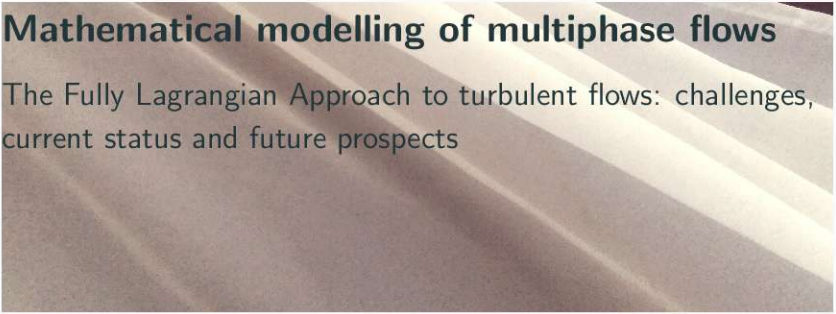


Mathematical modelling of multiphase flows

The Fully Lagrangian Approach to turbulent flows: challenges, current status and future prospects

Andreas Papoutsakis, Ricardo LTD

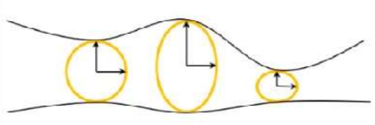
10 May 2018

University of Brighton

Table of contents

Osiptsov method: The Fully Lagrangian Approach

Osiptsov method



Cloud motion:

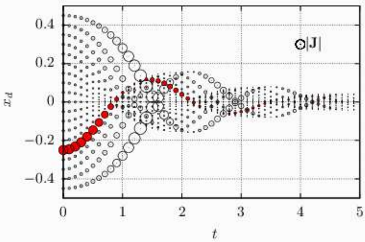
$$\frac{d\mathbf{x}^d}{dt} = \mathbf{V_d} \quad , \quad m_d \frac{d\mathbf{V}_d}{dt} = \mathbf{f}$$

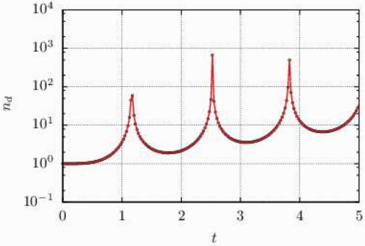
Mass conservation:

$$\frac{d}{dt}\int_{V_L(t)} n_d d\mathbf{x}^d = 0 \quad \Rightarrow \frac{d}{dt}\int_{V_0} n_d(\mathbf{x_0}, t)\det\left(J_{ij}(\mathbf{x}_0, t)\right) d\mathbf{x}_0 = 0$$

Expression for the number density n_d:

$$n_d(\mathbf{x}_0, t) = \frac{n_d(\mathbf{x}_0, 0)}{||\mathbf{J}(\mathbf{x}_0, t)||} \quad , \quad J_{ij} = \frac{\partial x_i^d}{\partial x_{0,j}^d}$$





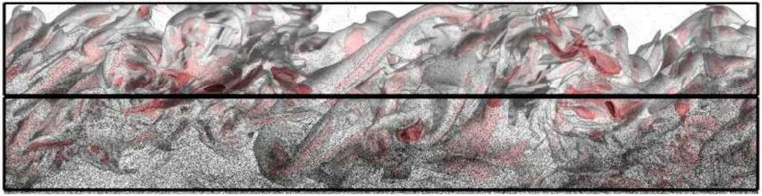
The initial value problem for the calculation of J:

$$\frac{\partial}{\partial t}\begin{bmatrix} J \\ \omega \end{bmatrix} = \begin{bmatrix} \omega \\ \frac{1}{\tau_d}\left(\frac{\partial U}{\partial x} J - \omega\right) \end{bmatrix}, \quad \text{with} \quad \begin{bmatrix} J \\ \omega \end{bmatrix}_{t=0} = \begin{bmatrix} 1 \\ \frac{\partial V}{\partial x} \end{bmatrix}$$

