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A coupled Eulerian interface capturing and Lagrangian particle method for multiscale simulation.

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Abstract

A new Eulerian-Lagrangian coupling on a staggered fluid mesh is proposed to simulate multiscale atomization. This coupling relies on a sharp interface capturing method (ICM) to transport the resolved fluid structures and a Lagrangian tracking algorithm to model the under-resolved Eulerian droplets. The Lagrangian droplets momentum is spread to the source terms of the incompressible fluid momentum equations through a spatial filtering operation, and the flow velocity around the Lagrangian droplets is corrected to account for their local flow disturbance. This allows accurate transport of Lagrangian droplets that are both smaller and larger than the fluid mesh spacing. The implementation of the algorithm for switching from an Eulerian toward a Lagrangian framework is discussed, along with criteria validating a transformation. Then the Eulerian-Lagrangian coupling is applied to several test cases from the literature, and is compared to our in-house pure ICM solver on the atomization of a liquid jet. The results show that the Eulerian-Lagrangian coupling improves the physical analysis of the atomization, and achieves more accurate results for poorly resolved droplets.

Keywords: DNS, Two Phase Flow, Atomization, ICM, Eulerian-Lagrangian coupling

1. Introduction

Two phase flow atomization is involved in several natural and industrial applications, such as geyser eruption [1], jet sprinkler applications [2], liquid fuel injection in combustion chambers [3], and many others [4]. The analysis of atomization within a combustion chamber relies upon an accurate description of flow injection. Indeed, the injection and fragmentation of the jet create the initial conditions for the development of the spray, and therefore, allow for the estimation of important statistics such as total surface area. Thus, the scientific community has

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8 put considerable efforts to describe liquid jet breakup, referred now as the primary atomization
9 area [5]. This area involves complex phenomena such as turbulence, high momentum exchanges
10 and break up events. Hence, robust experimental [6, 7], and numerical techniques [8–10], are
11 required for a thorough understanding and description of the primary atomization area.

12 Direct numerical simulation (DNS) is an ideal tool to numerically investigate atomization.
13 Interface capturing method (ICM) are often used to transport the interface between fluid and
14 gas phases [11]. Several ICM have been successfully applied to analyze the primary atomization
15 area, such as level set [12, 13], volume of fluid (VOF) [14, 15], or a coupling of both level set and
16 VOF (CLSVOF) [16, 17]. With these methods, it is possible to accurately describe the liquid
17 structure resulting from the breakup of the liquid jet, such as ligaments or large droplets. In
18 particular, the CLSVOF method accurately represents the interface topology changes through
19 the level set while taking advantage from the mass conservation properties of the VOF. In
20 previous studies, our group applied the CLSVOF to several multiphase flows applications with
21 complex interface topology change [18–20].

22 Ligaments and large droplets arising from primary breakup can experience successive break-
23 ups downstream to the jet [21]. Therefore, DNS must provide an accurate description of both
24 the primary atomization and subsequent fragmentation, referred to as the secondary atomiza-
25 tion [22]. Droplets in the secondary atomization area are several orders of magnitude smaller
26 than the injected liquid jet. This leads to a significant scale range, from μm for droplets to
27 mm for the liquid jet, that is too consequent to provide a complete description of a spray using
28 current numerical resources. In addition to a poor physical representation of the secondary at-
29 omization, the transport of under-resolved droplets can generate numerical instabilities, known
30 as *flotsam* or *jetsam*. Several solutions exist to circumvent this multiscale issue: to couple the
31 fluid solver with an adaptive mesh refinement method [23], to model the transport of small fluid
32 structures using a Lagrangian method [24], or, to simply remove these droplets from the DNS
33 simulations [25]. Within the scope of this manuscript, small fluid structures are modeled.

34 This modeling approach, referred here to as the Eulerian-Lagrangian coupling [26, 27], com-
35 bines the resolved transport of larger structures (ICM), and the modeling of under-resolved
36 droplets (Lagrangian). A Lagrangian method is used to track these droplets, herein after called
37 Lagrangian droplets. Semi-empirical correlations are used to transport Lagrangian droplets,
38 relying upon instantaneous local fluid properties [28]. One of the challenges of this framework
39 is to ensure a stable and conservative coupling at the transformation of an Eulerian droplet

40 toward a Lagrangian droplet, and vice-versa, without including artificial source terms to both
41 frameworks. This goes with the definition of numerical and physical criteria of transformation
42 and modification of the Eulerian fields.

43 In the pioneer works of Herrmann [26] and Tomar et al. [27], the Eulerian-Lagrangian frame-
44 work is coupled with an adaptive mesh refinement (AMR). The Lagrangian framework is used to
45 transport all Eulerian droplets far from the primary atomization. A two way Lagrangian coup-
46 ling is used to transport Lagrangian droplets, accounting for both the transport of Lagrangian
47 droplets and the fluid-droplets interphases momentum in the source terms of the fluid equations.
48 After transformation, the fluid mesh is coarsened and the Lagrangian droplets are smaller than
49 the fluid mesh. To distinguish between droplets, several criteria of transformation are used such
50 as the distance between Eulerian droplets and other structures, or, the sphericity of Eulerian
51 droplet. The latter enables transport of Lagrangian droplets using semi-empirical correlations
52 derived from spherical shape [28]. The implementation of the Eulerian-Lagrangian coupling
53 of Herrmann [26] and Tomar et al. [27] reduces the computational cost of the simulation while
54 conserving an accurate description of the droplets' statistics downstream to the jet. However,
55 results of Zuzio et al. [29] show that the coarsening of the fluid mesh during the transformation
56 step can yield to numerical instabilities. They propose to first transport Eulerian droplet as a
57 resolved solid particle, where all interactions between the fluid and the particle are resolved, en-
58 suring a smooth transition toward coarser levels of the Eulerian fluid grid. This method requires
59 adaptive mesh refinement which is challenging to implement.

60 In Ling et al. [30] an Eulerian-Lagrangian coupling for fixed Eulerian grid is proposed simpli-
61 fying the Eulerian-Lagrangian coupling strategy. The transformation on a constant grid implies
62 that Lagrangian droplets are larger than the fluid mesh spacing, yielding to a large local dis-
63 turbance on the resolved flow. In the work of Ling et al. [30], this disturbance is filtered using a
64 regularized weighted function to spread the coupling force over several droplets' diameter [31].
65 Despite the regularization of the Lagrangian droplets' feedback force, the local flow disturbance
66 for Lagrangian droplets larger than the fluid mesh spacing are not filtered [32, 33]. This disturb-
67 ance affects both the resolved flow and the Lagrangian droplets, as it yields to an inaccurate
68 estimation of local fluid forces acting on Lagrangian droplets. Moreover, this flow disturbance is
69 shown to be proportional to the number of cells across the diameter of the Lagrangian droplet,
70 which deteriorates the accuracy of the Eulerian-Lagrangian coupling on a constant grid.

71 To circumvent large local disturbances on the resolved flow when dealing with particles

72 larger than the fluid mesh spacing, Evrard et al. [34] propose an Eulerian-Lagrangian coupling
73 based on the filtering of the governing equations [35, 36]. It relies upon the filtering of the
74 volume fraction, the drag force experienced by the particles, and the fluid velocity, as well as
75 exchanges between the Eulerian and the Lagrangian frameworks. The results presented in the
76 work of Evrard et al. [34] drastically improve the accuracy of the transport of the dispersed phase
77 within the Lagrangian framework, however it requires the transport of the volume fraction as
78 well as modification of the Poisson solver resolution.

79 Another solution to improve the Lagrangian transport of the particles larger than the fluid
80 mesh spacing is to subtract the local flow disturbance by recovering the local undisturbed velocity
81 through an analytical analysis of the Stokes and Oseen flow solutions [37, 38]. In Balachandar
82 et al. [37] and Evrard et al. [38], the flow disturbance correction enables accurate transport
83 of Lagrangian droplets larger than the fluid mesh. In addition, this method does not require
84 the modification of the fluid solver. Thus, it is an ideal solution to transport the dispersed
85 phase within the Lagrangian framework in the Eulerian-Lagrangian coupling. The fundamental
86 originality of our study is the implementation, validation, and analysis of this coupling.

87 The present method couples a resolved transport of large fluid structures with the CLSVOF
88 method of Ménard et al. [16] and a modeling of the small droplets with a Lagrangian two way
89 coupling on the same grid level. A spatial filtering operation through a regularization of the
90 force coupling is used [30], along with the correction of local flow disturbance derived in Evrard
91 et al. [38] to transport Lagrangian droplets larger than the fluid mesh spacing. Although the im-
92 plementation is straightforward because both Eulerian and Lagrangian solvers are independent,
93 the analysis of the transformation step shows a mass inconsistency in the Lagrangian toward Eu-
94 lerian transformation. A cost-efficient solution based on a minimization algorithm is proposed,
95 reducing the error of several orders of magnitude. Additionally, all criteria of transformation
96 implemented within this work are discussed along with their algorithms of implementation to
97 provide a guideline for future implementations. The new method, as well as the new transform-
98 ation criteria, are validated among reference cases from the literature, and successfully applied
99 to two phase flow atomization of a liquid jet.

100 The manuscript is organized as follows. Section 2 presents the general framework, the in-
101 terface capturing (ICM) and the Lagrangian particle tracking methods. In Section 3, limits of
102 the ICM are investigated, as the basis of Eulerian-Lagrangian coupling. Section 4 presents the
103 general Eulerian-Lagrangian coupling framework, and focuses on the criteria used to validate

104 both transformations. The Eulerian-Lagrangian coupling is thoroughly studied over a series of
 105 numerical examples in Section 5, validating the conservation of mass and momentum. In Sec-
 106 tion 6 the Eulerian-Lagrangian coupling is applied to the study of two phase flow atomization of
 107 a cross flow configuration, previously studied in the work of Herrmann [39]. Concluding remarks
 108 are outlined in Section 7.

109 2. Methodology

110 2.1. Eulerian framework

111 2.1.1. Interface Capturing Method

112 The transport of the interface is done by coupling the level set with the Volume of Fluid
 113 method (VOF), referred to as CLSVOF [40]. The motivation of this coupling is to benefit from
 114 both the second order geometrical accuracy of the level set and the mass conservative properties
 115 of the VOF. In this section, the methodology is briefly introduced, and the reader is referred
 116 to Ménard et al. [16] for a meticulous description of the CLSVOF and its implementation within
 117 our flow solver.

118 The location of the interface is defined from the signed level set distance function $\phi(\mathbf{x})$,
 119 where $\phi(\mathbf{x}) < 0$ indicates the gas fluid phase, $\phi(\mathbf{x}) > 0$ the liquid fluid phase, and $\phi(\mathbf{x}) = 0$
 120 the interface. The volume occupied by the fluid phase (VOF), F , in a cell is obtained from
 121 the *VOFTools* library [41]. Then, the VOF and the level set, F and ϕ , are advected using a
 122 transport equation. For the level set field, it reads

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = 0, \tag{1}$$

123 with \mathbf{u} the fluid velocity vector. The VOF being a passive scalar, the same transport
 124 equation, Eq. 1 is used to advect F . Eq. 1 is solved with a second order conservative operator
 125 split advection scheme [40]. To conserve the numerical stability of our solver, a volume restriction
 126 algorithm is implemented that removes small numerical artifacts of VOF from the computational
 127 domain. It reads for the k th fluid cell as

$$F_k = \begin{cases} 0 & \text{if } F_k < \epsilon_F \quad \text{or} \quad \text{No interface in all neighbor cells} \\ 1 & \text{if } F_k > 1 - \epsilon_F \quad \text{or} \quad \text{No interface in all neighbor cells} \\ F_k & \text{otherwise} \end{cases} \quad (2)$$

128 where ϵ_F is the numerical threshold for the VOF quantity, set to $\epsilon_F = 1 \times 10^{-12}$ and ϵ_ϕ the
129 numerical threshold for the level set distance, set to $\epsilon_\phi = \frac{3}{4}\sqrt{3}\Delta x$, with Δx the mesh spacing.
130 Each time step, the position of the level set at the interface is corrected from the VOF updated
131 field, ensuring conservation of geometric properties and mass. To preserve the sign distance
132 properties of the level set function, a redistancing algorithm is applied at the end of each time
133 step

$$\frac{\partial d}{\partial \tau} = \text{sign}(\phi^n) (1 - |\nabla d|), \quad \text{where } d(\mathbf{x}, \tau)_{\tau=0} = \phi^n(\mathbf{x}, t) \quad (3)$$

134 where τ is a fictitious time, and d is used to ensure the distance property. After solving Eq. 3, the
135 level set field is updated, setting $\phi^{n+1} = d$. Finally, the classical projection method is applied,
136 updating the velocity and the pressure fields (Section 2.1.2).

137 2.1.2. Projection method

138 The fluid phase is considered an incompressible Newtonian fluid subject to the Navier-Stokes
139 equations and reads as

$$\nabla \cdot \mathbf{u} = 0, \quad (4)$$

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) = -\nabla P + \nabla \cdot \mathcal{D} + \mathbf{f}, \quad (5)$$

where ρ is the density, P the pressure, \mathcal{D} the strain rate tensor, and \mathbf{f} , a volume force accounting for the presence of particles, surface tension force, and external forces such as gravity \mathbf{g} . The strain rate tensor is defined as

$$\mathcal{D} = \mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T), \quad (6)$$

140 with μ the dynamic viscosity.

141 A standard projection method is used to solve the system after the interface transport. The
142 first step is to solve the momentum equation excluding the pressure terms at the current time
143 step n . This predictor step reads

$$\mathbf{u}^* = \mathbf{u}^n + \Delta t \left(-(\mathbf{u}^n \cdot \nabla) \mathbf{u}^n + \frac{1}{\rho^{n+1}} (\nabla \cdot \mathcal{D} + \mathbf{f}^n) \right), \quad (7)$$

144 where Δt is the n th time step. The pressure is obtained from the intermediate velocity field \mathbf{u}^*
145 as a solution of an implicit system (Poisson equation)

$$\nabla \cdot \left(\frac{1}{\rho^{n+1}} (\nabla P^{n+1}) \right) = \nabla \cdot \mathbf{u}^*. \quad (8)$$

146 Finally, the velocity at the next time step is obtained as

$$\mathbf{u}^{n+1} = \mathbf{u}^* + \frac{1}{\rho^{n+1}} (-\nabla P^{n+1}). \quad (9)$$

147 The momentum flux computation is discretized with a fifth-order WENO scheme in a con-
148 servative form [18]. The viscous term is discretized with the algorithm of Sussman and Puckett
149 [40]. The pressure, density and viscous jumps across the interface are handled using a ghost fluid
150 method, that consists of extrapolating fluid quantities on both sides of the interface, preventing
151 discontinuities in the derivation of fluid variables for a sharp interface method [42]. The Poisson
152 equation is solved with a Conjugate Gradient preconditioned by a Multi-grid Method coupled
153 with a Red-Black Gauss-Seidel algorithm [43]

154 2.1.3. Time integration

155 The temporal integration is done with a second order TVD Runge-Kutta explicit time
156 scheme. An adaptive time stepping is used based on the convection, viscosity, surface ten-
157 sion and gravity. The adaptive time step, Δt , is estimated from these constraints as in Kang
158 et al. [42]. In the present work, the CFL condition is fixed to $K_{CFL} = 0.3$ to ensure the stability
159 of the approach.

160 *2.2. Lagrangian framework*

161 To circumvent the shortcomings of the ICM, under-resolved droplets are modeled with a
 162 Lagrangian tracking method (Section 2.2.1), and the droplets' momentum is transferred toward
 163 the source terms of the fluid momentum equation (Section 2.2.2). A flow disturbance correction is
 164 coupled with a spatial filtering of the feedback force to prevent over estimation of hydrodynamic
 165 forces experienced by Lagrangian droplets (Section 2.2.3).

