Cours INSTN CFD diphasique du STMF – Partie 1.C

Approche thermodynamique des interfaces : les modèles à champ de phase (4h30)

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Pré-requis pour la partie 1.C

Physique

- Bases de *Mécanique des fluides monophasiques*
  - E. Guyon, J.-P. Hulin, L. Petit, Hydrodynamique Physique, EDP Sciences, 2012 (724 pages)
  - S. Candel, Mécanique des Fluides, Dunod, 2002 (451 pages)
- Bases de *Thermodynamique* (rappels des principaux concepts utiles en Section 1)
  - J.-Ph. Ansermet, S. Bréchet, Thermodynamique, EPFL Press, 3e Ed, 2024 (516 pages).

Outils mathématiques

- Introduction au *Calcul des variations* (quelques rappels en annexe A)
  - Ex. vidéos youtube : ex. `https://www.youtube.com/watch?v=VCHFCXgYdvY`
- Calculs algébriques en notations indicielles (pratiqués dans ce cours)
- Introduction aux *Méthodes numériques* des Equations aux Dérivées Partielles (ex. diff finies)

Informatique

- Pour la pratique sur ordinateur : commandes Linux de base (rappels en Section 1)

Table of contents

1. Introduction

Purpose, basic thermodynamics and `LBM_Saclay` code

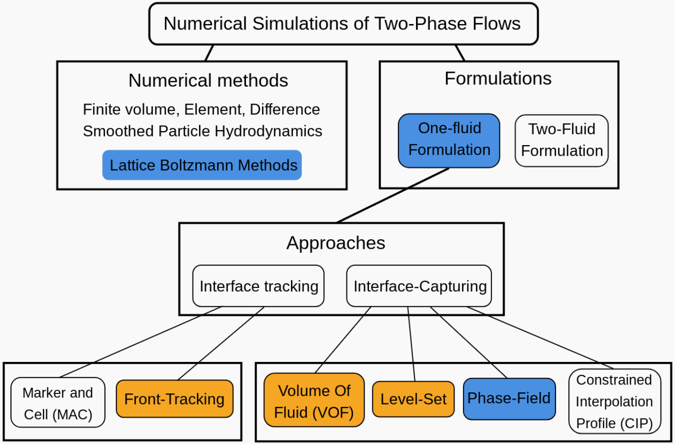
Outline section 1

1 Introduction

a. Purpose of this Part 1.C

Interface methods with one-fluid formulation

Overview of interface-tracking and interface-capturing methods



Motivation: revisit two-phase flows in energy framework

Two-phase flows with capillarity

- Two immiscible fluids
  - Water-Oil (liquid A-liquid B)
  - Water-air (liquid-gas)
  - etc.
- Examples
  - Coalescence and break-up
  - Rayleigh-Taylor instability
  - Rising bubbles, etc.

Two-phase flows with capillarity & coupling with T and c

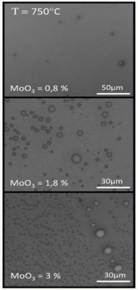
- Phase change (solid/liquid & liquid/gas)
  - Liquid-vapor (phase change)
  - Solidification (e.g. crystal growth)
  - Dissolution of porous media
- Multi-component mixtures: composition transfer through interfaces of two fluids
  - Phenomena in *glass* (e.g. next slide)
  - *corium* at high temp
  - etc.
- Phenomena
  - Ostwald ripening
  - Marangoni flows
  - Two-phase flows with surfactant
  - etc.
- Applications
  - Microfluidics
  - Flow and transport in porous media
  - Severe accidents
  - etc.

One example of CEA observations

Nuclear glass: a multi-phase/multi-components system

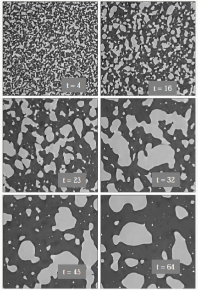
Liquid – Liquid interface

Demixing of immiscible fluids



S. Schuller (ISEC/DPME), 2013

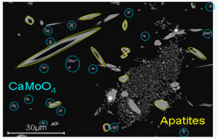
Spinodal decomposition



D. Bouttes (PhD 2015)

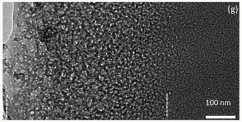
Solid – Liquid interface

Crystal growth



E. Régnier (DPME), 2011

Maturation of gels



S. Gin (DPME), 2015

Objectives: Modeling and simulations of those phenomena

The models need to **capture an interface** and need to **be thermodynamically-consistent**

Energy framework: example of least action principle

Energetic interpretation of Newton's 2nd law

Action $\mathscr{A}[q_i(t)]$ for $i = 1, 2, 3$ (t ind var)

$$\mathscr{A}[q_i(t)] = \int_{t_1}^{t_2} \mathscr{L}\left(q_i(t), \dot{q}_i(t)\right) dt$$

$$\begin{aligned}
\delta\mathscr{A} &= \int_{t_1}^{t_2} \delta\mathscr{L}\left(q_i(t), \dot{q}_i(t)\right) dt \\
&= \int_{t_1}^{t_2} \left[\frac{\partial\mathscr{L}}{\partial q_i}\delta q_i + \underbrace{\frac{\partial\mathscr{L}}{\partial \dot{q}_i}\delta \dot{q}_i}_{\text{ibp}}\right] dt \\
&= \int_{t_1}^{t_2} \left[\frac{\partial\mathscr{L}}{\partial q_i} - \frac{d}{dt}\left(\frac{\partial\mathscr{L}}{\partial \dot{q}_i}\right)\right] \delta q_i dt
\end{aligned}$$

$$\boxed{\frac{\partial\mathscr{L}}{\partial q_i} - \frac{d}{dt}\left(\frac{\partial\mathscr{L}}{\partial \dot{q}_i}\right) = 0} \qquad (1)$$

Lagrangian:

$$\mathscr{L}\left(x, y, z, \dot{x}, \dot{y}, \dot{z}\right) = \mathcal{K}(\dot{x}, \dot{y}, \dot{z}) - \mathcal{V}(x, y, z)$$

Kinetic energy:

$$\begin{aligned}
\mathcal{K}(\dot{x}, \dot{y}, \dot{z}) &= \frac{1}{2} m \left|v\right|^2 \\
&= \frac{1}{2} m \left[\left(\dot{x}^2 + \dot{y}^2 + \dot{z}^2\right)^{1/2}\right]^2
\end{aligned}$$

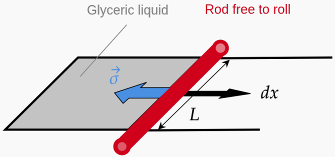
Application of Euler-Lagrange Eq. (1):

$$\begin{aligned}
m\ddot{x} &= -\partial_x \mathcal{V}(\boldsymbol{x}) \\
m\ddot{y} &= -\partial_y \mathcal{V}(\boldsymbol{x}) \\
m\ddot{z} &= -\partial_z \mathcal{V}(\boldsymbol{x})
\end{aligned}$$

Energy interpretation of surface tension

Capillary force

- Glyceric liquid: water, soap, glycerine



- As soon as the device is removed from the liquid, the mobile rod moves spontaneously in the direction of $\vec{\sigma}$ in order to decrease the surface area of the liquid.
- If the rod is displaced by dx, the work done is

$$d\mathcal{W} = F dx = 2\sigma L dx$$

- $\vec{\sigma} \equiv \boldsymbol{\sigma}$ is a force (per unit length) normal to the rod in the plane of the surface and directed toward the liquid.

In this part 1.C: energetic approach of interface “surface energy”

- Work required to increase the liquid surface of dA is proportional to σ:

$$d\mathcal{W} = \sigma dA$$

- σ is the energy that must be supplied to increase the surface area by one unit.

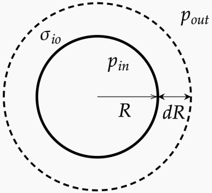
$$[\sigma] = \frac{[\mathrm{E}]}{[\mathrm{L}]^2}$$

This thermodynamic (energetic) approach of capillarity was first proposed by VAN DER WAALS (1874)
See translation by ROWLINSON (1979)

Energy interpretation of Laplace's law

Derivation of Laplace's law for a sphere

Sphere of radius R



Variation of work $d\mathcal{W}$ for an increased radius $R + dR$

$$d\mathcal{W} = -p_{in} dV_{in} - p_{out} dV_{out} + \sigma_{io} dA$$

- $\mathcal{W}$: work done by pressure and surface tension
- V_{in}, V_{out}: volume of spheres *in* and *out*
- σ_{io}: surface tension between phases *in* and *out*
- A: sphere area

- Volume of sphere

$$V_{in} = \frac{4}{3}\pi R^3$$
$$dV_{in} = 4\pi R^2 dR$$
$$dV_{out} = -dV_{in}$$

- Sphere area

$$A = 4\pi R^2$$
$$dA = 8\pi R dR$$

- Equilibrium: $d\mathcal{W} = 0$

$$\boxed{p_{in} - p_{out} = \frac{2\sigma_{io}}{R}}$$

Equilibrium between volume energy and surface energy

Pedagogical objective of this Part 1.C

In this part 1.C: energy (or thermodynamic) approach of two-phase flows with interface

How to

- Analyse the phenomenology behind each observation
- Derive a mathematical model (set of coupled Partial Derivative Equations – PDEs)
- Understand the physical meaning of each term of PDEs
- ~~How to simulate the PDEs~~ (not here see course “Lattice Boltzmann Methods” – LBM)

Illustrations with videos of simulations and practice with CEA code `LBM_Saclay`

- Fluid–Fluid interface (Two-phase flows, three-phase flows, phase separation, surfactant, etc.)
- Liquid–Solid interface (crystal growth, dissolution)

Finally

- Become familiar on interface modelling with thermodynamics
- Know what math equations and terms must be simulated for those phenomena

b. Basic thermodynamics

Reminder of useful concepts

Variables of state & equilibrium

Extensive (proportional to the system size)

Name	Symb	Dim (SI)
Volume	V	$[\mathrm{m}]^3$
Entropy	S	[J]/[K]
Moles of substance	N	[mol]
$\vdots$	$\vdots$	$\vdots$

Use: conservation equations

Intensive (conjugate variable) ▸ Appendix

Name	Symb	Dim (SI)
Pressure	P	[Pa]
Temperature	T	[K]
Molar chemical potential	μ_c	[J]/[mol]
$\vdots$	$\vdots$	$\vdots$

Use: equilibrium

Mechanic and thermodynamic equilibrium or "equilibrium"

At equilibrium:

- The intensive variables are homogeneous in space and constant in time
- For two phases: equality of intensive variables

e.g. for $\Phi = 0, 1$ or $\Phi = l, g$ or $\Phi = A, B$:

$$\boxed{\begin{aligned} \mu_0^{eq} &= \mu_1^{eq} = \mu^{eq} \\ P_0^{eq} &= P_1^{eq} = P^{eq} \\ T_0^{eq} &= T_1^{eq} = T^{eq} \end{aligned}}$$

Functions of state: total energy $\mathscr{E}_{tot}$ and internal energy $\mathcal{U}$

Total energy $\mathscr{E}_{tot}$ as a function of state variables

Total energy as a function of extensive variables $\mathscr{E}_{tot}(\mathbb{P}, \mathbb{L}, S, V, N_1, \ldots, N_r)$

Impulsion: $\mathbb{P} = m\mathbb{U}$ (extensive variable)

Velocity: $\mathbb{U} = \dfrac{\partial \mathscr{E}_{tot}}{\partial \mathbb{P}}$ (intensive: conjugate variable)

- $\mathbb{L}$: kinetic moment
- $N_1, \ldots, N_r$: number of moles
- $\mathbb{P}, \mathbb{U}, \mathbb{L}$ are vectors

Total energy $\mathscr{E}_{tot}$ of a system with impulsion $\mathbb{P}$ and internal energy $\mathcal{U}$

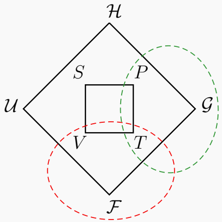
Differential: $$d\mathscr{E}_{tot} = \underbrace{\frac{\partial \mathscr{E}_{tot}}{\partial \mathbb{P}} \cdot d\mathbb{P} + \overbrace{\frac{\partial \mathscr{E}_{tot}}{\partial \mathbb{L}} \cdot d\mathbb{L}}^{\text{neglected here}}}_{\text{dependent on movement}} + \underbrace{d\mathscr{E}_{tot}(S, V, N_1, \ldots, N_r)}_{\text{independent on movement } \equiv d\mathcal{U}}$$

After integration: $$\mathscr{E}_{tot}(\mathbb{P}, \mathbb{L}, S, V, N_1, \ldots, N_r) = \underbrace{\frac{\mathbb{P}^2}{2m}}_{\text{kinetic energy}} + \underbrace{\cancel{\frac{\mathbb{L}^2}{2I}}}_{\text{neglected}} + \underbrace{\mathcal{U}(S, V, N_1, \ldots, N_r)}_{\text{internal energy}}$$

Thermodynamic potentials and second principle

Thermo potential: Legendre transform of internal energy $\mathcal{U}(S, V, \{N_k\})$

- $\mathcal{U}(S, V)$
- $\mathcal{F}(T, V)$
- $\mathcal{G}(T, P)$
- $\mathcal{H}(S, P)$



Born thermodynamic diagram

Potentials:

- $\mathcal{U}$: internal energy
- **$\mathcal{F}$: (Helmholtz) free energy**
- $\mathcal{G}$: Gibbs free energy
- $\mathcal{H}$: enthalpy

Variables:

- P: pressure
- V: volume
- S: entropy
- T: temperature

$\mathcal{G}$ood Physicists $\mathcal{H}$ave Studied $\mathcal{U}$nder Very $\mathcal{F}$ine Teachers

Evolution of free energy $\mathscr{F}$: 2nd principle of thermodynamics

Notations for free energy	Math	Dim
Local free energy density	f	$[E]/[L]^3$
Non-local free energy density	$\mathcal{F}$	$[E]/[L]^3$
Functional	$\mathscr{F}$	$[E]$

- Evolution condition (adia closed)

$$d\mathscr{S} \geqslant 0 \Longleftrightarrow \boxed{d\mathscr{F} \leqslant 0}$$

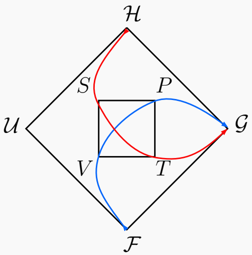
- Equilibrium condition: $\mathscr{F}$ minimum

Derivation rules from Born diagram

See: "A mnemonic scheme for thermodynamics", ZHAO (2009)

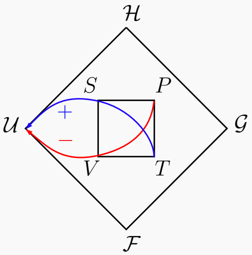
Derivation rules from Born diagram

Legendre transforms



- $\mathcal{U} - ST = \mathcal{F}$
- $\mathcal{F} + VP = \mathcal{G}$
- $\mathcal{H} - ST = \mathcal{G}$
- $\mathcal{U} + VP = \mathcal{H}$

Differential equations



- $+TdS - PdV = d\mathcal{U}$
- $VdP + TdS = d\mathcal{H}$
- $-SdT - PdV = d\mathcal{F}$
- $-SdT + VdP = d\mathcal{G}$

Sign conventions: upward direction $+$ (blue) and downward direction $-$ (red)

Local quantities 1/2: from global to local variables

Local extensive variables: ex. with $\mathfrak{p}(\boldsymbol{x}, t)$ and $s(\boldsymbol{x}, t)$

$$\underbrace{\mathbb{P}(t)}_{\text{global impulsion}} = \int_V \underbrace{d\mathbb{P}(\boldsymbol{x}, t)}_{\text{infinitesimal}} = \int_V \frac{d\mathbb{P}(\boldsymbol{x}, t)}{dV(\boldsymbol{x})} dV(\boldsymbol{x})$$

$$\equiv \int_V \underbrace{\mathfrak{p}(\boldsymbol{x}, t)}_{\text{local}} dV = \int_V \rho(\boldsymbol{x}, t)\boldsymbol{u}(\boldsymbol{x}, t) dV$$

$$\underbrace{\mathscr{S}(t)}_{\text{global entropy}} = \int_V \underbrace{dS(\boldsymbol{x}, t)}_{\text{infinitesimal}} = \int_V \frac{dS(\boldsymbol{x}, t)}{dV(\boldsymbol{x})} dV(\boldsymbol{x})$$

$$\equiv \int_V \underbrace{s(\boldsymbol{x}, t)}_{\text{local}} dV$$

Other extensive variables: nb of moles $n(\boldsymbol{x}, t)$ and composition $c(\boldsymbol{x}, t)$

- Total nb of moles:

$$N(t) = \int_V n(\boldsymbol{x}, t) dV$$

- Nb of moles of specie k

$$N_k(t) = \int_V n_k(\boldsymbol{x}, t) dV \quad \text{with} \quad N = \sum_{k=1}^{r} N_k$$

- Composition of specie k:

$$c_k(\boldsymbol{x}, t) \triangleq \frac{n_k}{n}$$

- with

$$\sum_{k=1}^{r} c_k = 1$$

Local quantities 2/2: local free energy $f(\rho, T, c)$

Dynamic local variables

Selected individually or together as main variables

Name	Math	Dim	Sections
Composition	$c(\boldsymbol{x}, t)$	$[-]$	2,3,4,6
Phase-field	$\phi(\boldsymbol{x}, t)$	$[-]$	

Name	Math	Dim	Sections
Temperature	$T(\boldsymbol{x}, t)$	$[\Theta]$	4,5
Density	$\rho(\boldsymbol{x}, t)$	$[M]/[L]^3$	5

Global free energy $\mathscr{F}(t)$ and local free energy density $f(\rho, T, c)$

$$\underbrace{\mathscr{F}[\rho, T, c]}_{\equiv \mathscr{F}(t)} = \int_V f(\rho, T, c) dV$$

Once $f(\rho, T, c)$ is defined, all other quantities can be derived such as pressure $p(\boldsymbol{x}, t)$, chemical potential $\mu(\boldsymbol{x}, t)$, specific internal energy and entropy (see next slides),

$\mathscr{F}(t)$ is a functional i.e. a function of functions $\rho(\boldsymbol{x}, t)$, $T(\boldsymbol{x}, t)$ and $c(\boldsymbol{x}, t)$

$$\frac{d\mathscr{F}}{dt} \leqslant 0$$

From 2nd principle, its evolution is such that the free energy decreases during time. At equilibrium $\mathscr{F}$ is minimum.

Definition of intensive μ and p with local free energy f

Chemical potential (*loc* means local)

If density ρ is the main variable

$$\mu^{loc}(\rho) \equiv \mu_\rho^{(0)} \triangleq \frac{\partial f(\rho)}{\partial \rho} \qquad (2)$$

If composition c is the main variable

$$\mu^{loc}(c) \equiv \mu_c^{(0)} \triangleq \frac{\partial f(c)}{\partial c} \qquad (3)$$

$\mu_\rho^{(0)}$ (resp. $\mu_c^{(0)}$) is the conjugate variable of ρ (resp. c): the dimension of $\mu_\rho \rho$ is $[E]/[L]^3$

Local pressure

- Equation Of State (*eos*) if ρ main variable

$$p^{loc}(\rho) \equiv p^{eos}(\rho) \triangleq \rho\mu^{(0)}(\rho) - f(\rho) \qquad (4)$$

- Osmotic pressure if c main variable

$$p^{loc}(c) \equiv p(c) \triangleq c\mu^{(0)}(c) - f(c) \qquad (5)$$

Laplace law for curved interface

Sphere of radius R and surf tension σ:

$$p_{in}(\phi) - p_{out}(\phi) = \frac{2\sigma}{R} \qquad (6)$$

with $\phi = \rho, c$ and curvature $\kappa = 2/R$

Derivation of other local quantities

Other derived quantities

Name	Math	Dim
Internal specific energy	$e(\rho, s)$	$[E]/[M]$
Specific entropy	$s(\rho, T)$	$[E]/[\Theta].[M]$
Grand potential	$\omega(\mu_c)$	$[E]/[L]^3$
Specific volume	v	$[L]^3/[M]$
Specific Gibbs enthalpy	$g(p, T)$	$[E]/[M]$
Specific enthalpy	$h(p, s)$	$[E]/[M]$

- Specific entropy with f (section 5)

$$s(\rho, T) \triangleq -\frac{1}{\rho}\frac{\partial f}{\partial T}$$

- Grand potential density (section 6)

$$\omega(\mu_c) \triangleq f(c) - \mu_c c$$

- Specific volume $v \triangleq 1/\rho$

Local specific internal energy $e(\rho, s)$

- Legendre transform of $f(\rho, T)$:

$$e(\rho, s) \triangleq \frac{f(\rho, T)}{\rho} + Ts \qquad (7) \qquad \longrightarrow$$

- Differential

$$\rho de = \frac{1}{\rho}\underbrace{\left[\rho\frac{\partial f}{\partial \rho} - f\right]}_{\triangleq p(\rho, T)} d\rho + \rho T ds \qquad (8)$$

Relations for phase change

Properties

- Specific heat (dim [E]/([M].[Θ]))

$$C_P \triangleq T\left(\frac{\partial s}{\partial T}\right)_P \qquad C_v \triangleq T\left(\frac{\partial s}{\partial T}\right)_\rho \tag{9}$$

- Latent heat (dim [E]/[M])

Melting (section 4)

$$\mathcal{L} \triangleq T(s_l - s_s) \tag{10}$$

Vaporization (section 5)

$$\mathcal{L} \triangleq h_g^{sat} - h_l^{sat} = T(s_g^{sat} - s_l^{sat}) \tag{11}$$

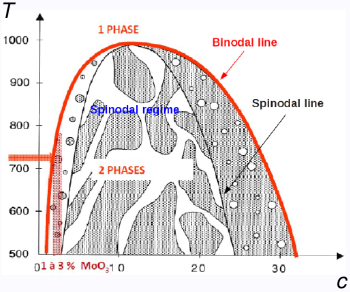
Thermodynamic Maxwell relations (proof see appendix A)

$$\left(\frac{\partial T}{\partial v}\right)_s = -\left(\frac{\partial P}{\partial s}\right)_v \qquad -\left(\frac{\partial s}{\partial v}\right)_T = -\left(\frac{\partial P}{\partial T}\right)_v$$

$$-\left(\frac{\partial s}{\partial P}\right)_T = \left(\frac{\partial v}{\partial T}\right)_P \qquad \left(\frac{\partial T}{\partial P}\right)_s = -\left(\frac{\partial v}{\partial s}\right)_P$$

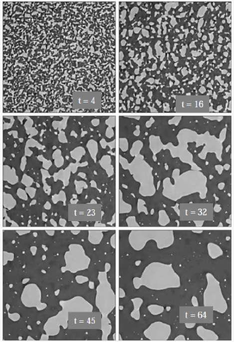
Two-phase 1/3: demixing regimes of binary mixtures

Binary phase diagram



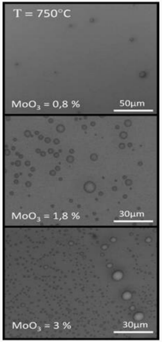
- Homogeneous mixture of SiO_2 and MoO_3 for $T > T_c$ (T_c critical temperature)
- For $T < T_c$ the system is unstable; SiO_2 and MoO_3 start to separate.

Inside spinodal line



Observation of spinodal decomposition

Outside spinodal line

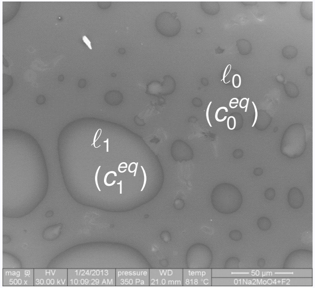


Observation of nucleation and growth

Two-phase with interface, capillarity and thermodynamic

Two-phase 2/3: introduction of a phase-field $\phi(\boldsymbol{x}, t)$

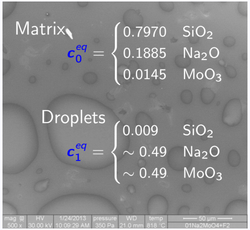
Binary case: e.g. SiO_2–MoO_3



Equilibrium compositions c_0^{eq} and c_1^{eq}

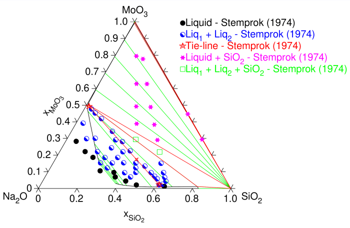
Ternary case: e.g. SiO_2Na_2O–MoO_3 (2 phases + 3 comp)

Observation



S. Schuller (DPME, 2013)

Gibbs triangle



S. Bordier (PhD, 2015)

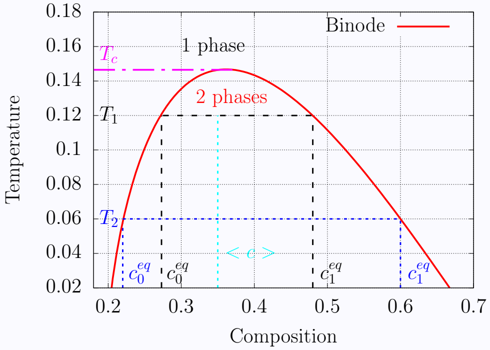
Phase diagrams with thermocalc and Open-Calphad

In order to capture the interface, introduction of an extensive phase-field $\phi(\boldsymbol{x}, t)$ of value c_0^{eq} in phase ℓ_0 (matrix) and c_1^{eq} in phase ℓ_1 (droplets)

Two-phase 3/3: double-well free energy density $f_{dw}(\phi)$

Equilibrium compositions of two-phases

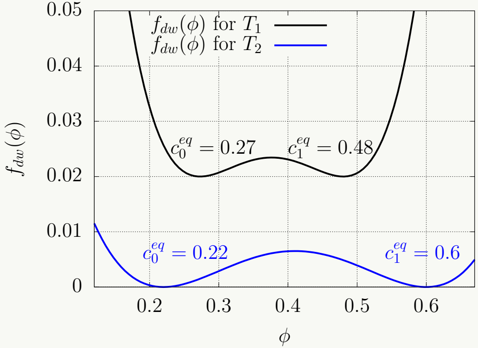
Equilibrium compositions c_0^{eq} and c_1^{eq} for 2 temperatures T_1 (black) and T_2 (blue)



Local free-energy for two-phase

Double-well (*dw*) free energy density

$$f_{dw}(\phi) \triangleq H(\phi - c_0^{eq})^2(\phi - c_1^{eq})^2 \qquad (12)$$



Overview of the phase-field (φ) theory

Concepts of phase-field method

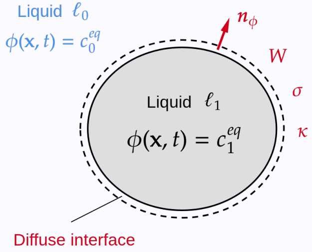
- Interface captured with a *phase-field* $\phi(\boldsymbol{x}, t)$
- Coupled to balance PDE (mass, impulsion, ...)
- Their evolutions minimize a *non local thermo potential*

  ex. *global free energy* $\mathscr{F}[\phi, c]$ (or *Gibbs*, etc.)

$$\mathscr{F}[\phi, c] = \int_V \left[\underbrace{f_{dw}(\phi)}_{\text{double-well}} + \underbrace{\frac{\zeta}{2}(\nabla\phi)^2}_{\text{section 2}} + \underbrace{f_{bulk}(\phi, c)}_{\text{section 4}} \right] dV$$

- Out-of-equilibrium thermo: i.e. constitutive laws of PDE are derived such as

$$\underbrace{\frac{d\mathscr{F}}{dt} \leqslant 0}_{\text{section 2}} \quad \text{or} \quad \underbrace{\frac{d\mathscr{E}_{tot}}{dt} \leqslant 0}_{\text{section 3, 5}}$$



Interface nomenclature

- $\boldsymbol{n}_\phi(\boldsymbol{x}, t)$ unit normal vector
- W interface width
- σ surface tension
- $\kappa(\boldsymbol{x}, t)$ curvature

History of “phase-field” theory and bibliography

History of “phase-field concept”

- van der Waals (1878): thermodynamic theory of capillarity (see translation 1979)
- Landau (1938): phase transition of 2nd order
- Landau–Ginzburg (1950) free energy functional for supraconductors
- Cahn-Hilliard (1958): non-uniform composition system

Since then: wide areas of applications

- Hydrodynamics: two- and multi-phase flows (introduction in this course)
- Materials science (see book ELDER/PROVATAS):
  - solidification, crystal growth (see M. PLAPP, CISM 2012)
  - fractures, etc.
- Polymers and biophysics (see J.-F. JOANNY)
- etc.

Pros and cons of using phase-field theory

Pros

- Derivation of thermodynamically consistent model (Sections 2, 3, 4, 5)
- One single eulerian grid for simulations ($\neq$ Front-Tracking)
- Modeling mass transfer through interfaces (e.g. Ostwald ripening)
- Straightforward generalization for multi-phase and multi-components (see Section 6)

Cons

- Diffuse interface: two additional parameters (interface width W and mobility M_ϕ)
- Requires many parameters (c_0^{eq}, c_1^{eq}, D_0, D_1, μ^{eq}) and more for multi-components

C. CEA code `LBM_Saclay`

Overview of Lattice Boltzmann Methods

Classical numerical methods for PDEs

Numerical methods

- Finite difference
- Finite volume
- Finite element

System to solve for NS

$$\nabla \cdot \boldsymbol{u}^{n+1} = 0$$

$$\frac{\boldsymbol{u}^{n+1} - \boldsymbol{u}^{n}}{\delta t} = -\frac{1}{\rho}\nabla p^{n+1} + \boldsymbol{F}^{n}$$

Unknown: $\boldsymbol{u}^{n+1}$ and p^{n+1}

Algorithm: Prediction-Correction

- Prediction of $\boldsymbol{u}^\star$

$$\frac{\boldsymbol{u}^\star - \boldsymbol{u}^{n}}{\delta t} = \boldsymbol{F}^{n}$$

- Poisson equation for pressure p^{n+1}

$$\nabla \cdot \left[\frac{1}{\rho}\nabla p^{n+1}\right] = \frac{\nabla \cdot \boldsymbol{u}^\star}{\delta t}$$

- Correction of $\boldsymbol{u}^\star$ with p^{n+1}

$$\boldsymbol{u}^{n+1} = \boldsymbol{u}^\star - \frac{\delta t}{\rho}\nabla p^{n+1}$$

In this part 1.C: simulation of PDEs with Lattice Boltzmann Methods (LBM)

What is the “Lattice Boltzmann Method” (LBM) ?

- “Lattice” Boltzmann is one discretization (among other) of the “Boltzmann equation” in the kinetic theory of gases
- “Lattice Boltzmann Methods” are a set of numerical methods used as NS solver and other conservative PDEs (e.g. Advection-Diffusion Eq.)

Popular

- Easy implementation (simple algo)
- Parallelization
- But non necessarily consistent
- Boltzmann Eq.

In Appendix E Appendix

- Introduction of basic concepts of LBM on single-phase applications
- ~~Extend them for *two-phase flows* with an *interface-capturing method*~~
- ~~Practice few of them with a C++ code `LBM_Saclay`~~

Practice with CEA code `LBM_Saclay`

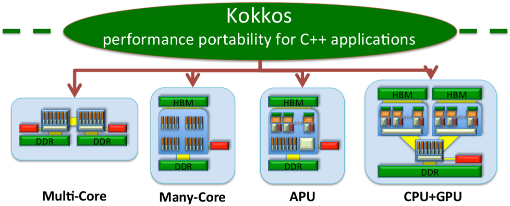
Main features of `LBM_Saclay`

- 2D/3D **Lattice Boltzmann Methods** (LBM)
  Collision BGK, TRT, MRT; lattices D3Q19, D3Q27, etc.
- **Multi-architecture HPC**
  - multi-CPUs and multi-GPUs
  - `Kokkos` (//intra-node - `OpenMP/Cuda`)
  - `MPI` (domain decomposition)
- `C++`, `CMAKE`, `Git`, post-pro with `paraview & python`

Simulations run on

Jean-Zay (V100) Topaze (A100)

+ Orcus (H100)



OpenSource: `GitLab`, licence CECILL

Documentation: Developers' guide `GitLab`, PhD and presentations

Programmers: P. Kestener, W. Verdier, T. Boutin, E. Stavropoulos, C. Méjanès, T. Duez, H. Keraudren, C. Elharti, S. Dupuy, C. Bardet, S. Cappe, A. Laurens, A. Cartalade

Summary of two-phase simulations with LBM

- ▶ φ-theory
  - Section 2

Phase-field models (ϕ-models)

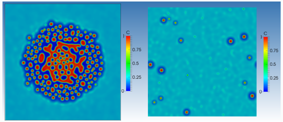
- ▶ Assumptions
- ▶ Writing PDEs

- ▶ NS/ϕ-models
  - Section 3

Lattice Boltzmann Methods

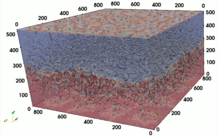
- ▶ LBM schemes
- ▶ C++ implementation
- ▶ HPC simulations

Binary demixing



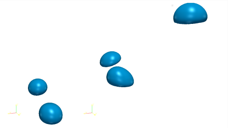
Cahn-Hilliard (C-H) model

Phase inversion



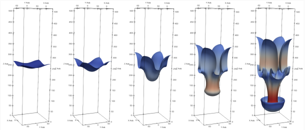
CAC / NS

Buoyancy & coalescence



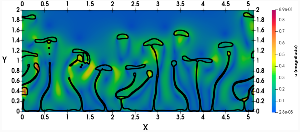
C-H / Navier-Stokes (NS)

Rayleigh-Taylor instability



Conservative Allen-Cahn (CAC) / NS

Liquid/gas phase change



AC / NS / T

Advanced applications

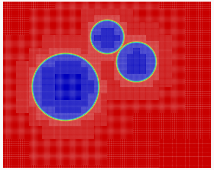
Advanced ϕ-models

- **Crystal growth**
  - Anisoptropy function
  - Coupling with flow
- **Three-phase flow**
- **Dissolution**
  - Anti-trapping current
- **Surfactant**

LB Methods

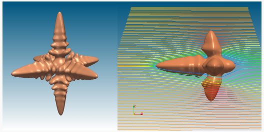
- **Advanced collision**
  - Central moment
  - Cumulant
- **Modif of streaming**
  - Adaptative Mesh Refinement (AMR)
- **Diffuse boundary cond**

AMR



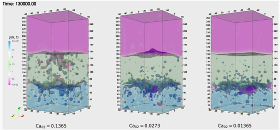
Section 6

Crystal growth



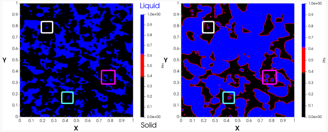
Sections 4 and 6

Three-phase flows



Section 6

Dissolution of porous media



Section 6

Advantages and drawbacks

Pros

- **Simplicity and efficiency**
  - No Poisson Equation
  - Local collisions: parallelization
- **Multiphase and multicomponent flows**
  - Wide range of methods
  - Multiphase simulations in complex geometry
- **Geometry**
  - Well suited to mass-conserving flows in complex geometries (porous media)
  - Attractive for moving boundaries that conserve mass (e.g. IBC)

Cons

- **Simplicity and efficiency**
  - Memory intensive (e.g. D3Q27)
  - Time-dependent (steady state flows)
- **Multiphase and multicomponent flows**
  - Similar than conventional CFD
  - Special methods needed for wide range of densities and viscosities
- **Sound and compressibility**
  - Not appropriate for long-range propagation of sound
  - Not appropriate for transonic and supersonic

Content of LBM training session (ED – SMEMaG)

Training session 16h – ED SMEMaG (U Paris-Saclay)

Part 1.A	Part 1.B	Part 2
Theory	**Practice with `LBM_Saclay`**	**Advanced applications**
▶ Discretization of Boltzmann eq, algorithm ▶ Boundary conditions, law of similarity, etc. ▶ Stability, consistency, accuracy, Chapman-Enskog ▶ Two-phase applications with interface-capturing	▶ Datafile and kernels description ▶ Compilation and run on GPU ▶ Accuracy with BGK and MRT ▶ Rayleigh-Taylor instability, rising droplets ▶ etc.	▶ Crystal growth with fluid flows ▶ Dissolution of porous media ▶ Two-phase with surfactant ▶ Three-phase flows ▶ Ostwald ripening ▶ Intro AMR ▶ etc.

February 17th – 21th, 2025

P. Practice with `LBM_Saclay`

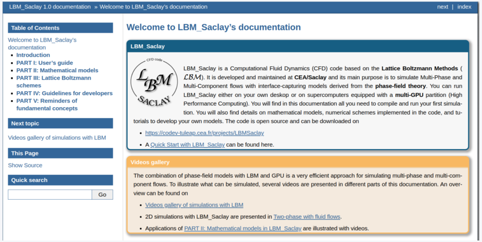
Documentation and connexion on Orcus

Documentation LBM_Saclay

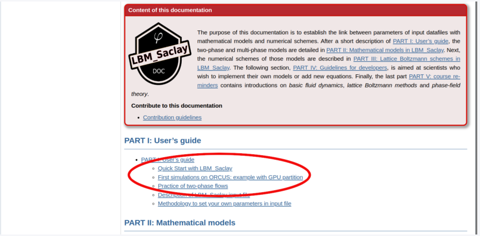
Open html documentation

```
$ google-chrome /tmpformation/LBM_Saclay/LBM_Saclay_Doc/_build/html/index.html
```

Main page



User's guide



For practicing: "copy-paste" commands of red boxes inside a terminal

Folder `run_training_lbm` 1/2: list of test cases

Single phase

	Name
1.	Lid driven cavity flow
2.	Poiseuille water
6a.	Gaussian Hill

Two-phase without fluid flow

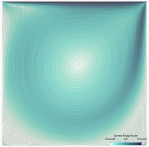
	Name
3.	Zalesak disk
4.	Interface deformation inside a vortex
5.	Spinodal decomposition
6b.	Stefan problem

Two-phase with fluid flow

	Name
7.	Double-Poiseuille
8.	Rayleigh-Taylor instability
9.	Capillary wave
10.	Falling droplet
11.	Rising bubble
12.	Taylor bubble
13.	Splashing droplet
14.	Dam-Break
⋮	⋮
20.	Moving-Container-Hole

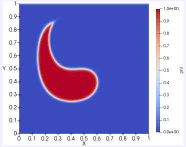
Folder `run_training_lbm` 2/2: overview of test cases

Single phase flow

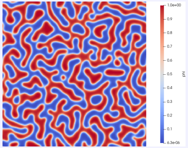


Cavity flow

Two-phase without fluid flow

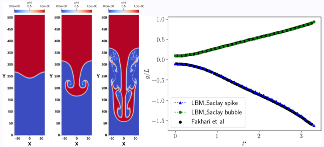


Interface deformation



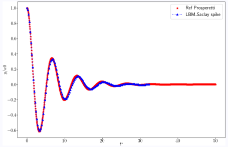
▸ Spinodal decomposition

Two-phase with fluid flow

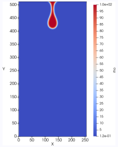


▸ Rayleigh-Taylor instability

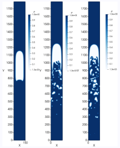
Two-phase with fluid flow



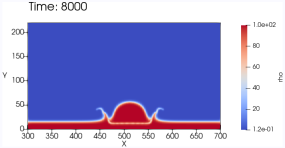
Capillary wave



▸ Falling droplet



▸ Taylor bubble



▸ Splashing droplet

Input datafile 1/2: law of similarity for simulations

Two incompressible flow systems are dynamically similar if they have the same Reynolds number and geometry.

Same Reynolds number

$$\mathrm{Re} = \frac{\left|\boldsymbol{u}^{phys}\right| L^{phys}}{\nu^{phys}} = \frac{\left|\boldsymbol{u}^{sim}\right| L^{sim}}{\nu^{sim}}$$

u_{sim}, L_{sim} and ν_{sim} can be the dimensionless quantities $(^\star)$ with ℓ_{ref} and t_{ref} and ρ_{ref}:

$$\mathrm{Re} = \frac{u^\star L^\star}{\nu^\star} \qquad \text{with} \qquad L^\star = \frac{L}{\ell_{ref}}, \quad u^\star = \frac{u}{C_u}, \quad \nu^\star = \frac{\nu}{C_\nu}, \quad g^\star = \frac{g}{C_g}$$

$$C_u = \frac{\ell_{ref}}{t_{ref}}, \quad C_\nu = \frac{\ell_{ref}^2}{t_{ref}}, \quad C_g = \frac{\ell_{ref}}{t_{ref}^2}$$

Single-phase example on Poiseuille flow ▸ Appendix

Input datafile 2/2: dimensionless quantities

Conversion coefficients

- Basic quantities: references of length (ℓ_{ref}), time (t_{ref}) and mass (ρ_{ref})

$$\ell_{ref} \text{ choose}, \qquad t_{ref} \text{ choose}, \qquad \rho_{ref} \text{ choose}$$

- Derived coefficients of conversion

$$\underbrace{C_u = \frac{\ell_{ref}}{t_{ref}},}_{\text{Velocity}} \qquad \underbrace{C_\nu = \frac{\ell_{ref}^2}{t_{ref}},}_{\text{Viscosity}} \qquad \underbrace{C_g = \frac{\ell_{ref}}{t_{ref}^2},}_{\text{Gravity}} \qquad \underbrace{C_p = \frac{C_\rho \ell_{ref}^2}{t_{ref}^2}}_{\text{Pressure}}$$

Example with $\ell_{ref} = \delta x$ and $t_{ref} = \delta t$ (lattice units in LB methods)

$$C_u = \frac{\delta x}{\delta t}, \qquad C_\nu = \frac{\delta x^2}{\delta t}, \qquad C_g = \frac{\delta x}{\delta t^2}, \qquad C_p = \rho_{ref} \frac{\delta x^2}{\delta t^2}$$

Finally post-process the results for recovering the physical quantities

$$L = L^\star \ell_{ref}, \qquad u = u^\star C_u, \qquad \nu = \nu^\star C_\nu, \qquad g = g^\star C_g, \qquad p = p^\star C_p$$

Guidelines for running and post-processing

Example on single-phase "Lid driven cavity flow"

- The output files will be written inside the folder «`RUN/TestCase01_LidDrivenCavityFlow`» :

```
$ cd TestCase01_LidDrivenCavityFlow
```

- Running

```
$ LBM_saclay/build_openmp/src/LBM_saclay TestCase01_Lid_driven_cavity_flow_Re1000.ini
```

- Post-processing with `paraview` (version $\geq$ `5.12.0`). Here `5.13.0-RC1`

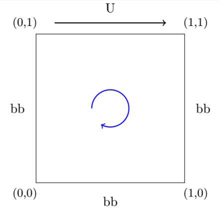
```
$ paraview&
```

- Export the velocity profiles in "`.csv`" files
- Run the python script comparing the LBM profiles ("`.csv`" files) with GHIA *et al.* results

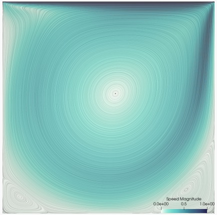
```
$ python Post-Pro_Lid_Driven_Cavity_Flow_Profile_Ux_y_Re1000.py
```

Example of results

Streamlines with `paraview`



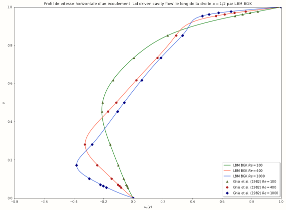
bb=bounce-back



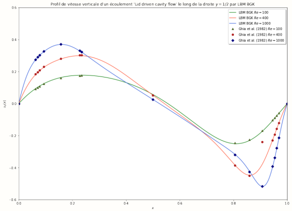
Streamlines
Re=?

`paraview` option:
“`Surface LIC`”

Comparison of profiles $Re = 100, 400, 1000$



$u_x(x_c = 0.5, y)$



$u_y(x, y_c = 0.5)$

Run on Orcus: connexion, run and transfer

Guidelines

- Connexion: change `train1` with your login name

```
$ ssh -XY S-SAC-DM2S-train1@orcusloginamd2
```

- Copy folder of test cases `run_training_lbm`

```
$ cp -r /tmpformation/LBM_Saclay/LBM_Saclay_Rech-Dev/run_training_lbm .
```

- Go to one test case (see previous slide) and submit your job

```
$ sbatch /tmpformation/LBM_Saclay/JOB_H100_GPU.slurm test-case-name.ini
```

- Files transfer on local computer

```
$ scp -r S-SAC-DM2S-train1@orcusloginamd2:~/run_training_lbm/test-case-name .
```

References

Books

- G.A. Bird, Molecular Gas Dynamics and Direct Simulation of Gas Flows, Oxford sci pub (1994)
- P.G. de Gennes, F. Brochard-Wyart, D. Quéré, Capillarity and wetting phenomena, Springer (2004)
- J.M. Delhaye, Thermohydraulique des réacteurs, EDP Sciences, (2008).
- N. Provatas, K. Elder, Phase-Field Methods in Materials Science and Engineering, Wiley-VCH (2010)
- Krüger *et al.*, The Lattice Boltzmann Method Principles and Practice, Springer (2017)
- J.-Ph. Ansermet, S. Bréchet, Thermodynamique, EPFL Press, 3e Ed, 2024 (516 pages).

Articles

- Historical articles

  - J.D. van der Waals (trans J.D. Rowlinson), *Journal of Statistical Physics*, vol 20 (2), 1979.
  - J.W. Cahn, J.E. Hilliard. *The journal of chemical physics*, vol 28 (2), 1958.

- Born diagram of Thermodynamics

  - J.C. Zhao. A mnemonic sheme for Thermodynamics. *MRS bulletin*, vol 34, 2009.

2. Phase-field theory

Energy approach of interfaces

Outline section 2

a. Fundamentals

Variational formulation and equilibrium properties

Free energy functional of an interface

Free energy and free energy density

- Main idea: the free energy is a function of two independent variables $\phi(\boldsymbol{x}, t)$ and $\boldsymbol{\nabla}\phi(\boldsymbol{x}, t)$

$$\underbrace{\mathscr{F}[\phi]}_{\text{Functional}} = \int_V \underbrace{\mathcal{F}(\phi, \boldsymbol{\nabla}\phi)}_{\text{Non-local free energy density}} dV \tag{13}$$

- Taylor expansion:

$$\mathcal{F}(\phi, \boldsymbol{\nabla}\phi, \nabla^2\phi) \approx \mathcal{F}_0(\phi) + \zeta_1 \boldsymbol{\nabla}^2\phi + \zeta_2(\boldsymbol{\nabla}\phi)^2 + \ldots \tag{14}$$

- After simplifying hypotheses (see Cahn & Hilliard (1958))

$$\mathscr{F}[\phi] = \int_V \left[\underbrace{\mathcal{F}_0(\phi)}_{\text{Local term}} + \underbrace{\frac{\zeta}{2}(\boldsymbol{\nabla}\phi)^2}_{\text{Non-local term}} \right] dV \tag{15}$$

In this section 2.a: implication of non-local term on equilibrium solution

Double-well and physical dimensions

Simplest free energy density of interface

- Local part (min of double-well: 0 and $+1$)

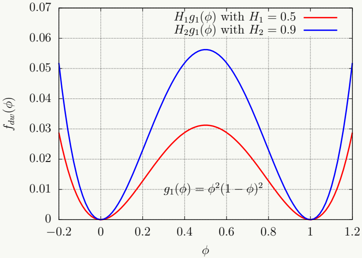
$$\mathcal{F}_0(\phi) \equiv \underbrace{f_{dw}(\phi)}_{\text{double-well}} = H \underbrace{\phi^2(1-\phi)^2}_{\equiv g_1(\phi)} \qquad (16)$$

Other choices for $f_{dw}(\phi)$: see next slides

- Non-local free energy density

$$\boxed{\mathcal{F}(\phi, \boldsymbol{\nabla}\phi) = H\phi^2(1-\phi)^2 + \frac{\zeta}{2}(\boldsymbol{\nabla}\phi)^2 \qquad (17)}$$

Representation of $f_{dw}(\phi)$



Physical dimensions

- $\mathscr{F}$: free energy, $[\mathscr{F}] = [\mathrm{E}]$
- f_{dw} double-well density, $[f_{dw}] = [\mathrm{E}]/[\mathrm{L}]^3$
- H: height of double-well, $[H] = [\mathrm{E}]/[\mathrm{L}]^3$
- ζ: capillary coefficient, $[\zeta] = [\mathrm{E}]/[\mathrm{L}]$

Minimum of $\mathscr{F}$ at equilibrium: stationary condition

First-order condition at equilibrium (see “Variational calculus” Appendix)

Application of δ-operator Appendix :

$$\delta\mathscr{F} = \int_V \left\{ \frac{\partial \mathcal{F}}{\partial \phi} - \boldsymbol{\nabla}\cdot\left[\frac{\partial \mathcal{F}}{\partial(\boldsymbol{\nabla}\phi)}\right]\right\}\delta\phi dV \quad (18)$$

First-order condition:

$$\frac{\delta\mathscr{F}}{\delta\phi} = 0 \iff \frac{\partial \mathcal{F}}{\partial \phi} - \boldsymbol{\nabla}\cdot\left[\frac{\partial \mathcal{F}}{\partial(\boldsymbol{\nabla}\phi)}\right] = 0 \quad (19)$$

Proof of Eq. (18)

$$\begin{aligned}
\delta\mathscr{F} &= \delta\int_V \mathcal{F}(\phi,\boldsymbol{\nabla}\phi)dV \\
&= \int_V \delta\mathcal{F}(\phi,\boldsymbol{\nabla}\phi)dV \\
&= \int_V \left[\frac{\partial \mathcal{F}}{\partial\phi}\delta\phi + \frac{\partial \mathcal{F}}{\partial(\boldsymbol{\nabla}\phi)}\underbrace{\delta(\boldsymbol{\nabla}\ \ \phi)}_{\text{intervert}}\right]dV
\end{aligned}$$

$$\begin{aligned}
\delta\mathscr{F} &= \int_V \frac{\partial \mathcal{F}}{\partial\phi}\delta\phi dV + \underbrace{\int_V \frac{\partial \mathcal{F}}{\partial(\boldsymbol{\nabla}\phi)}\boldsymbol{\nabla}(\delta\phi)dV}_{\text{integration by parts}} \\
&= \int_V \frac{\partial \mathcal{F}}{\partial\phi}\delta\phi dV + \underbrace{\cancel{\int_{\partial V} \boldsymbol{\mathcal{F}}\cdot\boldsymbol{n}\delta\phi d(\partial V)}}_{\text{hyp: } \boldsymbol{\mathcal{F}}\cdot\boldsymbol{n}=0 \text{ on } \partial V} - \int_V \boldsymbol{\nabla}\cdot\left[\frac{\partial \mathcal{F}}{\partial(\boldsymbol{\nabla}\phi)}\right]\delta\phi dV
\end{aligned} \quad (20)$$

Remark: if $\int_{\partial V} \neq 0$ see boundary condition with Contact angle

Euler-Lagrange equation and chemical potential

Equilibrium condition (necessary cond)

At equilibrium, if $\phi(\boldsymbol{x})$ is an extremal of

$$\mathscr{F}[\phi] = \int_V \mathcal{F}(\phi, \boldsymbol{\nabla}\phi) dV$$

then it satisfies the Euler-Lagrange Eq:

$$\boxed{\underbrace{\frac{\partial \mathcal{F}}{\partial \phi}}_{\text{Local part}} - \boldsymbol{\nabla} \cdot \underbrace{\left[\frac{\partial \mathcal{F}}{\partial(\boldsymbol{\nabla}\phi)}\right]}_{\text{Non-local part}} = 0 \qquad (21)}$$

- The local part is the classic thermo def of $\mu_\phi^{(0)}$
- The non-local part is non-zero because of gradient energy term $\zeta(\boldsymbol{\nabla}\phi)^2/2$

Def of non-local chemical potential μ_ϕ

- Conjugate variable of $\phi(\boldsymbol{x}, t)$:

$$\begin{aligned} \mu_\phi(\boldsymbol{x}, t) \triangleq \frac{\delta \mathscr{F}}{\delta \phi} &= \frac{\delta \mathcal{F}}{\delta \phi} \qquad (22) \\ &= \frac{\partial \mathcal{F}}{\partial \phi} - \boldsymbol{\nabla} \cdot \left[\frac{\partial \mathcal{F}}{\partial(\boldsymbol{\nabla}\phi)}\right] \end{aligned}$$

- At equilibrium $\mu_\phi(\boldsymbol{x}) = \mu^{eq}$
- $\phi\mu_\phi$ is homogeneous to [E]/[L]^3
- Application with $\mathcal{F}$ def by Eq. (17):

$$\boxed{\mu_\phi = f'_{dw}(\phi) - \zeta\boldsymbol{\nabla}^2\phi}$$

where f'_{dw} is the deriv of f_{dw} wrt ϕ

Fundamental solution of 1D Euler-Lagrange equation

Equilibrium solution ($\mu^{eq} = 0$)

- Euler-Lagrange 1D:

$$\zeta \frac{d^2\phi^{eq}}{dx^2} - H \frac{dg_1(\phi^{eq})}{d\phi} = 0 \qquad (23)$$

- which can be solved (see next slide):

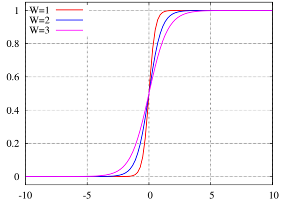
$$\boxed{\phi^{eq}(x) = \frac{1}{2}\left[1 + \tanh\left(\frac{2x}{W}\right)\right] \qquad (24)}$$

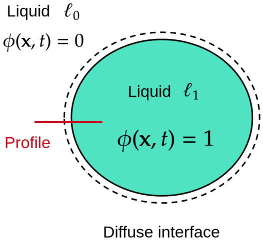
- W is the interface width:

$$W = \sqrt{\frac{8\zeta}{H}} \qquad (25)$$

At equilibrium, the profile $\phi^{eq}(x)$ is **continuous with a diffuse interface**

Hyperbolic tangent solution $\phi^{eq}(x)$





Derivation of 1D solution: proof of Eq. (24)

