# Reconstruction of the Droplet Size Distribution in Polydisperse Sprays Using the Generalised Fully Lagrangian Approach

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**Abstract**
In the present paper, it is proposed to use kernel regression to map the Lagrangian droplet data, droplet number density in particular, to Eulerian distribution fields. In this approach, the domain of influence of a kernel is linked to the local droplet deformation field, which is provided by the fully Lagrangian approach (FLA) or generalised fully Lagrangian approach. The advantages of this approach include its ability to retain the structures (caustics and voids) in the droplet cloud, computational efficiency when compared to conventional methods based on counting droplets, for example Cloud-In-Cell, and flexibility to be applied to polydisperse droplets. The proposed methodology has been implemented as additional libraries for the open-source computational fluid dynamics software OpenFOAM, and applied to benchmark steady state and transient flow around a cylinder. The results are in agreement with previously reported observations. It is demonstrated that the new method achieves significant reduction in computational costs if compared with the Cloud-In-Cell approach, this is due to $\sim 10^3$ times fewer droplet data being required to reconstruct the droplet fields.

**Keywords**
Droplet size distribution, fully Lagrangian approach, kernel regression, polydisperse droplets.

## Introduction

Gas-droplet flows are widely observed in engineering and environmental settings [1], including during fuel injection in internal combustion engines [2]. In such flows, the admixture forms high concentration regions with folds (local zones of crossing particle/droplet trajectories, hereafter referred to as droplets) and caustics. The fully Lagrangian approach (FLA) has been known for its potential to capture such complex structures in gas-droplet flows while providing number density values in Lagrangian droplet positions [3, 4]. Moreover, it has been demonstrated that the FLA is an efficient method for calculating droplet distributions in comparison to other Lagrangian approaches [4]. In [5], a generalised FLA (gFLA) was applied to polydisperse evaporating sprays. At the edge of a local region of crossing particle trajectories (caustics), the particle number density has a singularity. This is a well-known feature of the mathematical model of the collisionless continuum of point particles (see details in [6], where typical examples of flows with singularities in the particle number density field were analysed). It was shown that for an integrable singularity of particle number density, at the singular points the mean distance between the particles remains finite and the model of collisionless particles remains valid. The goal of the present study is to develop a robust remapping method for droplet parameters onto an Eulerian field, especially for the droplet number density calculated using the FLA or gFLA. The paper is arranged as follows, Section 1 is dedicated to the description of the FLA and gFLA, kernel regression and its implementation are presented in Section 2, Section 3 is dedicated to discussion and results, finally the study outcomes are summarised in Conclusions (Section 4).

## The fully Lagrangian approach for droplet distribution calculations

In this section, only mathematical formalism for admixture in gas-droplet flow is presented as this is the focus of the study. The carrier phase is described using a conventional approach such as a numerical solution to the Navier–Stokes equations.

The governing equations and corresponding initial conditions for droplet motion and evaporation are:

$$\ddot{\mathbf{x}}_d(t) = \mathbf{f}(\mathbf{x}_d(t), \mathbf{v}_d(t), r_d(t), t), \qquad \begin{aligned} \mathbf{x}_d(t_0) &= \mathbf{x}_0, \\ \dot{\mathbf{x}}_d(t_0) &= \mathbf{v}_0, \end{aligned} \tag{1a}$$

$$\dot{r}_d(t) = \varphi(\mathbf{x}_d(t), \mathbf{v}_d(t), r_d(t), t), \qquad r_d(t_0) = r_0, \tag{1b}$$

where $\mathbf{f}$ is the force per unit mass exerted on a droplet, which is usually a known function of the droplet size, droplet velocity, and other parameters; $\dot{r}_d = \varphi$ is the rate of droplet size change, which is usually a known function of the droplet size and thermodynamic parameters, and the subscript $d$ denotes droplet parameters.
According to the fully Lagrangian approach, the droplet cloud is represented as a continuum with continuous parameters. The Lagrangian variables are the droplet initial position coordinates $\mathbf{x}_0$, which together with time $t$ define the droplet current location. Extending the set of the Lagrangian variables to include the initial size $r_0$ makes it possible to describe polydisperse and evaporating droplets [3, 5]. The droplet distribution function $p(\mathbf{x}_d, r_d, t)$ can be found from the Lagrangian form of the continuity equation