166 *2.2.1. Lagrangian transport*

167 The motion of a rigid Lagrangian droplet obeys Newton's second law

$$\frac{d\mathbf{X}_p}{dt} = \mathbf{U}_p, \quad (10)$$

$$m_p \frac{d\mathbf{U}_p}{dt} = \sum \mathbf{F}_p, \quad (11)$$

168 where m_p , \mathbf{X}_p , \mathbf{U}_p , and \mathbf{F}_p are the mass, coordinates, velocity, and sum of the forces acting on
 169 a Lagrangian droplet. The resultant of forces reads

$$\mathbf{F}_p = \mathbf{F}_{p,ext} + \mathbf{F}_{p,fluid}, \quad (12)$$

170 with $\mathbf{F}_{p,ext}$ accounting for the action of external forces on Lagrangian droplets, reduced to the
 171 gravitational acceleration in this work, and $\mathbf{F}_{p,fluid}$ the action of the fluid which reads

$$\mathbf{F}_{p,fluid} = \frac{3}{4} \frac{\rho_f V_p C_D}{D_p} |\mathbf{U}_{slip}| \mathbf{U}_{slip}, \quad (13)$$

172 where V_p and D_p are the volume and diameter of the Lagrangian droplet, \mathbf{U}_{slip} is the difference
 173 between the velocity of the Lagrangian droplet, \mathbf{U}_p , and the velocity of the fluid phase inter-
 174 polated at the position of the droplet, $\mathbf{u}_{f@p}$. The coefficient C_D is a drag coefficient obtained from
 175 the correlation of Schiller and Naumann [44] and varies with respect to the Lagrangian droplet's
 176 Reynolds number

$$Re_p = \frac{\rho_f D_p |\mathbf{U}_{slip}|}{\mu_f}. \quad (14)$$

177 *2.2.2. Momentum coupling*

178 The feedback force accounting for the presence of the droplets is transferred toward the fluid
179 with a smooth regularized kernel function [31]. A Gaussian kernel is used

$$G(\mathbf{x}) = (2\pi\sigma)^{-2/3} e^{-\frac{|\mathbf{x}|^2}{2\sigma^2}}, \quad (15)$$

180 where σ is the length controlling the region of the force spreading. Ideally, the support of the
181 Gaussian kernel is of infinite length, but, for computational efficiency the support is considered
182 of finite length, referred to as compact support. This assumption is valid because the Lagrangian
183 droplet mostly affects its local surrounding. The main drawback of a compact support with a
184 Gaussian kernel is that the momentum transfer is not fully conservative, however by adequately
185 choosing σ we can ensure that at least 99% of the energy is transferred over this compact support.
186 The volume force \mathbf{f}_p in Eq. 5 reads

$$\mathbf{f}_p = \sum_{i=1}^{N_p} \mathbf{F}_{p,i} G(|\mathbf{x} - \mathbf{X}_{p,i}|). \quad (16)$$

187 The analytical discretization of the Gaussian filter for a Cartesian uniform grid is used [38]. It
188 reads for an arbitrary 2D cell $k_{i,j}$

$$G(\mathbf{X}_p) = \frac{1}{V_K} \int_{V_K} G(|\mathbf{x} - \mathbf{X}_p|) d\mathbf{x} = \frac{\left[\operatorname{erf} \left(\frac{x - X_p}{\sigma\sqrt{2}} \right) \right]_{x_i}^{x_{i+1}} \left[\operatorname{erf} \left(\frac{y - Y_p}{\sigma\sqrt{2}} \right) \right]_{y_j}^{y_{j+1}}}{4(x_{i+1} - x_i)(y_{j+1} - y_j)}, \quad (17)$$

189 where $V_k = [x_i, x_{i+1}] \times [y_j, y_{j+1}]$ is the discretized volume of the cell k .

190 *2.2.3. Velocity disturbance correction*

191 The velocity interpolation at the position of the Lagrangian droplet, $\mathbf{u}_{f@p}$, can be decom-
192 posed between two contributions as

$$\mathbf{u}_{f@p} = \tilde{\mathbf{u}}_{f@p} + \mathbf{u}'_{f@p}, \quad (18)$$

193 where $\mathbf{u}'_{f@p}$ is the estimation of velocity disturbance arising from the momentum coupling at
 194 the position of the droplet, and, $\tilde{\mathbf{u}}_{f@p}$ is the reconstruction of the interpolated velocity, $\mathbf{u}_{f@p}$,
 195 filtering the velocity disturbance.

196 An analytical correction to the flow disturbance in Eq. 18 is derived for the Stokes flow
 197 through the regularized momentum contribution of the Lagrangian droplet, and, extended to
 198 finite Reynolds number accounting for the Oseen's approximation of the Navier-Stokes equa-
 199 tions [37, 38]. In the respective works of Balachandar et al. [37] and Evrard et al. [38], a
 200 point-wise correction and an averaged velocity correction based are derived, respectively. Both
 201 methods have been coupled and tested within our flow solver, the averaged correction is con-
 202 served for numerical stability reasons. This correction reads as

$$\tilde{\mathbf{u}}_{f@p} = A(\mathbf{u}_{f@p})_\lambda - \frac{\mathbf{f}_p \psi_{St}(\lambda/\delta) \psi_{Os}(Re_G)}{2\pi\mu_f\delta}, \quad (19)$$

203 where δ is the compact support of integration for a Wendland kernel, linked to the Gaussian
 204 kernel by

$$\delta = \frac{\sigma}{\sqrt{2/9\pi}}, \quad (20)$$

205 used as controlling length in Eq. 17. λ is the size of the averaging regularized support and is
 206 chosen as

$$\lambda = \max(\delta, 2\Delta x), \quad (21)$$

207 and the averaged velocity over the length λ , $A(\mathbf{u}_{f@p})_\lambda$ obtained through the convolution of the
 208 velocity through the regularized kernel function defined in Eq. 15,

$$A(\mathbf{u}_{f@p})_\lambda = \frac{1}{V_\Omega} \int_\Omega G(|\mathbf{x} - \mathbf{X}_p|) \mathbf{u}(\mathbf{x}) d\mathbf{x}, \quad (22)$$

209 with Ω the domain of convolution of the regularized kernel function and V_Ω its equivalent volume.

210 The corrections ψ_{St} and ψ_{Os} are the Stokes and Oseen corrections given in Appendix A.

211 2.2.4. Time integration

212 The Lagrangian quantities are temporally integrated with a second order Runge-Kutta tem-
 213 poral schemes. The coupling between Lagrangian and Eulerian frameworks is split, which gives
 214 more flexibility for both implementations. The coupling follows the steps listed in algorithm 1
 215 for a first order time scheme, where Capital letters indicate Lagrangian quantities.

Algorithm 1: Lagrangian solver coupling with flow solver

```

foreach Lagrangian droplet do
  Interpolate  $\mathbf{u}_{f@p}$  from  $\mathbf{u}^n$ 
  Apply flow disturbance corrections (Section 2.2.3)
  Compute fluid forces  $\mathbf{F}_p^n$ 
  Transport Lagrangian droplets ( $\mathbf{U}_p^{n+1}, \mathbf{X}_p^{n+1}$ , Section 2.2.1)
  Regularize  $\mathbf{F}_p^n$  and add to source terms  $\mathbf{f}^n$  (Section 2.2.2)
end
Add  $\mathbf{f}^n$  to predictor step (Eq. 7).

```

216 3. Analysis of the numerical limits of the ICM

217 In this section, we study the limits of the ICM methods in the simulation of under-resolved
 218 droplets on a classical test case, a sedimented droplet falling in a box [29, 30, 34]. The config-
 219 uration is also used to validate the implementation of the Lagrangian framework (Section 2.2).

220 3.1. Numerical configuration

We analyze the temporal evolution of a sedimented spherical droplet falling in a box under gravity. The computational domain is a rectangular box of size $Lx \times Ly \times Lz$ with $Lx = Lz = Ly/2$ and $Lx = 1 \times 10^{-3} m$. Wall boundary conditions are used everywhere but the top face along y which is set to a outflow boundary condition. The physical properties are taken from Ling et al. [30], $D_p/Lx = 0.1$, with D_p the diameter of the Lagrangian droplet, $\rho^* = \rho_l/\rho_g = 100$, with ρ_l and ρ_g the density of the liquid and the gas, respectively, and $\mu^* = \mu_l/\mu_g = 10$, the viscous ratio, only relevant to the Eulerian droplet. Surface tension forces are not considered in

the Eulerian droplet [29]. The gravitational acceleration is set to $\mathbf{g} = 9.81 \text{ m/s}^2$. The terminal velocity of the droplet is obtained by balancing gravity and drag forces (Eq. 13). To account for the confined environment, the terminal velocity of the droplet is multiplied by a semi-empirical parameter modeling the confined environment [45], giving

$$V_{\tau_p} k_\eta = 4.112 \times 10^{-2} \text{ m/s}, \quad (23)$$

221 with k_η set to $k_\eta = 0.824$ for this configuration. This set of parameters gives a particles' Reynolds
 222 number of $Re_p = 0.4112$.

223 The Eulerian droplet can be compared to the Lagrangian droplet only if it remains spherical.
 224 Subsequent snapshots of the interface of the Eulerian droplet falling in the box are presented in
 225 figure 1. The results show that these physical parameters almost maintain the spherical shape
 226 of the Eulerian droplet, allowing the comparison of both methods.



Figure 1: Successive representations of the interface of the sedimented Eulerian droplet falling within a box. Interface is shown at distances $\phi(x) = [-\Delta x; 0; \Delta x]$, in green, red, green, respectively. Results are obtained at $D_D/\Delta x = 6.4$ at $t/\tau_p = [0, 1.8, 3.6, 4.5]$, from top to bottom.

227 Since we are interested in the performance of ICM method in the coarse regime, we vary the
 228 numerical resolution of ICM simulation in the range $D_D/\Delta x = 3.2, 4.8, 6.4, 8$ and 16, with D_D
 229 the diameter of the droplet. Simulations with finer resolution are used to compute a reference
 230 solution for the ICM method. Simulations below the numerical resolution $D_D/\Delta x = 3.2$ are
 231 unstable. On the other hand, the two way method employed in the present Eulerian-Lagrangian
 232 coupling is also tested. Thus, the two way approach simulations vary over the range $D_p/\Delta x =$
 233 $0.4, 0.8, 1.6, 3.2$ and 4.8. This corresponds to the numerical resolution where the resolved ICM

234 cannot accurately transport the droplets. The size of the regularized kernel support affects the
 235 drag force experienced by the Lagrangian droplet. Therefore, we vary the length of the Gaussian
 236 regularized kernel support, δ , over several Lagrangian droplets' radii (R_p) $\delta = 3R_p, 5R_p, 7R_p$ and
 237 $10R_p$, where the upper bounds are given by the size of the box. The two way coupling results
 238 without flow disturbance corrections are obtained with the method presented in Ling et al. [30]
 239 to transport the small droplets in the Eulerian-Lagrangian coupling. The averaging kernel length
 240 varies accordingly to δ (Eq. 21).

241 3.2. Results

242 3.2.1. Lagrangian solver

243 The temporal evolution of the Lagrangian droplets' velocity scaled by the terminal velocity,
 244 Eq. 23, is presented in figure 2. The simulation time is scaled by the particles' characteristic
 245 time $\tau_p = \frac{\rho_p D_p^2}{18\mu_f}$. This figure is organized as follows, the columns present the results with the self-
 246 disturbance correction (left), and without (right). In the latter, a trilinear interpolation is used
 247 to obtain $\mathbf{u}_{f@p}$. The four rows show the evolution of length of the Gaussian regularized kernel
 248 support δ (increases from top to bottom). The color map indicates the numerical resolution,
 249 and, the solid black line shows the results for the equivalent one way coupling. The one way
 250 results are used as a numerical reference solution because flow disturbance is null, $\mathbf{u}'_{f@p} = 0$.

251 For both two way approaches, the number of fluid cells across the diameter of the particle
 252 affects the temporal evolution of the particle and its terminal velocity. We observe an overestim-
 253 ation of the terminal velocity proportional to the number of fluid cells across the diameter, the
 254 worst results are obtained at $D_p/\Delta x = 4.8$. These observations agree with the literature [37, 38].

255 The results with the self-disturbance correction reduces the influence of the flow disturbance
 256 in the two way coupling. For example, at $\delta = 3R_p$ and $D_p/\Delta x = 4.8$, the correction prevents the
 257 solver from diverging (the results without correction are numerically unstable). Yet, at $\delta = 3R_p$
 258 and $D_p/\Delta x = 4.8$ the terminal velocity is overestimated by a factor 1.5. To increase accuracy
 259 at high $D_p/\Delta x$ the size of the spatial filter, δ , can be increased. For example at $\delta = 10R_p$, the
 260 reference results are recovered. Nonetheless, the larger is the support of the regularized function,
 261 the more expensive is the two way coupling, i.e. integration of the flow variable and spreading
 262 of the particles' momentum on a larger compact support. Therefore, the choice of δ results from
 263 a trade-off between physical accuracy and computational cost.

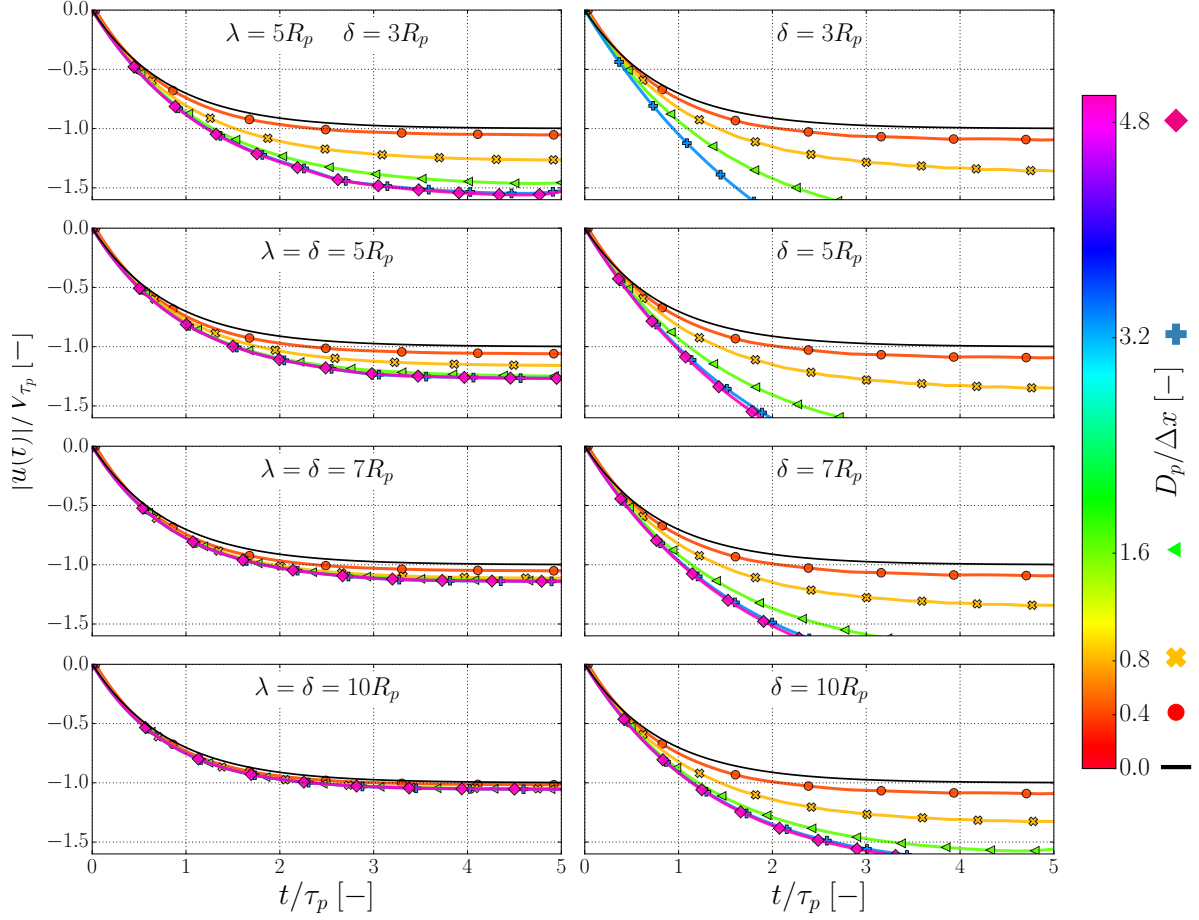
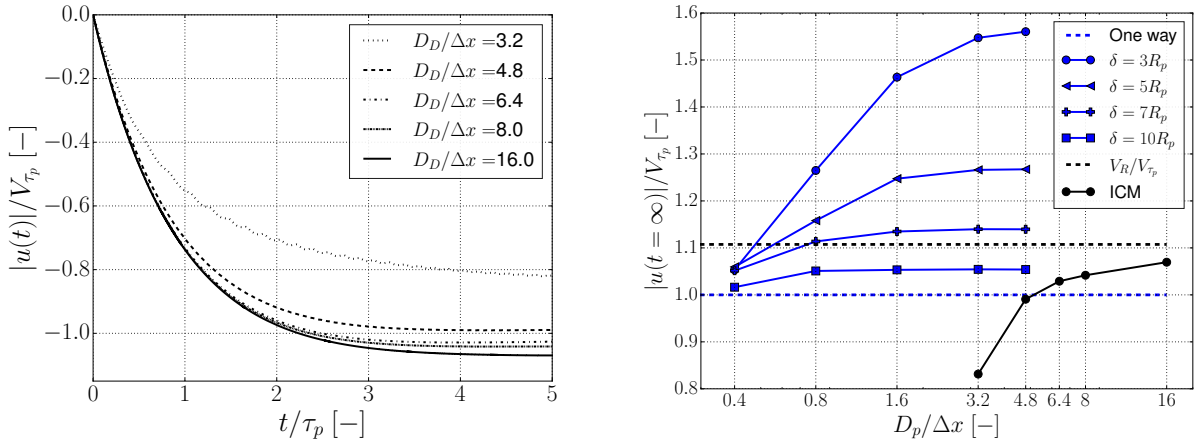


Figure 2: Temporal velocity evolution of the sedimented free-falling particle scaled by the terminal velocity V_{τ_p} using the two way Lagrangian coupling. Left column: two way coupling including self-disturbance corrections on the averaged velocity interpolation Eq. 19. Right column: without corrections using a trilinear interpolation. Results are obtained for four support size, $\delta = [3R_p; 5R_p; 7R_p; 10R_p]$ (from top to bottom) and numerical resolutions $D_p/\Delta x = [0.4; 0.8; 1.6; 3.2; 4.8]$ (color map and symbols). Black solid line shows the one way coupling evolution.

