Robust interpolation for momentum coupling of dispersed multiphase flows in OpenFOAM using the Full Lagrangian Approach

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The simulation of dispersed multiphase flows has evolved into an area of continued importance, with a diverse range of industrial and environmental applications leading to the development of a variety of computational approaches for modelling the behaviour of droplets and particles. Of central importance in the modelling of such flows is the accurate representation of the spatial distribution of droplets, which can exhibit wide variation in unsteady or turbulent flows. Whilst an important metric in its own right, the spatial distribution also plays a key role within simulations for interphase momentum and energy coupling in dilute suspensions, and for this reason accurate determination of the dispersed phase concentration field is paramount to ensuring physically correct behaviour can be reproduced within simulations.

The present work seeks to address this need by utilizing a mathematical model known as the Full Lagrangian Approach (FLA). Unlike existing simulation approaches, the FLA is able to calculate the local concentration of droplets along their trajectories and thereby include detail of the behaviour experienced by individual droplets [1]. This is realised through computation of the Eulerian-Lagrangian transformation along trajectories with respect to an initial position $\mathbf{x}_0$, as given by the Jacobian tensor $\mathbf{J}$, defined as

$$\mathrm{J}_{ij}(\mathbf{x}_0, t) = \frac{\partial x_{di}(t)}{\partial \mathrm{x}_{0j}} \tag{1}$$

For trajectories $\boldsymbol{x}_d(t)$ of spherical droplets which move according to a linear drag law, the equation of evolution for $\mathbf{J}$ is given by

$$\ddot{\mathrm{J}}_{ij} = \beta \frac{\partial \mathrm{u}_i}{\partial \mathrm{x}_k}(\boldsymbol{x}_d(t), t)\mathrm{J}_{kj} - \beta \dot{\mathrm{J}}_{ij} \tag{2}$$

where β is the droplet inertia parameter. The droplet number density n_d is then evaluated directly using the Lagrangian form of conservation of mass

$$n_d(\mathbf{x}, t) = \frac{n_d(\mathbf{x}_0, t_0)}{|\det(\mathbf{J}(\mathbf{x}_0, t))|} \tag{3}$$

The advantage of this method is that relatively few droplets need to be tracked in order to reproduce a faithful representation of the droplet number density field, when compared to conventional box-counting methods such as the Cloud-In-Cell approach [2]. Reconstruction of the number density field does however require that a suitable numerical scheme is used to interpolate the Lagrangian data between trajectories. The novelty of the present research comes from using a statistical learning approach through the use of a kernel estimator to accumulate the contributions from individual trajectories and reconstruct the droplet number density field, which enables a high level of detail to be retained at a reduced computational cost. Furthermore, the FLA has recently been generalized to account for polydispersity by including the droplet radius as an additional variable within the formulation [3], and the kernel estimator has the advantage of being able to straightforwardly extend to this framework, and reproduce the dispersed phase spatial distribution across a range of droplet radii.

The developed methodology has been implemented into a custom OpenFOAM solver that has been developed on top of the Lagrangian library, allowing it to be coupled to all OpenFOAM solvers for the carrier flow [4]. Benchmark simulations for flow past a cylinder of radius R have been conducted in steady ($Re = 20$, Figure. 1) and unsteady ($Re = 100$, Figure. 2) cases for both monodisperse and polydisperse droplets, and the kernel estimator is shown to provide a reliable means of reconstructing the number density field across this range of flow configurations. When compared to a Cloud-In-Cell procedure, this is seen to come at a decreased computational cost due to the ability of the kernel estimator to directly make use of the Lagrangian number density data provided by Eq. (3), and demonstrates the potential of the FLA methodology for upscaling to the simulation of industrially relevant spray systems.