- FLA predicts n_d using a single cloud and identifies the infinitesimally small scales of the critical points (caustics)
- The ODE for J summarises the history of the droplet cloud trajectory
- The critical points of $1/J$ do not degenerate the ODE for J

Challenges of implementing the FLA to turbulent flows

Challenges of implementing the FLA to turbulent flows



- Mass transport
- Momentum transport
- Turbulent diffusion modelling for inertia droplets
- Filtered number density, integrability of the point-wise FLA number density
- Modelling of higher moments of number density

Current status

Mass transport

From the mass conservation equation in Eulerian form:

$$\frac{\partial \overline{n_d}}{\partial t} + \mathrm{div}(\overline{n_d \mathbf{V_d}}) = 0$$

we obtain

$$\frac{\partial \overline{n_d}}{\partial t} + \mathrm{div}(\overline{n_d}\,\overline{\mathbf{V_d}}) = -\mathrm{div}\mathbf{j_T}$$

by introducing the turbulent difussion flux $\mathbf{j_T}$

$$\mathbf{j_T} = \overline{n_d' \mathbf{v_d'}} = \overline{n_d \mathbf{V_d}} - \overline{n_d}\,\overline{\mathbf{V_d}}$$

for a Lagrangian volume

$$\frac{D}{Dt}\int_{V_L} \overline{n_d}(\mathbf{x}, t) d\mathbf{x} = -\int_{V_L} \mathrm{div}\,(\mathbf{j_T})\, d\mathbf{x}$$

Mass transport

Trasforming from the Lagrangian volume

$$\frac{D}{Dt}\int_{V_L} \overline{n_d}(\mathbf{x},t)d\mathbf{x} = -\int_{V_L} \mathrm{div}\left(\mathbf{j_T}\right)d\mathbf{x}$$

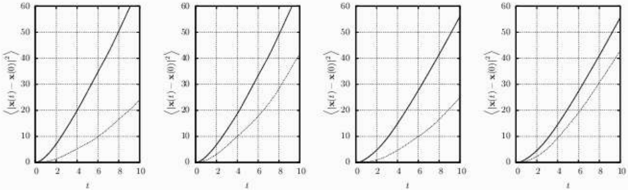
To the initial Lagrangian volume at $t=0$

$$\frac{d}{dt}\int_{V_0} n_d(\mathbf{x_0},t)\left|det\left(\overline{J_{ij}}(\mathbf{x}_0,t)\right)\right| d\mathbf{x}_0 = -\int_{V_0} \mathrm{div}(\mathbf{j_T})\left|det\left(\overline{J_{ij}}(\mathbf{x}_0,t)\right)\right| d\mathbf{x}_0 \,.$$

we obtain the FLA expression for the mass conservation in a filtered turbulent flow field

$$\frac{d}{dt}\left[n_d(\mathbf{x}_0,t)\left|det\left(\overline{J_{ij}}\right)\right|\right] = -\left|det\left(\overline{J_{ij}}\right)\right|\mathrm{div}(\mathbf{j_T})$$

Turbulent diffusion modelling for inertia droplets



The analogy to Brownian motion (Xia 2013) supports the use of the Fick's law for the modelling of turbulent diffusion

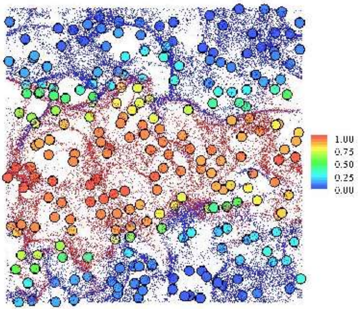
$$\mathbf{j}_T = -D_T \nabla n_s \ , \ \ D_T = \langle v_i^2 \rangle T_l = \sqrt{\langle v_i^2 \rangle} \mathcal{L}$$

$$\frac{d\mathcal{V}^2}{dt} = \frac{1}{3}\frac{d}{dt}\overline{v_i' v_i'} = \frac{1}{3}\overline{2v_i'\frac{dv_i'}{dt}} = \frac{2}{\tau_d}\left(\frac{1}{3}\overline{v_i' u_i'} - \frac{1}{3}\overline{v_i' v_i'}\right) = \frac{2}{\tau_d}\left(\mathcal{U}^2 e^{-B\frac{\tau_d}{\tau_t}} - \mathcal{V}^2\right)$$

