Derivation of compressible two-phase flow models with surface tension

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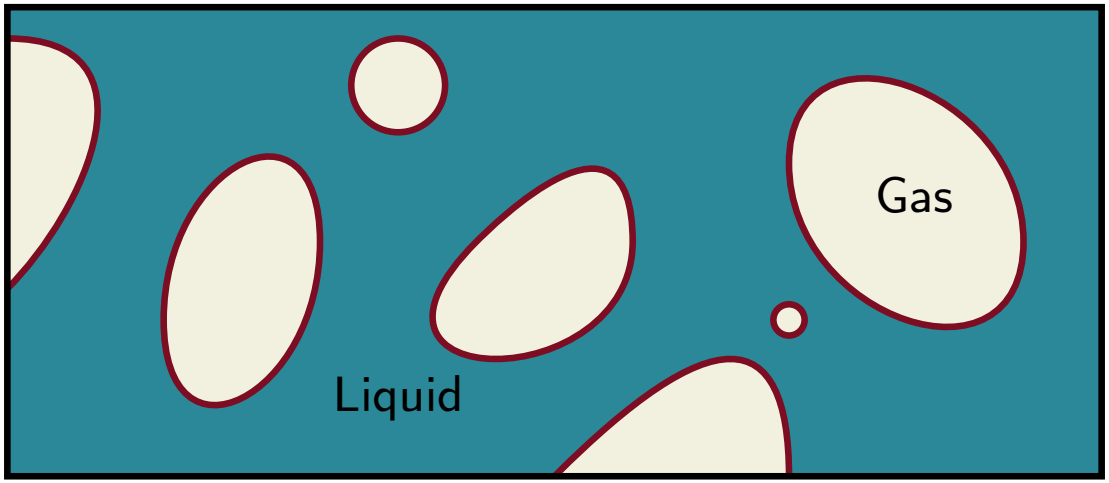
Séminaire - SISMA - CEA DAM - Mai 2024

Motivations



Context

- Nuclear safety: accident situation in pressurized water reactor
- High temperature and pressure conditions
- Compressible two-phase flows (or multiphase flows) with heterogeneities (bubbles, droplets...)
  - Complex interface
- Thermodynamical (dis)equilibrium
  - Thermal, mechanical, mass transfers through the interface
- Complex wave interactions (shocks, phase transition...)

The richest model [Baer, Nunziato '86]

- Euler system for two immiscible phases $k = 1, 2$ with coupling terms
- Phasic state $w_k = (\rho_k, u_k, e_k)$, $w = (w_1, w_2)$
- Pressure $p_k = p_k(\rho_k, e_k)$, total energy $E_k = e_k + \dfrac{u_k^2}{2}$, chemical potential $\mu_k = \mu_k(\rho_k, e_k)$
- Volume fraction $\alpha_k \in [0, 1]$

