

# Diffuse Interface Models and two Phases Flow Simulations with Free Surface

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# Diffuse Interface Models and SPH

- SPH naturally multimaterial
- Difficulties for equilibrium in the vicinity of contact line of materials with high density ratio
- Needs of interface forces such as surface tension
- General framework for mixture models (Baer Nunziato)
- Connection with incompressible limits used as a numerical tool for solving free surface flow problems
- Alternative to Standard SPH
- Originally developed for Sloshing application in space engineering

## Models and Numerical tools

2001- 2003 (PhD Thesis of G. Chantepedrix) : Finite Volume and Riemann solvers

SLOSH 2D code of ONERA 2004-2005 : SLOSH 3D

2003-2006 : Mixture models for SPH (IFP Thesis of PV Cueille)

Hybrid FV SPH version for miscible fluids

## Physical and Mathematical Background of the models – Diffuse Interface and Thermodynamics

# MIXTURE MODEL (1)

## Dynamic equations

Gas volume fraction

$$(D) \begin{cases} \frac{\partial \tilde{\rho}_1}{\partial t} + \operatorname{div}(\tilde{\rho}_1 V) = 0 & \text{Gas mass conservation} \\ \frac{\partial \tilde{\rho}_2}{\partial t} + \operatorname{div}(\tilde{\rho}_2 V) = 0 & \text{Liquid mass conservation} \\ \frac{\partial \rho V}{\partial t} + \operatorname{div}(\rho V \otimes V + p I_d - \Sigma_v) = \rho g + F_i + F_c & \text{Momentum balance} \end{cases}$$

↑ viscosity    
 ↑ gravity    
 ↑ inertia    
 ↑ Surface tension

$$\tilde{\rho}_1 = \alpha \rho_1 \quad \tilde{\rho}_2 = (1 - \alpha) \rho_2 \quad \rho = \tilde{\rho}_1 + \tilde{\rho}_2$$

## MIXTURE MODEL(2)

### Closure laws

Pressure :

$$p(\alpha, \tilde{\rho}_1, \tilde{\rho}_2) = \alpha p_1 \left( \frac{\tilde{\rho}_1}{\alpha} \right) + (1 - \alpha) p_2 \left( \frac{\tilde{\rho}_2}{1 - \alpha} \right)$$

Dynamic viscosity :

$$\mu = \alpha \mu_1 + (1 - \alpha) \mu_2$$

Gas volume fraction :

$$p_1 \left( \frac{\tilde{\rho}_1}{\alpha} \right) = p_2 \left( \frac{\tilde{\rho}_2}{1 - \alpha} \right) \Rightarrow \alpha = \alpha^* (\tilde{\rho}_1, \tilde{\rho}_2)$$

Linear pressure laws :

$$\begin{aligned} p_1(\rho_1) &= p_{01} + c_1^2 (\rho_1 - \rho_{01}) \\ p_2(\rho_2) &= p_{02} + c_2^2 (\rho_2 - \rho_{02}) \end{aligned}$$

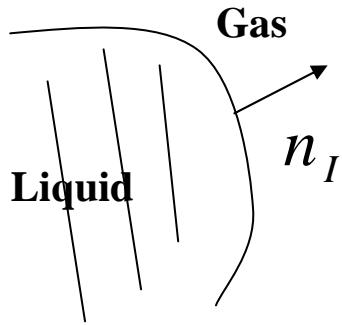
Choice of  $c_i$ :

$$T_a = L/c_i \ll T$$

$$\frac{\Delta \rho_i}{\rho_{0i}} \approx \frac{1}{c_{0i}^2} \Delta p \ll 1$$

# MIXTURE MODEL(3)

## Capillary forces I



$$F_C = \sigma \kappa n_I \approx -\sigma \operatorname{div} \left( \frac{\nabla \alpha}{\|\nabla \alpha\|} \right) \nabla \alpha$$

$$F_C = \nabla \cdot \left( \sigma \|\nabla \alpha\| \mathbf{I}_d - \frac{\sigma \nabla \alpha}{\|\nabla \alpha\|} \otimes \nabla \alpha \right)$$

conservation form

Integration over a boundary cell of the second term gives :

$$\frac{\nabla \alpha}{\|\nabla \alpha\|} \bullet \vec{n}_{\text{wall}} = -\cos \theta$$

Dynamic contact angle model

$$\theta_d = f(V, \theta_s),$$

(from de Gennes *et al*

“Gouttes, bulles, perles et ondes”)

$$\begin{cases} 3 \text{ Ca } \ell = \tan \theta_d (\cos \theta_s - \cos \theta_d) \\ \text{Ca} = \frac{\mu V}{\sigma}, \quad \ell = \log \left( \frac{L}{a} \right) \text{ length scale ratio} \end{cases}$$

Conservation form of  $F_C$  allows for an efficient implementation

# MIXTURE MODEL(3)

## Thermal effects (Boussinesq type model)

Momentum

$$\frac{\partial \rho V}{\partial t} + \text{div}(\rho V \otimes V + p I_d - \Sigma_v) = \rho_0 g - \rho g \beta (T - T_0) + F_c$$

