Some tools for modeling two-phase flows multiple scales phenomena: bridges between disperse separate phase flows

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Outline

1. Introduction
2. Two-scale multi-material continuous medium: specification attempt
3. Numerical results
4. Conclusion and perspectives

Introduction

Results based on the Ph.D thesis work of A. Loison + M. Massot, T. Pichard, SK

Ongoing work by W. Haegeman and G. Orlando

Sequel to a long series of works with **many** people: F. Caro, F. Coquel, D. Jamet, F. Drui, A. Larat, P. Cordesse, R. Di Battista, S. Jay

(+ endless and stimulating discussions with many (inspiring) people: S. Gavrilyuk, H. Mathis, N. Seguin, C. Perrin, V. Perrier. . .)

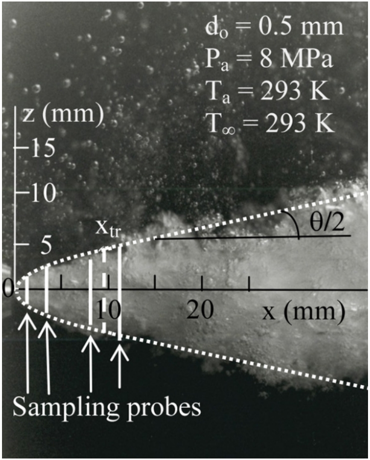
Long term goals

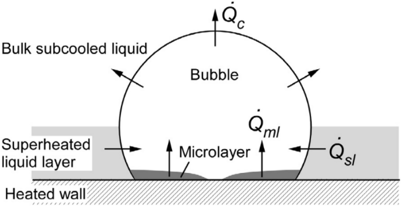
Better understand two-phase flows involving phenomena spanning over multiple (two!) scales.

Example: separate phase / disperse phase.

No turbulence! (yet?)

A few two-phase modeling nightmares...





Possible approaches

Classical approaches

Coupling different models dedicated to each scale across different regions of the computation domain

- Model coupling
- Numerical coupling

(see Lebas, Herrmann, Le Touze)

Present attempt

Working (incrementally) towards a unified model that encompasses scale coupling

(see Devassy, Cordesse, Di Battista)

Guideline element

Coupling strategy independant from the discretization strategy

Two driving questions in this work

Q1: How can we have a model that describes the coexistence of large scale features and small scale features?

Q2: How can we transfer information across scales?
(here: transfer large $\rightarrow$ small)

Preliminary remarks

The present work relies on a modeling "routine"

- no magic bullet: not an infallible method that yields "perfect models"
- get a clear picture of the hypotheses at play
- provide a "raw material" that require further study

Strategy modeled after many previous contributions of the literature:
Herivel, Dunn, Serrin, Berdischevski, Salmon, Gavrilyuk, Germain, Gouin, Romenski, Serrin, Gurtin, Lhuillier, Coleman, Noll, Truskinovsky, Jamet, Ruggieri, Burtea, Perrin, Peshkov . . .

Describing a multi-material continuous medium

Definition attempt of a continuous multi-material medium

- Continuous collection of "fluid elements (particles)"
- Each fluid element (possibly) contains all materials $a = 1, \dots, N$
- Elements are labeled using a continuous index $\boldsymbol{X} \in \mathbb{R}^d$
- Natural choice: $\boldsymbol{X} \in \mathbb{R}^d =$ initial position of the fluid el$^{\text{t}}$

  $=$ Lagrangian coordinates

Describing a multi-material continuous medium

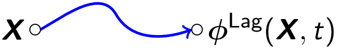
Equip the system with kinematics: how does motion or deformation occur?

(very) strong hypothesis

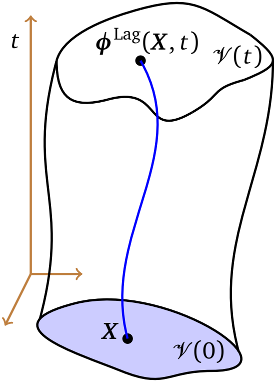
At the bulk scale: shared velocity $\mathbf{u}(\mathbf{x}, t)$ shared by all materials across all scales

$\mathbf{u}(\mathbf{x}, t)$ enables the definition of fluid el$^{\mathrm{t}}$ trajectories:

$$\partial_t \phi^{\mathrm{Lag}}(\boldsymbol{X}, t) = \mathbf{u}(\phi^{\mathrm{Lag}}(\boldsymbol{X}, t), t), \qquad \phi^{\mathrm{Lag}}(\boldsymbol{X}, t = 0) = \boldsymbol{X}$$



Motion of a portion of medium $\mathscr{V}(0) \in \mathbb{R}^d$ for $t \in [0, T]$



$X \in \mathscr{V}(0) =$ position of a fluid el$^{\mathrm{t}}$ at $t = 0$

$\phi^{\mathrm{Lag}}(X, t) \in \mathscr{V}(t) =$ position at instant t of the el$^{\mathrm{t}}$ initially located at X

$$\mathscr{V}(t) = \phi^{\mathrm{Lag}}(\mathscr{V}(0), t)$$

$\mathscr{V}(t) \subset \mathbb{R}^d$: volume of space occupied by the portion of medium at $t \in [0, T]$

$$\Omega = \{(\mathbf{x}, t) \in \mathbb{R}^d \times [0, T] \mid \mathbf{x} \in \mathscr{V}(t), 0 \leq t \leq T\}$$

3-step modeling routine

How shall we proceed now?

3 steps

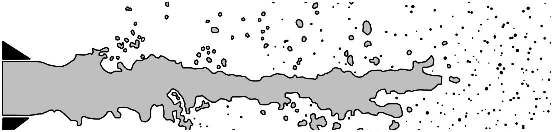
1. Characterize the system
2. Model conservative structures of the system
3. Model dissipative structures of the system

$$\text{step 1} + \text{step 2:} \begin{cases} \text{Co-existence of two scales of interface:} \\ \text{no mass transfer across scales} \end{cases}$$

step 3 : mass transfer across scales

In the sequel: an "abstract" generic system that will be used that fits our problem.

Characterizing the system



Fluid 1 (liquid in gray)
Fluid 2 (gas)

What can I see/measure?

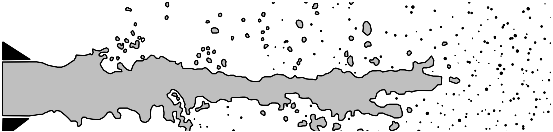
Standard two-phase approach: for each material $k = 1, 2$

- mass (per unit of volume): m_k
- volume fraction for each material: $\alpha_k \in [0, 1]$,
- thermodynamic characteristics (*e.g.* pressure)
- ...

Multiscale description of the interface?

What do we mean?

Characterizing the system



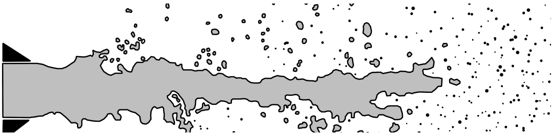
Fluid 1 (liquid in gray)
Fluid 2 (gas)

What can I see/measure?

Given some length scale threshold ℓ (yet to be clarified...)

- single out droplets whose size $< \ell$ into a fluid 1^d
- "non fluid 2" and "non fluid 1^d" = fluid 1
- mass for the droplets: m_1^d
- volume fraction for the droplets: α_1^d
- interface topology information for the droplets...

Characterizing the system



Fluid 1 (liquid in gray)
Fluid 2 (gas)

What can I see/measure?

Two-phase+two-scale "mixture" mass and volume parameters

mass of the medium $\rho = m_1 + m_2 + m_1^d$

$$m_k = \alpha_k \rho_k$$

spatial configuration (volume fractions) $\alpha_1 + \alpha_2 + \alpha_1^d = 1$

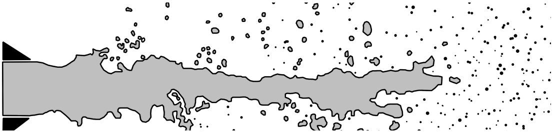
Constraints: postulate balance of masses

$$(m_1)_t + \mathrm{div}(m_1 \mathbf{u}) = 0$$

$$(m_1)_t + \mathrm{div}(m_2 \mathbf{u}) = 0$$

$$(m_1^d)_t + \mathrm{div}(m_1^d \mathbf{u}) = 0$$

Characterizing the system



Fluid 1 (liquid in gray)
Fluid 2 (gas)

What can I see/measure?

Two-scale interface "geometry" ??

$$\alpha_1 + \alpha_2 + \alpha_1^d = 1$$

$$\overline{\alpha}_1 + \overline{\alpha}_2 = 1, \qquad \overline{\alpha} = \overline{\alpha}_1 = \frac{\alpha_1}{1-\alpha_1^d}, \qquad \overline{\alpha}_2 = \frac{\alpha_2}{1-\alpha_1^d}$$

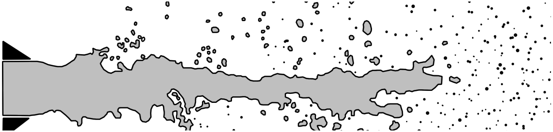
Large scale interface features

bulk scale variation of $\overline{\alpha}_1$
curvature $H = -\operatorname{div}(\nabla\overline{\alpha}/\|\nabla\overline{\alpha}\|)$

Small scale interface features

$\alpha_1^d \leftarrow$ underlying kinetic model

Characterizing the system: small scale model



(simple) Kinetic model for the small scale

Droplets distribution given by a Number Density Function (NDF): $n(x', t', \mathfrak{m}')$

(as physicists would say)

$$n(x', t', \mathfrak{m}')\mathrm{d}x'\mathrm{d}t'\mathrm{d}\mathfrak{m}' = \text{nb of droplets} \begin{cases} \text{located within } [x' - \frac{\mathrm{d}x'}{2}, x' + \frac{\mathrm{d}x'}{2}] \\ \text{instants within } [t' - \frac{\mathrm{d}t'}{2}, t' + \frac{\mathrm{d}t'}{2}] \\ \text{mass within } [\mathfrak{m}' + \frac{\mathrm{d}\mathfrak{m}'}{2}, \mathfrak{m}' + \frac{\mathrm{d}\mathfrak{m}'}{2}] \end{cases}$$

$$\text{Hyp.} + \text{moments of } n \rightarrow \begin{cases} \text{Eulerian fields for small scale topology} \\ \text{informations} \end{cases}$$

