and relative velocities (via their PDF) in statistically stationary isotropic turbulence. From these results, we can predict particle collision rates, and thereby the growth of the droplet size distribution [8].

The DNS is also used to develop the experimental techniques of our collaborators at SUNY Buffalo. The fluid parameters (i.e., the Reynolds number R_λ) and particle parameters (i.e., the Stokes number St) in our simulations are parametrically matched to those of experiments in an analagous turbulent flow. Using the insight afforded by our DNS, we determine the optimum camera settings for accurate measurement of particle positions and velocities. We conclude by discussing practical applications to open questions regarding cloud growth and aerosol transport.

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