Coupling term

Low velocity flow =>

$$\Delta p \approx 1/2 \rho_0 \Delta(V^2) \ll \rho_0 c_p \Delta T$$

Let :  $T' = T - T_0$

Enthalpy balance

Enthalpy

$$\frac{\partial \rho c_p T'}{\partial t} + \text{div}(\rho c_p T' V) = \text{div}(\lambda \nabla T') + \Sigma_v : \nabla V$$

$$\rho \frac{Dh}{Dt}$$

$$\Phi_c$$

$$W_f$$

Additional closure

$$c_p = \alpha_* c_{p1} + (1 - \alpha_*) c_{p2}$$

# MIXTURE MODEL(3)

## Numerical Tools

Finite Volume scheme based upon Riemann Solvers

Relaxation procedure to achieve mechanical equilibrium

Explicit treatment of Surface tension and viscous effects

Quasi incompressibility or low mach number approach for incompressible fluid

Natural extension to SPH with hybrid ALE formulation

# PHYSICAL BACKGROUND

## Least action Principle (1)

The mixture is characterized by a total energy :  $E = \frac{1}{2} \rho \|\mathbf{u}\|^2 + \sum_i (\tilde{\rho}_i e_i) + \Phi$

where  $e_i(\rho_i, s_i)$  is the internal energy of the fluid i given as a function of the density and the specific entropy of fluid i

and  $\Phi$  a functional which may represent an internal energy related with surface tension and mixture energy :

$$\Phi = \Phi(\alpha_1, \alpha_2, \nabla \alpha_1, \nabla \alpha_2, s_1, s_2) \quad \alpha_1 + \alpha_2 = 1 \quad \text{or} \quad \Phi = G(\alpha, \nabla \alpha, s_1, s_2) \quad \alpha_1 = \alpha, \alpha_2 = 1 - \alpha$$

- The least action principle states that any motion  $(x^\varepsilon, t^\varepsilon)$  minimize the integral of action defined as

$$\mathbf{A}(\varepsilon) = \int_Q L(\tilde{\rho}_1^\varepsilon, \tilde{\rho}_2^\varepsilon, \alpha^\varepsilon, \nabla \alpha^\varepsilon, \mathbf{u}^\varepsilon, s_1^\varepsilon, s_2^\varepsilon) dx^\varepsilon dt^\varepsilon$$

where Q is the space – time domain of definition of the motion and

$$L(\tilde{\rho}_1, \tilde{\rho}_2, \alpha, \nabla \alpha, \mathbf{u}, s_1, s_2) = \frac{1}{2} \rho \|\mathbf{u}\|^2 - \sum_i (\tilde{\rho}_i e_i(\rho_i, s_i)) - G(\alpha, \nabla \alpha, s_1, s_2)$$

under the constraints of mass conservation given by:  $\frac{\partial \tilde{\rho}_i}{\partial t} + \text{div}(\tilde{\rho}_i \mathbf{u}) = 0$



## Least action Principle (2)

- Virtual Motions in agreement with mass conservation are given by a space time diffeomorphism of

$$Q = [t_0, t_1] \times \Omega \quad \Omega \text{ domain in } \mathbf{R}^d \quad \mathbf{x} = (x_0, x_1, \dots, x_d)^T \quad x_0 = t$$

$\mathbf{a}(x)$  Vector field defined on Q is transformed by the diffeomorphism  $\mathbf{g}$  ( $\mathbf{h} = \mathbf{g}^{-1}$ )

$$(\mathbf{a}^g)^T = J_g(\mathbf{a}^T \cdot \nabla(\mathbf{h}^T)) \circ \mathbf{g} \quad \int_{\mathbf{g}(A)} \text{div}_x(\mathbf{a}(x)) dx = \int_A \text{div}_{x'}(\mathbf{a}^g(x')) dx'$$

$$\mathbf{a}^g = J_g(D\mathbf{h} \cdot \mathbf{a}) \circ \mathbf{g}$$

Mass conservation of each constituent reads

$$\frac{\partial \tilde{\rho}_i}{\partial t} + \text{div}(\tilde{\rho}_i \mathbf{u}) = 0$$

Taking  $\mathbf{a}(x) = \begin{pmatrix} \tilde{\rho}_i(x) \\ \tilde{\rho}_i(x) \mathbf{u}(x) \end{pmatrix}$  mass conservation is also

$$\text{div}_x(\mathbf{a}(x)) = 0$$

Transformation rules for  $\mathbf{a}$  and over fields ( $s$  and  $\alpha$ ) are

$$\mathbf{h} = \begin{pmatrix} h_0 \\ h_x \end{pmatrix} \quad \tilde{\rho}_i^\varepsilon(\mathbf{x}^\varepsilon) = J_{g^\varepsilon}(\mathbf{x}^\varepsilon) \tilde{\rho}_i(\mathbf{x}) \left( \frac{\partial h_0}{\partial t} + (\nabla h_0)^T \mathbf{u}(\mathbf{x}) \right) \quad \mathbf{u}^\varepsilon(\mathbf{x}^\varepsilon) = \frac{\frac{\partial h_x}{\partial t} + (\nabla^T h_x)^T \mathbf{u}(\mathbf{x})}{\frac{\partial h_0}{\partial t} + (\nabla h_0)^T \mathbf{u}(\mathbf{x})}$$

$$\alpha_i^\varepsilon(\mathbf{x}^\varepsilon) = \alpha_i(\mathbf{x}) \quad s_i^\varepsilon(\mathbf{x}^\varepsilon) = s_i(\mathbf{x})$$