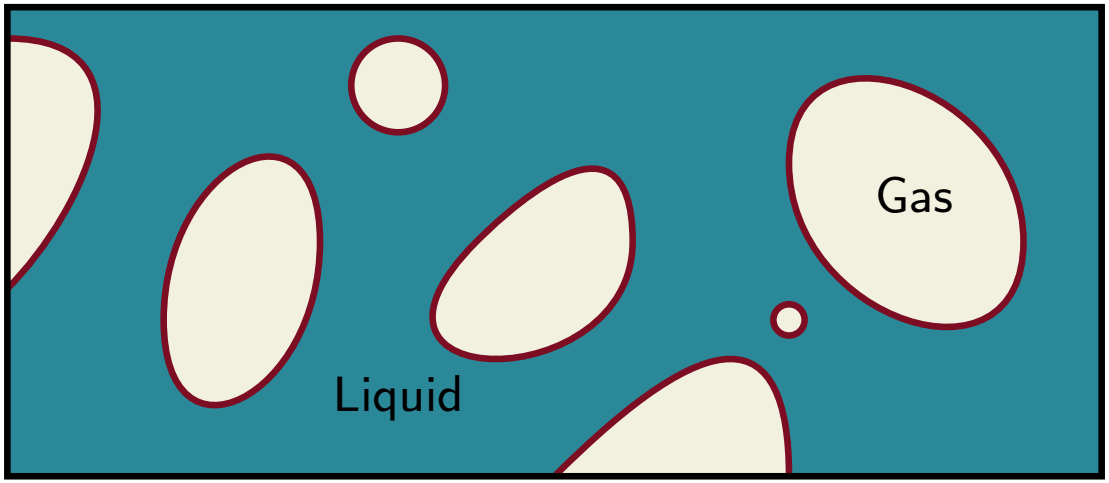
$$\alpha_1 + \alpha_2 = 1 \qquad \rho = \alpha_1\rho_1 + \alpha_2\rho_2$$
$$\partial_t\alpha_1 + u_i(w)\partial_x\alpha_1 = \lambda_p(w)(p_1 - p_2)$$
$$\partial_t(\alpha_k\rho_k) + \partial_x(\alpha_k\rho_k u) = \lambda_\rho(w)(\mu_l - \mu_k)$$
$$\partial_t(\alpha_k\rho_k u_k) + \partial_x(\alpha_k\rho_k u_k^2 + \alpha_k p_k) - p_i(w)\partial_x\alpha_k = \lambda_u(w)(u_l - u_k)$$
$$\partial_t(\alpha_k\rho_k E_k) + \partial_x((\rho_k E_k + p_k)\alpha_k u) + p_i(w)\partial_t\alpha_k = \lambda_u(w)u_i(w)(u_l - u_k)$$

✓ Well-posedness although nonconservative: hyperbolicity, symmetrizable, jump conditions...

✗ Heuristic closure laws for interfacial quantities $u_i(w)$ and $p_i(w)$

✗ Empirical relaxation time scales $\lambda_{p,\rho,u}(w)$ and source terms, possibly depending on interfacial area...