First part

- Euler-Lagrange 1D:

$$\zeta \frac{d^2\phi}{dx^2} - H\frac{dg_1(\phi)}{d\phi} = 0$$

- Multiply by $d\phi/dx$, gather under d/dx:

$$\zeta \frac{d\phi}{dx}\frac{d^2\phi}{dx^2} - H\underbrace{\frac{d\phi}{dx}\frac{dg_1(\phi)}{d\phi}}_{\text{chain rule}} = 0$$

$$\frac{\zeta}{2}\frac{d}{dx}\left(\frac{d\phi}{dx}\right)^2 - H\frac{dg_1(\phi)}{dx} = 0$$

$$\frac{\zeta}{2}\left(\frac{d\phi}{dx}\right)^2 = Hg_1(\phi) \qquad (26)$$

Second part

- Positive root of Eq. (26)

$$\frac{d\phi}{dx} = \underbrace{\sqrt{\frac{2H}{\zeta}}}_{\equiv C}\phi(1-\phi)$$

$$\frac{d\phi}{\phi(1-\phi)} = Cdx$$

$$\ln\phi - \ln(1-\phi) = Cx$$

$$\frac{\phi}{1-\phi} = \exp\left[\frac{2C}{2}x\right]$$

- Use $\tanh X = (e^{2X}-1)/(e^{2X}+1)$, finally

$$2\phi - 1 = \tanh\left(\frac{Cx}{2}\right)$$

Interface properties: surface tension σ and interface width W

Surface tension: excess of free energy at equilibrium

Calculation of surface tension

$$\sigma \hat{=} \int_{-\infty}^{+\infty} \mathcal{F}(\phi^{eq}, \frac{d\phi^{eq}}{dx}) dx \tag{27}$$

$$= \int_{-\infty}^{+\infty} \zeta \left(\frac{d\phi^{eq}}{dx}\right)^2 dx$$

$$= \int_{-\infty}^{+\infty} 2Hg_1(\phi^{eq}) dx$$

$$= \int_{\phi^{min}}^{\phi^{max}} \sqrt{2\zeta H g_1(\phi)} d\phi$$

For $g_1(\phi) = \phi^2(1-\phi)^2$: $\phi^{min} = 0$ and $\phi^{max} = 1$:

$$\sigma = \sqrt{2\zeta H} \int_0^1 \phi(1-\phi) d\phi = \frac{1}{6}\sqrt{2\zeta H}$$

Interface properties

- Surface tension σ

$$\boxed{\sigma = \frac{1}{6}\sqrt{2\zeta H}} \tag{28}$$

Dimension $[\sigma] = [\mathrm{E}]/[\mathrm{L}]^2$

- Interface width W

$$\boxed{W = \sqrt{\frac{8\zeta}{H}}} \tag{29}$$

Dimension $[W] = [\mathrm{L}]$

Double-well: inflection points and concave part

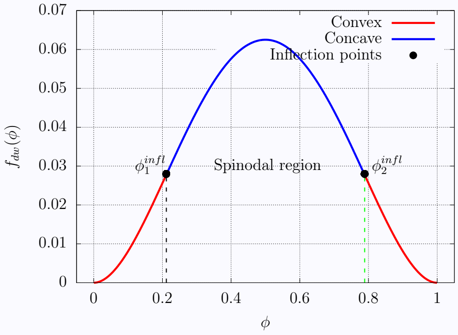
Inflection points of local free energy $f_{dw}(\phi) = \phi^2(1-\phi)^2$

- Definition of inflection points: points ϕ^{infl} such as

$$\boxed{\left.\frac{\partial^2 f_{dw}(\phi)}{\partial \phi^2}\right|_{\phi=\phi^{infl}} \equiv f''_{dw}(\phi^{infl}) = 0}$$

- e.g. for $f_{dw}(\phi) = g_1(\phi)$:

$$\begin{aligned} f''_{dw}(\phi) &= 2(6\phi^2 - 6\phi + 1) \\ \phi_1^{infl} &= 0.2113248654051871 \\ \phi_1^{infl} &= 0.788675134594813 \end{aligned}$$



Convex part: $f''_{dw}(\phi) > 0$
when $\phi < \phi_1^{infl}$ and $\phi_2^{infl} < \phi$

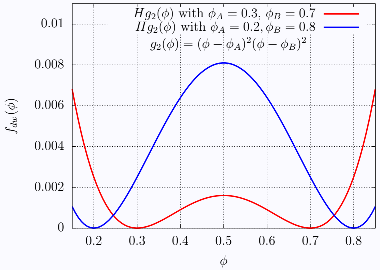
Concave part: $f''_{dw}(\phi) < 0$
when $\phi_1^{infl} < \phi < \phi_2^{infl}$

Alternative forms of double-wells $g_2(\phi)$ and $g_3(\phi)$

For $g(\phi) \equiv g_1(\phi)$ the two minima are $\phi_A = 0$, $\phi_B = 1$ and $g_1(\phi_A) = g_1(\phi_B) = 0$

Modification of minima ϕ_A and ϕ_B

Function $g_2(\phi) = (\phi - \phi_A)^2(\phi - \phi_B)^2$

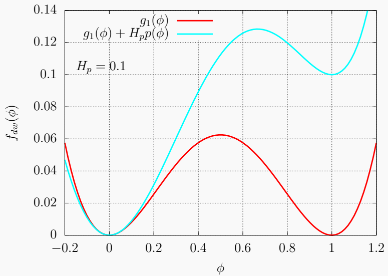


Special case $\phi_A = +\phi^\star$ and $\phi_B = -\phi^\star$

$$g_3(\phi) = (\phi - \phi^\star)^2(\phi + \phi^\star)^2$$

Modification of height

Function $g_1(\phi)$ and $p(\phi) = \phi^3(10 - 15\phi + 6\phi^2)$



Properties of interpolation function $p(\phi)$

$$p(0) = 0,\ p(1) = 1 \quad \text{and} \quad p'(0) = p'(1) = 0$$

Summary of $\phi^{eq}(x)$, W and σ as function of $f_{dw}(\phi)$

Interface width W

Double-well	Solution	Interface width W
$g_1(\phi) = \phi^2(1-\phi)^2$	$\phi_1^{eq}(x) = \frac{1}{2}\left[1 + \tanh\left(\frac{2x}{W}\right)\right]$	$W_1 = \sqrt{\frac{8\zeta}{H}}$
$g_2(\phi) = (\phi_l - \phi)^2(\phi - \phi_g)^2$	$\phi_2^{eq}(x) = \frac{\phi_l+\phi_g}{2} + \frac{\phi_l-\phi_g}{2}\tanh\left[\frac{2x}{W}\right]$	$W_2 = \frac{4}{(\phi_l-\phi_g)}\sqrt{\frac{\zeta}{2H}}$
$g_3(\phi) = (\phi^\star - \phi)^2(\phi + \phi^\star)^2$	$\phi_3^{eq}(x) = \phi^\star \tanh\left(\frac{2x}{W}\right)$	$W_3 = \frac{1}{\phi^\star}\sqrt{\frac{2\zeta}{H}}$

Surface tension σ

Surface tension expression $\sigma = I\sqrt{2\zeta H}$

Double-well	Bounds	Factor I
$g_1(\phi) = \phi^2(1-\phi)^2$	$0 < \phi < 1$	$I_1 = 1/6$
$g_2(\phi) = (\phi_l - \phi)^2(\phi - \phi_g)^2$	$\phi_g < \phi < \phi_l$	$I_2 = (\phi_l - \phi_g)^3/6$
$g_3(\phi) = (\phi^\star - \phi)^2(\phi + \phi^\star)^2$	$-\phi^\star < \phi < \phi^\star$	$I_3 = 4\phi^{\star 3}/3$
$g(\phi) = 8g_1(\phi) = 8\phi^2(1-\phi)^2$	$0 < \phi < 1$	$I = 2\sqrt{2}/6$

Equilibrium μ^{eq} 1/2: common tangent for flat interface

Common tangent construction

- Equilibrium conditions

$$\mu_0^{eq}(\phi_0) = \mu_1^{eq}(\phi_1) = \mu^{eq} \tag{30a}$$
$$p_0(\phi_0) = p_1(\phi_1) \tag{30b}$$

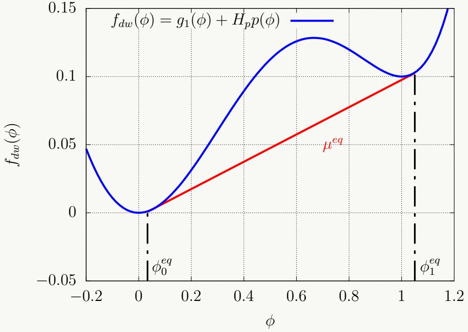
- With its def (Eq. (5)), Eq. (30b) writes

$$\phi_0 \underbrace{\mu_0^{eq}}_{\text{Eq. (30}a)} - f_{dw}(\phi_0) = \phi_1 \underbrace{\mu_1^{eq}}_{\text{Eq. (30}a)} - f_{dw}(\phi_1)$$

- We find:

$$\boxed{\mu^{eq} = \frac{f_{dw}(\phi_1) - f_{dw}(\phi_0)}{\phi_1 - \phi_0} \quad (31)}$$

Graphical interpretation



μ^{eq} is the slope of the red line which is the common tangent of f_{dw}

Equilibrium μ_i^{eq} 2/2: Gibbs-Thomson for curved interface

Gibbs-Thomson condition for a curved interface

- Equilibrium conditions (Laplace for p)

$$\mu_{in}^{eq}(\phi_{in}) = \mu_{out}^{eq}(\phi_{out}) = \mu_i^{eq} \tag{32a}$$
$$p_{in}(\phi_{in}) - p_{out}(\phi_{out}) = \sigma\kappa \tag{32b}$$

where i is for interface

- With its def (Eq. (5)), Eq. (32b) writes

$$\phi_{in} \underbrace{\mu_{in}^{eq}}_{\text{Eq. (32}a\text{)}} - f(\phi_{in}) - \phi_{out} \underbrace{\mu_{out}^{eq}}_{\text{Eq. (32}a\text{)}} + f(\phi_{out}) = \sigma\kappa$$

- Using common tangent construction Eq. (31) for $f(\phi_{out}) - f(\phi_{in})$:

$$\mu_i^{eq}(\phi_{in} - \phi_{out}) + \mu^{eq}(\phi_{out} - \phi_{in}) = \sigma\kappa$$

- Finally:

$$\boxed{\mu_i^{eq} = \mu^{eq} + \frac{\sigma\kappa}{(\phi_{out} - \phi_{in})} \qquad (33)}$$

This is the Gibbs-Thomson condition

Remarks

- Gibbs-Thomson condition exists for temperature and is quite similar (see section 4)
- Sign of $(\phi_{out} - \phi_{in})$ can change depending on the def of bulk phases: < 0 if $\phi_{out} = 0$ and $\phi_{in} = 1$

Spherical Euler-Lagrange with $\mu^{eq} \neq 0$

Laplace relation for a sphere of radius R

- Euler-Lagrange with spherical Laplacian

$$\frac{df_{dw}}{d\phi} - \zeta\frac{d^2\phi}{dr^2} - \zeta\frac{2}{r}\frac{d\phi}{dr} = \mu^{eq} \quad \xrightarrow{\times d\phi/dr} \quad \frac{d}{dr}\left[f_{dw} - \frac{\zeta}{2}\left(\frac{d\phi}{dr}\right)^2 - \mu^{eq}\phi\right] - \zeta\frac{2}{r}\left(\frac{d\phi}{dr}\right)^2 = 0$$

- After 2 integrations $\int_0^r dr$ and $\int_r^{+\infty} dr$:

$$f_{dw}(\phi) - f_{dw}(\phi_0) - \mu^{eq}(\phi - \phi_0) = \frac{\zeta}{2}\left(\frac{d\phi}{dx}\right)^2 + \int_0^r \zeta\frac{2}{\varrho}\left(\frac{d\phi}{d\varrho}\right)^2 d\varrho$$

$$f_{dw}(\phi_1) - f_{dw}(\phi) - \mu^{eq}(\phi_1 - \phi) = -\frac{\zeta}{2}\left(\frac{d\phi}{dx}\right)^2 + \int_r^{+\infty} \zeta\frac{2}{\varrho}\left(\frac{d\phi}{d\varrho}\right)^2 d\varrho$$

- After summing

$$\underbrace{\mu^{eq}\phi_0 - f_{dw}(\phi_0)}_{=P_0} - (\underbrace{\mu^{eq}\phi_1 - f_{dw}(\phi_1)}_{=P_1}) \approx \frac{2}{R}\underbrace{\int_0^{+\infty} \zeta\left(\frac{d\phi}{d\varrho}\right)^2 d\varrho}_{\equiv\sigma} \longrightarrow$$

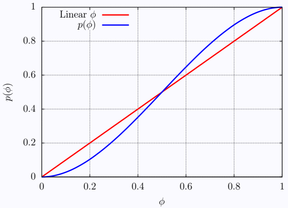
Laplace law

$$\boxed{P_0(\phi_0) - P_1(\phi_1) \approx \sigma\kappa}$$

Interpolation function $p(\phi)$ in the diffuse interface

Interpolation function $p(\phi)$ for $0 \leqslant \phi \leqslant 1$

$$\boxed{p(\phi) \triangleq \phi^2(3-2\phi)} \quad \text{such as} \quad \begin{cases} p(0) & = 0 \\ p(1) & = 1 \\ p'(0) = p'(1) & = 0 \end{cases}$$

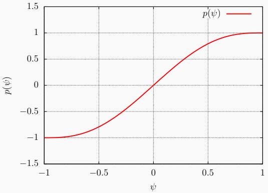


Example with bulk free energy:

$$f_{bulk}(\phi, c) = f_s(c)p(\phi) + f_l(c)[1 - p(\phi)]$$

Interpolation function $p(\psi)$ for $-1 \leqslant \psi \leqslant +1$ (section 4)

$$\boxed{p(\psi) \triangleq \frac{15}{8}\left[\psi - \frac{2}{3}\psi^3 + \frac{\psi^5}{5}\right]} \quad \text{such as} \quad \begin{cases} p(-1) & = -1 \\ p(1) & = 1 \\ p'(-1) = p'(1) & = 0 \end{cases}$$



Remark: μ_ϕ seen as a Lagrange multiplier

Remark for conserved order parameter (e.g. composition $\phi \equiv c$ or density $\phi \equiv \rho$)

- For conserved order parameter ϕ :

$$\int_V \phi(\boldsymbol{x}, t) dV = \int_V \phi_0(\boldsymbol{x}) dV$$

- We can introduce the Lagrange multiplier $\mu_\phi(\boldsymbol{x}, t)$ associated to the constraint $\phi(\boldsymbol{x}, t) - \phi_0(\boldsymbol{x}) = 0$,

$$\mathscr{F}[\phi] = \int_V \left\{ \mathcal{F}(\phi, \boldsymbol{\nabla}\phi) - \mu_\phi(\phi - \phi_0) \right\} dV$$

- After applying the delta operator δ:

$$\delta\mathscr{F}[\phi] = \int_V \left\{ \left[\frac{\partial \mathcal{F}}{\partial \phi} - \boldsymbol{\nabla} \cdot \left(\frac{\partial \mathcal{F}}{\partial (\boldsymbol{\nabla}\phi)} \right) - \mu_\phi \right] \delta\phi - (\phi - \phi_0)\delta\mu_\phi \right\} dV$$

- Stationnary conditions:

$$\left.\begin{aligned} \frac{\delta \mathscr{F}}{\delta \phi} &= 0 \\ \frac{\delta \mathscr{F}}{\delta \mu_\phi} &= 0 \end{aligned}\right. \quad \Longrightarrow \quad \boxed{\begin{aligned} \mu_\phi &= \frac{\partial \mathcal{F}}{\partial \phi} - \boldsymbol{\nabla} \cdot \left[\frac{\partial \mathcal{F}}{\partial (\boldsymbol{\nabla}\phi)} \right] \\ \phi &= \phi_0 \end{aligned}}$$

b. Time-evolution

Constitutive laws of Cahn-Hilliard and Allen-Cahn models

Cahn-Hilliard equation 1/2: definition of flux $\boldsymbol{j}_{CH}$

Derivation of constitutive law $\boldsymbol{j}_{diff}$

- Conservation equation:

$$\frac{\partial \phi(\boldsymbol{x},t)}{\partial t} = -\boldsymbol{\nabla}\cdot \boldsymbol{j}_{diff}(\boldsymbol{x},t)$$

- Pb: define flux $\boldsymbol{j}_{diff}$ such as:

$$\frac{d\mathscr{F}}{dt} \leqslant 0$$

- Method:

$$\begin{aligned}
\frac{d\mathscr{F}}{dt} &= \int_V \frac{\delta \mathscr{F}}{\delta \phi}\frac{\partial \phi}{\partial t} dV && \text{Chain rule} \\
&= -\int_V \frac{\delta \mathscr{F}}{\delta \phi}\boldsymbol{\nabla}\cdot \boldsymbol{j}_{diff} dV && \text{Conserv eq} \\
&= \int_V \boldsymbol{j}_{diff}\cdot \boldsymbol{\nabla}\frac{\delta \mathscr{F}}{\delta \phi} dV && \text{Integ by parts}
\end{aligned}$$

Simplest choice for $\boldsymbol{j}_{diff}$

Constitutive law:

$$\underbrace{\boldsymbol{j}_{diff}(\boldsymbol{x},t)}_{\equiv \boldsymbol{j}_{CH}} \triangleq -\mathcal{M}_\phi \boldsymbol{\nabla}\frac{\delta \mathscr{F}}{\delta \phi}$$

Because:

$$\frac{d\mathscr{F}}{dt} = -\int_V \mathcal{M}_\phi \left[\boldsymbol{\nabla}\frac{\delta \mathscr{F}}{\delta \phi}\right]^2 dV \leqslant 0$$

where:

- $\mathcal{M}_\phi$: positive proportionality coefficient
- $\frac{\delta \mathscr{F}}{\delta \phi} = \mu_\phi$: chemical potential (Eq. (22))

$$\boxed{\boldsymbol{j}_{CH}(\boldsymbol{x},t) = -\mathcal{M}_\phi \boldsymbol{\nabla}\mu_\phi \quad (34)}$$

Cahn-Hilliard equation 2/2: model with advection

Mass balance for conserved order parameter

- Mass balance

$$\frac{\partial\phi(\boldsymbol{x},t)}{\partial t} = -\boldsymbol{\nabla}\cdot\boldsymbol{j}_{tot}(\boldsymbol{x},t) \qquad (35)$$

$$\boldsymbol{j}_{tot}(\boldsymbol{x},t) = \boldsymbol{j}_{adv}(\boldsymbol{x},t) + \boldsymbol{j}_{CH}(\boldsymbol{x},t)$$

- Assumptions on fluxes

$$\boldsymbol{j}_{adv}(\boldsymbol{x},t) = \boldsymbol{u}(\boldsymbol{x},t)\phi(\boldsymbol{x},t) \qquad (36)$$

$$\boldsymbol{j}_{CH}(\boldsymbol{x},t) = -\mathcal{M}_\phi\boldsymbol{\nabla}\mu_\phi(\boldsymbol{x},t) \qquad (37)$$

Cahn-Hilliard model (for conserved order parameter): eq. of 4th order

$$\frac{\partial\phi}{\partial t} + \boldsymbol{\nabla}\cdot(\boldsymbol{u}\phi) = \mathcal{M}_\phi\boldsymbol{\nabla}^2\mu_\phi \qquad (38a)$$

$$\mu_\phi = \underbrace{2H\phi(1-\phi)(1-2\phi)}_{f'_{dw}(\phi)} - \zeta\boldsymbol{\nabla}^2\phi \qquad (38b)$$

ϕ plays two roles:

- composition
- Interface tracking

The Cahn-Hilliard model is useful for phenomena occuring in mixtures: demixing, nucleation-growth, spinodal decomposition and Ostwald ripening

Consequence of Gibbs-Thomson and $\boldsymbol{j}_{CH}$: Ostwald ripening

Remark on Gibbs-Thomson condition with $\boldsymbol{j}_{CH}$

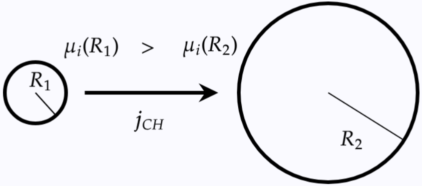
- The Gibbs-Thomson condition writes:

$$\mu_i = \mu^{eq} + \frac{1}{(\phi_{out} - \phi_{in})} \frac{2\sigma}{R} \qquad (39)$$

- With $R_1 < R_2$, Eq. (39) implies:

$$\mu_i(R_2) < \mu_i(R_1)$$

- Two bubbles of radius R_1 and R_2 with $R_1 < R_2$



- There exists a flow from $\mu_i(R_1)$ to $\mu_i(R_2)$ because $\boldsymbol{j}_{CH} \propto -\boldsymbol{\nabla}\mu_\phi(\boldsymbol{x}, t)$
- Consequence: the smaller bubble disappears and the bigger one grows.

This is the Ostwald ripening (see section 6 for simulations).

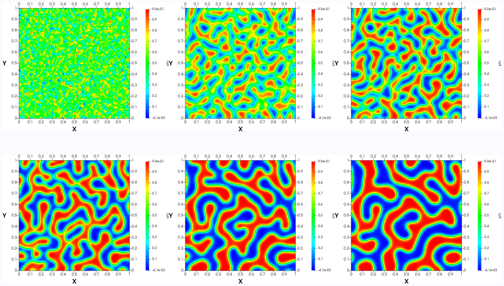
Simulations with Cahn-Hilliard 1/2

Spinodal decomposition 50-50

Initial conditions

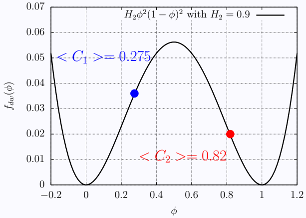
r random number (uniform distrib): $0 \leq r \leq 1$

$\phi(\boldsymbol{x}, 0) = r, \quad$ for all nodes

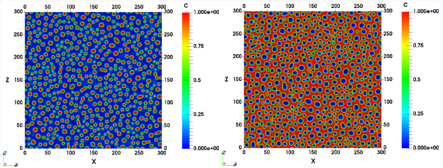


Video

Other initializations



Demixing $\langle C_1 \rangle = 0.275$, $\langle C_2 \rangle = 0.67$



Video

Simulations with Cahn-Hilliard 2/2

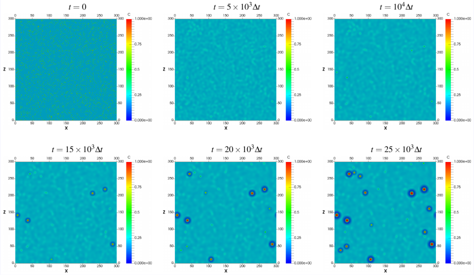
Nucleation-growth

Video

Initial condition

r random number (uniform distrib): $0 \leq r \leq 1$

$$\phi(\boldsymbol{x}, 0) = \begin{cases} 0.2 & \text{for 97\% of nodes} \\ \frac{(9+r)}{10} & \text{for 3\%} \end{cases}$$



Phase separation

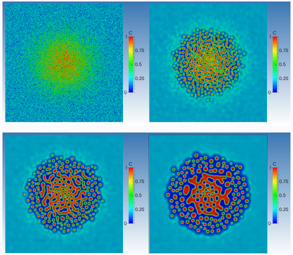
Video

Initial condition: gaussian distrib

r random number (uniform distrib): $0 \leq r \leq 1$

$$\phi(\boldsymbol{x}, 0) = \begin{cases} \frac{3}{10} r & \text{for 90\% of nodes} \\ \frac{9+r}{10} & \text{for 10\%} \end{cases}$$

Gaussian distrib for 10% nodes $\boldsymbol{x}_g = (x_g, y_g)$



Allen-Cahn equation 1/2: definition of source term

Source definition for evolution equation

- Evolution equation:

$$\frac{\partial \phi(\boldsymbol{x},t)}{\partial t} = \mathcal{S}_{AC}(\boldsymbol{x},t)$$

- Define source term $\mathcal{S}_{AC}(\boldsymbol{x},t)$ such as

$$\frac{d\mathscr{F}}{dt} \leqslant 0$$

- Method:

$$\begin{aligned}\frac{d\mathscr{F}}{dt} &= \int_V \frac{\delta \mathscr{F}}{\delta \phi}\frac{\partial \phi}{\partial t} dV \\ &= -\int_V \frac{\delta \mathscr{F}}{\delta \phi}\mathcal{S}_{AC} dV\end{aligned}$$

Simplest and minimal choice for $\mathcal{S}$

Constitutive law:

$$\mathcal{S}_{AC}(\boldsymbol{x},t) = -\mathscr{M}_\phi \frac{\delta \mathscr{F}}{\delta \phi}$$

Because:

$$\frac{d\mathscr{F}}{dt} = -\int_V \mathscr{M}_\phi \left[\frac{\delta \mathscr{F}}{\delta \phi}\right]^2 dV \leqslant 0$$

where:

- $\mathscr{M}_\phi$: positive proportionality coefficient
- $\frac{\delta \mathscr{F}}{\delta \phi} = \mu_\phi$: chemical potential

$$\boxed{\mathcal{S}_{AC}(\boldsymbol{x},t) = -\mathscr{M}_\phi \mu_\phi}$$

Allen-Cahn equation 2/2: model with advection

Allen-Cahn equation (for non conserved order parameter)

$$\frac{\partial \phi}{\partial t} + \boldsymbol{\nabla} \cdot (\boldsymbol{u}\phi) = -\mathscr{M}_\phi \mu_\phi \tag{40a}$$

$$\mu_\phi = 2H\phi(1-\phi)(1-2\phi) - \zeta \boldsymbol{\nabla}^2 \phi \tag{40b}$$

The Allen-Cahn equation tracks the interface for phase change problems. It must be derived and considered coupled with (at least) one supplementary eq which is responsible for the interface displacement: temperature, solute, etc. Illustrations are given on “phase change” in Section 4, “crystal growth” and “dissolution” in Section 6

Remark: diffusivity coefficient M_ϕ in CH and AC eqs

We can make appear a diffusivity coefficient M_ϕ of dimension $[M_\phi] = [\mathrm{L}]^2/[\mathrm{T}]$

Cahn-Hilliard Eq. (CH) – conserved ϕ

Diffusivity parameter $M_\phi = \mathcal{M}_\phi H$

$$\begin{aligned}\mathcal{M}_\phi \nabla^2 \mu_\phi &= \mathcal{M}_\phi \nabla^2 \left[H g_1'(\phi) - \zeta \nabla^2 \phi \right] \\ &= \mathcal{M}_\phi H \nabla^2 \left[g_1'(\phi) - \frac{\zeta}{H} \nabla^2 \phi \right] \\ &= M_\phi \nabla^2 \left[g_1'(\phi) - \frac{W^2}{8} \nabla^2 \phi \right]\end{aligned}$$

$$\frac{\partial \phi}{\partial t} + \nabla \cdot (\boldsymbol{u}\phi) = M_\phi \nabla^2 \left[g_1'(\phi) - \frac{W^2}{8} \nabla^2 \phi \right] \quad (41)$$

Allen-Cahn Eq. (AC) – non-conserved ϕ

Diffusivity parameter $M_\phi = \mathscr{M}_\phi \zeta$

$$\begin{aligned}-\mathscr{M}_\phi \mu_\phi &= -\mathscr{M}_\phi \left[H g_1'(\phi) - \zeta \nabla^2 \phi \right] \\ &= -\mathscr{M}_\phi \zeta \left[\frac{H}{\zeta} g_1'(\phi) - \nabla^2 \phi \right] \\ &= M_\phi \left[\nabla^2 \phi - \frac{8}{W^2} g_1'(\phi) \right]\end{aligned}$$

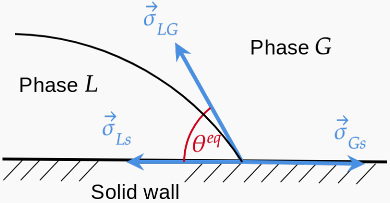
$$\frac{\partial \phi}{\partial t} + \nabla \cdot (\boldsymbol{u}\phi) = M_\phi \left[\nabla^2 \phi - \frac{8}{W^2} g_1'(\phi) \right] \quad (42)$$

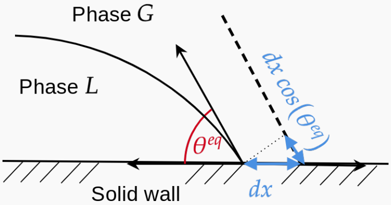
Double-well derivative $g_1'(\phi)$

$$g_1'(\phi) = 2\phi(1-\phi)(1-2\phi) \quad (43)$$

Contact angle 1/2: concept

Law of Young-Dupré (see book de Gennes *et al.*, 2004)





- σ_{Ls}: surface tension between Liquid/solid
- σ_{Gs}: surface tension between Gas/solid
- σ_{LG}: surface tension between Liquid/Gas
- θ^{eq}: equilibrium angle (contact angle)

- Work for a small displacement dx

$$d\mathcal{W} = (\sigma_{Gs} - \sigma_{Ls})dx - \sigma_{LG}dx\cos(\theta^{eq})$$

- At equilibrium $d\mathcal{W} = 0$

$$\boxed{\cos(\theta^{eq}) = \frac{\sigma_{Gs} - \sigma_{Ls}}{\sigma_{LG}}} \tag{44}$$

Contact angle 2/2: boundary condition for diffuse interface

Free energy of wall

- Minimization of $\mathscr{F} + \mathscr{F}_w$
- With wall free energy defined by

$$\mathscr{F}_w = \int_{\partial V} [(\sigma_{Gs} - \sigma_{Ls})p(\phi) + \sigma_{Ls}]d(\partial V)$$

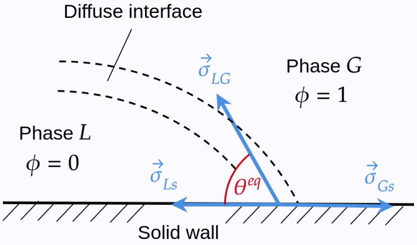
$$p(\phi) = \phi^2(3 - 2\phi)$$

- Properties of interpolation $p(\phi)$:

$$p(0) = 0,\ p(1) = 1,\ p'(0) = p'(1) = 0$$

- Variation $\delta(\mathscr{F} + \mathscr{F}_w)/\delta\phi$ (see Eq. (20)):

$$\int_{\partial V} \left[\zeta \boldsymbol{\nabla}\phi \cdot \boldsymbol{n} + \underbrace{(\sigma_{Gs} - \sigma_{Ls})}_{\text{use Eq. (44)}} p'(\phi)\right] d(\partial V) = 0$$



- Boundary condition at solid surface:

$$\boxed{\zeta \boldsymbol{\nabla}\phi \cdot \boldsymbol{n} = -\sigma_{LG} \cos(\theta^{eq}) p'(\phi)}$$

- Remark: if $\theta^{eq} = 90^\circ$ then $\boldsymbol{\nabla}\phi \cdot \boldsymbol{n} = 0$

C. Conservative Allen-Cahn (CAC) model

Also called "Advected field" or "conservative level-set"

Properties of derivatives of ϕ^{eq}

Hyperbolic tangent solution (see section 2)

$$\mathscr{F}[\phi] = \int \left[H\phi^2(1-\phi)^2 + \frac{\zeta}{2}|\nabla\phi|^2 \right] dV$$

$$\mu_\phi = \frac{\delta \mathscr{F}}{\delta \phi} = 2H\phi(1-\phi)(1-2\phi) - \zeta\nabla^2\phi$$

Equilibrium 1D

$$\mu_\phi = 0 \implies \phi^{eq} = \frac{1}{2}\left[1 + \tanh\left(\frac{2s}{W}\right)\right]$$

- s normal coordinate at interface
- $W = \sqrt{\frac{8\zeta}{H}}$ interface width

Derivatives of 1D equilibrium $\phi^{eq}(x)$

First derivative

$$\partial_x \phi^{eq} = \frac{4}{W}\phi^{eq}(1-\phi^{eq}) \qquad (45)$$

Second derivative

$$\partial_{xx}\phi^{eq} = \frac{16}{W^2}\phi^{eq}(1-\phi^{eq})(1-2\phi^{eq}) \qquad (46)$$

Summary of useful relationships

Normal vector $\boldsymbol{n}_\phi \equiv \boldsymbol{n}_\phi(\boldsymbol{x}, t)$

$$\boxed{\boldsymbol{n}_\phi = \frac{\boldsymbol{\nabla}\phi}{|\boldsymbol{\nabla}\phi|}} \quad (47)$$

Dimension $[\boldsymbol{n}_\phi] = [-]$

Curvature $\kappa \equiv \kappa(\boldsymbol{x}, t)$

$$\boxed{\kappa = \boldsymbol{\nabla}\cdot\boldsymbol{n}} \quad (48)$$

Dimension $[\kappa] = 1/[\mathrm{L}]$

Counter Term (CT)

$$\boxed{\mathrm{CT} = M_\phi \kappa\,|\boldsymbol{\nabla}\phi|} \quad (49)$$

Dimension $[\mathrm{CT}] = 1/[\mathrm{T}]$

See details in html documentation

3D equilibrium (kernel function $|\boldsymbol{\nabla}\phi|^{eq}$)

$$\boxed{|\boldsymbol{\nabla}\phi|^{eq} = \frac{4}{W}\phi^{eq}(1-\phi^{eq})} \quad (50)$$

we can derive:

$$\boldsymbol{\nabla}\,|\boldsymbol{\nabla}\phi|^{eq} = \frac{4}{W}(1-2\phi^{eq})\boldsymbol{\nabla}\phi^{eq} \quad (51a)$$

after scalar product with $\boldsymbol{n}_\phi$

$$\boldsymbol{n}_\phi\cdot\boldsymbol{\nabla}\,|\boldsymbol{\nabla}\phi|^{eq} = \frac{16}{W^2}\phi^{eq}(1-\phi^{eq})(1-2\phi^{eq}) \quad (51b)$$

Advected field with curvature

Transport of ϕ

- Hyperbolic equation:

$$\frac{\partial \phi}{\partial t} + \boldsymbol{V} \cdot \boldsymbol{\nabla} \phi = 0 \tag{52}$$

- Hypothesis on total velocity $\boldsymbol{V}$:

$$\boldsymbol{V} = \boldsymbol{u} + \boldsymbol{v}$$

$\boldsymbol{u}$: fluid velocity, $\boldsymbol{v}$: velocity of interface

- Advective term:

$$\begin{aligned}\boldsymbol{V} \cdot \boldsymbol{\nabla}\phi &= \boldsymbol{u} \cdot \boldsymbol{\nabla}\phi + \boldsymbol{v} \cdot \boldsymbol{\nabla}\phi \\ &= \boldsymbol{u} \cdot \boldsymbol{\nabla}\phi + \boldsymbol{v} \cdot \boldsymbol{\nabla}\phi \times \frac{|\boldsymbol{\nabla}\phi|}{|\boldsymbol{\nabla}\phi|} \\ &= \boldsymbol{u} \cdot \boldsymbol{\nabla}\phi + v_n |\boldsymbol{\nabla}\phi|\end{aligned}$$

Velocity due to curvature

$v_n = \boldsymbol{v} \cdot \boldsymbol{n}_\phi$: normal velocity of interface

$$v_n = -M_\phi \kappa \tag{53}$$

Remarks

- The product is homogenous to a velocity
- Origin: curvature-driven motion
- Simplified form of AC eq 2nd member

Advected field with curvature

Transport of ϕ with Eq. (53)

$$\frac{\partial \phi}{\partial t} + \boldsymbol{u} \cdot \boldsymbol{\nabla}\phi = M_\phi \kappa |\boldsymbol{\nabla}\phi| \tag{54}$$

Objective: add a new term that cancels the 2nd member of Eq. (54)

Conservative Allen-Cahn model 1/3: counter term

Cancelling the curvature-driven motion of interface: add the counter term $-M_\phi \kappa \left|\nabla\phi\right|$

$$\frac{\partial\phi}{\partial t} + \nabla\cdot(\boldsymbol{u}\phi) = \overbrace{M_\phi\left[\nabla^2\phi - \underbrace{\frac{16}{W^2}\phi(1-\phi)(1-2\phi)}_{\text{Eq. }(51b)}\right]}^{\text{standard Allen-Cahn Eq (42) with Eq. (43)}} - \overbrace{M_\phi \underbrace{\kappa}_{\text{Eq. (48)}} \left|\nabla\phi\right|}^{\text{Counter Term}}$$

$$= M_\phi\left[\nabla^2\phi - \boldsymbol{n}\cdot\nabla\left|\nabla\phi\right| - \left|\nabla\phi\right|\nabla\cdot\boldsymbol{n}\right]$$

$$= M_\phi\left[\nabla^2\phi - \nabla\cdot\left(\underbrace{\left|\nabla\phi\right|}_{\text{Eq. (50)}}\boldsymbol{n}\right)\right]$$

$$= M_\phi\left[\nabla^2\phi - \nabla\cdot\left(\frac{4}{W}\phi(1-\phi)\boldsymbol{n}\right)\right]$$

Conservative Allen-Cahn model (CAC) or “advected field”

$$\frac{\partial\phi}{\partial t} + \nabla\cdot(\boldsymbol{u}\phi) = \nabla\cdot\left\{M_\phi\left[\nabla\phi - \frac{4}{W}\phi(1-\phi)\boldsymbol{n}_\phi\right]\right\} \tag{55}$$

Conservative Allen-Cahn model 2/3: flux $\boldsymbol{j}_{CAC}$

Transport equation

$$\partial_t \phi = -\boldsymbol{\nabla} \cdot \boldsymbol{j}_{tot} \qquad (56)$$

$$\boldsymbol{j}_{tot} = \boldsymbol{j}_{Adv} + \underbrace{\boldsymbol{j}_{diff} + \boldsymbol{j}_{CT}}_{\equiv \boldsymbol{j}_{CAC}} \qquad (57)$$

- $\boldsymbol{j}_{Adv} = \phi \boldsymbol{u}$
- $\boldsymbol{j}_{diff} = -M_\phi \boldsymbol{\nabla} \phi$ (std diffusive flux)
- $\boldsymbol{j}_{CT}$? (Counter Term)

$\boldsymbol{j}_{diff}$ at equilibrium:

$$\begin{aligned}
\boldsymbol{j}_{diff}^{eq} &= -M_\phi \boldsymbol{\nabla} \left\{ \frac{1}{2} \left[1 + \tanh\left(\frac{2s}{W} \right) \right] \right\} \\
&= -M_\phi \boldsymbol{n}_\phi \frac{\partial}{\partial s} \left\{ \frac{1}{2} \left[1 + \tanh\left(\frac{2s}{W} \right) \right] \right\} \\
&= -M_\phi \frac{4}{W} \phi^{eq} (1 - \phi^{eq}) \boldsymbol{n}_\phi
\end{aligned}$$

At equilibrium $\boldsymbol{j}_{CT}^{eq}$ cancels $\boldsymbol{j}_{diff}^{eq}$

- Counter flux: $\boldsymbol{j}_{CT}^{eq} = -\boldsymbol{j}_{diff}^{eq}$

$$\boldsymbol{j}_{CT} = +M_\phi \frac{4}{W} \phi (1 - \phi) \boldsymbol{n}_\phi$$

- Finally, $\boldsymbol{j}_{CAC}$ writes:

$$\boxed{\boldsymbol{j}_{CAC} = -M_\phi \left[\boldsymbol{\nabla} \phi - \frac{4}{W} \phi (1 - \phi) \boldsymbol{n}_\phi \right] \qquad (58)}$$

Conservative Allen-Cahn model 3/3: remarks

The Conservative Allen-Cahn model must be considered coupled with the Navier-Stokes equations. It is useful for simulations of two immiscible and incompressible fluids. Examples are given in Section 3 and extension for three phases in section 6.

Link with one particular Level-Set (LS) method: "conservative Level-Set"

- See e.g. E. Olsson & G. Kreiss JCP (2005)
- Splitting of Eq. (55) with 2 stages (adv and diff):

$$\partial_t \varphi + \boldsymbol{\nabla} \cdot (\boldsymbol{u}\varphi) = 0 \qquad (59a)$$

$$\partial_\tau \varphi + \boldsymbol{\nabla} \cdot (\varphi(1-\varphi)\boldsymbol{n}) = \epsilon \boldsymbol{\nabla} \cdot (\nabla \varphi) \qquad (59b)$$

- ϵ is equiv to W (interface width)
- Computationaly more expensive because the steady state solution of Eq. (59b) is required

Kernel function of LS is equiv to tanh solution:

$$\varphi = \frac{1}{1+\exp(-s/\epsilon)} = \frac{1}{2}\left[1+\tanh\left(\frac{s}{2\epsilon}\right)\right] = \phi^{eq}$$

Proof: set $x = s/2\epsilon$ and use def

$$\tanh(x) = \frac{e^{2x}-1}{e^{2x}+1}$$

LBM for CAC: ADE equilibrium with source term

LBM for CAC

- **LB equation**

$$g_i(\boldsymbol{x} + \boldsymbol{c}_i\delta t, t + \delta t) = g_i(\boldsymbol{x}, t) - \frac{1}{\tau_g + 1/2}\left[g_i(\boldsymbol{x}, t) - \overline{g}_i^{eq,ADE}(\boldsymbol{x}, t)\right] + \delta t \mathcal{G}_i$$

$$\overline{g}_i^{eq,ADE}(\boldsymbol{x}, t) = w_i\phi\left[1 + \frac{\boldsymbol{c}_i \cdot \boldsymbol{u}}{c_s^2}\right] - \frac{\delta t}{2}\mathcal{G}_i$$

$$\mathcal{G}_i = \frac{4}{W}\phi(1-\phi)w_i\boldsymbol{c}_i \cdot \boldsymbol{n}_\phi$$

- **Moment**

$$\phi = \sum_i g_i + \frac{\delta t}{2}\mathcal{G}_i$$

- **Mobility**

$$M_\phi = \tau_g c_s^2 \delta t$$

- **Computation of normal vector $\boldsymbol{n}_\phi = \boldsymbol{\nabla}\phi / |\boldsymbol{\nabla}\phi|$**

Directional derivatives:

$$\boldsymbol{\nabla}\phi = \frac{1}{e^2}\sum_{i=0}^{N_{pop}} w_i \boldsymbol{e}_i \left(\boldsymbol{e}_i \cdot \boldsymbol{\nabla}\phi\big|_x\right) \qquad \text{with} \qquad \boldsymbol{e}_i \cdot \boldsymbol{\nabla}\phi\big|_x = \frac{1}{2\delta x}\left[\phi(\boldsymbol{x} + \boldsymbol{e}_i\delta x) - \phi(\boldsymbol{x} - \boldsymbol{e}_i\delta x)\right]$$

Norm:

$$|\boldsymbol{\nabla}\phi| = \sqrt{(\partial_x\phi)^2 + (\partial_y\phi)^2 + (\partial_z\phi)^2}$$

V. Validations

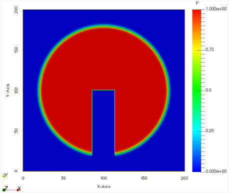
Zalesak's disk and serpentine

«Zalesak's slotted disk» 1/2: setup

Initial condition: diffusive slotted disk

$$\phi(\boldsymbol{x},0) = \frac{1}{2}\left[1+\tanh\left(\frac{R-d_c}{W\sqrt{2}}\right)\right] \qquad \text{with} \qquad d_c = \sqrt{(x-x_c)^2+(y-y_c)^2+(z-z_c)^2}$$

$$\phi(\boldsymbol{x},0) = 0 \qquad \text{if } x_c - R/6 \le x \le x_c + R/6 \text{ and } y_c - 1.1R \le y \le y_c$$



Parameters of domain
$N_x = 201$, $N_y = 201$, $N_z = 3$
$L_x = 1$, $L_y = 1$, $L_z = 0.01$
$\delta x = 5\times 10^{-3}$, $\delta t = 10^{-4}$

Parameters of initial condition
$x_c = 100$, $y_c = 100$, $z_c = 1$ (l.u.)
$W = 2$
$R = 80$ (l.u.)

Analytical expression for velocity *u*

$$u_x(x,\,y) = u_0(2y-1)$$
$$u_y(x,\,y) = u_0(1-2x)$$

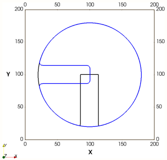
with $u_0 = 0.7853975$ (value for a full rotation of disk at $T_f = 4$)

«Zalesak's slotted disk» 2/2: comparison between CAC/CH

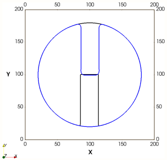
Iso $\phi = 0.5$ for several times and init cond (in black)

Allen-Cahn: lattice D3Q19, $M_\phi = 5 \times 10^{-4}$, $W = 0.03$

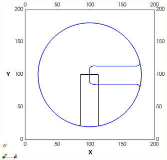
(a) $t = T_f/4$



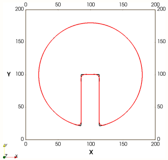
(b) $t = T_f/2$



(c) $t = 3T_f/4$

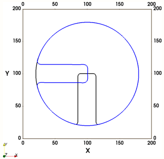


(d) $t = T_f$

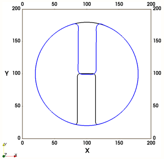


Cahn-Hilliard: lattice D3Q15, $M_\phi = 2 \times 10^{-2}$, $W = 0.015$

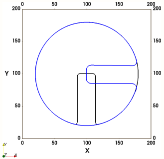
(a) $t = T_f/4$



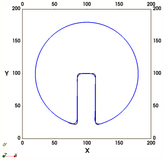
(b) $t = T_f/2$



(c) $t = 3T_f/4$



(d) $t = T_f$



Interface inside a vortex 1/2: setup

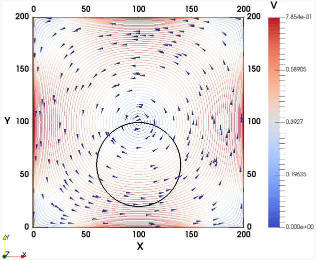
Initial condition: diffuse disk

- Initial condition

$$\phi(\boldsymbol{x},0) = \frac{1}{2}\left[1 + \tanh\left(\frac{R - d_c}{\sqrt{2W}}\right)\right]$$

with d_c defined previously

- Parameters of initial condition
$x_c = 100,\ y_c = 60,\ z_c = 1$ (l.u.)
$W = 2,\ R = 40$ (l.u.)



Imposed velocity $\boldsymbol{u}(\boldsymbol{x})$ and parameters

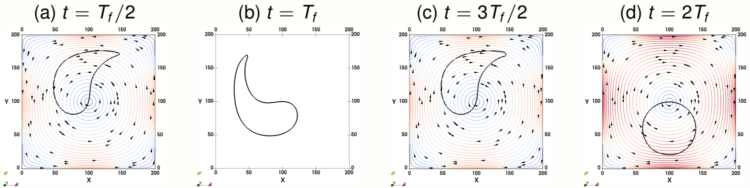
Video

$$u_x(x,\ y) = -u_0 \cos\left[\pi(x - 0.5)\right] \sin\left[\pi(y - 0.5)\right]$$
$$u_y(x,\ y) = u_0 \sin\left[\pi(x - 0.5)\right] \cos\left[\pi(y - 0.5)\right]$$

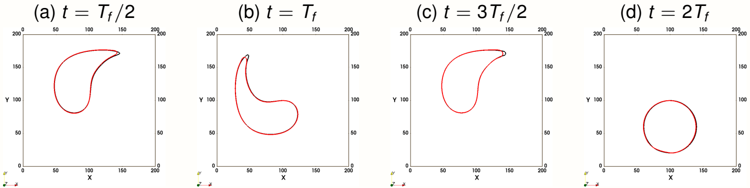
- Lattice D3Q19
- $M_\phi = 5 \times 10^{-4},\ W = 0.03,\ T_f = 4$
- $u_0 = 0.7853975$

Interface inside a vortex 2/2: comparison between CAC/CH

With $\boldsymbol{u}'(\boldsymbol{x}, t) = \boldsymbol{u}(\boldsymbol{x}) \times \cos(\pi t / 2T_f)$ for inverting the flow at T_f



Superposition Cahn-Hilliard (red) and Conservative Allen-Cahn (black)



P. Cahn-Hilliard simulation

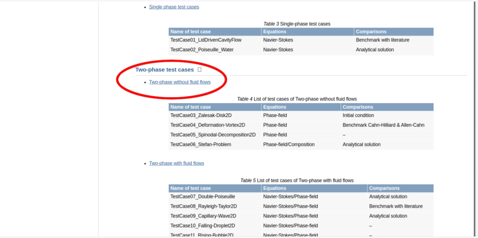
Spinodal decomposition

Return

Run spinodal decomposition

Guidelines in documentation

In page `Practice of two-phase flows`



- Single phase test cases

Table 3 Single-phase test cases

Name of test case	Equations	Comparisons
TestCase01_LidDrivenCavityFlow	Navier-Stokes	Benchmark with literature
TestCase02_Poiseuille_Water	Navier-Stokes	Analytical solution

Two-phase test cases

- Two-phase without fluid flows

Table 4 List of test cases of Two-phase without fluid flows

Name of test case	Equations	Comparisons
TestCase03_Zalesak-Disk2D	Phase-field	Initial condition
TestCase04_Deformation-Vortex2D	Phase-field	Benchmark Cahn-Hilliard & Allen-Cahn
TestCase05_Spinodal-Decomposition2D	Phase-field	–
TestCase06_Stefan-Problem	Phase-field/Composition	Analytical solution

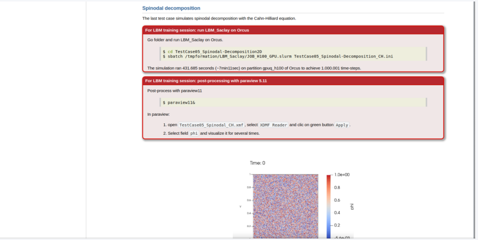
- Two-phase with fluid flows

Table 5 List of test cases of Two-phase with fluid flows

Name of test case	Equations	Comparisons
TestCase07_Double-Poiseuille	Navier-Stokes/Phase-field	Analytical solution
TestCase08_Rayleigh-Taylor2D	Navier-Stokes/Phase-field	Benchmark with literature
TestCase09_Capillary-Wave2D	Navier-Stokes/Phase-field	Analytical solution
TestCase10_Falling-Droplet2D	Navier-Stokes/Phase-field	–
TestCase11_Rising-Bubble2D	Navier-Stokes/Phase-field	–

clic on `Two-phase without fluid flow`

Go to section `Spinodal decomposition`



Spinodal decomposition

The last test case simulates spinodal decomposition with the Cahn-Hilliard equation.

For LBM training session: run LBM_Saclay on Orcus

Go folder and run LBM_Saclay on Orcus.

```
$ cd TestCase05_Spinodal-Decomposition2D
$ sbatch /tmpformation/LBM_Saclay/JOB_H100_GPU.slurm TestCase05_Spinodal-Decomposition_CH.ini
```

The simulation ran 431.685 seconds (~7min11sec) on partition gpuq_h100 of Orcus to achieve 1.000.001 time-steps.