$$p(\mathbf{x}_d, r_d, t) = \frac{p(\mathbf{x}_0, r_0, t_0)}{|\det(\mathbf{J}(\mathbf{x}_0, r_0, t))|}, \tag{2}$$

where the Jacobian tensor $\mathbf{J}(\mathbf{x}_0, r_0, t)$ is defined by

$$\mathbf{J}(\mathbf{x}_0, r_0, t) = \begin{bmatrix} \mathbf{J}^{\mathbf{xx}} & \mathbf{J}^{\mathbf{x}r} \\ \mathbf{J}^{r\mathbf{x}} & J^{rr} \end{bmatrix} = \begin{bmatrix} \frac{\partial \mathbf{x}_d}{\partial \mathbf{x}_0} & \frac{\partial \mathbf{x}_d}{\partial r_0} \\ \frac{\partial r_d}{\partial \mathbf{x}_0} & \frac{\partial r_d}{\partial r_0} \end{bmatrix}. \tag{3}$$

The equations for the Jacobian components are obtained by taking partial derivatives of Eqs. (1) with respect to the Lagrangian variables

$$\ddot{\mathbf{J}}^{\mathbf{xx}} = \frac{\partial \mathbf{f}_d}{\partial \mathbf{x}} \cdot \mathbf{J}^{\mathbf{xx}} + \frac{\partial \mathbf{f}_d}{\partial \mathbf{v}} \cdot \dot{\mathbf{J}}^{\mathbf{xx}} + \frac{\partial \mathbf{f}_d}{\partial r} \mathbf{J}^{r\mathbf{x}}, \qquad \begin{aligned} \mathbf{J}^{\mathbf{xx}}(\mathbf{x}_0, r_0, t_0) &= \mathbf{I}, \\ \dot{\mathbf{J}}^{\mathbf{xx}}(\mathbf{x}_0, r_0, t_0) &= \partial \mathbf{v}_0 / \partial \mathbf{x}_0, \end{aligned} \tag{4a}$$

$$\ddot{\mathbf{J}}^{\mathbf{x}r} = \frac{\partial \mathbf{f}_d}{\partial \mathbf{x}} \cdot \mathbf{J}^{\mathbf{x}r} + \frac{\partial \mathbf{f}_d}{\partial \mathbf{v}} \cdot \dot{\mathbf{J}}^{\mathbf{x}r} + \frac{\partial \mathbf{f}_d}{\partial r} J^{rr}, \qquad \begin{aligned} \mathbf{J}^{\mathbf{x}r}(\mathbf{x}_0, r_0, t_0) &= \mathbf{0}, \\ \dot{\mathbf{J}}^{\mathbf{x}r}(\mathbf{x}_0, r_0, t_0) &= \mathbf{0}, \end{aligned} \tag{4b}$$

$$\dot{\mathbf{J}}^{r\mathbf{x}} = \frac{\partial \varphi_d}{\partial \mathbf{x}} \cdot \mathbf{J}^{\mathbf{xx}} + \frac{\partial \varphi_d}{\partial \mathbf{v}} \cdot \dot{\mathbf{J}}^{\mathbf{xx}} + \frac{\partial \varphi_d}{\partial r} \mathbf{J}^{r\mathbf{x}}, \qquad \mathbf{J}^{r\mathbf{x}}(\mathbf{x}_0, r_0, t_0) = \mathbf{0}, \tag{4c}$$

$$\dot{J}^{rr} = \frac{\partial \varphi_d}{\partial \mathbf{x}} \cdot \mathbf{J}^{\mathbf{x}r} + \frac{\partial \varphi_d}{\partial \mathbf{v}} \cdot \dot{\mathbf{J}}^{\mathbf{x}r} + \frac{\partial \varphi_d}{\partial r} J^{rr}, \qquad J^{rr}(\mathbf{x}_0, r_0, t_0) = 1, \tag{4d}$$

where $\mathbf{I}$ is the identity matrix. The initial conditions for the system (4) are found from the initial conditions associated with the governing equations (1).
In the case of monodisperse droplets (standard FLA), the probability density $p(\mathbf{x}_d, r_d, t)$ reduces to the number density $n(\mathbf{x}_d, t)$, which is a function of droplet position $\mathbf{x}_d$ only.