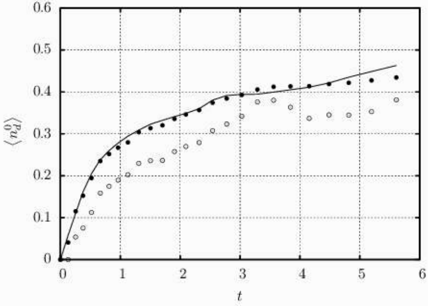
Simplistic closure (Chen 1994), actually D_T changes with L

$$\frac{1}{3}\overline{v_i' u_i'} = \mathcal{U}^2 e^{-B\tau_d/\tau_t}.$$

Turbulent diffusion modelling for inertia droplets



(a)



(b)

Mass conservation:

$$n_d(\mathbf{x}_0, t) = \frac{n_d(\mathbf{x}_0, 0)}{||\mathbf{J}(\mathbf{x}_0, t)||} + \frac{\int_{\tau=0}^{\tau=t} ||\mathbf{J}(\mathbf{x}_0, \tau)|| \, \nabla \cdot (D_T \nabla n_d(\mathbf{x}_0, \tau)) \, d\tau)}{||\mathbf{J}(\mathbf{x}_0, t)||}$$

Momentum transport

The momentum trasport equation (Marble 1970):

$$\frac{\partial \overline{n_d \mathbf{V_d}}}{\partial t} + \operatorname{div}\left(\overline{n_d \mathbf{V_d} \cdot \mathbf{V_d^T}}\right) = \frac{1}{\tau_d}\overline{\left(\mathbf{U} - \mathbf{V}\right) n_d} \, .$$

Assumming that $d\mathbf{j_T}/dt = 0$ and $\frac{1}{\tau_d}\overline{\left(\mathbf{U} - \mathbf{V}\right) n_d} = \frac{1}{\tau_d}\overline{n_d}\left(\overline{\mathbf{U}} - \overline{\mathbf{V}}\right)$

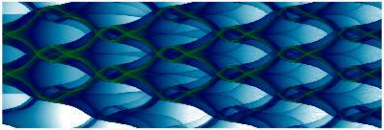
$$\frac{\partial \overline{n_d}\overline{\mathbf{V_d}}}{\partial t} + \operatorname{div}\left(\overline{n_d}\overline{\mathbf{V_d}} \cdot \overline{\mathbf{V_d^T}}\right) = \frac{1}{\tau_d}\overline{n_d}\left(\overline{\mathbf{U}} - \overline{\mathbf{V}}\right) + \operatorname{div}\mathbf{p} \, .$$

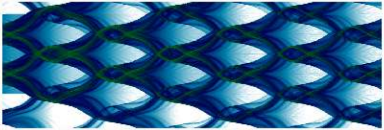
where $\mathbf{p}$ is the pressure term:

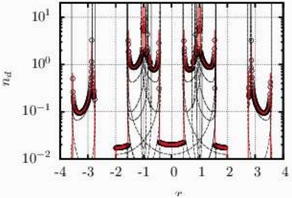
$$p_{ij} = \overline{n_d V_{d,i} V_{d,j}} - \overline{n_d}\,\overline{V_{d,i}}\;\overline{V_{d,j}}$$

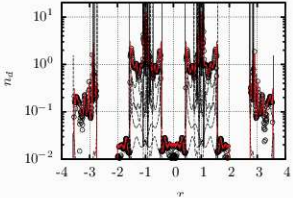
Momentum transport

Assessment of the importance of the pressure term



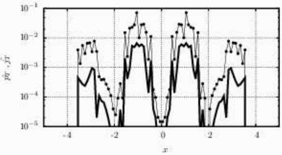






$$\hat{j}_T = \left| |\widetilde{n_d v_d}| - |\widetilde{\overline{n}_d \overline{v}_d}| \right| / |\widetilde{n_d \overline{v}_d}| \,,$$

$$\hat{p}_T = \left| \widetilde{n_d v_d^2} - \widetilde{\overline{n}_d \overline{v}_d^2} \right| / \widetilde{n_d \overline{v}_d^2} \,,$$



