MODELLING PARTICLE-LADEN TURBULENT FLOWS WITH NEURAL STOCHASTIC DIFFERENTIAL EQUATIONS

JOSH WILLIAMS

Turbulent particle-laden flows appear in many medical applications including inhaler drug deposition. In these applications, aerosolised solid drug particles or liquid droplets (henceforth called ‘particles’) are transported. The particles have low inertia and are influenced by fluctuations in carrier fluid motion. In turbulent flows, it is computationally expensive to fully resolve all length and timescales. Therefore, the fluid phase is simulated with a large-eddy simulation (LES) where only the largest scales are resolved and the fluctuating motion smaller than the cell size (subgrid scales) is modelled. To account for the effect of fluid fluctuations on the particle dynamics, models based on stochastic differential equations (SDEs) have been proposed for the fluid velocity ‘seen’ by a particle which is used to compute the particle drag force. We propose to learn drift and diffusion terms for a Langevin equation using neural networks (‘neural SDEs’), based on fully resolved direct numerical simulations (DNS) of particles in turbulence at varying Reynolds numbers. The trained model is then implemented in OpenFOAM to evaluate the model efficacy a posteriori with a focus on particle velocity and kinetic energy predictions at varying level of particle inertia. We observe good agreement with DNS data for low to high inertia particles. The model correctly recovers the particle kinetic energy lost by filtering the subgrid scales. Neural SDEs are therefore a suitable approach for creating coarse-grained models for multiphase flow modelling, and may be extended to include particle-particle interactions.