264 *3.2.2. Eulerian solver*

265 The ICM results are shown in the figure 3a. The ICM results converge at a terminal velocity
 266 higher than the reference one. This is because the reference terminal velocity is given for a solid
 267 spherical particle and the ICM resolves two-phase flow.

268 A new reference velocity is computed for these results using a Richardson extrapolation
 269 from the results obtained at $D_D/\Delta x = 6.4, 8$ and 16 . This value is $V_R = 4.55 \times 10^{-2}$ m/s. At
 270 low resolution, the reference terminal velocity of the droplet is underestimated by the coarse
 271 numerical resolution. For example, at $D_D/\Delta x = 3.2$, we observe an underestimation of 26.3%
 272 of the terminal velocity. For numerical resolutions higher than $4.8D_D/\Delta x$ the error drops below
 273 10%, and the ICM method recovers the reference results under spatial refinement.



(a) Temporal evolution of the Eulerian droplet (ICM) velocity against characteristic time for several numerical resolutions.

(b) Spatial convergence of the terminal velocity for the Eulerian droplet and two way Lagrangian coupling with self-disturbance correction varying the support size δ . Reference: dashed line.

Figure 3

274 *3.2.3. Numerical limits*

275 The snapshots of the velocity fields are extracted at the same time step for the three studied
 276 configuration, at $D_p/\Delta x = 4.8$, and are reported in figure 4. The main differences are the
 277 location of the droplet at the same time step and the local velocity field in the surrounding of
 278 the droplets. The fluid velocity reaches a higher magnitude with the ICM method, meanwhile
 279 it is significantly lower with the two way coupling without corrections. These differences do
 280 not alter the main velocity pattern: the recirculation in-between the droplet and the walls is
 281 observed for all cases. The location of the droplets agrees with the temporal evolution of the
 282 velocity of the droplets, see figure 2 and left figure 3b; this shows the importance of the velocity
 283 disturbance correction in the two way coupling.

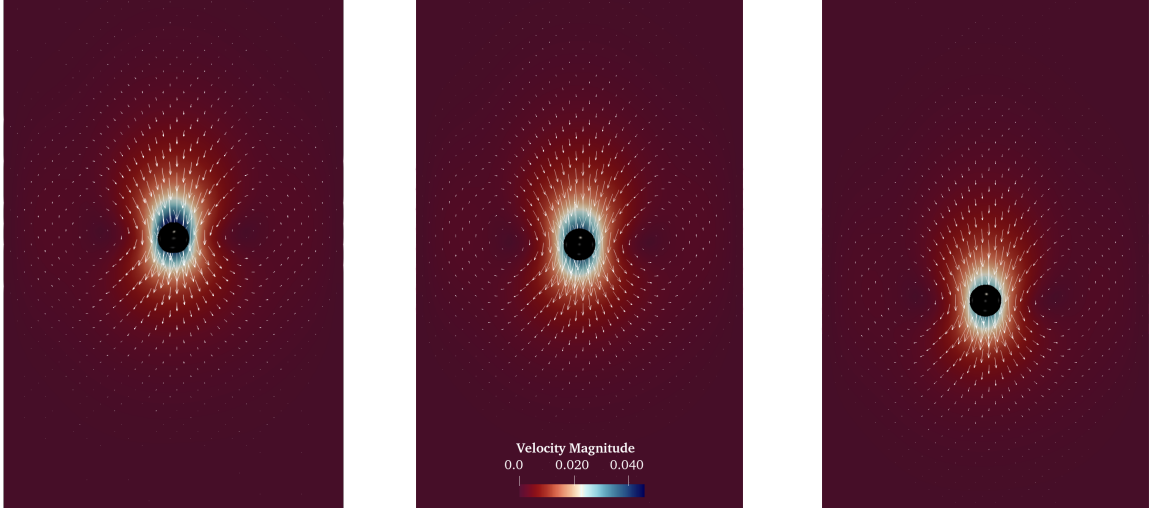


Figure 4: Velocity field around the free-falling sedimented droplet at $D_p/\Delta x = 4.8$ at time $t/\tau_p = 1.8$. Left: CLSVOF, Center: two way Lagrangian method with correction, Right: two way Lagrangian method without correction (filter length $\delta = 7R_p$).

284 The terminal velocity obtained with the ICM and the two way Lagrangian coupling, including
 285 the self-disturbance corrections, are compared for the entire spectra of numerical resolutions.
 286 The terminal velocity is scaled by the reference velocity V_{τ_p} , and the results are shown in
 287 figure 3b. The reference velocity of the ICM method obtained from the Richardson extrapolation
 288 of our results is also reported. Above 4.8 fluid cells across the diameter, the ICM accurately
 289 transports the droplets and the results are close to the Richardson's reference velocity. For
 290 $D_p/\Delta x = 4.8$, only the two way results obtained with the length $\delta = 10R_p$ improves the results
 291 of ICM method. At $D_p/\Delta x = 3.2$, the necessary filter width to improve the ICM method is of
 292 $\delta = 7R_p$. In addition, the results below $\delta = 7R_p$ do not improve the transport of the droplets
 293 in the range $D_p/\Delta x \geq 3.2$. Therefore, the filter length δ is always set to $\delta = 7R_p$ if not stated
 294 otherwise in the manuscript.

295 4. Eulerian-Lagrangian coupling

296 4.1. From the Eulerian droplet toward the Lagrangian particle

297 This section discusses the steps, from the selection of criteria of transformation toward the
 298 reconstruction of the Eulerian fields after transformation, required to switch from Eulerian
 299 framework toward the Lagrangian one, and vice-versa. The first step consists in the detection
 300 of all Eulerian and Lagrangian droplets in the computational domain.

301 While the knowledge of the Lagrangian droplets' coordinates is natural in the Lagrangian
 302 framework, this is not straightforward for the ICM. A labeling algorithm is used to identify all

303 the fluid structures by associating a group of neighboring fluid cells [26, 27], that can represent
 304 the liquid core of an atomized jet, a ligament, a droplet, etc.

305 From this algorithm can be derived Lagrangian statistics, such as the volume of the droplet,
 306 used to define a numerical resolution criterion, the distance to other structures, or to qualify the
 307 droplet as spherical under a morphological analysis. These steps are summarized in algorithm 2.

Algorithm 2: Eulerian-Lagrangian coupling: Eulerian droplet transformation.

```

  Get labeling field (Section 4.1.1)
  foreach Labelled structure j do
    Compute structure volume  $V_j$  and equivalent diameter  $D_{eq,j}$  (Section 4.1.1)
    if Droplet under resolved then
      Compute distance to other fluid structures  $\mathcal{L}_D$  (Section 4.1.3)
      if Droplet isolated then
        Compute morphological parameters  $\alpha_j$  and  $\iota_j$  (Section 4.1.4)
        if Droplet is spherical then
          | Add  $j$  to the droplets' transformation list
        end
      end
    end
  end
  foreach Droplet in transformation list do
    Update VOF and level set fields (Section 4.1.5)
    Update Velocity field (Section 4.1.6)
    Remove Eulerian droplet and add it to Lagrangian droplet list
  end

```

308 *4.1.1. Detection of fluid structures*

309 **General algorithm**

310 The implementation of the labeling algorithm combines both the VOF and level set fields,
 311 and is applied for the k th cell as

$$\mathcal{X}_k = \begin{cases} i_k & \text{if } F_k \geq \epsilon_F \text{ and } \phi_k \geq -\epsilon_\phi \\ 0 & \text{otherwise} \end{cases} \quad (24)$$

312 where \mathcal{X} is the label field, i is the value associated to the k th fluid cell, and ϵ_F and ϵ_ϕ are
 313 thresholds based on the desired accuracy. Here ϵ_F is set to 10×10^{-10} and ϵ_ϕ to $\sqrt{\frac{3}{4}\Delta x^2}$ (being
 314 the distance from the edge of a cube to its center). The level set is used to filter small VOF
 315 artifacts. From the labelled field a linked list connects all labelled fluid cells with a value strictly
 316 superior to 0 to its neighbors. Following the required MPI communications, all the labelled

317 belonging to the fluid cells in a fluid structure are switched to the smallest value to provide a
 318 unique label to each droplet.

319 Figure 5 shows the three steps of the algorithm, 1) identification of the fluid structures based
 320 on the VOF and level set fields, 2) labeling of all the fluid cells \mathcal{X} , 3) fix the label of all fluid
 321 cells in the same fluid structure to the minimum value after MPI communications. The last
 322 step illustrates the configuration where a small droplet, $\mathcal{X} = 3$, is grouped with a neighboring
 323 structure because of the poor numerical resolution.

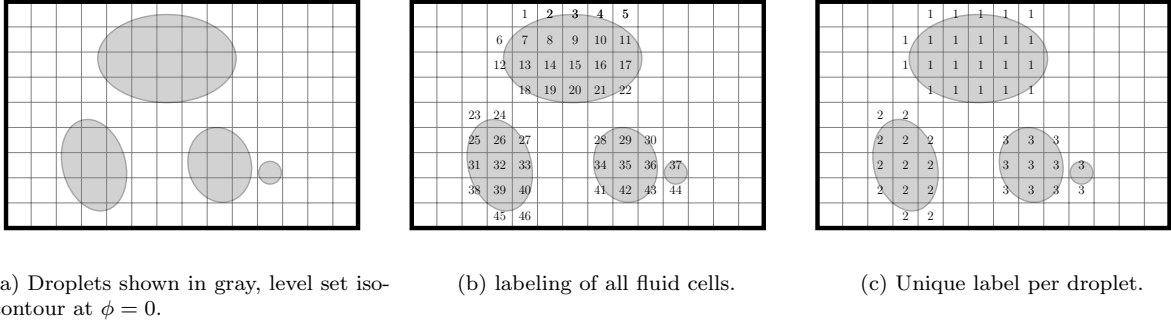


Figure 5: Labeling algorithm.

324 Eulerian droplets tracking

325 The label field \mathcal{X} is used to track Eulerian droplets coordinates, and to detect coalescence
 326 and break up events. The volume-based centroid of the droplets is obtained as

$$\mathbf{X}_j = \sum_{k=1}^{N_{cells}} F_k \mathbf{x}_k \delta_{k,j}, \quad (25)$$

327 with \mathbf{X}_j the center of the j th fluid structure, F_k , \mathbf{x}_k and \mathcal{X}_k being the volume fraction, the
 328 center and the label of the k th fluid cell, respectively. $\delta_{k,j}$ is the Kronecker-Delta set to $\delta_{k,j} = 1$
 329 if $k = j$ and 0 if $k \neq j$.

330 To track the spatial evolution of these structures, the Euclidean distance between the center
 331 of the j th fluid structure at time step n and the i th structures at the previous time step is
 332 computed. To reduce uncertainties a first order temporal integration scheme is used to advect
 333 the center of all the i th fluid structures at the previous time step $(n - 1)$, and the comparison
 334 reads

$$|\mathbf{X}_j^n - \mathbf{X}_i^{n-1} + \Delta t \mathbf{V}_i^{n-1}| < \eta \Delta x, \quad (26)$$

335 with η a constant adapting to the calling frequency. This constant is set to $\eta = 1/2$ when the
 336 algorithm is employed at every time step.

337 In addition to the center-to-center distance computation, the volume variation is computed
 338 between two paired structures to ensure an accurate tracking. For the j th structure, the volume
 339 is obtained with

$$V_j = \sum_{k=1}^{N_{cells}} F_k \Delta x^3 \delta_{k,j} \quad (27)$$

340 An unpaired structure often results from a breakup or a coalescence event. To enhance the
 341 statistics, two algorithms are implemented to detect these events, and are given in Appendix B
 342 and Appendix C.

343 4.1.2. Numerical resolution criterion

344 A numerical resolution criterion, based on the fluid mesh spacing and the numerical size of
 345 the droplet, is defined. The volume-based-equivalent diameter of the studied droplet is used
 346 to compute the numerical size of the droplet. It is obtained from the volume of the j th fluid
 347 structure (see Eq. 27)

$$D_{eq} = 2 \left(\frac{3}{4\pi} V_j \right)^{1/3}, \quad (28)$$

348 used to discriminate under resolved droplets,

$$D_{eq}/\Delta x \leq \epsilon_V,$$

349 with ϵ_V a numerical-resolution-based accuracy threshold.

350 Based on the analysis of the limits of the present ICM method in the simulation of under-
 351 resolved droplets, see Section 3, the value of ϵ_V is set to $\epsilon_V = 4$ if not stated otherwise in the
 352 manuscript.

353 *4.1.3. Distance criterion \mathcal{L}_D*

354 The distance criterion, \mathcal{L}_D , ensures that the Eulerian droplet is isolated before an eventual
 355 transformation. This prevents topology changes for the surrounding droplets resulting from the
 356 modification of the Eulerian fields, discussed in the Sections 4.1.5 and 4.1.6. From numerical
 357 experiment, the minimum distance \mathcal{L}_D must satisfy

$$\mathcal{L}_D \geq D_{eq}, \quad (29)$$

358 to consider the Eulerian droplet isolated. This value prevents topology changes at the trans-
 359 formation from Eulerian droplet toward Lagrangian droplet.

The inequality in Eq. 29 consists of looping over the fluid cells near the droplet to detect any other fluid structure. The distance criterion is validated for the j th structure if all the fluid cells in a box given by

$$|x_{x,k} - (X_{x,j} + D_{eq,j}/2)| \leq D_{eq,j}, \quad |x_{y,k} - (X_{y,j} + D_{eq,j}/2)| \leq D_{eq,j}, \quad |x_{z,k} - (X_{z,j} + D_{eq,j}/2)| \leq D_{eq,j},$$

360 have a label equal to zero or to the structure label. In the previous equation, \mathbf{X}_j is the center
 361 of mass of the j th structure and \mathbf{x}_k the center of the Eulerian grid.