Density of the disperse phase : $m_1^d = \alpha_1^d \rho_1^d$

Additional hypotheses pertaining to the disperse phase

- $\mathrm{D}_t\, \rho_1^d = 0$ (neglecting compression effects within droplets)
- isoperimetric ratio $q = \dfrac{(\text{surface of the droplet})^3}{(\text{volume of the droplet})^2} = \mathrm{C}^{\text{st}}$
- Definition of the Interfacial Area Density (IAD)
$$\Sigma(x,t) = \int_{\mathfrak{m}'} q^{1/3} (\rho_1^d)^{-2/3} (m')^{2/3} n(x,t,\mathfrak{m}') \mathrm{d}\mathfrak{m}'$$
- No breakup of coalescence of droplets: $n_t + \operatorname{div}(n\mathbf{u}) = 0$

Evolution of the IAD

$$\Sigma_t + \operatorname{div}(\Sigma \mathbf{u}) = \frac{2}{3} \Sigma \operatorname{div}(\mathbf{u}) + \frac{2}{3} \Sigma\, \mathrm{D}_t\, \alpha_1^d$$

equivalent to (for smooth solutions)

$$\mathrm{D}_t\, z = 0, \qquad z = (\rho_1^d)^{2/3} \Sigma / m_1^d$$

Summing up parameters and related constraints

$$m_k = \rho_k \alpha_k, \qquad k = 1, 2, 1^d$$

$$\overline{\alpha}_1 + \overline{\alpha}_2 = 1, \qquad \overline{\alpha}_k (1 - \alpha_1^d) = \alpha_k, \qquad k = 1, 2$$

$$\begin{tikzcd}
(m_1)_t + \operatorname{div}(m_1 \mathbf{u}) = 0 & \\
(m_2)_t + \operatorname{div}(m_2 \mathbf{u}) = 0 & \\
(m_1^d)_t + \operatorname{div}(m_1^d \mathbf{u}) = 0 \arrow[dr, bend left] & \\
\mathrm{D}_t \, \rho_1^d = 0 \arrow[r] & (\alpha_1^d)_t + \operatorname{div}(\alpha_1^d \mathbf{u}) = 0 \\
\mathrm{D}_t \, z = 0 &
\end{tikzcd}$$

The medium is described by the Eulerian mappings

$$(\mathbf{x}, t) \mapsto (\mathbf{u}, m_1, m_2, \alpha_1^d, \rho_1^d, z, \overline{\alpha})$$

Two categories of parameters/constraints

$$(m)_t + \operatorname{div}(m\mathbf{u}) = 0, \qquad m \in \mathcal{M} = \{m_1, m_2, \alpha_1^d\}$$

$$\mathrm{D}_t \, b = 0, \qquad b \in \mathcal{B} = \{\rho_1^d, z\}$$

Modeling conservative structures

Postulate the energies involved in the evolution of the system:

- kinetic energies: E_{kin}
- potential energies: E_{pot}

Build a Lagrangian $\mathscr{L} = E_{\mathrm{kin}} - E_{\mathrm{pot}}$

We will assume here the general form

$$\mathscr{L} = \mathscr{L}\Big(\mathbf{u}, \overline{\alpha}, \boldsymbol{\nabla}\overline{\alpha}, (m)_{m\in\mathcal{M}}, (b)_{b\in\mathcal{B}}\Big) \overset{\text{noted}}{\sim} \mathscr{L}(\mathbf{u}, \overline{\alpha}, \boldsymbol{\nabla}\overline{\alpha}, m, b)$$

We are ready to apply the Hamilton Stationary Action Principle (SAP)

SAP $\simeq$ $(\mathbf{u}, \overline{\alpha}, \boldsymbol{\nabla}\overline{\alpha}, m, b)$ is a "physically relevant" transformation if it extremalizes some function $\mathscr{A}$ (yet to be defined)

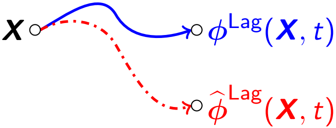
SAP decorum

Consider a transformation of the medium + associated material trajectories

$$\mathcal{T} : (\mathbf{x}, t) \mapsto (\mathbf{u}, \overline{\alpha}, \boldsymbol{\nabla}\overline{\alpha}, m, b), \quad (\boldsymbol{X}, t) \mapsto \phi^{\mathsf{Lag}}$$

Consider: a family of perturbations: $\zeta \in [-1, 1]$

$$\widehat{\mathcal{T}} : (\mathbf{x}, t, \zeta) \mapsto (\widehat{\mathbf{u}}, \widehat{\overline{\alpha}}, \boldsymbol{\nabla}\widehat{\overline{\alpha}}, \widehat{m}, \widehat{b}), \quad (\boldsymbol{X}, t, \zeta) \mapsto \widehat{\phi}^{\mathsf{Lag}}$$



The family of transformation $(\widehat{\mathcal{T}}, \widehat{\phi}^{\mathsf{Lag}})$ is chosen so that it satisfies the following constraints

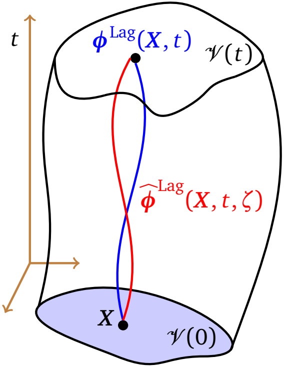
$$\widehat{\phi}^{\mathsf{Lag}} = \phi^{\mathsf{Lag}} \quad \text{for} \quad \begin{cases} (\boldsymbol{X}, t) \in \mathscr{V}(0) \times [0, T], \zeta = 0 \\ (\boldsymbol{X}, t) \in \partial \mathscr{V}(0) \times [0, T], \zeta \in [-1, 1] \end{cases}$$

$$\widehat{\mathcal{T}} = \mathcal{T} \quad \text{for} \quad \begin{cases} (\mathbf{x}, t) \in \Omega, \zeta = 0 \\ (\mathbf{x}, t) \in \partial\Omega, \zeta \in [-1, 1] \end{cases}$$

$$\partial_t \widehat{m} + \mathrm{div}_{\mathbf{x}}(\widehat{m}\widehat{\mathbf{u}}) = 0, \qquad m \in \mathcal{M}$$

$$\partial_t \widehat{b} + (\partial_{\mathbf{x}} \widehat{b})\widehat{\mathbf{u}} = 0, \qquad b \in \mathcal{B}$$

$$\widehat{\mathfrak{f}^{\mathsf{Lag}}}(\boldsymbol{X}, t, \zeta) = \widehat{\mathfrak{f}}(\widehat{\phi}^{\mathsf{Lag}}(\boldsymbol{X}, t, \zeta), t, \zeta)$$



Infinitesimal variations

Lagrangian infinitesimal variations of trajectories

$$\delta\phi^{\mathsf{Lag}}(\boldsymbol{X},t)=\left(\frac{\partial\widehat{\phi^{\mathsf{Lag}}}}{\partial\zeta}\right)_{\boldsymbol{X},t}(\boldsymbol{X},t,\zeta=0)$$

Eulerian infinitesimal variations of trajectories

Enables the definition of $(\mathbf{x},t)\mapsto\delta\phi$ by setting

$$\delta\phi\Big(\mathbf{x}=\phi^{\mathsf{Lag}}(\boldsymbol{X},t),t\Big)=\delta\phi^{\mathsf{Lag}}(\boldsymbol{X},t)$$

Eulerian infinitesimal variations associated with a fluid parameter $\mathfrak{f}$

Consider

$$(\mathbf{x},t)\mapsto\mathfrak{f},\qquad(\boldsymbol{X},t)\mapsto\mathfrak{f}^{\mathsf{Lag}}$$

and the associated perturbations

$$(\mathbf{x},t,\zeta)\mapsto\widehat{\mathfrak{f}},\qquad(\boldsymbol{X},t,\zeta)\mapsto\widehat{\mathfrak{f}}^{\mathsf{Lag}}$$

$$\delta\mathfrak{f}(\mathbf{x},t)=\left(\frac{\partial\widehat{\mathfrak{f}}}{\partial\zeta}\right)_{\mathbf{x},t}(\mathbf{x},t,\zeta=0),$$

$$\delta\mathfrak{f}^{\mathsf{Lag}}(\boldsymbol{X},t)=\left(\frac{\partial\widehat{\mathfrak{f}}}{\partial\zeta}\right)_{\boldsymbol{X},t}(\boldsymbol{X},t,\zeta=0)$$

Infinitesimal variations and constraints

Unconstrained variations

$$\delta\overline{\alpha}$$

Variations connected to $\delta\phi$

$$\begin{aligned}
\delta\mathbf{u} &= D_t(\delta\phi) - (\partial_x \mathbf{u})\delta\phi && (\Longleftarrow \mathbf{u}^{\mathsf{Lag}})\\
m\in\mathcal{M} : \delta m + \mathrm{div}_{\mathbf{x}}(m\delta\phi) &= 0 && (\Longleftarrow m \text{ conservation})\\
b\in\mathcal{B} : \quad \delta b &= -(\partial_{\mathbf{x}} b)\delta\phi && (\Longleftarrow D_t b = 0)
\end{aligned}$$

Stationary action principle

Hamiltonian action

$$\widehat{\mathscr{A}}(\zeta) = \int_{\Omega} \mathscr{L}(\widehat{\mathbf{u}}, \widehat{\overline{\alpha}}, \boldsymbol{\nabla}\widehat{\overline{\alpha}}, \widehat{m}, \widehat{b})\mathrm{d}\mathbf{x}\mathrm{d}t$$

Stationary action principle

The transformation $(\mathbf{u}, \overline{\alpha}, \boldsymbol{\nabla}\overline{\alpha}, m, b)$ is "admissible" (*i.e.* this a "genuine physical transformation") if

$$\delta\mathscr{A} = \left[\frac{\mathrm{d}\widehat{\mathscr{A}}}{\mathrm{d}\zeta}\right](\zeta = 0) = 0$$

$\delta\mathscr{A} = 0$ will yield the motion equations (PDEs)...