Momentum transport

Dropping the pressure term

$$\frac{\partial \overline{n_d}\overline{\mathbf{V_d}}}{\partial t} + \mathrm{div}\left(\overline{n_d}\overline{\mathbf{V_d}} \cdot \overline{\mathbf{V_d^T}}\right) = \frac{1}{\tau_d}\overline{n_d}\left(\overline{\mathbf{U}} - \overline{\mathbf{V}}\right) \ .$$

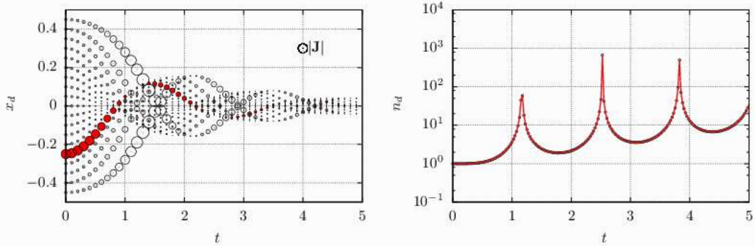
and applying the Reynolds transport theorem

$$\frac{D}{Dt}\int_{V_L} \overline{n}_d(\mathbf{x},t)\overline{\mathbf{V}}_\mathbf{d} dV = \int_{V_L} \overline{n}_d \frac{1}{\tau_d}\left(\overline{\mathbf{U}} - \overline{\mathbf{V}}_\mathbf{d}\right) dV$$

we obtain the simplified momentum transport equation having assummed that $d\mathbf{j_T}/dt = 0$, $\frac{1}{\tau_d}\overline{(\mathbf{U}-\mathbf{V})\,n_d} = \frac{1}{\tau_d}\overline{n_d}\left(\overline{\mathbf{U}} - \overline{\mathbf{V}}\right)$ and $\mathbf{p} = \mathbf{0}$

$$\frac{d\overline{\mathbf{V_d}}}{dt} = \frac{1}{\tau_d}\left(\overline{\mathbf{U}} - \overline{\mathbf{V_d}}\right) \ .$$

Integrability of the point-wise FLA number density



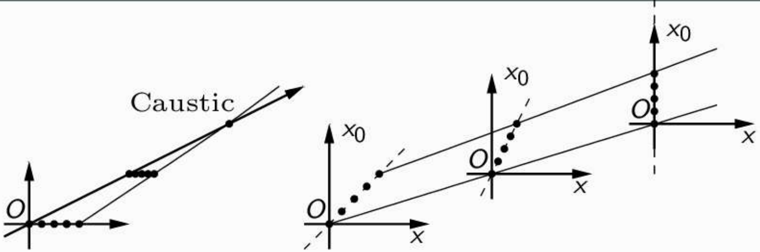
Inertia particles accumulate in Caustic regions where $J = 0$, for which the number density is considered integrable (Osiptsov 1984)

$$n_d = \frac{n_d^0}{\mathbf{J}}$$

Attempting to expand the number density did not result to the calculation of the finite number density within V

$$\int_V n_d d\mathbf{x} = \int_V \frac{1}{\mathbf{J}} d\mathbf{x} = \int_V \left(\frac{1}{J}\bigg|_0 + \frac{\partial}{\partial x}\frac{1}{J}\bigg|_0 x \ldots \right) dx$$