**Kernel regression in application to reconstruction of the droplet number density field**

The FLA described in the previous section is used to calculate the droplet parameters, droplet number density values in particular, along trajectories (in Lagrangian coordinates). This data is then required to be remapped onto an Eulerian field. We propose to use kernel regression for droplet data interpolation due to the flexibility of this approach. There is no limit on the minimal number of data points needed (one is suffice), and it can be extended to the case of multivalued droplet parameter fields and the case of polydisperse droplets. In our study, we consider the Nadaraya-Watson estimator [7]

$$n(\mathbf{x}, t) = \frac{\sum_{i=1}^{N} K_{\mathbf{H}}(\mathbf{x}, \mathbf{x}_d^i) n(\mathbf{x}_d^i, t)}{\sum_{j=1}^{N} K_{\mathbf{H}}(\mathbf{x}, \mathbf{x}_d^j)}, \tag{5}$$

where $n(\mathbf{x}_d^i, t)$ is the instantaneous number density along the trajectory $\mathbf{x}_d^i$ associated with the $i^{\text{th}}$ droplet at time $t$ as obtained from the FLA, $n(\mathbf{x}, t)$ is the Eulerian number density field, $N$ is the number of droplets that contribute at the point $\mathbf{x}$, and $K_{\mathbf{H}}(\mathbf{x}, \mathbf{x}_d^i)$ is the kernel. A multivariate Gaussian form is chosen in this work, and a corresponding kernel can be defined as

$$K_{\mathbf{H}}(\mathbf{x}, \mathbf{x}_d^i) = \frac{1}{\sqrt{\det(\mathbf{H})}} \exp\left[-\frac{1}{2}\left(\mathbf{x} - \mathbf{x}_d^i\right)^\top \cdot \mathbf{H}^{-1} \cdot \left(\mathbf{x} - \mathbf{x}_d^i\right)\right], \tag{6}$$

where $\mathbf{H}$ is the bandwidth matrix that contains information about the smoothing lengths in different directions, e.g. $\mathbf{H} = h^2\mathbf{I}$ corresponds to a spherical kernel with a smoothing length $h$. In the case of polydisperse droplets, which includes the behaviour of the droplet radius $r_d$, the bandwidth matrix $\mathbf{H}$ is defined as

$$\mathbf{H}(\mathbf{x}_0, r_0, t) = \begin{bmatrix} h_{\mathbf{x}0}^2 |J^{\mathbf{xx}}(\mathbf{x}_0, r_0, t)|^{2/n}\mathbf{I} & \mathbf{0} \\ \mathbf{0} & h_{r0}^2 |J^{rr}(\mathbf{x}_0, r_0, t)|^2 \end{bmatrix} \tag{7}$$

where $h_{\mathbf{x}0}$ and $h_{r0}$ are the initial smoothing lengths in physical and radial space respectively, and $n$ is the spatial dimensionality of the problem. This form of the bandwidth matrix takes into account information about local deformation in the droplet phase by including the Jacobian blocks.

**Results and Discussion**

The developed approach of combined gFLA and kernel regression has been implemented in an open-source CFD code OpenFOAM as additional libraries. In this section we discuss 2D steady-state and periodic gas-droplet flows around a cylinder with mono- and polydisperse droplets. The gas (carrier phase) parameters are calculated using the OpenFOAM pimpleFoam solver, whereas the droplet parameters are reconstructed using the newly implemented library. For the purposes of verification of the implementation and testing the functionality, we limit our study to Stokes's drag law, neglecting other forces and assuming low droplet Reynolds numbers. Also, it is assumed that droplets evaporate into their own vapour and all heat at the droplet surface is spent on its evaporation. These assumptions lead to simplified expressions for the force $\mathbf{f}$ and evaporation rate $\varphi$ used in Eq. (1). The above assumptions on physical models can be relaxed by replacing expressions for $\mathbf{f}$ and $\varphi$ by the ones corresponding to more realistic flow scenarios.