"but there is no such thing as magic" (unlike Harry Potter)

SAP: where are my PDEs?

The PDEs are hidden in $\delta\mathscr{A} = 0$. Let us express $\delta\mathscr{A}$.

Notations

$$(\partial\mathscr{L}/\partial\mathbf{u}) = \mathbf{K}^T, \qquad (\partial\mathscr{L}/\partial\boldsymbol{\nabla}\overline{\alpha}) = \mathbf{D}$$

$$\delta\mathscr{A} = \delta\mathscr{A}_{\mathbf{u}} + \delta\mathscr{A}_{\overline{\alpha}} + \delta\mathscr{A}_{\boldsymbol{\nabla}\overline{\alpha}} + \delta\mathscr{A}_m + \delta\mathscr{A}_b$$

$$\delta\mathscr{A}_m = \sum_m \int_\Omega \left(\frac{\partial\mathscr{L}}{\partial m}\right)\delta m, \qquad \delta\mathscr{A}_{\mathbf{u}} = \int_\Omega \left(\frac{\partial\mathscr{L}}{\partial\mathbf{u}}\right)\delta\mathbf{u} = \int_\Omega \mathbf{K}^T\delta\mathbf{u}$$

$$\delta\mathscr{A}_{\overline{\alpha}} = \int_\Omega \left(\frac{\partial\mathscr{L}}{\partial\overline{\alpha}}\right)\delta\overline{\alpha},$$

$$\delta\mathscr{A}_b = \sum_b \int_\Omega \left(\frac{\partial\mathscr{L}}{\partial b}\right)\delta b, \qquad \delta\mathscr{A}_{\boldsymbol{\nabla}\overline{\alpha}} = \int_\Omega \left(\frac{\partial\mathscr{L}}{\partial\boldsymbol{\nabla}\overline{\alpha}}\right)\delta(\boldsymbol{\nabla}\overline{\alpha}) = \int_\Omega \mathbf{D}^T\delta(\boldsymbol{\nabla}\overline{\alpha})$$

$$\delta\mathscr{A} = \textstyle\int_\Omega \delta\boldsymbol{\phi}^T(\cdots) + \delta\overline{\alpha}(\cdots)$$

$$\mathsf{CV}\left(\mathfrak{f}\right) = \partial_t \mathfrak{f} + \operatorname{div}_{\mathbf{x}}(\mathfrak{f}\mathbf{u}^T), \qquad \mathscr{L} + \mathscr{L}^* = \sum_{m\in\mathcal{M}} m\Big(\frac{\partial \mathscr{L}}{\partial m}\Big)$$

$\delta\mathscr{A}_m$

$$\begin{aligned}\delta\mathscr{A}_m &= \sum_{m\in\mathcal{M}} \int_\Omega \left(\frac{\partial\mathscr{L}}{\partial m}\right)\delta m = -\int_\Omega \sum_{m\in\mathcal{M}} \left(\frac{\partial\mathscr{L}}{\partial m}\right) \operatorname{div}_{\mathbf{x}}(m\delta\boldsymbol{\phi})\\ &= \int_\Omega \sum_{m\in\mathcal{M}} \delta\boldsymbol{\phi}^T m \boldsymbol{\nabla}_{\mathbf{x}}\Big(\frac{\partial\mathscr{L}}{\partial m}\Big)\\ &= \int_\Omega \delta\boldsymbol{\phi}^T\left[\boldsymbol{\nabla}\mathscr{L} + \boldsymbol{\nabla}\mathscr{L}^* - \sum_{m\in\mathcal{M}} \boldsymbol{\nabla} m\Big(\frac{\partial\mathscr{L}}{\partial m}\Big)\right]\end{aligned}$$

$\delta\mathscr{A}_{\mathbf{u}}$

$$\delta\mathscr{A}_{\mathbf{u}} = \int_\Omega \mathbf{K}^T\delta\mathbf{u} = \int_\Omega \delta\boldsymbol{\phi}^T[\mathsf{CV}\left(\mathbf{K}\right) + (\boldsymbol{\nabla}_{\mathbf{x}}\mathbf{u})\mathbf{K}]$$

$\delta\mathscr{A}_{\boldsymbol{\nabla}\overline{\alpha}}$

using $\delta(\boldsymbol{\nabla}\overline{\alpha}) = \boldsymbol{\nabla}(\delta\overline{\alpha})$

$$\delta\mathscr{A}_{\boldsymbol{\nabla}\overline{\alpha}} = \int_\Omega \mathbf{D}^T\delta(\boldsymbol{\nabla}\overline{\alpha}) = -\int_\Omega \mathrm{div}_{\mathbf{x}}(\mathbf{D})\delta\overline{\alpha}$$

$\delta\mathscr{A}_{\overline{\alpha}}$

$$\delta\mathscr{A}_{\overline{\alpha}} = \int_\Omega \left(\frac{\partial\mathscr{L}}{\partial\overline{\alpha}}\right)\delta\overline{\alpha}$$

$\delta\mathscr{A}_b$

using $\delta b = -\delta\boldsymbol{\phi}^T\boldsymbol{\nabla}b,\ b\in\mathcal{B}$

$$\delta\mathscr{A}_b = \int_\Omega \sum_{b\in\mathcal{B}}\left(\frac{\partial\mathscr{L}}{\partial b}\right)\delta b = -\int_\Omega \delta\boldsymbol{\phi}^T\sum_{b\in\mathcal{B}}\boldsymbol{\nabla}b\left(\frac{\partial\mathscr{L}}{\partial b}\right)$$

$$
\begin{aligned}
\delta\mathscr{A} = \int_\Omega \delta\boldsymbol{\phi}^T \Big[\mathsf{CV}(\mathbf{K}) - \boldsymbol{\nabla}\mathscr{L} - \boldsymbol{\nabla}\mathscr{L}^* + (\boldsymbol{\nabla}_{\mathbf{x}}\mathbf{u})\mathbf{K} \\
+ \sum_{m\in\mathcal{M}} \boldsymbol{\nabla} m \frac{\partial\mathscr{L}}{\partial m} + \sum_{b\in\mathcal{B}} \boldsymbol{\nabla} b \frac{\partial\mathscr{L}}{\partial b} \Big] \\
+ \int_\Omega \delta\overline{\alpha}\Big[-\left(\frac{\partial\mathscr{L}}{\partial\overline{\alpha}}\right) + \mathrm{div}(\mathbf{D}) \Big]
\end{aligned}
$$

$$\mathrm{CV}(\mathbf{K}) - \boldsymbol{\nabla}\mathscr{L} - \boldsymbol{\nabla}\mathscr{L}^* + \sum_m \boldsymbol{\nabla} m \left(\frac{\partial \mathscr{L}}{\partial m}\right) + (\boldsymbol{\nabla}_{\mathbf{x}}\mathbf{u})\mathbf{K}$$

$$\sum_b \boldsymbol{\nabla} b \left(\frac{\partial \mathscr{L}}{\partial b}\right) = 0$$

$$-\left(\frac{\partial \mathscr{L}}{\partial \overline{\alpha}}\right) + \mathrm{div}(\mathbf{D}) = 0$$

Conservative system

$$\mathrm{CV}(\mathbf{K}) - \boldsymbol{\nabla}\mathscr{L}^* - \mathrm{div}_{\mathbf{x}}[(\boldsymbol{\nabla}\overline{\alpha})\mathbf{D}^T] = 0$$

$$-\left(\frac{\partial \mathscr{L}}{\partial \overline{\alpha}}\right) + \mathrm{div}(\mathbf{D}) = 0$$

$$\mathrm{CV}\,(\mathfrak{f}) = \partial_t \mathfrak{f} + \mathrm{div}_{\mathbf{x}}(\mathfrak{f}\mathbf{u}^T), \quad \mathscr{L} + \mathscr{L}^* = \sum_{m \in \mathcal{M}} \boldsymbol{\nabla} m \left(\frac{\partial \mathscr{L}}{\partial m}\right)$$

$$(\partial \mathscr{L}/\partial \mathbf{u}) = \mathbf{K}^T, \quad (\partial \mathscr{L}/\partial \boldsymbol{\nabla}\overline{\alpha}) = \mathbf{D}^T$$

Conservative structure of the system

$$(\partial\mathscr{L}/\partial\mathbf{u}) = \mathbf{K}^T \text{ : momentum associated with } \mathbf{u}$$

$$-\mathscr{L}^* = \mathscr{L} - \sum_{m\in\mathcal{M}} \boldsymbol{\nabla} m \left(\frac{\partial\mathscr{L}}{\partial m}\right) \text{ : pressure term}$$

$$\mathrm{CV}(\mathfrak{f}) = \partial_t\mathfrak{f} + \mathrm{div}_{\mathbf{x}}(\mathfrak{f}\mathbf{u}^T) \text{ : convection operator}$$

$$(\partial\mathscr{L}/\partial\boldsymbol{\nabla}\overline{\alpha}) = \mathbf{D}^T \text{ : associated to \"capillary-like\" terms}$$

Conservative system

$$\begin{aligned} \mathrm{CV}(\mathbf{K}) - \boldsymbol{\nabla}\mathscr{L}^* - \mathrm{div}_{\mathbf{x}}[(\boldsymbol{\nabla}\overline{\alpha})\mathbf{D}^T] &= 0 \quad \text{(impulsion balance)} \\ -\left(\frac{\partial\mathscr{L}}{\partial\overline{\alpha}}\right) + \mathrm{div}(\mathbf{D}) &= 0 \quad \text{(equilibrium relation)} \end{aligned}$$