For LBM training session: post-processing with paraview 5.11

Post-process with paraview11

```
$ paraview11&
```

In paraview:

1. open `TestCase05_Spinodal_CH.xmf`, select `XDMF Reader` and clic on green button `Apply`.
2. Select field `phi` and visualize it for several times.

copy-paste commands of red boxes

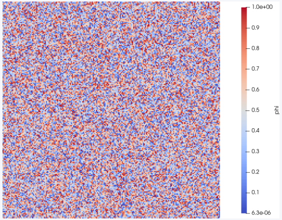
- Run one simulation
- Make a video with paraview

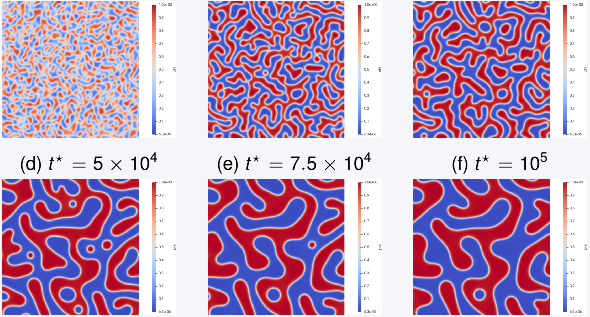
Results

With $t^\star = t/\delta t$

- Periodic boundary conditions
- Initial condition
  r random number (uniform distrib):
  $0 \leq r \leq 1$

$$\phi(\boldsymbol{x}, 0) = r, \quad \text{for all nodes}$$





(a) $t^\star = 10^3$ (b) $t^\star = 5 \times 10^3$ (c) $t^\star = 10^4$

(d) $t^\star = 5 \times 10^4$ (e) $t^\star = 7.5 \times 10^4$ (f) $t^\star = 10^5$

Conclusion of section 2

Summary in this section

- The thermodynamic formulation of interface implies:
  - Diffuse interface with a hyperbolic tangent solution at equilibrium
  - With a double-well algebraic relations for σ and W
- For time-evolution, the dynamics is described such as $d\mathscr{F}/dt \leqslant 0$
  - Cahn-Hilliard, Allen-Cahn and Conservative Allen equations were derived
  - Validations and Simulations

Notations of phase index (or order parameter) in following sections

Notations	Nb Interface	Type of interface	Double-well	Sections
ϕ	1	Fluid/Fluid	$g_1(\phi)$	3
ψ	1	Solid/Liquid	$g_3(\psi)$	4
ρ	1	Liquid/Gas	$g_2(\rho)$	5
ϕ_0, ϕ_1, ϕ_2	3	Fluid/Fluid/Fluid	$g_1(\phi)$	6
ϕ, φ, ψ	3	Liquid/Gas/Solid	$g_1(\phi)$	6

3. Two-phase flows

Coupling with incompressible Navier-Stokes

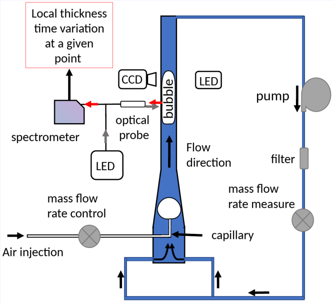
Outline section 3

One example of two-phase flows

Taylor bubble of two immiscible fluids

CEA experimental device (Saclay/ISAS/DM2S)

Air injection inside a column filled with water



Picture measured by the CCD

- Study of thin liquid film
- Applications
  - Compact heat exchanger
  - Evaporator in mini-channels

From C. Tecchio (STMF/LE2H, 2025)

Nomenclature

Main variables and parameters

Dynamic variables

Name	Math	Dim
Hydrodynamic pressure	$p_h(\boldsymbol{x}, t)$	$[E]/[L]^3$
Velocity	$\boldsymbol{u}(\boldsymbol{x}, t)$	$[L]/[T]$
Phase index	$\phi(\boldsymbol{x}, t)$	[–]
Viscous stress tensor	$\overline{\overline{\tau}}(\boldsymbol{x}, t)$	$[M]/([L].[T]^2)$

Interface parameters

Name	Math	Dim
Surface tension	σ	$[E]/[L]^2$
Interface width	W	$[L]$
Mobility coefficient of interface	M_ϕ	$[L]^2/[T]$
Curvature	κ	$1/[L]$

Bulk parameters

Bulk densities ($\Phi = A, B$)	ρ_Φ	$[M]/[L]^3$
Bulk viscosities	ν_Φ	$[L]^2/[T]$
Gravity	$\boldsymbol{g}$	$[L]/[T]^2$

Interpolate parameters

Density	$\rho(\phi)$	$[M]/[L]^3$
Kinematic viscosity	$\nu(\phi)$	$[L]^2/[T]$
Dynamic viscosity	$\eta(\phi)$	$[M]/([L].[T])$

a. Derivation of math model

Two immiscible fluids at constant temperature

Local densities of two incompressible fluids

Density of bulk phases: constant ρ_A and ρ_B

Local densities $\widetilde{\rho}_\Phi(\boldsymbol{x}, t)$

- Local densities $\tilde{\rho}_A(\boldsymbol{x}, t)$ and $\tilde{\rho}_B(\boldsymbol{x}, t)$

$$\tilde{\rho}_B(\boldsymbol{x}, t) = \rho_B \phi(\boldsymbol{x}, t)$$
$$\tilde{\rho}_A(\boldsymbol{x}, t) = (1 - \phi(\boldsymbol{x}, t))\rho_A$$

- Total density

$$\rho(\boldsymbol{x}, t) = \rho_B \phi(\boldsymbol{x},\ t) + (1 - \phi(\boldsymbol{x}, t))\rho_A$$

- Viscosity

$$\nu(\phi) = \nu_B \phi(\boldsymbol{x},\ t) + (1 - \phi(\boldsymbol{x}, t))\nu_A$$
$$\nu(\phi) = \frac{\nu_A \nu_B}{\phi(\boldsymbol{x}, t)\nu_A + (1 - \phi(\boldsymbol{x}, t))\nu_B}$$

Mass balance

- Balance on $\tilde{\rho}_A$ and $\tilde{\rho}_B$

$$\frac{\partial \tilde{\rho}_B}{\partial t} + \boldsymbol{\nabla} \cdot (\tilde{\rho}_B \boldsymbol{u} + \rho_B \boldsymbol{j}_B) = +\dot{m}''' \tag{60}$$
$$\frac{\partial \tilde{\rho}_A}{\partial t} + \boldsymbol{\nabla} \cdot (\tilde{\rho}_A \boldsymbol{u} + \rho_A \boldsymbol{j}_A) = -\dot{m}''' \tag{61}$$

- $\dot{m}'''$: source (or sink) at interface
- Hyp on fluxes

$$\boldsymbol{j}_\phi = \boldsymbol{j}_B = -\boldsymbol{j}_A$$

Mass balance and interface for one-fluid formulation

Expressed with ϕ

Eqs. (60) and (61) expressed with ϕ:

$$\frac{\partial \phi}{\partial t} + \boldsymbol{\nabla} \cdot (\boldsymbol{u}\phi + \boldsymbol{j}_\phi) = +\frac{\dot{m}'''}{\rho_B}$$
$$\frac{\partial (1-\phi)}{\partial t} + \boldsymbol{\nabla} \cdot (\boldsymbol{u}(1-\phi) - \boldsymbol{j}_\phi) = -\frac{\dot{m}'''}{\rho_A}$$

Sum

$$\boldsymbol{\nabla} \cdot \boldsymbol{u} = \dot{m}''' \left(\frac{1}{\rho_B} - \frac{1}{\rho_A} \right)$$

Material derivative

$$\boxed{\frac{d}{dt} \hat{=} \frac{\partial}{\partial t} + \boldsymbol{u} \cdot \boldsymbol{\nabla} \qquad (62)}$$

With $\dot{m}''' = 0$

- Mass balance

$$\boldsymbol{\nabla} \cdot \boldsymbol{u} = 0$$

- Interface tracking

$$\frac{\partial \phi}{\partial t} + \boldsymbol{\nabla} \cdot (\boldsymbol{u}\phi) = -\boldsymbol{\nabla} \cdot \boldsymbol{j}_\phi$$

  - where $\boldsymbol{j}_\phi$ to be determined
  - With material derivative Eq. (62)

$$\frac{\partial \phi}{\partial t} + \boldsymbol{u} \cdot \boldsymbol{\nabla}\phi + \phi \boldsymbol{\nabla} \cdot \boldsymbol{u} = -\boldsymbol{\nabla} \cdot \boldsymbol{j}_\phi$$
$$\frac{d\phi}{dt} + \phi \boldsymbol{\nabla} \cdot \boldsymbol{u} = -\boldsymbol{\nabla} \cdot \boldsymbol{j}_\phi$$

Total energy $\mathscr{E}_{tot}$ with ϕ and $\boldsymbol{u}$

Previously: minimization of global free energy

$$\mathscr{F}[\phi] = \int_V \mathcal{F}(\phi, \nabla\phi) dV \qquad (63)$$

In section 2: determination of $\boldsymbol{j}_\phi$ such as $d\mathscr{F}/dt \leqslant 0$

Now: total energy $\mathscr{E}_{tot}$ with new variable $\boldsymbol{u}$

$$\mathscr{E}_{tot}[\phi, \boldsymbol{u}] = \int_V \left[\underbrace{\frac{1}{2}\rho_0 |\boldsymbol{u}|^2}_{\text{kinetic energy}} + \underbrace{\mathcal{F}(\phi, \nabla\phi)}_{\text{potential energy}} \right] dV \qquad (64)$$

$$\mathcal{F}(\phi, \nabla\phi) = f_{dw}(\phi) + \frac{\zeta}{2}|\nabla\phi|^2 \qquad (65)$$

- $\rho_0 |\boldsymbol{u}|^2/2$: kinetic energy
- $f_{dw}(\phi)$ is the double-well
- ρ_0: constant density
- ζ is a constant parameter

Objective: derivation of constitutive laws $\overline{\overline{\boldsymbol{T}}}$ and $\boldsymbol{j}_\phi$

Balance equations

$$\frac{d\rho_0}{dt} = -\rho_0 \nabla \cdot \boldsymbol{u} \qquad (66)$$

$$\rho_0 \frac{d\boldsymbol{u}}{dt} = \nabla \cdot \overline{\overline{\boldsymbol{T}}} \qquad (67)$$

$$\frac{d\phi}{dt} + \phi \nabla \cdot \boldsymbol{u} = -\nabla \cdot \boldsymbol{j}_\phi \qquad (68)$$

Objective

Determine the constitutive laws $\boldsymbol{j}_\phi$ and $\overline{\overline{\boldsymbol{T}}}$ such as

$$\frac{d\mathscr{E}_{tot}}{dt} - \int_V \underbrace{\lambda \nabla \cdot \boldsymbol{u}}_{\hat{=}\mathscr{L}} \leqslant 0$$

λ: lagrange multiplier of constraint $\nabla \cdot \boldsymbol{u} = 0$

Method

Express

$$\frac{d\mathscr{E}_{tot}}{dt} = \frac{d}{dt} \int_V \left[\mathcal{F}(\phi, \nabla\phi) + \frac{1}{2}\rho_0 |\boldsymbol{u}|^2 \right] dV$$

on the form

$$\frac{d\mathscr{E}_{tot}}{dt} = -\mathcal{D}(V) + \underbrace{\mathcal{W}(V) + \Phi(\partial V)}_{\text{neglected here}} \leqslant 0$$

- $\mathcal{D}$: dissipation with $\mathcal{D} \geqslant 0$
- $\mathcal{W}$: work of external forces
- Φ: Flux through surface

Methodology 1/2: Reynolds transport theorem

Reynolds transport theorem for Ψ

$$\frac{d}{dt}\left[\int_V \Psi dV\right] \triangleq \int_V \left[\frac{d\Psi}{dt} + \Psi\nabla\cdot\boldsymbol{u}\right] dV \tag{69}$$

Example with Eq. (64)

$$\begin{aligned}
\frac{d\mathscr{E}_{tot}}{dt} &= \frac{d}{dt}\int_V \left[\mathcal{F}(\phi,\nabla\phi) + \frac{1}{2}\rho_0\left|\boldsymbol{u}\right|^2\right] dV\\
&= \int_V \left\{\frac{d}{dt}\left[\mathcal{F} + \frac{1}{2}\rho_0\left|\boldsymbol{u}\right|^2\right] + \left[\mathcal{F} + \frac{1}{2}\rho_0\left|\boldsymbol{u}\right|^2\right]\nabla\cdot\boldsymbol{u}\right\} dV\\
&= \int_V \left\{\left[\frac{d\mathcal{F}}{dt} + \mathcal{F}\nabla\cdot\boldsymbol{u}\right] + \left[\cancel{\frac{1}{2}\frac{d\rho_0}{dt}\left|\boldsymbol{u}\right|^2} + \frac{1}{2}\rho_0\frac{d\left|\boldsymbol{u}\right|^2}{dt} + \cancel{\frac{1}{2}\rho_0\left|\boldsymbol{u}\right|^2\nabla\cdot\boldsymbol{u}}\right]\right\}dV
\end{aligned}$$

$$\frac{d\mathscr{E}_{tot}}{dt} = \int_V \left\{\underbrace{\left[\frac{d\mathcal{F}}{dt} + \mathcal{F}\nabla\cdot\boldsymbol{u}\right]}_{\triangleq\mathcal{I}} + \underbrace{\frac{1}{2}\rho_0\frac{d\left|\boldsymbol{u}\right|^2}{dt}}_{\triangleq\mathcal{K}}\right\}dV \tag{70}$$

- Make appear balance equations in $\mathcal{I}$ and $\mathcal{K}$
- Evaluation of differentials
  - $d\mathcal{F}$
  - $d\left|\boldsymbol{u}\right|^2$

Methodology 2/2: differentials

Term $\mathcal{I}$: differential of free energy density $\mathcal{F}$

- Differential

$$d\mathcal{F}(\phi, \boldsymbol{\nabla}\phi) = \frac{\partial \mathcal{F}}{\partial \phi} d\phi + \underbrace{\frac{\partial \mathcal{F}}{\partial(\boldsymbol{\nabla}\phi)}}_{\triangleq \boldsymbol{\mathcal{F}}} \cdot d(\boldsymbol{\nabla}\phi)$$

- Divide by dt:

$$\frac{d\mathcal{F}(\phi, \boldsymbol{\nabla}\phi)}{dt} = \frac{\partial \mathcal{F}}{\partial \phi} \underbrace{\frac{d\phi}{dt}}_{\text{Eq. (68)}} + \boldsymbol{\mathcal{F}} \cdot \underbrace{\frac{d(\boldsymbol{\nabla}\phi)}{dt}}_{\text{re-write}} \tag{71}$$

- Replace $d\phi/dt$ by Eq. (68) and re-write $d(\boldsymbol{\nabla}\rho)/dt$ (next slide)

Term $\mathcal{K}$ kinetic energy: use impulsion balance Eq. (67)

$$\frac{1}{2}\rho_0 \frac{d|\boldsymbol{u}|^2}{dt} = \rho_0 \boldsymbol{u} \cdot \frac{d\boldsymbol{u}}{dt} = \boldsymbol{u} \cdot \boldsymbol{\nabla} \cdot \overline{\overline{\boldsymbol{T}}}$$

Algebraic tricks for calculations 1/2

Algebraic calculation: usual tips and tricks

- Trick 1

$$f\nabla g = \nabla(fg) - g\nabla f \tag{72}$$

- Trick 2

$$f\nabla f = \frac{1}{2}\nabla f^2 \tag{73}$$

- Chain rule

$$\nabla f(\phi) = \frac{\partial f}{\partial \phi}\nabla\phi = f'(\phi)\nabla\phi \tag{74}$$

- Use of index notations

Example 1

$$\mu_\phi \nabla\phi = \nabla f_{dw} - \zeta\nabla^2\phi\nabla\phi \tag{75}$$

Demo

$$\begin{aligned}\mu_\phi \nabla\phi &= \left[\partial_\phi f_{dw} - \zeta\nabla^2\phi\right]\nabla\phi \\ &= \underbrace{\partial_\phi f_{dw}\nabla\phi}_{\text{chain rule}} - \zeta\nabla^2\phi\nabla\phi \\ &= \nabla f_{dw} - \zeta\nabla^2\phi\nabla\phi\end{aligned}$$

Example 2

$$\nabla\cdot(\nabla\phi\otimes\nabla\phi) = \frac{1}{2}\nabla\left(|\nabla\phi|^2\right) + (\nabla^2\phi)\nabla\phi \tag{76}$$

Demo

$$\begin{aligned}\partial_\beta(\partial_\alpha\phi\partial_\beta\phi) &= (\underbrace{\partial_\beta\partial_\alpha}_{\text{intervert}}\phi)(\partial_\beta\phi) + (\partial_\alpha\phi)(\partial^2_{\beta\beta}\phi) \\ &= \underbrace{[\partial_\alpha(\partial_\beta\phi)](\partial_\beta\phi)}_{\text{form } f\nabla f = \nabla f^2/2} + (\partial_\alpha\phi)(\partial^2_{\beta\beta}\phi) \\ &= \partial_\alpha(\partial_\beta\phi)^2/2 + (\partial_\alpha\phi)(\partial^2_{\beta\beta}\phi)\end{aligned}$$

Algebraic tricks for calculations 2/2

Relation 1

$$\boxed{\frac{d}{dt}(\nabla\phi) = \nabla\left(\frac{d\phi}{dt}\right) - (\nabla\boldsymbol{u})(\nabla\phi)} \qquad (77)$$

Demo

$$\begin{aligned}
\frac{d}{dt}(\nabla\phi) &= \frac{d}{dt}(\partial_\alpha\phi) \\
&= (\partial_t + u_\beta\partial_\beta)(\partial_\alpha\phi) \\
&= \underbrace{\partial_t(\partial_\alpha\,\phi)}_{\text{intervert}} + u_\beta\,\underbrace{\partial_\beta(\partial_\alpha\,\phi)}_{\text{intervert}} \\
&= \partial_\alpha(\partial_t\phi) + \underbrace{u_\beta\partial_\alpha(\partial_\beta\phi)}_{\text{trick}} \\
&= \partial_\alpha(\partial_t\phi) + \partial_\alpha[u_\beta(\partial_\beta\phi)] - (\partial_\alpha u_\beta)(\partial_\beta\phi) \\
&= \partial_\alpha[(\partial_t\phi) + u_\beta(\partial_\beta\phi)] - (\partial_\alpha u_\beta)(\partial_\beta\phi) \\
&= \nabla\left(\frac{d\phi}{dt}\right) - (\nabla\boldsymbol{u})(\nabla\phi)
\end{aligned}$$

Remark: 2nd term of Eq. (71)

$$\boxed{\boldsymbol{\mathcal{F}}\cdot\frac{d}{dt}(\nabla\phi) = \boldsymbol{\mathcal{F}}\cdot\nabla\left(\frac{d\phi}{dt}\right) - \boldsymbol{\mathcal{F}}\otimes\nabla\phi : \nabla\boldsymbol{u}} \qquad (78)$$

Demo (use Eq. (77))

$$\begin{aligned}
\boldsymbol{\mathcal{F}}\cdot\frac{d}{dt}(\nabla\phi) &= \boldsymbol{\mathcal{F}}\cdot\nabla\left(\frac{d\phi}{dt}\right) - \mathcal{F}_\alpha(\partial_\alpha u_\beta)(\partial_\beta\phi) \\
&= \boldsymbol{\mathcal{F}}\cdot\nabla\left(\frac{d\phi}{dt}\right) - \underbrace{\mathcal{F}_\alpha(\partial_\beta\phi)}_{\equiv\boldsymbol{\mathcal{F}}\otimes\nabla\phi}\,\underbrace{(\partial_\alpha u_\beta)}_{\equiv\nabla\boldsymbol{u}}
\end{aligned}$$

Relation 2

$$\boxed{\nabla\cdot\boldsymbol{u} = \bar{\bar{\boldsymbol{I}}} : \nabla\boldsymbol{u}} \qquad (79)$$

Demo

$$\begin{aligned}
\bar{\bar{\boldsymbol{I}}} : \nabla\boldsymbol{u} &= \delta_{\alpha\beta}\partial_\alpha u_\beta \\
&= \partial_\alpha(u_\beta\delta_{\alpha\beta}) - u_\beta\cancel{\partial_\alpha\delta_{\alpha\beta}} \\
&= \partial_\alpha u_\alpha
\end{aligned}$$

Derivation 1/3

Terms $\mathcal{I}$ and $\mathcal{K}$ of Eq. (70)

$$\int_V \mathcal{I} dV = \int_V \left[\frac{\partial \mathcal{F}}{\partial \phi} \frac{d\phi}{dt} + \underbrace{\boldsymbol{\mathcal{F}} \cdot \boldsymbol{\nabla} \left(\frac{d\phi}{dt} \right)}_{\text{integration by parts}} - \boldsymbol{\mathcal{F}} \otimes \boldsymbol{\nabla}\phi : \boldsymbol{\nabla} \boldsymbol{u} + \mathcal{F} \boldsymbol{\nabla} \cdot \boldsymbol{u} \right] dV \tag{80}$$

$$\int_V (\mathcal{K} + \mathscr{L}) dV = \int_V \underbrace{[\boldsymbol{u} \cdot \boldsymbol{\nabla} \cdot \overline{\overline{\boldsymbol{T}}}]}_{\text{ibp}} - [\lambda \boldsymbol{\nabla} \cdot \boldsymbol{u}] dV \tag{81}$$

Results of integration by parts

$$\int_V \left[\boldsymbol{\mathcal{F}} \cdot \boldsymbol{\nabla} \left(\frac{d\phi}{dt} \right) \right] dV = \int_{\partial V} \frac{d\phi}{dt} \boldsymbol{\mathcal{F}} \cdot \boldsymbol{n} d(\partial V) - \int_V \boldsymbol{\nabla} \cdot \boldsymbol{\mathcal{F}} \frac{d\phi}{dt} dV$$

$$- \int_V \frac{\partial \mathcal{F}}{\partial \phi} \boldsymbol{\nabla} \cdot \boldsymbol{j}_\phi dV = - \int_{\partial V} \frac{\partial \mathcal{F}}{\partial \phi} \boldsymbol{j}_\phi \cdot \boldsymbol{n} d(\partial V) + \int_V \boldsymbol{j}_\phi \cdot \boldsymbol{\nabla} \left(\frac{\partial \mathcal{F}}{\partial \phi} \right) dV$$

$$\int_V \boldsymbol{u} \cdot \boldsymbol{\nabla} \cdot \overline{\overline{\boldsymbol{T}}} dV = \int_{\partial V} \boldsymbol{u} \cdot \overline{\overline{\boldsymbol{T}}} \boldsymbol{n} d(\partial V) - \int_V \overline{\overline{\boldsymbol{T}}} : \boldsymbol{\nabla} \boldsymbol{u} dV$$

Hyp: all $\int_{\partial V} d(\partial V)$ terms are neglected

Derivation 2/3

Group terms $\cdot\nabla\mu_\phi$ and $:\nabla \boldsymbol{u}$

Sum Eq. (80)+Eq. (81)

$$\int_V (\mathcal{I}+\mathcal{K}+\mathcal{L})dV = \int_V \left\{ \underbrace{\left[\frac{\partial \mathcal{F}}{\partial \phi} - \nabla\cdot\boldsymbol{\mathcal{F}}\right]}_{\equiv \mu_\phi} \underbrace{\frac{d\phi}{dt}}_{\text{Eq. (68)}} - \boldsymbol{\mathcal{F}}\otimes\nabla\phi : \nabla\boldsymbol{u} + \mathcal{F}\nabla\cdot\boldsymbol{u} - \overline{\overline{\boldsymbol{T}}} : \nabla\boldsymbol{u} - \lambda\nabla\cdot\boldsymbol{u} \right\} dV$$

$$= \int_V \left\{ \mu_\phi \left[-\phi\nabla\cdot\boldsymbol{u} - \nabla\cdot\boldsymbol{j}_\phi \right] - \boldsymbol{\mathcal{F}}\otimes\nabla\phi : \nabla\boldsymbol{u} + \mathcal{F}\nabla\cdot\boldsymbol{u} - \overline{\overline{\boldsymbol{T}}} : \nabla\boldsymbol{u} - \lambda\nabla\cdot\boldsymbol{u} \right\} dV$$

$$= \int_V \left\{ (-\mu_\phi\phi + \mathcal{F} - \lambda) \underbrace{\nabla\cdot\boldsymbol{u}}_{\text{Eq. (79)}} - \left[\boldsymbol{\mathcal{F}}\otimes\nabla\phi + \overline{\overline{\boldsymbol{T}}} \right] : \nabla\boldsymbol{u} - \mu_\phi\nabla\cdot\boldsymbol{j}_\phi \right\} dV$$

$$= \int_V \left\{ \left[(-\mu_\phi\phi + \mathcal{F} - \lambda)\overline{\overline{\boldsymbol{I}}} - \boldsymbol{\mathcal{F}}\otimes\nabla\phi - \overline{\overline{\boldsymbol{T}}} \right] : \nabla\boldsymbol{u} - \underbrace{\mu_\phi\nabla\cdot\boldsymbol{j}_\phi}_{\text{ibp}} \right\} dV$$

$$= -\int_V \left\{ \left[\underbrace{(\mu_\phi\phi - \mathcal{F} + \lambda)\overline{\overline{\boldsymbol{I}}} + \boldsymbol{\mathcal{F}}\otimes\nabla\phi + \overline{\overline{\boldsymbol{T}}}}_{\overline{\overline{\boldsymbol{T}}} \text{ def such as } = -\overline{\overline{\boldsymbol{P}}} + \overline{\overline{\boldsymbol{\tau}}}} \right] : \nabla\boldsymbol{u} dV + \int_V \underbrace{\boldsymbol{j}_\phi\cdot\nabla\mu_\phi}_{\boldsymbol{j}_\phi \text{ def such as } \propto -\nabla\mu_\phi} dV$$

Derivation 3/3

Appropriate choice of $\boldsymbol{j}_\phi$ and $\overline{\overline{\boldsymbol{T}}}$

$$\boldsymbol{j}_\phi = -\mathcal{M}_\phi \boldsymbol{\nabla}\mu_\phi$$

$$\overline{\overline{\boldsymbol{T}}} = -\overline{\overline{\boldsymbol{P}}} + \overline{\overline{\boldsymbol{\tau}}}$$

$$\overline{\overline{\boldsymbol{\tau}}} = \eta(\boldsymbol{\nabla}\boldsymbol{u} + \boldsymbol{\nabla}\boldsymbol{u}^T)$$

Tensor pressure $\overline{\overline{\boldsymbol{P}}}$ and hydrodynamic pressure p_h

$$\overline{\overline{\boldsymbol{P}}} = (p_h - \mathcal{F})\overline{\overline{\boldsymbol{I}}} - \boldsymbol{\mathcal{F}} \otimes \boldsymbol{\nabla}\phi$$

$$p_h = \lambda + \phi\mu_\phi$$

are appropriate constitutive laws such as the dissipation is positive

$$\mathcal{D} = \int_V \overline{\overline{\boldsymbol{T}}} : \boldsymbol{\nabla}\boldsymbol{u} dV - \int_V \boldsymbol{j}_\phi \cdot \boldsymbol{\nabla}\mu_\phi dV \geqslant 0$$

Remarks

- $\overline{\overline{\boldsymbol{\tau}}}$: viscous stress tensor is such as $\overline{\overline{\boldsymbol{\tau}}} : \boldsymbol{\nabla}\boldsymbol{u} \geqslant 0$
- External force $\rho\boldsymbol{g}$ could have been considered and set in $\mathcal{W}(V)$
- If the integrals of surface are not neglected they must be considered in $\Phi(\partial V)$

Expressions of $\overline{\overline{\boldsymbol{T}}}$ and $\boldsymbol{j}_\phi$ with $\mathcal{F}$ defined by Eq. (65)

With $\mathcal{F}$ defined by Eq. (65): $\mathcal{F} = \zeta\boldsymbol{\nabla}\phi$

$$\mu_\phi = f'_{dw}(\phi) - \zeta\boldsymbol{\nabla}^2\phi \tag{82}$$

$$\boldsymbol{j}_\phi = -\mathcal{M}_\phi\boldsymbol{\nabla}\mu_\phi \tag{83}$$

$$\overline{\overline{\boldsymbol{T}}} = -\overline{\overline{\boldsymbol{P}}} + \eta(\boldsymbol{\nabla}\boldsymbol{u} + \boldsymbol{\nabla}\boldsymbol{u}^T) \tag{84}$$

$$\overline{\overline{\boldsymbol{P}}} = \left[(p_h - \mathcal{F})\overline{\overline{\boldsymbol{I}}} + \zeta\boldsymbol{\nabla}\phi\otimes\boldsymbol{\nabla}\phi\right] \tag{85}$$

Potential form of pressure tensor $\overline{\overline{\boldsymbol{P}}}$ (use Eq. (76))

$$\boxed{-\boldsymbol{\nabla}\cdot\overline{\overline{\boldsymbol{P}}} = -\boldsymbol{\nabla}p_h + \mu_\phi\boldsymbol{\nabla}\phi} \tag{86}$$

- $\overline{\overline{\boldsymbol{P}}}$: pressure tensor
- p_h: hydrodynamic pressure
- $\mu_\phi\boldsymbol{\nabla}\phi$: capillary force

$$\begin{aligned}
-\boldsymbol{\nabla}\cdot\overline{\overline{\boldsymbol{P}}} &= -\boldsymbol{\nabla}p_h + \boldsymbol{\nabla}\mathcal{F} - \zeta\boldsymbol{\nabla}\cdot(\boldsymbol{\nabla}\phi\otimes\boldsymbol{\nabla}\phi) \\
&= -\boldsymbol{\nabla}p_h + \boldsymbol{\nabla}\left[f_{dw} + \frac{\zeta}{2}|\boldsymbol{\nabla}\phi|^2\right] - \zeta\boldsymbol{\nabla}\cdot(\boldsymbol{\nabla}\phi\otimes\boldsymbol{\nabla}\phi) \\
&= -\boldsymbol{\nabla}p_h + \boldsymbol{\nabla}f_{dw} + \cancel{\frac{\zeta}{2}\boldsymbol{\nabla}(|\boldsymbol{\nabla}\phi|^2)} - \cancel{\frac{\zeta}{2}\boldsymbol{\nabla}(|\boldsymbol{\nabla}\phi|^2)} - \zeta(\boldsymbol{\nabla}^2\phi)\boldsymbol{\nabla}\phi \\
&= -\boldsymbol{\nabla}p_h + \underbrace{\left[f'_{dw} - \zeta(\boldsymbol{\nabla}^2\phi)\right]}_{\equiv\mu_\phi}\boldsymbol{\nabla}\phi
\end{aligned}$$

Navier-Stokes/Cahn-Hilliard for binary fluids

See for example D. JACQMIN JCP (1999)

Incompressible Navier-Stokes (iNS)

$$\nabla \cdot \boldsymbol{u} = 0 \tag{87}$$

$$\underbrace{\rho(\phi)\left[\frac{\partial \boldsymbol{u}}{\partial t} + \nabla \cdot (\boldsymbol{u}\boldsymbol{u})\right]}_{\text{Acceleration}} = \underbrace{-\nabla p_h}_{\text{Pressure force}} + \underbrace{\nabla \cdot \left[\rho(\phi)\nu(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T)\right]}_{\text{Viscous force}} + \underbrace{\mu_\phi \nabla \phi}_{\text{Capillary force } \boldsymbol{F}_c} + \underbrace{\rho(\phi)\boldsymbol{g}}_{\text{Buoyancy}} \tag{88}$$

Cahn-Hilliard with advection

$$\frac{\partial \phi}{\partial t} + \underbrace{\nabla \cdot (\phi \boldsymbol{u})}_{\text{Advective term}} = \underbrace{M_\phi \nabla^2 \mu_\phi}_{\text{"Diffusive" term}} \tag{89}$$

$$\mu_\phi = \frac{3}{2}\sigma\left[\frac{16}{W}\phi(1-\phi)(1-2\phi) - W\nabla^2\phi\right] \tag{90}$$

Interpretation of term $\mu_\phi \nabla \phi$: capillary force

$\boldsymbol{F}_c$ contains σ, κ and $\boldsymbol{n}_\phi = \nabla\phi / |\nabla\phi|$

$$\boldsymbol{F}_c = \mu_\phi \nabla \phi = -\delta_d \sigma \kappa \boldsymbol{n}_\phi$$

$$\delta_d \equiv \delta_d(\phi) = \frac{3}{2} W |\nabla \phi|^2$$

$\sigma\kappa\boldsymbol{n}_\phi$ is spread over δ_d prop to interface thickness W

Demo using Eq. for μ_ϕ

$$\boldsymbol{F}_c = \mu_\phi \nabla \phi = \Big[4 \underbrace{H}_{\text{Eq. (91)}} \phi(\phi-1)(\phi-1/2) - \underbrace{\zeta}_{\text{Eq. (92)}} \nabla^2\phi \Big] \nabla \phi$$

$$= -\frac{3}{2} W\sigma \underbrace{\left[\Delta\phi - \frac{16}{W^2}\phi(1-\phi)(1-2\phi) \right]}_{\kappa|\nabla\phi| \text{ Eq (93)}} \nabla\phi$$

$$= -\frac{3}{2} W\sigma\kappa |\nabla\phi| \nabla\phi$$

$$= -\delta_d(\phi)\sigma\kappa\boldsymbol{n}_\phi \qquad \text{with } \delta_d = \frac{3}{2} W |\nabla\phi|^2$$

See BRACKBILL *et al*, JCP (1992) (Continuous Surface tension Force)

We can check that

- Thermo coefficients

$$H = 12\frac{\sigma}{W} \tag{91}$$

$$\zeta = \frac{3}{2} W\sigma \tag{92}$$

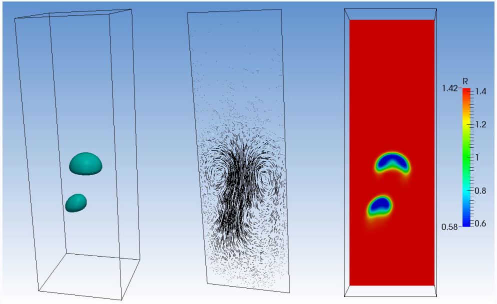
- Curvature

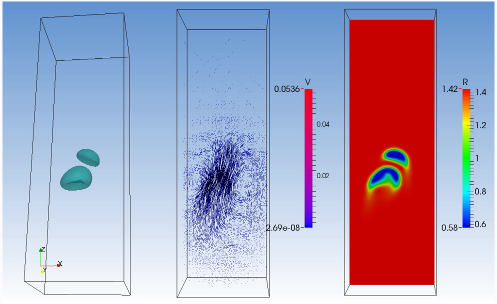
$$\begin{aligned} \kappa|\nabla\phi| &= (\nabla\cdot\boldsymbol{n})|\nabla\phi| \\ &= \nabla\cdot(|\nabla\phi|\boldsymbol{n}) - \boldsymbol{n}\cdot\nabla|\nabla\phi| \\ &= \nabla\cdot\left(\cancel{|\nabla\phi|}\frac{\nabla\phi}{\cancel{|\nabla\phi|}}\right) - \boldsymbol{n}\cdot\nabla|\nabla\phi| \\ &= \Delta\phi - \frac{16\phi}{W^2}(1-\phi)(1-2\phi) \end{aligned} \tag{93}$$

Illustration of Navier-Stokes/Cahn-Hilliard model

Simulation of model Eqs. (87)–(90)

Rising bubbles inside a channel





Video Video

NS/Conservative Allen-Cahn for immiscible fluids

See P.-H. CHIU & Y.-T. LIN JCP (2011)

Incompressible Navier-Stokes (unchanged)

$$\nabla \cdot \boldsymbol{u} = 0 \tag{94}$$

$$\rho(\phi)\left[\frac{\partial \boldsymbol{u}}{\partial t} + \nabla \cdot (\boldsymbol{u}\boldsymbol{u})\right] = -\nabla p_h + \nabla \cdot \left[\rho(\phi)\nu(\phi)\left(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T\right)\right] + \mu_\phi \nabla \phi + \rho(\phi)\boldsymbol{g} \tag{95}$$

$$\mu_\phi = \frac{3}{2}\sigma\left[\frac{16}{W}\phi(1-\phi)(1-2\phi) - W\nabla^2\phi\right] \tag{96}$$

Conservative Allen-Cahn (or levelset)

$$\frac{\partial \phi}{\partial t} + \nabla \cdot (\boldsymbol{u}\phi) = \nabla \cdot \left[M_\phi\left(\nabla \phi - \frac{4}{W}\phi(1-\phi)\boldsymbol{n}_\phi\right)\right] \tag{97}$$

$$\boldsymbol{n}_\phi = \frac{\nabla \phi}{|\nabla \phi|} \tag{98}$$

Capillarity and gravity

Capillary length ℓ_c

Determination of ℓ_c:

- Capillary pressure: $p_c = \sigma/\ell_c$
- Hydrostatic pressure: $p_h = \rho g \ell_c$
- ℓ_c is the particular length such as $p_c = p_h$ (equilibrium)

Capillary length:

$$\boxed{\ell_c \triangleq \sqrt{\frac{\sigma}{\rho g}}} \qquad (99)$$

- σ: surface tension
- g: gravity
- ρ: density

For one system of size L (e.g. bubble diameter $\equiv D$ or wavelength $\equiv \lambda$):

- If $L < \ell_c \rightarrow p_h < p_c$: capillary effects dominate and gravity is negligible
- If $L > \ell_c \rightarrow p_h > p_c$: gravity regime

We also define its inverse:

$$\boxed{k_c \triangleq \frac{1}{\ell_c} = \sqrt{\frac{\rho g}{\sigma}}}$$

Application: see Rayleigh-Taylor instability (see next slides)

Dimensionless number involving σ 1/2: Bond (or Eötvös)

Bond number

First method

$$\text{Bo} = \frac{\Delta p_h}{\Delta p_c} = \frac{\rho g(2R)}{2\sigma/R} = \frac{\rho g R^2}{\sigma}$$

- Δp_h: difference of hydrostatic pressure
- Δp_c: difference of capillary pressure

Second method

$$\text{Bo} = \frac{L^2}{\ell_c^2} = \frac{L^2}{\sigma/\rho g} = \frac{\rho g L^2}{\sigma}$$

- ℓ_c: capillary length $\sqrt{\sigma/\rho g}$
- L: characteristic length (e.g. radius R)

Nomenclature

- σ: surface tension $[\text{E}]/[\text{L}]^2 = [\text{M}]/[\text{T}]^2$
- ρ: density $[\text{M}]/[\text{L}]^3$
- or $\Delta\rho$: diff of density $[\text{M}]/[\text{L}]^3$
- g: gravity $[\text{L}]/[\text{T}]^2$
- L: characteristic length [L]
- R: bubble radius [L]

Dimensionless number involving σ 2/2: We, Ca, La, Oh, Mo

Weber number

$$\mathrm{We} = \frac{\rho U^2 L}{\sigma}$$

- U: characteristic velocity

Capillary number

$$\mathrm{Ca} = \frac{\mathrm{We}}{\mathrm{Re}} = \frac{\rho U^2 L/\sigma}{UL/\nu} = \frac{\eta U}{\sigma}$$

- η: dynamic viscosity

Laplace number

$$\mathrm{La} = \frac{\sigma L \rho}{\eta^2}$$

Ohnesorge number

$$\mathrm{Oh} = \frac{1}{\sqrt{\mathrm{La}}} = \frac{\eta}{\sqrt{\sigma L \rho}}$$

Froude number

$$\mathrm{Fr} = \frac{U}{\sqrt{gL}}$$

Morton number

$$\mathrm{Mo} = \frac{\mathrm{We}^3}{\mathrm{Fr}^2\mathrm{Re}^4} = \frac{gL\left(\rho U^2 L/\sigma\right)^3}{U^2(\rho UL/\eta)^4} = \frac{g\eta^4}{\rho\sigma^3}$$

b. Validations

Static and dynamic test cases

V. Static validations

Double-Poiseuille and Laplace law

Comparison with Double-Poiseuille analytical solution

Analytical solution with viscosity ratio η_A and η_B

$$u_x(y) = \begin{cases} \frac{Gh^2}{2\eta_A}\left[-\left(\frac{y}{h}\right)^2 - \frac{y}{h}\left(\frac{\eta_A-\eta_B}{\eta_A+\eta_B}\right) + \frac{2\eta_A}{\eta_A+\eta_B}\right] & \text{if } 0 \leq y \leq h \\ \frac{Gh^2}{2\eta_B}\left[-\left(\frac{y}{h}\right)^2 - \frac{y}{h}\left(\frac{\eta_A-\eta_B}{\eta_A+\eta_B}\right) + \frac{2\eta_B}{\eta_A+\eta_B}\right] & \text{if } -h \leq y \leq 0 \end{cases}$$

Numerical LBM (mesh $101 \times 101 \times 3$)

- BC periodic and «no slip» top and bottom
- Force term $\boldsymbol{F} = G\boldsymbol{i}$ with:

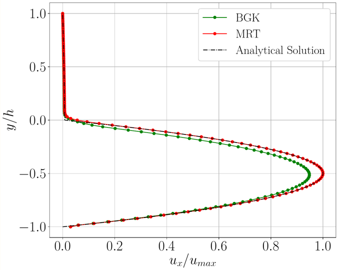
$$G = \frac{u_c}{h^2}(\eta_A + \eta_B) \text{ and } u_c = 5 \times 10^{-5}$$

- Interpolation of viscosity:

$$\eta(\phi) = \frac{\eta_A\eta_B}{\phi(\boldsymbol{x},t)\eta_A + (1-\phi(\boldsymbol{x},t))\eta_B}$$

- $\rho_A = \rho_B = 1$
- IC for Allen-Cahn : $\phi(\boldsymbol{x},0) = \frac{1}{2}\left[\tanh\left(\frac{y_0-y}{\xi}\right)\right]$

From C. Méjanès

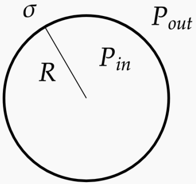


Laplace's law

Laplace's law

Spherical droplet of

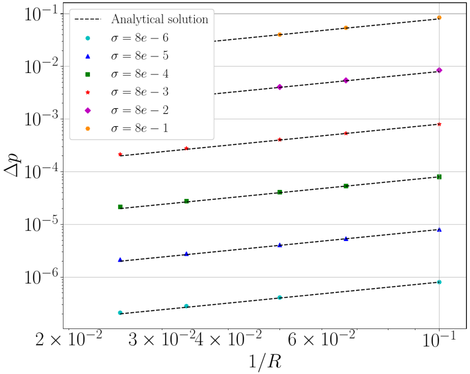
- Radius R
- Surface tension σ



Laplace's law

$$\underbrace{P_{in} - P_{out}}_{\Delta P} = \frac{2\sigma}{R}$$

`LBM_Saclay` simulations



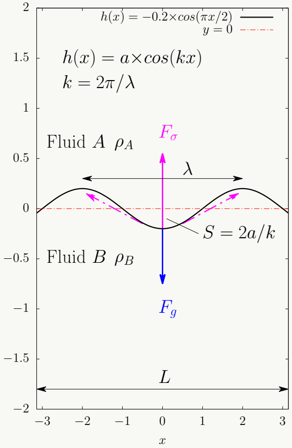
V. Dynamic validations

Rayleigh-Taylor instability and capillary wave

Return

Physical analysis of Rayleigh-Taylor instability

Competition between F_g and F_σ



Height of interface ($hyp. h_0 = 0$)

$$h(x) = h_0 + a\cos(kx) \tag{100}$$

Wave number k

$$k = \frac{2\pi}{\lambda} \tag{101}$$

$\Delta F = F_\sigma - F_g$ with $\Delta\rho = \rho_A - \rho_B$

$$\Delta F = \frac{\lambda a^2}{4}\sigma\left[k^2 - \frac{\Delta\rho g}{\sigma}\right] \tag{102}$$

Proof see next slide

Derivation of Eq. (102)

Forces

$$\Delta F = \underbrace{\int_0^\lambda \sigma(ds - dx)}_{F_\sigma} - \underbrace{\int_0^\lambda \frac{1}{2}\Delta\rho g h^2(x) dx}_{F_g}$$

$$= \frac{1}{2}a^2 \int_0^\lambda \left[\sigma k^2 \sin^2(kx) - \Delta\rho g \cos^2(kx)\right] dx$$

$$= \frac{a^2}{2}\int_0^\lambda \left[(\sigma k^2 + \Delta\rho g)\sin^2(kx) - \Delta\rho g\right] dx$$

$$= \frac{\lambda a^2}{4}\left[\sigma k^2 - \Delta\rho g\right]$$

$$= \frac{\lambda a^2}{4}\sigma\left[k^2 - \frac{\Delta\rho g}{\sigma}\right]$$

Remarks on surface tension forces

- $\int_0^\lambda \sigma ds$ is the force for curved interface
- $\int_0^\lambda \sigma dx$ is the force for flat interface (at equilibrium)

Intermediate stages

- Use Eqs. (100), (103) and (104)
- Use $\cos^2(kx) = 1 - \sin^2(kx)$

Hyp $dh \ll dx$

$$ds^2 = dx^2 + dh^2$$

$$ds = dx\sqrt{1 + (dh/dx)^2}$$

$$\sim dx\left[1 + 1/2(dh/dx)^2\right]$$

$$ds - dx = \frac{1}{2}\left(\frac{dh}{dx}\right)^2 dx \qquad (103)$$

dh/dx

$$\left(\frac{dh}{dx}\right)^2 = a^2k^2\sin^2(kx) \qquad (104)$$

Particular cases depending on sign of $\Delta\rho$

$$\Delta F = \frac{\lambda a^2}{4}\sigma\left[k^2 - \frac{\Delta\rho g}{\sigma}\right] \qquad (105)$$

Case $\rho_A < \rho_B$ ($\Delta\rho < 0$) then

$F_\sigma > F_g$ (flat interface)

Case $\rho_A > \rho_B$ ($\Delta\rho > 0$) then

Case $\lambda = 2\pi\ell_c$ (equilibrium)

k_c is the value such as $F_\sigma = F_g$ i.e.

$$k_c = \sqrt{\frac{\Delta\rho g}{\sigma}} \qquad (106)$$

Where the capillary length is

$$\ell_c = \frac{1}{k_c} = \sqrt{\frac{\sigma}{g\Delta\rho}} \qquad (107)$$

Case $\lambda > 2\pi\ell_c$ (gravity regime)

Then

$$F_g > F_\sigma$$

The gravitational force is greater than the surface tension force. The interface is unstable.

Atwood and dimensionless numbers with $U = \sqrt{gL}$

Hypothesis

- $\lambda = L$ where L is the length of the domain
- $\rho_A \equiv \rho_h$ density of *h*eavy fluid
- $\rho_B = \rho_l$ density of *l*ight fluid

Characteristic velocity U

$$U = \sqrt{gL}$$

Re and Ca with $U = \sqrt{gL}$

$$\text{Re} = \frac{L\sqrt{gL}}{\nu}$$

$$\text{Ca} = \frac{\eta_h\sqrt{gL}}{\sigma}$$

η_h: dyn visc of *h*eavy fluid

Atwood number

$$\text{At} = \frac{\rho_h - \rho_l}{\rho_h + \rho_l}$$

Validation of time-evolution: 2D Rayleigh-Taylor instability

Simulations of Rayleigh-Taylor

Numerical parameters

$N_x = 128 \quad L = 128 \quad \delta x = 1 \quad W = 4\delta x \quad \delta t = 1$

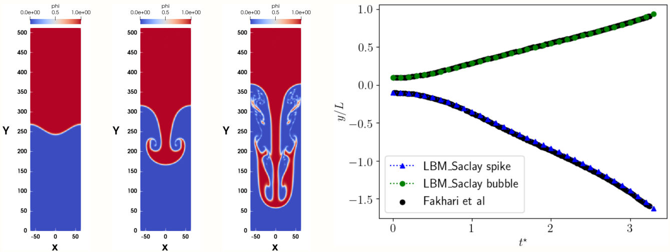
Dimensionless numbers

- Pe $= 1000$ At $= 0.5$, $t_c = \sqrt{L/g\mathrm{At}} = 1.6 \times 10^4 \delta t$ ($\Longleftrightarrow g = 10^{-6}$)

- Re $= 100$, Ca $= 10$
- Re $= 300$, Ca $= 2.6$
- **Re** $= 3000$, **Ca** $= 0.26$

Simulation and validation (Théo Duez, 2023)

$\bar{t}_0 = 0$ $\quad \bar{t}_1 = 1.7$ $\quad \bar{t}_2 = 3.2$ $\quad$ Spike and bubble positions vs time



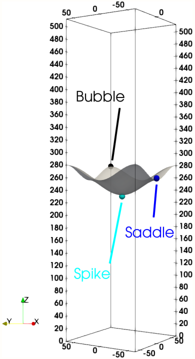
For three-phase simulations:

- Re, Ca, At, Pe, t_c are set
- Varying ρ_k, $\sigma_{k\ell}$, ν_k around those dimensionless numbers
- Definition

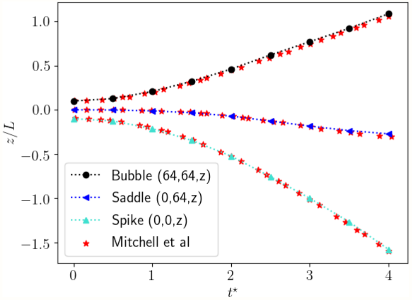
$$\rho_1^\star = \frac{\rho_1}{\rho_0}, \quad \rho_2^\star = \frac{\rho_2}{\rho_0}$$

3D Rayleigh-Taylor instability

3D validation of NS/CAC



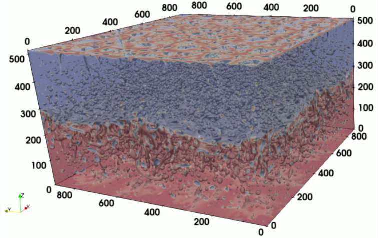
Mesh: 128×128×512 (∼8.4M nodes)



At $= 0.5$, Re $= 128$, $\eta^\star = 3$, Ca $= 9.1$, Pe $= 744$

3D simulation on Topaze-A100

Mesh: 900×900×512 (∼415M nodes)



Video 144 GPUs

- Init wavelength: $L_x/2 = L_y/2$
- 24h for 2.680.000 time-it

Capillary wave 1/4: analytical solution of Prosperetti

Amplitude of oscillation $a(t)$

$$a(t) = \frac{4(1-4\beta)\nu^2k^4}{8(1-4\beta)\nu^2k^4+\omega_0^2}a_0\mathrm{erfc}(\nu k^2 t)^{1/2} + \sum_{i=1}^{4}\frac{z_i}{Z_i}\left(\frac{\omega_0^2 a_0}{z_i^2-\nu k^2}-u_0\right)\times\exp[(z_i^2-\nu k^2)t]\mathrm{erfc}(z_i t^{1/2})$$

where coefficients β and the inviscid natural frequency ω_0 are given by

$$\beta = \frac{\rho_l\rho_g}{(\rho_l+\rho_g)^2}, \qquad \omega_0 = \frac{\rho_l-\rho_g}{\rho_l+\rho_g}gk + \frac{\sigma k^3}{\rho_l+\rho_g}$$

z_i's are the four roots of the algebric equation

$$z^4 - 4\beta(k^2\nu)^{1/2}z^3 + 2(1-6\beta)k^2\nu z^2 + 4(1-3\beta)(k^2\nu)^{3/2}z + (1-4\beta)\nu^2k^4 + \omega_0^2 = 0$$

and Z_i are defined by

$$Z_1 = (z_2-z_1)(z_3-z_1)(z_4-z_1)$$

Capillary wave 2/4: setup

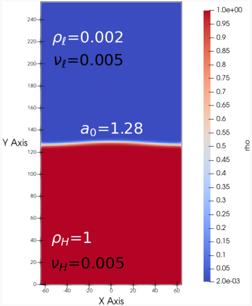
Input parameters

- Mesh 128×256

Name	Symb	Value	Dim
Heavy fluid density	ρ_H	1	–
Light fluid density	ρ_ℓ	0.01	–
Kin viscosity	$\nu_H = \nu_\ell$	5×10^{-3}	–
Surface tension	σ	10^{-4}	–
Mobility	M_ϕ	0.02	–
Interf width	W	5	–
Gravity	g_y	0	–

- Boundary conditions
  - xmin & xmax: periodic
  - ymin & ymax: wall

Initial condition

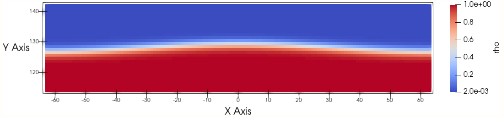


- Comparison with analytical solution of “spike position”

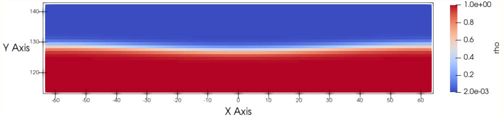
Capillary wave 3/4: density ratio 100

Simulation and validation

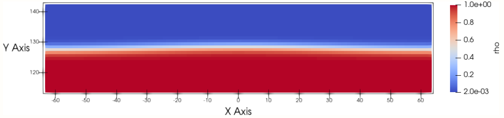
$t = 0$



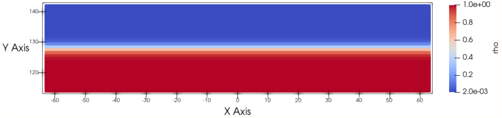
$t = 3 \times 10^4$



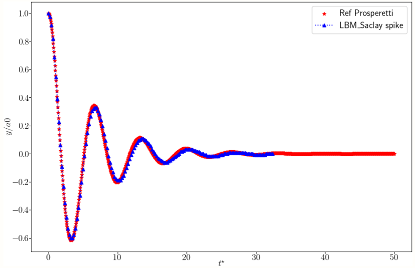
$t = 6 \times 10^4$



$t = 1.48 \times 10^5$



Spike positions vs time

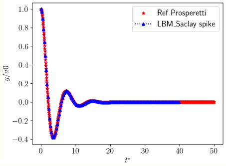


Capillary wave 4/4: density ratio 500

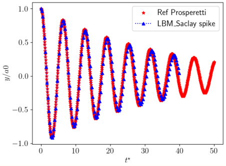
Validation from H. KERAUDREN (2023)

Mesh 256×512

Validation for ν_0

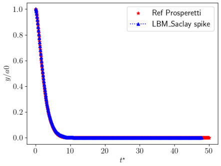


Validation for ν_1

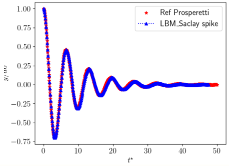


Mesh 400×800

Validation for ν_0



Validation for ν_1



C. Bubbles and droplets

Simulations with `LBM_Saclay`

Dimensionless numbers for interface Eq.