We start our analysis with a steady-state flow of gas with monodisperse droplets. Three cases have been considered, $St = 0.1,\ 1,\ 10$, representing small, medium-size, and large droplets. The number density distributions for the three cases are presented in Fig 1, left column. The results obtained using the combined FLA and kernel regression approach are compared with conventional Cloud-In-Cell approach (see Fig 1, middle column), and the relative error is presented in Fig 1, right column. The error values are acceptable in the most of the domain, and are high on the edges of two-phase regions behind the cylinder, where areas devoid of droplets are formed. This discrepancy is attributable to the following two factors. Firstly, kernel regression smooths sharp gradients over the support area. Secondly, the Cloud-In-Cell (CIC) approach requires about 100 times more droplet trajectories and 10 times more sampling data along the trajectories than the proposed combined FLA and kernel regression method. This leads to extra data used in the CIC approach, which is not accounted for in the combined FLA and kernel regression method. Overall, the CIC approach requires about 1000 times more droplet data, which significantly increases the computational time and storage required..

The results for polydisperse droplets in periodic flow around a cylinder are shown in Fig 2. Since the approach makes it possible to reconstruct the droplet distribution field, apart from the number density across all droplet sizes, the average droplet size, variance in sizes, and other higher order statistics can also be calculated. The results presented in the figure demonstrate that the proposed approach correctly represents the thin droplet accumulation structures, as well as brings an insight into droplet size (re-)distributions in the flow.

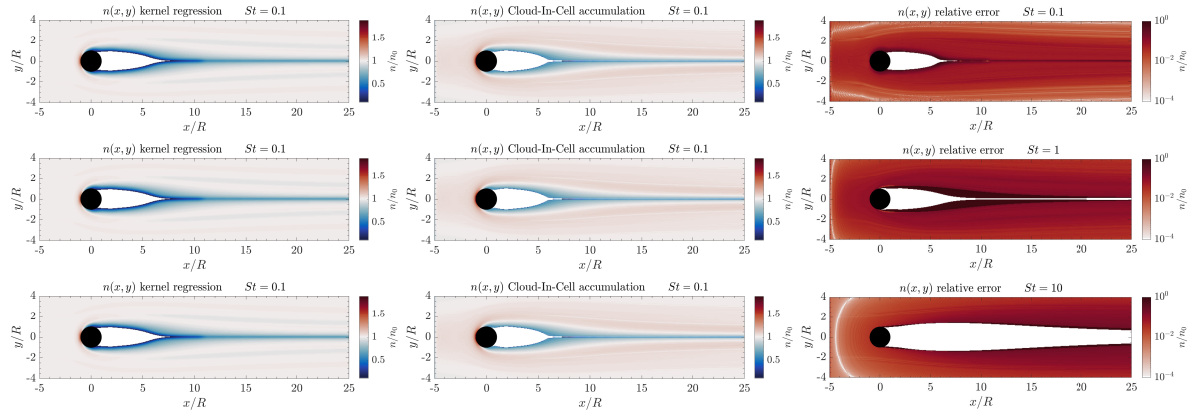


**Figure 1.** Reconstruction of droplet number density $n(x, y)$ using kernel regression in monodisperse steady-state flow around a cylinder at $Re = 20$ for $St = 0.1$ (top row); $St = 1$ (middle row); and $St = 10$ (bottom row). Second column: the same but obtained using the Cloud-In-Cell (CIC) approach. Third column: relative difference between the combined FLA and kernel regression method and the CIC approach.