Integrability of the point-wise FLA number density



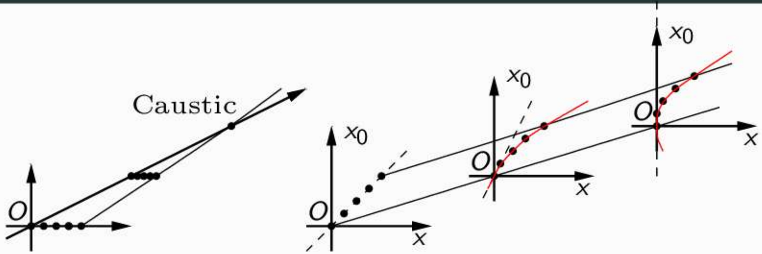
The FLA can be seen as a first order (linear) approximation of the structure for the dispersed continuum

$$n_d = \frac{\partial x_0}{\partial x}$$

where for $\delta = x_0 - x_0^C$ and $\epsilon = x - x^C$

$$\epsilon = J\delta \;\; with \;\; J = \left.\frac{\partial \epsilon}{\partial \delta}\right|_0$$

Integrability of the point-wise FLA number density



Introducing a second order description for the dispersed continuum

$$\epsilon(\delta) = J\delta + \frac{1}{2}H\delta^2.$$

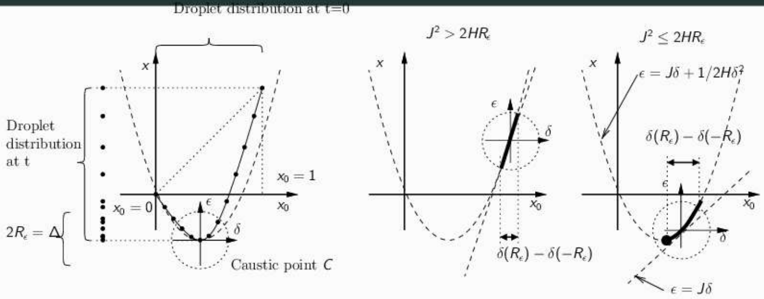
the filtered number density defined in a finite volume R_ϵ

$$\hat{n}_d = \frac{1}{2R_\epsilon}\int_{-R_\epsilon}^{R_\epsilon} n_d \, d\epsilon = \left| \frac{\delta(\epsilon = R_\epsilon) - \delta(\epsilon = -R_\epsilon)}{2R_\epsilon} \right| ,$$

where H is the Hessian of the transformation

$$H = \frac{\partial^2 \epsilon}{\partial \delta^2} = \frac{\partial^2 x}{\partial x_0^2}$$

Integrability of the point-wise FLA number density



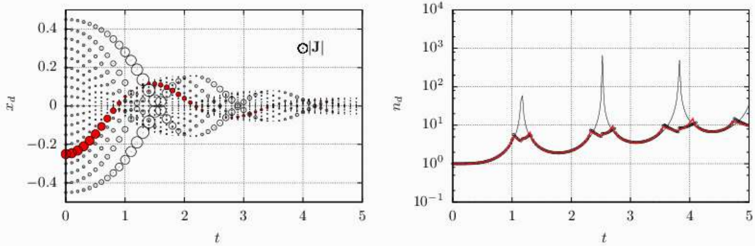
From the expression of the current coordinate ϵ

$$\delta(\epsilon) = \frac{-J + \sqrt{J^2 + 2H\epsilon}}{H}$$

we obtain $\hat{n}_d = \left|\left(\delta(\epsilon = R_\epsilon) - \delta(\epsilon = -R_\epsilon)\right)/(2R_\epsilon)\right|$

$$\hat{n}_d = \begin{cases} \frac{2}{\sqrt{J^2+2HR_\epsilon} + \sqrt{J^2-2HR_\epsilon}} & \text{if } J^2 - 2HR_\epsilon > 0 \\ \\ \frac{\sqrt{J^2+2HR_\epsilon}}{2R_\epsilon H} & \text{if } J^2 - 2HR_\epsilon < 0\,. \end{cases}$$

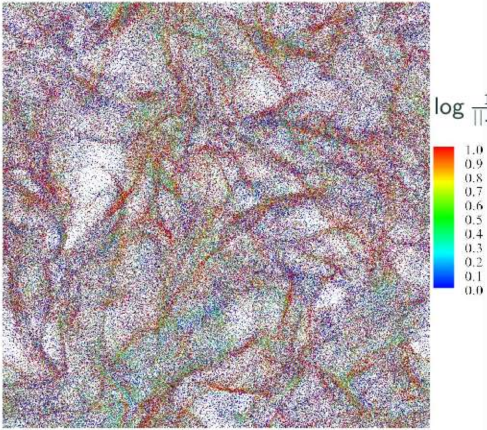
Integrability of the point-wise FLA number density



To calculate the filtered number density we need to solve an ODE of the Hessian too.