Motivations

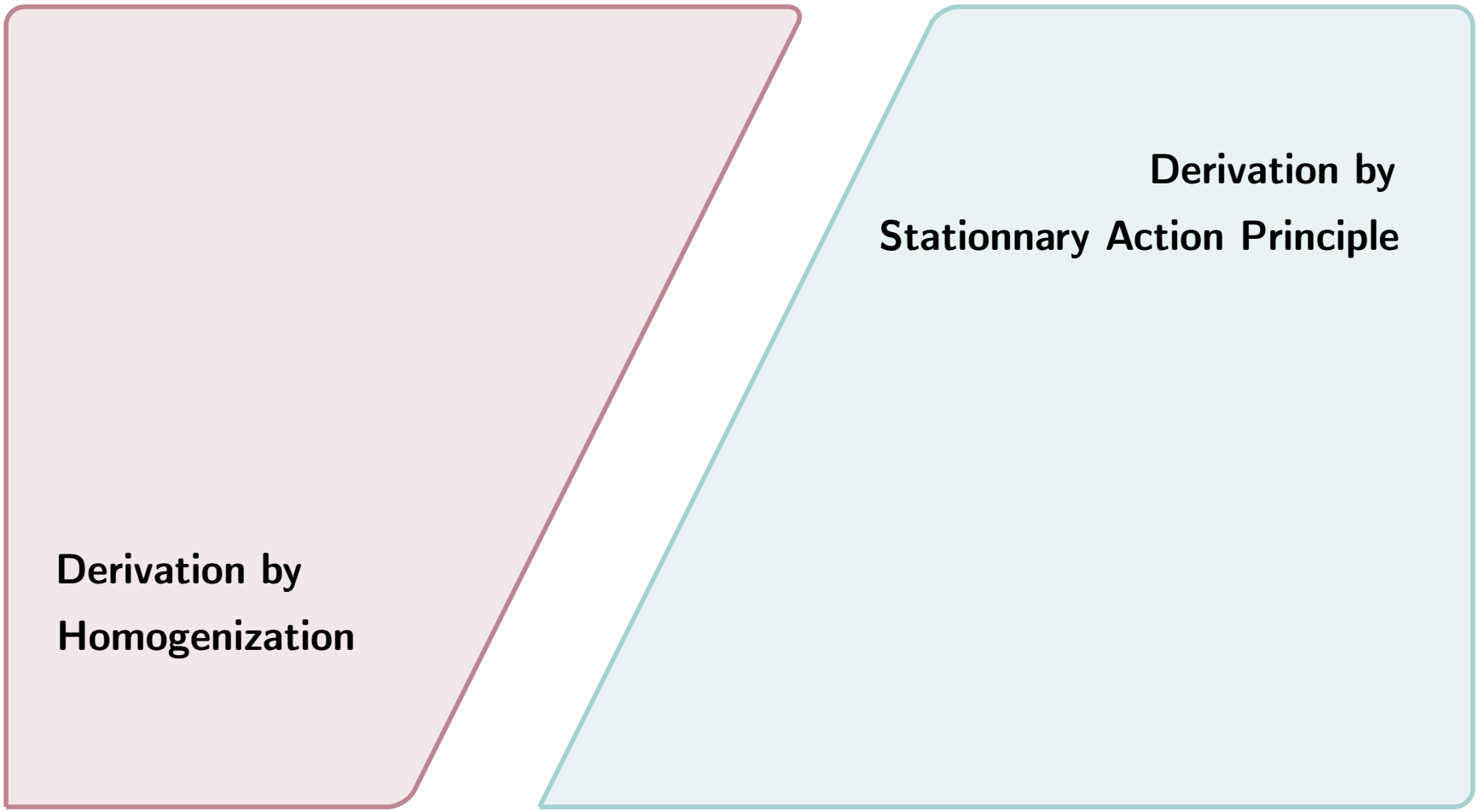


Derivation of consistent models

- Macroscopic description
  - Derive average models
- Conserve informations from the interface scale
  - Interfacial area, surface tension...
- Mathematical structure
  - Well-posedness (smooth solutions, discontinuities...)

Comparison of two possible derivations

- One-velocity framework



Derivation by homogenization

[Serre '91 & '01, E '92, Hillairet '07, Bresch & Huang '11, Bresch & Hillairet '15 & '19, Hillairet '18, Bresch, Burtea & Lagoutière '20]

From micro to macro...

- Microscopic description of the mixture
  - Viscous flows (smooth enough solutions) for both phases
  - Conditions through the interfaces ("perfect transducers")
- One-fluid model with high-oscillatory density solutions
- Pass to the limit to deduce macroscopic quantities $\alpha_{1,2}, \rho_{1,2}, \rho$ and u

Pros & Cons

✓ Fully rigorous

✗ Restrictive interface conditions

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- One-fluid model with high-oscillatory density solutions ✗
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Pros & Cons

✓ Fully rigorous

✗ Restrictive interface conditions

Goal [Hillairet, M. & Seguin '23]

✓ Introduce more complex interface behavior $\rightsquigarrow$ surface tension

✓ Couple different fluid models

The one-dimensional microscopic model

Assumptions for the microscopic model (first in 3D)

- Fluid f, N bubbles of gas g, $n \in \{1, \dots, N\}$
- Compressible Navier-Stokes equations for both phases
- Bubbles remain spherical (translation, dilatation, rotation)
- Interface conditions
  - Continuity of the velocity field $u_f = u_n$
  - Surface tension $(\Sigma_f - \Sigma_n)\nu = \kappa_n \nu$

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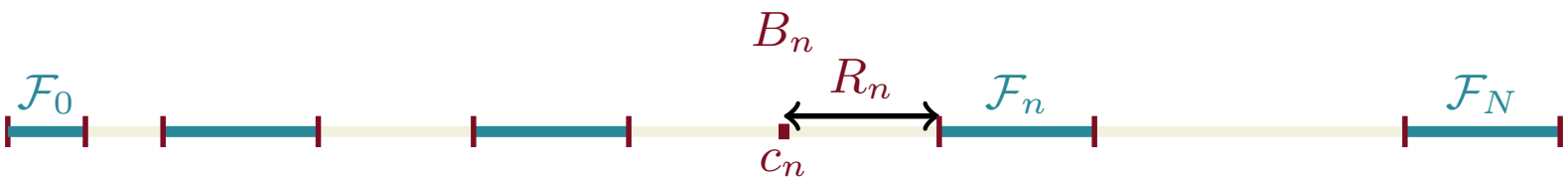
In 1D