Energy evolution

Let us define the Hamiltonian $\mathscr{H}$

$$\mathscr{H} + \mathscr{L} = \mathbf{K}^T \mathbf{u}$$

Then we have

$$\mathrm{CV}(\mathscr{H}) - \mathrm{div}(\mathscr{L}^* \mathbf{u} + \mathbf{D}\overline{\alpha}_t) = 0$$

Conservative structure: sum up

$$\partial_t m + \mathrm{div}_{\mathbf{x}}(m\mathbf{u}) = 0, \quad m \in \mathcal{M}$$
$$\partial_t b + (\partial_{\mathbf{x}} b)\mathbf{u} = 0, \quad b \in \mathcal{B}$$

$$\partial_t \mathbf{K} + \mathrm{div}_{\mathbf{x}}(\mathbf{K}\mathbf{u}^T) - \boldsymbol{\nabla}\mathscr{L}^* - \mathrm{div}_{\mathbf{x}}[(\boldsymbol{\nabla}\overline{\alpha})\mathbf{D}^T] = 0$$
$$-\left(\frac{\partial \mathscr{L}}{\partial \overline{\alpha}}\right) + \mathrm{div}(\mathbf{D}) = 0$$

$$(\implies) \qquad \partial_t \mathscr{H} + \mathrm{div}_{\mathbf{x}}(\mathscr{H}\mathbf{u}) - \mathrm{div}(\mathscr{L}^*\mathbf{u} + \mathbf{D}\overline{\alpha}_t) = 0$$

$(\partial\mathscr{L}/\partial\mathbf{u}) = \mathbf{K}^T$: momentum associated with $\mathbf{u}$

$(\partial\mathscr{L}/\partial D_t\overline{\alpha}) = \mathscr{M}$: "momentum" associated with $D_t\overline{\alpha}$

$-\mathscr{L}^* = \mathscr{L} - \sum_{m\in\mathcal{M}} \boldsymbol{\nabla} m \left(\frac{\partial \mathscr{L}}{\partial m}\right)$: pressure term

$(\partial\mathscr{L}/\partial\boldsymbol{\nabla}\overline{\alpha}) = \mathbf{D}^T$: associated to "capillary-like" terms

$\mathscr{H}$: total energy

Modeling dissipative structures

$$\partial_t m + \mathrm{div}_{\mathbf{x}}(m\mathbf{u}) = 0, \quad m \in \mathcal{M}$$
$$\partial_t b + (\partial_{\mathbf{x}} b)\mathbf{u} = 0, \quad b \in \mathcal{B}$$

$$\begin{aligned} \partial_t \mathbf{K} + \mathrm{div}_{\mathbf{x}}(\mathbf{K}\mathbf{u}^T) - \boldsymbol{\nabla}\mathscr{L}^* - \mathrm{div}_{\mathbf{x}}[(\boldsymbol{\nabla}\overline{\alpha})\mathbf{D}^T] &= 0 \\ -\left(\frac{\partial \mathscr{L}}{\partial \overline{\alpha}}\right) + \mathrm{div}(\mathbf{D}) &= 0 \end{aligned}$$

$$(\implies) \qquad \partial_t \mathscr{H} + \mathrm{div}_{\mathbf{x}}(\mathscr{H}\mathbf{u}) - \mathrm{div}(\mathscr{L}^*\mathbf{u} + \mathbf{D}\overline{\alpha}_t) = 0$$

Modeling dissipative structures

$$\begin{aligned}\partial_t m + \mathrm{div}_{\mathbf{x}}(m\mathbf{u}) &\xcancel{=} 0, \quad m \in \mathcal{M}\\ \partial_t b + (\partial_{\mathbf{x}} b)\mathbf{u} &\xcancel{=} 0, \quad b \in \mathcal{B}\end{aligned}$$

$$\begin{aligned}\partial_t \mathbf{K} + \mathrm{div}_{\mathbf{x}}(\mathbf{K}\mathbf{u}^T) - \boldsymbol{\nabla}\mathscr{L}^* - \mathrm{div}_{\mathbf{x}}[(\boldsymbol{\nabla}\overline{\alpha})\mathbf{D}^T] &\xcancel{=} 0\\ -\left(\frac{\partial\mathscr{L}}{\partial\overline{\alpha}}\right) + \mathrm{div}(\mathbf{D}) &\xcancel{=} 0\end{aligned}$$

$$(\Longrightarrow) \qquad \partial_t \mathscr{H} + \mathrm{div}_{\mathbf{x}}(\mathscr{H}\mathbf{u}) - \mathrm{div}(\mathscr{L}^*\mathbf{u} + \mathbf{D}\overline{\alpha}_t) \xcancel{=} 0$$

Modeling dissipative structures

$$\begin{aligned} \partial_t m + \mathrm{div}_{\mathbf{x}}(m\mathbf{u}) &= R_m, \qquad m \in \mathcal{M} \\ \partial_t b + (\partial_{\mathbf{x}} b)\mathbf{u} &= R_b, \qquad b \in \mathcal{B} \end{aligned}$$

$$\begin{aligned} \partial_t \mathbf{K} + \mathrm{div}_{\mathbf{x}}(\mathbf{K}\mathbf{u}^T) - \boldsymbol{\nabla}\mathscr{L}^* - \mathrm{div}_{\mathbf{x}}[(\boldsymbol{\nabla}\overline{\alpha})\mathbf{D}^T] &= R_{\mathbf{u}} \\ -\left(\frac{\partial \mathscr{L}}{\partial \overline{\alpha}}\right) + \mathrm{div}(\mathbf{D}) &= \varepsilon\, \mathrm{D}_t\, \overline{\alpha} \end{aligned}$$

$$(\implies) \qquad \partial_t \mathscr{H} + \mathrm{div}_{\mathbf{x}}(\mathscr{H}\mathbf{u}) - \mathrm{div}(\mathscr{L}^*\mathbf{u} + \mathbf{D}\overline{\alpha}_t) = \mathscr{Q}$$

$$\mathscr{Q} = \mathbf{u}^T R_{\mathbf{u}} - \sum_{m\in\mathcal{M}} \frac{\partial \mathscr{L}}{\partial m} R_m - \sum_{b\in\mathcal{B}} \frac{\partial \mathscr{L}}{\partial b} R_b - \left[\left(\frac{\partial \mathscr{L}}{\partial \overline{\alpha}}\right) - \mathrm{div}(\mathbf{D})\right] D_t\overline{\alpha}$$

Constraints on the source terms

- no mass transfer between materials: $R_{m_2} = 0$
- mass conservation for fluid 1: $R_{m_1} = -R_{m_1^d}$
- no density variation within droplets: $R_{\rho_1^d} = 0$ and $R_{m_1^d} = \rho_1^d R_{\alpha_1^d}$
- by taking moments of the kinetic equation on n: $R_z = -\dfrac{(\rho_1^d)^{2/3}\Sigma}{m_1^2} R_{m_1}$
- mass conservation for fluid 1: $R_{m_1} = -R_{m_1^d} = -\rho_1^d R_{\alpha_1^d}$

Source yet to be specified boils down to: $R_{\mathbf{u}}$ and R_{m_1}

Lagrangian specification: choice of energies

Framework: mixture of 2 barotropic compressible fluids $k = 1, 2$

EOS for fluid $k = 1, 2$: $\rho_k \mapsto e_k$, $p_k = \rho_k^2(\mathrm{d}e_k/\mathrm{d}\rho_k)$

Choosing energies

$$\text{kinetic energy:} \quad E_{\text{kin}} = \sum_{k=1,2,1^d} \frac{1}{2} m_k |\mathbf{u}|^2$$

$$\text{potential energy:} \quad E_{\text{pot}} = \sum_{k=1,2,1^d} m_k e_k(\rho_k) + \sigma \|\boldsymbol{\nabla}\overline{\alpha}\| + \sigma\Sigma(z, \rho_1^d, \alpha_1^d)$$

Lagrangian

$$\begin{aligned}\mathscr{L} &= E_{\text{kin}} - E_{\text{pot}} \\ &= \sum_{k=1,2,1^d} \frac{1}{2} m_k |\mathbf{u}|^2 - \sum_{k=1,2,1^d} m_k e_k(\rho_k) - \sigma \|\boldsymbol{\nabla}\overline{\alpha}\| - \sigma \Sigma(z, \rho_1^d, \alpha_1^d)\end{aligned}$$

So that the previous esoteric terms now read

$$\mathbf{K} = \rho \mathbf{u}, \quad \mathbf{D} = -\sigma \frac{\boldsymbol{\nabla}\overline{\alpha}}{\|\boldsymbol{\nabla}\overline{\alpha}\|}, \quad \frac{\partial \mathscr{L}}{\partial \overline{\alpha}} = (1 - \alpha_1^d)(p_1 - p_2)$$

$$\begin{aligned}-\mathscr{L}^* &= \overline{\alpha}_1 p_1 + \overline{\alpha}_2 p_2 - \sigma \|\boldsymbol{\nabla}\overline{\alpha}\| \\ \mathscr{H} &= \frac{1}{2} \rho |\mathbf{u}|^2 + \sum_{k=1,2,1^d} m_k e_k(\rho_k) + \sigma \|\boldsymbol{\nabla}\overline{\alpha}\| + \sigma \Sigma(z, \rho_1^d, \alpha_1^d)\end{aligned}$$

Equilibrium: Laplace relation

$$-\left(\frac{\partial \mathscr{L}}{\partial \overline{\alpha}}\right) = +\operatorname{div}(\mathbf{D}) \Longleftrightarrow p_1 - p_2 - \frac{\sigma H}{1 - \alpha_1^d} = 0$$