## Least action Principle (3)

For a given smooth field  $\mathbf{v}$  in  $Q$ , we define a family of diffeomorphism  $\mathbf{g}(\mathbf{x}, \varepsilon)$  depending smoothly on the parameter  $\varepsilon$

$$\begin{cases} \frac{d\mathbf{g}}{d\varepsilon} = \mathbf{g} \circ \mathbf{v} \\ \mathbf{g}|_{\varepsilon=0} = Id_Q \end{cases} \quad \frac{d\mathbf{g}}{d\varepsilon} \Big|_{\varepsilon=0} = \frac{d\mathbf{x}^\varepsilon}{d\varepsilon} \Big|_{\varepsilon=0} = \mathbf{v} = \begin{pmatrix} v_0 \\ \mathbf{w} \end{pmatrix} = - \frac{d\mathbf{h}}{d\varepsilon} \Big|_{\varepsilon=0}$$

$$\frac{d\mathbf{x}^\varepsilon}{d\varepsilon} \Big|_{\varepsilon=0} = \mathbf{v} := \delta\mathbf{x}$$

$$\frac{dJ^\varepsilon}{d\varepsilon} \Big|_{\varepsilon=0} = \frac{\partial v_0}{\partial t} + \text{div}(\mathbf{w}) := \delta J$$

$$\frac{ds_i^\varepsilon}{d\varepsilon} \Big|_{\varepsilon=0} = 0$$

$$\frac{d\alpha_i^\varepsilon}{d\varepsilon} \Big|_{\varepsilon=0} = 0$$

$$\frac{d\tilde{\rho}_i^\varepsilon}{d\varepsilon} \Big|_{\varepsilon=0} = \tilde{\rho}_i (\text{div}(\mathbf{w}) - \mathbf{u}^T \cdot \nabla(v_0)) := \delta\tilde{\rho}_i$$

$$\frac{d\mathbf{u}^\varepsilon}{d\varepsilon} \Big|_{\varepsilon=0} = - \left( \frac{\partial w_\alpha}{\partial t} + \sum_{\beta=1,d} u_\beta \frac{\partial w_\alpha}{\partial x_\beta} \right) + \mathbf{u}_\alpha(\mathbf{x}) \left( \frac{\partial v_0}{\partial t} + (\nabla v_0)^T \cdot \mathbf{u} \right) := \delta\mathbf{u}_\alpha$$

$$\frac{d\nabla_{x^\varepsilon} \alpha_i^\varepsilon}{d\varepsilon} \Big|_{\varepsilon=0} = \frac{\partial \alpha_i}{\partial t} \nabla(v_0) + (\nabla^T \mathbf{w})^T \nabla \alpha_i := \delta \nabla \alpha_i$$

The Action  $\mathcal{A}(\varepsilon) = \int_Q L(\tilde{\rho}_i^\varepsilon, \alpha_i^\varepsilon, \nabla \alpha_i^\varepsilon, \mathbf{u}^\varepsilon, s_i^\varepsilon) dx^\varepsilon dt^\varepsilon$  is differentiable with respect to  $\varepsilon$  at  $\varepsilon=0$

and its derivative is given by

$$\frac{d\mathcal{A}(\varepsilon)}{d\varepsilon} \Big|_{\varepsilon=0} = \int_Q \left( \left( \frac{\partial L}{\partial \mathbf{u}} \right)^T \delta \mathbf{u} + \sum_i \left( \frac{\partial L}{\partial \tilde{\rho}_i} \delta \tilde{\rho}_i + \frac{\partial L}{\partial \nabla \alpha_i} \delta \nabla \alpha_i \right) - L \delta J \right) dx dt$$

Least Action Principle says Action is minimal among all the virtual motions, thus

$$\frac{d\mathcal{A}(\varepsilon)}{d\varepsilon} \Big|_{\varepsilon=0} = 0$$

## Least action Principle (4)

The above computation gives

$$\begin{aligned} \frac{d\mathcal{A}(\varepsilon)}{d\varepsilon}\Big|_{\varepsilon=0} &= \int_Q \left( (-P + \Phi) \operatorname{div}(\mathbf{w}) - \sum_i \frac{\partial \Phi_i}{\partial \nabla \alpha_i} (\nabla^T \mathbf{w})^T \nabla \alpha - \rho \mathbf{u}^T \left( \frac{\partial \mathbf{w}}{\partial t} + (\mathbf{u}^T \cdot \nabla \mathbf{w}^T)^T \right) \right. \\ &\quad \left. + \left( \frac{1}{2} \rho \|\mathbf{u}\|^2 + \sum_i (\tilde{\rho}_i e_i) + \Phi \right) \frac{\partial v_0}{\partial t} \right. \\ &\quad \left. - \left( \sum_i \frac{\partial \alpha_i}{\partial t} \frac{\partial \Phi}{\partial \nabla \alpha_i} - \left( \frac{1}{2} \rho \|\mathbf{u}\|^2 + P + \sum_i \tilde{\rho}_i e_i \right) \mathbf{u}^T \right) \nabla(v_0) \right) dxdt \end{aligned}$$