362 *4.1.4. Morphological criterion*

363 **Parameters definition**

364 The morphological analysis of a fluid structure in 2D has been widely analyzed, see the
 365 detailed literature review of existing parameters of Ghaemi et al. [46]. On the other hand,
 366 few parameters exist to characterize fluid structures in 3D, such as the eccentricity parameter
 367 defined in Herrmann [26] who scales the maximal distance to the interface from the center of the
 368 droplet by the volume-based-equivalent radius of the droplet, or the sphericity parameter defined
 369 in Zuzio et al. [29], Arienti et al. [47] who scales the minimum distance to the interface from
 370 the center of the droplet by the volume-based-equivalent radius of the droplet. In a previous
 371 work [48], our research group analyzed 3D morphological parameters, and showed that the aspect
 372 ratio [49], and the irregularity [50], are relevant morphological parameters to study the shape of
 373 a 3D droplet. The aspect ratio, α , reads

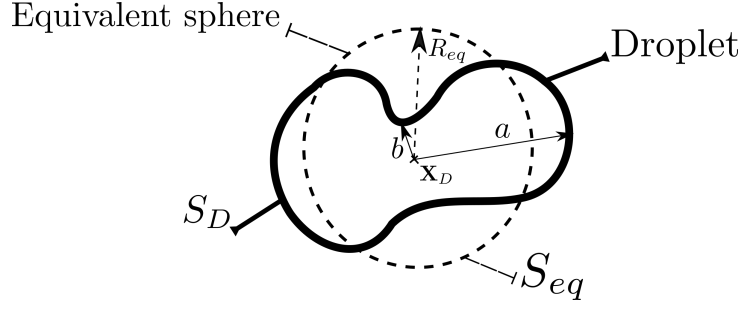


Figure 6: Construction of the aspect ratio α and irregularity ι from the lengths a , b and quantities of surface S_D , $S_{eq} = 4\pi R_{eq}^2$, for a peanut like droplet.

$$\alpha = \frac{b}{a}, \quad (30)$$

374 with a and b the maximum and minimum distances from the center of mass of the droplet to
 375 its interface. The irregularity ι reads

$$\iota = \frac{S_S}{S_D}, \quad (31)$$

376 with S_S the surface of the volume-based-equivalent sphere of radius R_{eq} , see Eq. 28, and S_D the
 377 surface of the droplet. The computation of the quantities a , b , S_D for a droplet and R_{eq} for the
 378 equivalent sphere is schemed in figure 6. These two parameters are bounded over $[0; 1]$ with 1
 379 for a perfect sphere and 0 for an infinite cylinder.

380 **Parameter thresholds**

381 The goal of this numerical test case is to provide a value for the parameter thresholds based
 382 on the irregularity and the aspect ratio. The Eulerian droplets candidate to transformation are
 383 under-resolved, see Section 4.1.2; Chéron et al. [48] show that it results in an overestimation of
 384 the deformation of the droplets. Thus, the numerical accuracy of the aspect ratio and irregularity
 385 is studied for realistic droplets in a spray by extending the spatial convergence analysis of Chéron
 386 et al. [48] to spheroidal shapes. The results of this numerical test case is used to provide a
 387 value for the parameters thresholds based on the irregularity and the aspect ratio, ϵ_ι and ϵ_α ,
 388 respectively.

389 In this numerical test, the spheroid is created using an analytical equation, and is centered
 390 in a cubic domain of size $4D_{eq}$. The morphological parameters are directly computed without

391 solving the fluid equations. For coarse resolution, the location of the centroid of the spheroid
 392 affects the estimation of the morphological parameters, creating a mesh dependency. Thus,
 393 several simulations are performed varying the location of the centroid of the spheroid, and
 394 averaged, maximum and minimum values are reported.

395 The initial shape of the spheroids is based on the aspect ratio and varies in the range $\alpha = 0.5$
 396 to 1 with an increment of 0.05. The numerical resolution of the spheroids varies in the range
 397 $D_{eq}/\Delta x = 2$ to 36, with a volume

$$V_D = \frac{4}{3}\pi ab^2 \quad \text{with } a \geq b. \quad (32)$$

398 The averaged, maximum and minimum values are reported in figure 7a for the aspect ratio,
 399 α , and in figure 7b for the irregularity, ι (for clarity not all the results are shown). The two
 400 parameters converge toward their expected values for well resolved interfaces, regardless of the
 401 initial deformation of the spheroid. At coarse resolution, the mean of both parameters always
 402 underestimate the expected value, thus over-estimating the deformation of the droplets. For the
 403 aspect ratio, the more flattened is the spheroid the higher is the overestimation. For instance,
 404 at $\alpha = 0.5$, 10 fluid cells across the diameter are required to reach an error of 1%, meanwhile
 405 accurate results are obtained with 4 fluid cells across the equivalent diameter when $\alpha \geq 0.85$.
 406 The same variation is observed for the extreme values. In opposition to the aspect ratio, the
 407 spatial convergence of the mean, minimum, and maximum irregularity parameter does not show
 408 a dependence to the shape. For example at $D_{eq}/\Delta x = 4$, a mean error below 10% is reached for
 409 all spheroids.

410 The average values of aspect ratio and irregularity show an over-estimation of the deforma-
 411 tions of the droplets in the coarse regime. To circumvent the over-estimation of the shape de-
 412 formation, the criteria of transformations based on the morphological parameters α and ι must
 413 allow ‘non-spherical’ droplets to be transformed. To do so, their values are set to $\epsilon_\alpha = 0.65$ for
 414 the aspect ratio based threshold, and $\epsilon_\iota = 0.85$ for the irregularity based threshold.

415 4.1.5. Eulerian transformation: reconstruction of the level set and VOF

416 At the transformation from Eulerian droplet toward Lagrangian droplet, the level set and
 417 VOF fields represent an Eulerian droplet that no longer exist in the Eulerian framework. In
 418 the literature, the methodologies to reconstruct the VOF and level set fields vary. In our flow

419 solver, the VOF field is updated setting

$$F_k = \begin{cases} 0 & \text{if } \mathcal{X}_k = \mathcal{X}_j \\ F_k & \text{otherwise,} \end{cases} \quad (33)$$

420 and the level set, setting

$$\phi(\mathbf{x})^{rec} = \min \left(\phi(\mathbf{x}), \sqrt{|\mathbf{x}_D - \mathbf{x}|^2} - 6D_{eq} \right), \quad (34)$$

421 over the entire computational domain to conserve the continuous description of the level set.

422 In Eq. 34 the negative signed distance ensures that the fluid phase is removed (in our solver

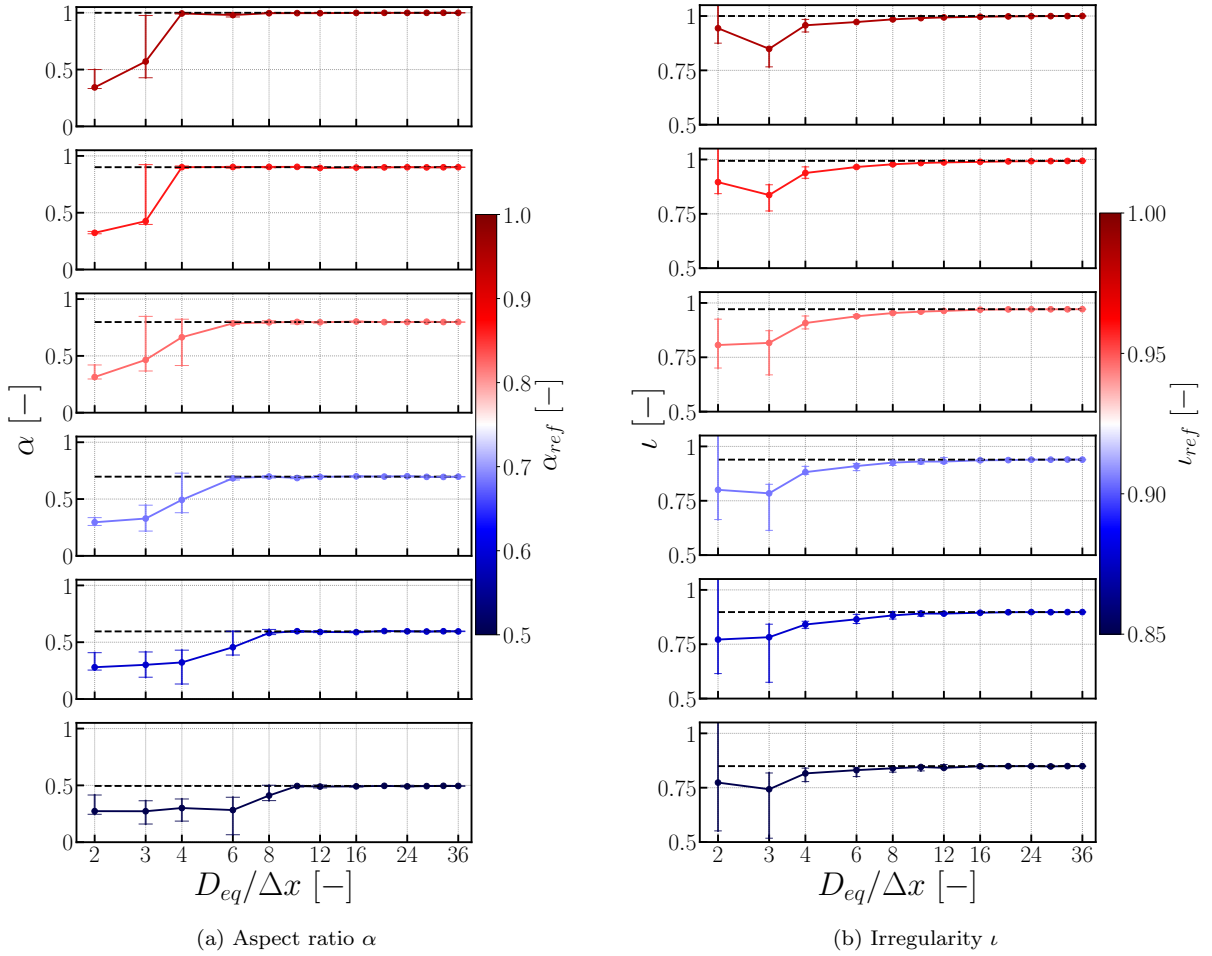


Figure 7: Spatial convergence of the aspect ratio α , figure 7a, and the irregularity ν , figure 7b, for a spheroid varying $a : b$. Black dashed line is the reference value of the morphological parameter. The error bar indicates the maximum and minimum values obtained varying the location of the spheroid center.

423 $\phi > 0$ is for the liquid phase). The coefficient 6 has been fixed after some numerical test in our
 424 numerical solver. It prevents the reconstruction of a liquid droplet during the redistance step
 425 (Eq. 3).

426 4.1.6. Eulerian transformation: reconstruction of the velocity field

427 The transformation of the Eulerian droplet toward the Lagrangian droplet breaks the conser-
 428 vation of the momentum. Hereby reconstruction of the velocity field, Ling et al. [30] circumvent
 429 this inconsistency in the momentum equation. Their solution consists of defining a box centered
 430 on the particle and to modify the velocity field inside this box using a first order linear interpola-
 431 tion from the fluid cells' velocity at the faces of the box. This updated velocity field is divergence
 432 free only if the velocity at the faces of the box is divergence free and the divergence components
 433 are constant within the area of reconstruction. Figure 8 illustrates the reconstruction of the
 434 velocity field after the transformation of an Eulerian droplet.

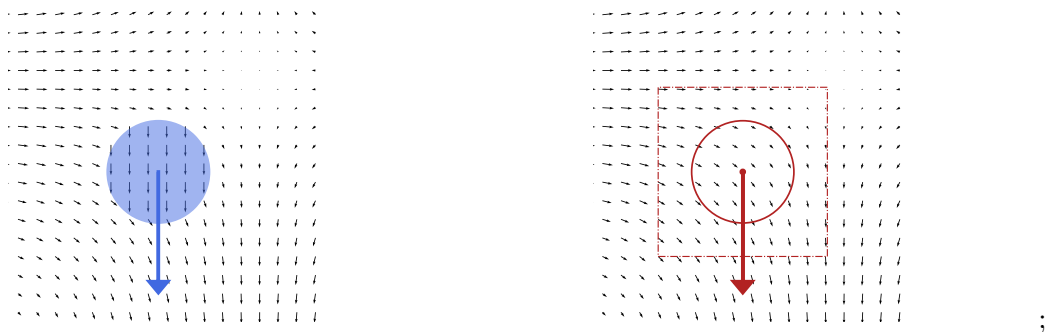


Figure 8: Reconstruction of the velocity field after the transformation of an Eulerian droplet (in blue) toward a Lagrangian droplet (in red). Red box indicates the area of reconstruction.

435 Although this transformation does not guarantee a solenoid vector field at the transformation
 436 step, it provides satisfactory results and is shown to enhance momentum conservation.

437 4.2. From the Lagrangian particle toward the Eulerian droplet

438 The Lagrangian droplets are allowed to transform toward Eulerian droplet to capture the
 439 interface topology changes arising from the coalescence of droplets in spray. The implementation
 440 is discussed within Section 4.2, with a special care on the reconstruction of the Eulerian fields
 441 at the transformation, and the main steps are summarized in algorithm 3.

442 4.2.1. Distance criterion \mathcal{L}_P

443 The distance from the center of the particle toward the closest interface is obtained through
 444 a linear interpolation at the position of the particle toward the level set field $\phi(\mathbf{X}_p)$. From

Algorithm 3: Eulerian-Lagrangian coupling: Lagrangian droplet transformation.

```
foreach Lagrangian droplet  $j$  do
  Compute distance to Eulerian droplets (Section 4.2.1)
  if Lagrangian droplet near Eulerian droplet then
    | Add  $j$  to the Lagrangian droplets' transformation list
  end
end
foreach Lagrangian droplet in transformation list do
  Update VOF and level set fields (Section 4.2.2)
  Update Velocity field (Section 4.2.3)
  Remove Lagrangian droplet and add it to Eulerian droplet list
end
```

445 our analysis, the distance criterion \mathcal{L}_P and \mathcal{L}_D cannot be equal in order to avoid successive
446 transformations from the Eulerian toward the Lagrangian frameworks. Therefore, the distance
447 criterion \mathcal{L}_P and \mathcal{L}_D are set to

$$\mathcal{L}_D = 2\mathcal{L}_P,$$

448 to favor the transformation from Eulerian droplet toward Lagrangian particle.

449 *4.2.2. Lagrangian transformation: reconstruction of the level set and the VOF*

450 **Reconstruction of the Eulerian fields**

451 The reconstruction of the ICM fields at the Lagrangian toward Eulerian transformation has
452 not been of particular interest in the literature. The update of the ICM method follows the
453 general algorithm of the CLSVOF [16] (Section 2.1.1). The level set is reconstructed using a
454 sphere equation, based on the radius of the Lagrangian droplet R_p . Next, the VOF is integrated
455 over the new level set field, and the redistancing algorithm is used to recover the level set
456 distance properties. This procedure is shown for a Lagrangian droplet (in red) moving toward
457 an Eulerian droplet (in blue) in figure 9. Step 1 computes \mathcal{L}_P from a linear interpolation of
458 $\phi(\mathbf{X}_p)$. Following the transformation, Step 2 updates the Eulerian fields to account for the new
459 Eulerian droplet. Step 3 is to iterate the redistancing algorithm until the level set distance
460 properties are recovered.

461 **Mass conservation improvement**

462 The transformation from Lagrangian droplet toward Eulerian droplet yields to an over-
463 estimation of the volume occupied by the droplet at the reconstruction of the interface step.

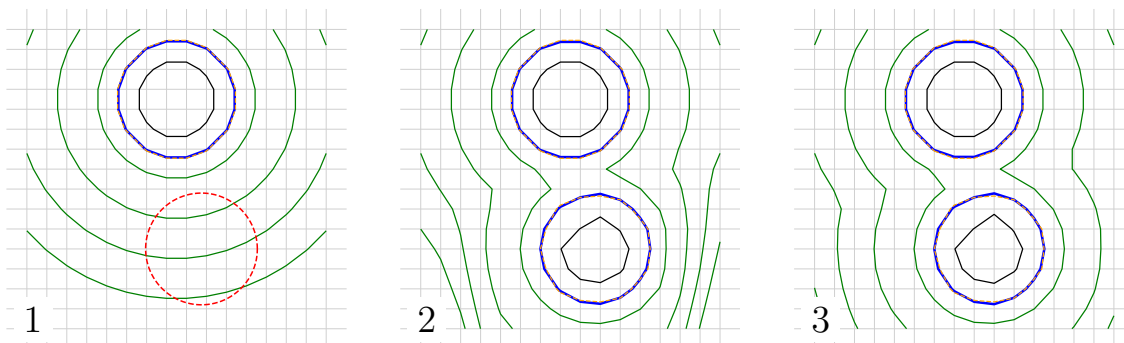
464 A line, or plane equation in 3D, is used to reconstruct the VOF based on the level set of a
 465 sphere. Although a minimization algorithm over a 9-point stencil, in 2D, is used to minimize
 466 the distance between the level set and the reconstructed line equation, a line equation cannot
 467 represent a parabolic surface. Therefore, the error on F for the k th cell is proportional to the
 468 numerical resolution, as illustrated in left figure 10 for a cell k .