Resulting model

$$\partial_t m + \mathrm{div}_{\mathbf{x}}(m\mathbf{u}) = R_m, \qquad m \in \mathcal{M} = \{m_1, m_2, \alpha_1^d\}$$

$$\partial_t b + (\partial_{\mathbf{x}} b)\mathbf{u} = R_b, \qquad b \in \mathcal{B} = \{z, \rho_1^d\}$$

$$\partial_t(\rho\mathbf{u}) + \mathrm{div}_{\mathbf{x}}(\rho\mathbf{u}\mathbf{u}^T) + \boldsymbol{\nabla}[\overline{\alpha}_1 p_1 + \overline{\alpha}_2 p_2 - \sigma\|\boldsymbol{\nabla}\overline{\alpha}\|] + \mathrm{div}\left[\frac{\sigma\boldsymbol{\nabla}\overline{\alpha}\boldsymbol{\nabla}\overline{\alpha}^T}{\|\boldsymbol{\nabla}\overline{\alpha}\|}\right] = R_{\mathbf{u}}$$

$$D_t\overline{\alpha} = \frac{1}{\varepsilon}\left[p_1 - p_2 - \frac{\sigma}{1-\alpha_1^d}H(\overline{\alpha})\right]$$

$$\mathscr{Q} = \mathbf{u}^T R_{\mathbf{u}} - \sum_{m\in\mathcal{M}} \frac{\partial\mathscr{L}}{\partial m} R_m - \sum_{b\in\mathcal{B}} \frac{\partial\mathscr{L}}{\partial b} R_b - \left[p_1 - p_2 - \frac{\sigma H}{1-\alpha_1^d}\right] D_t\overline{\alpha}$$

The source terms $R_{\mathbf{u}}$, R_{m_1} are yet to be defined so that $\mathscr{Q} \leq 0$

$$\mathscr{Q} = \mathbf{u}^T R_{\mathbf{u}} - \sum_{m \in \mathcal{M}} \frac{\partial \mathscr{L}}{\partial m} R_m - \sum_{b \in \mathcal{B}} \frac{\partial \mathscr{L}}{\partial b} R_b - \left[p_1 - p_2 - \frac{\sigma H}{1 - \alpha_1^d} \right] D_t \overline{\alpha}$$

Accouting for the constraints on the source terms:

$$\mathscr{Q} = \mathbf{u}^T R_{\mathbf{u}} - R_{m_1} \left[\frac{\overline{\alpha}_1 p_1 + \overline{\alpha}_2 p_2}{\rho_1^d} + e_1^d - \frac{p_1}{\rho_1} - e_1 + \frac{2\sigma\Sigma}{m_1^d} \right]$$
$$- \left[p_1 - p_2 - \frac{\sigma H}{1 - \alpha_1^d} \right] D_t \overline{\alpha}$$

Introducing mass transfer across scales

How can we implement mass transfer between scales in the model?

We discard the possibility of small droplets coalescing into a large scale interface

Purpose of mass transfer in the present case

1. prevent $\overline{\alpha}$ from describing "too small" interface features
2. feed fluid 1^d with information coming from the large interface

1: achieved by altering the equilibrium of $\overline{\alpha}$

$$D_t\overline{\alpha} = \frac{1}{\varepsilon}\left[p_1 - p_2 - \frac{\sigma H(\overline{\alpha})}{1-\alpha_1^d}\right] \text{ replaced by } D_t\overline{\alpha} = \frac{1}{\varepsilon}\left[p_1 - p_2 - \frac{\sigma H^{\text{lim}}}{1-\alpha_1^d}\right]$$

2: achieved by defining R_{m_1} and $R_{\mathbf{u}}$ so that $\mathscr{Q} \leq 0$.

$$\mathscr{Q} = \mathbf{u}^T R_{\mathbf{u}} - R_{m_1} \left[\frac{\overline{\alpha}_1 p_1 + \overline{\alpha}_2 p_2}{\rho_1^d} + e_1^d - \frac{p_1}{\rho_1} - e_1 + \frac{2\sigma\Sigma}{m_1^d} \right] - \frac{1}{\varepsilon} \left[p_1 - p_2 - \frac{\sigma H}{1-\alpha_1^d} \right] \left[p_1 - p_2 - \frac{\sigma H^{\text{lim}}}{1-\alpha_1^d} \right]$$

Possible choice:

- Very meticulous rearrangement of terms in the expression of $\mathscr{Q}$...
- Set $R_{m_1} = \dfrac{-\sigma\rho_1}{(1-\overline{\alpha})\varepsilon}(H - H^{\text{lim}})$
- Suppose that $R_{\mathbf{u}} = -\dfrac{\sigma(H - H^{\text{lim}})}{\varepsilon}\widetilde{R}_{\mathbf{u}}\mathbf{u}$, now seek for $\widetilde{R}_{\mathbf{u}}$ as our source of dissipation

Introducing

$$h = \frac{\rho_1}{\overline{\alpha}_2(p_2 - p_1)} \left[\frac{\overline{\alpha}_1 p_1 + \overline{\alpha}_2 p_2}{\rho_1^d} + e_1^d - \frac{p_1}{\rho_1} - e_1 \right] - 1$$

Possible choice

$$\widetilde{R}_{\mathbf{u}} = \frac{-1}{\|\mathbf{u}\|^2} \left[\frac{\sigma H^{\mathrm{lim}}}{1 - \alpha_1^d} + (p_1 - p_2)h - \frac{2\sigma\rho_1\Sigma}{\overline{\alpha}_2 m_1^d} \right]$$

Division by $\|\mathbf{u}\|^2$ is delicate to handle but we can suppose that no mass transfer occurs when $\mathbf{u} = \mathbf{0}$.

Relaxed system (without mass transfer): a few properties

$$
\begin{aligned}
(k=1,2,1^d) \qquad (m_k)_t + \operatorname{div}(m_k\mathbf{u}) &= 0\\
(\alpha_1^d)_t + \operatorname{div}(\alpha_1^d\mathbf{u}) &= 0\\
z_t + \mathbf{u}^T\boldsymbol{\nabla} z &= 0\\
\partial_t(\rho\mathbf{u}) + \operatorname{div}_{\mathbf{x}}(\rho\mathbf{u}\mathbf{u}^T) + \boldsymbol{\nabla}[\overline{\alpha}_1 p_1 + \overline{\alpha}_2 p_2 - \sigma\|\boldsymbol{\nabla}\overline{\alpha}\|] + \operatorname{div}\left[\frac{\sigma\boldsymbol{\nabla}\overline{\alpha}\boldsymbol{\nabla}\overline{\alpha}^T}{\|\boldsymbol{\nabla}\overline{\alpha}\|}\right] &= \mathbf{0}\\
D_t\overline{\alpha} - \frac{1}{\varepsilon}\left[p_1 - p_2 - \frac{\sigma}{1-\alpha_1^d}H(\overline{\alpha})\right] &= 0
\end{aligned}
$$

Properties

When $\sigma = 0$: hyperbolicity

Sound velocity $c_W^d = \frac{1}{1-\alpha_1^d}\left[\rho\left(\frac{\alpha_1}{\rho_1 c_1^2} + \frac{\alpha_2}{\rho_2 c_2^2}\right)\right]^{-1/2}$

Equilibrium system (without mass transfer): a few properties

$$
\begin{aligned}
(k=1,2,1^d)\qquad (m_k)_t+\mathrm{div}(m_k\mathbf{u})&=0\\
(\alpha_1^d)_t+\mathrm{div}(\alpha_1^d\mathbf{u})&=0\\
z_t+\mathbf{u}^T\boldsymbol{\nabla} z&=0\\
\partial_t(\rho\mathbf{u})+\mathrm{div}_{\mathbf{x}}(\rho\mathbf{u}\mathbf{u}^T)+\boldsymbol{\nabla}[\overline{\alpha}_1p_1+\overline{\alpha}_2p_2-\sigma\|\boldsymbol{\nabla}\overline{\alpha}\|]+\mathrm{div}\left[\frac{\sigma\boldsymbol{\nabla}\overline{\alpha}\boldsymbol{\nabla}\overline{\alpha}^T}{\|\boldsymbol{\nabla}\overline{\alpha}\|}\right]&=\mathbf{0}\\
p_1-p_2-\frac{\sigma}{1-\alpha_1^d}H(\overline{\alpha})&=0
\end{aligned}
$$

Properties

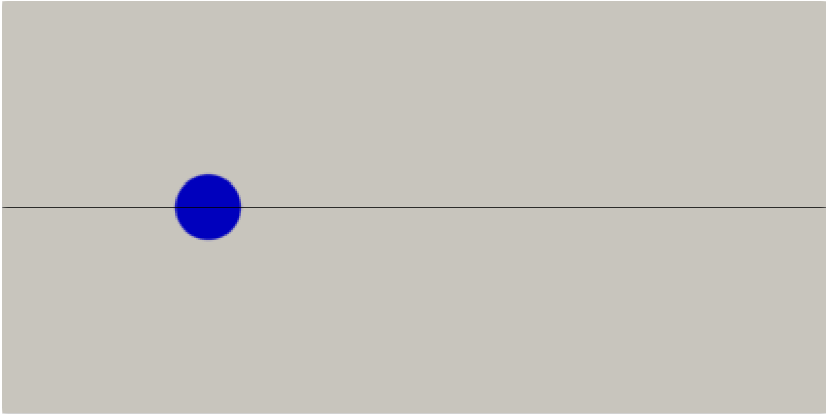
When $\sigma=0$: hyperbolicity

Sound velocity $c_F^d=\frac{1}{1-\alpha_1^d}\left[\frac{\rho_1\alpha_1}{\rho}c_1^2+\frac{\rho_2\alpha_2}{\rho}c_2^2\right]^{1/2}$

Numerical results

- Simulation performed by A. Loison (`josiepy` simulation code)
- Two-dimensional test: a water column destabilized by a gas inlet from the left of the domain.
- Mesh $=$ 400$\times$200
- Numerical method: extended system including capillary effects $+$ Godunov-type solver (see Schmidmayer et al.)
- EOS $=$ barotropic stiffened gas
- numerical goldsmithing for the mass transfer...