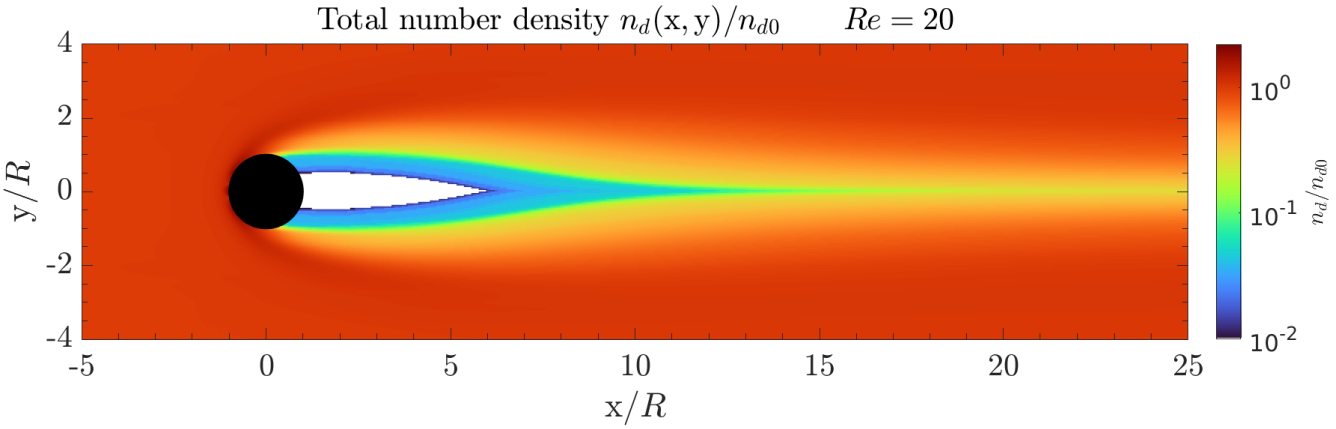

Figure 1: Total number density field $n_d(\mathrm{x},\mathrm{y})/n_{d0}$ for steady-state flow past a cylinder at $Re = 20$

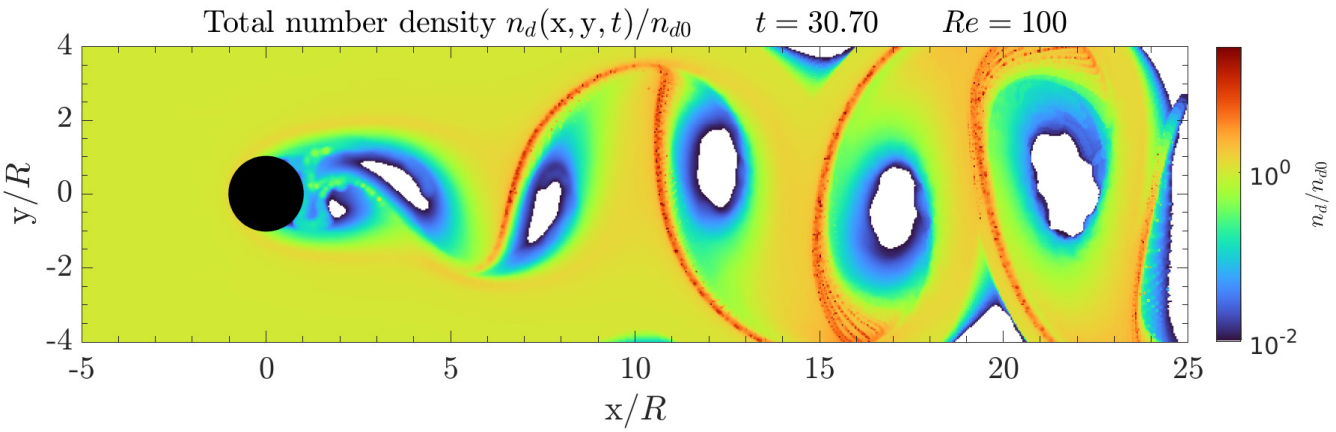

Figure 2: Total number density field $n_d(\mathrm{x},\mathrm{y},t)/n_{d0}$ for transient flow past a cylinder at $Re = 100$ for time $t = 30.70$

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