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DIRECT SIMULATION OF DISPERSED LIQUID DROPLETS IN ISOTROPIC TURBULENCE

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EXECUTIVE SUMMARY:

The objective of our research is to enhance understanding of the two-way interactions between liquid droplets and a turbulent flow by performing direct numerical simulations (DNS). The freely moving deformable liquid droplets are fully resolved in three spatial dimensions and time and all the scales of the turbulent motion are simultaneously resolved down to the smallest relevant length and time scales. Our DNS solve the unsteady 3D Navier–Stokes and continuity equations throughout the whole computational domain, including the interior of the liquid droplet. The droplet surface motion and deformation are captured accurately by using the level set method. Discontinuous density and viscosity are smoothed out across the interface by means of the continuous surface force approach. A variable-density projection method imposes the incompressibility constraint.

INTRODUCTION

The two-way interactions between liquid droplets and turbulent flows are important in nature and engineering applications, for example cloud formation and burning of liquid fuel in internal combustion (reciprocating and jet) engines and rockets. Understanding the physical details of the vaporization and mixing processes in a turbulent flow is an essential prerequisite to understanding the chemical reaction and the eventual control/optimization of energy conversion.

METHODS & RESULTS

The freely-moving deformable liquid droplets are fully resolved in time and 3D space, and all the scales of the turbulent motion are simultaneously resolved down to the smallest relevant length and time scales. Our direct numerical simulations (DNSs) solve the unsteady 3D Navier–Stokes and continuity equations throughout the whole computational domain, including the interior of the liquid droplet. The droplet surface motion and deformation are captured accurately by using the level set method (LSM). The discontinuous density and viscosity are smoothed out across the interface by means of the continuous surface force (CSF) approach. A variable density projection method is used to impose the incompressibility constrain.

So far we focused on validating our numerical solution method. We compared our simulation results of an initially spherical liquid water droplet settling in stagnant air, under the effect of gravity and surface tension, with available experimental data. We monitored the shape changes, the terminal velocity, and the conservation of both mass and momentum. Once this validation is completed we will simulate the motion of a number of liquid droplets in isotropic turbulence. This will allow us to examine the dispersion statistics of the droplets and their effects on the carrier flow turbulence (two-way coupling).

WHY BLUE WATERS?

DNS of turbulent flows is very demanding in terms of computational power and memory. The computational grids need to be fine enough to resolve the smallest flow structures accurately; this requirement becomes more and more stringent as the Reynolds number, based on the Taylor microscale, increases. In addition, we seek an accurate time history of the flow in order to compute time-dependent statistics, thus limiting the time-step size (time interval) for advancing the solution in time. For example, DNS of single-phase isotropic turbulence at Reynolds number 300 requires a grid of $2{,}048^3$ mesh points, and about 12 hours on 65,536 processors to cover seven large eddy turnover times.

The demand for computational power is even larger if a multiphase flow (e.g., liquid droplets in air) is considered; the standard projection method for incompressible flows must be replaced by a variable-density projection method. The latter results in a variable-coefficients Poisson's equation that is not solvable by means of a fast Fourier transform, thus requiring an iterative solver. We use the multigrid-preconditioned conjugate gradient solver provided by the PETSc library. Given the requirements outlined above, Blue Waters is a necessary tool for our research.

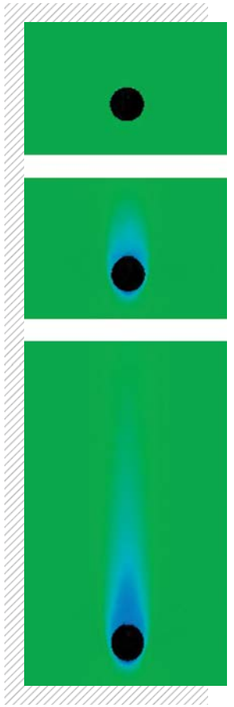

FIGURE 1: A liquid water droplet with initial diameter 0.6 mm is falling in stagnant air under the effect of gravity (=10 times gravity). The droplet's initial spherical shape changes with time due to the effects of acceleration, surface tension, and drag forces. Time (a) 0.0s; (b) 0.001 s; (c) 0.005 s. The velocity contours in the wake region are shown in blue.