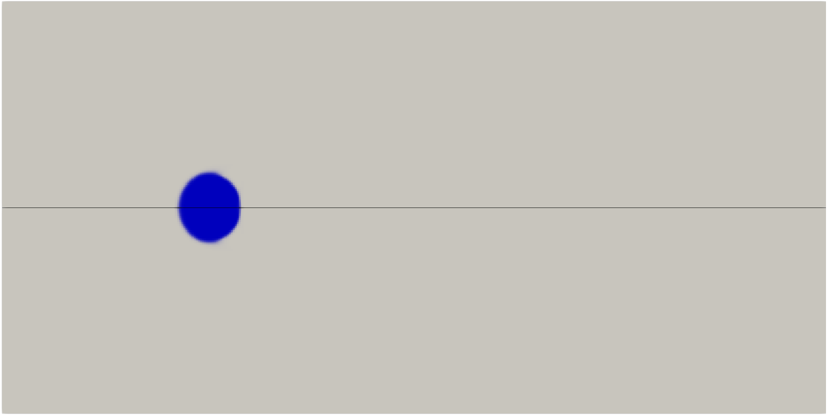
Numerical results



Mapping of $\overline{\alpha}$

top (~~mass transfer~~)
bottom (mass transfer)

Numerical results



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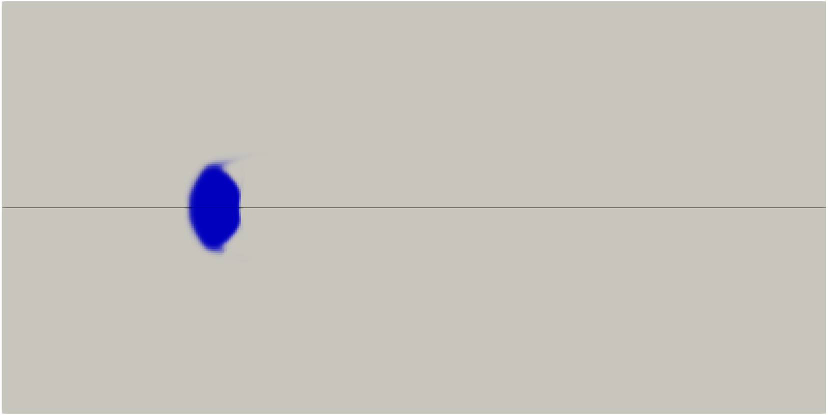

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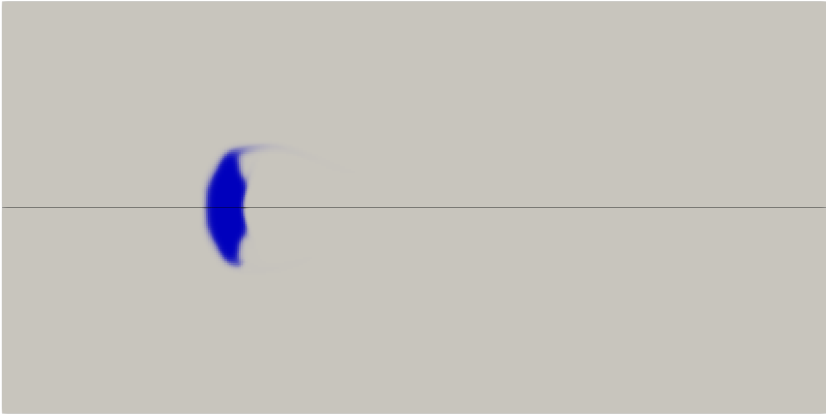

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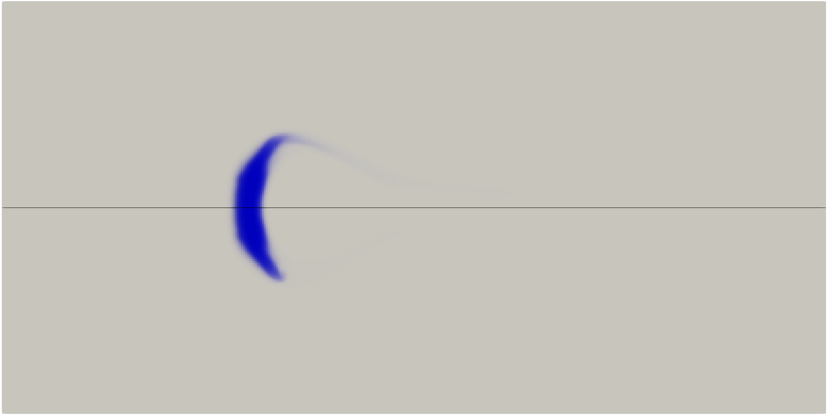

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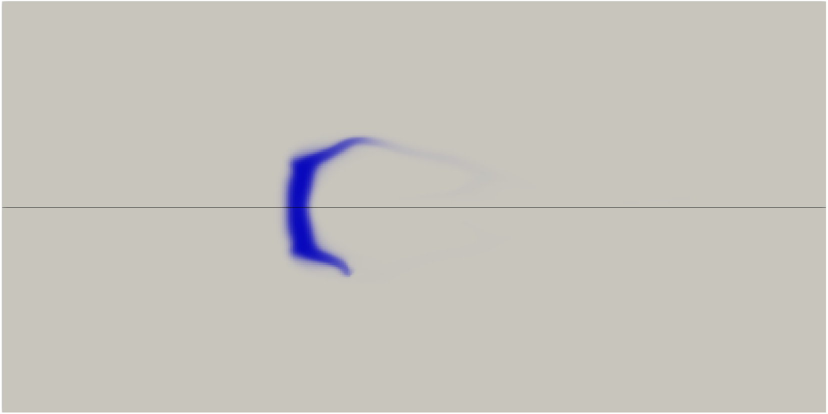

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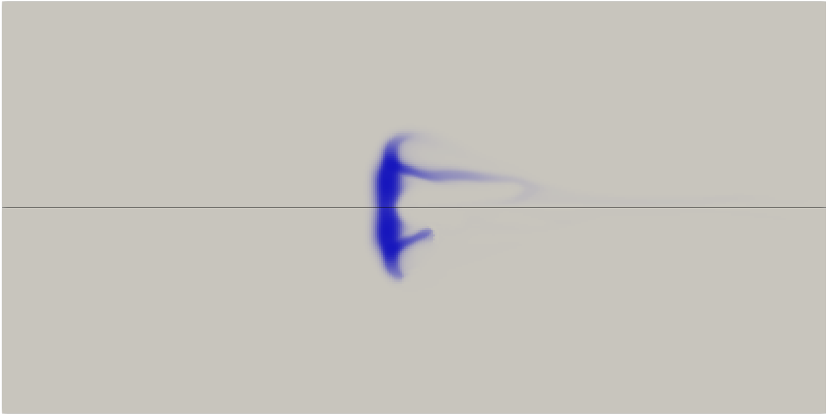

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Numerical results

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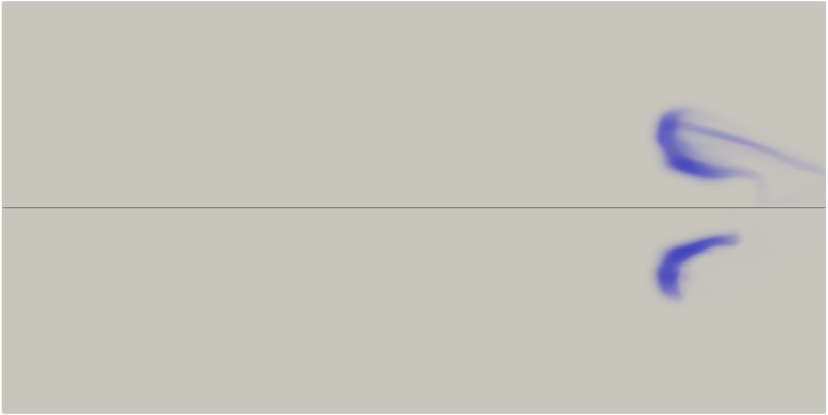
Numerical results

Mapping of $\overline{\alpha}$



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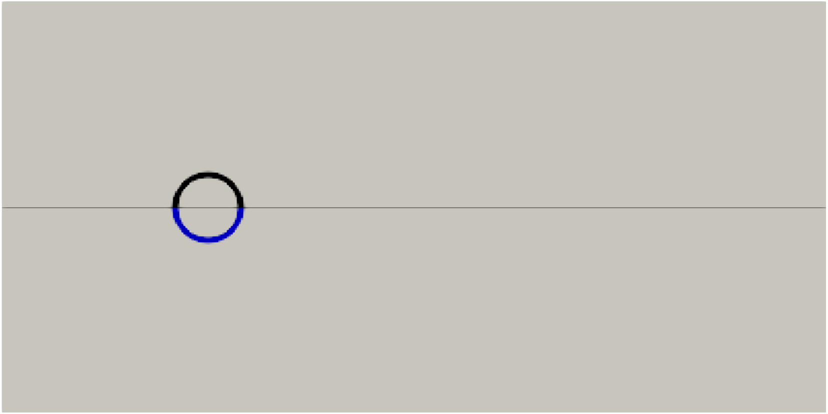
Numerical results



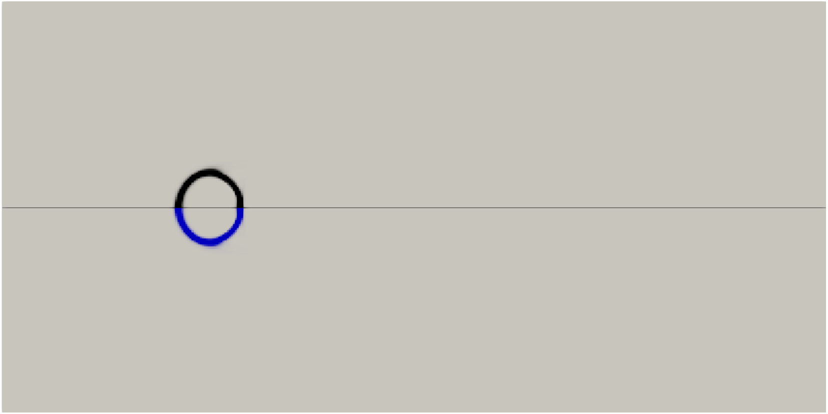
Large scale $\|\boldsymbol{\nabla}\overline{\alpha}\|$ and small scale IAD Σ