For fluid flow

Bond or Eötvös

$$\mathrm{Bo} = \frac{\Delta\rho g R^2}{\sigma}$$

Morton

$$\mathrm{Mo} = \frac{g\eta^4}{\rho\sigma^3}$$

Capillary number

$$\mathrm{Ca} = \frac{\rho\nu U}{\sigma}$$

For interface tracking

Peclet number

$$\mathrm{Pe} = \frac{UL}{M_\phi}$$

Cahn number

$$\mathrm{Cahn} = \frac{W}{L}$$

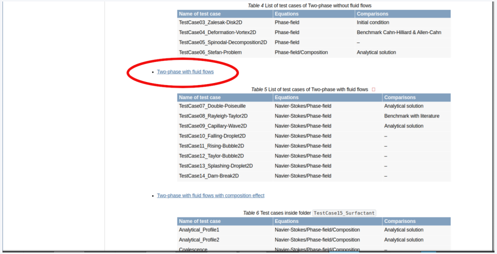
Nomenclature

- ν: kinematic viscosity $[L]^2/[T]$
- $\eta = \rho\nu$: dynamic viscosity $[M]/[L][T]$
- σ: surface tension $[E]/[L]^2 = [M]/[T]^2$
- $\Delta\rho$: density diff $[M]/[L]^3$
- M_ϕ: interface diffusivity $[L]^2/[T]$
- g: gravity $[L]/[T]^2$
- U: characteristic velocity $[L]/[T]$
- L: characteristic length [L]
- R: bubble radius [L]

Simulation with `LBM_Saclay`: choose one test case

Guidelines in documentation

In page `Practice of two-phase flows`



clic on `Two-phase with fluid flows`

Inside folder `run_training_lbm`

Directory
`TestCase07_Double-Poiseuille`
`TestCase08_Rayleigh-Taylor2D`
`TestCase09_Capillary-Wave2D`
`TestCase10_Falling-Droplet2D`
`TestCase11_Rising-Bubble2D`
`TestCase12_Taylor-Bubble2D`
`TestCase13_Splashing-Droplet2D`
`TestCase14_Dam-Break2D`

Choose one test case

- Copy-paste commands in red boxes inside a terminal

P. Rising bubble

Density ratio: 829 – Dynamic viscosity ratio: 53

Rising bubble 1/4: air – water properties

Physical parameters (20 ℃)

Name	Symb	Value	Dim
Water density	ρ_l	998.29	kg/m^3
Kin viscosity	ν_l	1.003×10^{-6}	m^2/s
Air density	ρ_a	1.204	kg/m^3
Kin viscosity	ν_a	1.56×10^{-5}	m^2/s
Surface tension	σ	7.28×10^{-2}	N/m
Gravity	g	9.81	m/s^2
Dyn viscos water	η_l	10^{-3}	Pa.s
Dyn viscos air	η_a	1.878×10^{-5}	Pa.s

Adim nb for air bubble in water

Hypotheses

Name	Sym	Value	D
Bubble diameter	D	2×10^{-3}	m
Width	L	0.01066	m

$$\mathrm{Bo} = \frac{g \Delta\rho D^2}{\sigma} = 5.37 \times 10^{-3}$$

$$\mathrm{Mo} = \frac{g \Delta\rho \eta_l^4}{\rho_l^2 \sigma^3} = 2.561 \times 10^{-11}$$

python script for input parameters

```
$ python Pre-Pro_InputParam_Rising-Bubble_Water-Air.py
```

Rising bubble 2/4: dimensionless numbers

Length of reference: D_b bubble diameter

Charac velocity

$$U = \sqrt{gD_b}$$

Bond nb

$$\mathrm{Bo} = \frac{g\Delta\rho D_b^2}{\sigma}$$

Morton nb

$$\mathrm{Mo} = \frac{g\Delta\rho\eta_l^4}{\rho_l^2\sigma^3}$$

python script

- Input parameters: adim input parameters
- Target adim numbers: Bo=339, Mo=43.1
- Derivation of $g^\star$ and $\sigma^\star$ for `LBM_Saclay`:

```
$ python Pre-Pro_Bo-Mo_2_AdimParam_Rising-Bubble.py
```

Rising bubble 3/4: setup

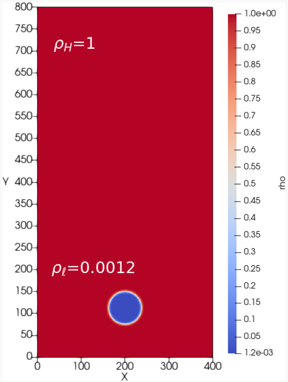
Parameters and dimensionless numbers

- Mesh 400×800

Name	Symb	Value	Dim
Water density	ρ_l	1	–
Kin viscosity	ν_l	3.333333×10^{-3}	–
Air density	ρ_a	1.206062×10^{-3}	–
Kin viscosity	ν_a	5.183943×10^{-2}	–
Surface tension	σ	2.935737×10^{-5}	–
Mobility	M_ϕ	5.6×10^{-3}	–
Interf width	W	8	–
Gravity	g_y	-1.682575×10^{-7}	–

- Boundary conditions
  - xmin & xmax: periodic
  - ymin & ymax: wall

Initial condition

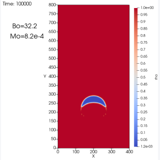


Rising bubble 4/4: comparison of Bo & Mo effects

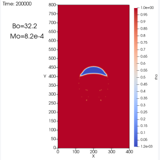
Bo $= 32.2$, Mo $= 8.2 \times 10^{-4}$ – mesh 400×800

Video

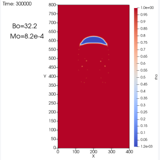
$t = 10^5$



$t = 2 \times 10^5$

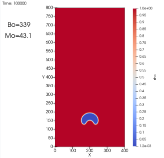


$t = 3 \times 10^5$

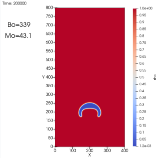


Bo $= 339$, Mo $= 43.1$ – mesh 400×800

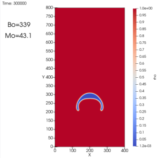
$t = 10^5$



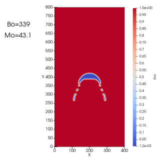
$t = 2 \times 10^5$



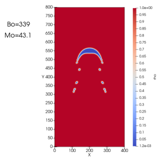
$t = 3 \times 10^5$



$t = 5 \times 10^5$



$t = 7.5 \times 10^5$



P. Taylor bubble

Density ratio: 744 – Dynamic viscosity ratio: 4236 ▸ Return

Taylor bubble 1/6: air bubble in olive oil

Physical parameters (~15 ℃)

Name	Symb	Value	Dim
Oil density	ρ_l	911.4	kg/m^3
Kin viscosity	ν_l	9.216×10^{-5}	m^2/s
Air density	ρ_a	1.225	kg/m^3
Kin viscosity	ν_a	1.618×10^{-5}	m^2/s
Surface tension	σ	0.032	N/m
Gravity	g	9.81	m/s^2
Dyn viscos oil	η_l	0.08399988	Pa.s
Dyn viscos air	η_a	1.983×10^{-5}	Pa.s

Adim number

Hypotheses			
Name	**Sym**	**Value**	**D**
Tube diameter	D_t	1.9×10^{-3}	m

$$\mathrm{Bo} = \frac{g\Delta\rho D_t^2}{\sigma} = 1.00728$$

$$\mathrm{Mo} = \frac{g\eta_l^4}{\Delta\rho\sigma^3} = 0.01637$$

python script for input parameters

```
$ python Pre-Pro_InputParam_Taylor-Bubble_OliveOil-Air.py
```

Taylor bubble 2/6: dimensionless numbers

Length of reference: D_t tube diameter

Charac velocity

$$U_c = \sqrt{gD_t}$$

Reynolds

$$\mathrm{Re}_t = \frac{U_c D_t}{\nu_l}$$

Bond nb

$$\mathrm{Bo} = \frac{g\Delta\rho D_t^2}{\sigma}$$

Morton nb

$$\mathrm{Mo} = \frac{g\eta_l^4}{\Delta\rho\sigma^3}$$

python script

- Input parameters: adim input parameters
- Target adim numbers: Bo=100 with 5 Morton numbers $\mathrm{Mo} = 1, 10^{-2}, 10^{-4}, 10^{-5}, 10^{-6}$
- Derivation of ν_l and σ for `LBM_Saclay`:

```
$ python Pre-Pro_BoMo_2_AdimNb_Taylor-Bubble.py
```

Taylor bubble 3/6: setup

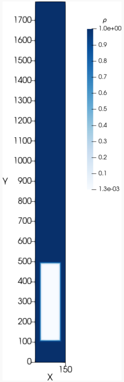
Objective: comparison of 5 Morton numbers

- Mesh 150×1792
- Input parameters

Name	Symb	Value	Bo	Dim
Oil density	ρ_l	1		–
Kin viscosity	ν_l	$\nu_1, \nu_2, \nu_3, \nu_4, \nu_5$		–
Air density	ρ_a	1.344086×10^{-3}		–
Kin viscosity	ν_a	6.666666×10^{-3}		–
Surface tension	σ_1	2.246975×10^{-4}	100	–
	σ_2	1.123487×10^{-4}	200	–
Mobility	M_ϕ	0.1		–
Interf width	W	8		–
Gravity	g_y	-10^{-6}		–

- Boundary conditions: wall for xmin, xmax, ymin & ymax

- Comparison for 5 Mo nbs

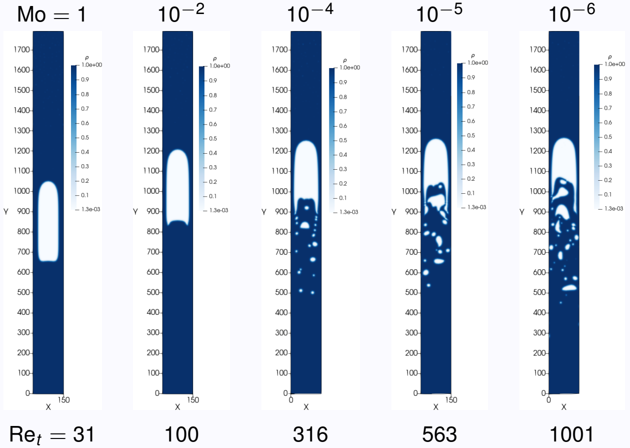


Initial condition

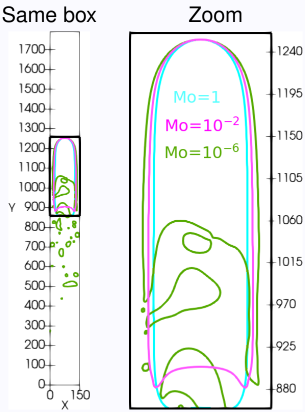
Taylor bubble 4/6: results for Bo $= 100$

Density at $t = 3 \times 10^5$

Video



$\phi_{1,2,5} = 0.5$ in the same box

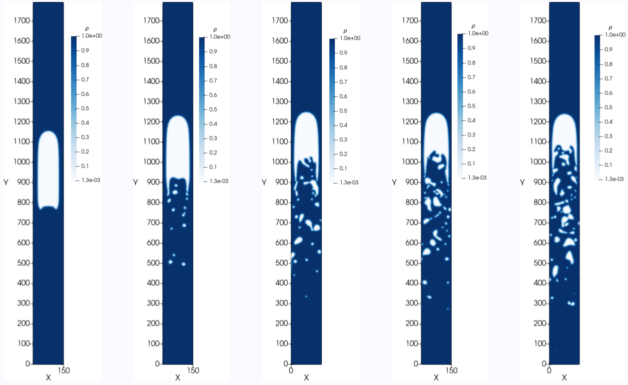


Comparison of $\phi = 0.5$ for 3 Mo

Taylor bubble 5/6: results for Bo $= 200$

Density at $t = 3 \times 10^5$ (10min on 1 GPU H100 for 800.000 time it)

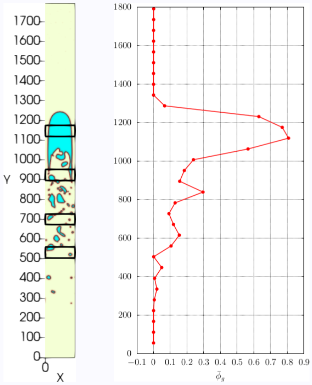
Mo $= 1$ | 10^{-2} | 10^{-4} | 10^{-5} | 10^{-6}



Re$_t = 53$ | 168 | 532 | 947 | 1684

$\bar{\phi}_g$ profile for Mo $= 10^{-5}$ at t_1

32 boxes | Mean profile

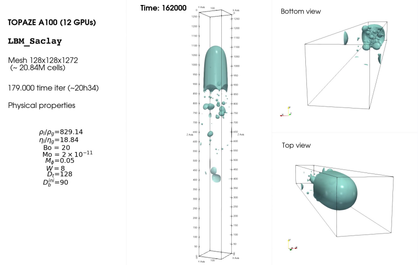


Box size: 150×56

Taylor bubble 6/6: 3D simulations

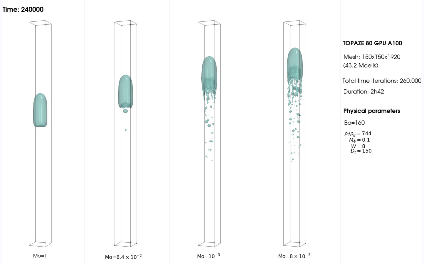
Bo $= 20$, $t = 1.62 \times 10^5$ ▶ Video

Mesh: 128×128×1272



Bo $= 160$, $t = 2.4 \times 10^5$ ▶ Video

Mesh: 150×150×1920



- TOPAZE: 80 GPUs A100
- Duration: 2h42 (4h58 on 20 GPUs)
- Total time iterations: 260.000
- MPI blocks: $2 \times 2 \times 20$

P. Falling and splashing droplet

Density ratio: 829 – Dynamic viscosity ratio: 53

Return

Falling droplet 1/2: setup

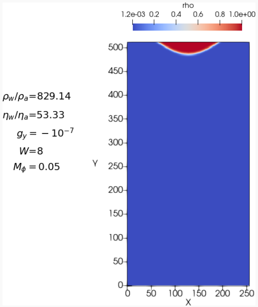
Input parameters

- Mesh 256×512
- Parameters

Name	Symb	Value	Dim
Water density	ρ_l	1	–
Air density	ρ_a	1.20606×10^{-3}	–
Kin viscosity	ν_l	3.33333×10^{-3}	–
Kin viscosity	ν_a	5.18394×10^{-2}	–
Mobility	M_ϕ	0.05	–
Interf width	W	8	–
Gravity	g_y	-10^{-7}	–

- Boundary conditions
  - xmin & xmax: periodic
  - ymin & ymax: wall

Initial condition



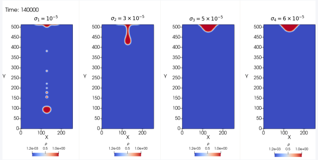
- Sensitivity of 4 values of σ

Falling droplet 2/2: results

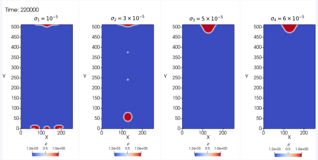
2D sensitivity on σ

Video

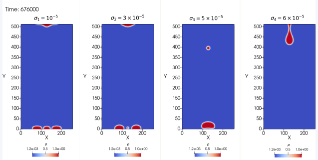
$t = 1.4 \times 10^5$



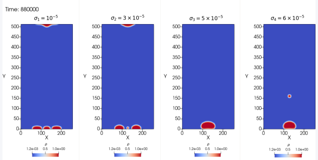
$t = 2.2 \times 10^5$



$t = 6.76 \times 10^5$

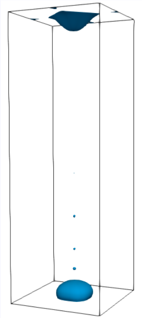


$t = 8.8 \times 10^5$



3D simulation

Video



$128 \times 128 \times 384$

600.000 time it
4h on Topaze A100 – 16 GPUs

Splashing droplet 1/3: air – water properties

Adim nb

Hypotheses

Name	Sym	Value	D
Bubble diameter	D	2×10^{-3}	m
Width	L	0.01066	m

$$\mathrm{Re} = \frac{UD}{\nu_l}$$

$$\mathrm{We} = \frac{\rho_l U^2 D}{\sigma}$$

python script for input parameters

```
$ python Pre-Pro_InputParam_Splash_Water-Air.py
```

Splashing droplet 2/3: setup

Parameters and dimensionless numbers

- Numerical parameters, mesh A: 1024×220

  $\delta x^\star = 1 \qquad W = 8\delta x^\star \qquad \delta t^\star = 1 \qquad R^\star = 30$

- Physical parameters of water and air

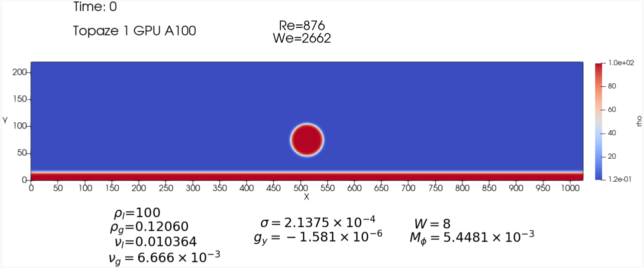
  Density ratio 829, dynamic viscosity ratio 53.33

- Sensitivity of Re and We numbers

$$\mathrm{Re} = \frac{UD}{\nu_l} \qquad \mathrm{We} = \frac{\rho_l U^2 D}{\sigma}$$

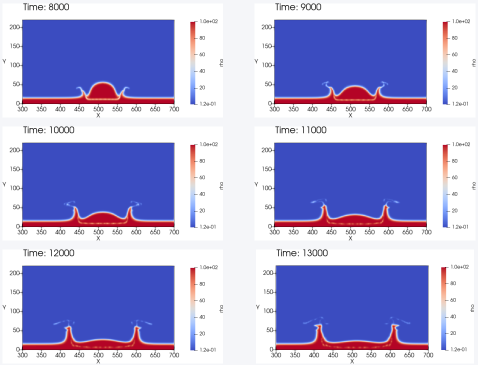
- Simulations for various ν_l and σ

Initial condition

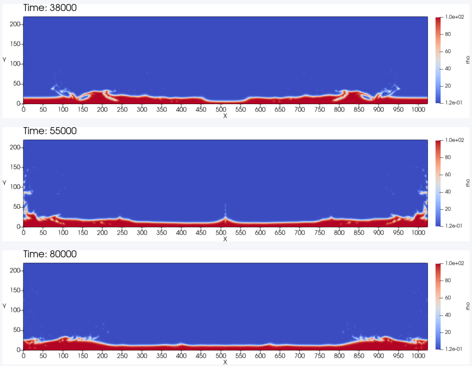


Splashing droplet 3/3: results

Short times



Longer times



Video

References of section 3

Incompressible Navier-Stokes/phase-field model

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  - D. JACQMIN, *J. Comp. Phys.* 155 (1999), 96-127, doi:10.1006/jcph.1999.6332
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  - P.-H. CHIU, Y.-T. LIN *J. Comp. Phys.* 230 (2011) 185–204, doi:10.1016/j.jcp.2010.09.021

4. Coupling with T and c

Marangoni, phase change and surfactant

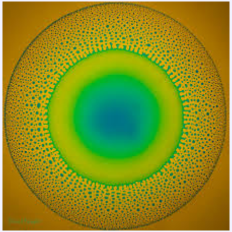
Outline section 4

a. Marangoni force

Effet Marangoni effect

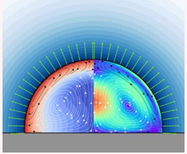
Marangoni effect

- Because of surface tension gradient
- Force toward strong surf tension
- Gradient of σ because of temperature or concentration gradient
- e.g. Marangoni bursting

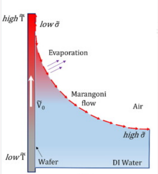


Applications

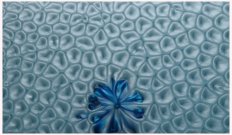
Microgravity convection



Sechage de wafer



Bénard-Marangoni instability



Ordres de grandeur

Dimensionless numbers

Characteristic velocity:

$$U = \frac{\frac{d\sigma}{dT}\,|\nabla T|\,L}{\eta}$$

Marangoni number:

$$\mathrm{Ma} = \frac{UL}{\alpha} = \frac{\text{thermocapillary}}{\text{dissipation}}$$

$$\mathrm{Re} = \frac{\rho UL}{\eta} = \frac{\text{inertia}}{\text{viscosity}}$$

Numerical values

Thin water layer under gradient of T

Grandeur	Value	Unit
$\frac{d\sigma}{dT}$	$-2.0 \cdot 10^{-4}$	$N.m^{-1}K^{-1}$
η	$1.0 \cdot 10^{-3}$	$Pa.s$
α	$0.144 \cdot 10^{-6}$	$m^2.s^{-1}$
Ma	$\sim$100	–

Droplet migration

Grandeur	Value	Unit
$\frac{d\sigma}{dT}$	$-1.06 \cdot 10^{-4}$	$\mathrm{N.m^{-1}K^{-1}}$
η	$3.52 \cdot 10^{-3}$	Pa.s
α	$9.14 \cdot 10^{-6}$	$\mathrm{m^2.s^{-1}}$
Ma	~1	–

Marangoni force

Balance of normal stress

$$(\overline{\overline{\boldsymbol{T}}}_L - \overline{\overline{\boldsymbol{T}}}_A) \cdot \boldsymbol{n} = \boldsymbol{\nabla} \cdot (\sigma(\overline{\overline{\boldsymbol{I}}} - \boldsymbol{n} \otimes \boldsymbol{n})) = -\sigma\kappa\boldsymbol{n} + \boldsymbol{\nabla}_S\sigma \quad (108)$$

- $\overline{\overline{\boldsymbol{T}}}_\Phi = -p\overline{\overline{\boldsymbol{I}}} + \eta_\Phi(\boldsymbol{\nabla}\boldsymbol{u} + \boldsymbol{\nabla}\boldsymbol{u}^T)$: viscous stress tensor
- $\boldsymbol{n}$: normal vector at interface
- $\kappa = \boldsymbol{\nabla} \cdot \boldsymbol{n}$: interface curvature
- $\boldsymbol{\nabla}_S \hat{=} \boldsymbol{\nabla} - \boldsymbol{n}(\boldsymbol{n} \cdot \boldsymbol{\nabla})$: gradient along surface

if $\sigma = cst$

$$\boldsymbol{F}_c = -\delta_\Sigma \sigma\kappa\boldsymbol{n}$$

if $\sigma = \sigma(c(\boldsymbol{x}, t))$ or $\sigma(T(\boldsymbol{x}, t))$

$$\boldsymbol{F}_s = \boldsymbol{F}_c + \boldsymbol{F}_M = \delta_\Sigma(-\sigma\kappa\boldsymbol{n} + \boldsymbol{\nabla}_S\sigma)$$

σ as a function of c

Linear

$$\sigma(c) = \sigma_{ref} + \frac{d\sigma}{dc}(c - c_{ref})$$

$$\frac{d\sigma}{dc} = \sigma_c < 0$$

Log

$$\sigma = \sigma_0 \left[1 + \beta \ln(1 - \frac{c}{c_\infty})\right]$$

Marangoni force in phase-field framework

$\boldsymbol{F}_c$ and $\boldsymbol{F}_M$ expressed with ϕ

- Surface tension force

$$\boldsymbol{F}_s = \delta_d(\phi)[-\sigma\kappa(\phi)\boldsymbol{n}_\phi + \boldsymbol{\nabla}_s\sigma]$$

- Capillary and Marangoni forces

$$\boldsymbol{F}_c = \mu_\phi \boldsymbol{\nabla}\phi$$

$$\boldsymbol{F}_M = \frac{3W}{2}\left[|\boldsymbol{\nabla}\phi|^2\boldsymbol{\nabla}\sigma - (\boldsymbol{\nabla}\phi\cdot\boldsymbol{\nabla}\sigma)\boldsymbol{\nabla}\phi\right]$$

Final expression of Marangoni's force

with chain rule for $\boldsymbol{\nabla}\sigma = (\partial\sigma/\partial c)\boldsymbol{\nabla}c$

$$\boxed{\boldsymbol{F}_M = \frac{3W}{2}\frac{\partial\sigma}{\partial c}\left[|\boldsymbol{\nabla}\phi|^2\boldsymbol{\nabla}c - (\boldsymbol{\nabla}\phi\cdot\boldsymbol{\nabla}c)\boldsymbol{\nabla}\phi\right] \qquad (109)}$$

Proof for $\boldsymbol{F}_M$

- For $\boldsymbol{F}_c$ see section 3
- For $\boldsymbol{F}_M$ use def of

$$\boldsymbol{\nabla}_s \hat{=} \boldsymbol{\nabla} - \boldsymbol{n}(\boldsymbol{n}\cdot\boldsymbol{\nabla})$$

$$\boldsymbol{n}_\phi \hat{=} \frac{\boldsymbol{\nabla}\phi}{|\boldsymbol{\nabla}\phi|}$$

$$\delta_d \hat{=} \frac{3W}{2}|\boldsymbol{\nabla}\phi|^2$$

$$\begin{aligned}
\boldsymbol{F}_M &= \delta_d\boldsymbol{\nabla}_s\sigma \\
&= \frac{3W}{2}|\boldsymbol{\nabla}\phi|^2[\boldsymbol{\nabla}\sigma - \boldsymbol{n}_\phi(\boldsymbol{n}_\phi\cdot\boldsymbol{\nabla}\sigma)] \\
&= \frac{3W}{2}|\boldsymbol{\nabla}\phi|^2\left[\boldsymbol{\nabla}\sigma - \frac{\boldsymbol{\nabla}\phi}{|\boldsymbol{\nabla}\phi|}\left(\frac{\boldsymbol{\nabla}\phi}{|\boldsymbol{\nabla}\phi|}\cdot\boldsymbol{\nabla}\sigma\right)\right] \\
&= \frac{3W}{2}\left[|\boldsymbol{\nabla}\phi|^2\boldsymbol{\nabla}\sigma - (\boldsymbol{\nabla}\phi\cdot\boldsymbol{\nabla}\sigma)\boldsymbol{\nabla}\phi\right]
\end{aligned}$$

Navier-Stokes/CAC + composition

Navier-Stokes + conservative Allen-Cahn model

$$\nabla \cdot \boldsymbol{u} = 0,$$

$$\rho \left[\frac{\partial \boldsymbol{u}}{\partial t} + \nabla \cdot (\boldsymbol{u}\boldsymbol{u}) \right] = -\nabla p_h + \nabla \cdot \left[\eta (\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T) \right] + \boldsymbol{F}_{tot} + \boldsymbol{F}_M$$

$$\frac{\partial \phi}{\partial t} + \nabla \cdot (\boldsymbol{u}\phi) = \nabla \cdot \left[M_\phi \left(\nabla \phi - \frac{4}{W} \phi (1 - \phi) \boldsymbol{n} \right) \right],$$

Transport equation for composition (or temperature)

$$\frac{\partial c}{\partial t} + \nabla \cdot (c\boldsymbol{u}) = \nabla \cdot (M_c \nabla c)$$

Forces

Total force:

$$\boldsymbol{F}_{tot} = \boldsymbol{F}_c + \boldsymbol{F}_g$$

Capillary and gravity forces:

$$\boldsymbol{F}_c = \mu_\phi \nabla \phi \quad \text{and} \quad \boldsymbol{F}_g = \rho \boldsymbol{g}$$

Marangoni force $\boldsymbol{F}_M$

Previous slide Eq. (109)

Droplet migration by thermocapillarity 1/2: analytical velocity

Theoretical final velocity

$$U_{YGB} = -\frac{D\frac{d\sigma}{dT}\,|\nabla T_\infty|}{(3\mu' + 2\mu)(2 + \frac{\alpha'}{\alpha})} \qquad (110)$$

(Young,Goldstein,Block 1959,Fedosov 1948)

Hypotheses:

- Re $<<$ 1 (Stokes regime)
- Ma $<<$ 1(T and σ stationnary)
- Spherical droplet
- $\sigma = \sigma_{ref} + \frac{d\sigma}{dT}(T - T_{ref})$
- $g = 0$

Two contributions

Decomposition of terminal velocity:

$$U_{YGB} = U_{\sigma\kappa n} + U_{\nabla_\Sigma\sigma}$$

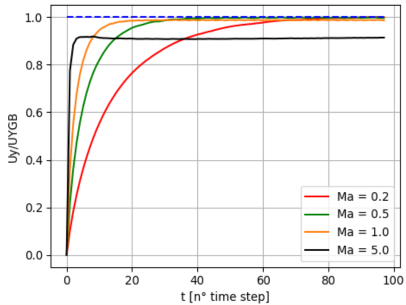
$$U_{\sigma\kappa n} = -\frac{2R\frac{d\sigma}{dT}\nabla T(3\mu + 2\mu')}{\mu(2\mu + 3\mu')\,(2 + \frac{\alpha'}{\alpha})}$$

$$U_{\nabla_\Sigma\sigma} = \frac{4R\frac{d\sigma}{dT}\nabla T(\mu + \mu')}{\mu(2\mu + 3\mu')\,(2 + \frac{\alpha'}{\alpha})}$$

Droplet migration by thermocapillarity 2/2: validation

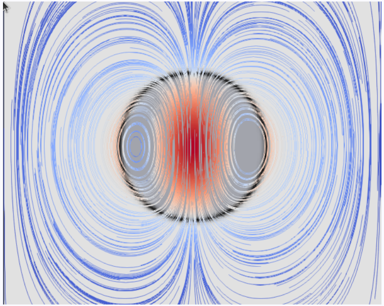
Validation: Simon Cappe (2024)

Comparisons with `LBM_Saclay`



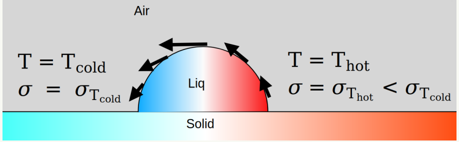
Effect of Marangoni number

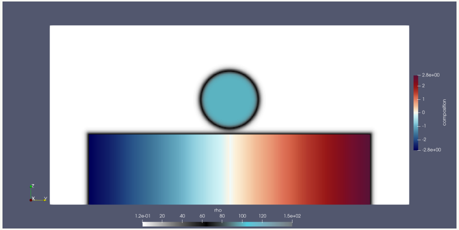
Simulation



Droplet migration on solid surface

Simulation





Video

b. Phase change model

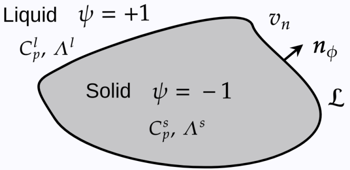
Stefan's problem and phase-field model

Thermodynamics of solidification

Phenomenology

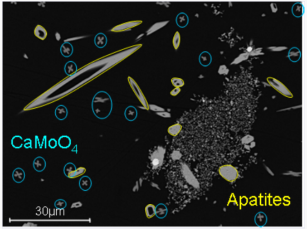
If the temperature T is lowered below the melting temperature T_m :

- Solidification occurs: «A liquid yields A solid and releases the latent heat $\mathcal{L}$ at interface».



- Problem: calculate the interface position and the temperature field

Observation of crystal growth in glass



- Borosilicate glass
- Heated between 600° and 900℃ during ~120h

Stefan's problem of phase change

Sharp interface model of phase change

$$C_p \frac{\partial T}{\partial t} = \Lambda_\Phi \nabla^2 T \qquad \text{Heat eq for } \Phi = s, l \qquad (111a)$$

$$\mathcal{L} v_n = \boldsymbol{n} \cdot \left(C_p \Lambda \nabla T|_{sol} - C_p \Lambda \nabla T|_{liq} \right) \qquad \text{Stefan condition} \qquad (111b)$$

$$T_i = T_m - \frac{\sigma T_m}{\mathcal{L}} \kappa - \frac{v_n}{m_k} \qquad \text{Gibbs-Thomson cond} \qquad (111c)$$

Two conditions at interface

- Flux
- Curvature

Nomenclature

- T: temperature
- Λ_Φ: thermal conductivity
- C_p: specific heat
- $\mathcal{L}$: latent heat
- v_n: normal velocity at interface
- T_i: interface temperature
- T_m: melting temperature
- σ: interfacial energy
- κ: curvature
- m_k: interface mobility

Free energy functional for phase change

Free energy of interface and bulk thermodynamics: dependance with ψ and T

$$\mathscr{F}[\psi, T] = \int \Big[\underbrace{\mathcal{F}_{int}(\psi, \boldsymbol{\nabla}\psi)}_{\text{Standard interface free energy}} + \underbrace{f_{bulk}(\psi, T)}_{\text{Thermodynamic of bulks}} \Big] dV$$

Interface free energy

Defined with minima $\psi^\star = \pm 1$ (next slide)

Thermodynamic of bulks

$$f_{bulk}(\psi, T) = p_s(\psi) f_s(T) + [1 - p_s(\psi)]\, f_l(T)$$

- $f_{l,s}(T)$: free energy of liquid (resp. solid) bulk
- $p_s(\psi)$: interpol function (next slide)

Variation

$$\delta\mathscr{F} = \int \left\{ -\zeta \boldsymbol{\nabla}^2\psi + f'_{dw}(\psi) + \frac{p'(\psi)}{2}\left[f_s(T) - f_l(T)\right] \right\} \delta\psi + \left\{ p_s(\psi)\frac{\partial f_s(T)}{\partial T} + [1 - p_s(\psi)]\frac{\partial f_l(T)}{\partial T} \right\} \delta T dV$$

Double-well and interpolation function

Interface free energy

$$\mathcal{F}_{int}(\psi, \nabla\psi) = f_{dw}(\psi) + \frac{\zeta}{2}(\nabla\psi)^2$$

Double-well $f_{dw}(\psi)$ with $\psi^\star = 1$

$$\boxed{f_{dw}(\psi) = Hg_3(\psi) = H(\psi^\star - \psi)^2(\psi + \psi^\star)^2}$$

Equilibrium (see section 2.a)

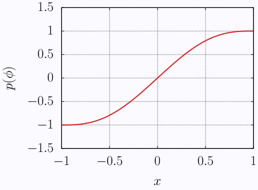
$$\psi^{eq}(x) = \psi^\star \tanh\left(\frac{2x}{W}\right)$$

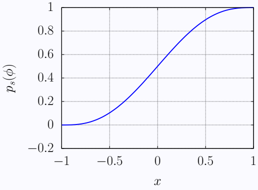
$$W = \frac{1}{\psi^\star}\sqrt{\frac{2\zeta}{H}} \qquad \sigma = \frac{4}{3}\sqrt{2\zeta H}$$

Interpolation function $p(\psi)$

$$p(\psi) = \frac{15}{8}\left[\psi - \frac{2}{3}\psi^3 + \frac{\psi^5}{5}\right]$$

$$p_s(\psi) = \frac{1 + p(\psi)}{2}$$





Derivation of math model 1/2: temperature equation

Starting point

Conservation of internal energy density:

$$\frac{\partial e}{\partial t} = \nabla \cdot (\Lambda \nabla T) \qquad (113)$$

Pb: express $e(\phi, s)$ as a function of T

$\downarrow$ see proof

Temperature equation

Finally combining Eq. (113) and (115)

$$\boxed{C_p \frac{\partial T}{\partial t} = \nabla \cdot (\Lambda \nabla T) - \underbrace{\frac{1}{2} p'(\psi) \mathcal{L} \frac{\partial \psi}{\partial t}}_{\text{Latent heat at interface}}}$$

Proof

- Variation of $\mathscr{F}$ wrt T: opposite of entropy

$$s(\psi, T) = -\frac{\delta \mathscr{F}}{\delta T} = -\frac{\partial f_{bulk}(\psi, T)}{\partial T}$$
$$= -p_s(\psi) \underbrace{\frac{\partial f_s}{\partial T}}_{s_s(T)} - [1 - p_s(\psi)] \underbrace{\frac{\partial f_l}{\partial T}}_{s_l(T)} \qquad (114)$$

- Thermo identity ($de = Tds$) and chain rule

$$de = Tds(\psi, T)$$
$$= \underbrace{T \frac{\partial s}{\partial T}}_{C_p\text{: specific heat}} dT + T \underbrace{\frac{\partial s}{\partial \psi}}_{\text{use Eq. (114)}} d\psi$$
$$\frac{\partial e}{\partial t} = C_p \frac{\partial T}{\partial t} + p_s'(\psi) \underbrace{T [s_l(T) - s_s(T)]}_{\equiv \mathcal{L}\text{: latent heat}} \frac{\partial \psi}{\partial t} \qquad (115)$$

Derivation of math model 2/2: phase-field equation

Variation wrt ϕ: Allen-Cahn (see section 2)

$$\begin{aligned}\frac{1}{\mathscr{M}_\psi}\frac{\partial\psi}{\partial t} &= -\frac{\delta\mathscr{F}}{\delta\psi}\\ &= -\frac{\delta\mathscr{F}_{int}(\psi,\nabla\psi)}{\delta\psi} - \frac{\partial f_{bulk}(\psi,T)}{\partial\psi}\\ &= \zeta\nabla^2\psi - f'_{dw}(\psi) - \underbrace{\frac{p'(\psi)}{2}\left[f_s(T) - f_l(T)\right]}_{\text{Thermodynamic driving source}}\end{aligned}$$

Common hypothesis: $T \sim T_m$

- For $\Phi = s, l$

$$f_\Phi(T) \sim f_\Phi(T_m) + \left.\frac{\partial f_\Phi}{\partial T}\right|_{T_m}(T - T_m)$$

- Properties at T_m

$$\begin{aligned} f_s(T_m) &= f_l(T_m)\\ \mathcal{L} &= T_m[s_l(T_m) - s_s(T_m)]\end{aligned}$$

Phase-field equation

$$\frac{1}{\mathscr{M}_\psi}\frac{\partial\psi}{\partial t} = \zeta\nabla^2\psi - Hg'_3(\psi) - \frac{p'(\psi)}{2}\frac{\mathcal{L}}{T_m}(T - T_m) \tag{117}$$

Phase-field model for solid-liquid phase change

See M. Plapp, CISM 2012

Phase-field Eq.: coefficients W, τ_ϕ and λ

In Eq. (117), set H in factor in right-hand side:

$$\frac{1}{\mathscr{M}_\psi}\frac{\partial \psi}{\partial t} = H\left[\frac{\zeta}{H}\boldsymbol{\nabla}^2\psi - g_3'(\psi) - \frac{1}{H}\frac{p'(\psi)}{2}\frac{\mathcal{L}}{T_m}(T-T_m)\right]$$

$$\tau_0 = 1/(H\mathscr{M}_\psi)$$
$$W_0 = \sqrt{\zeta/H}$$
$$\lambda = 1/H$$

Phase-field model for pure substance

$$C_p\frac{\partial T}{\partial t} = \boldsymbol{\nabla}\cdot(\Lambda\boldsymbol{\nabla}T) - \frac{1}{2}p'(\psi)\mathcal{L}\frac{\partial \psi}{\partial t}$$

$$\tau_0\frac{\partial \psi}{\partial t} = W_0^2\boldsymbol{\nabla}^2\psi - g_3'(\psi) - \lambda\frac{p'(\psi)}{2}\frac{\mathcal{L}}{T_m}(T-T_m)$$

Equivalence between phase-field model and Stefan's problem

Stefan's problem with $\overline{T} = (T - T_m)C_p/\mathcal{L}$

$$\frac{\partial \overline{T}}{\partial t} = D\boldsymbol{\nabla}^2\overline{T}$$
$$v_n = D\boldsymbol{n}\cdot(\boldsymbol{\nabla}\overline{T}|_{sol} - \boldsymbol{\nabla}\overline{T}|_{liq})$$
$$\overline{T}_i = -d_0\kappa - \beta v_n$$

$\Updownarrow$ Matched asymptotic expansions

Phase-field model for pure substance

$$\frac{\partial \overline{T}}{\partial t} = D\boldsymbol{\nabla}^2\overline{T} - \frac{1}{2}p'(\psi)\frac{\partial \psi}{\partial t}$$
$$\tau_0\frac{\partial \psi}{\partial t} = W_0^2\boldsymbol{\nabla}^2\psi - g_3'(\psi) - \lambda\frac{p'(\psi)}{2}\overline{T}$$

Equivalence conditions

- $\overline{T}$: dimensionless temperature
- $d_0 = \sigma_0 T_m C_p/\mathcal{L}^2$: capillary length
- $\beta = C_p/\mathcal{L}m$: kinetic coefficient

$$d_0 = a_1\frac{W_0}{\lambda} \tag{119}$$
$$\beta = a_1\left[\frac{\tau_0}{\lambda W_0} - a_2\frac{W_0}{D}\right] \tag{120}$$

- $a_1 = 0.8839$, $a_2 = 0.6267$
- Right-hand side: λ, W_0 and τ_0 are the parameters of the phase-field model.

V. Comparison with solution of Stefan's problem

First Stefan problem 1/2: analytical solutions

1D Problem (see Hahn & Özişik sec 12-3)

Mathematical problem in bulks

$$\frac{\partial T_l}{\partial t} = \alpha_l \frac{\partial^2 T_l}{\partial x^2} \quad \text{for }]0, x_i(t)[\tag{121a}$$

$$\frac{\partial T_g}{\partial t} = \alpha_g \frac{\partial^2 T_g}{\partial x^2} \quad \text{for }]x_i(t), \infty[\tag{121b}$$

$$T_g(x, t=0) = T_\infty \quad \text{Init Cond} \tag{122}$$

BC

$$T_l(x,\, t)|_{x=0} = T_w \quad \text{for } x = 0 \tag{123a}$$

$$T_g(x \to \infty,\, t) = T_\infty \quad \text{for } x \to \infty \tag{123b}$$

Interface conditions at $x = x_i(t)$

$$T_l(x,\, t) = T_g(x,\, t) = T_i, \tag{124a}$$

$$\mathcal{K}_l \frac{\partial T_l}{\partial x} - \mathcal{K}_g \frac{\partial T_g}{\partial x} = \rho \mathcal{L} \frac{dx_i(t)}{dt} \tag{124b}$$

Analytical solution with $\theta = C_p(T - T_{sat})/\mathcal{L}$

Temperatures of liquid and gas

$$\theta_l(x,t) = \theta_w + (\theta_i - \theta_w)\frac{\operatorname{erf}(x/2\sqrt{\alpha_l t})}{\operatorname{erf}(\xi)} \tag{125}$$

$$\theta_g(x,t) = \theta_\infty + (\theta_i - \theta_\infty)\frac{\operatorname{erfc}(x/2\sqrt{\alpha_g t})}{\operatorname{erfc}(\xi\sqrt{\alpha_l/\alpha_g})} \tag{126}$$

Interface position $x_i(t)$

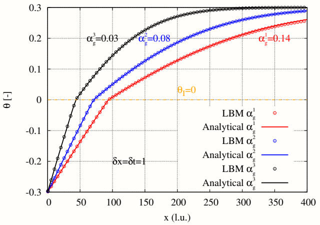
$$x_i(t) = 2\xi\sqrt{\alpha_l t} \tag{127}$$

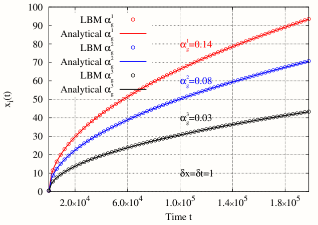
with ξ solution of transcendental Eq.:

$$\frac{e^{-\xi^2}}{\operatorname{erf}(\xi)} + \left(\frac{\alpha_g}{\alpha_l}\right)^{1/2} \frac{\theta_i - \theta_\infty}{\theta_i - \theta_w} \frac{e^{-\xi^2(\alpha_l/\alpha_g)}}{\operatorname{erfc}(\xi\sqrt{\alpha_l/\alpha_g})} = -\frac{\xi\sqrt{\pi}}{\theta_w} \tag{128}$$

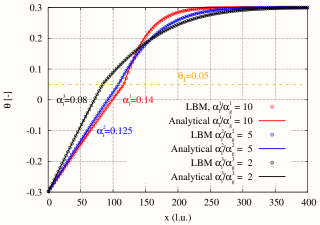
First Stefan problem 2/2: validation `LBM_Saclay`

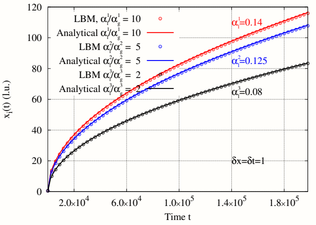
Case 1





Case 2





Surface tension anisotropy and anisotropy function

See KARMA & RAPPEL PRE (1998)

Dependence of properties with normal vector $\boldsymbol{n}$

- Properties

$$\sigma \equiv \sigma(\boldsymbol{n}) = \sigma_0 a_s(\boldsymbol{n})$$
$$\beta \equiv \beta(\boldsymbol{n}) = \beta_0 a_s(\boldsymbol{n})$$
$$W \equiv W(\boldsymbol{n}) = W_0 a_s(\boldsymbol{n})$$

- Gibbs-Thomson

$$\overline{T}_i = -d_0 \sum_{\xi=1,2} \left[a_s(\boldsymbol{n}) + \frac{\partial^2 a_s(\boldsymbol{n})}{\partial \theta_\xi} \right] \frac{1}{R_\xi} - \beta(\boldsymbol{n}) v_n$$

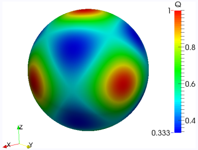
- Normal vector

$$\boldsymbol{n} = -\frac{\boldsymbol{\nabla}\phi}{|\boldsymbol{\nabla}\phi|}$$

Anisotropy function $a_s(\boldsymbol{n})$

$$a_s(\boldsymbol{n}) = 1 + \epsilon_s \left[4(n_x^4 + n_y^4 + n_z^4) - 3 \right]$$

where ϵ_s is a parameter



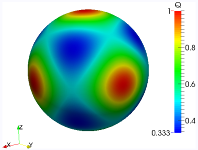
Simulations of crystal growth 1/2: anisotropy function $a_s(\boldsymbol{n})$

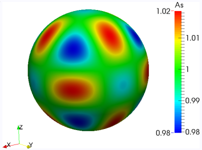
From Younsi *et al.* CAMWA (2016)

Video

$$a_s(\mathbf{n}) = 1 - 3\varepsilon_s + 4\varepsilon_s \sum_\alpha n_\alpha^4$$

$$a_s(\mathbf{n}) = 1 + \varepsilon_s\left(\sum_\alpha n_\alpha^4 - \frac{3}{5}\right) + \delta\left(3\sum_\alpha n_\alpha^4 + 66 n_x^2 n_y^2 n_z^2 - \frac{17}{7}\right)$$





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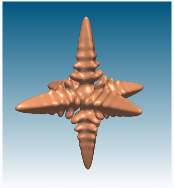
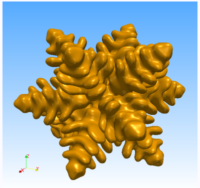
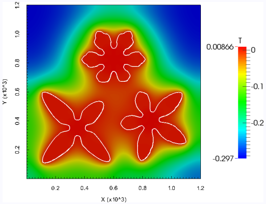
[110]



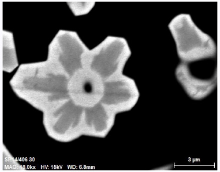


Interaction between crystals

Video



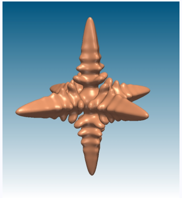
CEA/Mar – DE2D



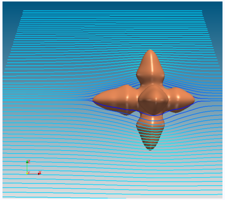
Simulations of crystal growth 2/2: flow effects

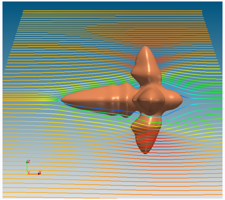
Flow effects

Without fluid flow



With fluid flow:

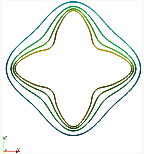




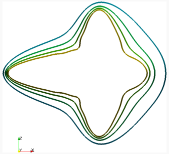
Video

Iso-values of temperature and sensitivity to V_i: ($\psi = 0$)

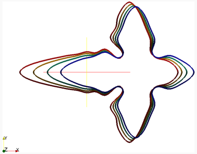
$V_i = 0$



$V_i = 4V_0$



$V_i = 4V_0$ (red) et $V_i = V_0$ (blue)



Faster growth with bigger initial velocity

C. Fluid flow with phase change

Incompressible model

Mass balance for one-fluid formulation

Mass balance for $\tilde{\rho}_l$ and $\tilde{\rho}_g$

Mass balance

- Balance on $\tilde{\rho}_l$ and $\tilde{\rho}_g$

$$\frac{\partial \tilde{\rho}_g}{\partial t} + \nabla \cdot (\tilde{\rho}_g \boldsymbol{u} + \rho_g \boldsymbol{j}_g) = +\dot{m}''' \quad (129)$$

$$\frac{\partial \tilde{\rho}_l}{\partial t} + \nabla \cdot (\tilde{\rho}_l \boldsymbol{u} + \rho_l \boldsymbol{j}_l) = -\dot{m}''' \quad (130)$$

- $\dot{m}'''$: source (or sink) at interface
- Hyp on fluxes

$$\boldsymbol{j}_\phi = \boldsymbol{j}_g = -\boldsymbol{j}_l$$

Expressed with ϕ

- Eqs. (129) expressed with ϕ:

$$\frac{\partial \phi}{\partial t} + \nabla \cdot (\boldsymbol{u}\phi + \boldsymbol{j}_\phi) = +\frac{\dot{m}'''}{\rho_g} \quad (131)$$

- Sum Eq.(129) + Eq. (130)

$$\nabla \cdot \boldsymbol{u} = \dot{m}''' \left(\frac{1}{\rho_g} - \frac{1}{\rho_l} \right)$$

Objective: determine the production term $\dot{m}'''$

Advected field with curvature and phase change

Transport of ϕ (see section 2)

- Hyperbolic equation:

$$\frac{\partial \phi}{\partial t} + \boldsymbol{V} \cdot \boldsymbol{\nabla} \phi = 0$$

- Advective term: 2 terms

$$\boldsymbol{V} \cdot \boldsymbol{\nabla} \phi = \boldsymbol{u} \cdot \boldsymbol{\nabla} \phi + v_n \left| \boldsymbol{\nabla} \phi \right|$$

Normal velocity of interface

- Normal velocity: curvature and phase change

$$v_n = -M_\phi \kappa + \tilde{v}_n \tag{132}$$

$\tilde{v}_n$: velocity due to phase change

- Transport of ϕ with Eq. (132)

$$\frac{\partial \phi}{\partial t} + \boldsymbol{u} \cdot \boldsymbol{\nabla} \phi = M_\phi \kappa \left| \boldsymbol{\nabla} \phi \right| - \tilde{v}_n \left| \boldsymbol{\nabla} \phi \right| \tag{133}$$

Source term of production

By comparing Eq. (131) and (133)

$$\frac{\dot{m}'''}{\rho_g} = -\tilde{v} \left| \boldsymbol{\nabla} \phi \right|$$

Model for production source $\dot{m}'''$

Remark on Stefan condition

Stefan condition at interface

$$\tilde{v}_n = \frac{C_p}{\mathcal{L}}\left[\alpha\nabla T\big|_l - \alpha\nabla T\big|_g\right]\cdot\boldsymbol{n}$$

Approximation with T_i saturation temperature

$$\tilde{v}_n = \frac{\alpha}{\mathscr{A}}\frac{C_p}{\mathcal{L}}\frac{T_i - T}{W} \qquad \text{with } \alpha = \frac{\Lambda}{C_p}$$

Source term of Eq. (131)

With

$$|\nabla\phi| = \frac{4}{W}\phi(1-\phi)$$

$$\overline{T} = \frac{C_p}{\mathcal{L}}T$$

$$\mathscr{A} = 0.21$$

$$\begin{aligned}\frac{\dot{m}'''}{\rho_g} &= -\tilde{v}_n\,|\nabla\phi| \\ &= -\left[\frac{\alpha}{\mathscr{A}}\frac{\overline{T}_i - \overline{T}}{W}\right]\times\left[\frac{4}{W}\phi(1-\phi)\right]\end{aligned}$$

$$\boxed{\dot{m}''' = -\frac{4\alpha\rho_g}{\mathscr{A}W^2}(\overline{T}_i - \overline{T})\phi(1-\phi)}$$

Incompressible model with phase change

Navier-Stokes + interface tracking + Temperature

$$\nabla \cdot \boldsymbol{u} = \dot{m}''' \left(\frac{1}{\rho_g} - \frac{1}{\rho_l} \right),$$

$$\rho(\phi) \left[\frac{\partial \boldsymbol{u}}{\partial t} + \nabla \cdot (\boldsymbol{u}\boldsymbol{u}) \right] = -\nabla p + \nabla \cdot \left[\eta (\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T) \right] + \mu_\phi \nabla \phi + \rho(\phi) \boldsymbol{g}$$

$$\frac{\partial \phi}{\partial t} + \nabla \cdot (\boldsymbol{u}\phi) = \nabla \cdot \left[M_\phi \left(\nabla \phi - \frac{4}{W} \phi (1 - \phi) \boldsymbol{n} \right) \right] + \frac{\dot{m}'''}{\rho_g},$$

$$\frac{\partial \overline{T}}{\partial t} + \nabla \cdot (\boldsymbol{u} \overline{T}) = \alpha \nabla^2 \overline{T} - \left[\frac{\partial \phi}{\partial t} + \nabla \cdot (\boldsymbol{u}\phi) \right].$$

Relationships for μ_ϕ and $\dot{m}'''$

Chemical potential:

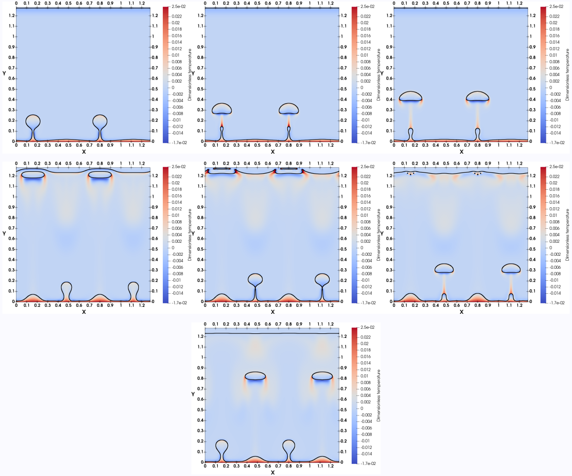
$$\mu_\phi = 4H\phi(\phi - 1)(\phi - 1/2) - \zeta \nabla^2 \phi$$

Phase change production (with $\mathscr{A} = 0.21$)**:**

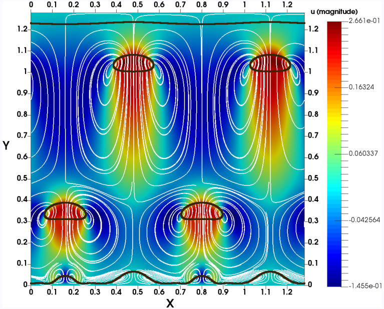
$$\dot{m}''' = -\frac{4\alpha \rho_g}{\mathscr{A} W^2} (\overline{T}_i - \overline{T}) \phi (1 - \phi)$$

Simulation of film boiling

Phase-field and temperature



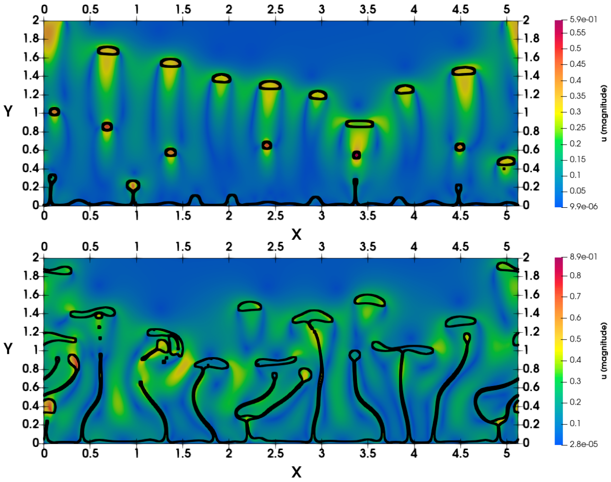
Streamlines and velocity magnitude



Video

From W. VERDIER *et al.* (2020)

Simulations of Film boiling on 8 GPUs



$T_w = T_1$
(Ja=0.025)

Mesh size 4096×3072

Video 1a

5.33×10^5 time iterations: 80 min

$T_w = T_2 > T_1$
(Ja=0.1)

Video 1b

Warning about incompressible model with phase change

No thermodynamic pressure for incompressible fluids

- Because the pressure has no thermodynamic meaning for incompressible fluids (no relation between pressure and density), that incompressible model is necessarily an approximation for modeling and simulating two-phase flows with phase change.
- It has been presented here as an extension of NS–CH/CAC models for incompressible fluids to make easier the comparison with Navier-Stokes/Korteweg models of section 5.

In section 5: Navier-Stokes/Korteweg models

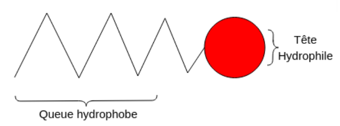
One thermodynamically consistent model for phase change will be presented in section 5 with:

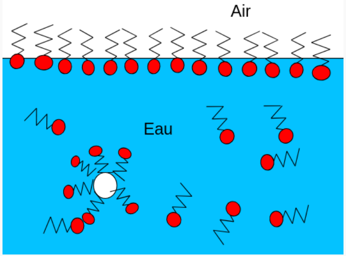
- A low Mach formulation of NS equations
- An equation of state that relates pressure and density
- A derivation of math model for Korteweg tensor and coupling with temperature
- etc.

d. Two-phase with surfactant

Surfactant

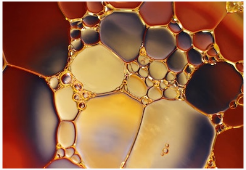
Surface Active Agents





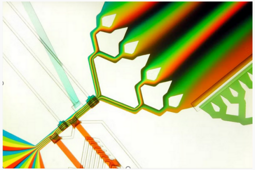
Applications

Emulsions



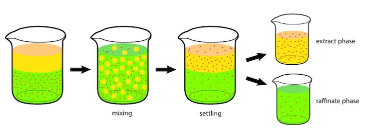
Detergents

Microfluidic devices



Example of CEA application: liquid-liquid extraction

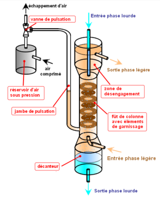
Principle of liquid-liquid extraction



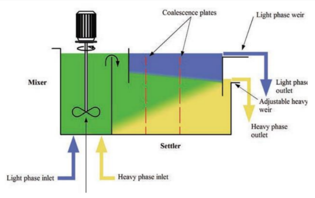
Transfer one chemical specie (red dots) from one phase (green) to another one (yellow) after mixing both fluids. A surfactant is used to lower the surface tension, promote emulsification and increase the surface of exchange.