469 To reduce the overestimation, we seek for the radius of reconstruction that minimizes the
 470 error $|V_D - V_p|$, with V_D and V_p the volumes of the reconstructed Eulerian droplet and Lagrangian
 471 droplet, respectively, considering two methodologies. The first one substitutes R_p by a radius
 472 R_p^* , obtained from a parametrization

$$R_p^* = R_p - \frac{1}{4}\Delta x^3,$$

473 schemed in the left figure 10. The second relies upon an iterative Newton minimization algorithm
 474 to substitute R_p by an optimal value R_p^* that minimizes the error $|V_D - V_p|$. It consists in the
 475 reconstruction of the Eulerian fields, level set and VOF, over a fictitious domain, centered on the
 476 Lagrangian droplet centroid, of length $2D_{eq}$, to estimate the reconstructed volume V_D , satisfying
 477 an accuracy threshold.

478 Both implementations are tested along with the reconstruction of the ICM fields based on the
 479 true radius of the Lagrangian droplet. The numerical experiment consists of the transformation
 480 of a Lagrangian droplet varying both its numerical resolution, here in the range $D_p = 2\Delta x$ to
 481 $D_p = 12\Delta x$, and the centroid location (the center varies over the mesh spacing, as in the spatial
 482 convergence analysis of Section 4.1.4). The accuracy criterion of the Newton algorithm is set to



(a) Step 1: A Lagrangian particle in the vicinity of an Eulerian droplet. (b) Step 2: modification of the Eulerian fields after Lagrangian transformation. (c) Step 3: redistancing algorithm is used to recover the level set distance properties.

Figure 9: Transformation of a Lagrangian particle toward Eulerian droplet. Particle surface: red dashed line, level set levels: $\phi < 0$ solid green, $\phi = 0$ solid blue, $\phi > 0$ solid black, VOF planes: orange dashed line.

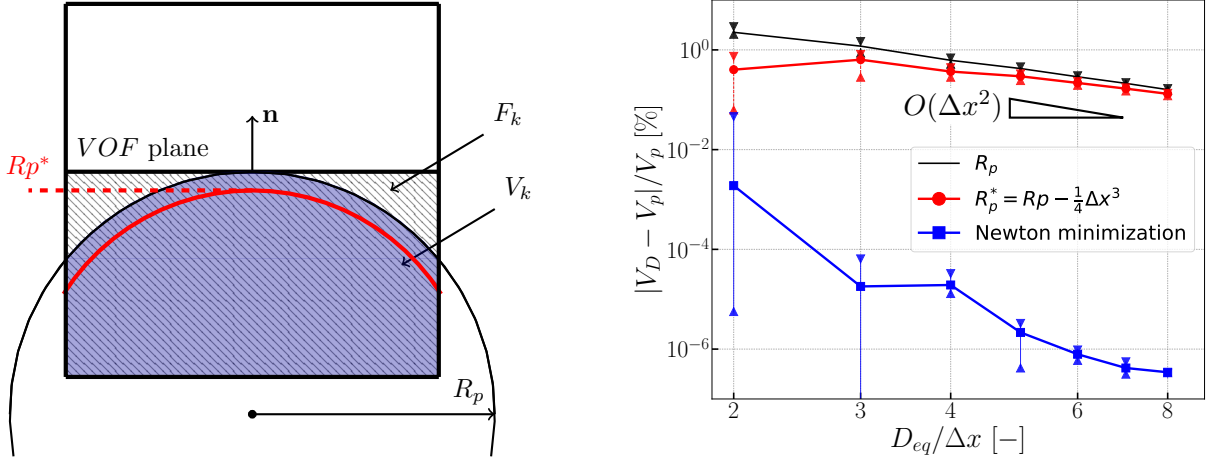


Figure 10: Error on the volume conservation. Left: volume fraction reconstruction from the level set (Section 2.1.1). Right: Spatial convergence error $|V_D - V_p|$.

483 10^{-5} , the maximum number of iterations to 10.

484 The results of the spatial convergence of the volume variation $|V_D - V_p|$ is shown in figure 10.
 485 The results of the ICM and the R_p^* substitution converge with a second order of spatial accuracy.
 486 In addition, the results using R_p^* always improves the volume conservation, for example at coarse
 487 numerical resolution, $D_p/\Delta x = 2$, the error is reduced of one order of magnitude with respect
 488 to the ICM. The results obtained with the Newton minimization algorithm always significantly
 489 improve the mass conservation regardless of the numerical resolution for a reasonable number
 490 of iterations.

491 In the manuscript, the Newton minimization algorithm is used for the simulations of valida-
 492 tion. For the analysis of the jet, the retraction of the radius methodology is used to reduce the
 493 overall computational cost in massively parallel simulations.

494 4.2.3. Lagrangian transformation: reconstruction of the velocity field

495 At Lagrangian transformation, the velocity field is reconstructed as in Ling et al. [30]. It
 496 consists in setting the velocity of the particle within the fluid cells *inside* the reconstructed
 497 Eulerian droplet. They also account for the flow disturbance induced by the two-way coupling
 498 and propose a correction to filter this disturbance. This correction is natural to our framework
 499 because the flow disturbance correction derived in Evrard et al. [38] is used.

500 4.3. Eulerian-Lagrangian coupling with the two phase flow solver

501 The coupling between the flow solver and the Eulerian-Lagrangian framework is presented as
 502 a flow chart in figure 11. The classical time loop for our flow solver, that includes the transport

503 of interfaces, transport of Lagrangian droplets, resolution of the Navier-Stokes equations with
 504 the projection method, the Eulerian-Lagrangian coupling is applied.

505 The methodology follows the organization of Section 4.1 for the Eulerian droplets and Sec-
 506 tion 4.2 for the Lagrangian droplets. The values used for the criteria of transformation, presented
 507 in Sections 4.1 and 4.2 are summarized in table 1. The droplets qualifying for transformation
 508 are stored in a general list, used to reconstruct the Eulerian fields. Then, the list storing the
 509 droplets' information is updated and shared with neighboring processors. This step concludes
 510 the current time step.

Criterion	Symbol	Value	Definition
<i>From Eulerian droplet toward Lagrangian droplet</i>			
Numerical resolution	ϵ_V	4.	Section 4.1.2
Distance from other Eulerian droplets	\mathcal{L}_D	$2D_{eq} \geq \mathcal{L}_D$	Section 4.1.3
Aspect ratio	ϵ_α	0.65	Section 4.1.4
Irregularity	ϵ_t	0.85	Section 4.1.4
<i>From Lagrangian droplet toward Eulerian droplet</i>			
Distance from other droplet	\mathcal{L}_P	$\mathcal{L}_P \leq \mathcal{L}_D/2$	Section 4.2.1

Table 1: Summary of the criteria of transformation for Eulerian toward Lagrangian droplets transformation, and vice-versa.

511 5. Validation

512 5.1. Particle to Droplet and Droplet to Particle transformations

513 5.1.1. Numerical configuration

514 In this numerical experiment successive transformations from Lagrangian droplets to Eu-
 515 lerian ones are studied to validate the reconstruction of the interface for a large number of
 516 transformations in both directions. The coupling with the flow solver is deactivated and only
 517 the level set and the VOF fields are modified at the transformation.

518 100,000 mono dispersed Lagrangian droplets are randomly initialized within a unit cubic box,
 519 allowing the particle to overlap but to touch the borders of the domain. The total number of
 520 cells is 384^3 , with $D_p/\Delta x = 3.84$. The thresholds used for the transformation are listed in table 1.
 521 In order to emphasize transformation, both distance distance criteria are set to $\mathcal{L}_P = 2\Delta x$ and
 522 $\mathcal{L}_D = 2\Delta x$.

523 5.1.2. Results

524 The fields at initialization, after transformation toward Eulerian droplets, and after the
 525 reverse transformation from Eulerian toward Lagrangian droplets, are shown in figure 12. From

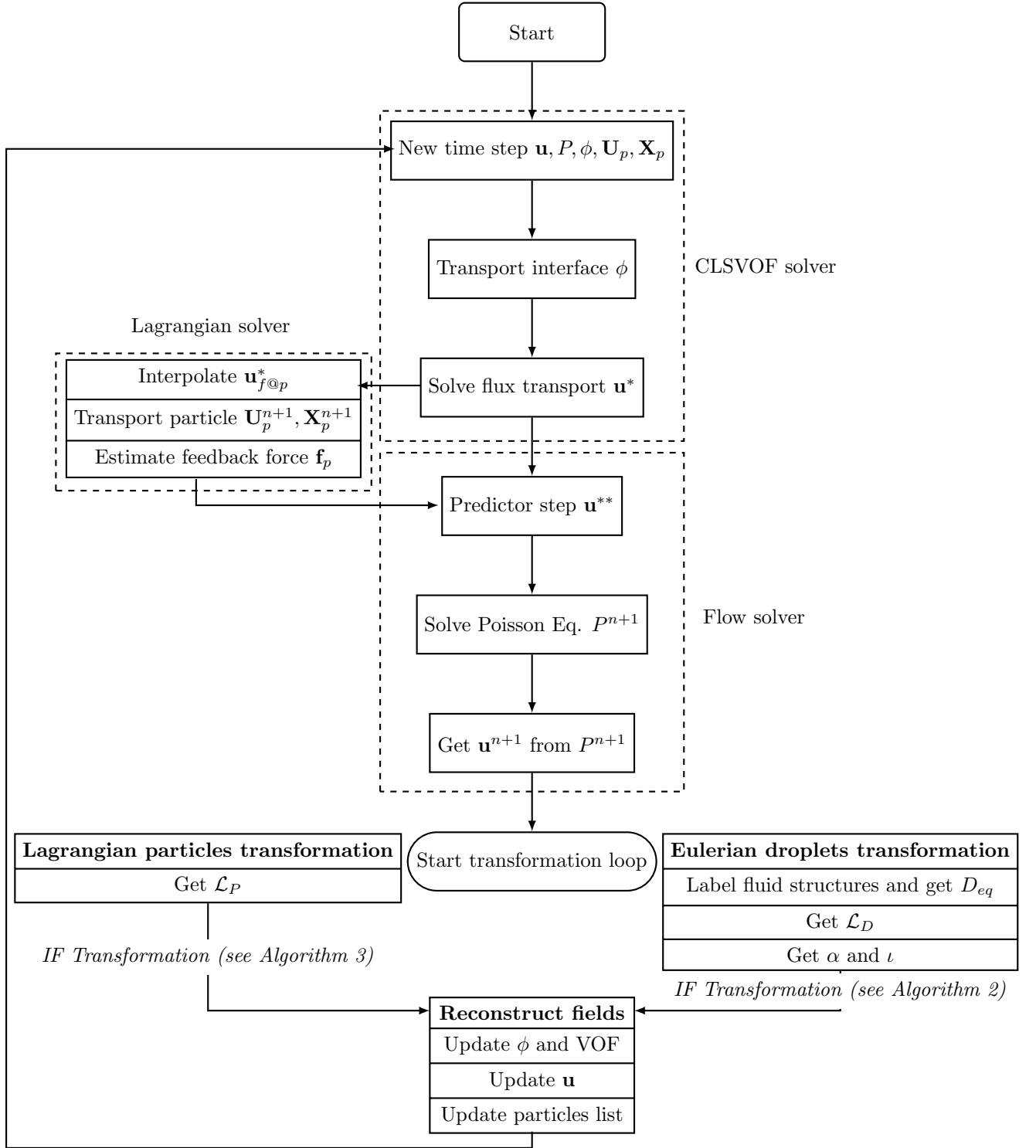


Figure 11: Flow chart of the Eulerian-Lagrangian coupling within the flow solver.

526 the 100,000 initialized Lagrangian droplets, only 26,640 isolated structures are identified after
527 Eulerian transformation and structure detection through the labeling algorithm because of the
528 initial overlaps. An example of overlapping liquid structure is given in figure 13.

529 The shape analysis of the 26,640 Eulerian droplets is plotted in figure 14. From the scattering

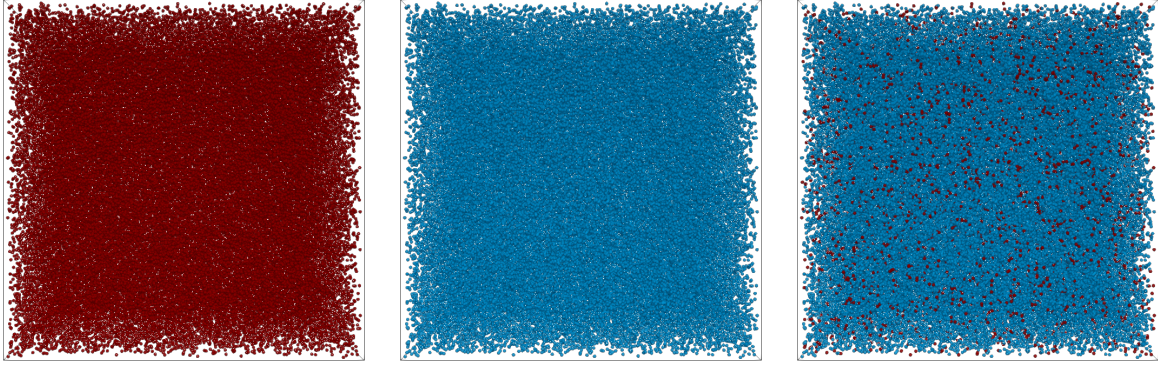


Figure 12: Left: Initialization of Lagrangian droplets (in red), center: Lagrangian droplets are transformed to droplets (in blue), right: selected droplets are transformed back toward Lagrangian droplets.

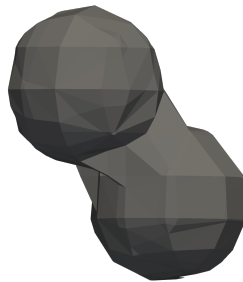


Figure 13: Overlapping liquid structures identified after transformation from Lagrangian toward Eulerian droplet.

530 of points, the droplets are classified in three populations, i) droplets qualifying for transform-
 531 ation, ii) droplets within the range $0.2 < \alpha \leq 0.65$, iii) droplets with $\alpha \leq 0.2$ and $\iota \leq 0.8$. In
 532 population i) the droplets are close to the initial sphere, as seen with their volume in the range
 533 $1 \leq V_D/V_P < 1.2$. At $V_D/V_P = 1$, the minor deviations from the ideal value of ι and α for a
 534 sphere are to be expected due to the numerical resolution (Section 4.1.4). In population ii) most
 535 of the droplets have a volume in the range $1.2 \leq V_D/V_P < 10$ (see extracted structure from the
 536 numerical simulation in figure 13), the morphological criteria do not qualify these droplets for
 537 transformation. Population iii) is composed of large overlapping structures, or groups of struc-
 538 tures. The combination of the two morphological criteria allows us to accurately discriminate
 539 against these structures.

540 The transformation from Eulerian toward Lagrangian droplets identifies 31.6% of Lagrangian
 541 droplets and 68.4% of isolated Eulerian droplets (right figure 12). The average radius of these
 542 Lagrangian droplets is 5.11×10^{-3} , this represents an increase of 2.2% with respect to the initial
 543 Lagrangian droplet.

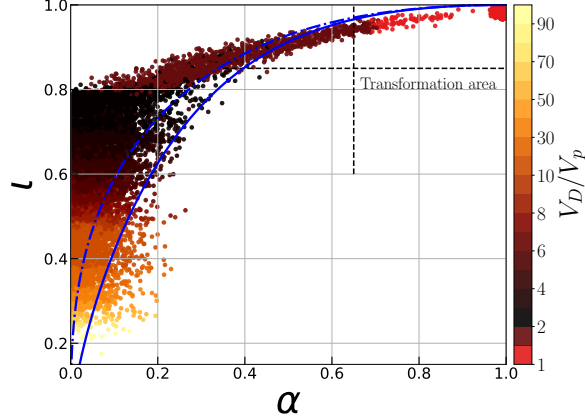


Figure 14: Irregularity parameter, ι , against aspect ratio, α , for all the transformed droplets. The color map represents the volume of the droplet scaled by the maximum volume identified. Dashed black line represents the value set for the two morphological criteria. Blue solid and dashed lines are the analytical relation between α and ι for a prolate and an oblate spheroid, respectively [51].

544 5.2. Transformation of a free-falling confined droplet

545 5.2.1. Numerical configuration

546 The second validation case considers the transformation of a free-falling Eulerian droplet
 547 toward a Lagrangian droplet. The numerical configuration is similar to Section 3. The Eu-
 548 lerian droplet is transformed toward Lagrangian droplet at three transformation times, $t_{trans} =$
 549 $1.25t/\tau_p$, $3.125t/\tau_p$ and $5t/\tau_p$, which corresponds to two distinct stages of acceleration evolu-
 550 tion and a stationary droplet, respectively. The motivation is to study the influence of the
 551 transformation over the free-falling droplet evolution and its terminal velocity.