Top (~~mass transfer~~): $\|\boldsymbol{\nabla}\overline{\alpha}\| \in (0, 1.6)$

Bottom (mass transfer): $\|\boldsymbol{\nabla}\overline{\alpha}\| \in (0, 1.6)$ + $\Sigma \in (0, 3.4)$

Numerical results

Large scale $\|\boldsymbol{\nabla}\overline{\alpha}\|$ and small scale IAD Σ



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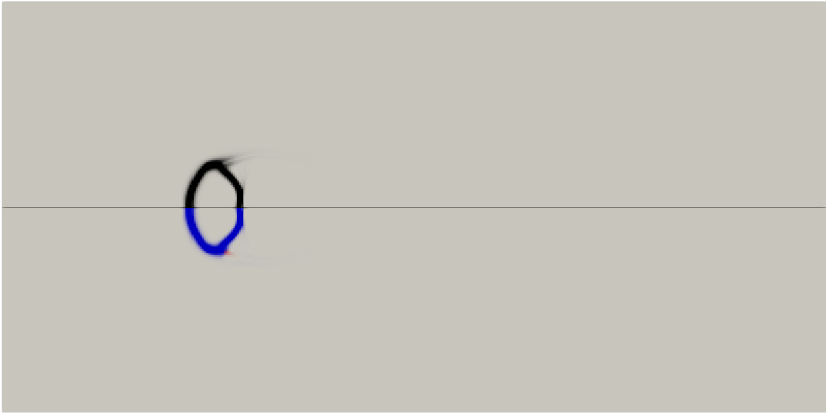

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Numerical results

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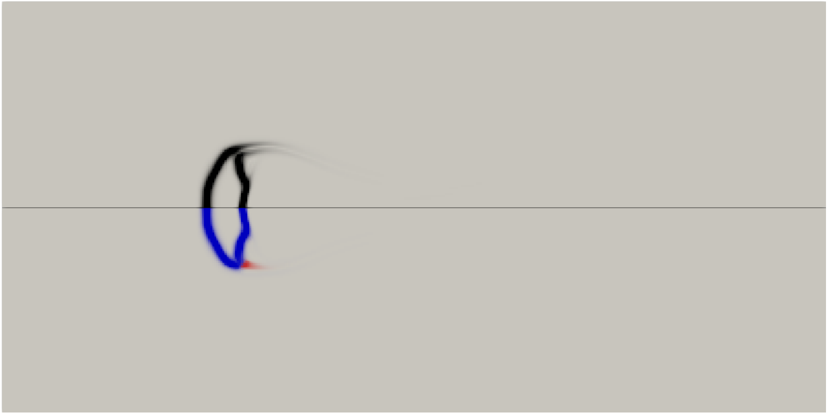

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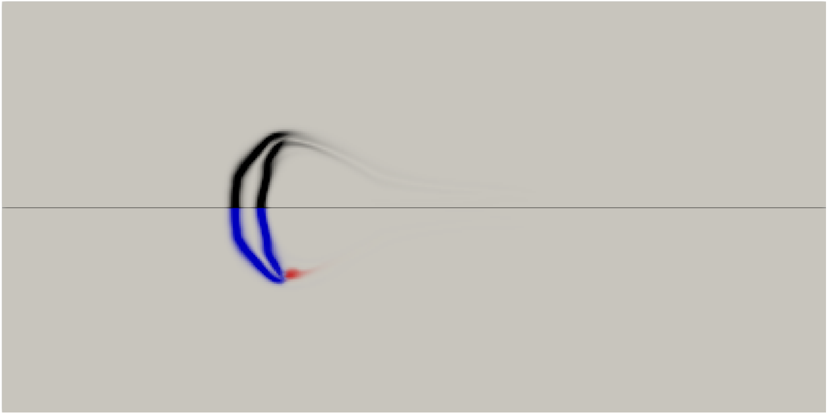

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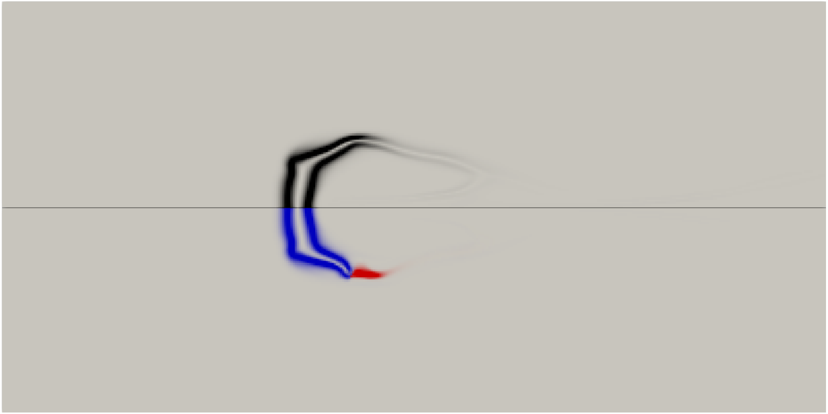

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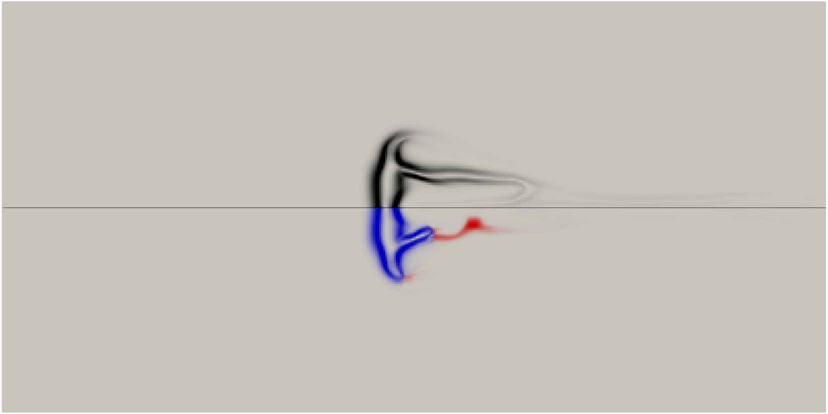

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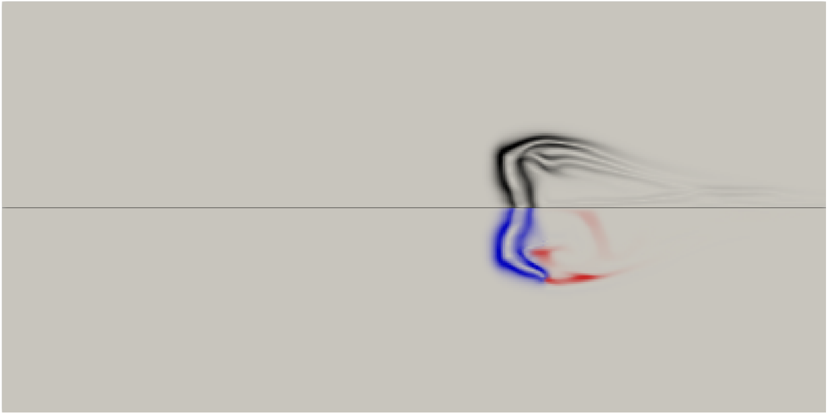

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Numerical results

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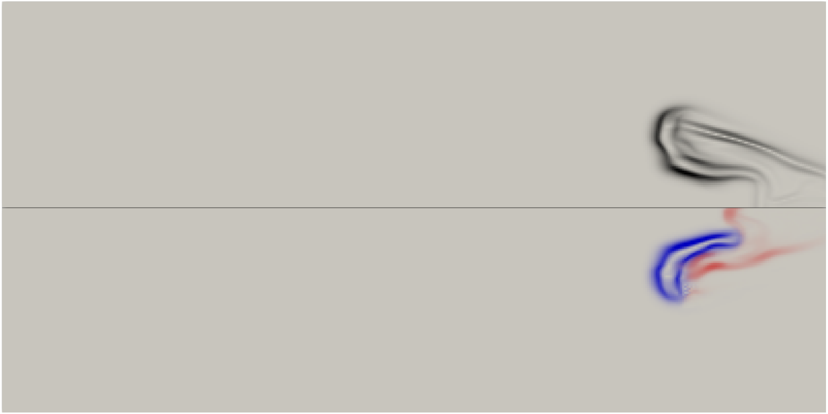

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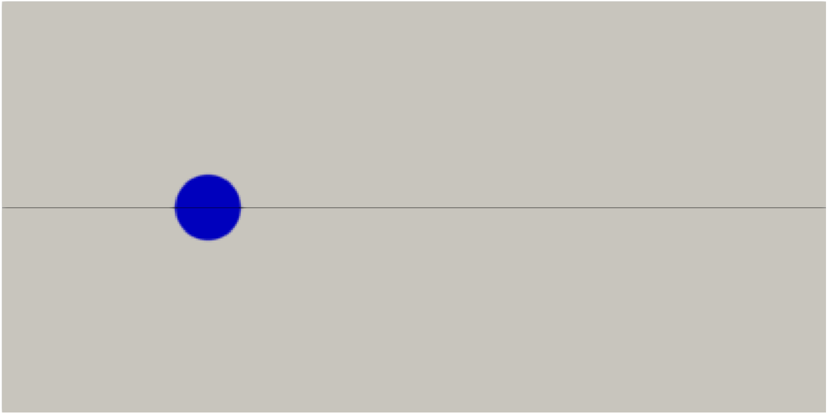
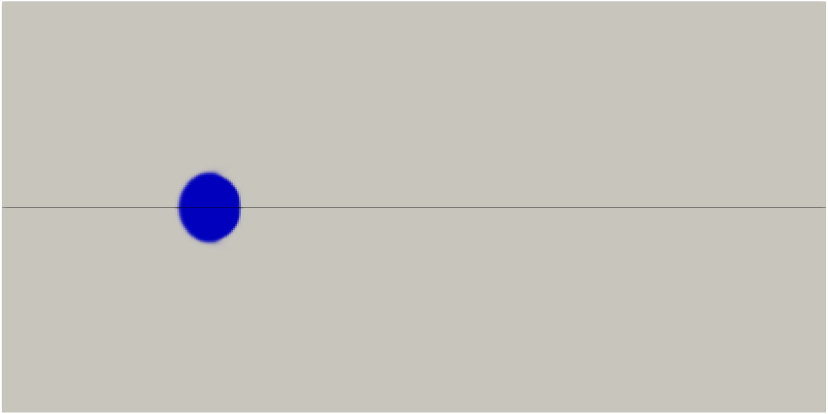
Large scale mass m_1 and small scale mass m_1^d