- In the fluid domain $\mathcal{F}(t)$
  - ρ_f, u_f, $\Sigma_f = \lambda_f \partial_x u_f - \mathrm{p}_f(\rho_f)$
- In each buble $B_n(t) = B(c_n(t), R_n(t))$
  - Constant mass m_n and Newton laws

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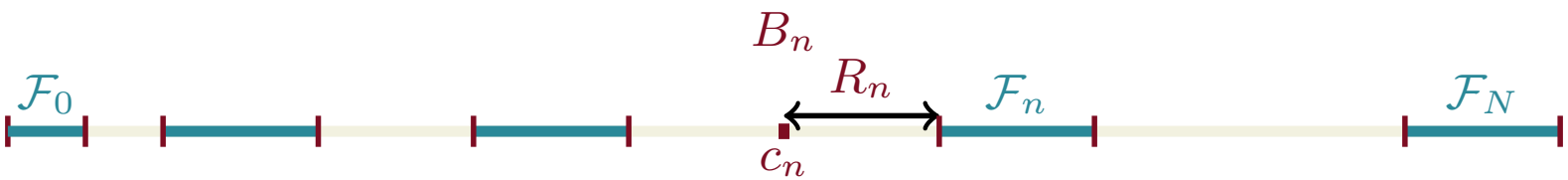

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- In each buble $B_n(t) = B(c_n(t), R_n(t))$
  - Constant mass m_n and Newton laws
- Well posedness of the Cauchy problem for a time $T > 0$, depending on N...

Microscopic initial data

Provide the initial gas-bubble distribution

- Probability distribution of the bubbles, in position x and radius r

$$S_g^0 = S_g^0(x, r) \in L^1(\Omega \times \mathbb{R}^+)$$

- First moments of S_g^0
  - $1-$st order moment $\rightsquigarrow$ volume fraction

$$\alpha_g^0(x) = \int_{\mathbb{R}^+} (2r) S_g^0(x, r) \mathrm{d}r$$

  - $0-$th order moment ($\rightsquigarrow$ gas covolume, "interfacial area")

$$a^0(x) = \int_{\mathbb{R}^+} S_g^0(x, r) \mathrm{d}r$$

Family of microscopic initial data to be constructed from S_g^0, ρ_f^0 and u_f^0

- For any bubble number $N \geq 1$:
  1. From S_g^0 deduce $(c_n^{(N),0}, R_n^{(N),0})_{n=1,\dots,N}$
  2. Use velocity continuity to define $\dot{c}_n^{(N),0}$, $\dot{R}_n^{(N),0}$

Solve the microscopic model

Scaling

- m_n, R_n^0, $|\mathcal{F}_n^0|$ and γ behave as N^{-1}

Microscopic Cauchy problem independent of N [Hillairet, M., Seguin '23]

Consider compatible initial data and the above scaling. Then there exists $T_\infty > 0$, independent of N, such that

$$\left(\rho_f^{(N)}, u_f^{(N)}, (c_n^{(N)}, R_n^{(N)})_{n=1,\dots,N}\right)$$

exists and is unique

- T_∞ taken smaller and smaller along the proof
- Combine energy and regularity estimates, independent of N
- Smoothness of the velocity $u_f^{(N)}$ obtained by extended stress tensors

Pass to the limit $N \to \infty$ to deduce macroscopic quantities

Fluid unknowns

- Characteristic function of the fluid domain $\chi^{(N)} = \mathbf{1}_{\mathcal{F}^{(N)}}$, density $\rho_1^{(N)} = \rho_f^{(N)}$

Gas unknowns

- Density $\rho_2^{(N)} = \sum_{n=1}^{N} \rho_n^{(N)} \mathbf{1}_{B_n}$ with $\rho_n^{(N)} = m_n^{(N)}/(2R_n^{(N)})$
- Interfacial area/covolume $a^{(N)} = \sum_{n=1}^{N} a_n^{(N)} \mathbf{1}_{B_n}$ with $a_n^{(N)} = 1/(2NR_n)$