552 The numerical resolution of the Eulerian droplet is $D_D/\Delta x = 4.8$. The transformation is
 553 done toward both the one way and two way coupling, using the best parameters resulting from
 554 Section 3, *i.e.* an interpolation/spreading kernel as large as the computational domain permits
 555 coupled with the correction of the self-disturbance in the two way coupling.

556 5.2.2. Results

557 The temporal evolution of the transformed free-falling droplet is reported in figure 15, for the
 558 three characteristic times of transformation and both methods. A zoom on the transformation
 559 time is added for each graph showing the temporal evolution of the position, velocity, and
 560 acceleration of the particle for a few time steps after transformation.

561 For all transformation times, the one way method accelerates the Lagrangian droplet, res-
 562 ulting in increasing the speed of the droplets after transformation. The transformation toward
 563 the two way coupling ensures the continuity of the velocity profile at the transformation time;

564 a continuous evolution for both the acceleration and the velocity of the Lagrangian droplet is
 565 observed.

566 For all test cases the transformation from Eulerian toward Lagrangian reduces the compu-
 567 tational time of the simulation. The CFL restriction defined on the curvature being the most
 568 restrictive, removing the interface allows larger time steps.

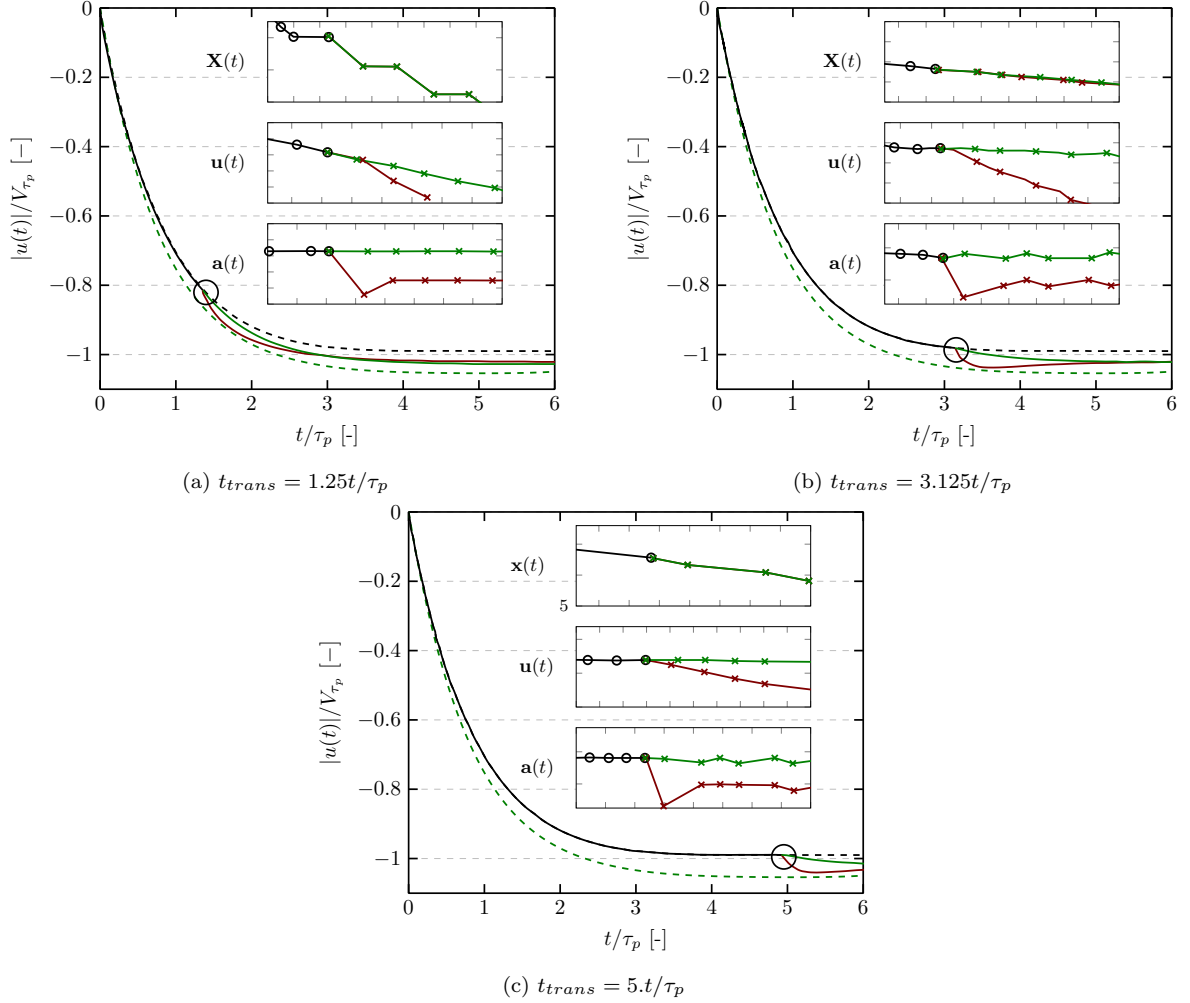


Figure 15: Temporal evolution of the velocity of a transformed free-falling droplet. Three transformation time are shown $t_{trans} = 1.25, 3$ and $5t/\tau_p$. A zoom on the transformation time is proposed, showing the temporal evolution of the acceleration, the velocity, and the position of the particle for a few time steps. Solid black line: ICM, solid green line: two way, solid red line: one way. The dash lines are the pure ICM and two way references.

569 5.3. Decaying Homogeneous Isotropic Turbulence

570 5.3.1. Numerical configuration

571 This validation case considers the transformation of Eulerian droplets subject to complex
 572 flows. The goal is to compare the results of the Eulerian-Lagrangian coupling method to the
 573 coarse ICM in a complex flow. The turbulent flow field is generated as in Duret et al. [52]
 574 and Canu et al. [19] using a linear forcing [53]. The mean kinetic energy \bar{k}_c is set to $\bar{k}_c = 3.6$

575 m^2/s^2 , the fluctuating velocity u' to $u' = \sqrt{\frac{2}{3}\overline{k}_c}$, and the eddy turnover time T_e to $T_e = u'/\Lambda$ with
576 Λ being the Taylor length scale set to half the domain length. The physical size of the domain,
577 and the physical properties of both phases are reported in table 2. This set of physical parameters
578 gives an inertial Taylor length scale based Reynolds number of $Re_\Lambda = \Lambda\sqrt{\frac{2\overline{k}_c}{3}}/\nu_f = 37.77$, a
579 liquid Weber number of $We_D = \frac{\rho_f D_D (u')^2}{\sigma} = 1.60$, which ensures that the droplets remain
580 spherical, and a Stokes number of $St = \tau_p/T_e = \rho_f D_D^2/18\mu_g \times \overline{u'}/L_c = 2.58$.

581 These non-dimensional numbers are reported in table 3 along with the relevant characteristic
582 times: the eddy turnover time T_e , the particle relaxation time τ_p and, the collision time $\tau_c =$
583 $\left[4N_D D_D^2 \sqrt{\pi(\overline{u'})^2}\right]^{-1}$, where N_D is the total number of droplets. To limit coalescence the liquid
584 volume fraction is set to 0.1%, giving $N_D = 64$. The total number of fluid cells is 128^3 , it results
585 in 4 fluid cells across the diameter of the Eulerian droplets.

ρ_f [$\frac{kg}{m^3}$]	ρ_g [$\frac{kg}{m^3}$]	μ_f [$\frac{kg}{m.s}$]	μ_g [$\frac{kg}{m.s}$]	σ [$\frac{kg}{s^2}$]	L [m]	Δx [-]	D_D [m]	$D_D/\Delta x$ [-]
1945.0	65.0	5.650×10^{-4}	1.879×10^{-5}	1.35×10^{-2}	1.5×10^{-4}	1.172×10^{-6}	4.69×10^{-6}	4

Table 2: Physical parameters employed in the Decaying Homogeneous Isotropic Turbulence configuration.

Re_Λ [-]	Λ [m]	ϕ [%]	N_D [-]	We_D [-]	T_e [s]	τ_p [s]	τ_c [s]	St [-]	\overline{k}_c [$\frac{m^2}{s^2}$]
37.77	7.064×10^{-6}	0.10	64	1.60	4.885×10^{-5}	1.25×10^{-4}	1.5×10^{-8}	2.58	3.6

Table 3: Relevant non dimensional parameters of the Decaying Homogeneous Isotropic turbulence configuration.

586 A specific methodology is employed to initialize the two phase flow turbulence in order to
587 prevent strong shear at the Eulerian droplets' interface [54]. A single phase flow is initialized
588 forcing the gas phase during $5T_e$. Then 64 equally spaced fixed resolved particles are added in
589 the domain using the immersed boundary method of Uhlmann [55] that resolves all fluid-surface
590 interactions. The forcing scheme is held during $2T_e$ to adapt the flow to the particles. Then, the
591 forcing is stopped and the resolved particles are transformed toward moving Eulerian droplets.
592 At $8T_e$ the Eulerian droplets are transformed toward Lagrangian droplets, and statistics over
593 three realizations performed per method are studied, until the turbulent kinetic energy drops to
594 50% of the energy at $8T_e$.

595 5.3.2. Results

The trajectory of Eulerian/Lagrangian droplets starting at the transformation time is shown
in figure 16. The position at the transformation, $\mathbf{X}_{p,trans}$ is used as a reference to normalize the

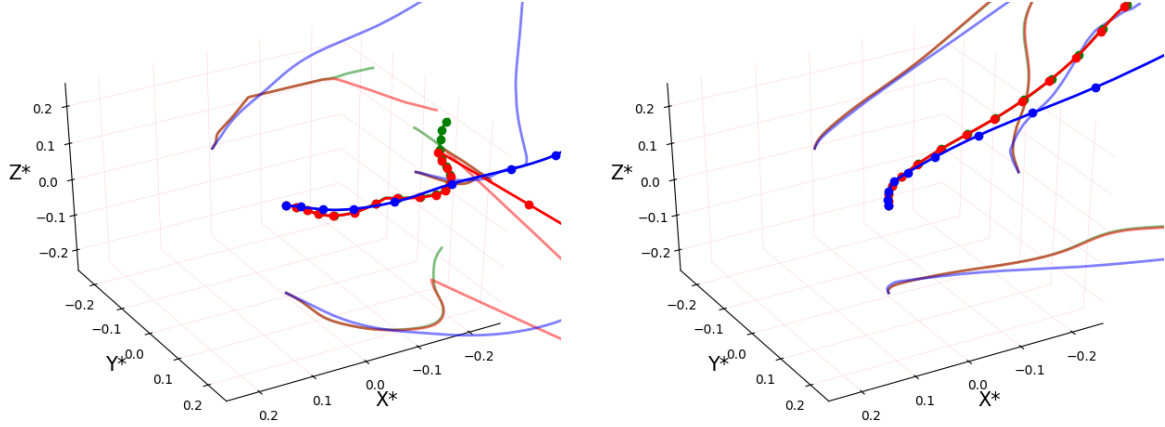


Figure 16: The droplets temporal position evolution after transformation for the ICM (blue), Eulerian-Lagrangian coupling one way (red) and two way (green). The solid lines with markers: 3D trajectory, solid lines without markers: 2D projection.

spatial evolution

$$\mathbf{X}^* = (X_p(t) - X_{p,trans}) / L. \quad (35)$$

596 The trajectory of the droplets at the time after the transformation is similar for all methods.
 597 However, the trajectory of the ICM droplets deviates from the trajectory of the droplets trans-
 598 ported within the Lagrangian framework several time steps after the transformation. Differences
 599 in trajectory are also observed between both Lagrangian frameworks.

The temporal evolution of the averaged dispersion, defined

$$\langle |\mathbf{X}_D(t) - \mathbf{X}_D(t_{trans})| \rangle = \frac{1}{N_D} \sqrt{\left[\sum_{i=1}^{N_D} |\mathbf{X}_{D,i}(t) - \mathbf{X}_{D,i}(t_{trans})| \right]^2}, \quad (36)$$

and the root-mean-square velocity, V_{RMS} ,

$$V_{RMS}(t) = \frac{1}{N_D} \sqrt{\left[\sum_{i=1}^{N_D} |\mathbf{u}_{D,i}(t)| \right]^2}, \quad (37)$$

600 are reported in figure 17. The Eulerian-Lagrangian coupling increases the dispersion of the
 601 Lagrangian droplets with respect to the ICM. The comparison of both Lagrangian approaches
 602 show that the Lagrangian droplets transported within the one way framework have a lower
 603 dispersion than the two way framework; this is a result of the modeling approach. The V_{RMS}
 604 analysis shows that the ICM method reaches a higher peak, meanwhile the results obtained with
 605 the Eulerian-Lagrangian coupling overlap. Thus, in complex flow configuration, the comparison

606 of the Eulerian-Lagrangian coupling with the under-resolved ICM shows a modification of the
 607 droplets' statistics that can be impeded to the poor resolution of the ICM droplets.

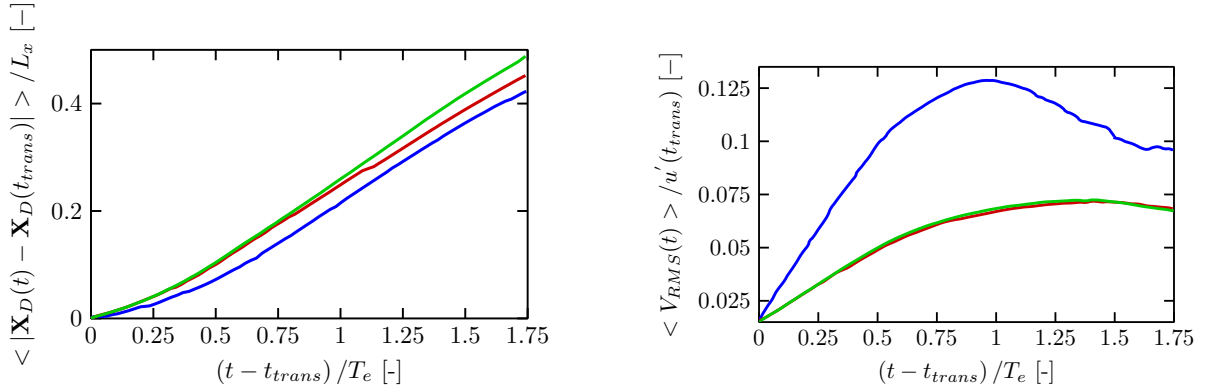


Figure 17: Mean position evolution (left) and V_{RMS} (right) against characteristic time. ICM (blue), Eulerian-Lagrangian coupling one way (red) and two way (green).

608 6. Eulerian-Lagrangian coupling applied to cross flow atomization

609 6.1. Numerical configuration

610 The Eulerian-Lagrangian coupling is applied to the analysis of a jet in cross flow, relevant
 611 to several industrial applications [56]. The configuration consists of the injection of a turbulent
 612 liquid jet bent under the action of a perpendicularly injected uniform flow. This configuration
 613 produces a large number of droplets, as reported both experimentally in Aalburg et al. [57],
 614 Brown and McDonnell [58] and numerically in the work of Herrmann [59], Xiao et al. [60] as well
 615 as within our research group [20].

616 The fluid physical properties are set to $\rho_f = 12.25 \text{ kg/m}^3$, $\mu_f = 1.11 \times 10^{-4} \text{ kg/(m.s)}$, and the
 617 gas carrier phase to $\rho_g = 1.225 \text{ kg/m}^3$, $\mu_g = 1.82 \times 10^{-5} \text{ kg/(m.s)}$. The surface tension is set to
 618 $\sigma = 7 \times 10^{-2} \text{ N/m}^2$. The size of the computational domain is $[-10 \times D_{inj} : 30 \times D_{inj}, -5 \times D_{inj} :$
 619 $5 \times D_{inj}, 0 : 20 \times D_{inj}] \text{ m}$, where D_{inj} is the diameter of injection set to $D_{inj} = 1.3 \times 10^{-3} \text{ m}$. The
 620 injection point is located at $[0, 0, 0]$. The turbulent pipe flow profile is obtained using filter based
 621 turbulent data generation [61], with a mean velocity of $U_{inj} = 97.84 \text{ m/s}$. The carrier velocity
 622 is uniform and set to $U_c = 120.4 \text{ m/s}$. This set of physical parameters gives the characteristic
 623 numbers reported in table 4.