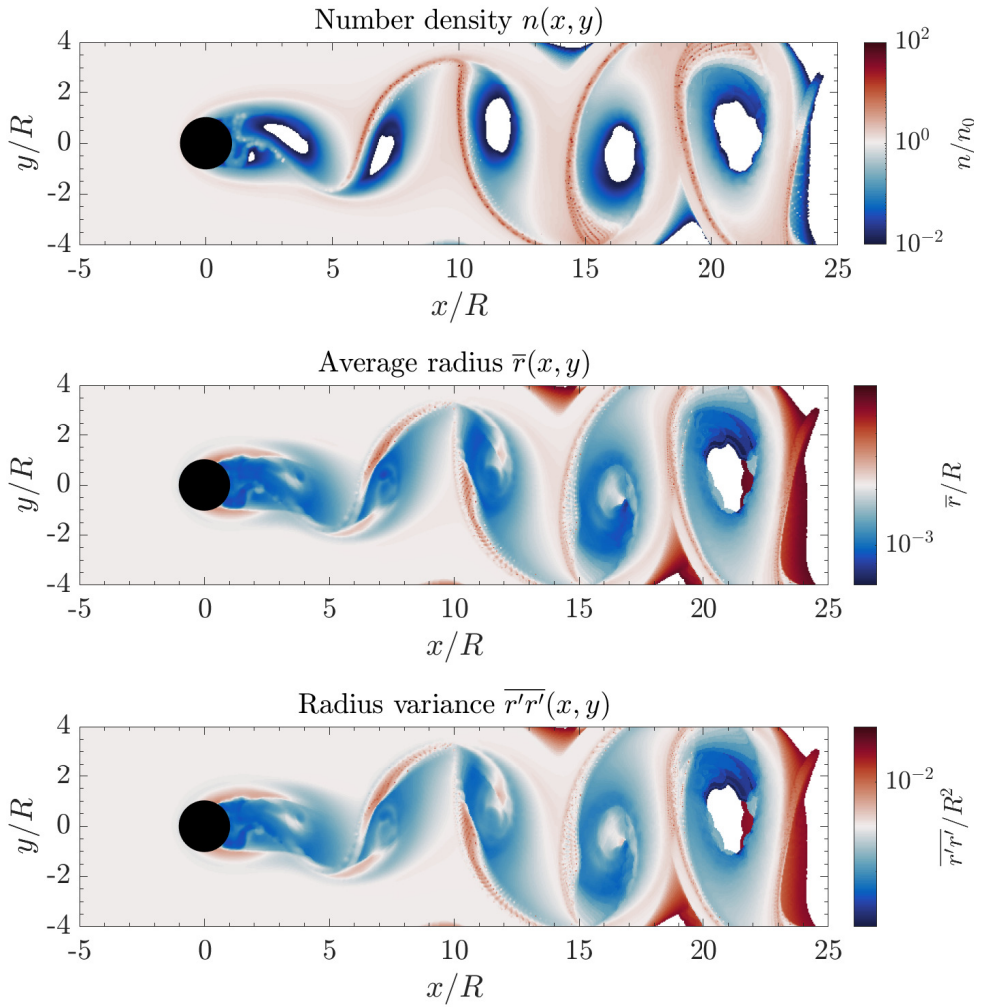


**Figure 2.** Reconstruction of the droplet number density $n(x, y)$ across all droplet sizes (top); average droplet size distribution (middle); and variance in droplet size (bottom) for polydisperse transient flow around a cylinder at $Re = 100$.

## Conclusions

In this study, we propose a novel approach for reconstruction of droplet parameter fields calculated using the fully Lagrangian approach on an Eulerian grid. The focus of the study is on reconstruction of number density distributions and distributions in size. This approach is based on kernel regression and is linked to the salient FLA property of tracking the droplet field defor-

mation. This information is used to inform the size and the shape of the kernel support. The model has been coupled with OpenFOAM and applied to steady-state and transient flow around a cylinder, for the cases of mono- and polydisperse droplets. It has been demonstrated that the new approach might lead to significant savings in computational resources when compared with the conventional Cloud-In-Cell approach. The new approach supports reconstruction of useful statistics, for example average droplet size and variance in sizes, which are used in experimental observations.

**Acknowledgements**
The authors are grateful to the UKRI Future Leaders Fellowship (Grant MR/T043326/1) for the financial support.

**Nomenclature**

| | |
|---|---|
| CIC | Cloud-In-Cell |
| $\mathbf{f}$ | force per unit mass |
| FLA | fully Lagrangian approach (also known as Osiptsov's method) [3] |
| $\mathbf{H}$ | bandwidth matrix |
| $h$ | smoothing length |
| $\mathbf{I}$ | identity matrix |
| $\mathbf{J}$, $J$ | Jacobian tensor and Jacobian components |
| $K$ | kernel |
| $m$ | mass of a particle/droplet |
| $N$ | number of droplets that contribute at the point $\mathbf{x}$ |
| $n$ | particle/droplet number density or spatial dimensionality of the problem (1D, 2D or 3D) |
| $p$ | droplet distribution function |
| $t$ | time |
| $\mathbf{v} = (v_x, v_y, v_z)$ | velocity |
| $r$ | droplet radius |
| $\mathbf{x} = (x, y, z)$ | position vector |
| *Subscripts* | |
| $d$ | dispersed phase parameter |
| $i, j$ | indices |
| $0$ | initial value |
| *Superscripts* | |
| $i$ | index |
| $\mathbf{x}$ | index corresponding to the space variables |
| $r$ | index corresponding to the droplet radius |

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