Mixture unknowns

- Density $\rho^{(N)}$ and velocity $u^{(N)}$

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Methodology

- Using relative compactness (up to extraction of subsequences)
- Pass to the limit in nonlinear combinations of $\chi^{(N)}(t,x)$, $\rho^{(N)}(t,x)$ and $a^{(N)}(t,x)$

✓ Nonlinear convergence in the sense of Young measures

$\rightsquigarrow$ Evolution equations on fluid, bubble and mixture unknowns

The macroscopic model

Macroscopic closed system

$$
\begin{cases}
\alpha_1 + \alpha_2 = 1, \qquad \rho = \alpha_1\rho_1 + \alpha_2\rho_2 \\
\partial_t\alpha_1 + u\partial_x\alpha_1 = \dfrac{\alpha_2\alpha_1}{\alpha_1\lambda_2 + \alpha_2\lambda_1}\left[(\lambda_2 - \lambda_1)\partial_x u + (\mathrm{p}_1(\rho_1) - \mathrm{p}_2(\rho_2)) - \bar{\gamma}\dfrac{a}{\alpha_2}\right] \\
\partial_t a + \partial_x(au) = 0 \\
\partial_t(\alpha_1\rho_1) + \partial_x(\alpha_1\rho_1 u) = 0, \qquad \partial_t(\alpha_2\rho_2) + \partial_x(\alpha_2\rho_2 u) = 0 \\
\partial_t(\rho u) + \partial_t(\rho^2 u) = \partial_x\Sigma \\
\text{with } \Sigma = \frac{\lambda_2\lambda_1}{\alpha_1\lambda_2+\alpha_2\lambda_1}\left[\partial_x u - \left(\frac{\alpha_1}{\lambda_f}\mathrm{p}_1(\rho_1) + \frac{\alpha_2}{\lambda_2}\mathrm{p}_2(\rho_2)\right) - \frac{\bar{\gamma}}{\lambda_2}a\right]
\end{cases}
$$

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Additional kinetic equation (Boltzmann-Williams)

- Distribution function in position and radius $S_t^{(N)} = \dfrac{1}{N}\sum_{k=1}^{N}\delta_{c_k(t),NR_k(t)}$
- Converges towards the probability distribution S_g satisfying

$$\partial_t S_g - \partial_x(S_g\bar{u}) + \frac{1}{\lambda_2}\partial_r\big((r(\Sigma_2 + \mathrm{p}_2(\rho_2)) + \bar{\gamma}/2)S_g\big) = 0$$

- 0-th order moment $a(t,x) = \int_{\mathbb{R}^+} S_g(t,x,r)\mathrm{d}r$

Comments on the macroscopic model

✓ Mechanical relaxation

Surface tension

a interfacial area in 3D(?)

Additional kinetic equation

✗ 3D extension

Viscous flows

1 velocity/temperature

Derivation by Homogenization

Two possible derivations

✓ Mechanical relaxation

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Derivation by Homogenization

Derivation by Stationnary Action Principle

Derivation by Stationary Action Principle

[Bedford '85, Gavrilyuk & Gouin '99, Gavrilyuk & Saurel '02, Berdichevsky '09, Belozerov, Peshkov & Romenski '15...]

- Set up the assumptions that govern the physical phenomenon
  i.e. define kinetic and potential energies
- Lagrangian L whose integral over space-time gives the Hamiltonian Action of the system
- Evolution of the system along possible trajectories
- SAP postulate: the physical trajectory optimizes the action

✓ Hamiltonian and entropy structure

✗ Reversible processes

SAP for two-phase flows with surface tension

Main ingredient

$$L = \text{kinetic energy} - \text{potential energy}$$

State of art

[Gavrilyuk & Saurel '02, Drui '17, Essadki '18, Cordesse '20, Di Battista '21, Kokh '21...]