$$P = \sum_i \alpha_i p_i$$

and  $\frac{d\mathcal{A}(\varepsilon)}{d\varepsilon}\Big|_{\varepsilon=0} = 0$

$$\forall \mathbf{w} \in \mathcal{C}^\infty(Q, \mathbb{R}^d)$$

$$\int_Q \left( \rho \mathbf{u}^T \left( \frac{\partial \mathbf{w}}{\partial t} + (\mathbf{u}^T \cdot \nabla \mathbf{w}^T)^T \right) + (P - \Phi) \operatorname{div}(\mathbf{w}) + \sum_i \frac{\partial \Phi_i}{\partial \nabla \alpha_i} (\nabla^T \mathbf{w})^T \nabla \alpha \right) dxdt = 0$$

$$\forall v_0 \in \mathcal{C}^\infty(Q, \mathbb{R})$$

$$\begin{aligned} &\int_Q \left( \left( \frac{1}{2} \rho \|\mathbf{u}\|^2 + \sum_i (\tilde{\rho}_i e_i) + \Phi \right) \frac{\partial v_0}{\partial t} \right. \\ &\quad \left. + \left( \left( \frac{1}{2} \rho \|\mathbf{u}\|^2 + P + \sum_i \tilde{\rho}_i e_i \right) \mathbf{u}^T - \sum_i \frac{\partial \alpha_i}{\partial t} \frac{\partial \Phi}{\partial \nabla \alpha_i} \right) \cdot \nabla(v_0) \right) dxdt = 0 \end{aligned}$$

## Least action Principle (5)

Which are variationnal (or weak) formulation of momentum and energy conservation of the mixture

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \text{div}(\rho \mathbf{u} \otimes \mathbf{u}) + \nabla(P - \Phi) + \text{div}\left(\sum_i \frac{\partial \Phi}{\partial \nabla \alpha_i} \otimes \nabla \alpha_i\right) = \mathbf{0} \quad P = \sum_i \alpha_i p_i$$

$$\frac{\partial(\frac{1}{2}\rho\|\mathbf{u}\|^2 + \sum_i(\tilde{\rho}_i e_i) + \Phi)}{\partial t} + \text{div}\left(\left(\frac{1}{2}\rho\|\mathbf{u}\|^2 + P + \sum_i \tilde{\rho}_i e_i\right)\mathbf{u} - \sum_i \frac{\partial \alpha_i}{\partial t} \frac{\partial \Phi}{\partial \nabla \alpha_i}\right) = 0$$

And we recover the capillary tensor

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \text{div}(\rho \mathbf{u} \otimes \mathbf{u}) = \text{div} \boldsymbol{\tau} \quad \boldsymbol{\tau} = -(P - \Phi) \mathbf{1}_d - \left(\sum_i \frac{\partial \Phi}{\partial \nabla \alpha_i} \otimes \nabla \alpha_i\right) \quad \boldsymbol{\tau} = -(P - \Phi) \mathbf{1}_d - \frac{\partial G}{\partial \nabla \alpha} \otimes \nabla \alpha$$

$$\frac{\partial E}{\partial t} + \text{div}(E \mathbf{u}) = \text{div} \boldsymbol{\pi} + \text{div} \mathbf{W} \quad E = \frac{1}{2}\rho\|\mathbf{u}\|^2 + \sum_i(\tilde{\rho}_i e_i) + \Phi$$

$$\mathbf{W} = \sum_i \frac{\partial \Phi}{\partial \nabla \alpha_i} \left(\frac{\partial \alpha_i}{\partial t} + \mathbf{u}^T \nabla \alpha_i\right) = \sum_i \frac{\partial \Phi}{\partial \nabla \alpha_i} \frac{d \alpha_i}{dt} \quad \mathbf{W} = \frac{\partial G}{\partial \nabla \alpha} \frac{d \alpha}{dt} = \frac{\partial G}{\partial \nabla \alpha} \left(\frac{\partial \alpha}{\partial t} + \mathbf{u} \nabla \alpha\right)$$

$\mathbf{W}$  is the interstitial work

The unknowns are  $(\tilde{\rho}_1, \tilde{\rho}_2, \mathbf{u}, \alpha, s_1, s_2)$ , system has  $d+5$  unknowns. We only have  $d+3$  equations.

We need 2 additionnal closures

## Least action Principle (6)

We define 2 additional families of virtual motion (mechanical equilibrium and thermodynamical equilibrium)

### Virtual motion for mechanical equilibrium

$(\tilde{\rho}_i(\mathbf{x}), s_i(\mathbf{x}), \mathbf{u}(\mathbf{x}))$  unchanged with

$$\begin{cases} \frac{d\alpha_i^\varepsilon}{d\varepsilon} = \varphi_i \\ \alpha_i^\varepsilon|_{\varepsilon=0} = \alpha_i \end{cases}$$

where  $\varphi_i(\mathbf{x})$  are smooth functions such that

$$\sum_i \varphi_i(\mathbf{x}) = 0$$

Then the non null derivatives are

$$\frac{d\alpha_i^\varepsilon}{d\varepsilon}|_{\varepsilon=0} = \varphi_i$$

$$\frac{d\nabla_x \alpha_i^\varepsilon}{d\varepsilon}|_{\varepsilon=0} = \nabla \varphi_i$$