Examples of liquid/liquid extraction devices (CEA/Marcoule/ISEC/DMRC)

Pulsed column



Mixer-decanter



From T. RANDRIAMANANTENA (SASP/LSPS)

First approach: Conservative Allen-Cahn and counter term

Free energy

$$\mathscr{F}[\phi, c] = \underbrace{\int_V \left[H\phi^2(1-\phi)^2 + \frac{\zeta}{2}(\nabla\phi)^2 \right] dV}_{\text{usual free energy for phase-field } \equiv \mathscr{F}[\phi]} + \int_V \underbrace{f_c(\phi, \nabla\phi, c)}_{\text{free energy for surfactant}} \; dV$$

$$f_c(\phi, \nabla\phi, c) = \frac{1}{\beta} \underbrace{\left[c \ln(c) + (1-c)\ln(1-c) \right]}_{(I)} - \underbrace{\frac{\epsilon}{2} c \left| \nabla\phi \right|^2}_{(II)} + \underbrace{\frac{k}{2} c \left[\phi - \frac{1}{2} \right]^2}_{(III)}$$

Physical meaning of each term

- (I): Mixing entropy, penalization of homogeneous mixtures ($c = 0$ or $c = 1$)
- (II): Energetic preferency for composition at interface (neg sign because $c \nearrow$ when $\mathscr{F} \searrow$)
- (III): Penalization of high compositions in the bulk

Chemical potential $\mu_c(\boldsymbol{x}, t)$ and bulk μ_c^b

Derivation of μ_c

$$\mathscr{F}[\phi, c] = \mathscr{F}[\phi] + \int \left\{ \frac{1}{\beta}[c\ln(c) + (1-c)\ln(1-c)] - \frac{\epsilon}{2} c\left|\boldsymbol{\nabla}\phi\right|^2 + \frac{k}{2} c \left[\phi - \frac{1}{2}\right]^2 \right\} dV$$

$$\begin{aligned} \mu_c(\boldsymbol{x}, t) &= \frac{\delta \mathscr{F}}{\delta c} = \frac{\partial f_c(\phi, \boldsymbol{\nabla}\phi, c)}{\partial c} \\ &= \frac{1}{\beta}\ln\left(\frac{c}{1-c}\right) - \frac{\epsilon}{2}\left|\boldsymbol{\nabla}\phi\right|^2 + \frac{k}{2}\left[\phi - \frac{1}{2}\right]^2 \end{aligned} \tag{134}$$

Bulk chemical potential

with $\begin{cases} c_b \ll 1 & \text{(input param)} \\ \phi_b = 0 \text{ or } \phi_b = 1 \\ \left|\boldsymbol{\nabla}\phi\right| = 0 \end{cases}$

Eq. (134) becomes

$$\boxed{\mu_c^b = \frac{1}{\beta}\ln(c_b) + \frac{k}{8}} \tag{135}$$

1D analytical solution at equilibrium $c^{eq}(x)$

Equilibrium: equality of chemical potential $\mu_c^b = \mu_c(x)$ (Eq. (135) = Eq. (134))

$$\frac{1}{\beta}\ln(c_b) + \frac{k}{8} = \frac{1}{\beta}\ln\left[\frac{c^{eq}(x)}{1-c^{eq}(x)}\right] - \frac{\epsilon}{2}\underbrace{|\partial_x\phi^{eq}|^2}_{\text{Eq. (50)}} + \frac{k}{2}\left(\phi^{eq}-\frac{1}{2}\right)^2$$

$$\frac{1}{\beta}\left\{\ln(c_b) - \ln\left[\frac{c^{eq}(x)}{1-c^{eq}(x)}\right]\right\} = \underbrace{-\frac{\epsilon}{2}\left[\frac{4}{W}\phi(1-\phi)\right]^2 + \frac{k}{2}\phi(\phi-1)}_{\equiv -G(\phi)}$$

$$\ln\left[\frac{1-c^{eq}(x)}{c^{eq}(x)}c_b\right] = -\beta G(\phi)$$

Finally

$$\boxed{c^{eq}(x) = \frac{c_b}{c_b + exp(-G(\phi))} \quad \text{with} \quad G(\phi) = \beta\phi(1-\phi)\left[\frac{8\epsilon}{W^2}\phi(1-\phi) + \frac{k}{2}\right]}$$

Remark for next slide:

$$\partial_x c^{eq} = \underbrace{\partial_x G(\phi^{eq})}_{\mathcal{P}(\phi^{eq})} c^{eq}(1-c^{eq})$$

Counter Term for composition equation

Transport equation

Conservation

$$\partial_t c = -\boldsymbol{\nabla} \cdot \boldsymbol{j}$$
$$\boldsymbol{j} = \boldsymbol{j}_{Adv} + \boldsymbol{j}_{Diff} + \boldsymbol{j}_{CT}$$

Fluxes

$$\boldsymbol{j}_{Adv} = c\boldsymbol{u} \qquad \text{(advection)}$$
$$\boldsymbol{j}_{Diff} = -M_c \boldsymbol{\nabla} c \qquad \text{(diffusion)}$$
$$\boldsymbol{j}_{Diff}^{eq} = -M_c \boldsymbol{\nabla} c^{eq} \qquad \text{(counter term)}$$

$\boldsymbol{j}_{CT}$ cancels $\boldsymbol{j}_{Diff}$ at equilibrium

$$\begin{aligned}
\boldsymbol{j}_{Diff}^{eq} &= -M_c \boldsymbol{\nabla}\left[\frac{c_b}{c_b + c_0(s)}\right] \\
&= -M_c \boldsymbol{n}_\phi \frac{\partial}{\partial s}\left[\frac{c_b}{c_b + c_0(s)}\right] \\
&= -M_c c^{eq}(1 - c^{eq})\mathcal{P}(\phi^{eq})\boldsymbol{n}_\phi
\end{aligned}$$

Finally

$$\boldsymbol{j}_{CT} = +M_c c(1 - c)\mathcal{P}(\phi)\boldsymbol{n}_\phi \qquad (136)$$

Mathematical model with surfactant

Navier-Stokes + Conservative Allen-Cahn

$$\boldsymbol{\nabla}\cdot\boldsymbol{u}=0,$$

$$\rho\left[\frac{\partial\boldsymbol{u}}{\partial t}+\boldsymbol{\nabla}\cdot(\boldsymbol{u}\boldsymbol{u})\right]=-\boldsymbol{\nabla}p_h+\boldsymbol{\nabla}\cdot\left[\eta(\boldsymbol{\nabla}\boldsymbol{u}+\boldsymbol{\nabla}\boldsymbol{u}^T)\right]+\boldsymbol{F}_{tot}$$

$$\frac{\partial\phi}{\partial t}+\boldsymbol{\nabla}\cdot(\boldsymbol{u}\phi)=\boldsymbol{\nabla}\cdot\left[M_\phi\left(\boldsymbol{\nabla}\phi-\frac{4}{W}\phi(1-\phi)\boldsymbol{n}_\phi\right)\right],$$

Composition equation for surfactant

$$\frac{\partial c}{\partial t}+\boldsymbol{\nabla}\cdot(c\boldsymbol{u})=\boldsymbol{\nabla}\cdot\left[M_c\left(\boldsymbol{\nabla}c-c(1-c)\mathcal{P}(\phi)\boldsymbol{n}_\phi\right)\right]$$

$$\mathcal{P}(\phi)=\beta\frac{4}{W}\phi(1-\phi)(1-2\phi)\left[\frac{k}{2}+\frac{16}{W^2}\epsilon(1-\phi)\phi\right]$$

Forces

Total force:

$$\boldsymbol{F}_{tot}=\boldsymbol{F}_c+\boldsymbol{F}_g+\boldsymbol{F}_M$$

Capillary and gravity forces:

$$\boldsymbol{F}_c=\mu_\phi\boldsymbol{\nabla}\phi \quad\text{and}\quad \boldsymbol{F}_g=\rho\boldsymbol{g}$$

Marangoni force $\boldsymbol{F}_M$

Previous slide Eq. (109)

Lattice Boltzmann scheme for composition

PDE

$$\frac{\partial \overbrace{c}^{\mathcal{M}_0}}{\partial t} + \nabla \cdot \overbrace{(c\boldsymbol{u})}^{\boldsymbol{\mathcal{M}}_1} + \nabla \cdot \overbrace{\left[M_c c(1-c)\mathcal{P}(\phi)\boldsymbol{n}_\phi\right]}^{\boldsymbol{j}_{CT}=\boldsymbol{\mathcal{M}}_1} = \nabla \cdot \left(M_c \nabla \cdot \underbrace{c\boldsymbol{I}}_{\boldsymbol{\mathcal{M}}_2}\right)$$

Equilibrium distribution function

$$h_i^{eq} = \underbrace{w_i c\left(1 + \frac{\boldsymbol{u}\cdot\boldsymbol{c}_i}{c_s^2}\right)}_{h_i^{eq,ADE}} + \underbrace{\overbrace{M_c c(1-c)\mathcal{P}(\phi)\boldsymbol{n}_\phi}^{\boldsymbol{j}_{CT}} \cdot \left(\frac{w_i \boldsymbol{c}_i}{c_s^2}\right)}_{h_i^{eq,CT}} \tag{137}$$

V. Comparison with analytical solutions

Validation with analytical solutions

Equilibrium phase-field

$$\phi^{eq}(x) = \frac{1}{2}\left[1 + \tanh\left(\frac{2x}{W}\right)\right]$$

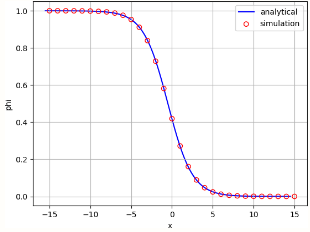
Equilibrium composition

$$c^{eq}(x) = \frac{c_b}{c_b + exp\left[-G(\phi^{eq}(x))\right]}$$

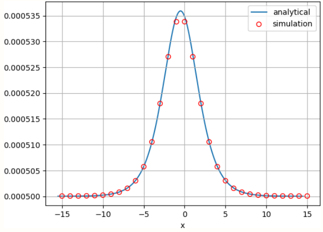
$$G(\phi) = \beta\phi(1-\phi)\left[\frac{8\epsilon}{W^2}\phi(1-\phi) + \frac{k}{2}\right]$$

Verifications from S. Cappe (2024)

ϕ-profile



c-profile



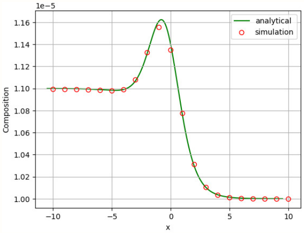
Expansion with different solubilities in bulk phases

Sman & Meinder (2016)

$$\mathscr{F}_{SG}[\phi, c] = \underbrace{\mathscr{F}_{SM}[\phi, c]}_{(I,II,III,IV)} + \int \underbrace{2\gamma\phi c}_{(V)} d\boldsymbol{x}$$

- (V) $\rightarrow$ For different compositions in the bulks
- $G_{bis}(\phi) = \beta\phi(1-\phi)\left(\frac{8\epsilon}{W^2}\phi(1-\phi) + \frac{k}{2}\right) - 2\beta\gamma\phi$
- $\mathcal{P}_{bis}(\phi) = \frac{4\beta}{W}\phi(1-\phi)\left[\frac{k}{2}(1-2\phi) + \frac{16\epsilon}{W^2}\phi(1-\phi)(1-2\phi) - 2\gamma\right]$
- $\gamma = \frac{1}{2\beta}\ln\left(\frac{c_{b,1}}{c_{b,0}}\right)$

From S. Cappe (2024)



Analytical solution

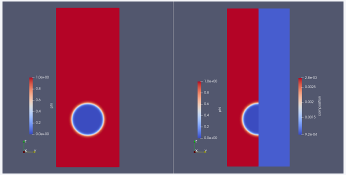
$$c^{analytical}(x) = \frac{c_b^0}{c_b^1 + exp\left\{\beta\phi(1-\phi)\left[\frac{8\epsilon}{W^2}\phi(1-\phi) + \frac{k}{2}\right] - 2\beta\gamma\phi\right\}}$$

P. Simulations with and without surfactant

Run `TestCase15_Surfactant`

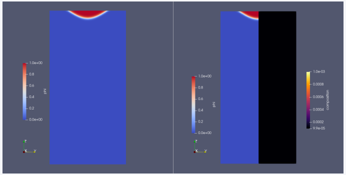
Surfactant effect on two-phase flows

Rising bubble



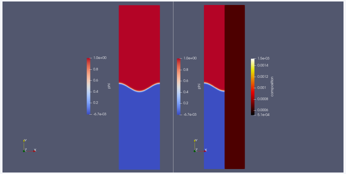
Video

Falling droplet



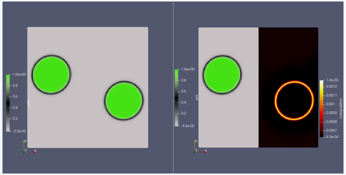
Video

Rayleigh-Taylor



Video

Coalescence of two droplets inside flow



Video

Second approach: Cahn-Hilliard and surfactant equation

Free energy with phase-field ϕ and c composition of surfactant

$$\mathscr{F}[\phi, c] = \underbrace{\int_V \mathcal{F}_\phi(\phi, \nabla\phi) dV}_{\text{unchanged}} + \underbrace{\int_V [f_s(\phi, c) + f_b(\phi, c)]\, dV}_{\text{surfactant}}$$

- Composition at interface (surfactant)

$$f_s(\phi, c) = -\frac{\alpha}{2} c\phi^2 (1-\phi)^2$$

Negative sign because $c \nearrow$ when $\mathscr{F} \searrow$ and α positive coefficient

- Composition in bulk phases

$$f_b(\phi, c) = \underbrace{\theta[c \log c + (1-c)\log(1-c)]}_{\text{entropy of mixing}\equiv f_c^{mix}} + \underbrace{p(\phi) f_{\ell_1}(c) + (1-p(\phi)) f_{\ell_2}(c)}_{\text{bulks interpolated by } p(\phi)}$$

Free energy of bulks

Composition

- Free energy of bulks

$$\begin{cases} f_{\ell_1}(c) & = \frac{1}{2}(\beta c^2 + 2\gamma c) \\ f_{\ell_2}(c) & = \frac{1}{2}(\beta c^2 - 2\gamma c) \\ p(\phi) & = \phi^2(3-2\phi) \end{cases} \longrightarrow \quad p(\phi) f_{\ell_1}(c) + (1-p(\phi)) f_{\ell_2}(c) = \frac{\beta}{2}c^2 + 2\gamma c p(\phi) - \gamma c$$

- The free energy $f_b(\phi, c)$ writes:

$$f_b(\phi, c) = \underbrace{\theta[c \log c + (1-c)\log(1-c)]}_{\text{entropy of mixing} \equiv f_c^{mix}} + \underbrace{\frac{\beta}{2}c^2}_{\text{diffusive term}} + 2\gamma c \underbrace{\phi^2(3-2\phi)}_{p(\phi)} - \gamma c$$

Mathematical model: Cahn-Hilliard + composition Eq

Cahn-Hilliard equation

$$\frac{\partial \phi}{\partial t} + \nabla \cdot (\boldsymbol{u}\phi) = \nabla \cdot [M_\phi \nabla \mu_\phi]$$

$$\mu_\phi = \frac{\delta \mathscr{F}}{\delta \phi} = \underbrace{4H\phi(\phi-1)(\phi-\frac{1}{2}) - \zeta \nabla^2 \phi}_{\text{stand. C-H.}} + \underbrace{2\gamma c p'(\phi) - 2\alpha c \phi(\phi-1)(\phi-1/2)}_{\text{coupling with term involving } c}$$

Surfactant equation

$$\frac{\partial c}{\partial t} + \nabla \cdot (\boldsymbol{u}c) = \nabla \cdot [M_c \nabla \mu_c]$$

$$\mu_c = \frac{\delta \mathscr{F}}{\delta c} = \underbrace{\theta[\log c - \log(1-c)]}_{\partial_c f_c^{mix}} + \underbrace{\beta c}_{\text{diffusive term}} + \underbrace{2\gamma p(\phi) - \frac{\alpha}{2} g_1(\phi)}_{\text{term involving } \phi} - \gamma$$

Thermodynamic equilibrium: c-profile

Equilibrium chemical potentials

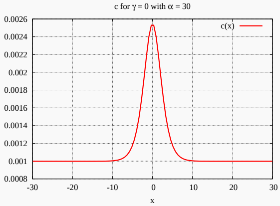
The concentration of surfactant in bulk phases $c_b \ll 1$. The chemical potential is

$$\mu_c^b = \theta \log(c_b) \; + \; 2\gamma\phi_b^2(3 - 2\phi_b) \; - \; \gamma$$

Analytical solution of composition c at equilibrium

At equilibrium $\mu_c(x) = \mu_c^b$, we obtain

$$c(x) = \frac{c_b}{c_b + c_0(x)e^{\frac{\beta}{\theta}c(x)}}$$

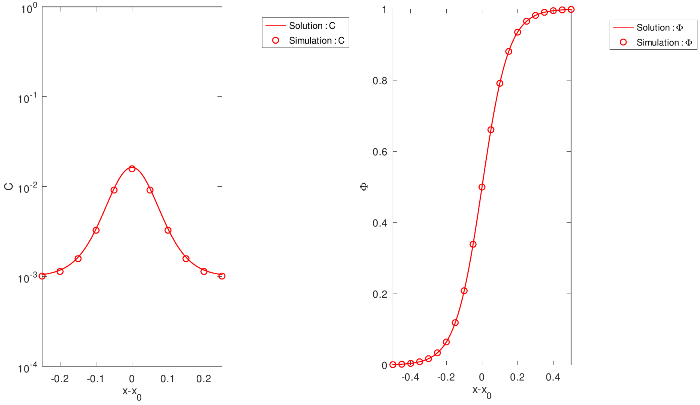


with

$$c_0(x) = \exp\left\{\frac{1}{\theta}\left[2\gamma(\phi_0(x)^2(3 - 2\phi_0(x)) - \phi_b^2(3 - 2\phi_b)) \; - \; \frac{\alpha}{2}\phi_0(x)^2(1 - \phi_0(x))^2\right]\right\}$$

Verification: ϕ and c

Comparison with analytical solution



- Mesh

  $\delta x = 10^{-3}, \ \delta t = 5 \times 10^{-6}$

  $n_x = 500, \ n_y = 10$

- Phase-field

  $M_\phi = 1.2 \times 10^{-2}$

  $W = 0.003, \ \sigma = 5 \times 10^{-6}$

- Composition

  $M_C = 1.2 \times 10^{-2}$

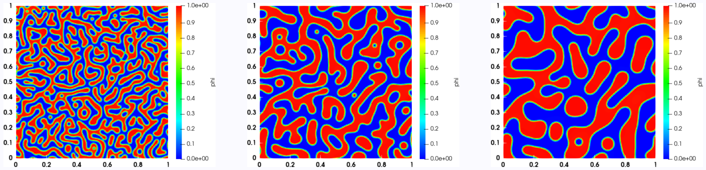
  $C_0 = 0.1$

Spinodal decomposition with surfactant

From H. De Gieter (2022)

Cahn-Hilliard for phase-field $\phi(\boldsymbol{x}, t)$

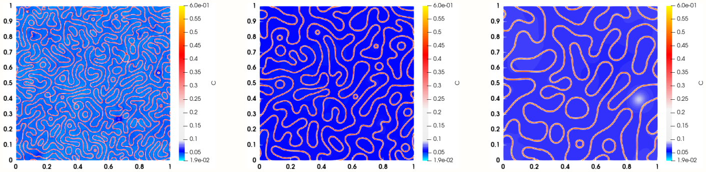
$t_0 = 0$ $\quad$ $t_1 = 10\delta t$ $\quad$ $t_2 = 10^3\,\delta t$



Two immiscible liquids demixing

Composition $c(\boldsymbol{x}, t)$ for surfactant

$t_0 = 0$ $\quad$ $t_1 = 10\delta t$ $\quad$ $t_2 = 10^3\,\delta t$



Sorption of the chemical specie at the interface between both fluids ▸ Video

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5. van der Waals fluids

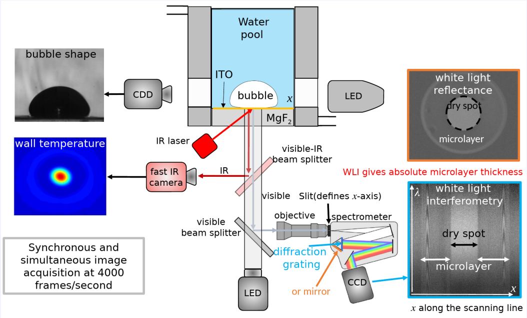
The Navier-Stokes/Korteweg model of phase change

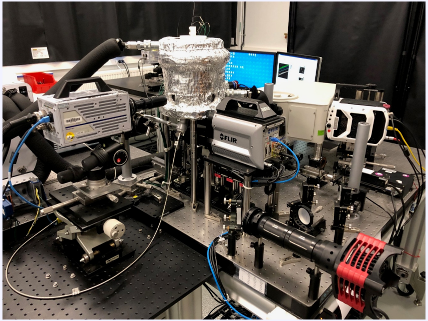
Outline section 5

Example of liquid/vapor phase change experiment

CEA device for studying phase change (Saclay/ISAS/DM2S)

A vapor bubble grows inside a pool filled with liquid water. The surface is heated by a laser.



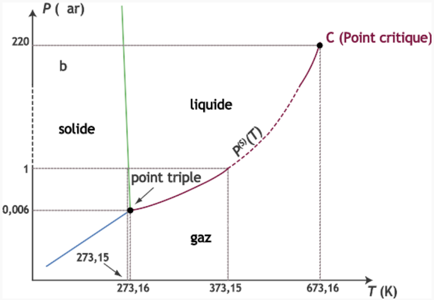


From C. TECCHIO (STMF/LE2H, 2022)

Phase diagrams of water

Phase diagram $P - T$ of water

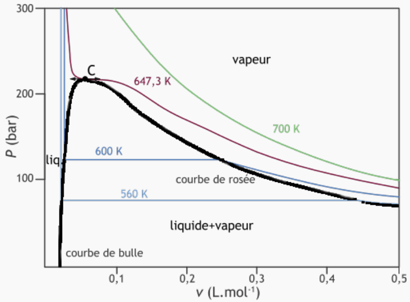
Solid/liquid/gas phases



The liquid and vapor coexist at saturation curve $P^{sat}(T)$ which is invertible: $T^{sat}(P)$

Clapeyron diagram

Saturation curve and Andrews isotherms



The liquid and vapor coexist within the area delimited by the saturation curve (black)

Clapeyron relation

Clapeyron relation

$$\frac{dP^{sat}}{dT} = \frac{h_g^{sat} - h_l^{sat}}{T(v_g^{sat} - v_l^{sat})} = \frac{\mathcal{L}}{T(v_g^{sat} - v_l^{sat})} \qquad (138)$$

Proof

At equilibrium

$$\mu_l^{eq}(T, P^{sat}(T)) = \mu_g^{eq}(T, P^{sat}(T))$$

Derivation for

$$\mu_l^{eq}(T + dT, P^{sat} + dP^{sat}) = \mu_g^{eq}(T + dT, P^{sat} + dP^{sat})$$

Taylor expansions for $\Phi = l, g$

$$\mu_\Phi^{eq}(T + dT, P^{sat} + dP^{sat}) \simeq \mu_\Phi^{eq}(T, P^{sat}(T)) + \underbrace{\frac{\partial \mu_\Phi^{eq}}{\partial T}}_{-s_\Phi^{sat}} dT + \underbrace{\frac{\partial \mu_\Phi^{eq}}{\partial P}}_{v_\Phi^{sat}} dP^{sat}$$

Equality

$$-s_l^{sat} dT + v_l^{sat} dP^{sat} = -s_g^{sat} dT + v_g^{sat} dP^{sat}$$

$$\frac{dP^{sat}}{dT} = \frac{(s_g^{sat} - s_l^{sat})}{(v_g^{sat} - v_l^{sat})}$$

And finally, relation for $s_g^{sat} - s_l^{sat}$

$$g_l = g_g$$
$$h_l - Ts_l = h_g - Ts_g$$
$$s_g - s_l = (h_g - h_l)/T = \mathcal{L}/T$$

Low Mach Navier-Stokes equations (NS)

Low Mach Navier-Stokes with "equation of state" (eos)

$$\partial_t \rho + \boldsymbol{\nabla} \cdot (\rho \boldsymbol{u}) = 0 \tag{139}$$

$$\partial_t (\rho \boldsymbol{u}) + \boldsymbol{\nabla} \cdot (\rho \boldsymbol{u}\boldsymbol{u}) = -\boldsymbol{\nabla} p + \boldsymbol{\nabla} \cdot \left[\eta (\boldsymbol{\nabla} \boldsymbol{u} + (\boldsymbol{\nabla} \boldsymbol{u})^T) + \left(\eta_B - \frac{2}{3}\eta \right) (\boldsymbol{\nabla} \cdot \boldsymbol{u}) \boldsymbol{I} \right] + \boldsymbol{F} \tag{140}$$

- **Isothermal EoS** $p = \rho R T_0$ where T_0 constant temperature and R specific gas constant
- **Unknown**: density $\rho \equiv \rho(\boldsymbol{x}, t)$, velocity $\boldsymbol{u} \equiv \boldsymbol{u}(\boldsymbol{x}, t)$ and pressure $p \equiv p(\boldsymbol{x}, t)$
- **Parameters**: dynamic viscosity $\eta = \nu \rho$ (kinematic viscos ν), bulk viscos η_B, force $\boldsymbol{F}$

In this section: two-phase by modification of Equation of State

Nomenclature of this section

Thermodynamics

Functions				Parameters		
Name	Local	Non-local	Dim	Name	Local	Dim
Free energy density	$f(\rho, T)$	$\mathcal{F}(\rho, \boldsymbol{\nabla}\rho, T)$	$[E]/[L]^3$	Latent heat	$\mathcal{L}$	$[E]/[M]$
Specific internal energy	$e(\rho, T)$	$\mathcal{E}(\rho, \boldsymbol{\nabla}\rho, T)$	$[E]/[M]$	Thermal conductivity	Λ	$[E]/[\Theta].[T].[L]$
Specific entropy	$s(\rho, T)$	$\mathcal{S}(\rho, \boldsymbol{\nabla}\rho, T)$	$[E]/([M].[\Theta])$	Specific heat	C_V	$[E]/[M].[\Theta]$
Dissipation		$\mathcal{D}(\rho, \boldsymbol{\nabla}\rho, T)$	$[E]/([L]^3.[T].[\Theta])$	Capillary coefficient	ζ	$[E].[L]^5/[M]^2$
Chemical potential	$\mu^{(0)}(\rho, T)$	$\mu(\rho, \boldsymbol{\nabla}\rho, T)$	$[E]/[M]$	Specific gas constant	R	$[E]/[M].[\Theta]$
Pressure	$p^{eos}(\rho, T)$	$\mathcal{P}(\rho, \boldsymbol{\nabla}\rho, T)$	$[E]/[L]^3$	Attractive interactions coeff	a	$[E].[L]^3/[M]^2$
Pressure tensor		$\overline{\overline{\boldsymbol{P}}}(\rho, \boldsymbol{\nabla}\rho, T)$	$[E]/[L]^3$	Excluded volume	b	$[L]^3/[M]$
Material time derivative	$d/dt = \partial_t + \boldsymbol{u}\cdot\boldsymbol{\nabla}$		$1/[T]$			

a. Constant temperature T_0

Eq of state, non-local pressure and Korteweg's tensor

Free energy functional with density ρ

Free energy with order parameter ρ

$$\mathscr{F}[\rho] = \int_V \underbrace{f(\rho) + \frac{\zeta}{2}\left|\boldsymbol{\nabla}\rho\right|^2}_{\equiv \mathcal{F}(\rho, \boldsymbol{\nabla}\rho)} dV \tag{141}$$

- The new phase index is the density ρ
- $f(\rho)$ is the local free energy density
- $\left|\boldsymbol{\nabla}\rho\right|^2/2$ is the gradient energy term
- ζ is the capillary coefficient

Remarks

- Here f has a dimension [E]/[L]^3
- But we could have defined a specific f (dim [E]/[M]) and

$$\mathcal{F}(\rho, \boldsymbol{\nabla}\rho) = \rho f(\rho) + \frac{\zeta}{2}\left|\boldsymbol{\nabla}\rho\right|^2$$

Chemical potential μ_ρ

Euler-Lagrange

$$\begin{aligned}\mu_\rho &= \frac{\partial \mathcal{F}}{\partial \rho} - \boldsymbol{\nabla}\cdot\left[\frac{\partial \mathcal{F}}{\partial(\boldsymbol{\nabla}\rho)}\right] \\ &= \partial_\rho f(\rho) - \boldsymbol{\nabla}\cdot(\zeta\boldsymbol{\nabla}\rho) \\ &= f'(\rho) - \zeta\boldsymbol{\nabla}^2\rho\end{aligned} \tag{142}$$

Free energy density close to the critical point

Classical double-well

Close to the critical point we can approximate:

$$f(\rho) \approx f_{dw}(\rho) = H(\rho - \rho_l)^2(\rho - \rho_g)^2 = Hg_2(\rho)$$

Equilibrium interface properties (see slide section 2a)

$$\rho(x) = \frac{\rho_l + \rho_g}{2} + \frac{\rho_l - \rho_g}{2} \tanh\left[\frac{2x}{W}\right] \qquad \text{Density profile}$$

$$W = \frac{4}{\rho_l - \rho_g}\sqrt{\frac{\zeta}{2H}} \qquad \text{Interface width}$$

$$\sigma = \int_{-\infty}^{+\infty} \zeta(\partial_x \rho)^2 dx = \frac{1}{6}(\rho_l - \rho_g)^3 \sqrt{2\zeta H} \qquad \text{Surface tension}$$

In what follows: alternative way to define the free energy density $f(\rho)$

Beyond the perfect gas: the van der Waals eq. of state

Internal energy e_{vdW} of a van der Waals fluid (pg: perfect gas)

$$e_{vdW} = \underbrace{e_{pg}}_{\text{int energy}} - \underbrace{aN\varrho}_{\text{pot. en. of molecular interaction}}$$

$$\underbrace{\frac{\partial e_{vdW}}{\partial V}}_{\equiv -p_{vdW}} = \underbrace{\frac{\partial e_{pg}}{\partial V}}_{\equiv -p_{pg}} + \frac{aN^2}{V^2}$$

$$p_{pg} = p_{vdW} + \frac{aN^2}{V^2} \qquad (143)$$

$$V = V_{pg} + \underbrace{Nb}_{\text{vol occupied by } N \text{ moles}}$$

$$V_{pg} = V - Nb \qquad (144)$$

- N: number of moles
- ϱ: volumic density of molecules $\varrho = N/V$
- a: attractive interaction coeff
- b: excluded volume

Perfect gas Eq. of State

$$p_{pg} V_{pg} = NRT \qquad (145)$$

Rq: Eq. (146) can be expressed with ρ with $v = V/N$ and $\rho = 1/v$ (see next slide)

van der Waals Eq. of state

use Eqs. (143) & (144) in (145):

$$\left(p_{vdW} + \frac{aN^2}{V^2}\right)(V - Nb) = NRT \qquad (146)$$

Thermodynamic pressure $p^{eos}(\rho, T)$

Thermodynamic pressure: $p^{eos}(\rho, T) = \rho\partial_\rho f(\rho, T) - f(\rho, T)$

van der Waals (vdW) Equation of State (*eos*)

$$p^{eos}_{vdW}(\rho, T) = \frac{\rho RT}{1-\rho b} - a\rho^2 \qquad (147)$$

Free energy density

$$f(\rho, T) = \rho \int \frac{p^{eos}(\rho, T)}{\rho^2} d\rho \qquad (148)$$

The van der Waals *eos* explains phase transition ($v = 1/\rho$ is the specific volume)

Diagram $p - v$

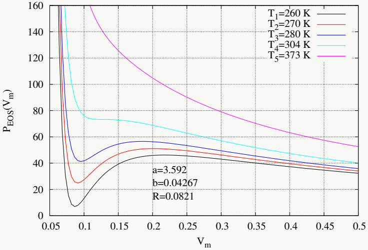
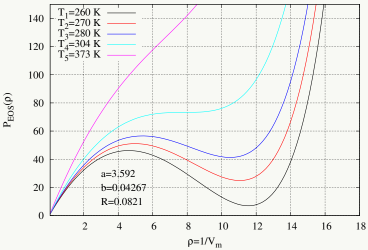


Diagram $p - \rho$ with $\rho = 1/v$



Critical point

Critical point

The critical point corresponds to the presence of an inflexion point on the curve $p(v)$:

$$\frac{\partial p^{eos}}{\partial v} = 0 \qquad \text{and} \qquad \frac{\partial^2 p^{eos}}{\partial v^2} = 0$$

Critical point for van der Waals eq. of state p_{vdW}^{eos}

$$v_c = 3b, \qquad T_c = \frac{8}{27}\frac{a}{Rb}, \qquad p_c = \frac{1}{27}\frac{a}{b^2}$$

If T_c and P_c are known for a pure substance, the relations can be interverted to obtain a and b:

$$b = \frac{RT_c}{8p_c}, \qquad a = \frac{27}{64}\frac{R^2 T_c^2}{p_c}$$

Densities of coexistence 1/2: Maxwell construction

Maxwell construction for eq densities ρ_l and ρ_g

- Solutions P^{sat}, v_l and v_g are such as $S_1 = S_2$

$$\underbrace{\int_{v_l}^{v_g} p^{eos}(v)dv}_{S_1} = \underbrace{P^{sat}(v_g - v_l)}_{S_2} \qquad (149)$$

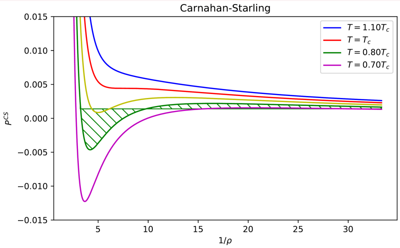
- e.g. for van der Waals eos:

$$p^{eos}_{vdW}(v) = \frac{RT}{v-b} - a\left(\frac{1}{v}\right)^2$$

$$S_1 = \left[RT\ln(v_g - b) + \frac{a}{v_g}\right] - \left[RT\ln(v_l - b) + \frac{a}{v_l}\right]$$

$$S_2 = P^{sat}(v_g - v_l)$$

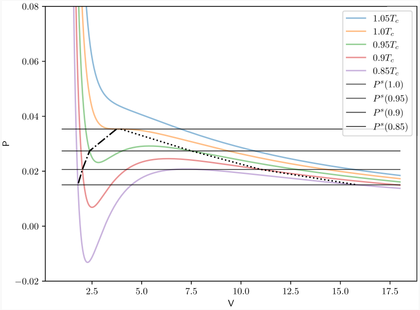
- Geometric interpretation: for a given isotherm (e.g. green one),the solutions are such as the areas above and below P^{sat} are equal



Densities of coexistence 2/2: saturation curve

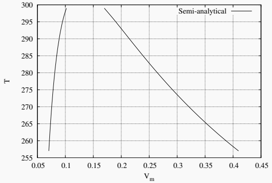
Solutions ρ_l and ρ_g for van der Waals *eos*

Diagram P–v

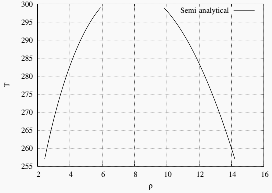


- Remark: diagram $\rho(T)$ corresponds to the binodal line of diagram $c(T)$ section 1

v_g and v_l function of T



ρ_l and ρ_g function of T



Common tangent construction

Equilibrium conditions for two phases

- Equality of intensive variables

$$\mu^{loc}(\rho_g) = \mu^{loc}(\rho_l) = \mu^{eq}$$
$$p^{eos}(\rho_g) = p^{eos}(\rho_l) = P^{sat}$$

- Expressed with their definitions with f:

$$\left.\frac{\partial f}{\partial \rho}\right|_{\rho_g} = \left.\frac{\partial f}{\partial \rho}\right|_{\rho_l} = \mu^{eq} \qquad (150)$$
$$\rho_g \mu^{eq} - f(\rho_g) = \rho_l \mu^{eq} - f(\rho_l) \qquad (151)$$

- Conditions (151) and (150):

Common tangent construction

$$\frac{f(\rho_g) - f(\rho_l)}{\rho_g - \rho_l} = \mu^{eq}$$

with

$$\mu^{eq} = f'(\rho_g) = f'(\rho_l)$$

Equivalence Maxwell construction and common tangent

Maxwell construction for eq densities ρ_l and ρ_g

- Equilibrium condition

$$P^{sat} = p^{eos}(\rho_l) = p^{eos}(\rho_g)$$

- Definitions

$$\frac{f(\rho)}{\rho} \hat{=} \int \frac{p^{eos}(\rho)}{\rho^2} d\rho$$

$$p^{eos}(\rho_l) \hat{=} \rho_l f'(\rho_l) - f(\rho_l)$$

$$p^{eos}(\rho_g) \hat{=} \rho_g f'(\rho_g) - f(\rho_g)$$

- Maxwell construction expressed with ρ:

$$\frac{\rho_l \rho_g}{\rho_l - \rho_g} \int_{\rho_g}^{\rho_g} \frac{p^{eos}(\varrho)}{\varrho^2} d\varrho = P^{sat}$$

$$\frac{\rho_l \rho_g}{\rho_l - \rho_g} \left[\frac{f(\rho_l)}{\rho_l} - \frac{f(\rho_g)}{\rho_g} \right] = P^{sat}$$

$$\frac{\rho_l \rho_g}{\rho_l - \rho_g} \left[\frac{f(\rho_l)}{\rho_l} - \frac{f(\rho_g)}{\rho_g} \right] = \rho_l \mu^{eq} - f(\rho_l)$$

- Finally:

$$\boxed{\mu^{eq} = \frac{f(\rho_l) - f(\rho_g)}{\rho_l - \rho_g}}$$

Eq. of State and chemical potentials

van der Waals (*vdW*)

$$p_{vdW}^{eos}(\rho, T) = \frac{\rho RT}{1 - \rho b} - a\rho^2 \tag{152a}$$

$$f_{vdW}(\rho, T) = \rho RT \ln\left(\frac{\rho}{1 - b\rho}\right) - a\rho^2 \tag{152b}$$

$$\mu_\rho^{vdW}(\rho, T) = RT\left[\ln\left(\frac{\rho}{1 - b\rho}\right) + \frac{1}{1 - b\rho}\right] - 2a\rho - \kappa\boldsymbol{\nabla}^2\rho \tag{152c}$$

Carnahan-Starling (*CS*)

$$p_{CS}^{eos}(\rho, T) = \rho RT\frac{1 + b\rho/4 + (b\rho/4)^2 - (b\rho/4)^3}{(1 - b\rho/4)^3} - a\rho^2 \tag{153a}$$

$$f_{CS}(\rho, T) = \rho RT\left[\frac{3 - b\rho/2}{(1 - b\rho/4)^2} + \ln(b\rho/4)\right] - a\rho^2 \tag{153b}$$

$$\mu_\rho^{CS}(\rho, T) = RT\left[\frac{3 - b\rho/4}{(1 - b\rho/4)^3} + \ln(b\rho/4) + 1\right] - 2a\rho - \kappa\boldsymbol{\nabla}^2\rho \tag{153c}$$

Other popular cubic Eq. of State

Redlich-Kwong (*RK*)

$$p^{eos}_{RK}(\rho, T) = \frac{\rho R T}{1 - b\rho} - \frac{a\alpha(T)\rho^2}{1 + b\rho}$$

$$\alpha(T) = 1/\sqrt{T}$$

$$\text{Soave modif } \alpha(T) = [1 + (\alpha_1 + \alpha_2\omega - \alpha_3\omega^2)(1 - \sqrt{T/T_c})]^2$$

$$\text{coeff}\alpha_1 = 0.480, \quad \alpha_2 = 1.574, \quad \alpha_3 = 0.176$$

Peng-Robinson (*PR*)

$$p^{eos}_{PR}(\rho, T) = \frac{\rho R T}{1 - b\rho} - \frac{a\alpha(T)\rho^2}{1 + 2b\rho - b^2\rho^2}$$

$$\alpha(T) = [1 + (\alpha_1 + \alpha_2\omega + \alpha_3\omega^2)(1 - \sqrt{T/T_c})]^2$$

$$\text{coeff}\alpha_1 = 0.37464, \quad \alpha_2 = 1.54226, \quad \alpha_3 = 0.26992$$

b. Navier-Stokes/Korteweg model

Non-local pressure and pressure tensor

Consequence of $|\boldsymbol{\nabla}\rho|^2$ in $\mathcal{F}(\rho, \boldsymbol{\nabla}\rho)$

- Def of thermo pressure with $\boldsymbol{\nabla}\rho$:

$$\mathcal{P}(\rho, \boldsymbol{\nabla}\rho) = \rho \frac{\delta \mathcal{F}(\rho, \boldsymbol{\nabla}\rho)}{\delta \rho} - \mathcal{F}(\rho, \boldsymbol{\nabla}\rho)$$

- Application: non-local pressure $\mathcal{P}(\rho, \boldsymbol{\nabla}\rho)$

$$\boxed{\mathcal{P}(\rho, \boldsymbol{\nabla}\rho) = p^{eos}(\rho) - \zeta\rho\boldsymbol{\nabla}^2\rho - \frac{\zeta}{2}|\boldsymbol{\nabla}\rho|^2} \qquad (154)$$

In an inhomogeneous system, the variations in ρ contribute

Noether's theorem and pressure tensor $\overline{\overline{\boldsymbol{P}}}$ (see GOLDSTEIN Sec 12-3 & 12-7)

Noether's theorem: because $\mathcal{F}$ does not depend on $\boldsymbol{x}$, there exists a quantity $\overline{\overline{\boldsymbol{P}}}$ that is conserved:

$$\boldsymbol{\nabla} \cdot \overline{\overline{\boldsymbol{P}}} = \boldsymbol{0}$$

where

$$\overline{\overline{\boldsymbol{P}}} = \mathscr{L}\overline{\overline{\boldsymbol{I}}} - \boldsymbol{\nabla}\rho \otimes \frac{\partial \mathscr{L}}{\partial(\boldsymbol{\nabla}\rho)}$$

$$\mathscr{L}(\rho, \boldsymbol{\nabla}\rho) = \mathcal{F}(\rho, \boldsymbol{\nabla}\rho) - \rho\mu_\rho$$

$$\overline{\overline{\boldsymbol{P}}} = \mathcal{P}(\rho, \boldsymbol{\nabla}\rho)\overline{\overline{\boldsymbol{I}}} + \underbrace{\zeta\boldsymbol{\nabla}\rho \otimes \boldsymbol{\nabla}\rho}_{\text{Korteweg's tensor}} \qquad (155)$$

- The surface tension comes from Korteweg's tensor

Interpretation of Korteweg tensor

Equilibrium

No fluid motion, no friction, and eq conditions:

$$\nabla \cdot \overline{\overline{\boldsymbol{P}}}^{eq} = \boldsymbol{0}$$

Hypothesis: planar interface

$$\overline{\overline{\boldsymbol{P}}}^{eq} = \mathcal{P}\overline{\overline{\boldsymbol{I}}} + \zeta(\partial_z\rho)^2 \boldsymbol{e}_z \otimes \boldsymbol{e}_z$$

Force balance along z:

$$\partial_z P_{zz} = 0 \longrightarrow \mathcal{P}(z) + \zeta(\partial_z\rho)^2 = P_b$$

$$\mathcal{P}(z) = P_b - \zeta(\partial_z\rho)^2$$

where P_b is bulk pressure

Interface force

- Normal force to the interface (ind z)

$$\begin{aligned}\boldsymbol{F}_z &= \overline{\overline{\boldsymbol{P}}}^{eq} \cdot \boldsymbol{e}_z \\ &= [P_b - \cancel{\zeta(\partial_z\rho)^2} + \cancel{\zeta(\partial_z\rho)^2}]\, \boldsymbol{e}_z \\ &= P_b \boldsymbol{e}_z\end{aligned}$$

- Tangential force: depends on z

$$\begin{aligned}\boldsymbol{F}_x &= \overline{\overline{\boldsymbol{P}}}^{eq} \cdot \boldsymbol{e}_x \\ &= \left[P_b - \zeta(\partial_z\rho)^2\right] \boldsymbol{e}_x\end{aligned}$$

- Surface tension:

$$\sigma = \int_{-\infty}^{+\infty} \zeta(\partial_z\rho)^2 dz$$

Isothermal Navier-Stokes/Korteweg model

Conservation equations

$$\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla} \cdot (\rho \boldsymbol{u}) = 0 \quad (156a)$$

$$\frac{\partial (\rho \boldsymbol{u})}{\partial t} + \boldsymbol{\nabla} \cdot (\rho \boldsymbol{u}\boldsymbol{u}) = -\boldsymbol{\nabla} \cdot \overline{\overline{\boldsymbol{P}}} + \boldsymbol{\nabla} \cdot \overline{\overline{\boldsymbol{\tau}}} \quad (156b)$$

Closures

- Viscous stress tensor:

$$\overline{\overline{\boldsymbol{\tau}}} = \eta \left(\boldsymbol{\nabla} \boldsymbol{u} + \boldsymbol{\nabla} \boldsymbol{u}^T \right) + \left(\eta_B - \frac{2}{3}\eta \right) (\boldsymbol{\nabla} \cdot \boldsymbol{u}) \overline{\overline{\boldsymbol{I}}} \quad (157)$$

- Tensor pressure

$$\overline{\overline{\boldsymbol{P}}} = \left[p^{eos} - \zeta \rho \boldsymbol{\nabla}^2 \rho - \frac{1}{2} \zeta |\boldsymbol{\nabla} \rho|^2 \right] \overline{\overline{\boldsymbol{I}}} + \zeta \boldsymbol{\nabla} \rho \otimes \boldsymbol{\nabla} \rho \quad (158)$$

- Equation of state for pressure:

$$p^{eos} \equiv p^{eos}(\rho, T) = \rho \partial_\rho f - f \quad (159)$$

- e.g. for f_{vdW} van der Waals:

$$p^{eos}_{vdW}(\rho, T_0) = \frac{\rho R T}{1 - b\rho} - a\rho^2 \quad (160)$$

Equivalence of pressure tensor 1/2: *eos* pressure and force

Equivalence 1

$$-\boldsymbol{\nabla}\cdot\overline{\overline{\boldsymbol{P}}} = -\nabla p^{eos} + \boldsymbol{F} \qquad \text{with} \qquad \boldsymbol{F} = \zeta\rho\boldsymbol{\nabla}(\boldsymbol{\nabla}^2\rho) \tag{161}$$

Demo

$$\begin{aligned}
\partial_\beta P_{\alpha\beta} &= \partial_\beta\left\{\left[p^{eos} - \zeta\rho\partial_\gamma\partial_\gamma\rho - \frac{1}{2}\zeta(\partial_\gamma\rho)^2\right]\delta_{\alpha\beta} + \zeta(\partial_\alpha\rho)(\partial_\beta\rho)\right\}\\
&= \partial_\alpha p^{eos} - \partial_\alpha(\zeta\rho\partial_\gamma\partial_\gamma\rho) - \frac{1}{2}\underbrace{\partial_\alpha(\zeta(\partial_\gamma\rho)^2)}_{\text{development}} + \underbrace{\partial_\gamma(\zeta(\partial_\alpha\rho)(\partial_\gamma\rho))}_{\text{index } \beta\rightarrow\gamma}\\
&= \partial_\alpha p^{eos} - \partial_\alpha(\zeta\rho\partial_\gamma\partial_\gamma\rho) - [\zeta(\partial_\gamma\rho)(\partial_\alpha\partial_\gamma\rho)] + \underbrace{\partial_\gamma(\zeta(\partial_\alpha\rho)(\partial_\gamma\rho))}_{\text{Development}}\\
&= \partial_\alpha p^{eos} - \underbrace{\partial_\alpha(\zeta\rho\partial_\gamma\partial_\gamma\rho)}_{\text{Development}} - [\cancel{\zeta(\partial_\gamma\rho)(\partial_\alpha\partial_\gamma\rho)}] + [\cancel{\zeta\partial_\gamma(\partial_\alpha\rho)(\partial_\gamma\rho)} + \zeta(\partial_\alpha\rho)\partial_\gamma(\partial_\gamma\rho)]\\
&= \partial_\alpha p^{eos} - [\cancel{\zeta(\partial_\alpha\rho)\partial_\gamma\partial_\gamma\rho} + \zeta\rho\partial_\alpha\partial_\gamma\partial_\gamma\rho] + \cancel{\zeta(\partial_\alpha\rho)\partial_\gamma(\partial_\gamma\rho)}\\
&= \partial_\alpha p^{eos} - \zeta\rho\partial_\alpha(\partial_\gamma\partial_\gamma\rho)
\end{aligned}$$

Equivalence of pressure tensor 2/2: chemical potential

Equivalence 2

$$-\nabla \cdot \overline{\overline{P}} = -\rho \nabla \mu_\rho \tag{162}$$

Demo

Chemical potential

$$\mu_\rho = f'(\rho) - \zeta \nabla^2 \rho$$

Thermodynamic pressure

$$p^{eos}(\rho) = \rho f'(\rho) - f(\rho)$$

$$\begin{aligned}
\rho \nabla \mu_\rho &= \rho \nabla \left[\frac{1}{\rho} \left(p^{eos} + f(\rho) \right) - \zeta \nabla^2 \rho \right] \\
&= \left(p^{eos} + f(\rho) \right) \rho \nabla \left(\frac{1}{\rho} \right) + \nabla \left(p^{eos} + f(\rho) \right) - \rho \zeta \nabla (\nabla^2 \rho) \\
&= \left(p^{eos} + f(\rho) \right) \cancel{\rho} \left(-\frac{1}{\rho^{\cancel{2}}} \right) \nabla \rho + \nabla p^{eos} + f'(\rho) \nabla \rho - \rho \zeta \nabla (\nabla^2 \rho) \\
&= \left[-p^{eos} \underbrace{- f(\rho) + \rho f'(\rho)}_{\equiv + p^{eos}} \right] \frac{\nabla \rho}{\rho} + \nabla p^{eos} - \rho \zeta \nabla (\nabla^2 \rho) \\
&= \nabla p^{eos} - \rho \zeta \nabla (\nabla^2 \rho)
\end{aligned}$$

Pseudo-potential LB method

Lattice Boltzmann equation with Kupershtokh's force

$$f_i(\boldsymbol{x}+\boldsymbol{c}_i\delta t,\ t+\delta t) = f_i(\boldsymbol{x},\ t) - \frac{1}{\tau}\left[f_i(\boldsymbol{x},\ t) - f_i^{eq}(\boldsymbol{x},\ t)\right] + \delta t\mathcal{F}_i(\boldsymbol{x}, t)$$

$$f_i^{eq}(\boldsymbol{x},\ t) = w_i\rho\left[1 + \frac{\boldsymbol{c}_i\cdot\boldsymbol{u}}{c_s^2} + \frac{(\boldsymbol{c}_i\cdot\boldsymbol{u})^2}{2c_s^4} - \frac{\boldsymbol{u}\cdot\boldsymbol{u}}{2c_s^2}\right]$$

$$\rho = \sum_i f_i \qquad \boldsymbol{u} = \frac{1}{\rho}\sum_i f_i\boldsymbol{c}_i + \frac{\delta t}{2}\boldsymbol{F}_{int}$$

Kupershtokh force term

$$\mathcal{F}_i(\boldsymbol{x}, t) = f_i^{eq}(\boldsymbol{u}^\star + \Delta\boldsymbol{u}) - f_i^{eq}(\boldsymbol{u}^\star)$$

$$\boldsymbol{u}^\star = \frac{1}{\rho}\sum_i f_i\boldsymbol{c}_i$$

$$\Delta\boldsymbol{u} = \frac{1}{\rho}\boldsymbol{F}_{int}\delta t$$

Pseudo-potential $\psi(\rho)$

Definition of the forcing term:

$$\boldsymbol{F}_{int} = \psi(\rho)\boldsymbol{\nabla}\psi(\rho)$$

$$\psi(\rho) = \sqrt{\frac{2(\rho c_s^2 - p^{eos}(\rho))}{c_s^2}}$$

Discrete force:

$$\boldsymbol{F}_{int}(\boldsymbol{x}, t) = \psi(\boldsymbol{x}, t)\frac{1}{\delta x}\sum_i w_i\psi(\boldsymbol{x}+\boldsymbol{c}_i\delta t, t)\boldsymbol{c}_i$$

Chapman-Enskog analysis

Macroscopic equation recovered

$$\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla} \cdot (\rho \boldsymbol{u}) = 0$$

$$\frac{\partial (\rho \boldsymbol{u})}{\partial t} + \boldsymbol{\nabla} \cdot (\rho \boldsymbol{u}\boldsymbol{u}) = -\boldsymbol{\nabla} \cdot \overline{\overline{\boldsymbol{P}}} + \boldsymbol{\nabla} \cdot \left[\eta \left(\boldsymbol{\nabla} \boldsymbol{u} + \boldsymbol{\nabla} \boldsymbol{u}^T\right) + \left(\eta_B - \frac{2}{3}\eta\right) (\boldsymbol{\nabla} \cdot \boldsymbol{u}) \boldsymbol{I}\right]$$

$$\overline{\overline{\boldsymbol{P}}} = p^{eos}(\rho, T)\overline{\overline{\boldsymbol{I}}} + \overline{\overline{\zeta}}$$

$$\overline{\overline{\zeta}} = \frac{c_s^4}{2}\left[\psi(\rho)\boldsymbol{\nabla}^2\psi(\rho) + \frac{1}{2}\left|\boldsymbol{\nabla}\psi(\rho)\right|^2\right]\overline{\overline{\boldsymbol{I}}} - \frac{c_s^4}{2}\boldsymbol{\nabla}\psi(\rho) \otimes \boldsymbol{\nabla}\psi(\rho)$$

- Approximation of the Korteweg tensor because ψ replaces ρ in $\overline{\overline{\zeta}}$

LBM with a potential form of pressure tensor

Lattice Boltzmann equation with GUO's force

$$f_i(\boldsymbol{x}+\boldsymbol{c}_i\delta t, t+\delta t) = f_i(\boldsymbol{x},t) - \frac{1}{\tau}\left[f_i(\boldsymbol{x},t) - f_i^{eq}(\boldsymbol{x},t)\right] + \delta t \mathcal{F}_i(\boldsymbol{x},t)$$

$$f_i^{eq}(\boldsymbol{x},t) = w_i\rho\left[1 + \frac{\boldsymbol{c}_i\cdot\boldsymbol{u}}{c_s^2} + \frac{(\boldsymbol{c}_i\cdot\boldsymbol{u})^2}{2c_s^4} - \frac{\boldsymbol{u}\cdot\boldsymbol{u}}{2c_s^2}\right]$$

$$\mathcal{F}_i(\boldsymbol{x},t) = w_i\left[\frac{\boldsymbol{c}_i-\boldsymbol{u}}{c_s^2} + \frac{(\boldsymbol{c}_i\cdot\boldsymbol{u})\boldsymbol{c}_i}{c_s^4}\right]\cdot\boldsymbol{F}_{tot}$$

$$\rho\boldsymbol{u} = \sum_i f_i\boldsymbol{c}_i + \frac{\delta t}{2}\boldsymbol{F}_{tot}$$

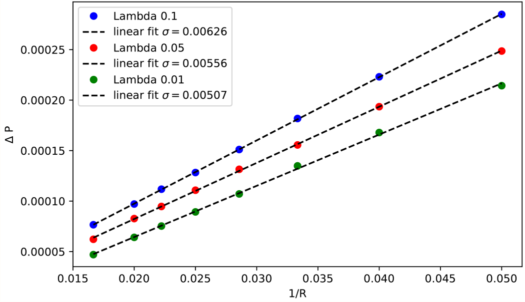
Forces

$$\boldsymbol{F}_{tot} = \boldsymbol{\nabla}\rho c_s^2 - \rho\boldsymbol{\nabla}\mu_\rho$$

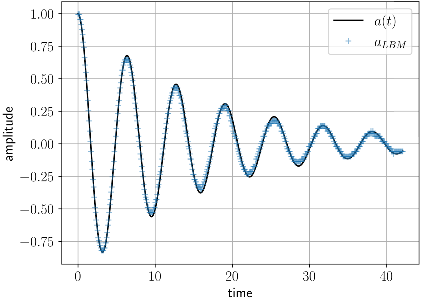
- where μ_ρ is defined by Eq. (152c) for van der Waals eos or Eq. (153c) for Carnahan-Starling eos
- $\boldsymbol{\nabla}\rho c_s^2$ is added to cancel the eos of perfect gas which arises from the Chapman-Enskog procedure

Validations

Laplace law



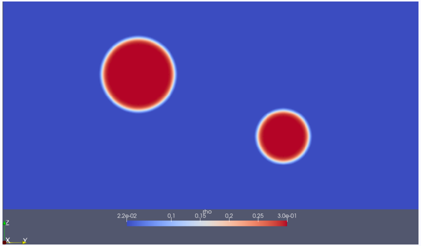
Capillary wave



Simulations with NS/K model

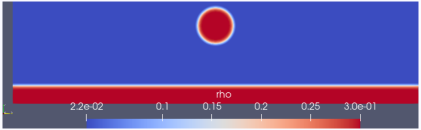
Coalescence of bubbles

▸ Video



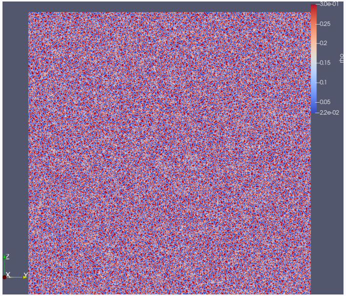
Splash

▸ Video



Spinodal decomposition

▸ Video



C. Coupling with temperature T

Derivation of NS/K model coupled with temperature

Free energy with ρ and T and total energy

Free energy with order parameter ρ

$$\mathscr{F}[\rho, T] = \int_V \mathcal{F}(\rho, \nabla\rho, T)dV \qquad \text{with} \qquad \mathcal{F}(\rho, \nabla\rho, T) = f(\rho, T) + \frac{\zeta}{2}|\nabla\rho|^2 \tag{163}$$

- $f(\rho, T)$: local free energy which can be derived from $p^{eos}(\rho, T)$ e.g. $f_{vdW}(\rho, T)$ or $f_{CS}(\rho, T)$
- Hypothesis: ζ is independent of T

Total energy $\mathscr{E}_{tot}$: kinetic energy and internal energy $\mathcal{U}$

$$\mathscr{E}_{tot}[\rho, \boldsymbol{u}, T] = \int_V \Bigg[\underbrace{\frac{1}{2}\rho|\boldsymbol{u}|^2}_{\text{kinetic energy}} + \underbrace{\mathcal{U}(\rho, \nabla\rho, \mathcal{S})}_{\text{Legendre transform of } \mathcal{F}(\rho,\nabla\rho,T)} \Bigg] dV \tag{164}$$

Use of $\mathcal{U}$ because there are conservation eqs on $\mathcal{U}$ and $\mathcal{S}$

Remark: in section 3, the constitutive laws $\boldsymbol{j}_\phi$ and $\overline{\overline{\boldsymbol{T}}}$ were derived such as $d\mathscr{E}_{tot}/dt \leqslant 0$. Here we use an alternative form of the 2nd principle of thermodynamics.