- ▶ Add terms in the kinetic energy, keep geometrical informations related to small scale interface features
- ✗ Consider surface tension as a kinetic feature
- ✗ No particular derivation of the potential energy
- ✗ Isothermal case

Aim

- ✓ Consider surface tension as a thermodynamic feature
- ✓ Provide a rigorous derivation of the potential energy

Fluid and gas phases

- Porous media literature [Smai '20, Kondepudi & Prigogine '98, Laudau & Lifshitz '78...]

Extensive description

- $k = 1, 2$
- Volume $V_k \geq 0$, entropy $S_k \geq 0$, mass $M_k \geq 0$
- Internal energy $E_k \in C^2((\mathbb{R}_+)^3)$
  - Convex and positively homogeneous: $\forall \lambda \in \mathbb{R}_+^*$

$$E_k(\lambda M_k, \lambda V_k, \lambda S_k) = \lambda E_k(M_k, V_k, S_k)$$

  - Gibbs form

$$\mathrm{d}E_k = T_k \mathrm{d}S_k - p_k \mathrm{d}V_k + \mu_k \mathrm{d}M_k$$

    - Pressure p_k, temperature $T_k > 0$, chemical potential μ_k

Intensive form : intensive variables relatively to the mass of the phase k

- Specific volume $\tau_k = V_k/M_k = (1/\rho_k)$ and entropy $s_k = S_k/M_k$
- Specific internal energy $e_k(\tau_k, s_k) = 1/M_k \, E_k(M_k, V_k, S_k)$

$$\mathrm{d}e_k = T_k \mathrm{d}s_k - p_k \mathrm{d}\tau_k$$

The interface

Assumptions

- Sharp, no volume, no mass

Extensive description

- Entropy $S_i \geq 0$, area $A \geq 0$
- Internal energy $E_i(S_i, A)$ convex and positively homogeneous
- Gibbs form

$$\mathrm{d}E_i = T_i \mathrm{d}S_i + \gamma \mathrm{d}A$$

  - Surface tension γ
  - Interfacial temperature T_i

Intensive description

- Intensive variables relatively to the volume V of the mixture
  - Interfacial area density $a = A/V$
- Intensive variables relatively to the interfacial area A
  - Interfacial intensive entropy $s_i = S_i/A$
  - Interfacial intensive energy $e_i = E_i/A$

The fluid-interface system

For a given state (M, V, E, A) of the system

Modeling constraints

- Fluid phases are immiscible, no vacuum, interface has no volume

$$1 = \alpha_1 + \alpha_2 \text{ with } \alpha_k = V_k/V \in [0, 1]$$

- Mass conservation, interface has no mass

$$1 = y_1 + y_2 \text{ with } y_k = M_k/M \in [0, 1]$$

- Entropy conservation (homogeneity)

$$1 = z_1 + z_2 + z_i \text{ with } z_k = S_k/S \in [0, 1], k = 1, 2, i$$

System extensive internal energy

$$E(M, V, S, A) = E_1(M_1, V_1, S_1) + E_2(M_2, V_2, S_2) + E_i(S_i, A)$$

Mixture potentials and equilibrium

Extended Gibbs form for the system

$$\begin{aligned}\mathrm{d}E = &(z_1T_1 + z_2T_2 + z_iT_i)\mathrm{d}S - (\alpha_1 p_1 + \alpha_2 p_2 - a\gamma)\mathrm{d}V + (y_1\mu_1 + y_2\mu_2)\mathrm{d}M \\ &+ S((T_1 - T_i)\mathrm{d}z_1 + (T_2 - T_i)\mathrm{d}z_2) - V((p_1 - p_2)\mathrm{d}\alpha_1 - \gamma\mathrm{d}a) + M(\mu_1 - \mu_2)\mathrm{d}y_1\end{aligned}$$

Consequences

- Definitions of the mixture potentials

$$\begin{cases} T := z_1T_1 + z_2T_2 + z_iT_i \\ p := \alpha_1 p_1 + \alpha_2 p_2 - a\gamma \\ \mu := y_1\mu_1 + y_2\mu_2 \end{cases}$$

- At thermodynamical equilibrium, for a given state (M, V, E, A), the mixture energy E reaches a minimum

$$\begin{cases} \mu_1 = \mu_2 \\ T_1 = T_2 = T_i \\ \gamma\mathrm{d}a - (p_1 - p_2)\mathrm{d}\alpha_1 = 0 \end{cases}$$