Least action principle gives as above  $\frac{d\mathcal{A}(\varepsilon)}{d\varepsilon}|_{\varepsilon=0} = 0$

with  $\frac{d\mathcal{A}(\varepsilon)}{d\varepsilon}|_{\varepsilon=0} = \int_Q \left( \sum_i \frac{\partial L}{\partial \alpha_i} \delta \alpha_i + \frac{\partial L}{\partial \nabla \alpha_i} \delta \nabla \alpha_i \right) dx dt$  which leads to

$\forall \varphi_i \in \mathbf{C}^\infty(Q, \mathbb{R}^d)$  such that  $\sum_i \varphi_i = 0$

$$\int_Q \left( \sum_i \left( p_i - \frac{\partial \Phi}{\partial \alpha_i} \right) \varphi_i - \frac{\partial \Phi}{\partial \nabla \alpha_i} \nabla \varphi_i \right) dx dt = 0$$

And consequently to

$$p_i - \frac{\partial \Phi}{\partial \alpha_i} + \text{div} \left( \frac{\partial \Phi}{\partial \nabla \alpha_i} \right) = P + \sum_j \alpha_j \text{div} \left( \frac{\partial \Phi}{\partial \nabla \alpha_j} \right)$$

or

$$p_2 - p_1 = -\frac{\partial G}{\partial \alpha} + \text{div} \left( \frac{\partial G}{\partial \nabla \alpha} \right)$$

Mixing Energy effect

Surface Tension effect

# PHYSICAL BACKGROUND

## Least action Principle (7)

### Virtual motion for thermodynamical equilibrium

The aim is to construct extremum for  $\mathcal{S} = \int_Q \sum_i \tilde{\rho}_i s_i dxdt$  in agreement with least action principle which requires extremum for the action  $\mathcal{A}(\varepsilon)$ .

Taking  $(\tilde{\rho}_i(x), \alpha_i(x), u(x))$  unchanged with  $\begin{cases} \frac{ds_i^\varepsilon}{d\varepsilon} = \varphi_i \\ s_i^\varepsilon|_{\varepsilon=0} = s_i \end{cases}$  where  $\varphi_i(x)$  are smooth functions.

We find  $\frac{d\mathcal{A}(\varepsilon)}{d\varepsilon}|_{\varepsilon=0} = -\int_Q \left( \sum_i \left( \tilde{\rho}_i T_i + \frac{\partial \Phi}{\partial s_i} \right) \varphi_i \right) dxdt$ . Taking  $\sum_i \left( \tilde{\rho}_i T_i + \frac{\partial \Phi}{\partial s_i} \right) \varphi_i = 0 \longrightarrow \frac{d\mathcal{A}(\varepsilon)}{d\varepsilon}|_{\varepsilon=0} = 0$

We also have  $\frac{d\mathcal{S}(\varepsilon)}{d\varepsilon}|_{\varepsilon=0} = \int_Q \left( \sum_i \tilde{\rho}_i \delta s_i \right) dxdt$  and  $\frac{d\mathcal{S}(\varepsilon)}{d\varepsilon}|_{\varepsilon=0} = 0$  requires  $\sum_i \tilde{\rho}_i \delta s_i = 0$

Which is possible iff we have a unique thermodynamical temperature  $T$  such that

$$T_i + \frac{1}{\tilde{\rho}_i} \frac{\partial \Phi}{\partial s_i} = T$$

# PHYSICAL BACKGROUND

## Least Action Principle. Final model

- The complete model is :

$$E = \frac{1}{2} \rho \|\mathbf{u}\|^2 + \sum_i (\tilde{\rho}_i e_i) + \Phi$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \operatorname{div}(\rho \mathbf{u} \otimes \mathbf{u}) = \operatorname{div} \boldsymbol{\tau}$$

$$\Phi = G(\alpha, \nabla \alpha, s_1, s_2)$$

$$P = \alpha p_1 + (1 - \alpha) p_2$$

$$\frac{\partial \mathbf{E}}{\partial t} + \operatorname{div}(\mathbf{E} \mathbf{u}) = \operatorname{div} \boldsymbol{\tau} + \operatorname{div} \mathbf{W}$$

$$\boldsymbol{\tau} = -(P - \Phi) \mathbf{I}_d - \frac{\partial G}{\partial \nabla \alpha} \otimes \nabla \alpha$$

with the additional constraints of mechanical equilibrium :

$$p_2 - p_1 = -\frac{\partial G}{\partial \alpha} + \operatorname{div}\left(\frac{\partial G}{\partial \nabla \alpha}\right)$$

and thermal equilibrium :

$$T_1 + \frac{1}{\tilde{\rho}_1} \frac{\partial \Phi}{\partial s_1} = T_2 + \frac{1}{\tilde{\rho}_2} \frac{\partial \Phi}{\partial s_2} = \theta$$

In the isothermal case we recover the model presented above where the capillary tensor is given here by

$$\boldsymbol{\tau}_c = \left( \Phi \mathbf{I} - \frac{\partial \Phi}{\partial \nabla \alpha} \otimes \nabla \alpha \right)$$

# PHYSICAL BACKGROUND

## Laplace relation and sharp interface limit

- Taking  $G(\alpha, \nabla \alpha, s_1, s_2) = \varphi(\alpha) + \mathbf{G}(\|\nabla \alpha\|)$

$$\operatorname{div} \left( -(P - \Phi) \mathbf{I}_d - \frac{\partial \mathbf{G}(\|\nabla \alpha\|)}{\partial \nabla \alpha} \otimes \nabla \alpha \right) = -\nabla(P - \varphi) - \left( \operatorname{div} \left( \mathbf{G}'(\|\nabla \alpha\|) \frac{\|\nabla \alpha\|}{\nabla \alpha} \right) \right) \nabla \alpha$$