Clausius-Duhem inequality

Alternative way of expressing the 2nd law

Balance of entropy

$$\rho \frac{ds}{dt} = -\nabla \cdot \boldsymbol{q}_s + \frac{\rho r}{T} + \mathcal{D} \tag{165}$$

- $s(\boldsymbol{x}, t)$ is the specific entropy
- $\boldsymbol{q}_s(\boldsymbol{x}, t)$ entropy flux
- $T(\boldsymbol{x}, t)$ temperature
- $r(\boldsymbol{x}, t)$: heat source per unit mass
- $\mathcal{D}(\boldsymbol{x}, t)$ source term of Eq.

Local form of Clausius-Duhem inequality

$$\mathcal{D} := \rho \frac{ds}{dt} + \nabla \cdot \boldsymbol{q}_s - \frac{\rho r}{T} \geqslant 0$$

$\mathcal{D}$ is the entropy production and $T\mathcal{D}$ is called “dissipation”

Derivation 1/6: general balance equations

Conservation equations (hyp $\boldsymbol{g} = 0$ and $r = 0$)

$$\frac{d\rho}{dt} = -\rho \boldsymbol{\nabla} \cdot \boldsymbol{u} \tag{166}$$

$$\rho \frac{d\boldsymbol{u}}{dt} = \boldsymbol{\nabla} \cdot \overline{\overline{\boldsymbol{T}}} \tag{167}$$

$$\rho \frac{d\mathcal{E}_{tot}}{dt} = -\boldsymbol{\nabla} \cdot \boldsymbol{q} + \boldsymbol{\nabla} \cdot (\overline{\overline{\boldsymbol{T}}} \cdot \boldsymbol{u}) \tag{168}$$

$$\rho \frac{d\mathcal{S}}{dt} = -\boldsymbol{\nabla} \cdot \boldsymbol{q}_s + \mathcal{D} \tag{169}$$

Balance for internal energy density $\mathcal{U}$

where $\mathcal{E}_{tot}$ is the total energy density

$$\mathcal{E}_{tot} = \mathcal{U} + \frac{1}{2}\left|\boldsymbol{u}\right|^2 \tag{170}$$

Eq. (168)$-\boldsymbol{u}\cdot$Eq. (167):

$$\rho \frac{d\mathcal{U}}{dt} = -\boldsymbol{\nabla} \cdot \boldsymbol{q} + \overline{\overline{\boldsymbol{T}}} : \boldsymbol{\nabla} \boldsymbol{u} \tag{171}$$

Coleman–Noll procedure (1963):

Close the model by determining the constitutive laws for $\overline{\overline{\boldsymbol{T}}}$, $\boldsymbol{q}$, $\boldsymbol{q}_s$, and source term $\mathcal{D}$ expressed with $\rho(\boldsymbol{x}, t)$, $T(\boldsymbol{x}, t)$ and $\mathcal{F}(\rho, \boldsymbol{\nabla}\rho, T)$ such as the dissipation $\mathcal{D} \geqslant 0$

Derivation 2/6: differential of internal energy $\mathcal{U}$

$\mathcal{U}(\rho, \nabla\rho, \mathcal{S})$: Legendre transform of $\mathcal{F}(\rho, \nabla\rho, T)$ wrt T

$$\mathcal{U}(\rho, \nabla\rho, \mathcal{S}) = \frac{\mathcal{F}(\rho, \nabla\rho, T)}{\rho} + T\mathcal{S}(\rho, \nabla\rho, T)$$

Differential (see local Eq. (8))

$$d\mathcal{U} = \frac{1}{\rho}\underbrace{\left[\rho\frac{\partial\mathcal{F}}{\partial\rho} - \mathcal{F}\right]}_{\equiv\mathcal{P}\text{ pressure}} d\rho + \rho T d\mathcal{S} + \underbrace{\frac{\partial\mathcal{F}}{\partial(\nabla\rho)} \cdot d(\nabla\rho)}_{\text{New term because of }\nabla\rho} \qquad (172)$$

Divide by dt:

$$\boxed{\frac{d\mathcal{U}}{dt} = \frac{\mathcal{P}}{\rho}\frac{d\rho}{dt} + \rho T\frac{d\mathcal{S}}{dt} + \boldsymbol{\mathcal{F}} \cdot \frac{d(\nabla\rho)}{dt}} \qquad (173)$$

Where we set in Eq. (172)

$$\boxed{\mathcal{S} = -\frac{1}{\rho}\frac{\partial\mathcal{F}}{\partial T} \equiv s(\rho, T)} \qquad (174)$$

Remarks:

- $(\partial\mathcal{F}/\partial T + \rho\mathcal{S})dT/dt$ could be added in $\mathcal{D}$ and canceled to insure $\mathcal{D} \geqslant 0$.
- $\mathcal{S} = -\rho^{-1}\partial_T f = s(\rho, T)$ because ζ is independent on T
- Notations:

$$\boldsymbol{\mathcal{F}} \hat{=} \frac{\partial\mathcal{F}}{\partial(\nabla\rho)} \quad \text{and} \quad \mathcal{P} = \rho\frac{\partial\mathcal{F}}{\partial\rho} - \mathcal{F}$$

Method: replace $d\rho/dt$, $d\mathcal{S}/dt$ and $d\mathcal{U}/dt$ by their balance equations Eqs. (166), (169), (171) and express dissipation $\mathcal{D}$.

Derivation 3/6: dissipation

Re-expression of Eq. (173) with balance equations

$$-\boldsymbol{\nabla}\cdot\boldsymbol{q}+\overline{\overline{\boldsymbol{T}}}:\boldsymbol{\nabla}\boldsymbol{u}=T(-\boldsymbol{\nabla}\cdot\boldsymbol{q}_s+\mathcal{D})-\mathcal{P}\boldsymbol{\nabla}\cdot\boldsymbol{u}+\boxed{\boldsymbol{\mathcal{F}}\cdot\frac{d(\boldsymbol{\nabla}\rho)}{dt}} \tag{175}$$

Last term of Eq. (175) (use Eq. (78) and trick)

$$\boxed{\boldsymbol{\mathcal{F}}\cdot\frac{d(\boldsymbol{\nabla}\rho)}{dt}}=\boldsymbol{\nabla}\cdot\left[\boldsymbol{\mathcal{F}}\frac{d\rho}{dt}\right]-\frac{d\rho}{dt}\boldsymbol{\nabla}\cdot\boldsymbol{\mathcal{F}}-\boldsymbol{\mathcal{F}}\otimes\boldsymbol{\nabla}\rho:\boldsymbol{\nabla}\boldsymbol{u} \tag{176}$$

Trick for $\boldsymbol{j}=\boldsymbol{q},\boldsymbol{\mathcal{F}}$ (tips 1 and chain rule):

$$-\frac{1}{T}\boldsymbol{\nabla}\cdot\boldsymbol{j}=-\boldsymbol{\nabla}\cdot\left[\frac{1}{T}\boldsymbol{j}\right]-\frac{1}{T^2}\boldsymbol{j}\cdot\boldsymbol{\nabla}T \tag{177}$$

Isolate dissipation and make appear terms proportional to $\cdot\boldsymbol{\nabla}T$ and $:\boldsymbol{\nabla}\boldsymbol{u}$

$$\mathcal{D}=\overbrace{-\frac{1}{T}\boldsymbol{\nabla}\cdot\boldsymbol{q}}^{\text{use Eq.(177)}}+\underbrace{\frac{1}{T}\overline{\overline{\boldsymbol{T}}}:\boldsymbol{\nabla}\boldsymbol{u}}_{\text{gather }:\boldsymbol{\nabla}\boldsymbol{u}}+\overbrace{\boldsymbol{\nabla}\cdot\boldsymbol{q}_s}^{\text{unchanged}}+\underbrace{\frac{1}{T}\mathcal{P}\boldsymbol{\nabla}\cdot\boldsymbol{u}}_{:\boldsymbol{\nabla}\boldsymbol{u}}\overbrace{-\frac{1}{T}\boldsymbol{\nabla}\cdot\left[\boldsymbol{\mathcal{F}}\frac{d\rho}{dt}\right]}^{\text{use Eq.(177)}}+\underbrace{\frac{1}{T}(-\rho\boldsymbol{\nabla}\cdot\boldsymbol{u})\boldsymbol{\nabla}\cdot\boldsymbol{\mathcal{F}}}_{:\boldsymbol{\nabla}\boldsymbol{u}}+\underbrace{\frac{1}{T}\boldsymbol{\mathcal{F}}\otimes\boldsymbol{\nabla}\rho:\boldsymbol{\nabla}\boldsymbol{u}}_{:\boldsymbol{\nabla}\boldsymbol{u}}$$

$$=-\boldsymbol{\nabla}\cdot\underbrace{\left\{\boldsymbol{q}_s-\frac{1}{T}\left(\boldsymbol{q}+\boldsymbol{\mathcal{F}}\frac{d\rho}{dt}\right)\right\}}_{\text{def such as }=0}-\frac{1}{T^2}\underbrace{\left[\boldsymbol{q}+\boldsymbol{\mathcal{F}}\frac{d\rho}{dt}\right]}_{\text{def such as }\propto-(\boldsymbol{\nabla}T)^2}\cdot\boldsymbol{\nabla}T+\frac{1}{T}\underbrace{\left[\overline{\overline{\boldsymbol{T}}}+(\mathcal{P}-\rho\boldsymbol{\nabla}\cdot\boldsymbol{\mathcal{F}})\overline{\overline{\boldsymbol{I}}}+\boldsymbol{\mathcal{F}}\otimes\boldsymbol{\nabla}\rho\right]}_{\text{def such as }=(-\overline{\overline{\boldsymbol{P}}}+\overline{\overline{\boldsymbol{\tau}}}):\boldsymbol{\nabla}\boldsymbol{u}\geqslant 0}:\boldsymbol{\nabla}\boldsymbol{u}$$

Complete proof of equality Eq. (176)

Objective: make appear conservative form for $\mathcal{F}$ and Korteweg's tensor

Use $d/dt = \partial_t + \boldsymbol{u}\cdot\boldsymbol{\nabla}$ and index notations

$$
\begin{aligned}
\boldsymbol{\mathcal{F}}\cdot\frac{d}{dt}(\boldsymbol{\nabla}\rho) &= \mathcal{F}_\alpha \frac{d}{dt}(\partial_\alpha\rho) \\
&= \mathcal{F}_\alpha\left[\partial_t(\partial_\alpha\rho) + \boldsymbol{u}\cdot\boldsymbol{\nabla}(\partial_\alpha\rho)\right] \\
&= \mathcal{F}_\alpha\left[\underbrace{\partial_t(\partial_\alpha}_{\text{intervert}}\rho) + u_\beta\,\underbrace{\partial_\beta(\partial_\alpha}_{\text{intervert}}\rho)\right] \\
&= \underbrace{\mathcal{F}_\alpha\partial_\alpha(\partial_t\rho)}_{\text{Term }1\equiv A} + \underbrace{\mathcal{F}_\alpha u_\beta\partial_\alpha(\partial_\beta\rho)}_{\text{Term }2\equiv B}
\end{aligned}
$$

- Term 1: use tips 1 Eq. (72)

$$
A = \underbrace{\partial_\alpha[\mathcal{F}_\alpha(\partial_t\rho)]}_{\text{group I}} - \underbrace{(\partial_t\rho)\partial_\alpha\mathcal{F}_\alpha}_{\text{group II}}
$$

- Term 2: use tips 1 Eq. (72)

$$
\begin{aligned}
B &= \partial_\alpha[\mathcal{F}_\alpha u_\beta\partial_\beta\rho] - \underbrace{\partial_\alpha(\mathcal{F}_\alpha u_\beta)}_{\text{expansion}}\partial_\beta\rho \\
&= \underbrace{\partial_\alpha[\mathcal{F}_\alpha u_\beta\partial_\beta\rho]}_{\text{group I}} - \underbrace{(\partial_\alpha\mathcal{F}_\alpha)u_\beta\partial_\beta\rho}_{\text{group II}} - \mathcal{F}_\alpha(\partial_\alpha u_\beta)\partial_\beta\rho
\end{aligned}
$$

Finally:

$$
\boldsymbol{\mathcal{F}}\cdot\frac{d}{dt}(\boldsymbol{\nabla}\rho) = \underbrace{\partial_\alpha\left\{\left[(\partial_t\rho) + u_\beta\partial_\beta\rho\right]\mathcal{F}_\alpha\right\}}_{\equiv\boldsymbol{\nabla}\cdot\left[\frac{d\rho}{dt}\boldsymbol{\mathcal{F}}\right]} - \underbrace{\left[(\partial_t\rho) + u_\beta\partial_\beta\rho\right](\partial_\alpha\mathcal{F}_\alpha)}_{\equiv\frac{d\rho}{dt}\boldsymbol{\nabla}\cdot\boldsymbol{\mathcal{F}}} - \underbrace{(\mathcal{F}_\alpha\partial_\beta\rho)(\partial_\alpha u_\beta)}_{\equiv(\boldsymbol{\mathcal{F}}\otimes\boldsymbol{\nabla}\rho):\boldsymbol{\nabla}\boldsymbol{u}}
$$

Derivation 4/6: constitutive laws

Appropriate solutions (but other choices are possible)

$$\boldsymbol{q} = -\Lambda \boldsymbol{\nabla} T - \boldsymbol{\mathcal{F}} \frac{d\rho}{dt}$$

$$\boldsymbol{q}_s = \frac{1}{T}\left(\boldsymbol{q} + \boldsymbol{\mathcal{F}}\frac{d\rho}{dt}\right)$$

$$\overline{\overline{\boldsymbol{T}}} = -\left(\mathcal{P} - \rho \boldsymbol{\nabla} \cdot \boldsymbol{\mathcal{F}}\right)\overline{\overline{\boldsymbol{I}}} - \boldsymbol{\mathcal{F}} \otimes \boldsymbol{\nabla}\rho + \overline{\overline{\boldsymbol{\tau}}}$$

$\overline{\overline{\boldsymbol{\tau}}}$: defined by Eq. (157)

Expressions with $\mathcal{F}$ defined by Eq. (163)

$$\boldsymbol{\mathcal{F}} = \zeta \boldsymbol{\nabla}\rho$$

$$\boldsymbol{q} = -\Lambda \boldsymbol{\nabla} T + \zeta\rho \boldsymbol{\nabla}\rho \boldsymbol{\nabla} \cdot \boldsymbol{u}$$

$$\boldsymbol{q}_s = -\frac{\Lambda}{T}\boldsymbol{\nabla} T$$

$$\mathcal{D} = \frac{\Lambda}{T^2}\left(\boldsymbol{\nabla} T\right)^2 + \frac{1}{T}\overline{\overline{\boldsymbol{\tau}}} : \boldsymbol{\nabla}\boldsymbol{u}$$

$$\mathcal{P} = \underbrace{\rho f'(\rho, T) - f(\rho, T)}_{\equiv p^{eos}(\rho, T)} - \frac{\zeta}{2}\left|\boldsymbol{\nabla}\rho\right|^2$$

$$\overline{\overline{\boldsymbol{T}}} = -\overline{\overline{\boldsymbol{P}}} + \overline{\overline{\boldsymbol{\tau}}}$$

$$\overline{\overline{\boldsymbol{P}}} = \left[p^{eos} - \frac{\zeta}{2}\left|\boldsymbol{\nabla}\rho\right|^2 - \rho\zeta\boldsymbol{\nabla}^2\rho\right]\overline{\overline{\boldsymbol{I}}} + \zeta\boldsymbol{\nabla}\rho \otimes \boldsymbol{\nabla}\rho$$

Derivation 5/6: temperature equation

Specific entropy equation

With their expressions of $\boldsymbol{q}_s$ and $\mathcal{D}$:

$$-\boldsymbol{\nabla}\cdot\boldsymbol{q}_s+\mathcal{D}=\frac{1}{T}\boldsymbol{\nabla}\cdot(\Lambda\boldsymbol{\nabla}T)+\frac{1}{T}\overline{\overline{\tau}}:\boldsymbol{\nabla}\boldsymbol{u}$$

Equation for entropy:

$$\rho T\frac{ds}{dt}=\boldsymbol{\nabla}\cdot(\Lambda\boldsymbol{\nabla}T)+\overline{\overline{\tau}}:\boldsymbol{\nabla}\boldsymbol{u}\qquad(178)$$

We also have:

$$\rho T ds=\underbrace{\rho\,T\left.\frac{\partial s}{\partial T}\right|_{\rho}}_{C_v}dT+\rho T\left.\frac{\partial s}{\partial\rho}\right|_{T}d\rho$$

$$\rho T\frac{ds}{dt}=\rho C_v\frac{dT}{dt}+\rho T\left.\frac{\partial s}{\partial\rho}\right|_{T}\frac{d\rho}{dt}\qquad(179)$$

$\mathcal{S}\equiv s(\rho,T)$ because independent on $\boldsymbol{\nabla}\rho$ (see Eq. (174))

Temperature equation Eq (178) = Eq. (179)

$$\rho C_v\frac{dT}{dt}=\underbrace{\boldsymbol{\nabla}\cdot(\Lambda\boldsymbol{\nabla}T)}_{\text{conduction}}+\underbrace{\overline{\overline{\tau}}:\boldsymbol{\nabla}\boldsymbol{u}}_{\text{viscous dissipation}}\underbrace{-\rho T\left.\frac{\partial s}{\partial\rho}\right|_{T}\frac{d\rho}{dt}}_{\text{next slide}}\qquad(180)$$

Remark on source term of temperature Eq.

Interpretation of last term in temperature Eq. (180) at saturation

The last term writes:

$$\rho T \left.\frac{\partial s^{sat}}{\partial \rho}\right|_T \frac{d\rho}{dt}$$

But:

$$\left.\frac{\partial s^{sat}}{\partial v}\right|_T \underset{\text{relation}}{\overset{\text{Maxwell}}{=}} \left.\frac{\partial P^{sat}}{\partial T}\right|_v \underset{\text{relation}}{\overset{\text{Clapeyron}}{=}} \frac{\mathcal{L}}{T(v_g^{sat} - v_l^{sat})}$$

with $v = 1/\rho$:

$$\left.\frac{\partial s^{sat}}{\partial v}\right|_T = \left.\frac{\partial s^{sat}}{\partial \rho}\frac{\partial \rho}{\partial v}\right|_T = -\rho^2 \left.\frac{\partial s^{sat}}{\partial \rho}\right|_T$$

$$\frac{\mathcal{L}}{T(v_g^{sat} - v_l^{sat})} = \frac{\mathcal{L}}{T}\frac{\rho_l^{sat}\rho_g^{sat}}{(\rho_l^{sat} - \rho_g^{sat})}$$

$$\longrightarrow \quad \boxed{\rho T \left.\frac{\partial s^{sat}}{\partial \rho}\right|_T \frac{d\rho}{dt} = -\frac{\mathcal{L}}{\rho}\frac{\rho_l^{sat}\rho_g^{sat}}{(\rho_l^{sat} - \rho_g^{sat})}\frac{d\rho}{dt}}$$

The last term represents the latent heat which is absorbed or released at interface during the phase change. The expression is quite identical than solid/liquid phase change (see Eq. (115)).

Derivation 6/6: NS/K model with phase change

Mathematical model

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) = 0 \tag{181}$$

$$\frac{\partial (\rho \boldsymbol{u})}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}\boldsymbol{u}) = -\nabla \cdot \overline{\overline{\boldsymbol{P}}} + \nabla \cdot \overline{\overline{\tau}} \tag{182}$$

$$\frac{\partial (\rho C_v T)}{\partial t} + \nabla \cdot (\rho C_v T \boldsymbol{u}) = \nabla \cdot (\Lambda \nabla T) + \overline{\overline{\tau}} : \nabla \boldsymbol{u} - \rho T \left.\frac{\partial s}{\partial \rho}\right|_T \frac{d\rho}{dt} \tag{183}$$

Closures

- $\overline{\overline{\tau}}$ defined by Eq. (157)
- $\overline{\overline{\boldsymbol{P}}}$ defined by Eq. (158)
- Choose one $f(\rho, T)$ (e.g. f_{vdW} Eq. (152b))
- $p^{eos}(\rho, T)$ defined Eq. (159) (e.g. p^{eos}_{vdW})
- Last term of Eq. (183): next slide
- Potential form of Eq. (182): next slide

Potential form of tensor pressure

Potential form of tensor pressure

$$-\nabla\cdot\overline{\overline{P}} = -\nabla\cdot\left[p^{eos} - \frac{\zeta}{2}|\nabla\rho|^2 - \zeta\rho\nabla^2\rho\right]\overline{\overline{I}} - \zeta\underbrace{\nabla\cdot(\nabla\rho\otimes\nabla\rho)}_{\text{Eq. (185)}}$$

$$= -\nabla p^{eos} + \cancel{\frac{\zeta}{2}\nabla(|\nabla\rho|^2)} + \underbrace{\nabla[\zeta\rho\nabla^2\rho]}_{\text{expansion}} - \cancel{\frac{\zeta}{2}\nabla(|\nabla\rho|^2)} - \zeta(\nabla^2\rho)\nabla\rho$$

$$= \underbrace{-\nabla p^{eos}}_{\text{Eq. (184)}} + \cancel{\zeta(\nabla\rho)(\nabla^2\rho)} + \zeta\rho\nabla(\nabla^2\rho) - \cancel{\zeta(\nabla^2\rho)\nabla\rho}$$

$$-\nabla\cdot\overline{\overline{P}} = -\rho\nabla[\partial_\rho f(\rho,T)] - \rho s\nabla T + \zeta\rho\nabla(\nabla^2\rho)$$

$$= -\rho\nabla\underbrace{[\partial_\rho f(\rho,T) - \zeta\nabla^2\rho]}_{\equiv\mu_\rho} - \rho s\nabla T$$

$$\boxed{-\nabla\cdot\overline{\overline{P}} = -\rho\nabla\mu_\rho - \rho s\nabla T}$$

Useful relations

$$-\nabla p^{eos}(\rho,T) = -\rho\nabla[\partial_\rho f(\rho,T)] - \rho s\nabla T \qquad (184)$$

$$\nabla\cdot(\nabla\rho\otimes\nabla\rho) = \frac{1}{2}\nabla(|\nabla\rho|^2) + (\nabla^2\rho)\nabla\rho \qquad (185)$$

Demo see Eq. (76)

Demo

$$-\partial_\alpha p^{eos} = -\partial_\alpha\underbrace{[\rho\partial_\rho f(\rho,T) - f(\rho,T)]}_{\text{def } p^{eos}}$$

$$= -\rho\partial_\alpha[\partial_\rho f] - \partial_\rho f\partial_\alpha\rho + \underbrace{\partial_\alpha f(\rho,T)}_{\text{chain rule}}$$

$$= -\rho\partial_\alpha(\partial_\rho f) - \cancel{\partial_\rho f\partial_\alpha\rho} + \underbrace{\partial_T f}_{\equiv-\rho s}\ \partial_\alpha T + \cancel{\partial_\rho f\partial_\alpha\rho}$$

Alternative source term formulation of temperature Eq.

Alternative formulation of source term

Maxwell relation with density

$$\rho^2 \left.\frac{\partial s}{\partial \rho}\right|_T = - \left.\frac{\partial p^{eos}}{\partial T}\right|_\rho$$

Source term of temperature Eq.:

$$-\rho T \left.\frac{\partial s}{\partial \rho}\right|_T \frac{d\rho}{dt} = \rho^2 T \left.\frac{\partial s}{\partial \rho}\right|_T \nabla \cdot \boldsymbol{u}$$

$$= -T \left.\frac{\partial p^{eos}}{\partial T}\right|_\rho \bar{\bar{\boldsymbol{I}}} : \nabla \boldsymbol{u}$$

Specific entropy

$$s = -\frac{1}{\rho} \left.\frac{\partial f}{\partial T}\right|_\rho \qquad (186)$$

$$\rho T \left.\frac{\partial s}{\partial \rho}\right|_T = -T \frac{\partial^2 f}{\partial \rho \partial T}$$

Example with van der Waals *eos*:

$$f(\rho, T) \equiv f_{vdW}(\rho, T) = \rho R T \ln\left(\frac{\rho}{1 - b\rho}\right) - a\rho^2$$

$$s = -R \ln\left(\frac{\rho}{1 - b\rho}\right) + a\rho$$

$$\rho T \left.\frac{\partial s}{\partial \rho}\right|_T = \frac{ab\rho^2 - a\rho + R}{b\rho - 1} T$$

d.

Coupling with composition c

Derivation of NS/K model for surfactant

Free energy with ρ and c

Free energy

$$\mathscr{F}[\rho, c] = \int_V \underbrace{f(\rho) + \frac{\zeta(c)}{2}\left|\nabla\rho\right|^2 + \frac{1}{2}\alpha c^2}_{\equiv\mathcal{F}(\rho,\nabla\rho,c)} dV \qquad (187)$$

- ζ is now a function of c
- New contribution: $\alpha c^2/2$

Total energy $\mathscr{E}_{tot}$

$$\frac{d\mathscr{E}_{tot}}{dt} = \frac{d}{dt}\int \left[\underbrace{\frac{1}{2}\rho\left|\boldsymbol{u}\right|^2}_{\text{kinetic energy}} + \underbrace{\mathcal{F}(\rho, \nabla\rho, c)}_{\text{potential energy}} \right] dV \qquad (188)$$

- $\mathcal{F}$: non-local free energy density
- $\rho\left|\boldsymbol{u}\right|^2/2$: kinetic energy

Derivation

Balance equations

$$\frac{d\rho}{dt} = -\rho \boldsymbol{\nabla} \cdot \boldsymbol{u} \qquad (189)$$

$$\rho \frac{d\boldsymbol{u}}{dt} = \boldsymbol{\nabla} \cdot \overline{\overline{\boldsymbol{T}}} \qquad (190)$$

$$\frac{dc}{dt} + c\boldsymbol{\nabla} \cdot \boldsymbol{u} = -\boldsymbol{\nabla} \cdot \boldsymbol{j}_c \qquad (191)$$

Objective

Determine the constitutive laws $\boldsymbol{j}_c$ and $\overline{\overline{\boldsymbol{T}}}$ such as

$$\frac{d\mathscr{E}_{tot}}{dt} \leqslant 0$$

Method

Express

$$\frac{d\mathscr{E}_{tot}}{dt} = \frac{d}{dt}\int \left[\mathcal{F}(\rho, \boldsymbol{\nabla}\rho, c) + \frac{1}{2}\rho|\boldsymbol{u}|^2\right] dV$$

on the form

$$\frac{d\mathscr{E}_{tot}}{dt} = -\mathcal{D}(V) + \mathcal{W}(V) + \Phi(\partial V) \leqslant 0$$

- $\mathcal{D}$: dissipation with $\mathcal{D} \geqslant 0$
- $\mathcal{W}$: work of external forces
- Φ: Flux through surface

Methodology of derivation 3/7

Kinetic energy

$$\frac{1}{2}\rho\frac{d\left|\boldsymbol{u}\right|^2}{dt} = \rho\boldsymbol{u}\cdot\frac{d\boldsymbol{u}}{dt} = \boldsymbol{u}\cdot\boldsymbol{\nabla}\cdot\overline{\overline{\boldsymbol{T}}}$$

Differential of free energy density $\mathcal{F}$

- Differential

$$d\mathcal{F}(\rho,\boldsymbol{\nabla}\rho,c) = \frac{\partial\mathcal{F}}{\partial\rho}d\rho + \underbrace{\frac{\partial\mathcal{F}}{\partial(\boldsymbol{\nabla}\rho)}}_{\hat{=}\boldsymbol{\mathcal{F}}}\cdot d(\boldsymbol{\nabla}\rho) + \frac{\partial\mathcal{F}}{\partial c}dc$$

- Divide by dt:

$$\frac{d\mathcal{F}(\rho,\boldsymbol{\nabla}\rho,c)}{dt} = \frac{\partial\mathcal{F}}{\partial\rho}\underbrace{\frac{d\rho}{dt}}_{\text{Eq. (189)}} + \boldsymbol{\mathcal{F}}\cdot\underbrace{\frac{d(\boldsymbol{\nabla}\rho)}{dt}}_{\text{re-write}} + \frac{\partial\mathcal{F}}{\partial c}\underbrace{\frac{dc}{dt}}_{\text{Eq. (191)}} \tag{192}$$

- Replace $d\rho/dt$, dc/dt by their balance equations and re-write $d(\boldsymbol{\nabla}\rho)/dt$ (see next slide)

Methodology of derivation 5/7

Terms $\mathcal{I}$ and $\mathcal{K}$ of Eq. (70)

$$\int_V \mathcal{I} dV = \int_V \left\{ \left[-\rho \frac{\partial \mathcal{F}}{\partial \rho} + \mathcal{F} \right] \nabla \cdot \boldsymbol{u} + \left[\underbrace{\boldsymbol{\mathcal{F}} \cdot \nabla \left(\frac{d\rho}{dt} \right)}_{\text{integration by parts}} - \boldsymbol{\mathcal{F}} \otimes \nabla \rho : \nabla \boldsymbol{u} \right] + \underbrace{\frac{\partial \mathcal{F}}{\partial c} (-\nabla \cdot \boldsymbol{j}_c}_{\text{ibp}} - c \nabla \cdot \boldsymbol{u}) \right\} dV$$

$$\int_V \mathcal{K} dV = \int_V \left[\underbrace{\boldsymbol{u} \cdot \nabla \cdot \overline{\overline{\boldsymbol{T}}}}_{\text{ibp}} \right] dV$$

Results of integration by parts

$$\int_V \left[\boldsymbol{\mathcal{F}} \cdot \nabla \left(\frac{d\rho}{dt} \right) \right] dV = \int_{\partial V} \frac{d\rho}{dt} \boldsymbol{\mathcal{F}} \cdot \boldsymbol{n} d(\partial V) - \int_V \nabla \cdot \boldsymbol{\mathcal{F}} \frac{d\rho}{dt} dV$$

$$- \int_V \frac{\partial \mathcal{F}}{\partial c} \nabla \cdot \boldsymbol{j} dV = - \int_{\partial V} \frac{\partial \mathcal{F}}{\partial c} \boldsymbol{j} \cdot \boldsymbol{n} d(\partial V) + \int_V \boldsymbol{j} \cdot \nabla \left(\frac{\partial \mathcal{F}}{\partial c} \right) dV$$

$$\int_V \boldsymbol{u} \cdot \nabla \cdot \overline{\overline{\boldsymbol{T}}} dV = \int_{\partial V} \boldsymbol{u} \cdot \overline{\overline{\boldsymbol{T}}} \boldsymbol{n} d(\partial V) - \int_V \overline{\overline{\boldsymbol{T}}} : \nabla \boldsymbol{u} dV$$

Methodology of derivation 6/7

Group terms : $\nabla \boldsymbol{u}$ and $\nabla \cdot \boldsymbol{j}$

Use Eq. (79)

$$\int_V (\mathcal{I}+\mathcal{K})dV = \int_V \left\{ \left[\left(\rho \underbrace{\left(-\partial_\rho \mathcal{F} + \boldsymbol{\nabla}\cdot\boldsymbol{\mathcal{F}}\right)}_{\equiv -\mu_\rho} + \mathcal{F} - c \underbrace{\frac{\partial \mathcal{F}}{\partial c}}_{\equiv \mu_c} \right) \overline{\overline{\boldsymbol{I}}} - \overline{\overline{\boldsymbol{T}}} - \boldsymbol{\mathcal{F}} \otimes \boldsymbol{\nabla}\rho \right] : \boldsymbol{\nabla u} + \boldsymbol{j} \cdot \boldsymbol{\nabla} \frac{\partial \mathcal{F}}{\partial c} \right\}$$

$$= -\int_V \left\{ \underbrace{\left[\left(\rho\mu_\rho - \mathcal{F} + c\mu_c\right) \overline{\overline{\boldsymbol{I}}} + \overline{\overline{\boldsymbol{T}}} + \boldsymbol{\mathcal{F}} \otimes \boldsymbol{\nabla}\rho \right]}_{\overline{\overline{\boldsymbol{T}}} \text{ def such as } = -\overline{\overline{\boldsymbol{P}}} + \overline{\overline{\boldsymbol{\tau}}}} : \boldsymbol{\nabla u} - \underbrace{\boldsymbol{j}_c \cdot \boldsymbol{\nabla} \frac{\partial \mathcal{F}}{\partial c}}_{\boldsymbol{j}_c \text{ def such as } \propto -\boldsymbol{\nabla}(\partial\mathcal{F}/\partial c)} \right\}$$

Appropriate choice of $\boldsymbol{j}$ and $\overline{\overline{\boldsymbol{T}}}$

$$\boldsymbol{j} = -\mathcal{M}_c \boldsymbol{\nabla}\mu_c$$

$$\overline{\overline{\boldsymbol{T}}} = -\left[\rho\mu_\rho - \mathcal{F} + c\mu_c\right]\overline{\overline{\boldsymbol{I}}} - \boldsymbol{\mathcal{F}} \otimes \boldsymbol{\nabla}\rho + \overline{\overline{\boldsymbol{\tau}}}$$

- $\overline{\overline{\boldsymbol{\tau}}}$: viscous stress tensor is such as $\overline{\overline{\boldsymbol{\tau}}} : \boldsymbol{\nabla u} \geqslant 0$

Methodology of derivation 7/7

With $\mathcal{F}$ defined by Eq. (187)

$$\boldsymbol{\mathcal{F}} = \frac{\partial \mathcal{F}}{\partial (\boldsymbol{\nabla}\rho)} = \zeta(c)\boldsymbol{\nabla}\rho$$

$$\mu_c = \frac{1}{2}\zeta'(c)\left|\boldsymbol{\nabla}\rho\right|^2 + \alpha c$$

$$\overline{\overline{\boldsymbol{T}}} = -\underbrace{\left[\rho\mu_\rho - \mathcal{F} + c\mu_c\right]}_{\equiv \mathcal{J}}\overline{\overline{\boldsymbol{I}}} - \underbrace{\zeta\boldsymbol{\nabla}\rho \otimes \boldsymbol{\nabla}\rho}_{\text{Korteweg tensor}} + \overline{\overline{\boldsymbol{\tau}}}$$

$$\begin{aligned}\mu_\rho &= \frac{\partial f}{\partial \rho} - \boldsymbol{\nabla}\cdot\left(\zeta(c)\boldsymbol{\nabla}\rho\right)\\ &= \partial_\rho f - \zeta(c)\boldsymbol{\nabla}^2\rho - \boldsymbol{\nabla}\rho\cdot\boldsymbol{\nabla}\zeta(c)\\ &= \partial_\rho f - \zeta(c)\boldsymbol{\nabla}^2\rho - \zeta'(c)\boldsymbol{\nabla}\rho\cdot\boldsymbol{\nabla}c\end{aligned}$$

Remarks on first term of $\overline{\overline{\boldsymbol{T}}}$

$$\mathcal{J}\overline{\overline{\boldsymbol{I}}} = \Bigg[\overbrace{\underbrace{\rho\partial_\rho f - f(\rho)}_{\equiv p^{eos}(\rho)} - \rho\zeta(c)\boldsymbol{\nabla}^2\rho - \frac{\zeta(c)}{2}\left|\boldsymbol{\nabla}\rho\right|^2}^{\equiv \mathcal{P}(\rho,\boldsymbol{\nabla}\rho)}\Bigg]\overline{\overline{\boldsymbol{I}}} + \underbrace{\left[\frac{\alpha}{2}c^2 + \zeta'(c)\left(\frac{c}{2}\left|\boldsymbol{\nabla}\rho\right|^2 - \rho\boldsymbol{\nabla}\rho\cdot\boldsymbol{\nabla}c\right)\right]\overline{\overline{\boldsymbol{I}}}}_{\equiv \overline{\overline{\boldsymbol{\zeta}}}_s}$$

References to go further with those approaches

Remark on NS/K model coupled with temperature

Also called "Second gradient theory"

see CASAL & GOUIN CRAS (1985) and JAMET *et al.* JCP (2001)

Books

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6. Advanced applications

Overview of three-phase flows, ternary mixture, etc.

Outline section 6

a. Three-phase flows

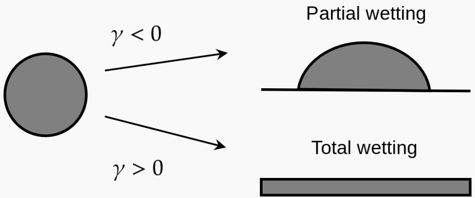
Three immiscible fluids

Spreading parameter

Two types of wetting

$$\gamma \hat{=} \sigma_{Gs} - (\sigma_{Ls} + \sigma_{LG})$$

- γ: spreading parameter
- σ_{ij}: surface tension between *i* and *j*



Assumptions and formulation for three phases

Phase-field model

- PDEs on ϕ_1 and ϕ_2
- Only one composition c (transfer between phases k and ℓ)
- Mass and impulsion balance for $\boldsymbol{u}$ and p_h

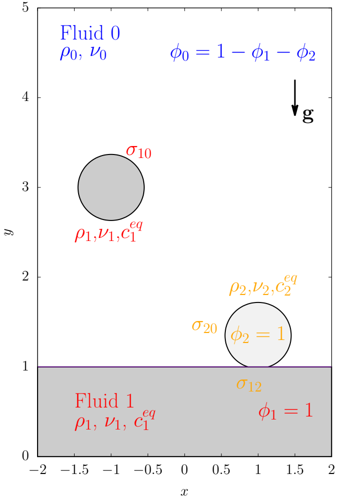
Origin: free energy (from BOYER *et al.* 2008)

$$\mathscr{F}[\phi_0,\phi_1,\phi_2]=\int f_{dw}(\phi_0,\phi_1,\phi_2)+\frac{3}{8}W\sum_{k=0}^{2}\gamma_k\left|\boldsymbol{\nabla}\phi_k\right|^2 dV$$

$$f_{dw}(\phi_0,\phi_1,\phi_2)=\sum_{k=0}^{2}\frac{12}{W}\left[\frac{\gamma_k}{2}\phi_k^2(1-\phi_k)^2\right]$$

Spreading coefficients γ_k (see book DE GENNES *et al.*, 2004)

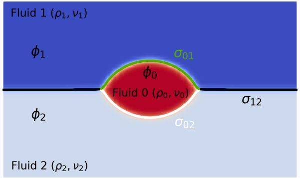
$$\gamma_0=\sigma_{10}+\sigma_{20}-\sigma_{12},\quad \gamma_1=\sigma_{10}+\sigma_{12}-\sigma_{20},\quad \gamma_2=\sigma_{20}+\sigma_{12}-\sigma_{01}$$



Notations of three-phase and equilibrium

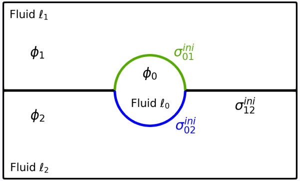
Mechanical equilibrium without composition effect

Notations (phase index $k = 0, 1, 2$)

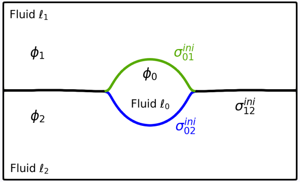


Phase-fields	: $\phi_k(\boldsymbol{x}, t)$
Surface tensions	: $\sigma_{k\ell}$
Bulk densities	: ρ_k
Kinematic viscosities	: ν_k
Total density	: $\varrho(\phi)$
Total viscosity	: $\vartheta(\phi)$

Initial setup

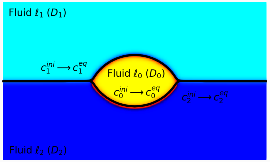


Without composition effect

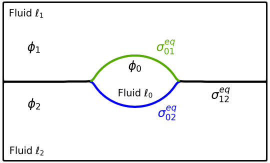


With composition effect

Studied but not presented here



Thermodynamic equilibrium



$\sigma_{k\ell}^{ini} \to \sigma_{k\ell}^{eq}$

Model of three-phase flow 1/2: EDPs

Three-phase interface capturing (see ABADI *et al.*, JCP 2018)

$$\frac{\partial \phi_1}{\partial t} + \nabla \cdot (\boldsymbol{u}\phi_1) = \nabla \cdot \left[M_\phi \left(\nabla \phi_1 - \left| \nabla \phi_1 \right|^{eq} \boldsymbol{n}_1 + \frac{1}{3} \sum_{k=0}^{2} \left| \nabla \phi_k \right|^{eq} \boldsymbol{n}_k \right) \right] \tag{193a}$$

$$\frac{\partial \phi_2}{\partial t} + \nabla \cdot (\boldsymbol{u}\phi_2) = \nabla \cdot \left[M_\phi \left(\nabla \phi_2 - \left| \nabla \phi_2 \right|^{eq} \boldsymbol{n}_2 + \frac{1}{3} \sum_{k=0}^{2} \left| \nabla \phi_k \right|^{eq} \boldsymbol{n}_k \right) \right] \tag{193b}$$

$$\phi_0(\boldsymbol{x}, t) = 1 - \phi_1(\boldsymbol{x}, t) - \phi_2(\boldsymbol{x}, t) \tag{193c}$$

$$\left| \nabla \phi_k \right|^{eq} = \frac{4}{W} \phi_k (1 - \phi_k) \tag{193d}$$

Flows: Navier-Stokes (articificial compressibility algorithm)

$$\nabla \cdot \boldsymbol{u} = 0 \tag{194a}$$

$$\frac{\partial \varrho \boldsymbol{u}}{\partial t} + \nabla \cdot (\varrho \boldsymbol{u}\boldsymbol{u}) = -\nabla p_h + \nabla \cdot \left[\varrho \vartheta \left(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T \right) \right] + \boldsymbol{F}_s + \boldsymbol{F}_g \tag{194b}$$

Model of three-phase flow 2/2: forces and closures

Force terms

$$\boldsymbol{F}_s + \boldsymbol{F}_g = \underbrace{\mu_{\phi_0}\boldsymbol{\nabla}\phi_0 + \mu_{\phi_1}\boldsymbol{\nabla}\phi_1 + \mu_{\phi_2}\boldsymbol{\nabla}\phi_2}_{\text{Capillary forces}} + \underbrace{\varrho(\phi)\boldsymbol{g}}_{\text{Gravity force}}$$

Capillary forces in the diffuse interface approximation ▸ Appendix

Chemical potentials μ_{ϕ_k} (sum conv over $k = 0, 1, 2$)

$$\mu_{\phi_k}(\boldsymbol{x}, t) = \frac{4\gamma_T}{W}\sum_{\ell\neq k}\left[\frac{1}{\gamma_\ell}\left(\frac{\partial f_{dw}}{\partial\phi_k} - \frac{\partial f_{dw}}{\partial\phi_\ell}\right)\right] - \frac{3}{4}W\gamma_k\boldsymbol{\nabla}^2\phi_k$$

$$\frac{3}{\gamma_T} = \sum_k \frac{1}{\gamma_k} \qquad (e.g.\ \gamma_1 = \sigma_{10} + \sigma_{12} - \sigma_{20})$$

Interpolations $\phi = (\phi_0, \phi_1, \phi_2)$

Total density

$$\varrho(\phi) = \sum_k \rho_k\phi_k(\boldsymbol{x}, t)$$

Total viscosity

$$\frac{1}{\vartheta(\phi)} = \sum_k \frac{\phi_k(\boldsymbol{x}, t)}{\nu_k}$$

Lattice Boltzmann keywords for the three-phase model

Lattices

- 2D: **D2Q9** ($i = 0, \dots, 8$)
- 3D: **D3Q27** ($i = 0, \dots, 26$)
- One layer of ghost cells (`MPI` sub-domains)

Navier-Stokes Eqs

- Distribution function: f_i for $\varrho \boldsymbol{u}$ and p
- Collision: BGK and MRT (compared)
- Additional gradients (force terms) with finite difference

Composition Eq.