Potential energy candidate

Potential energy accounting for interfacial informations [M. '24]

$$e(\tau, s, s_1, s_2, a, \alpha_1, y_1) = y_1 e_1\left(\frac{\alpha_1}{y_1}\tau, s_1\right) + (1-y_1)e_2\left(\frac{1-\alpha_1}{1-y_1}\tau, s_2\right) + a\tau e_i\left(\frac{s - y_1 s_1 - (1-y_1)s_2}{a\tau}\right)$$

where

- s is the system specific entropy

$$s = y_1 s_1 + (1-y_1)s_2 + a\tau s_i$$

Kinetic energy

$$\text{kinetic energy } = \frac{1}{2}\rho|\mathbf{u}|^2 + \theta$$

- Kinetic energy of translational motion +small scale kinetic energy
  - [Gavrilyuk & Saurel '02, Drui '17, Cordesse '18, Di Battista '21, Loison '23...]

$$\theta = m(a)|\mathrm{D}_t\alpha_1|^2 \quad \text{with } \mathrm{D}_t\cdot = \partial_t\cdot + \mathbf{u}\cdot\nabla\cdot$$

- Here consider

$$\theta = \frac{1}{2}m|D_t\alpha_1|^2 + \frac{1}{2}\nu|D_t a|^2$$

- Physical interpretation
  - Pulsation energy results in both volume and interfacial area variations
- (*A posteriori*) Mathematical argument
  - Mandatory to get evolution/transport equations on α_1 and a

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Moral

- Kinetic energy encodes the final set of PDEs
- Potential energy encodes the pressure and source terms (via the extended Gibbs form)

Lagrangian, assumptions and SAP

Lagrangian

$$L(\mathbf{B}) = \frac{1}{2}\rho|\mathbf{u}|^2 + \frac{1}{2}m|\mathrm{D}_t\alpha_1|^2 + \frac{1}{2}\nu|\mathrm{D}_t a|^2 - \rho e(\tilde{\mathbf{B}})$$

Some additional assumptions/constraints

- Mass conservations
  - Density of the system $\rho = 1/\tau$: $\partial_t\rho + \mathrm{div}(\rho\mathbf{u}) = 0$
  - Mass fraction y_1: $\mathrm{D}_t y_1 = 0$
- Specific entropy conservation along trajectories

$$\mathrm{D}_t s = 0 \quad \text{and} \quad \mathrm{D}_t s_k = 0, \qquad k = 1, 2$$

  $\rightsquigarrow$ Interface entropy s_i is not advected

Choice of variables to depict the system

$$(x, t) \mapsto \mathbf{B} = (\rho, s, s_1, s_2, a, \alpha_1, y_1, \mathbf{u}, \mathrm{D}_t\alpha_1, \mathrm{D}_t a)$$

Stationary Action Principle

- Integral of L defines the Hamiltonian Action of the system
- Family of transformations such that the constraints hold
- Physically relevant transformation optimizes the Action

Conservative PDE system

Evolution equations [Di Battista '21, M. '24]

SAP leads to

$$\begin{cases} \partial_t M + \mathrm{div}(M\mathbf{u}) - \dfrac{\partial L}{\partial \alpha_1} = 0 & \text{with } M = \dfrac{\partial L}{\partial (D_t \alpha_1)} \\ \partial_t P + \mathrm{div}(P\mathbf{u}) - \dfrac{\partial L}{\partial a} = 0 & \text{with } P = \dfrac{\partial L}{\partial (D_t a)} \\ \partial_t K + \mathrm{div}(K\mathbf{u}) - \nabla L^{*,\rho} = 0 & \text{with } K = \dfrac{\partial L}{\partial \mathbf{u}} \text{ and } L^{*,\rho} = \rho \dfrac{\partial L}{\partial \rho} - L. \end{cases}$$

Moreover if

$$E(\rho, K, M, P, s, s_1, s_2, y_1) = \text{kinetic energy} + \text{potential energy}$$

is convex, then the system is hyperbolic and symetrizable.