Static equilibrium requires 
$$\nabla(P - \varphi) = - \left( \operatorname{div} \left( \mathbf{G}'(\|\nabla \alpha\|) \frac{\|\nabla \alpha\|}{\nabla \alpha} \right) \right) \nabla \alpha$$

In the sharp interface limit  $\alpha(x) = Y_\varepsilon(r - R)$  where  $Y_\varepsilon$  is a regularisation of the heaviside function of thickness  $\varepsilon$

In the special case  $\mathbf{G}(\|\nabla \alpha\|) = \sigma \|\nabla \alpha\|$  we recover that the pressure jump across the interface layer is given by the Laplace relation.

$$p_2 - p_1 = \sigma C$$

In the more general case  $\mathbf{G}(\|\nabla \alpha\|) = k \|\nabla \alpha\|^m$ , the Laplace law is still valid, but the macroscopic surface tension coefficient depends also of the thickness of the layer (once we give the coefficient  $k$  of the microscopic energy)

The case  $m=1$  corresponds with CSF method of Brackbill,  $m=2$  corresponds with a more realistic Physics, but requires a correct resolution of interface layer (second gradient or Korteweg point of view)



## Dissipation and Thermodynamics of Irreversible Process (1)

- Least Action Principle ignore dissipative mechanisms. 2nd principle of Thermodynamics ( Clausius Duhem inequality) gives information on admissible dissipative process.

- Let  $\frac{da}{dt} = \frac{\partial a}{\partial t} + \mathbf{u} \nabla a$  the balance laws reads

$$(i) \quad \frac{d\tilde{\rho}_i}{dt} = -\tilde{\rho}_i \operatorname{div} \mathbf{u}$$

$$(ii) \quad \rho \frac{du}{dt} = \operatorname{div}(\Sigma) + \rho \mathbf{f}$$

$$(iii) \quad \rho \frac{de}{dt} = \Sigma \cdot D\mathbf{u} + \operatorname{div}(\mathbf{w}) - \operatorname{div}(\mathbf{q}) + \rho r$$

Clausius Duhem inequality  
is not the standart one



$$(iv) \quad \rho \left( \frac{d\psi}{dt} + s \frac{d\theta}{dt} \right) - \Sigma \cdot D\mathbf{u} - \operatorname{div}(\mathbf{w}) + \frac{\mathbf{q} \cdot \nabla \theta}{\theta} \leq 0$$

where  $\psi = e - \theta s$  is the free Helmolzt energy and  $\theta$  the thermodynamic temperature. In our case we postulate

$$\rho \psi = \rho \bar{\psi}(\tilde{\rho}_1, \tilde{\rho}_2, \alpha, \theta) + \Phi(\alpha, \theta, \|\nabla \alpha\|)$$

$$\rho \psi = \tilde{\rho}_1 e_1 \left( \frac{\tilde{\rho}_1}{\alpha}, s_1 \right) + \tilde{\rho}_2 e_2 \left( \frac{\tilde{\rho}_2}{\alpha}, s_2 \right) - \theta(\tilde{\rho}_1 s_1 + \tilde{\rho}_2 s_2) + \varphi(\alpha) + G(\theta, \|\nabla \alpha\|)$$

We also need a closure equation in order to relate the volume fraction with other unknowns.

We propose

$$\frac{d\alpha}{dt} = R$$

where R is an unknown fonctionnal.

## Dissipation and Thermodynamics of Irreversible Process (2)

- The flow process is determined by  $\pi = \{\tilde{\rho}_1, \tilde{\rho}_2, \alpha, R, \theta, e, s, \Sigma, \mathbf{u}, \mathbf{q}, \mathbf{w}, \mathbf{f}, r\}$  and we need to define unknown fluxes  $R, e, s, \Sigma, \mathbf{q}, \mathbf{w}$  as functional of some set of variables or auxiliary variables e.g. :

$$\Lambda^T = (\tilde{\rho}_1, \tilde{\rho}_2, \alpha, \mathbf{u}, \theta, \nabla \mathbf{u}, \nabla \theta, \nabla \alpha, \nabla \nabla \alpha)$$

As a consequence we have necessarily

$$s = s(\tilde{\rho}_1, \tilde{\rho}_2, \alpha, \theta, \|\nabla \alpha\|) = -\frac{\partial \psi}{\partial \theta}$$

and with the additional **material indifference principle** which states some rules for dependency of unknown fluxes with respect to  $\Lambda$  under a change of referential, we find that  $\mathbf{w}$  is given by

$$\mathbf{w} = \rho \frac{\partial \psi}{\partial \nabla \alpha} R(\tilde{\rho}_1, \tilde{\rho}_2, \alpha, \mathbf{u}, \theta, \nabla \mathbf{u}, \nabla \theta, \nabla \alpha, \nabla \nabla \alpha) + \gamma_2(\alpha, \theta, \|\nabla \alpha\|) \nabla \alpha \wedge \nabla \theta$$

where  $\gamma_2$  is a scalar valued functions. We also have a reduced Clausius – Duhem inequality

$$\left( \rho \frac{\partial \bar{\psi}}{\partial \alpha} - \operatorname{div} \left( \frac{\partial \Phi}{\partial \|\nabla \alpha\|} \frac{\nabla \alpha}{\|\nabla \alpha\|} \right) \right) R_{eq} \leq 0 \quad \text{where} \quad R_{eq} = R(\tilde{\rho}_1, \tilde{\rho}_2, \alpha, \theta, 0, 0, \nabla \alpha, \nabla \nabla \alpha)$$

$$\left( p_2 - p_1 + \frac{\partial \varphi}{\partial \alpha} - \operatorname{div} \left( \frac{\partial G}{\partial \|\nabla \alpha\|} \frac{\nabla \alpha}{\|\nabla \alpha\|} \right) \right) R_{eq} \leq 0$$