- Distribution function h_i for c
- Collision: BGK

Lattice Boltzmann schemes for all PDEs

Phase-field ϕ_1-eq and ϕ_2-eq

- Eq. ϕ_1 (details next slide)
  - Distribution function g_i^1 for ϕ_1
  - Collision: BGK
  - Computation of additional gradients with directional derivatives (e.g. $\boldsymbol{n} = \boldsymbol{\nabla}\phi / \left|\boldsymbol{\nabla}\phi\right|$ and μ_ϕ)
- Eq. ϕ_2 (same scheme but on g_i^2)

Lattice Boltzmann schemes 1/2: Navier-Stokes

LB scheme on f_i for $p^\star$ and $\boldsymbol{u}$ with $p^\star = p_h/\varrho c_s^2$ and MRT collision operator

$$\boldsymbol{f}(\boldsymbol{x}+\boldsymbol{c}_i\delta t, t+\delta t) = \boldsymbol{f}(\boldsymbol{x},t) - \boldsymbol{M}^{-1}\boldsymbol{S}\boldsymbol{M}\left[\boldsymbol{f}(\boldsymbol{x},t) - \boldsymbol{f}^{eq}(\boldsymbol{x},t)\right] + \delta t\boldsymbol{\mathcal{F}}$$

For $i=0,\dots,N_{pop}$
$$\begin{cases} f_i^{eq}(\boldsymbol{x},t) &= w_i\left[p^\star + \left(\dfrac{\boldsymbol{c}_i\cdot\boldsymbol{u}}{c_s^2} + \dfrac{(\boldsymbol{c}_i\cdot\boldsymbol{u})^2}{2c_s^4} - \dfrac{\boldsymbol{u}^2}{2c_s^2}\right)\right] - \dfrac{\delta t}{2}\mathcal{F}_i \\ \mathcal{F}_i(\boldsymbol{x},t) &= w_i\dfrac{\boldsymbol{c}_i\cdot\boldsymbol{F}_{tot}(\boldsymbol{x},t)}{\varrho(\phi)c_s^2} \end{cases}$$

with
$$\boldsymbol{F}_{tot}(\boldsymbol{x},t) = (\boldsymbol{F}_p + \boldsymbol{F}_v) + (\boldsymbol{F}_s + \boldsymbol{F}_g)$$

Macroscopic quantities

Force terms

$$\boldsymbol{F}_p = -p^\star c_s^2\boldsymbol{\nabla}\rho$$

$$\boldsymbol{F}_v = \vartheta(\phi)\left[\boldsymbol{\nabla}\boldsymbol{u} + (\boldsymbol{\nabla}\boldsymbol{u})^T\right]\cdot\boldsymbol{\nabla}\varrho(\phi)$$

$$\boldsymbol{F}_s + \boldsymbol{F}_g = \sum_{k=0}^{2}\mu_{\phi_k}\boldsymbol{\nabla}\phi_k + \varrho\boldsymbol{g}$$

Moments

$$p^\star = \sum_i f_i \qquad \text{pressure}$$

$$\boldsymbol{u} = \sum_i f_i\boldsymbol{c}_i + \frac{\delta t}{2\varrho}\boldsymbol{F}_{tot} \qquad \text{velocity}$$

Lattice Boltzmann schemes 2/2: phase-field

Distribution function g_i for $\phi_1 \equiv \phi$

LB equation

$$g_i(\boldsymbol{x}+\boldsymbol{c}_i\delta t, t+\delta t) = g_i(\boldsymbol{x},t) - \frac{1}{\tau_g+1/2}\left[g_i(\boldsymbol{x},t) - g_i^{eq}(\boldsymbol{x},t)\right] + \delta t \mathcal{G}_i$$

$$g_i^{eq}(\boldsymbol{x},t) = w_i\phi\left[1+\frac{\boldsymbol{c}_i\cdot\boldsymbol{u}}{c_s^2}\right] - \frac{\delta t}{2}\mathcal{G}_i$$

$$\mathcal{G}_i = \left[\frac{4}{W}\phi(1-\phi)+\mathscr{L}(\phi)\right] w_i \boldsymbol{c}_i\cdot\boldsymbol{n}$$

Moment

$$\phi = \sum_i g_i + \frac{\delta t}{2}\mathcal{G}_i$$

Mobility

$$M_\phi = \frac{1}{3}\tau_g\frac{\delta x^2}{\delta t}$$

Computation of normal vector $\boldsymbol{n}_k = \boldsymbol{\nabla}\phi_k/\left|\boldsymbol{\nabla}\phi_k\right|$:

Directional derivatives:

$$\boldsymbol{e}_i\cdot\boldsymbol{\nabla}\phi\big|_{\boldsymbol{x}} = \frac{1}{2\delta x}\left[\phi(\boldsymbol{x}+\boldsymbol{e}_i\delta x) - \phi(\boldsymbol{x}-\boldsymbol{e}_i\delta x)\right]$$

$$\boldsymbol{\nabla}\phi = \frac{1}{e^2}\sum_{i=0}^{N_{pop}} w_i\boldsymbol{e}_i\left(\boldsymbol{e}_i\cdot\boldsymbol{\nabla}\phi\big|_{\boldsymbol{x}}\right)$$

Norm:

$$\left|\boldsymbol{\nabla}\phi\right| = \sqrt{(\partial_x\phi)^2+(\partial_y\phi)^2+(\partial_z\phi)^2}$$

Dimensionless numbers

Return

For fluid flow

Reynolds numbers

$$\mathrm{Re}_k = \frac{U_c L_c}{\nu_k}$$

Capillary numbers

$$\mathrm{Ca}_{k\ell} = \frac{\eta_k U_c}{\sigma_{k\ell}}$$

Bond or Eötvös

$$\mathrm{Bo}_{k\ell} = \frac{(\Delta\rho)_{k\ell} g R^2}{\sigma_{k\ell}}$$

For Rayleigh-Taylor

Velocity U_c

$$U_c = \sqrt{g L_c}$$

Atwood numbers

$$\mathrm{At}_{k\ell} = \frac{\rho_k - \rho_\ell}{\rho_k + \rho_\ell}$$

Nomenclature 1/2

- L_c: domain width
- g: gravity
- ρ_k: heavy density

For interface tracking

Peclet number

$$\mathrm{Pe}_\phi = \frac{U_c L_c}{M_\phi}$$

Cahn number

$$\mathrm{Cahn} = \frac{W}{L_c}$$

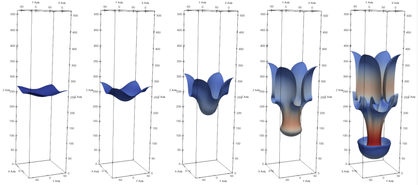
Nomenclature 2/2

- ν_k: kinematic visc
- $\sigma_{k\ell}$: surf tension between k and ℓ
- ρ_ℓ: light density

List of validations in `LBM_Saclay` (non exhaustive)

Two-phase

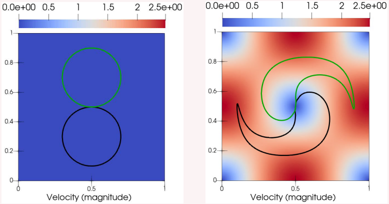
Equations	Name
$1\phi^{AC}$+1C	Stefan
$1\phi^{AC}$+NS	Double-Poiseuille
	Laplace law
	Rayleigh-Taylor instab
	Drag coeff of a droplet
	Splashing droplet



Rayleigh-Taylor instability (C. ELHARTI, 2023)

Three-phase

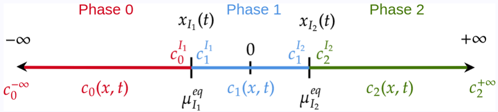
Equations	Name
$2\phi^{AC}$	Interface deformation
$2\phi^{AC}$+1C	Analytical solution
$2\phi^{AC}$+NS	Spreading capsule
$2\phi^{AC}$+NS	Spreading of liq lens
$2\phi^{AC}$+NS	Rayleigh-Taylor instability



Interface deformation inside a vortex ▸ Video

Verification 1/4: analytical solution for 2ϕ+1C

Stefan's solutions for three-phase

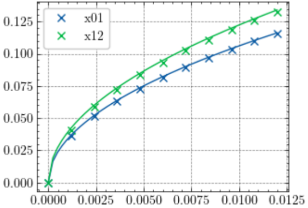


Analytical solutions of

- Two positions $x_{I_1}(t)$ and $x_{I_2}(t)$
- Three compositions $c_0(x,t)$, $c_1(x,t)$ and $c_2(x,t)$

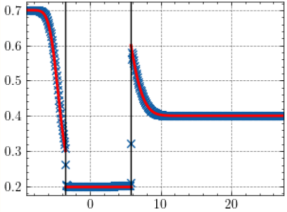
Comparisons with LBM (T. Boutin)

Positions $x_{I_1}(t)$ and $x_{I_2}(t)$ (LBM dots)



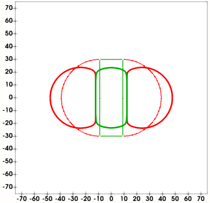
L^1-errors: 0.7% and 1.54%

Composition $c(x,t)$ at $t = 0.012$



Verification 2/4: steady state comparison of shapes

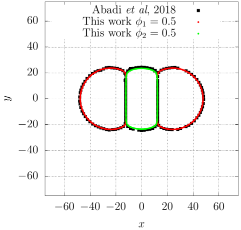
Spreading capsule



$\rho = (0.1, 10, 5)$
$\nu = 4.827 \times 10^{-3}$
$\sigma = 5 \times 10^{-4}$

t_i dash line
t_f solid line

▸ Video

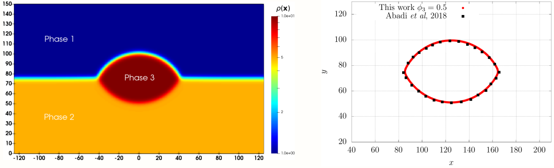


$W = 5$
$M_\phi = 5 \times 10^{-3}$

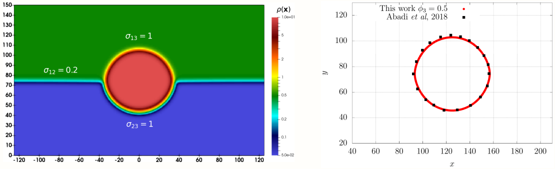
Comparison (JCP 2018)

Spreading liquid lens for $(\sigma_{12}, \sigma_{13}, \sigma_{23})$

Case A: $(1, 1, 1) \times 10^{-4}$



Case B: $(0.2, 1, 1) \times 10^{-4}$

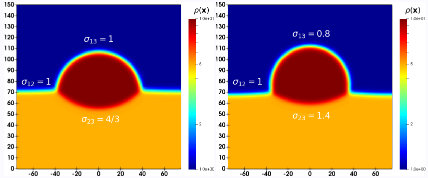


Initial conditions and parameters ▸ Appendix

Verification 3/4: theoretical and numerical contact angles

Spreading liquid lens

Case A2 **Case A3**

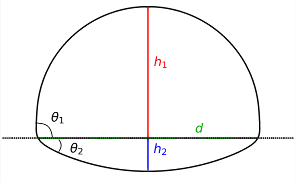


Theoretical contact angles $\theta^{th}_{1,2}$ depending on $\sigma_{k\ell}$

Theoretical $\theta^{th}_{1,2}$

$$\cos\theta_1^{th} = \frac{\sigma_{12}^2 + \sigma_{13}^2 - \sigma_{23}^2}{2\sigma_{12}\sigma_{13}}$$

$$\cos\theta_2^{th} = \frac{\sigma_{12}^2 + \sigma_{23}^2 - \sigma_{13}^2}{2\sigma_{12}\sigma_{23}}$$



Relative errors of numerical contact angles θ_1^{sim} and θ_2^{sim}

Simulations $\theta^{sim}_{1,2}$

$$\tan\left(\frac{\theta_1^{sim}}{2}\right) = \frac{2h_1}{d}$$

$$\tan\left(\frac{\theta_2^{sim}}{2}\right) = \frac{2h_2}{d}$$

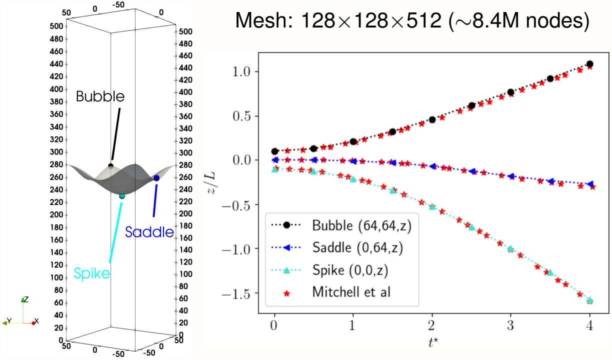
Case	$(\sigma_{12}, \sigma_{13}, \sigma_{23})$	θ_1^{th}	θ_1^{sim}	θ_2^{th}	θ_2^{sim}	Err(θ_1)	Err(θ_2)
A1	$(1, 1, 1)$	60°	62.161°	60°	59.767°	3.6026%	0.3879%
A2	$(1, 1, 4/3)$	83.621°	83.635°	48.189°	49.019°	0.0174%	1.7218%
A3	$(1, 0.8, 1.4)$	101.53°	101.32°	34.047°	33.256°	0.2094%	2.324%
B2	$(0.2, 1, 1)$	84.261°	83.684°	84.261°	84.133°	0.6847%	0.1519%

Verification 4/4: time-evolution of 3D Rayleigh-Taylor instability

Three-phase model degenerating into two-phase Rayleigh-Taylor: $\phi_0 = 0$ everywhere

3D validation of NS + 2 eqs for ϕ_1 and ϕ_2

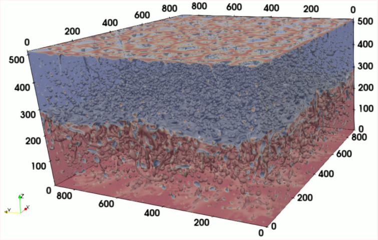
Mesh: 128×128×512 (∼8.4M nodes)



At $= 0.5$, Re $= 128$, $\eta^\star = 3$, Ca $= 9.1$, Pe $= 744$

Simulation on Topaze-A100

Mesh: 900×900×512 (∼415M nodes)



▶ Video 144 GPUs

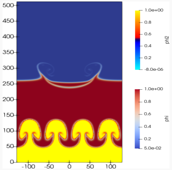
▶ Appendix dimensionless numbers

▶ Appendix 2D validation of R-T instab

Overview of three-phase simulations

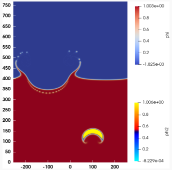
2D simulations

Rayleigh-Taylor/splashing



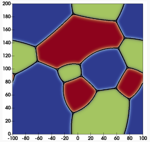
Video

Rising/splashing droplets



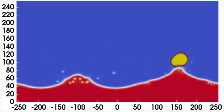
Video 1 Video 2

Spinodal decomposition



Video 1 Video 2

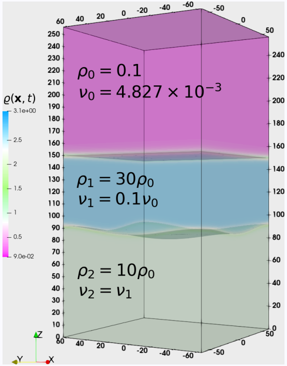
Splashing/falling droplets



Video 1 Video 2

3D simulation: initialization of three-phase

Lightest phase: magenta Heaviest phase: cyan



Adim nb

Re $= 3000$
Pe $= 1000$
Cahn $= 0.039$

$\mathrm{Ca}_{12} = 0.26$
$\mathrm{Ca}_{01} = 0.26$
$\mathrm{Ca}_{02} = 0.1365$

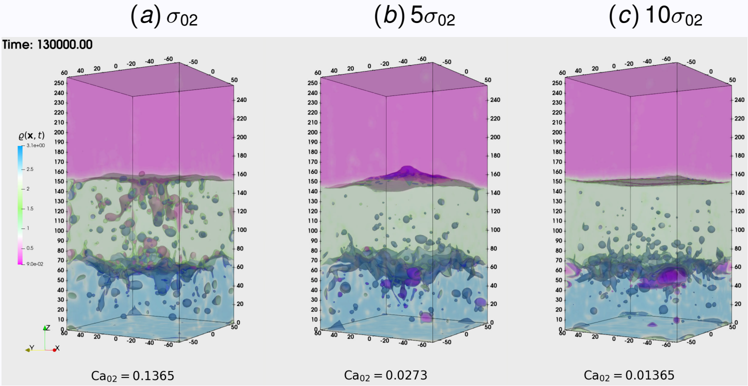
$\mathrm{At}_{12} = 0.5$
$\mathrm{At}_{01} = 0.9355$
$\mathrm{At}_{02} = 0.8181$

Interface height (cyan/green)

$$z(x, y) = A \times L\left[\cos(2\pi x/\lambda) + \cos(2\pi y/\lambda)\right]$$

3D three-phase simulations of surface tension effect

Simulations of surface tension effect: greater values of σ_{02} . . .



Jean-Zay (V100)

Mesh: 128×128×256 ($\sim$ 4.2M nodes)
16 GPUs

$\sigma_{02} = 4 \times 10^{-5}$

$W = 5$
$M_\phi = 1.44 \times 10^{-3}$
$\sigma_{01} = \sigma_{12} = 6.3 \times 10^{-5}$

Video

. . . imply that **bigger magenta bubbles are trapped between the cyan and green phases** . . .

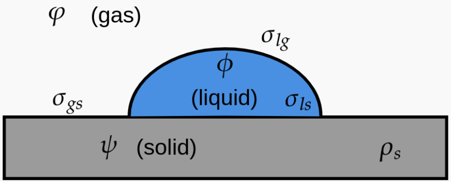
2D simulations of radius sensitivity Appendix

b. Two-phase interacting with a solid phase

Assumptions for two-phase interacting with a solid phase

Here the solid is not a boundary condition but it is considered as a new phase ψ

Add new phase-fields: ψ for solid phase and φ for gas phase



- ρ_s: solid density
- σ_{ij}: surface tension between i and j

Assumption: conservation of phases (no phase change)

$$\phi + \varphi + \psi = 1 \tag{195}$$

Consequence:

- one PDE on ϕ + one PDE on ψ
- Derivation of φ with Eq. (195)

Math model for solid phase interaction 1/2

Evolution for ψ

$$\frac{\partial\psi}{\partial t}+\boldsymbol{u}_s\cdot\boldsymbol{\nabla}\psi=0 \qquad (196)$$

$$\varphi=1-\phi-\psi \qquad (197)$$

Modification of interface-capturing eq.

- Evolution

$$\frac{\partial\phi}{\partial t}+\boldsymbol{\nabla}\cdot(\boldsymbol{u}\phi)=\boldsymbol{\nabla}\cdot\left\{M_\phi\left[\boldsymbol{\nabla}\phi-\frac{4}{W_\phi}\phi(1-\phi)\boldsymbol{n}_\phi+\boldsymbol{\mathcal{L}}(\phi,\varphi,\psi)\right]\right\} \qquad (198)$$

- Lagrange multiplier

$$\boldsymbol{\mathcal{L}}(\phi,\varphi,\psi)=\frac{1}{2}\left[\frac{4}{W_\psi}\psi(1-\psi)\boldsymbol{n}_\psi+\frac{4}{W_\phi}\phi(1-\phi)\boldsymbol{n}_\phi+\frac{4}{W_\varphi}\varphi(1-\varphi)\boldsymbol{n}_\varphi\right] \qquad (199)$$

- Normal vectors at interface: $\boldsymbol{n}_f=\frac{\boldsymbol{\nabla}f}{|\boldsymbol{\nabla}f|}$ (for $f=\psi,\phi,\varphi$)

Math model for solid phase interaction 2/2

Incompressible Navier-Stokes

- Mass and impulsion balance

$$\nabla \cdot \boldsymbol{u}' = -\boldsymbol{u}_s \cdot \nabla \psi \tag{200}$$

$$\varrho \left[\frac{\partial \boldsymbol{u}'}{\partial t} + \nabla \cdot (\boldsymbol{u}'\boldsymbol{u}) \right] = -(1-\psi)\nabla p_h + \nabla \cdot \left[\eta \left(\nabla \boldsymbol{u}' + (\nabla \boldsymbol{u}')^T \right) \right] + (1-\psi)\boldsymbol{F}_{tot} \tag{201}$$

$$\boldsymbol{u}' = (1-\psi)\boldsymbol{u} \tag{202}$$

- Interpolation

$$\varrho = \phi\rho_l + \varphi\rho_g + \psi\rho_s \tag{203}$$

$$\frac{1}{\eta} = \frac{\phi}{\eta_l} + \frac{(1-\phi)}{\eta_g} \tag{204}$$

- Forces

$$\boldsymbol{F}_{tot} = \boldsymbol{F}_c + \boldsymbol{F}_g \tag{205}$$

$$\boldsymbol{F}_c = \underbrace{\mu_\phi \nabla \phi + \mu_\varphi \nabla \varphi + \mu_\psi \nabla \psi}_{\propto f(\sigma_{lg}, \sigma_{ls}, \sigma_{gs})} \tag{206}$$

$$\boldsymbol{F}_g = \varrho \boldsymbol{g} \tag{207}$$

Cancel velocity in solid phase

LB scheme for fluid flow (initial scheme on $p^\star$ and $\boldsymbol{u}$)

$$\boldsymbol{f}(\boldsymbol{x}+\boldsymbol{c}_i\delta t, t+\delta t) = \boldsymbol{f}(\boldsymbol{x}, t) - \boldsymbol{M}^{-1}\boldsymbol{SM}\left[\boldsymbol{f}(\boldsymbol{x}, t) - \boldsymbol{f}^{eq}(\boldsymbol{x}, t)\right] + \delta t \boldsymbol{\mathcal{F}}$$

$$f_i^{eq}(\boldsymbol{x}, t) = w_i(1-\psi)\left[p^\star + \left(\frac{\boldsymbol{c}_i \cdot \boldsymbol{u}}{c_s^2} + \frac{(\boldsymbol{c}_i \cdot \boldsymbol{u})^2}{2c_s^4} - \frac{\boldsymbol{u}^2}{2c_s^2}\right)\right] - \frac{\delta t}{2}\mathcal{F}_i$$

$$\mathcal{F}_i = w_i \frac{\boldsymbol{c}_i \cdot \boldsymbol{F}_{tot}}{\varrho(\phi)c_s^2}$$

Macroscopic quantities

Force $\boldsymbol{F}_{tot}$

$$\boldsymbol{F}_{tot} = (1-\psi)(\boldsymbol{F}_p + \boldsymbol{F}_s + \boldsymbol{F}_g + \boldsymbol{F}_v) + \boldsymbol{F}_{p'}$$

Moments

$$p^\star = \sum_i f_i$$

$$\boldsymbol{u} = \sum_i f_i \boldsymbol{c}_i + \frac{\delta t}{2\varrho(\phi)}\boldsymbol{F}_{tot}$$

Force terms ($p^\star = p_h/\varrho c_s^2$ and $\boldsymbol{F}_{p'}$)

$$\boldsymbol{F}_p = -p^\star c_s^2 \boldsymbol{\nabla}\varrho$$

$$\boldsymbol{F}_{p'} = -p_h \boldsymbol{\nabla}\psi$$

$$\boldsymbol{F}_s = \mu_\phi \boldsymbol{\nabla}\phi$$

$$\boldsymbol{F}_g = \varrho \boldsymbol{g}$$

$$\boldsymbol{F}_v = \nu\left[\boldsymbol{\nabla u} + (\boldsymbol{\nabla u})^T\right]\cdot\boldsymbol{\nabla}\varrho(\phi)$$

Origin of the pressure force $\boldsymbol{F}_{p'}$

Pressure force $\boldsymbol{F}_{p'}$

The Chapman-Enskog expansion recovers the pressure term $-\boldsymbol{\nabla}\left[(1-\phi)p^\star c_s^2\right]$ with $p^\star = p_h/\varrho c_s^2$:

$$
\begin{aligned}
-\boldsymbol{\nabla}\left[(1-\phi)p^\star c_s^2\right] &= -\boldsymbol{\nabla}\left[(1-\phi)\frac{p_h}{\varrho \cancel{c_s^2}}\cancel{c_s^2}\right]\\
&= -\frac{(1-\phi)}{\varrho}\boldsymbol{\nabla} p_h - p_h\boldsymbol{\nabla}\left(\frac{1-\phi}{\varrho}\right)\\
&= -\frac{1-\phi_1}{\varrho}\boldsymbol{\nabla} p_h + (1-\phi_1)\frac{p_h}{\varrho^2}\boldsymbol{\nabla}\varrho + \frac{p_h}{\varrho}\boldsymbol{\nabla}\phi
\end{aligned}
$$

$$
-\boldsymbol{\nabla}\left[(1-\phi)p^\star c_s^2\right] + \frac{1}{\varrho}\left[-(1-\phi)\frac{p_h}{\varrho}\boldsymbol{\nabla}\varrho - p_h\boldsymbol{\nabla}\phi\right] = -\frac{1-\phi}{\varrho}\boldsymbol{\nabla} p_h
$$

Finally

$$
-\frac{1-\phi}{\varrho}\boldsymbol{\nabla} p_h = -\boldsymbol{\nabla}\left[(1-\phi)p^\star c_s^2\right] + \frac{1}{\varrho}\left[(1-\phi)\boldsymbol{F}_p + \boldsymbol{F}_{p'}\right] \qquad \text{with} \qquad \begin{cases} \boldsymbol{F}_p &= -\frac{p_h}{\varrho}\boldsymbol{\nabla}\varrho \\ \boldsymbol{F}_{p'} &= -p_h\boldsymbol{\nabla}\phi \end{cases}
$$

Contact angles 1/2: setup

Input dimensionless parameters

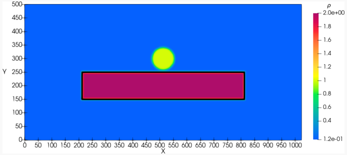
- Parameters

Name	Symb	Value	Dim
Water density	ρ_l	1	–
Air density	ρ_a	0.120606236	–
Kin viscosity	$\nu_l = \nu_a$	0.010364759	–
Surface tension	σ	0.1	–
Mobility	M_ϕ	0.08	–
Interf width	$W = W_s$	8	–
Gravity	g_y	-5×10^{-7}	–
Solid mobility	M_ψ	0.04	–
Solid density	ρ_s	2	–

- Boundary conditions
  - xmin & xmax: periodic
  - ymin & ymax: wall

- Mesh 1024$\times$500

Initial condition



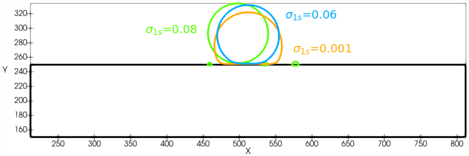
- Comparison for several values of σ_{1s} and σ_{2s}

Contact angles 2/2: results

Comparisons after 100.000 time-iterations

σ_{1s} effect

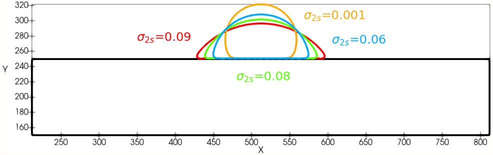
- $\sigma_{2s} = 10^{-9}$
- Sensitivity on $\sigma_{1s} = 0.08, 0.06, 0.001$



- σ_{1s} big for hydrophobic surface

σ_{2s} effect

- $\sigma_{1s} = 10^{-9}$
- Sensitivity on $\sigma_{2s} = 0.09, 0.08, 0.06, 0.001$



- σ_{2s} big for hydrophilic surface

P. Hydrophilic and hydrophobic surfaces

Run `TestCase17a_Hydrophobic-Solid`

Running “hydrophilic and hydrophobic surfaces” on ORCUS

command = sbatch /tmpformation/LBM_Saclay/JOB_H100_GPU.slurm

Guidelines

- Folder

```
$ cd TestCase17a_Hydrophobic-Solid
```

- For $\sigma_{1s} = 0.01$ and sensitivity on σ_{2s}

```
$ cd Sensib_Sigma1s_val1
$ command TestCase_Hydrophobic-Surface_val1.ini
```

- For $\sigma_{1s} = 0.5$ and sensitivity on σ_{2s}

```
$ cd Sensib_Sigma2s_val1
$ command TestCase_Wetting-solid-Rectangle_val1.ini
```

Hydrophilic and hydrophobic surfaces: setup

Input parameters

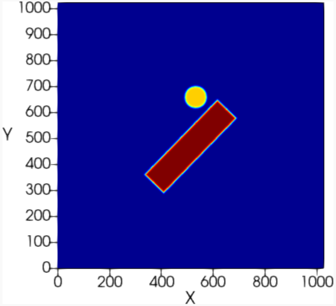
- Parameters

Name	Symb	Value	Dim
Water density	ρ_l	100	–
Air density	ρ_a	0.120606236	–
Kin viscosity	ν_l	6.666666×10^{-3}	–
Kin viscosity	ν_a	0.010364759	–
Surface tension	σ	0.5	–
Mobility	M_ϕ	0.08	–
Interf width	$W = W_s$	8	–
Gravity	g_y	-1.5×10^{-6}	–
Solid mobility	M_ψ	0.04	–
Solid density	ρ_s	150	–

- Boundary conditions
  - xmin & xmax: periodic
  - ymin & ymax: wall

- Mesh 1024×1024

Initial condition

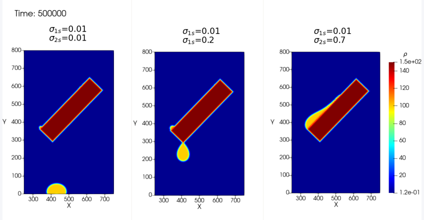


- Comparison for several values of σ_{1s} and σ_{2s}

Results

Wetting and no-wetting surface

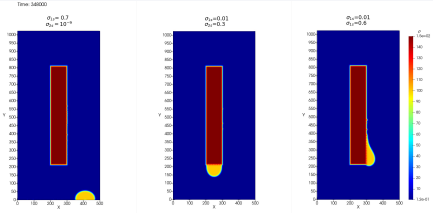
- $\sigma_{1s} = 0.01$
- Sensitivity to $\sigma_{2s} = 0.01, 0.2, 0.7$



Video

With a vertical wall

- $\sigma_{1s} = \sigma = 0.5$
- Sensitivity to $\sigma_{2s} = 0.1, 0.08, 0.05$



Video

P. Two-phase with container

Splash, leak, moving container

Running “Splash with container” on ORCUS

```
command = sbatch /tmpformation/LBM_Saclay/JOB_H100_GPU.slurm
```

Guidelines

- Folder:

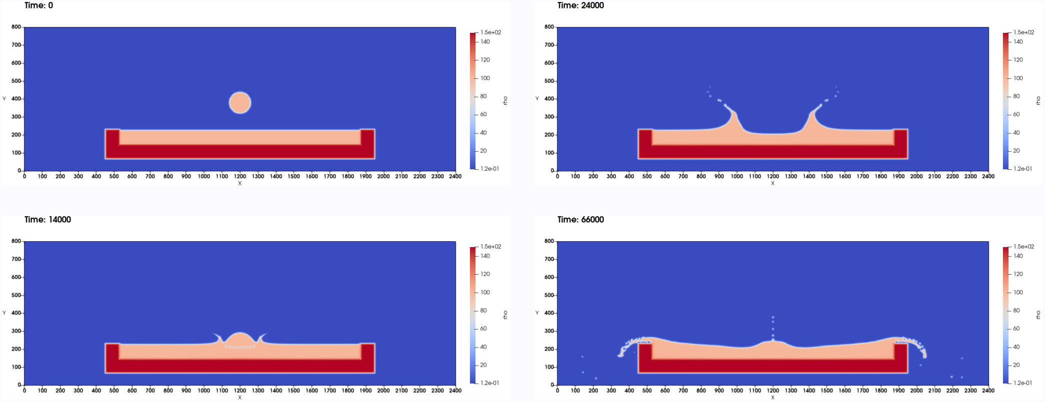
```
$ cd TestCase18_Container-Splash
```

- Run

```
$ command TestCase18_Container-Splash.ini
```

Results

Splash with a container – mesh 2400×800=1.92M nodes



Video

Running “Static and moving container leak” on ORCUS

Guidelines for “static container”

- Folder:

```
$ cd TestCase19_Static-Container-Hole
```

- Run

```
$ command TestCase19_Static-Container-Hole.ini
```

Guidelines for “Moving container”

- Folder:

```
$ cd TestCase20_Moving-Container-Hole
```

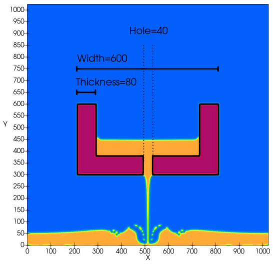
- Run

```
$ command TestCase20_Moving-Container-Hole.ini
```

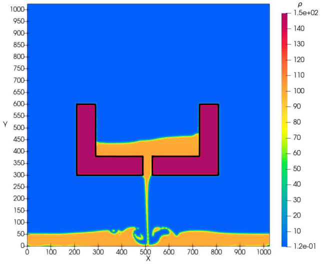
Results

Container leak – mesh 1024×1024

- 10^6 time-iterations
  - 1h20min (1 GPU A100)
  - 30min (1 GPU H100)



Static



Moving

Video

C. Crystal growth

Binary mixture and matched asymptotic expansions

Equivalence between ψ-model and sharp model

Sharp interface model

$$\frac{\partial \overline{T}}{\partial t} = D\nabla^2 \overline{T} \tag{208a}$$

$$v_n = D\boldsymbol{n} \cdot (\nabla \overline{T}|_{sol} - \nabla \overline{T}|_{liq}) \tag{208b}$$

$$\overline{T}_I = d_0 \sum_{\xi=1,2} \left[a_s(\boldsymbol{n}) + \frac{\partial^2 \gamma}{\partial \theta_\xi^2} \right] \frac{1}{R_\xi} - \beta(\boldsymbol{n}) v_n \tag{208c}$$

- $\overline{T} = (T - T_m)\mathcal{C}_p/\mathcal{L}$: dimensionless temperature
- $d_0 = \sigma_0 T_m \mathcal{C}_p/\mathcal{L}^2$: capillary length
- $\beta(\boldsymbol{n}) = \mathcal{C}_p/\mathcal{L}m(\boldsymbol{n})$: kinetic coefficient

$\Updownarrow$ Matched asymptotic expansion of the phase-field model

Conditions of equivalence

$$d_0 = a_1 \frac{W_0}{\lambda} \tag{209}$$

$$\beta(\boldsymbol{n}) = a_1 \left[\frac{\tau(\boldsymbol{n})}{\lambda W(\boldsymbol{n})} - a_2 \frac{W(\boldsymbol{n})}{\kappa} \right] \tag{210}$$

Right-hand side: λ, $W(\boldsymbol{n})$ and $\tau(\boldsymbol{n})$ are the parameters of the phase-field model.

Surface tension anisotropy and anisotropy function

Dependence of properties with normal vector *n*

- Properties

$$\sigma \equiv \sigma(\boldsymbol{n}) = \sigma_0 a_s(\boldsymbol{n})$$
$$\beta \equiv \beta(\boldsymbol{n}) = \beta_0 a_s(\boldsymbol{n})$$
$$W \equiv W(\boldsymbol{n}) = W_0 a_s(\boldsymbol{n})$$

- Gibbs-Thomson

$$\overline{T}_i = -d_0 \sum_{\xi=1,2} \left[a_s(\boldsymbol{n}) + \frac{\partial^2 a_s(\boldsymbol{n})}{\partial \theta_\xi} \right] \frac{1}{R_\xi} - \beta(\boldsymbol{n}) v_n$$

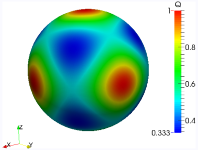
- Normal vector

$$\boldsymbol{n} = -\frac{\boldsymbol{\nabla}\phi}{|\boldsymbol{\nabla}\phi|}$$

Anisotropy function $a_s(\boldsymbol{n})$

$$\boxed{a_s(\boldsymbol{n}) = 1 + \epsilon_s \left[4(n_x^4 + n_y^4 + n_z^4) - 3 \right]}$$

where ϵ_s is a parameter



Phase-field model for crystal growth

Phase-field model for pure substance

$$\frac{\partial \overline{T}}{\partial t} = \kappa \boldsymbol{\nabla}^2 \overline{T} + \frac{1}{2}\frac{\partial \psi}{\partial t}$$

$$\tau_0 a_s^2(\boldsymbol{n}) \frac{\partial \psi}{\partial t} = W_0^2 \boldsymbol{\nabla} \cdot \left[a_s^2(\boldsymbol{n}) \boldsymbol{\nabla} \psi \right] + \boldsymbol{\nabla} \cdot \boldsymbol{\mathcal{N}}(\boldsymbol{n}) + (1 - \psi^2) \left[\psi - \lambda \overline{T} (1 - \psi^2) \right]$$

$$\boldsymbol{\mathcal{N}}(\boldsymbol{n}) = W_0^2 \left| \boldsymbol{\nabla} \psi \right|^2 a_s(\boldsymbol{n}) \frac{\partial a_s(\boldsymbol{n})}{\partial (\partial_\alpha \psi)}$$

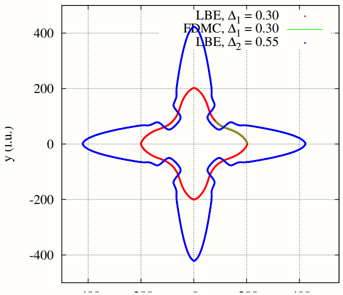
$$a_s(\boldsymbol{n}) = 1 - 3\epsilon_s + 4\epsilon_s \sum_\alpha n_\alpha^4$$

V. Benchmark

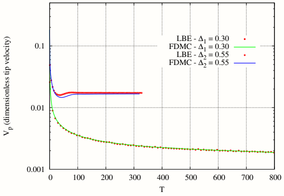
Comparison of dendrite tip velocity

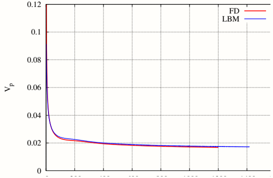
2D dendrite growth

2D dendrite for 2 undercoolings



Tip velocity V_p wrt t





Model of crystal growth for binary alloy

Dimensionless variables

$$\overline{T} = \frac{T - T_m - mc_\infty}{\mathcal{L}/C_p}, \qquad (211)$$

$$U = \frac{c - c_\infty}{(1-k)c_\infty}, \qquad (212)$$

$$U(c,\psi) = \frac{\frac{c/c_\infty}{\frac{1}{2}[1+k-(1-k)\phi]} - 1}{1-k}. \qquad (213)$$

$$a_s(\boldsymbol{n}) = 1 - 3\varepsilon_s + 4\varepsilon_s \sum_i n_i^4,$$

$$\tau(\boldsymbol{n}) = \tau_0 a_s^2(\boldsymbol{n})$$

$$\zeta(\psi) = \frac{1}{2}((1+k) - (1-k)\psi)$$

$$q(\psi) = \frac{1}{2}(1-\psi)$$

Anisotropy vector and anti-trapping current

$$\mathcal{N}(\boldsymbol{x},t) = |\boldsymbol{\nabla}\psi|^2 a_s(\mathbf{n}) \left(\frac{\partial a_s(\mathbf{n})}{\partial(\partial_x\psi)}, \frac{\partial a_s(\mathbf{n})}{\partial(\partial_y\psi)}, \frac{\partial a_s(\mathbf{n})}{\partial(\partial_z\psi)}\right)^T \qquad \text{Anisotropy vector} \qquad (214)$$

$$\boldsymbol{j}_{\mathrm{at}}(\boldsymbol{x},t) = -\frac{1}{2\sqrt{2}} W_0 \left[1 + (1-k)\, U\right] \times \frac{\partial\psi}{\partial t} \frac{\boldsymbol{\nabla}\psi}{|\boldsymbol{\nabla}\psi|} \qquad \text{Anti-trapping current} \qquad (215)$$

«ϕ-model» of crystal growth & fluid flow

Phase-field + supersaturation + Temperature

$$\tau(\boldsymbol{n})\frac{\partial\psi}{\partial t} = W_0^2\nabla\cdot\left(a_s^2(\boldsymbol{n})\nabla\psi\right) + W_0^2\sum_{i=1,2,3}\frac{\partial}{\partial x_i}\left(\left|\nabla\psi\right|^2 a_s(\boldsymbol{n})\frac{\partial a_s(\boldsymbol{n})}{\partial(\partial_{x_i}\psi)}\right) + (\psi-\psi^3) - \lambda\left(Mc_\infty U + \overline{T}\right)(1-\psi^2)^2$$

$$\zeta(\psi)\frac{\partial U}{\partial t} = \nabla\cdot\left(Dq(\psi)\nabla U + \frac{W_0}{2\sqrt{2}}\left[1+(1-k)\,U\right]\frac{\partial\psi}{\partial t}\frac{\nabla\psi}{|\nabla\psi|}\right) - q(\psi)\boldsymbol{V}\cdot\nabla U + \left[1+(1-k)\,U\right]\frac{1}{2}\frac{\partial\psi}{\partial t}$$

$$\frac{\partial\overline{T}}{\partial t} = \kappa\nabla^2\overline{T} - q(\psi)\boldsymbol{V}\cdot\nabla\overline{T} + \frac{1}{2}\frac{\partial\psi}{\partial t}$$

Hydrodynamics

$$\nabla\cdot q(\psi)\boldsymbol{V} = 0$$

$$\frac{\partial q(\psi)\boldsymbol{V}}{\partial t} + q(\psi)\boldsymbol{V}\cdot\nabla\boldsymbol{V} = -q(\psi)\nabla p/\rho + \nu\nabla^2 q(\psi)\boldsymbol{V} - \frac{\nu h}{2W_0^2}(1+\psi)^2 q(\psi)\boldsymbol{V}$$

d. Model of dissolution

Grand-potential and anti-trapping current

Grand-potential formulation $\Omega[\psi,\mu]$ of phase-field model

Why grand potential: easier way to ensure the equality of chemical potential at equilibrium (see M. PLAPP, *Phys. Rev E* 2011)

Thermodynamic functional of Grand-potential $\Omega[\psi,\mu]$

$$\Omega[\psi,\mu]=\int_V\left[\omega_{int}(\psi,\nabla\psi)+\omega_{bulk}(\psi,\mu)\right]dV \qquad \text{with} \begin{cases}\omega_{int}(\psi,\nabla\psi) & = H\psi^2(1-\psi)^2+\frac{\zeta}{2}|\nabla\psi|^2\\ \omega_{bulk}(\psi,\mu) & = p_{int}(\psi)\omega_l(\mu)+[1-p_{int}(\psi)]\,\omega_s(\mu)\\ p_{int}(\psi) & = \psi^2(3-2\psi)\end{cases}$$

Main assumptions: quadratic free energies for $\Phi = l, s$

$$\omega_\Phi(\mu)=f_\Phi-\mu c \qquad \text{(Legendre transform)}$$

$$f_\Phi(c)=\frac{\varepsilon_\Phi}{2}(c-m_\Phi)^2+f_\Phi^{min} \qquad \text{for} \quad \Phi=s,\ l$$

$$\varepsilon_s=\varepsilon_l$$

$\overline{\mu}^{eq}=\Delta\overline{f}^{min}/\Delta m$	Equil. chem. pot.
$c_l^{eq}=m_l+\overline{\mu}^{eq}$	Equil. liq. comp.
$c_s^{eq}=m_s+\overline{\mu}^{eq}$	Equil. sol. comp.

Sharp interface model of dissolution

Boundary conditions on solid/liquid interface Γ_{ls}

Hypothesis no diffusion in solid $D_s = 0$

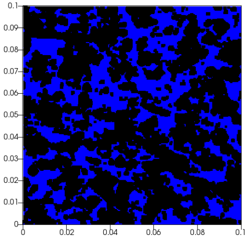
$$\frac{\partial c}{\partial t} + \boldsymbol{u}\cdot\boldsymbol{\nabla} c = \boldsymbol{\nabla}\cdot(D\boldsymbol{\nabla} c) \qquad \text{on } \Gamma_l(t) \qquad (216a)$$

$$(c - c_s)v_n = -D\boldsymbol{\nabla} c\cdot\boldsymbol{n}|_l + \cancel{D_s\boldsymbol{\nabla} c\cdot\boldsymbol{n}|_s} \qquad \text{on } \Gamma_{ls}(t) \qquad (216b)$$

$$\overline{\mu}_l - \overline{\mu}^{eq} = -d_0\kappa - \beta v_n \qquad \text{on } \Gamma_{ls}(t) \qquad (216c)$$

Notations

- c and c_s liquid and solid compos.
- $v_n = \boldsymbol{v}_s\cdot\boldsymbol{n}$ normal velocity of interface
- $\overline{\mu}$ dimensionless chemical potential
- $\overline{\mu}^{eq}$ equilibirum chem. pot.
- κ curvature; d_0 capillary length



Init cond:
solid (black)
liquid (blue)

Equivalent phase-field model

Phase-field equation (checked with "*matched asymptotic expansions*")

- Keep $-d_0\kappa$ in Eq. (216c): "standard" ψ-eq.

$$\frac{\partial \psi}{\partial t} = M_\psi \nabla^2 \psi - \frac{M_\psi}{W^2} 2\psi(1-\psi)(1-2\psi) + \frac{\lambda M_\psi}{W^2}\mathscr{S}_\psi(\psi, \overline{\mu}) \tag{217a}$$

- Cancel $\cancel{-d_0\kappa}$: add "counter term" $-M_\psi \kappa |\nabla\psi|$

$$\frac{\partial \psi}{\partial t} = \nabla \cdot \left[M_\psi \left(\nabla\psi - \frac{4}{W}\psi(1-\psi)\boldsymbol{n} \right) \right] + \frac{\lambda M_\psi}{W^2}\mathscr{S}_\psi(\psi, \overline{\mu}) \tag{217b}$$

Source term

$$\mathscr{S}_\psi(\psi, \overline{\mu}) = 6\psi(1-\psi)(c_s^{co} - c_l^{co})(\overline{\mu} - \overline{\mu}^{eq}) \tag{218}$$

Composition equation (checked with "*matched asymptotic expansions*")

$$\frac{\partial c}{\partial t} = \nabla \cdot \left[D_l \psi \nabla \overline{\mu} - \boldsymbol{j}_{at}(\psi, \overline{\mu}) \right] \qquad \text{Composition eq.} \tag{219a}$$

$$\overline{\mu} = \overline{\mu}^{eq} + c(\psi, \overline{\mu}) - \left[c_l^{co}\psi + c_s^{co}(1-\psi) \right] \qquad \text{Chemical potential} \tag{219b}$$

$$\boldsymbol{j}_{at} = \frac{1}{4} W \left(c_s^{co} - c_l^{co} \right) \frac{\partial \psi}{\partial t} \boldsymbol{n} \qquad \text{Anti-trapping current} \tag{219c}$$

Equivalent sharp interface model

Asymptotic expansions

$$\frac{\partial c}{\partial t} = D_{\Phi}\nabla^2 c \tag{220a}$$

$$D_l\partial_n c|_l - D_s\partial_n c|_s = -v_n\Delta c^{co} - \mathbb{E}_2\Delta\mathscr{H} - \mathbb{E}_3\Delta\mathscr{J} \quad \text{on } \Gamma_{ls} \tag{220b}$$

$$\left(\overline{\mu}_{\Phi} - \overline{\mu}^{eq}\right)\Delta c^{co} = -d_0\kappa - \beta_{\Phi}v_n + \mathbb{E}_1\left[\Delta\tilde{\mathscr{F}} - \Delta\mathscr{G}_{\Phi}\right]\Delta c^{co} \quad \text{on } \Gamma_{ls} \tag{220c}$$

Nomenclature

- $\mathbb{E}_1$, $\mathbb{E}_2$, $\mathbb{E}_3$: error terms arising from asymptotic analysis
- $\Delta\mathscr{H}$, $\Delta\mathscr{J}$, $\Delta\tilde{\mathscr{F}}$, $\Delta\mathscr{G}_{\Phi}$: integrals involving interpolation functions. Those integrals can be canceled with appropriate choices of interpolation functions.

LBM schemes for ψ-model of dissolution

LBM for $\psi(\boldsymbol{x}, t)$-equation

Evolution

$$\tilde{g}_k^{\star} = \tilde{g}_k - \frac{1}{\overline{\tau}_g + 1/2}\left[\tilde{g}_k - \tilde{g}_k^{eq}\right] + \mathcal{G}_k\delta t \qquad \text{with} \begin{cases} \tilde{g}_k^{eq} = & \psi w_k - \delta t \mathcal{G}_k/2 \\ \mathcal{G}_k = & w_k\left[-\frac{\lambda M_\psi}{W^2}\mathscr{S}_\psi(\psi, \overline{\mu}) + \frac{4}{W}\psi(1-\psi)\boldsymbol{\xi}_k\cdot\boldsymbol{n}\right] \\ \psi = & \sum_k \tilde{g}_k + \frac{\delta t}{2}\sum_k \mathcal{G}_k \end{cases}$$

Gradients

Mobility

$$\boldsymbol{e}_k\cdot\boldsymbol{\nabla}\phi\big|_{\boldsymbol{x}} = \frac{1}{2\delta x}\left[\psi(\boldsymbol{x}+\boldsymbol{e}_k\delta x) - \psi(\boldsymbol{x}-\boldsymbol{e}_k\delta x)\right] \quad \text{and} \quad \boldsymbol{\nabla}\psi\big|_{\boldsymbol{x}} = 3\sum_k w_k\boldsymbol{e}_k\left(\boldsymbol{e}_k\cdot\boldsymbol{\nabla}\psi\big|_{\boldsymbol{x}}\right) \quad M_\psi = \overline{\tau}_g\xi_s^2\delta t$$

LBM for $c(\boldsymbol{x}, t)$-equation

Evolution

$$\tilde{h}_k^{\star} = \tilde{h}_k - \frac{1}{\overline{\tau}_h + 1/2}\left[\tilde{h}_k - \tilde{h}_k^{eq}\right] + \mathcal{H}_k\delta t \qquad \text{with} \begin{cases} h_k^{eq} & = \begin{cases} c(\psi, \overline{\mu}) - (1-w_0)\gamma\mathcal{D}(\psi)\overline{\mu}(\boldsymbol{x}, t) & \text{if } k = 0 \\ w_k\gamma\mathcal{D}(\psi)\overline{\mu}(\boldsymbol{x}, t) & \text{if } k \neq 0 \end{cases} \\ \mathcal{H}_k & = \gamma w_k\boldsymbol{\xi}_k\cdot\left[\overline{\mu}\mathcal{D}'(\psi)\boldsymbol{\nabla}\psi + \boldsymbol{j}_{at}(\psi, \overline{\mu})\right] \\ c & = \sum_k \tilde{h}_k \end{cases}$$

Diffusion $\overline{\tau}_h = 3\delta t/(\gamma\delta x^2)$

Verifications `LBM_Saclay`: Stefan problem

From T. Boutin *et al.* (2022)

Analytical solutions (*as*)

- **Solid c_s and liquid c_l compositions**

$$c_s^{as}(x,\,t) = c_s^{\infty} + (c_s^{co} - c_s^{\infty})\frac{\operatorname{erfc}\left[-x/2\sqrt{D_s t}\right]}{\operatorname{erfc}\left[-\alpha/2\sqrt{D_s}\right]}$$

$$c_l^{as}(x,\,t) = c_l^{\infty} + (c_l^{co} - c_l^{\infty})\frac{\operatorname{erfc}\left[x/2\sqrt{D_l t}\right]}{\operatorname{erfc}\left[\alpha/2\sqrt{D_l}\right]}$$

- **Interface position**

$$x_i(t) = \alpha\sqrt{t}$$

with α computed with transcendental eq:

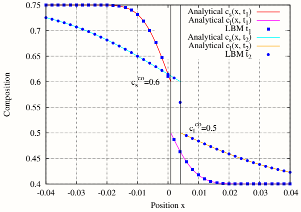
$$\alpha = 0.184841$$

- **Parameters**

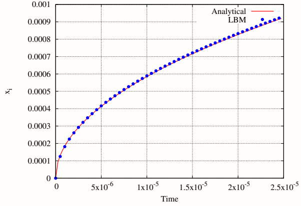
$D_s = 0.9$	$m_s = 0.2$
$D_l = 1$	$m_l = 0.1$
$c_s^{\infty} = 0.75$	$\Delta m = 0.1$
$c_l^{\infty} = 0.4$	$\Delta f^{min} = 0.04$

Comparisons with `LBM_saclay`

Compositions c_s and c_l

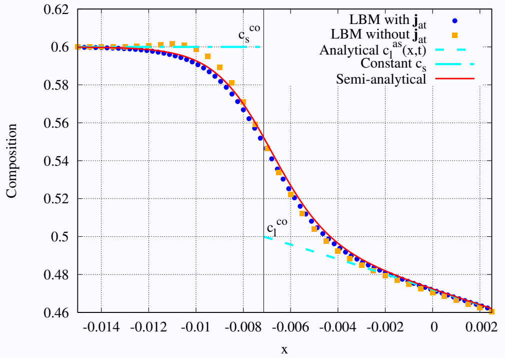


Interface position

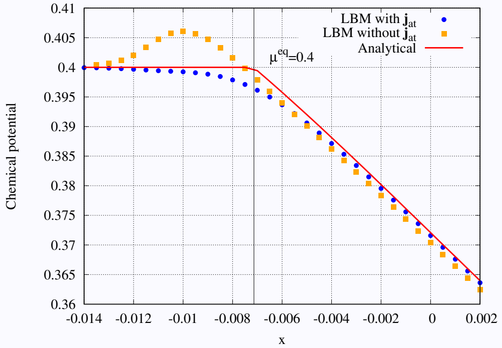


Effect of using or not the anti-trapping current $\boldsymbol{j}_{at}$

On composition



On chemical potential

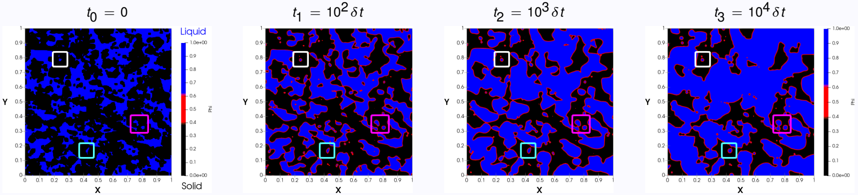


Using the anti-trapping current $\boldsymbol{j}_{at}$ Eq. (219c) in composition Eq. (219a) improves the numerical solution inside the diffuse interface

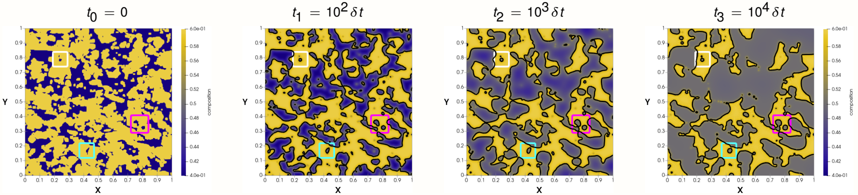
Simulation of dissolution (without curvature effect)

Phase-field $\psi(\boldsymbol{x}, t)$

Video



Composition field $c(\boldsymbol{x}, t)$



Simu with curvature effect

Appendix

$$c_s^{ini} = c_s^{co}$$
$$c_l^{ini} < c_l^{co}$$

Mesh
1024^2
$W = 20\delta x$

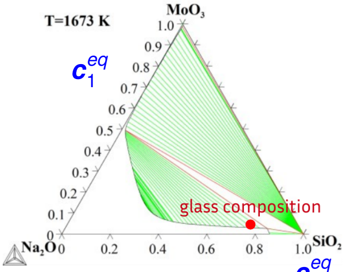
10^4 iterations
15 min
1 GPU V100

e. Ternary mixture

Two liquid phases with three components

Two-phase with three components SiO_2–Na_2O–MoO_3

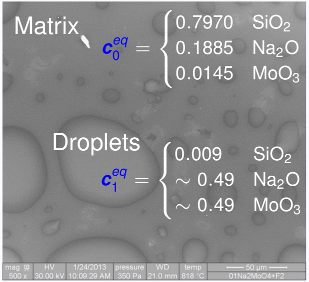
Phase diagram with Calphad modeling



c_1^{eq}

c_0^{eq}

Ternary glass equilibrium



$$c_0^{eq} = \begin{cases} 0.7970 & SiO_2 \\ 0.1885 & Na_2O \\ 0.0145 & MoO_3 \end{cases}$$

$$c_1^{eq} = \begin{cases} 0.009 & SiO_2 \\ \sim 0.49 & Na_2O \\ \sim 0.49 & MoO_3 \end{cases}$$

Three compositions (at 1152 °C) for each oxide:

SiO_2	: 78.79%	(C^A)
Na_2O	: 19.21%	(C^B)
MoO_3	: 2%	$(1 - C^A - C^B)$

Notations: vectors

$$\mathbf{c}^{glass} = (C^A, C^B)$$

$$\mathbf{c}_\Phi^{eq} = (c_\Phi^{A,eq}, c_\Phi^{B,eq})$$

Grand-potential formulation with vector $\boldsymbol{\mu}$

Grand-potential $\Omega[\phi, \boldsymbol{\mu}]$ with vector of two components $\boldsymbol{\mu} = (\mu_A, \mu_B)$

$$\Omega[\phi, \boldsymbol{\mu}] = \int_V \Big[\underbrace{\omega_{int}(\phi, \nabla\phi)}_{\text{interface}} + \underbrace{\omega_{bulk}(\phi, \boldsymbol{\mu})}_{\text{thermodynamics}}\Big] dV \qquad \text{with} \begin{cases} \omega_{int}(\phi, \nabla\phi) & = H\phi^2(1-\phi)^2 + \frac{\zeta}{2}\left|\nabla\phi\right|^2 \\ \omega_{bulk}(\phi, \boldsymbol{\mu}) & = p(\phi)\omega_0(\boldsymbol{\mu}) + [1 - p(\phi)]\,\omega_1(\boldsymbol{\mu}) \\ p(\phi) & = \phi^2(3 - 2\phi) \end{cases}$$

Assumption: quadratic free energies for f_Φ (2 parabolas)

- Grand potential densities with vectors $\boldsymbol{c}$ and $\boldsymbol{\mu}$:

$$\omega_\Phi(\boldsymbol{\mu}) = f_\Phi(\boldsymbol{c}) - \boldsymbol{\mu}\cdot\boldsymbol{c} \qquad \text{(Legendre transform of } f_\Phi\text{)}$$

- Free energy densities

$$f_\Phi(\boldsymbol{c}) = \frac{1}{2}\boldsymbol{K}_\Phi : (\boldsymbol{c} - \boldsymbol{c}_\Phi^{eq})^2 \qquad \text{where} \quad \boldsymbol{K}_\Phi = \begin{pmatrix} K_\Phi^{AA} & K_\Phi^{AB} \\ K_\Phi^{AB} & K_\Phi^{BB} \end{pmatrix} \quad \text{for } \Phi = 0, 1$$

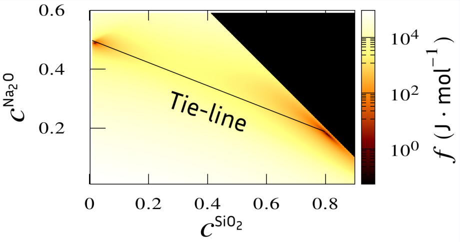
→ Determine $K_\Phi^{\alpha\beta}$ coefficients from the thermo landscape (Calphad)

Using the Calphad results for math model

1. Pre-processing

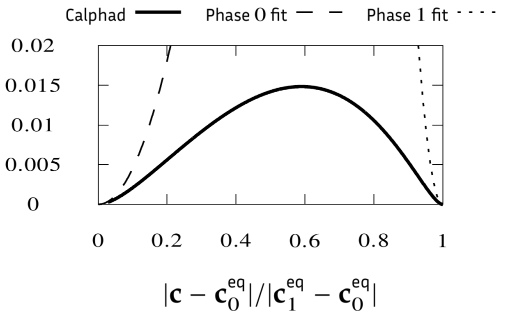
- Transform elements to oxides + global eq
- Turn off the grid minim (hyp local eq)
- interpolate the non-converging local eq

2. Free energy landscape from Calphad



Methodology (1, 2, 3) from R. Le Tellier, 2021

3. Fit the tie-line with two parabolas



→ We obtain the $K_\Phi^{\alpha\beta}$ coefficients

Phase-field model to simulate

Thermodynamics: compositional Allen-Cahn (ϕ^{AC}-model)

Interface tracking

$$\frac{\partial\phi}{\partial t}+\overbrace{\boldsymbol{\nabla}\cdot(\boldsymbol{u}\phi)}^{\text{Advective term}}=M_\phi\overbrace{\left[\boldsymbol{\nabla}^2\phi-\frac{1}{4W^2}\omega'_{dw}(\phi)\right]}^{\text{Curvature }\kappa\left|\boldsymbol{\nabla}\phi\right|}-\overbrace{\frac{\lambda M_\phi}{W^2}p'(\phi)\left[\omega_0(\boldsymbol{\mu})-\omega_1(\boldsymbol{\mu})\right]}^{\text{Thermodynamic}}\qquad(221)$$

Diffusion Eqs of SiO_2 and Na_2O

$$\frac{\partial c^A}{\partial t}+\boldsymbol{\nabla}\cdot(\boldsymbol{u}c^A)=\boldsymbol{\nabla}\cdot\left[D^A(\phi)\boldsymbol{\nabla}\mu^A\right]\qquad(222a)$$

$$\frac{\partial c^B}{\partial t}+\boldsymbol{\nabla}\cdot(\boldsymbol{u}c^B)=\boldsymbol{\nabla}\cdot\left[D^B(\phi)\boldsymbol{\nabla}\mu^B\right]\qquad(222b)$$

Relationship between $\boldsymbol{\mu}$ and $\boldsymbol{c}$

$$\boldsymbol{\mu}=\boldsymbol{K}(\phi)\left[\boldsymbol{c}-\boldsymbol{c}^{eq}(\phi)\right]\qquad(222c)$$

Initial conditions

using $\boldsymbol{c}_0^{eq}$, $\boldsymbol{c}_1^{eq}$ and $\boldsymbol{C}^{glass}$ (details in Part 3)

Illustration of ϕ^{AC}-model: Ostwald ripening

Phenomenon

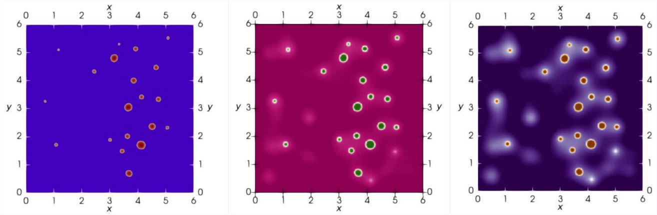
Smaller droplets vanish whereas the larger ones grow because

- Larger droplets have a lower μ (Gibbs-Thomson cond)
- Diffusion flux from lower to larger droplets ($\boldsymbol{j} \propto -\boldsymbol{\nabla}\mu$)

Expected mean radius: $\langle R\rangle \propto t^{1/3}$

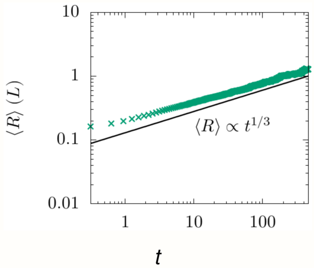
Simulation (from C. Méjanès)

Video



ϕ $\quad$ c^A $\quad$ c^B

Verification



Summary of phase-field simulations

^{NS}=Navier-Stokes ^{CH}=Cahn-Hilliard ^{AC}=Allen-Cahn ^{CAC}=Conservative Allen-Cahn

Phenomenology	Taken into account via						Currently neglected
1 phase	T	C	NS	ϕ	Nb comp	Examples	
☑ Thermics advective & diffusive	☑	☐	☐				Radiation
☑ Transport advective & diffusive	☐	☑	☐				$\geq$ 4 components
☑ Flows (incomp, lamin, viscous)	☐	☐	☑				Non-newtonian fluids
2 phases Fluid - Fluid							
☑ Demixing (phase separation)	☑	☑	☑	CH	2	Spinodal decomp	T coupling
☑ Coalescence & break-up	☑	☑	☑	CH	2	Rising bubbles	T coupling
☑ Phase change (liquid/gas)	☑	☑	☑	CAC	1	Film boiling	Big density ratios
☑ Exchange through interface	☑	☑	☑	AC	3	Ostwald ripening	T coupling
☑ Interface adsorption	☐	☑	☑	CH	1	Surfactant	Desorption
2 phases Fluid - Solid							
☑ Phase change (liquid/solid)	☑	☑	☑	AC	2	Crystal growth	Big Lewis nb
☑ Dissolution/precipitation	☐	☑	☑	AC	3	Dissolution phase solid	NS coupling
☑ Interface adsorption	☐	☑	☑	AC		Porous media retention	To be done
3 phases and more							
☑ 2 immisc fluids + solid	☐	☐	☑			Unsaturated porous media	To explore
☑ 3 immisc fluids	☐	☐	☐				To explore

7. Conclusion of Part 1.C

Conclusion of Part 1.C

Concept of phase-field

- Theory
  - Derivation of math models
  - Details on algebraic calculations
  - Constitutive laws such as
    - $d\mathscr{E}_{tot}/dt \leqslant 0$ or ($d\mathscr{F}/dt \leqslant 0$)
    - and $\mathcal{D} \geqslant 0$
- Various examples
  - Two immiscible fluids
  - Surfactant
  - Phase change (sol/liq and liq/gas)
  - Multi-phase, multi-component (intro)

Practice with `LBM_Saclay`

- Two-phase simulations
  - Spinodal decomposition
  - Rayleigh-Taylor instability
  - Rising bubbles and falling droplets
  - Surfactant effects
  - Two-phase interacting with solid
  - etc.
- Simulations on Graphic cards
- Post-processing with `paraview`

Not covered in this Part 1.C

Phase-field models

- Model derivation with an alternative potential (Gibbs or entropy, etc.)
- Additional gradient energy terms in $\mathscr{F}$: here only $|\boldsymbol{\nabla}\phi|^2$ but $|\boldsymbol{\nabla}c|^2$ also possible
- Matched asymptotic expansions (equivalence sharp/phase-field)
- Multi-component: link with thermo diagrams and database (Calphad)
- Multi-phase with phase change: e.g. liquid/gas interacting with a melting solid

Numerical methods

- e.g. see "An introduction to lattice Boltzmann Methods" (ED SMEMaG 16h)
- Adaptative Mesh Refinement around interfaces

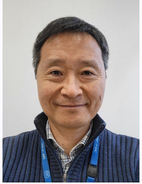
End of Part 1.C

Thank you for watching

APPENDICES

Présentation de l’auteur

À propos de l’auteur



Dr ALAIN CARTALADE
Physicien – Numéricien
Directeur de recherche au CEA
Expert senior au STMF/LDEL

Spécialités de R&D

- hydrodynamique
- sciences des matériaux
- calcul scientifique
- méthodes numériques

Activités de recherche en simulation numérique

Mes activités portent sur les modèles mathématiques de problèmes physiques impliquant des interfaces tels que les écoulements diphasiques (avec ou sans changement de phase), la démixtion, la croissance cristalline, les surfactants, la dissolution de milieux poreux, etc. Les schémas numériques sont adaptés aux EDPs et programmés dans le code C++ `LBM_Saclay`, un code HPC multi-GPUs et multi-CPUs basé sur les méthodes de Boltzmann sur réseaux. Ce cours est une introduction synthétique de ces activités.