- ▶ Godunov-Mock argument
- ✗ Sufficient criterion quite restrictive

Extended equations

- By definition of $L(\mathbf{B})$
- Equation on $K = \partial L / \partial \mathbf{u} = \rho \mathbf{u}$ gives the momentum equation

$$\partial_t(\rho \mathbf{u}) + \mathrm{div}(\rho \mathbf{u}^\top \mathbf{u}) + \nabla \left(p + \frac{m}{2} |D_t \alpha_1|^2 + \frac{\nu}{2} |D_t a|^2 \right) = 0$$

with

$$p = \alpha_1 p_1 + (1 - \alpha_1) p_2 - a\gamma$$

- Two second order conservative equations on $M = m D_t \alpha_1$ and $P = \nu D_t a$

$$\begin{cases} D_t \alpha_1 = \partial_t \alpha_1 + \mathbf{u} \cdot \nabla \alpha_1 = \dfrac{\rho y_1 w}{\sqrt{m}} \\ \partial_t w + \mathbf{u} \cdot \nabla w = \dfrac{1}{\sqrt{m} \rho y_1} (p_2 - p_1) \end{cases}$$

$$\begin{cases} D_t a = \partial_t a + \mathbf{u} \cdot \nabla a = \dfrac{\rho y_1 n}{\sqrt{\nu}} \\ \partial_t n + \mathbf{u} \cdot \nabla n = \dfrac{\gamma}{\sqrt{\nu} \rho y_1} \end{cases}$$

  - Equations on w and n refer to small scale momentum equation
  - Equations on α_1 and a connect small and large scales

Comparison to similar models

Final set of equations [M. '24]

$$\begin{cases} \alpha_1 + \alpha_2 = 1, \quad \rho = \alpha_1\rho_1 + \alpha_2\rho_2, \quad p = \alpha_1 p_1 + (1-\alpha_1)p_2 - a\gamma \\ \partial_t \rho + \operatorname{div}(\rho \mathbf{u}) = 0 \\ \partial_t(\rho\mathbf{u}) + \operatorname{div}\left(\rho \mathbf{u}^\top \mathbf{u} + \left(p + \frac{m}{2}(\rho y_1 w)^2 + \frac{\nu}{2}(\rho y_1 n)^2\right)\mathbf{Id}\right) = 0 \\ \partial_t \alpha_1 + \mathbf{u}^\top \nabla \alpha_1 = \dfrac{\rho y_1 w}{\sqrt{m}} \\ \partial_t a + \mathbf{u}^\top \nabla a = \dfrac{\rho y_1 n}{\sqrt{\nu}} \\ \partial_t w + \mathbf{u}^\top \nabla w = \dfrac{1}{\sqrt{m}\rho y_1}(p_2 - p_1) \\ \partial_t n + \mathbf{u}^\top \nabla n = \dfrac{\gamma}{\sqrt{\nu}\rho y_1} \end{cases}$$

- Formal asymptotics
  - $\gamma, \nu \to 0$ and isothermal case: [Drui *et al* '17]
  - $O(\sqrt{\nu}, \sqrt{m})$: [Kokh *et al* '19] , recover almost the model of part 1

Comments on the resulting model

✓ Mechanical relaxation

Surface tension

a interfacial area in 3D?

Additional kinetic equation

✗ 3D extension

Viscous flows

1 velocity/temperature

Derivation by

Homogenization

Derivation by

Stationnary Action Principle

✓ Mechanical relaxation

Surface tension, interfacial area

Two temperatures

Possibly two velocities

✗ Lack of dissipative terms

Provide relaxation terms to close the system

To sum up

✓ Mechanical relaxation
Surface tension
a interfacial area in 3D(?)
Additional kinetic equation

✗ 3D extension
Viscous flows
1 velocity/temperature

Derivation by
Homogenization

Derivation by
Stationnary Action Principle

✓ Mechanical relaxation
Surface tension, interfacial area
Two temperatures
Possibly two velocities

✗ Lack of dissipative terms
Provide relaxation terms to close the system

Thank you for your attention!