## Dissipation and Thermodynamics of Irreversible Process (3)

Any admissible process need to satisfy the above requirement. One acceptable choice is the following

$$\tau_c = -\left( \nabla \alpha \otimes \rho \frac{\partial \psi}{\partial \nabla \alpha} + \rho \frac{\partial \psi}{\partial \tilde{\rho}_i} \tilde{\rho}_i \mathbf{I} \right) \quad \Sigma = \tau_c + \Sigma_v \quad \mathbf{w} = \rho \frac{\partial \psi}{\partial \nabla \alpha} R$$

with

$$-\Sigma_v : \nabla \mathbf{u} \leq \mathbf{0} \quad R = -\frac{1}{\varepsilon} \left( \rho \frac{\partial \bar{\psi}}{\partial \alpha} - \operatorname{div} \left( \frac{\partial \Phi}{\partial \|\nabla \alpha\|} \frac{\nabla \alpha}{\|\nabla \alpha\|} \right) \right) \quad \frac{\mathbf{q} \cdot \nabla \theta}{\theta} \leq 0$$

and  $\varepsilon > 0$  in order to satisfy the Clausius Duhem inequality :

$$\begin{aligned} & -\left( \nabla \alpha \otimes \rho \frac{\partial \psi}{\partial \nabla \alpha} + \rho \frac{\partial \psi}{\partial \tilde{\rho}_i} \tilde{\rho}_i \mathbf{I} + \Sigma \right) : \nabla \mathbf{u} \\ & + \left( \rho \frac{\partial \bar{\psi}}{\partial \alpha} - \operatorname{div} \left( \frac{\partial \Phi(\alpha, \theta, \|\nabla \alpha\|)}{\partial \|\nabla \alpha\|} \frac{\nabla \alpha}{\|\nabla \alpha\|} \right) \right) R - \operatorname{div} \left( \mathbf{w} - \rho \frac{\partial \psi}{\partial \nabla \alpha} R \right) + \frac{\mathbf{q} \cdot \nabla \theta}{\theta} \leq 0 \end{aligned}$$

The above equations states the basis of our numerical models.

$$R_{eq} = -\frac{1}{\varepsilon} \left( p_2 - p_1 + \frac{\partial \varphi}{\partial \alpha} - \operatorname{div} \left( \frac{\partial G}{\partial \|\nabla \alpha\|} \frac{\nabla \alpha}{\|\nabla \alpha\|} \right) \right) \quad \text{is closely related to the previous notion of mechanical equilibrium}$$

Note that phase change phenomena can be included in such an approach. Strong connections of physical mechanism with relaxation procedure and energy transfer are one of the main characteristic of this approach.

# PHYSICAL BACKGROUND

## Dissipation and Thermodynamics of Irreversible Process (4)

Incompressible Limit and NS Cahn Hilliard formulation for partially miscible fluids

- Instead of  $\frac{d\alpha}{dt} = R$  we use  $\frac{d\alpha}{dt} = \text{div}(J)$
- With  $J = D\nabla\mu$   $\mu = p_2 - p_1 + \frac{\partial\phi}{\partial\alpha} - \text{div}\left(\frac{\partial G}{\partial\|\nabla\alpha\|} \frac{\nabla\alpha}{\|\nabla\alpha\|}\right)$

$$\mu R = \mu \text{div}(J) = \mu \text{div}(D\nabla\mu) = \text{div}(\mu D\nabla\mu) - D\|\nabla\mu\|^2$$

And a modified C.D. inequality is satisfied

$$-\left(\nabla\alpha \otimes \rho \frac{\partial\psi}{\partial\nabla\alpha} + \rho \frac{\partial\psi}{\partial\rho_i} \widehat{\rho}_i \mathbf{1} + \Sigma\right) : \nabla\mathbf{u}$$

$$+ \left(\rho \frac{\partial\bar{\psi}}{\partial\alpha} - \text{div}\left(\frac{\partial\Phi(\alpha, \theta, \|\nabla\alpha\|)}{\partial\|\nabla\alpha\|} \frac{\nabla\alpha}{\|\nabla\alpha\|}\right)\right) R - \text{div}\left(\mathbf{w} - \rho \frac{\partial\psi}{\partial\nabla\alpha} R\right) + \frac{\mathbf{q} \cdot \nabla\theta}{\theta} \leq 0$$

Example of planar interfaces

There is a competition relating TS and mixture energy which characterise the thickness of the interface