Top (~~mass transfer~~): large scale mass $m_1 \in (0, 10^3)$
Bottom (mass transfer): m_1 and $m_1^d \in (0, 3.8 \times 10^2)$

Large scale mass m_1 and small scale mass m_1^d



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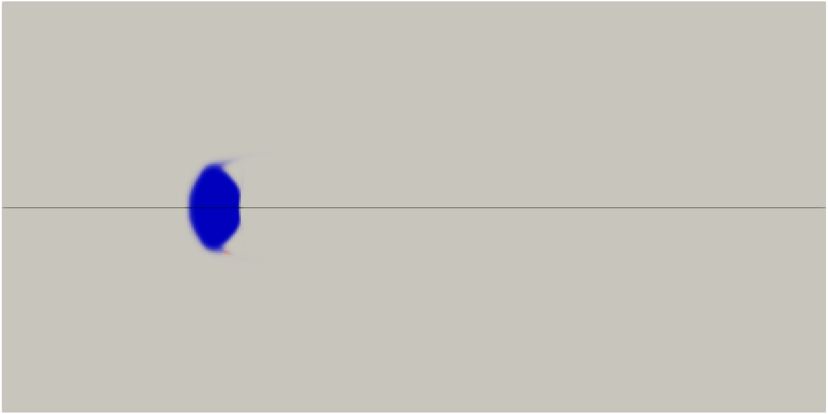

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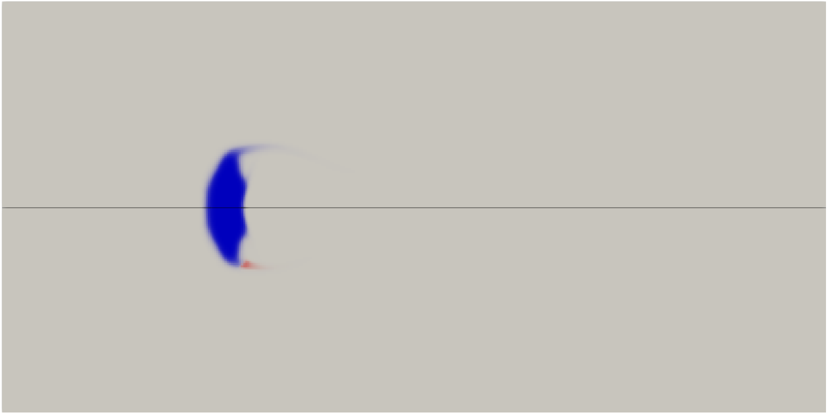

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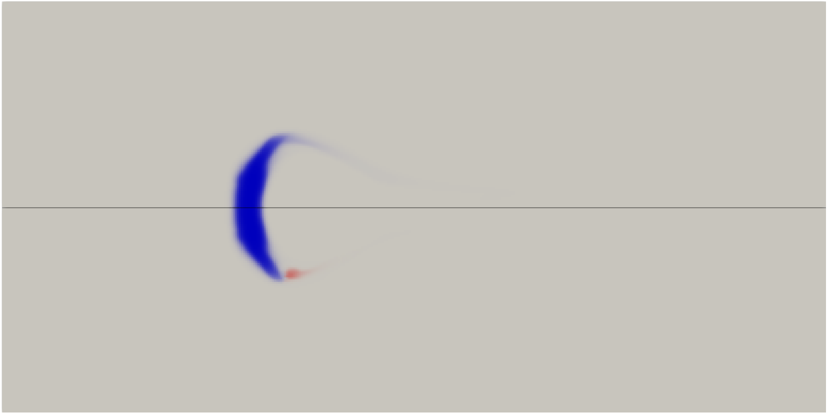

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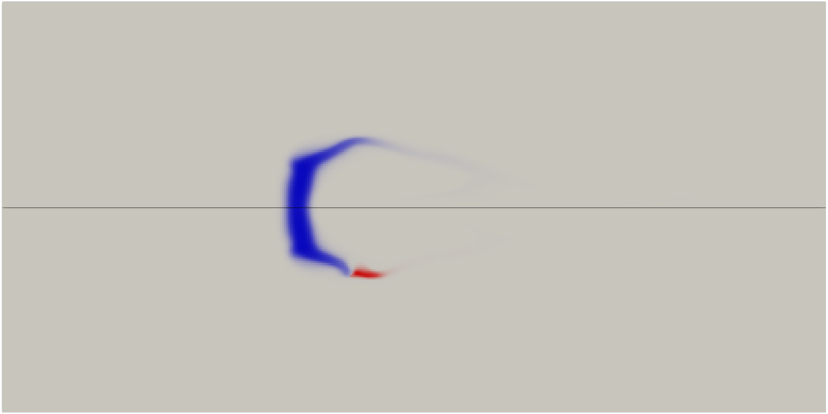

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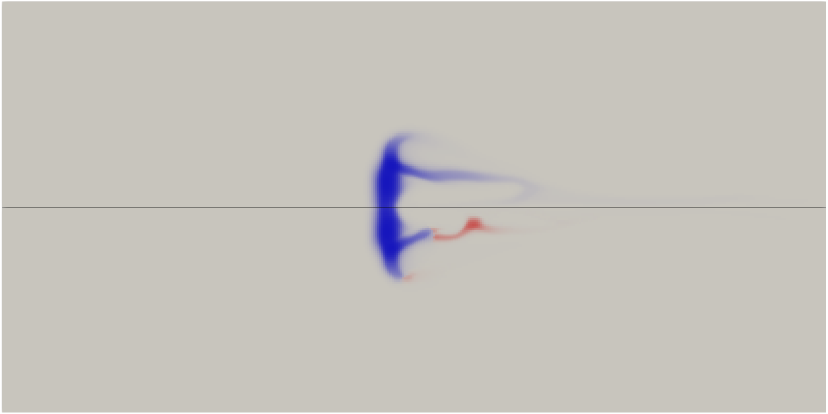

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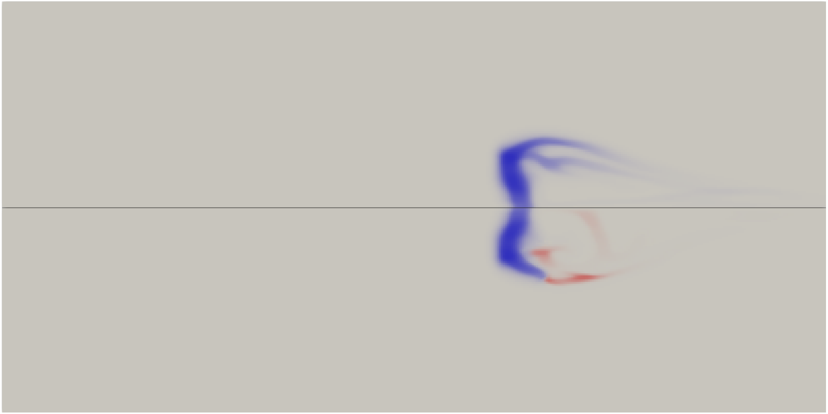
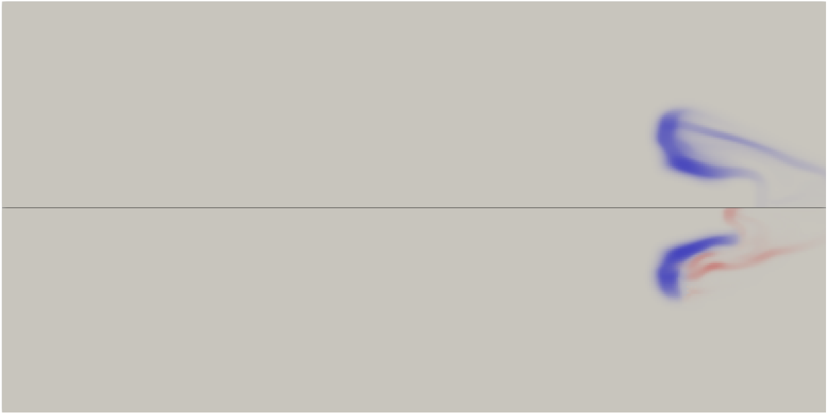
Bottom (mass transfer): m_1 and $m_1^d \in (0, 3.8 \times 10^2)$

Large scale mass m_1 and small scale mass m_1^d



Top (~~mass transfer~~): large scale mass $m_1 \in (0, 10^3)$
Bottom (mass transfer): m_1 and $m_1^d \in (0, 3.8 \times 10^2)$

Large scale mass m_1 and small scale mass m_1^d



Top (~~mass transfer~~): large scale mass $m_1 \in (0, 10^3)$
Bottom (mass transfer): m_1 and $m_1^d \in (0, 3.8 \times 10^2)$

Conclusion and perspectives

Conclusion

- model that can account for both small scale and large scale interfaces
- mass transfer mechanism large scale → small scale
- weakly hyperbolic system (extended system with capillarity)
- small scale coherent with a kinetic description of the disperse phase
- large scale interface topology regularizing property mecanism

Perspectives

- further comparison with DNS (G. Orlando, N. Grenier)
- AMR implementation (`SAMURAI` framework, G. Orlando, L. Gouarin)
- two-velocity kinematics (for the bulk phase)
- system with energy evolution (W. Haegeman, G.Orlando)
- mass transfer mechanism small scale → large scale
- ...