624 We use a total of 16.7×10^6 fluid cells, resulting in 14.5 cells across the diameter of injection.
 625 This results in a coarse description of the jet, but sufficient to our numerical analysis. The
 626 boundary conditions are: inflow and outflow in the streamwise direction (x-component), wall in

ρ^*	M	We_j	Re_j	We_c	Re_c
10	6.6	2178	14,079	330	10,652

Table 4: Cross flow atomization’s characteristic dimensionless numbers, density ratio $\rho^* = \rho_f/\rho_g$, momentum ratio $M = \rho_f U_{inj}^2/\rho_g U_c^2$, the injection Weber number $We_j = \rho_f D_{inj} U_{inj}^2/\sigma$, the injection Reynolds number $Re_j = \rho_f D_{inj} U_{inj}/\mu_f$, the carrier Weber number $We_c = \rho_g D_{inj} U_c^2/\sigma$ and the carrier Reynolds number $Re_c = \rho_g D_{inj} U_c/\mu_g$.

627 the direction of the liquid injection (y-component) except at the liquid jet injection (bottom)
628 and free slip in the spanwise direction (z-component). The simulation is performed during
629 $4 \times t^*$ where t^* is a characteristic time based on the droplets’ residence time in the domain,
630 $t^* = tU_c/(30D_{inj}) = 3.24 \times 10^{-4}$ s.

631 Three configurations are compared, the ICM approach, the Eulerian-Lagrangian coupling
632 with the one way and the two way methods. The criteria of transformation from droplets
633 toward particles and vice-versa are listed in table 1. The morphological parameters are not
634 checked when the droplet has less than 2 fluid cells across the diameter; these droplets are
635 directly transported within the Lagrangian framework.

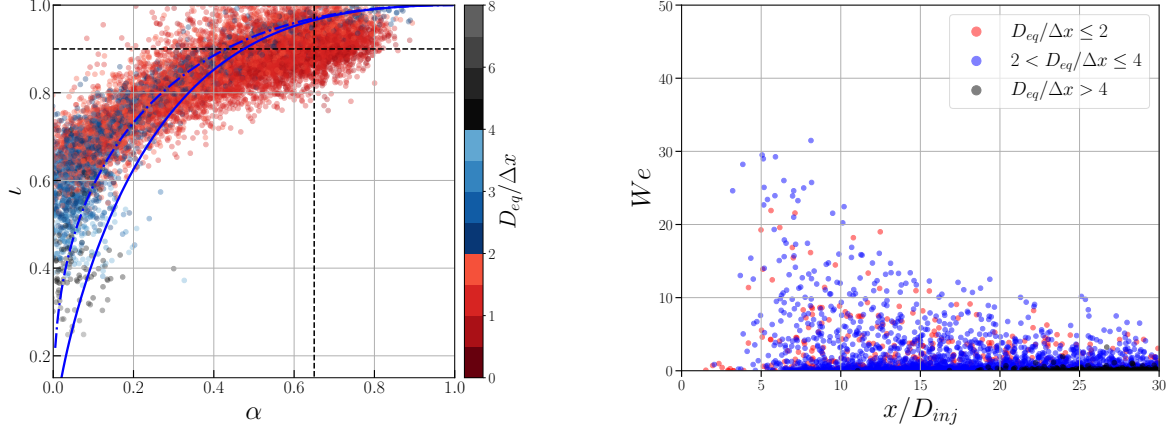
636 6.2. Analysis of the transformation criteria

637 To study the transformation criteria relying on the sphericity of the droplets, the irregularity
638 and the aspect ratio of all the droplets in the ICM simulation are computed. The results are
639 shown in figure 18a where the color map indicates the droplet diameter to fluid mesh size ratio
640 (here for clarity only 10% of the droplets are shown). The population of droplets within the range
641 $D_{eq}/\Delta x \leq 2$, (in red), spreads from $\alpha = 0$ to $\alpha = 0.85$. A large part of these droplets validate
642 the morphological criteria of transformation. The droplets in the range $2 < D_{eq}/\Delta x \leq 4$, (in
643 blue), spread along the spheroid relations derived in Chéron et al. [51], and are in the range
644 $\alpha = [0, 0.85]$, and $\iota = [0.4, 1.]$. Several droplets are identified within the transformation area,
645 these droplets are expected to be transported using the Lagrangian method within the Eulerian-
646 Lagrangian coupling. The largest droplets, (in black) are identified in the range $0.2 \leq \alpha \leq 0.4$;
647 $0.3 \leq \iota \leq 0.5$; they are large ligaments observed near the breakup area and are transported with
648 the resolved interface method.

The transformation criteria implies that the droplets remain spherical within the simulation time. The droplet Weber number can be used to indicate the probability to break of a droplet, defined as

$$We = \frac{\rho_g D_{eq} |\mathbf{u}_D - \mathbf{U}_c|^2}{\sigma},$$

649 where \mathbf{u}_D is the velocity of the droplet and, \mathbf{U}_c is the cross flow velocity. The Weber is plotted
 650 only for the droplets satisfying the morphological criteria of transformation against their distance
 651 to the injection point in figure 18b (here for clarity only 50% of the droplets are shown). The
 652 results indicate that the further from the injection point, the lower is the Weber number of the
 653 droplets. Moreover, most of the droplets have a Weber number below $We < 12$; thus these
 654 droplets are not likely to break [62], and are good candidates for transformation.



(a) Irregularity parameter, ι , against aspect ratio, α , for all structures in the spray. The color map represents the volume-based-equivalent diameter scaled by the mesh spacing. Blue solid and dashed lines are the analytical relation between α and ι for a prolate and an oblate spheroid, respectively [51]. Black dashed lines represents the morphological criteria limits.

(b) Spatial evolution of the droplets' Weber number for droplets validating morphological criteria (figure 18a). Colored markers indicate droplets candidate to transformation.

Figure 18: Morphological and physical analysis of the droplets produced in the reference ICM simulation.

655 6.3. Analysis of the Eulerian-Lagrangian coupling

656 6.3.1. Qualitative analysis

657 A snapshot of the developed atomized jet is presented in figure 19 for the ICM configuration
 658 and the Eulerian-Lagrangian coupling (one way). In this figure we observe the bending of the
 659 turbulent liquid jet under the action of the aerodynamic force induced by the cross flow [63], and
 660 the flattening of the jet in the direction normal to both the cross flow and the liquid injection.
 661 Two phase flow instabilities are observed on the liquid column. They propagate over the surface
 662 of the jet until the breakup of the liquid column, generating several large ligaments in the
 663 primary atomization area [64]. These large ligaments can further break into smaller droplets
 664 under aerodynamic shear effects. This results in a poly-dispersion of the droplets' size. In the
 665 bottom figure, corresponding to the Eulerian-Lagrangian coupling results, it can be seen that the
 666 majority of the small droplets are transported within the Lagrangian framework (white color),
 667 and the large structures are accurately resolved with the ICM (red color).

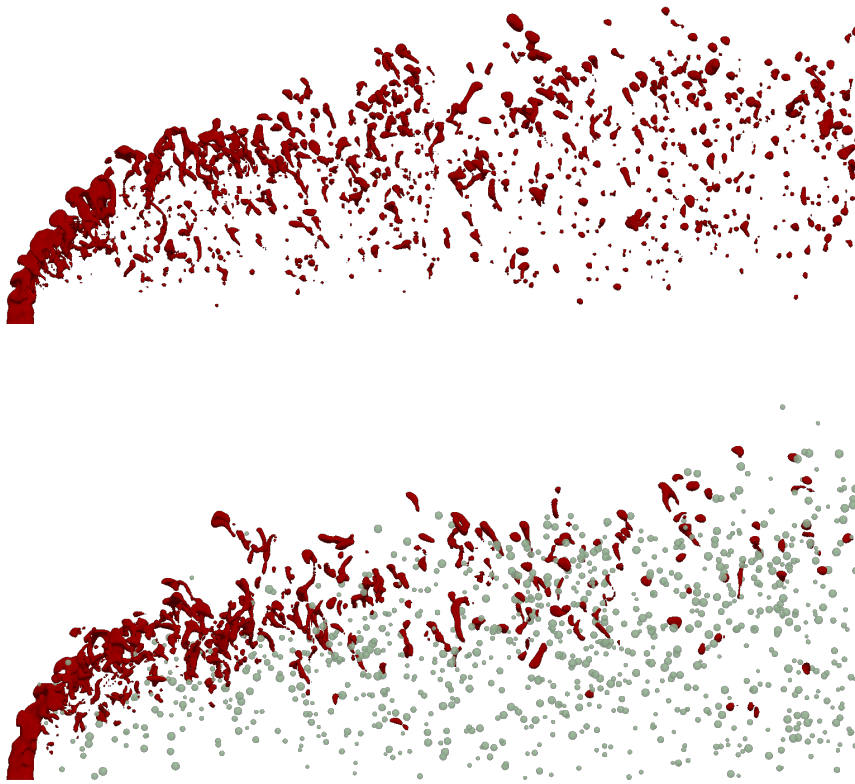


Figure 19: ICM (top) and Eulerian-Lagrangian coupling one way (bottom) snapshots of the side view of the cross flow atomization simulation. Dark color represents the iso-zero level of the ICM method, light color represents the surface of the spherical Lagrangian particles.

668 From figure 19 we identify three ‘states’, the liquid core that is the continuous liquid column
669 until breakage \mathcal{S}_{core} , the dispersed phase characterized by the droplets \mathcal{S}_D , and the carrier
670 phase \mathcal{S}_g . These three states are identified using the labeling algorithm, Section 4.1.1. They are
671 classified as follow

$$\begin{aligned} \mathcal{S}_g &= 1 - F_k \\ \mathcal{S}_{core} &= F_k \quad \text{if } \mathcal{X}_k = \mathcal{X}_{core} \\ \mathcal{S}_D &= F_k \quad \text{if } \mathcal{X}_k \neq \mathcal{X}_{core} \end{aligned}$$

672 where \mathcal{X}_{core} is the label of all the fluid cells connected to the jet injection.

673 In the Eulerian-Lagrangian coupling, the dispersed phase can be divided further among two
674 categories, the droplets transported within the ICM framework and the Lagrangian droplets.
675 The volume occupied by the liquid core, the ICM droplets and Lagrangian droplets is temporally
676 averaged, and, the results are reported in table 5 for the ICM, and the two Eulerian-Lagrangian
677 couplings. The liquid volume occupied per categories are similar for all configurations.

Method	Liquid Core [%]	ICM droplets [%]	Lagrangian particles [%]
ICM	36.76	63.23	-
Eul-Lag one way	32.05	35.58	32.37
Eul-Lag two way	35.54	34.68	29.78

Table 5: Liquid volume occupied by the liquid core, droplets transported within the ICM framework and droplets transported with the Lagrangian framework for the three studied configurations applied to the cross flow atomization.

678 6.3.2. Quantitative analysis

From the qualitative analysis of the primary atomization area, a quantitative analysis can be drawn using an entropy-based probability function [65], using the definition of ‘states’ to which the fluid cell belongs: \mathcal{S}_{core} , \mathcal{S}_G , \mathcal{S}_D . The number of states seen by each fluid mesh are temporally averaged over all the time steps to determine the probability of occurrence of each state, referred to as p_S . The regions upstream to the jet are more likely to see exclusively the carrier phase, therefore having a null entropy. The same comments hold for the area of the liquid jet injection. On the other hand, regions where the breakup occurs are more likely to identify the three states, and, the maximum entropy is reached when

$$p_{\mathcal{S}_{core}} \approx p_{\mathcal{S}_D} \approx p_{\mathcal{S}_g},$$

which is used to normalize the entropy field,

$$\text{Entropy} = \frac{-\sum_{\mathcal{S}} p_{\mathcal{S}} \ln p_{\mathcal{S}}}{\ln 3}.$$

679 To identify the primary atomization area the three state entropy threshold defined in Blaisot
 680 and Yon [65] is used, $\text{Entropy} = \frac{\ln 2}{\ln 3} \approx 0.631$, that captures the regions where each of the three
 681 states are located. The projection of the 3D Entropy field is done over the wall-normal and
 682 spanwise direction, see figure 20. The co-ordinates of the droplets transformed into particles
 683 for the two way Eulerian-Lagrangian coupling are also added (only 25% of the total number of
 684 events is shown for the readability of the figure). Only two way transformation co-ordinates are
 685 reported, since the one way and two way Eulerian-Lagrangian couplings' results do not vary.

686 The spanwise projection of the Entropy shows the conic shape of the liquid core ($\text{Entropy} =$
 687 0). The three states entropy contour indicates the presence of the three states near the injector,
 688 which corroborates the creation of droplets near the injector. This area expands from the liquid
 689 core limits to downstream to the jet. Also, the further from the injection point, the further the
 690 high entropy area is from the bottom wall. This agrees with the observations on the snapshot
 691 of the atomization in figure 19. Similarly to the spanwise projection, the wall-normal projection
 692 indicates a null entropy area where only the carrier phase is identified ($\text{Entropy} = 0$, bottom
 693 and top left corners). This area reduces along with the expansion of the jet, and thus the high
 694 entropy area. The co-ordinates of the Eulerian droplets' transformation indicate that there are
 695 few transformations near the liquid jet, and that the majority of the transformation occurs near
 696 or within the high entropy area.

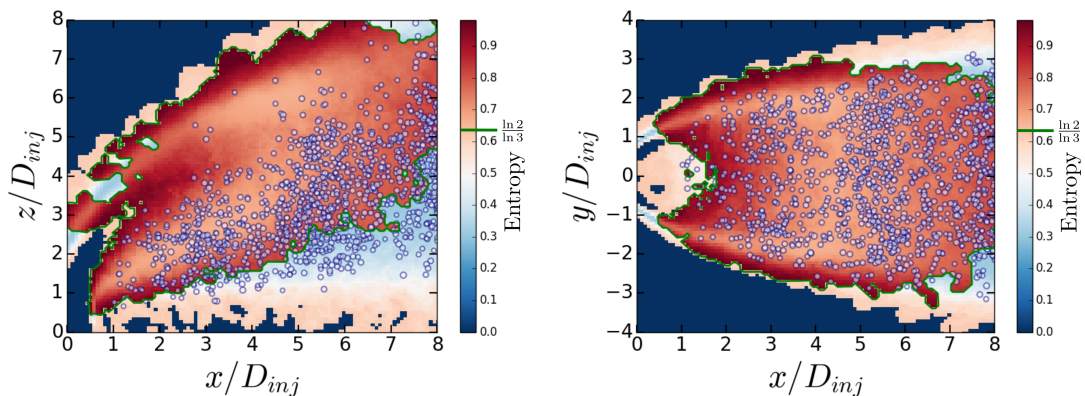


Figure 20: Entropy projection over the spanwise (left) and wall-normal (right) directions. Solid green: contour of the three state entropy threshold $\text{Entropy} \approx 0.631$. Markers indicate the co-ordinates of transformation of the Eulerian droplets (two way Eulerian-Lagrangian coupling).

697 *6.3.3. Dispersed phase analysis*

698 The results reported in figure 19 show a larger number of Lagrangian particles near the
 699 end of the computational domain than the Eulerian droplets. To quantify these qualitative
 700 differences the droplets' size distributions functions at $x/D_{inj} = 5, 10$ and 20 , using a log-space
 701 base, are reported in figure 21 along with the results of the ICM configuration. At $x/D_{inj} = 5$
 702 and 10 several Eulerian droplets have been transformed into Lagrangian droplets, this coincides
 703 with the results shown in figure 20. These Lagrangian droplets are exclusively in the range
 704 $D_{eq}/\Delta x = [1; 4]$ and represent the majority of the droplets in this range. The comparison with
 705 the ICM results show similarities in the histograms. At $x/D_{inj} = 20$ the probability to find
 706 small Eulerian droplets in the ICM configuration decreases, meanwhile it remains constant in
 707 the Eulerian-Lagrangian coupling. The ICM fails to transport these small droplets downstream
 708 to the jet as they break into smaller structures that results in numerical artifacts, removed with
 709 the VOF restriction (Section 2.1.1). In the Eulerian-Lagrangian coupling these droplets are
 710 transported, it results in a larger number of small droplets in this simulation, which explains
 711 the higher probability to find large droplets in the ICM framework.