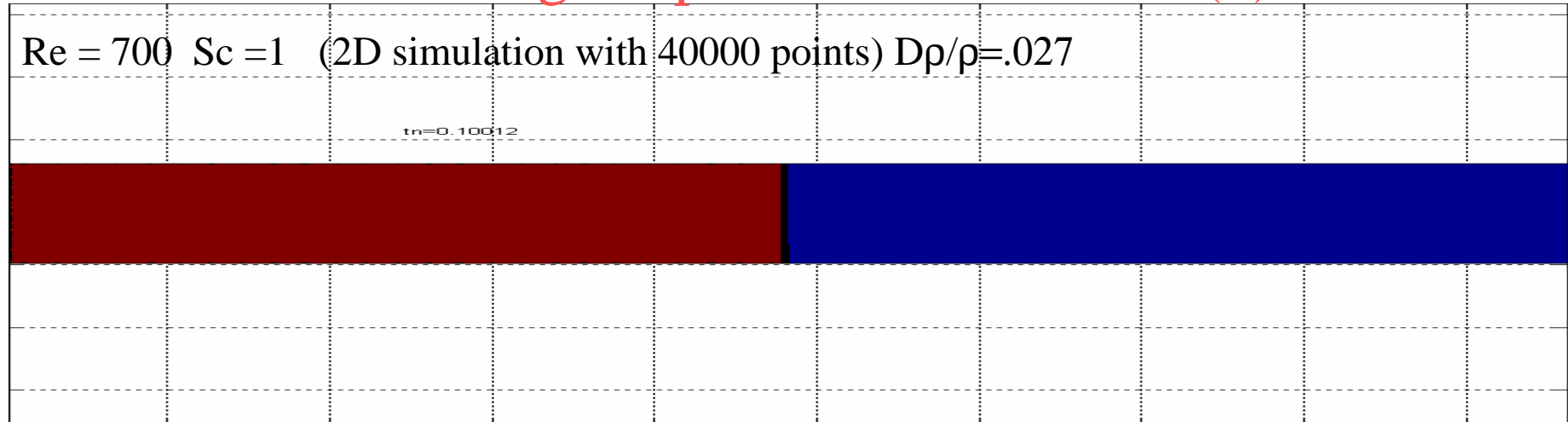
layer. Typically if 
$$\phi(\alpha) + G(\nabla\alpha) = \frac{K}{\varepsilon} \alpha^2 (1 - \alpha)^2 + \sigma\varepsilon \|\nabla\alpha\|^2$$

$\sigma$  is the macroscopic surface tension coeff. and  $\varepsilon$  the thickness of the interface

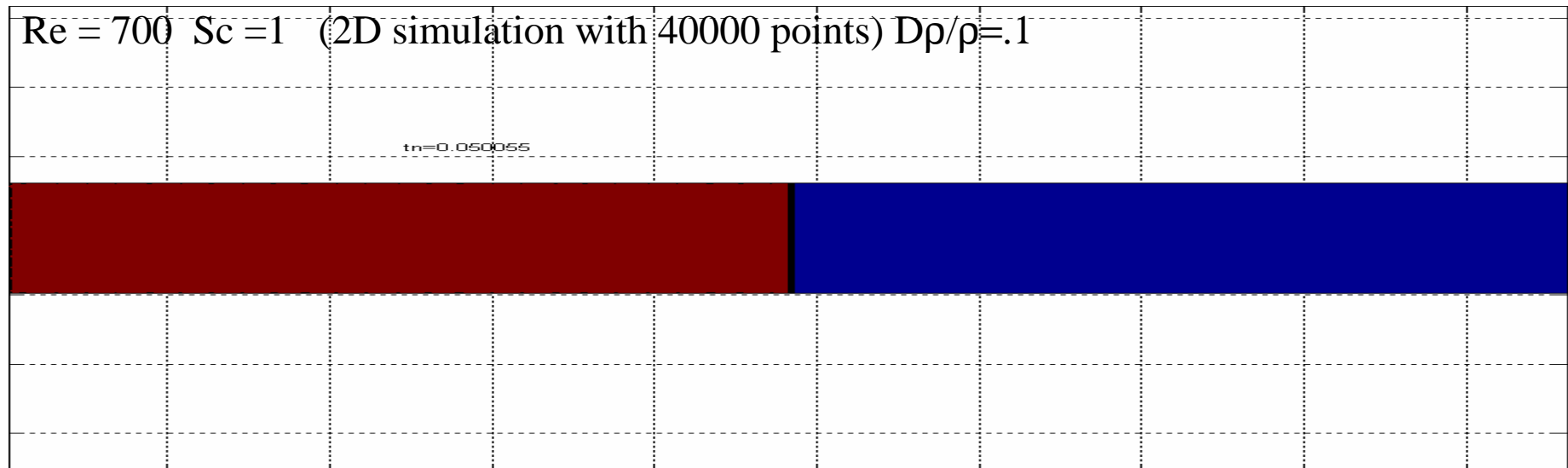
# Applications of the method to miscible Fluids

## Lock exchange experiment simulation (1)

- $Re = 700$   $Sc = 1$  (2D simulation with 40000 points)  $D\rho/\rho = .027$



- $Re = 700$   $Sc = 1$  (2D simulation with 40000 points)  $D\rho/\rho = .1$



# Applications of the method to miscible Fluids

## Lock exchange experiment simulation (2)

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- $Re = 10000$   $Sc = 1$  (2D simulation with 200000 points)