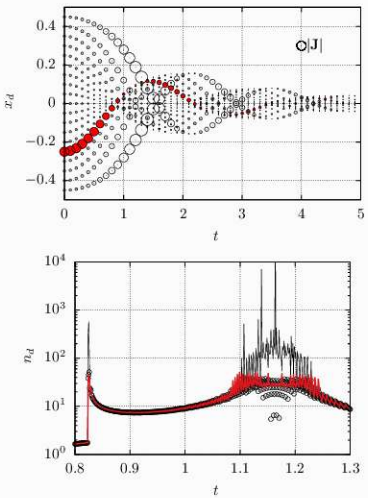
$$\frac{\partial}{\partial t}\begin{bmatrix} J \\ \omega \\ H \\ \psi \end{bmatrix} = \begin{bmatrix} \omega \\ \frac{1}{\tau_d}\left(\frac{\partial U}{\partial x} J - \omega\right) \\ \psi \\ \frac{1}{\tau_d}\left(\frac{\partial^2 U}{\partial x^2} J^2 + \frac{\partial U}{\partial x} H - \psi\right) \end{bmatrix}, \quad \text{with} \quad \begin{bmatrix} J \\ \omega \\ H \\ \psi \end{bmatrix}_{t=0} = \begin{bmatrix} 1 \\ \frac{\partial V}{\partial x} \\ 0 \\ \frac{\partial^2 V}{\partial x^2} \end{bmatrix}$$

Integrability of the point-wise FLA number density

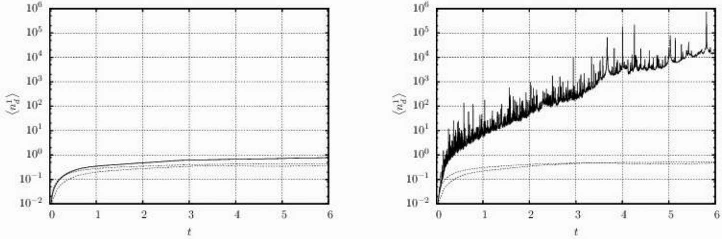


For 3D cases we currently assume that the caustic formations are 1D thus a primary direction can be defined for $\delta = x_0 - x_0^C$ and $\epsilon = x - x^C$

Integrability of the point-wise FLA number density



Modelling of higher moments of number density



Higher moments of the number density (Reeks 2014) in turbulent flow fields can be predicted using the second order FLA

$$\langle n_d^a \rangle = \left\langle \frac{n_d}{|\mathbf{J}|^{a-1}} \right\rangle$$

Closure

Future prespectives

- Use of the finite volume number density $\hat{n}_d$ for the modelling of higher moments for n_d in turbulent flows
- Extension of the second order FLA for the capturing of structues with more than one dimension (enlogated or collapsed caustic formations)
- Introduction of more advanced models for the turbulent diffussion of inertia droplets and particles
- Account for the pressure term in the conservation of momentum and/or the rate of the turbulent mass flux
- Calculation of the Jacobian and the Hessian matricies for non-Stokesian drag forces

Clonclusion

- FLA provides a robust and efficient method to calculating the fine structure of the dispersed continuum
- The Singularities of the FLA number density are important to identify caustic formations and do not affect the solution
- The second order FLA predicts the value of n_d on any finite volume with size R_ϵ providing a link to the filtering width of the LES framework, and converges to the standard FLA for $R_\epsilon \to 0$