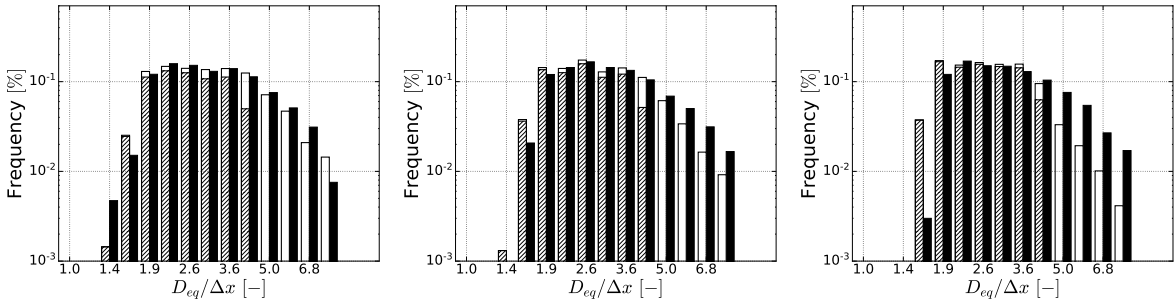


Figure 21: Frequency distribution of the volume-based-equivalent diameter scaled by the mesh spacing at several distances of injection $x/D_{inj} = [5, 10, 20]$. ICM: filled bars, Eulerian-Lagrangian coupling one way - ICM droplets: white bars, Lagrangian droplets: hatch bars.

712 The analysis of the temporal evolution of a free-falling confined particle shows that the
 713 method and the numerical resolution influence the velocity evolution, Section 3. Thus, we report
 714 in figure 22 the frequency distribution of the velocity of the Eulerian/Lagrangian droplets for
 715 the three studied configurations in the range $0. \leq D_{eq}\Delta x \leq 4.$ These figures show the velocity
 716 components in the cross flow direction (u_p) and the spanwise direction (w_p), respectively. Both
 717 plots are scaled by the cross flow velocity. For all methods, the u_p component is centered on
 718 $u_p/U_c = 1$ showing that the droplets evolve at the speed of the cross flow; these droplets behave
 719 as tracers and agrees with the previous observations of Herrmann [39]. The dispersion in the

720 spanwise direction, w_p/U_c , is centered on 0 for all methods, as observed in the work of Herrmann
721 [39]. However, their results show a larger dispersion of small droplets that is not found in our
722 work due to the low numerical resolution used. The use of the Eulerian-Lagrangian two way
723 coupling slightly reduces the concentration of the droplets at $w_p/U_c = 0$.

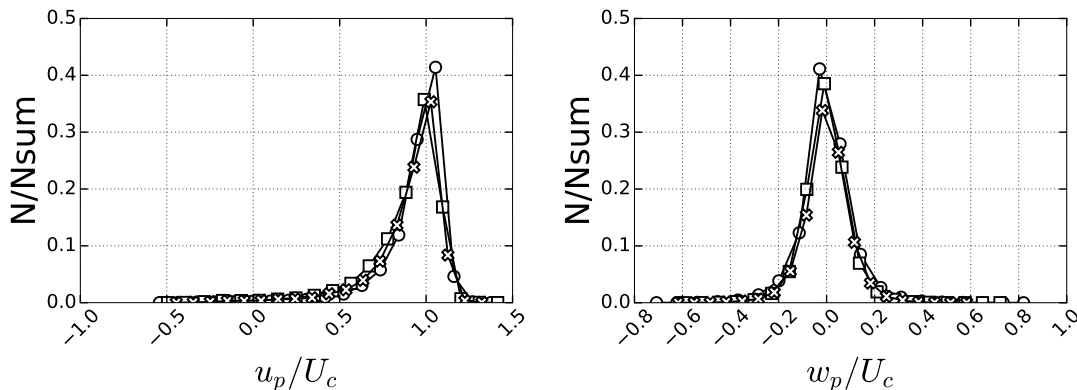


Figure 22: Velocity distribution in the streamwise (left) and the spanwise (right) directions scaled by cross flow injection velocity for the droplets in the range of transformation $0. \leq D_{eq}\Delta x \leq 4.$. ICM: circle markers, Eulerian-Lagrangian one way: square markers, Eulerian-Lagrangian two way: cross markers.

724 6.4. Computational cost

725 The computational time spent in the flow solver per configuration is analyzed for the fully
726 developed jet. Here the total CPU time is split in five main groups: the Lagrangian solver,
727 the transformations, the transport of the interface [18] (ICM), the iterative resolution of the
728 Poisson equation, and, the other functions related to the Eulerian framework such as the pro-
729 jection method or the time spent in the output writing (Others). The total time spent for $0.2t^*$
730 characteristic time per method and groups are reported in table 6. The methods considered
731 are the ICM and the Eulerian-Lagrangian couplings. For all configurations the most significant
732 computational efforts are in the transport of the interface/flux, the Other functions related to
733 the Eulerian framework, and the Poisson solver. The implementation of the transformation
734 algorithm from Eulerian toward Lagrangian and vice-versa is negligible compared to the total
735 CPU time.

736 The comparison between ICM and Eulerian-Lagrangian couplings do not exhibit a compu-
737 tational gain or increase for the transport of interface, or resolution of the solver. However, the
738 comparison of the Eulerian-Lagrangian couplings show that the time spent in the Lagrangian
739 function for the two way coupling significantly increases the CPU time, meanwhile the one way
740 coupling CPU computational cost is negligible. Most of this time is spent in sequential: in the

Method	ICM [s]	Trans. [s]	Lag. [s]	Poisson solver [s]	Others [s]	Total [s]
ICM	740.21	-	-	546.19	799.62	2102.38
- MPI	512.76	-	-	223.62	517.41	1253.79
Eul-Lag one way	727.25	0.09	0.24	515.79	787.07	2031.70
- MPI	474.98.27	0.04	0.05	198.61	485.33	1381.74
Eul-Lag two way	793.45	0.12	336.29	533.43	856.26	2520.12
- MPI	531.14	0.07	0.07	204.40	540.04	1488.39

Table 6: Computational time spent per block of functions in percent and total time spent for $0.2t^*$ characteristic time in second.

741 averaged interpolation and spreading operations between the Eulerian fluid mesh and the Lag-
742 rangian particles. Therefore, the spatial filtering operations implemented within our work must
743 be improved to reduce the computational cost of the Eulerian-Lagrangian two way coupling.

744 7. Conclusion

745 In this paper, a new Eulerian-Lagrangian coupling based on the resolved transport of the
746 interface through a sharp interface capturing method (ICM) and Lagrangian transport for mod-
747 eling under-resolved droplets for multiscale atomization is presented. The motivation of the
748 coupling is to improve the poor transport of under-resolved droplets in the ICM framework. In
749 this work, a threshold of 4 fluid cells across the volume-based-equivalent diameter is given for
750 our ICM method.

751 With the present Eulerian-Lagrangian coupling, the transformation from Eulerian droplet
752 toward Lagrangian droplet is done on the same fluid mesh, and thus the Lagrangian droplet
753 is larger than the local fluid mesh. In two way Lagrangian coupling, the spread of the source
754 terms induces a local flow disturbance, accelerating the Lagrangian particle. This results in a
755 poor representation of the forces experienced by Lagrangian droplets, resulting in an inaccurate
756 estimation of the drag force, or worst, a divergence of the solver. The present method circumvents
757 this inaccurate transport of Lagrangian droplets by spatially filtering the particles' momentum
758 across several fluid cells and correcting the local flow disturbance of the particle. The results of
759 the test case studying the free-falling sedimented droplet demonstrate the improvement of the
760 transport of an individual particle regardless of its diameter to fluid mesh spacing ratio.

761 The criteria of transformation from Eulerian droplet toward Lagrangian droplet, and vice-
762 versa, are meticulously detailed in the present paper, as well as a methodology to track individual
763 Eulerian droplet or ligament. The goal of these criteria is to ensure that the spherical assumption
764 used in the modeling of the transport of droplets is valid. The analysis of each one of the criteria

765 is necessary because it is computed for under-resolved droplets. In the morphological analysis,
766 this results in an overestimation of the droplet deformation. This must be acknowledged in the
767 choice of the threshold values. Similarly, the methodology to reconstruct the Eulerian fields is
768 also detailed, as well as the algorithms used to implement the transformation in both frameworks.

769 The coupled methodology is validated among several test cases from the literature. The
770 Eulerian-Lagrangian coupling is then successfully applied to the atomization of a liquid jet in a
771 cross flow configuration. The results using Eulerian-Lagrangian coupling and ICM method have
772 a similar accuracy, but the smallest droplets are conserved in the Eulerian-Lagrangian coup-
773 ling. However, the proposed Eulerian-Lagrangian coupling freezes the volume of the particles,
774 a secondary break-up modeling must be considered in an extension of this work. Although the
775 Eulerian-Lagrangian coupling conserves and improves the transport of the smallest droplets, to
776 our point of view, this method does not prevent *flotsam* or *jetsam* to occur.

777 Finally, the computational cost of the liquid jet simulation is slightly reduced with the
778 Eulerian-Lagrangian one way coupling. With the two way Lagrangian coupling, the simulation
779 becomes computationally more expensive. The convolution of the fluid variables at the location
780 of the Lagrangian droplet, as well as the spreading toward the source terms of the momentum
781 equation, are responsible for this increase. The computational cost of the simulation using the
782 two way Lagrangian coupling can be decreased by reducing the length of the compact support
783 of the Gaussian kernel.

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790 **Appendix A. Disturbed velocity corrections in the two way Lagrangian coupling**

In Section 2.2 the Stokes correction reads

$$\psi_{St}(x) = \frac{1}{2145} \begin{cases} 2145 - 1001x^2 + 910x^4 - 735x^5 + 250x^6 - 33x^7 & \text{if } x \in [0 : 1] \\ 2145/x - 1001/x^3 + 910/x^5 - 735/x^6 + 250/x^7 - 33/x^8 & \text{if } x > 1 \end{cases} \quad (\text{A.1})$$

and varies with respect to the averaging and spreading kernel lengths with $x = \lambda/\sigma$. The Oseen correction is

$$\psi_{Os}(Re_\sigma) = \frac{9\pi}{4Re_\sigma^3} \left(9\pi \left(1 - \text{erf}(Re_\sigma^3/3\sqrt{\pi}) \exp \frac{Re_\sigma^2}{9\pi} \right) - 6Re_\sigma + Re_\sigma^2 \right), \quad (\text{A.2})$$

791 and varies with Re_σ , a Reynolds number based on the length of the regularized kernel function
 792 (the characteristic length is the size of the compact support of the Gaussian kernel).

793 **Appendix B. Coalescence detection algorithm**

794 The detection of coalescence events is based on a balance of volume between two successive
 795 time steps in a fixed control volume. The droplets in this control volume are identified by $\mathcal{X}_k \neq 0$
 796 for the k th cell in the box, at the current time step and the previous one. Then, the volume
 797 of the droplets within this control volume is compared to the current droplet, and, an eventual
 798 coalescence is detected if the volume coincides.

799 The simulation of droplets' coalescence is done to illustrate this algorithm. Both droplets
 800 have the same diameter, are located at a normal surface-to-surface distance of one radius, and
 801 their velocity is initialized to force a coalescence. The field \mathcal{X} is given in figure Appendix B.1a,
 802 before and after coalescence. Before coalescence, the two fields have a unique non-zero label,
 803 1 and 2 for the lower and upper droplets, respectively. At coalescence, only one droplet is
 804 identified and former labels are stored for droplets' statistics, as shown in figure Appendix B.1b
 805 that shows the temporal evolution of the labels in the domain.

806 **Appendix C. Breakup detection algorithm**

807 The breakup algorithm is based on the field \mathcal{X} and aims to identify the droplet breaking
 808 into new droplets. Similarly to the coalescence detection, a control volume is used to identify
 809 all droplets in the new droplet vicinity where the volume balance is computed between two

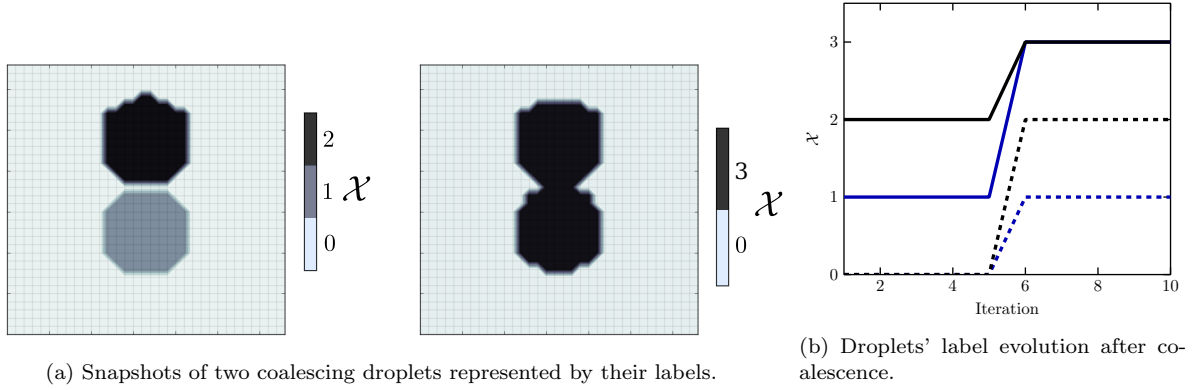


Figure Appendix B.1: Droplet coalescence.

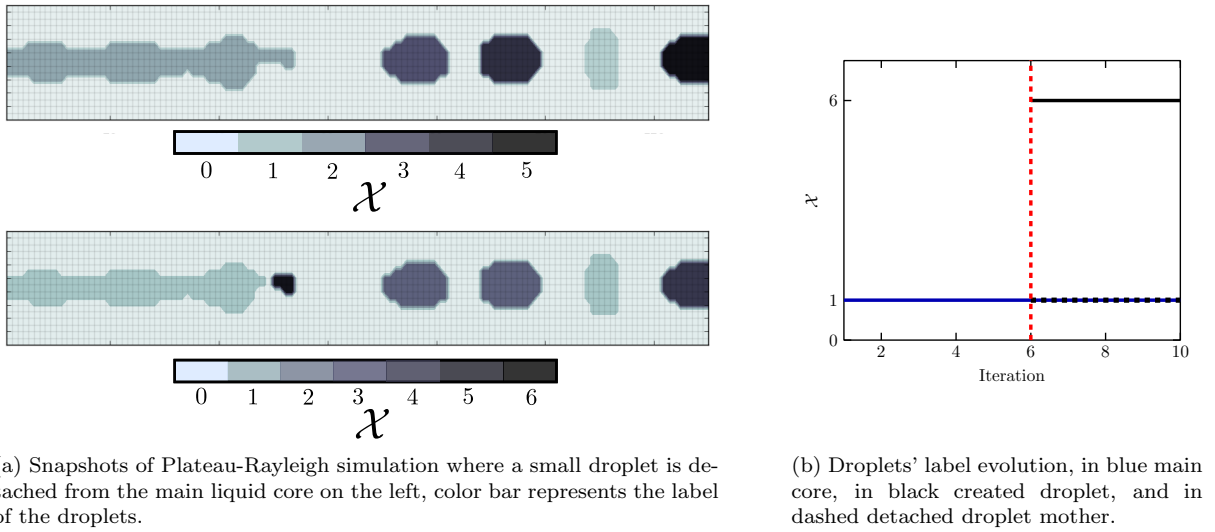


Figure Appendix C.1: Droplet breakup.

810 successive time steps. From the knowledge of volume variation the droplets that broke can be
 811 tracked to the newly formed droplet.

812 The breakup algorithm is illustrated through the simulation of the Plateau-Rayleigh atom-
 813 ization, using the numerical configuration of Denner et al. [66]. The simulation consists of the
 814 atomization of a pulsed liquid cylinder, which generates a single droplet at its tip. The breakup
 815 of the tip of the liquid cylinder into a droplet is shown in figure Appendix C.1a for two suc-
 816 cessive snapshots. Several droplets are identified with a varying label \mathcal{X} . The second snapshot
 817 shows the creation of a small droplet near the tip of the liquid cylinder with $\mathcal{X} = 6$. Here, a
 818 breakup event is identified through the breakup algorithm, as seen in the temporal evolution of
 819 the droplets' label in figure Appendix C.1b (here only the label of the liquid core and the new
 820 droplet are shown). At breakup, iteration 5, the new droplet is identified and the label of the
 821 breaking droplet is stored.

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