A. Thermodynamics & Hydrodynamics

Return

Fundamental thermodynamic relations

Gibbs relation

Differential of internal energy $\mathcal{U}(S, V, \{N_k\})$ where $\{N_k\} \equiv N_1, \ldots, N_r$:

$$d\mathcal{U} = TdS - PdV + \sum_{k=1}^{r} \mu_A dN_k \qquad (223)$$

with conjugate variables:

$$T(S, V, \{N_k\}) \triangleq \frac{\partial \mathcal{U}(S, V, \{N_k\})}{\partial S}$$
$$P(S, V, \{N_k\}) \triangleq -\frac{\partial \mathcal{U}(S, V, \{N_k\})}{\partial V}$$
$$\mu_k(S, V, \{N_k\}) \triangleq \frac{\partial \mathcal{U}(S, V, \{N_k\})}{\partial N_k}$$

Euler relation

$$\mathcal{U} = TS - PV + \sum_{k=1}^{r} \mu_k N_k \qquad (224)$$

Gibbs-Duhem relation

$$SdT - VdP + \sum_{k=1}^{r} N_k d\mu_k = 0 \qquad (225)$$

Free energy thermo potential $\mathcal{F}(T, V, \{N_k\})$

Free energy $\mathcal{F}$: Legendre transform of $\mathcal{U}$

- Legendre transform of $\mathcal{U}$ wrt S:

$$\begin{aligned}\mathcal{F}(T, V, \{N_k\}) &= \mathcal{U}(S, V, \{N_k\}) - \frac{\partial \mathcal{U}}{\partial S} S \\ &= \mathcal{U}(S, V, \{N_k\}) - TS\end{aligned}$$

- with Euler relation Eq. (224):

$$\mathcal{F} = -PV + \sum_{k=1}^{r} \mu_k N_k$$

Differential

Differential:

$$d\mathcal{F} = -SdT - PdV + \sum_{k=1}^{r} \mu_k dN_k$$

with

$$\begin{aligned}S(T, V, \{N_k\}) &\triangleq -\frac{\partial \mathcal{F}(T, V, \{N_k\})}{\partial T} \\ P(T, V, \{N_k\}) &\triangleq -\frac{\partial \mathcal{F}(T, V, \{N_k\})}{\partial V} \\ \mu_k(T, V, \{N_k\}) &\triangleq \frac{\partial \mathcal{F}(T, V, \{N_k\})}{\partial N_k}\end{aligned}$$

Thermodynamic relations

Thermodynamic Maxwell relations: examples with $\mathcal{U}(V,S)$ and $\mathcal{F}(V,T)$

$$\frac{\partial \mathcal{U}}{\partial V \partial S} = \frac{\partial \mathcal{U}}{\partial S \partial V} \iff \frac{\partial}{\partial V}\underbrace{\left(\frac{\partial \mathcal{U}}{\partial S}\right)}_{\equiv T} = \frac{\partial}{\partial S}\underbrace{\left(\frac{\partial \mathcal{U}}{\partial V}\right)}_{\equiv -P} \iff \left(\frac{\partial T}{\partial V}\right)_S = -\left(\frac{\partial P}{\partial S}\right)_V$$

$$\frac{\partial \mathcal{F}}{\partial V \partial T} = \frac{\partial \mathcal{F}}{\partial T \partial V} \iff \frac{\partial}{\partial V}\underbrace{\left(\frac{\partial \mathcal{F}}{\partial T}\right)}_{\equiv -S} = \frac{\partial}{\partial T}\underbrace{\left(\frac{\partial \mathcal{F}}{\partial V}\right)}_{\equiv -P} \iff -\left(\frac{\partial S}{\partial V}\right)_T = -\left(\frac{\partial P}{\partial T}\right)_V$$

Obtain thermo variable from potential and its conjugate variable

$$T = \left(\frac{\partial \mathcal{H}}{\partial S}\right)_P = \left(\frac{\partial \mathcal{U}}{\partial S}\right)_V \qquad V = \left(\frac{\partial \mathcal{H}}{\partial P}\right)_S = \left(\frac{\partial \mathcal{G}}{\partial P}\right)_T$$

$$S = -\left(\frac{\partial \mathcal{G}}{\partial T}\right)_P = -\left(\frac{\partial \mathcal{F}}{\partial T}\right)_V \qquad P = -\left(\frac{\partial \mathcal{U}}{\partial V}\right)_S = -\left(\frac{\partial \mathcal{F}}{\partial V}\right)_T$$

Gibbs phase rule

Gibbs phase rule (without chemical reactions)

$$N_f = N_s - N_p + 2$$

- N_f: number of freedom degree
- N_s: number of chemical species
- N_p: number of phases
- 2 external variables e.g. P and T (or ρ)

Examples with water

Liquid/vapor

- Nb of species: 1 $H_2O \rightarrow N_s = 1$
- Nb of phases: 1 liq + 1 gas $\longrightarrow N_p = 2$
- Two variables: P and T (or ρ)
- Finally: $N_f = 1$

Once P (or T) is set, T (or P) is fixed.

Triple point

- 1 $H_2O \rightarrow N_s = 1$
- 1 sol + 1 liq + 1 gas $\longrightarrow N_p = 3$
- Two variables: P and T (or ρ)
- Finally: $N_f = 0$

No freedom degree: only one P_{tp} and one T_{tp}

Incompressible and low Mach flows

Mach number

$$Ma = \frac{|\boldsymbol{u}|}{c_s}$$

$\boldsymbol{u}$: fluid velocity $\quad c_s$: speed of sound

Speed of sound (20 ℃)

Air	: 344 m/s	$\equiv$ 1240 km/h
Water	: 1500 m/s	$\equiv$ 5400 km/h

$\rho = \rho_0$ constant

$$\nabla \cdot \boldsymbol{u} = 0$$

Incompressible model
$Ma = 0$

Variable density $\rho(\boldsymbol{x}, t)$

$$\partial_t \rho + \nabla \cdot (\rho \boldsymbol{u}) = 0 \quad + \text{Equation of State (EoS)}$$

Low Mach model
$Ma \ll 1$

Pseudo-compressible
$Ma \simeq 0.1$

Momentun equation 1/2: stress and strain tensors

Stress tensor $\boldsymbol{T}$

Strain tensor

$$\boldsymbol{S} = \frac{1}{2}\left[\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^T\right]$$

$$\mathrm{tr}(\boldsymbol{S}) = \nabla \cdot \boldsymbol{u}$$

Linear constitutive eq

$$\boldsymbol{T} = -p\boldsymbol{I} + \zeta \mathrm{tr}(\boldsymbol{S})\boldsymbol{I} + 2\eta \boldsymbol{S}$$

$$\begin{aligned}
\boldsymbol{T} &= -p\boldsymbol{I} + \zeta \mathrm{tr}(\boldsymbol{S})\boldsymbol{I} + 2\eta\left[\boldsymbol{S} - \frac{1}{3}\mathrm{tr}(\boldsymbol{S})\boldsymbol{I} + \frac{1}{3}\mathrm{tr}(\boldsymbol{S})\boldsymbol{I}\right] \\
&= -p\boldsymbol{I} + \underbrace{\left(\zeta + \frac{2}{3}\eta\right)}_{\equiv \eta_B} \underbrace{\mathrm{tr}(\boldsymbol{S})}_{\equiv \nabla \cdot \boldsymbol{u}} \boldsymbol{I} + 2\eta\left[\boldsymbol{S} - \frac{1}{3}\underbrace{\mathrm{tr}(\boldsymbol{S})}_{\nabla \cdot \boldsymbol{u}}\boldsymbol{I}\right] \\
&= \underbrace{-p\boldsymbol{I} + \eta_B(\nabla \cdot \boldsymbol{u})\boldsymbol{I}}_{\text{Isotropic part}} + \underbrace{\eta\left[\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^T - \frac{2}{3}(\nabla \cdot \boldsymbol{u})\boldsymbol{I}\right]}_{\text{Traceless deviatoric part}}
\end{aligned}$$

- η dynamic viscosity
- η_B bulk viscosity
- ζ second viscosity
- $\mathrm{tr}(\boldsymbol{S})$ trace of tensor $\boldsymbol{S}$
- p pressure
- $\boldsymbol{I}$ identiy tensor

Momentum equation 2/2: Navier-Stokes momentum

Momentum equations

Cauchy momentum equation

$$\frac{\partial(\rho \boldsymbol{u})}{\partial t} + \boldsymbol{\nabla} \cdot \boldsymbol{\Pi} = \boldsymbol{F}$$

$$\boldsymbol{\Pi} = \rho \boldsymbol{u}\boldsymbol{u} - \boldsymbol{T}$$

$\boldsymbol{\Pi}$ momentum flux density tensor

Stress tensor with η and η_B

$$\boldsymbol{T} = -p\boldsymbol{I} + \left[\eta(\boldsymbol{\nabla}\boldsymbol{u} + (\boldsymbol{\nabla}\boldsymbol{u})^T + \left(\eta_B - \frac{2}{3}\eta\right)(\boldsymbol{\nabla}\cdot\boldsymbol{u})\boldsymbol{I}\right]$$

Stokes hypothesis $\eta_B = 0$

$$\boldsymbol{T} = -p\boldsymbol{I} + \eta\left[\boldsymbol{\nabla}\boldsymbol{u} + (\boldsymbol{\nabla}\boldsymbol{u})^T - \frac{2}{3}(\boldsymbol{\nabla}\cdot\boldsymbol{u})\boldsymbol{I}\right]$$

Navier-Stokes momentum equation with η and η_B

$$\partial_t(\rho\boldsymbol{u}) + \boldsymbol{\nabla}\cdot(\rho\boldsymbol{u}\boldsymbol{u}) = -\boldsymbol{\nabla}p + \boldsymbol{\nabla}\cdot\left[\eta(\boldsymbol{\nabla}\boldsymbol{u} + (\boldsymbol{\nabla}\boldsymbol{u})^T) + \left(\eta_B - \frac{2}{3}\eta\right)(\boldsymbol{\nabla}\cdot\boldsymbol{u})\bar{\bar{\boldsymbol{I}}}\right] + \boldsymbol{F}$$

PDEs 2/2: Advection-Diffusion type Eqs. (ADE)

"Levelset" or "phase-field" equations

$$\frac{\partial \phi}{\partial t} + \boldsymbol{\nabla} \cdot (\boldsymbol{u}\phi) = \boldsymbol{\nabla} \cdot \left[M_\phi \left(\boldsymbol{\nabla}\phi - \frac{4}{W}\phi(1-\phi)\boldsymbol{n} \right) \right] \tag{226}$$

- **Unknown**: phase-field $\phi \equiv \phi(\boldsymbol{x}, t)$
- **Parameters**: mobility M_ϕ, interface width W, velocity $\boldsymbol{u}$
- **Normal vector**: $\boldsymbol{n} \equiv \boldsymbol{n}(\boldsymbol{x}, t) = \frac{\boldsymbol{\nabla}\phi}{|\boldsymbol{\nabla}\phi|}$

Advection-Diffusion Equation – ADE: e.g. temperature and/or composition equation

$$C_p \frac{\partial T}{\partial t} + \boldsymbol{\nabla} \cdot (T\boldsymbol{u}) = \boldsymbol{\nabla} \cdot (\kappa \boldsymbol{\nabla} T) + \mathscr{S}_T \tag{227}$$

- **Unknown**: temperature $T \equiv T(\boldsymbol{x}, t)$
- **Parameters**: thermal conductivity κ , specific heat C_p and $\mathscr{S}_T$ source term. Diffusivity $\lambda = \kappa / C_p$

Boundary conditions (BC)

Navier-Stokes BC – x_b boundary position

Dirichlet

$$\boldsymbol{u}(\boldsymbol{x}_b, t) = \boldsymbol{U}_b(\boldsymbol{x}_b, t)$$

$$(\boldsymbol{u} - \boldsymbol{U}_b) \cdot \boldsymbol{n}_w = 0$$

$$(\boldsymbol{u} - \boldsymbol{U}_b) \cdot \boldsymbol{t}_w = 0 \qquad \text{(no-slip)}$$

- $\boldsymbol{n}_w$ normal boundary vector
- $\boldsymbol{t}_w$ tangential boundary vector

Neumann

$$\boldsymbol{n}_w \cdot \boldsymbol{\sigma}(\boldsymbol{x}_b, t) = \boldsymbol{T}_b(\boldsymbol{x}_b, t)$$

Generic boundary Eq. for ADE

$$a_1 \left.\frac{\partial f}{\partial n}\right|_{\boldsymbol{x}_b, t} + a_2 f(\boldsymbol{x}_b, t) = a_3$$

- f differentiable function
- a_1, a_2, a_3, three scalar values

Name	a_1	a_2	a_3
Dirichlet	0	–	–
Neumann	–	0	–
Robin	–	–	–

- –: non zero value

B. Variational calculus

Introduction

Finding a minimum

Return

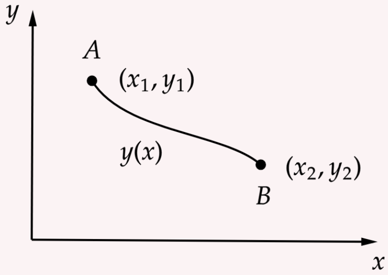
Regular calculus

- Problem: find the *point* x that makes *function* $f(x)$ minimum
- Necessary condition: $f'(x) = 0$

Variational calculus

Find the *function* $y(x)$ that makes the *integral* $\mathcal{I}$ (the *functional*) miminum (or stationary)

$$\mathcal{I}[y(x)] = \int_{x_1}^{x_2} \mathcal{F}(y, y')dx$$



- Boundary conditions

$$y(x_1) = y_1 \qquad \text{and} \qquad y(x_2) = y_2$$

- Remark: all functions have continuous 2nd derivatives

Standard derivation of Euler-Lagrange equation 1/2

Hypotheses

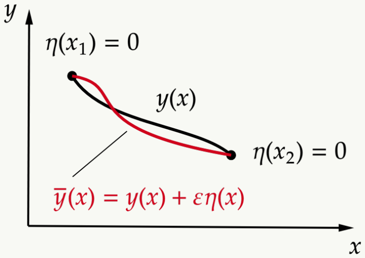
- Suppose $y(x)$ makes $\mathcal{I}$ stationary
- Introduce a function $\eta(x)$ such as

$$\eta(x_1) = \eta(x_2) = 0 \qquad (228)$$

- Define a varied path, ε small parameter

$$\overline{y}(x) = y(x) + \varepsilon\eta(x) \qquad (229)$$

$\overline{y}$ represents a family of curves



Problem

- Find the particular $\overline{y}(x)$ which makes stationary

$$\mathcal{I}[\varepsilon] = \int_{x_1}^{x_2} \mathcal{F}(\overline{y}, \overline{y}')dx \qquad (230)$$

- Stationary cond (at $\varepsilon = 0$ because $y(x)$ is assumed to make $\mathcal{I}$ stationary)

$$\boxed{\left.\frac{d\mathcal{I}}{d\varepsilon}\right|_{\varepsilon=0} = 0} \qquad (231)$$

Standard derivation of Euler-Lagrange equation 2/2

Derivation: replace Eq. (230) in Eq. (231)

$$\left.\frac{d}{d\varepsilon}\right|_{\varepsilon=0} \int_{x_1}^{x_2} \mathcal{F}(\overline{y}, \overline{y}')dx = 0$$

$$\int_{x_1}^{x_2} \left.\frac{d}{d\varepsilon}\mathcal{F}(\overline{y}, \overline{y}')\right|_{\varepsilon=0} dx = 0$$

$$\int_{x_1}^{x_2} \left.\left[\frac{\partial \mathcal{F}}{\partial \overline{y}}\frac{\partial \overline{y}}{\partial \varepsilon} + \frac{\partial \mathcal{F}}{\partial \overline{y}'}\frac{\partial \overline{y}'}{\partial \varepsilon}\right]\right|_{\varepsilon=0} dx = 0$$

$$\int_{x_1}^{x_2} \left.\left[\frac{\partial \mathcal{F}}{\partial \overline{y}}\eta + \underbrace{\frac{\partial \mathcal{F}}{\partial \overline{y}'}\eta'}_{\text{ibp}}\right]\right|_{\varepsilon=0} dx = 0$$

After ibp and using Eq. (228):

$$\int_{x_1}^{x_2} \left.\left[\frac{\partial \mathcal{F}}{\partial \overline{y}} - \frac{d}{dx}\left(\frac{\partial \mathcal{F}}{\partial \overline{y}'}\right)\right]\eta\right|_{\varepsilon=0} dx = 0$$

At $\varepsilon = 0$: $\overline{y} = y$

$$\int_{x_1}^{x_2} \left[\frac{\partial \mathcal{F}}{\partial y} - \frac{d}{dx}\left(\frac{\partial \mathcal{F}}{\partial y'}\right)\right]\eta dx = 0 \qquad (232)$$

Because η is an arbitrary function, this integral Eq. (232) is zero when

$$\boxed{\frac{\partial \mathcal{F}}{\partial y} - \frac{d}{dx}\left(\frac{\partial \mathcal{F}}{\partial y'}\right) = 0}$$

If $y(x)$ is an extremal of $\mathcal{I}$, then $y(x)$ must satisfy this differantial equation

Variational derivative: δ-operator

Return

Definition

From Eq. (229):

$$\delta y(x) \hat{=} \overline{y}(x) - y(x) = \varepsilon\eta(x) \longrightarrow \boxed{\overline{y}(x) = y(x) + \delta y(x)}$$

- $y(x)$: is the function that makes $\mathcal{I}$ stationary
- $\overline{y}(x)$: represents a family of curves
- $\eta(x)$ is an arbitrary curve
- ε is a small parameter

Example

$$\begin{aligned}
\delta\mathcal{F}(y(x), y'(x)) &= \mathcal{F}\left(\overline{y}(x), \overline{y}'(x)\right) - \mathcal{F}\left(y(x), y'(x)\right) \\
&= \mathcal{F}\left(y(x) + \delta y(x), y'(x) + \delta y'(x)\right) - \mathcal{F}\left(y(x), y'(x)\right) \\
&= \cancel{\mathcal{F}\left(y(x), y'(x)\right)} + \frac{\partial\mathcal{F}}{\partial y}\delta y + \frac{\partial\mathcal{F}}{\partial y'}\delta y' - \cancel{\mathcal{F}\left(y(x), y'(x)\right)} + \mathcal{O}(\delta^2)
\end{aligned}$$

Euler-Lagrange equation and chemical potential

Euler-Lagrange equation

$$\mathscr{F}[\phi] = \int_V \mathcal{F}(\phi, \boldsymbol{\nabla}\phi) dV \qquad (233)$$

Application of delta operator (variational derivative):

$\downarrow$ see next slide

$$\delta\mathscr{F}[\phi] = \int_V \left\{ \frac{\partial \mathcal{F}}{\partial \phi} - \underbrace{\partial_\alpha \left[\frac{\partial \mathcal{F}}{\partial(\partial_\alpha \phi)} \right]}_{\text{Einstein convention}} \right\} \delta\phi dV = C^t \qquad (234)$$

We obtain the Euler-Lagrange equation:

$$\boxed{\underbrace{\frac{\partial \mathcal{F}}{\partial \phi}}_{\text{Local part}} - \boldsymbol{\nabla} \cdot \underbrace{\left[\frac{\partial \mathcal{F}}{\partial(\boldsymbol{\nabla}\phi)} \right]}_{\text{Non-local part}} = C^t \qquad (235)}$$

Chemical potential $\mu_\phi \equiv \mu_\phi(\boldsymbol{x}, t)$

$$\begin{aligned} \mu_\phi &= \frac{\delta \mathscr{F}}{\delta \phi} \qquad (236) \\ &= \underbrace{\frac{\partial \mathcal{F}}{\partial \phi}}_{\hat{=}\mu^{(0)}} - \boldsymbol{\nabla} \cdot \left[\frac{\partial \mathcal{F}}{\partial(\boldsymbol{\nabla}\phi)} \right] \end{aligned}$$

$\mu^{(0)}$: classic thermo definition

Application

If $\mathcal{F}(\phi, \boldsymbol{\nabla}\phi)$ defined by Eq. (17), then:

$$\boxed{\mu_\phi = f'_{dw}(\phi) - \zeta \boldsymbol{\nabla} \cdot (\boldsymbol{\nabla}\phi)}$$

where f'_{dw} is the deriv of f_{dw} wrt ϕ

Remark on formulations of capillary force

Conservative formulation

- Equivalence:

$$-\nabla p_h + \mu_\phi \nabla \phi = -\nabla \cdot \overline{\overline{\boldsymbol{P}}}$$

- Where the pressure tensor

$$\overline{\overline{\boldsymbol{P}}} = \mathcal{P}(\phi, \nabla\phi)\overline{\overline{\boldsymbol{I}}} + \zeta(\nabla\phi \otimes \nabla\phi)$$

- Non-local pressure

$$\mathcal{P}(\phi, \nabla\phi) = p_h - \underbrace{\left[f_{dw} + \frac{\zeta}{2}(\nabla\phi)^2\right]}_{\equiv \mathcal{F}(\phi, \nabla\phi)}$$

- In section 5 the term $\zeta(\nabla\phi \otimes \nabla\phi)$ will be called the Korteweg's tensor

Proof

Eq. (76)$\times(-\zeta)$ and add ∇f_{dw} on both sides:

$$-\zeta\nabla \cdot (\nabla\phi \otimes \nabla\phi) + \nabla f_{dw} = -\frac{\zeta}{2}\nabla(\nabla\phi)^2 \underbrace{-\zeta(\nabla^2\phi)\nabla\phi + \nabla f_{dw}}_{\equiv \mu_\phi \nabla\phi}$$

Rearrange and add $-\nabla p_h$ on both sides

$$-\zeta\nabla \cdot (\nabla\phi \otimes \nabla\phi) + \nabla\left[f_{dw} + \frac{\zeta}{2}(\nabla\phi)^2\right] = \mu_\phi \nabla\phi$$

$$-\nabla p_h - \zeta\nabla \cdot (\nabla\phi \otimes \nabla\phi) + \nabla\left[f_{dw} + \frac{\zeta}{2}(\nabla\phi)^2\right] = -\nabla p_h + \mu_\phi \nabla\phi$$

$$-\nabla \underbrace{\left[p_h - f_{dw} - \frac{\zeta}{2}(\nabla\phi)^2\right]}_{\equiv \mathcal{P}(\phi, \nabla\phi)} - \zeta\nabla \cdot (\nabla\phi \otimes \nabla\phi) = -\nabla p_h + \mu_\phi \nabla\phi$$

$$-\nabla \cdot \underbrace{[\mathcal{P}(\phi, \nabla\phi)\overline{\overline{\boldsymbol{I}}} + \zeta(\nabla\phi \otimes \nabla\phi)]}_{\equiv \overline{\overline{\boldsymbol{P}}}} = -\nabla p_h + \mu_\phi \nabla\phi$$

C. Law of similarity

e.g. on single-phase Poiseuille flow

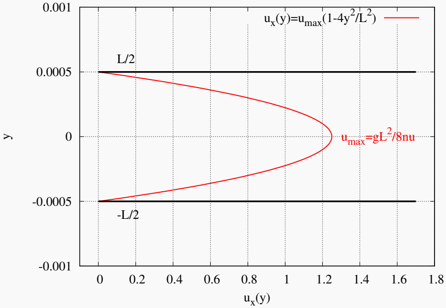
Example on Poiseuille flow

Return

Poiseuille analytical solution

$$u_x(y) = u_{max}\left(1 - \frac{4y^2}{L^2}\right)$$

$$u_{max} = \frac{gL^2}{8\nu}$$



Physical values

- Gravitational acceleration: $g = 9.81 \cong 10$ m/s^2
- Water properties at 20℃:
  - Density: $\rho_W = 998.29 \cong \rho = 1000$ kg/m^3
  - Kinematic viscosity: $\nu_W = 1.0034$ mm^2/s $\cong \nu = 10^{-6}$ m^2/s

Name	Symb	Value	Dim
Width	L	10^{-3}	m
Density	ρ	10^3	kg/m^3
Kinematic viscosity	ν	10^{-6}	m^2/s
Gravity	g	10	m/s^2

$$u_{max} = \frac{gL^2}{8\nu} = 1.25 \text{ m.s}^{-1}$$

$$\mathrm{Re} = \frac{u_{max} L}{\nu} = 1250$$

Choice of parameters δx and τ (1/2)

LBM parameters case 1

If we set (initial guess)

Name	Symb	Value	Dim
Space step	δx_1	5×10^{-5}	m
Collision rate	τ	0.6 (> 0.55)	–

then

$$L_1^\star = \frac{L}{\delta x_1} = 20 \quad \text{(number of nodes)}$$

$$\nu_1^\star = \frac{1}{3}(\tau - 0.5) = 0.03333$$

$$\delta t = \frac{1}{3}(\tau - 0.5)\frac{\delta x_1^2}{\nu} = 8.33 \times 10^{-5}$$

Law of similarity

$$\mathrm{Re} = \frac{u_{max}^\star L^\star}{\nu^\star} = 1250 \rightarrow u_{max}^\star = \frac{\nu^\star \mathrm{Re}}{L^\star} = 2.08$$

$u_{max}^\star \gg 0.4$!! (unstable simulation)

One solution: $u_{max}^\star/10$ and to keep Re constant: $L_1^\star \times 5$ with $\nu_1^\star/2$

Choice of parameters δx and τ (2/2)

LBM parameters case 2

If we set

Name	Symb	Value	Dim
Space step	δx $(= \delta x_1/5)$	10^{-5}	m
Collision rate	τ	0.55	–

then

$$L^\star = \frac{L}{\delta x} = 100 \quad (L^\star = 5L_1^\star)$$

$$\nu^\star = \frac{1}{3}(\tau - 0.5) = 0.016667 \quad (\nu^\star = \nu_1^\star/2)$$

$$\delta t = \frac{1}{3}(\tau - 0.5)\frac{\delta x^2}{\nu} = 1.6667 \times 10^{-6}$$

$$g^\star = g\frac{\delta t^2}{\delta x} = 2.777 \times 10^{-6}$$

Law of similarity

$$\mathrm{Re} = \frac{u^\star_{max} L^\star}{\nu^\star} = 1250 \rightarrow u^\star_{max} = \frac{\nu^\star \mathrm{Re}}{L^\star} = 0.208$$

$u^\star_{max} < 0.3$ (accurate) and $u^\star_{max} < 0.4$ (stable)

Pre-processing with python script

Follow instructions of html documention

Objectives

- Go to folder `TestCase02` of folder `run_training_lbm` and run python script

```
$ python Pre-Pro_Poiseuille.py
```

- Compare with parameters of `LBM_Saclay` input file

```
$ gedit TestCase02_Poiseuille_Water.ini
```

Other choice: $u^\star_{max}$ and τ

Alternative set of input parameters

If we set

Name	Symb	Value	Dim
Velocity	$u^\star_{max}$	0.1 (< 0.4)	–
Collision rate	τ	0.8 (> 0.55)	–

Relations to use

$$C_u = \frac{u_{max}}{u^\star_{max}} = \frac{\delta x}{\delta t}$$

$$\nu^\star = \frac{1}{3}(\tau - 0.5)$$

$$C_\nu = \frac{\nu}{\nu^\star} = \frac{\delta x^2}{\delta t}$$

$$\text{Re} = \frac{u^\star_{max} L^\star}{\nu^\star}$$

then

$$C_u = \frac{u_{max}}{u^\star_{max}} = 12.5$$

$$\nu^\star = \frac{1}{3}(\tau - 0.5) = 0.1$$

$$C_\nu = \frac{\nu}{\nu^\star} = 10^{-5}$$

$$L^\star = \frac{\text{Re}\nu^\star}{u^\star_{max}} = 1250$$

$$\delta x = \frac{C_\nu}{C_u} = 8 \times 10^{-7} \quad (\text{check } = L/L^\star)$$

$$\delta t = \frac{\delta x}{C_u} = 6.4 \times 10^{-8} \quad (\text{check } \nu = \nu^\star \delta x^2/\delta t)$$

$$g^\star = g\frac{\delta t^2}{\delta x} = 5.12 \times 10^{-8}$$

Other choice: $L^\star$ and $u^\star_{max}$

Alternative set of input parameters

If we set

Name	Symb	Value	Dim
Length	$L^\star$	5×10^2	–
Velocity	$u^\star_{max}$	0.1 (< 0.4)	–

Relations to use

$$\delta x = \frac{L}{L^\star}$$

$$C_u = \frac{u}{u^\star} = \frac{\delta x}{\delta t}$$

$$\mathrm{Re} = \frac{u^\star_{max} L^\star}{\nu^\star}$$

$$\nu = \frac{1}{3}(\tau - 0.5)\frac{\delta x^2}{\delta t}$$

then

$$\delta x = \frac{L}{L^\star} = 2\times 10^{-6}$$

$$C_u = \frac{u_{max}}{u^\star_{max}} = 12.5$$

$$\delta t = \frac{\delta x}{C_u} = 1.6\times 10^{-7}$$

$$\nu^\star = \frac{u^\star_{max} L^\star}{\mathrm{Re}} = 0.04 \quad (\text{check } \nu = \nu^\star \delta x^2/\delta t)$$

$$\tau = 3\nu^\star + 0.5 = 0.62\ (> 0.55)$$

$$g^\star = g\frac{\delta t^2}{\delta x} = 1.28\times 10^{-7}$$

If only Reynolds number is known

Example Re $= 1250$

If we set

Name	Symb	Value	Dim
Velocity	u_{sim}	0.1	–
Length	L_{sim}	100	–
Space-step	δx	1	–
Time-step	δt	1	–

then

$$\nu_{sim} = \frac{u_{sim} L_{sim}}{\mathrm{Re}} = 8 \times 10^{-3}$$

$$\tau = 3\nu_{sim}\frac{\delta t}{\delta x^2} + 0.5 = 0.524$$

$$g_{sim} = \frac{8\nu_{sim} u_{sim}}{L_{sim}^2} = 6.4 \times 10^{-7}$$

D. Practice of two-phase dimensionless numbers

Example of air bubble in water

Physical values

Water properties at 20 °C:

- Density: $\rho_l = 998.29$ kg/m^3
- Kinematic viscosity: $\nu_l = 1.0034 \times 10^{-6}$ m^2/s
- Water–Air surface tension: $\sigma = 0.0728$ N/m

- Gravitational acceleration: $g = 9.81$ m/s^2
- Domain between $[0, L]$

Name	Symb	Value	Dim
Width	L	0.001	m
Density	ρ_l	998.29	kg/m^3
Kinematic viscosity	ν_l	1.0034×10^{-6}	m^2/s
Gravity	g	9.81	m/s^2
Bubble radius	R	2×10^{-4}	m
Surface tension	σ	7.28×10^{-2}	N/m

$$u_{max} = \frac{gL^2}{2\nu} = 4.888 \text{ m.s}^{-1}$$

$$\text{Re} = \frac{u_{max} L}{\nu} = \frac{gL^3}{2\nu^2} = 4871.81$$

$$\text{Bo} = \frac{\Delta\rho g R^2}{\sigma} = 5.37 \times 10^{-3}$$

P. Practice with `python` scripts

Pre-processing with python script

Follow instructions of `html` documentation

Objectives

- Go to folder `TestCase11_Rising-Bubble2D/PYTHON_Scripts` and run

```
$ python Pre-Pro_InputParam_Rising-Bubble_Water-Air.py
```

- Derive $\sigma^{\star}$ and $g^{\star}$ for target Bo and Mo numbers

```
$ python Pre-Pro_Bo-Mo_2_AdimParam_Rising-Bubble.py
```

- Check that parameters of `LBM_Saclay` match with your dimensionless numbers

```
$ python Ini_2_AdimNb_Rising-Bubble_CASE-A2.py
```

LBM parameters with $R^\star$, τ_l and ρ_{ref}

Example of input parameters

If we set

Name	Symb	Value	Dim
Radius	$R^\star$	30	–
Reference density	ρ_{ref}	ρ_l	
Collision rate of air	τ_l	0.8	–

Then

$$\frac{g^\star}{\nu_l^{\star 2}} = \frac{2\mathrm{Re}}{L^{\star 3}} = 5.7425 \times 10^{-6}$$

$$\frac{\sigma^\star}{g^\star} = \frac{\Delta\rho^\star R^{\star 2}}{\mathrm{Bo}} = 288.46$$

$$\delta x = \frac{R}{R^\star} = 6.666 \times 10^{-6}$$

$$L^\star = L/\delta x = 150$$

$$\rho_l^\star = \rho_l/\rho_{ref} = 1.0$$

$$\rho_a^\star = \rho_a/\rho_{ref} = 1.206 \times 10^{-3}$$

$$\nu_l^\star = (\tau_l - 0.5)/3 = 1.166 \times 10^{-2}$$

$$g^\star = 2\mathrm{Re}\nu_l^{\star 2}/L^{\star 3} = 3.92953 \times 10^{-7}$$

$$\sigma^\star = \frac{\Delta\rho^\star R^{\star 2} g^\star}{\mathrm{Bo}} = 6.5724 \times 10^{-2}$$

$$\delta t = \sqrt{\frac{g^\star \delta x}{g}} = 5.167615 \times 10^{-7}$$

$$\nu_a^\star = (\tau_a^\star - 0.5)/3 = 0.1813832$$

Example of air bubble in glycerol

Physical values

Liquid glycerol properties at 20 °C:

- Density: $\rho_l = 1260$ kg/m^3
- Kinematic viscosity: $\nu_l = 8.49 \times 10^{-4}$ m^2/s
- Glycerol–Air surface tension: $\sigma = 6.34 \times 10^{-2}$ N/m

- Gravitational acceleration: $g = 9.81$ m/s^2
- Domain between $[0, L]$

Name	Symb	Value	Dim
Width	L	0.015	m
Density	ρ_l	1260	kg/m^3
Kinematic viscosity	ν_l	8.49×10^{-4}	m^2/s
Gravity	g	9.81	m/s^2
Bubble radius	R	4×10^{-3}	m
Surface tension	σ	6.34×10^{-2}	N/m

$$u_{max} = \frac{gL^2}{2\nu} = 1.3 \text{ m.s}^{-1}$$

$$\text{Re} = \frac{u_{max} L}{\nu} = \frac{gL^3}{2\nu^2} = 22.97$$

$$\text{Bo} = \frac{\Delta\rho g R^2}{\sigma} = 3.12$$

Running Taylor bubble

Guidelines

- Folder:

```
$ cd TestCase11_Taylor-Bubble2D
```

- Dimensionless input parameters

```
$ python Pre-Pro_InputParam_Taylor-Bubble_OliveOil-Air.py
```

- Set ν_l and σ in `.ini` file to respect the Bo&Mo nbs with python script

```
$ python Bo-Mo_2_AdimNb_Taylor-Bubble.py
```

- Running

```
$ LBM_saclay/build_openmp/src/LBM_saclay TestCase11_Taylor-Bubble_BoMo-A6.ini
```

- Post-processing with `paraview`. Make a video.

Running falling droplet

Guidelines

- Folder:

```
$ cd TestCase10_Falling-Droplet2D
```

- Running

```
$ LBM_saclay/build_openmp/src/LBM_saclay TestCase10_Rayleigh-Plateau.ini
```

- Post-processing with `paraview`

```
$ paraview&
```

Running splashing droplet

Guidelines

- Folder:

```
$ cd TestCase12_Splashing-Droplet2D
```

- Dimensionless input parameters

```
$ python Pre-Pro_InputParam_Splash_Water-Air.py
```

- Check with python script that the parameters in the `.ini` file respect the target Re & We nbs

```
$ python Ini_2_AdimNb_Splash_Re876-We2662.py
```

- Running

```
$ LBM_saclay TestCase12_SplashingDroplet_Re876-We2662_H15_1024x220.ini
```

- Post-processing with `paraview`. Make a video.

E. Lattice Boltzmann Methods

Return

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Overview of LBM 1/6: continuous Boltzmann equation

Kinetic theory (see BIRD's book, 1994)

Continuous Boltzmann equation

$$\frac{\partial f}{\partial t} + \boldsymbol{c} \cdot \nabla f + \boldsymbol{F} \cdot \nabla_{\boldsymbol{c}} f = \Omega(f, f^{eq}) \qquad (237)$$

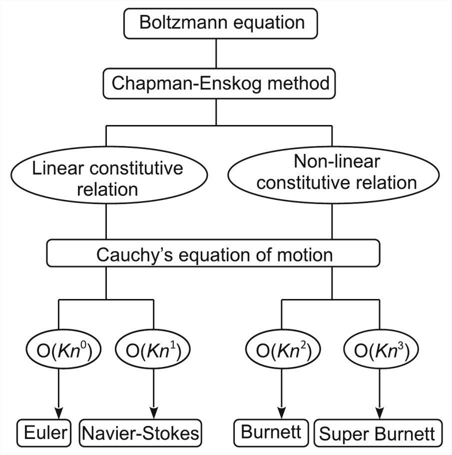
- f **distribution function** depending on pos $\boldsymbol{x}$, micro speeds $\boldsymbol{c}$ and time t : $f(\boldsymbol{x}, \boldsymbol{c}, t)$
- **Moments**:

$$\begin{cases} \rho & = \int f d\boldsymbol{c} \\ \rho \boldsymbol{u} & = \int f \boldsymbol{c} d\boldsymbol{c} \\ \rho\varepsilon & = \frac{1}{2} \int (\boldsymbol{c} - \boldsymbol{u})^2 f d\boldsymbol{c} \end{cases} \qquad (238)$$

- **Collision operator** $\Omega(f, f^{eq})$ and $\boldsymbol{F}$ ext forces
- Batnaghar-Gross-Krook (**BGK**) approximation:

$$\Omega(f, f^{eq}) \sim -\frac{1}{\lambda} \left[f - f^{eq} \right] \qquad (239)$$

Boltzmann eq and Navier-Stokes eqs



Overview of LBM 2/6: discretization $\boldsymbol{c}$, $\boldsymbol{x}$, t

Main quantity: $f(\boldsymbol{x}, \boldsymbol{c}, t)$ distribution function $\boldsymbol{x}$, $\boldsymbol{c}$ and t have to be discretized

Boltzmann equation

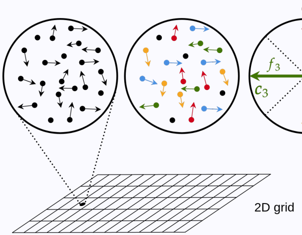
$$\frac{\partial f}{\partial t} + \boldsymbol{c} \cdot \nabla f + \boldsymbol{F} \cdot \nabla_{\boldsymbol{c}} f = \Omega(f, f^{eq})$$

Discrete $\boldsymbol{x}$ and $t \rightarrow \delta x, \delta t$

- Method of characteristics Appendix

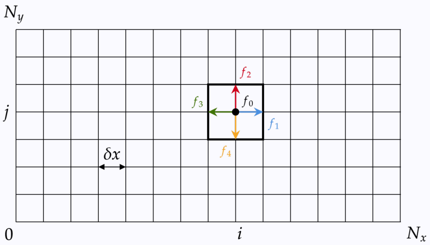
Discrete velocity space $\boldsymbol{c} \rightarrow \boldsymbol{c}_i$

Simplest 2D discrete velocity space



Lattice = Mesh + discrete speeds

Example of lattice “D2Q5”



Overview of LBM 3/6: lattices

Notations

- δx for space
- δt for time
- i for velocity space

The distribution function f is a function of $\boldsymbol{x}$, $\boldsymbol{c}$ and t

$$f(\boldsymbol{x}, \boldsymbol{c}, t) \to f_i(\boldsymbol{x}, t)$$

$$\boldsymbol{c} \to \boldsymbol{c}_i$$

$$\boldsymbol{c}_i = \boldsymbol{e}_i \frac{\delta x}{\delta t}$$

$\boldsymbol{e}_i$ moving direction

$$i = 0, \ldots, N_{pop}$$

One lattice is defined by a set of weights w_i and directions $\boldsymbol{e}_i$

e.g. most popular D2Q9

- Moving directions ($N_{pop} = 9$)

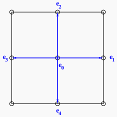
$$\begin{array}{lll} \boldsymbol{e}_0 = (0,0) & \boldsymbol{e}_3 = (-1,0) & \boldsymbol{e}_6 = (-1,1) \\ \boldsymbol{e}_1 = (1,0) & \boldsymbol{e}_4 = (0,-1) & \boldsymbol{e}_7 = (-1,-1) \\ \boldsymbol{e}_2 = (0,1) & \boldsymbol{e}_5 = (1,1) & \boldsymbol{e}_8 = (1,-1) \end{array}$$

- Weights

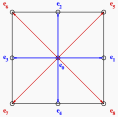
$$w_i = \begin{cases} 4/9 & i = 0 \\ 1/9 & i = 1, \ldots, 4 \\ 1/36 & i = 5, \ldots, 8 \end{cases}$$

Example of lattices – Def of 3D lattices

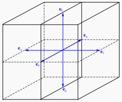
Lattice **D2Q5**



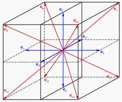
Lattice **D2Q9**



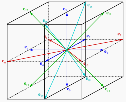
D3Q7



D3Q15



D3Q19



Overview of LBM 4/6: Lattice Boltzmann Equation (LBE)

After 3 discretizations of Boltzmann Eq. ($\boldsymbol{c}$, $\boldsymbol{x}$ and t)

Lattice Boltzmann for Navier-Stokes

Lattice Boltzmann Equation

$$f_i(\boldsymbol{x}+\boldsymbol{c}_i\delta t, t+\delta t) = \underbrace{f_i(\boldsymbol{x},t) - \frac{1}{\tau}\left[f_i(\boldsymbol{x},t) - f_i^{eq}(\boldsymbol{x},t)\right]}_{\equiv f_i^\star(\boldsymbol{x},t)} \qquad (240)$$

$$f_i^{eq}(\boldsymbol{x},t) = w_i\rho\left[1 + \frac{\boldsymbol{c}_i\cdot\boldsymbol{u}}{c_s^2} + \frac{(\boldsymbol{c}_i\cdot\boldsymbol{u})^2}{2c_s^4} - \frac{\boldsymbol{u}\cdot\boldsymbol{u}}{2c_s^2}\right] \qquad (241)$$

Discrete moments

$$\rho(\boldsymbol{x},t) = \sum_i f_i(\boldsymbol{x},t) \qquad (242)$$

$$\rho(\boldsymbol{x},t)\boldsymbol{u}(\boldsymbol{x},t) = \sum_i f_i(\boldsymbol{x},t)\boldsymbol{c}_i \qquad (243)$$

$$c_s = \frac{1}{\sqrt{3}}\frac{\delta x}{\delta t} \qquad (244)$$

Explicit algorithm

- Collision: $f_i(\boldsymbol{x},t) \to f_i^\star(\boldsymbol{x},t)$ (right-hand side of Eq. (240)) Local (same pos $\boldsymbol{x}$)
- Streaming: $f_i^\star(\boldsymbol{x},t) \to f_i(\boldsymbol{x}+\boldsymbol{c}_i\delta t, t+\delta t)$ (left-hand side)
- Updating the density (Eq. (242)) and impulsion (Eq. (243))

Overview of LBM 5/6: Chapman-Enskog expansion

«Standard LBM» for Navier-Stokes

Lattice Boltzmann Equation

$$f_i(\boldsymbol{x} + \boldsymbol{c}_i\delta t, t + \delta t) = f_i(\boldsymbol{x}, t) - \frac{1}{\tau}\left[f_i(\boldsymbol{x}, t) - f_i^{eq}(\boldsymbol{x}, t)\right] \qquad (245)$$

$$f_i^{eq}(\boldsymbol{x},\ t) = w_i\rho\left[1 + \frac{\boldsymbol{c}_i \cdot \boldsymbol{u}}{c_s^2} + \frac{(\boldsymbol{c}_i \cdot \boldsymbol{u})^2}{2c_s^4} - \frac{\boldsymbol{u} \cdot \boldsymbol{u}}{2c_s^2}\right] \qquad (246)$$

Discrete moments

$$\rho(\boldsymbol{x}, t) = \sum_i f_i(\boldsymbol{x}, t) \qquad (247)$$

$$\rho(\boldsymbol{x}, t)\boldsymbol{u}(\boldsymbol{x}, t) = \sum_i f_i(\boldsymbol{x}, t)\boldsymbol{c}_i \qquad (248)$$

$$c_s = \delta x/(\delta t\sqrt{3}) \qquad (249)$$

With Chapman-Enskog expansion (see LBM lecture) we can prove that

LB simulates with the condition $|\boldsymbol{u}| \ll c_s$

$$\partial_t\rho + \boldsymbol{\nabla} \cdot (\rho\boldsymbol{u}) = 0 \qquad (250)$$

$$\partial_t(\rho\boldsymbol{u}) + \boldsymbol{\nabla} \cdot (\rho\boldsymbol{u}\boldsymbol{u}) = -\boldsymbol{\nabla}p + \boldsymbol{\nabla} \cdot \left[\rho\nu(\boldsymbol{\nabla}\boldsymbol{u} + (\boldsymbol{\nabla}\boldsymbol{u})^T)\right] + \mathcal{O}(\rho u^3) \qquad (251)$$

Eq of state $\quad p = \rho c_s^2 \qquad (252)$

Kinematic viscosity $\quad \nu = (\tau - 1/2)c_s^2\delta t \qquad (253)$

Overview of LBM 6/6: algorithm with a forcing term

LBE with force term (2nd order accuracy)

$$f_i(\boldsymbol{x} + \boldsymbol{c}_i\delta t,\, t + \delta t) = f_i(\boldsymbol{x},\, t) - \frac{1}{\tau + 1/2}\left[f_i(\boldsymbol{x},\, t) - f_i^{eq}(\boldsymbol{x},\, t)\right] + \delta t\mathcal{F}_i(\boldsymbol{x}, t) \tag{254}$$

$$f_i^{eq}(\boldsymbol{x},\, t) = w_i\rho\left[1 + \frac{\boldsymbol{c}_i \cdot \boldsymbol{u}}{c_s^2} + \frac{(\boldsymbol{c}_i \cdot \boldsymbol{u})^2}{2c_s^4} - \frac{\boldsymbol{u} \cdot \boldsymbol{u}}{2c_s^2}\right] - \frac{\delta t}{2}\mathcal{F}_i \tag{255}$$

$$\mathcal{F}_i(\boldsymbol{x}, t) = w_i\left[\frac{\boldsymbol{c}_i - \boldsymbol{u}}{c_s^2} + \frac{(\boldsymbol{c}_i \cdot \boldsymbol{u})\boldsymbol{c}_i}{c_s^4}\right] \cdot \boldsymbol{F}_{tot} \tag{256}$$

$\boldsymbol{F}_{tot} \equiv \boldsymbol{F}_{tot}(\boldsymbol{x}, t)$ is the external force in the NS eq (e.g. $\boldsymbol{F}_{tot} = \rho\boldsymbol{g}$)

Macroscopic quantities

$$\rho(\boldsymbol{x}, t) = \sum_i f_i(\boldsymbol{x}, t) \quad \text{Density} \tag{257}$$

$$\rho(\boldsymbol{x}, t)\boldsymbol{u}(\boldsymbol{x}, t) = \sum_i f_i(\boldsymbol{x}, t)\boldsymbol{c}_i + \frac{\delta t}{2}\boldsymbol{F} \quad \text{Impulsion} \tag{258}$$

Origin of term $\delta t\boldsymbol{F}/2$

Kinematic viscosity

$$\nu = \tau c_s^2\delta t$$

Dim $[L]^2/[T]$

Discretization: method of characteristics ▸ Return

$$\text{Starting point} \qquad \partial_t f_i + \boldsymbol{c}_i \cdot \boldsymbol{\nabla} f_i = \Omega(f_i, f_i^{eq}) \qquad \text{(Discrete velocity Boltzmann Eq)} \tag{259}$$

Parametrization of $\boldsymbol{x}$ and t by ζ: $f_i \equiv f_i(\boldsymbol{x}(\zeta), t(\zeta))$

$$\text{Chain rule} \qquad \frac{df_i}{d\zeta} = \left(\frac{\partial f_i}{\partial t}\right)\frac{dt}{d\zeta} + (\boldsymbol{\nabla} f_i) \cdot \frac{\partial \boldsymbol{x}}{\partial \zeta} = \Omega_i\left(\boldsymbol{x}(\zeta), t(\zeta)\right) \tag{260}$$

Comparison of Eq. (260) with Eq. (259) requires $\frac{dt}{d\zeta} = 1$, and $\frac{d\boldsymbol{x}}{d\zeta} = \boldsymbol{c}_i$

Equiv to $dt = d\zeta$ and

$$\begin{aligned} d\boldsymbol{x} &= \boldsymbol{c}_i d\zeta \\ \boldsymbol{x}(t+\delta t) - \boldsymbol{x}(t) &= \boldsymbol{c}_i \delta t \\ \boldsymbol{x}(t+\delta t) &= \boldsymbol{x}(t) + \boldsymbol{c}_i \delta t \end{aligned}$$

Integration on ζ :

$$\int_t^{t+\delta t} \frac{df_i}{d\zeta} d\zeta = \int_t^{t+\delta t} \Omega_i\left(\boldsymbol{x}(\zeta), t(\zeta)\right) d\zeta$$

$$\begin{aligned} f_i(\boldsymbol{x}(t+\delta t), t+\delta t) - f_i(\boldsymbol{x}(t), t) &= \dots \\ f_i(\boldsymbol{x}(t) + \boldsymbol{c}_i\delta t, t+\delta t) - f_i(\boldsymbol{x}(t), t) &= \dots \\ f_i(\boldsymbol{x} + \boldsymbol{c}_i\delta t, t+\delta t) - f_i(\boldsymbol{x}, t) &= \dots \end{aligned}$$

Finally

$$f_i(\boldsymbol{x} + \boldsymbol{c}_i\delta t, t+\delta t) - f_i(\boldsymbol{x}, t) = \int_t^{t+\delta t} \Omega_i\left(\boldsymbol{x}(\zeta), t(\zeta)\right) d\zeta$$

Discretization 3/4: collision term

Starting point $$f_i(\boldsymbol{x}+\boldsymbol{c}_i\delta t, t+\delta t) - f_i(\boldsymbol{x}, t) = \int_t^{t+\delta t} \Omega_i\left(\boldsymbol{x}(\zeta), t(\zeta)\right) d\zeta$$

Integral of the right-hand side

First order

$$f_i(\boldsymbol{x}+\boldsymbol{c}_i\delta t, t+\delta t) - f_i(\boldsymbol{x}, t) = \delta t \Omega_i(\boldsymbol{x}, t)$$

Second order (trapezoïdal rule)

$$f_i(\boldsymbol{x}+\boldsymbol{c}_i\delta t, t+\delta t) - f_i(\boldsymbol{x}, t) = \frac{\delta t}{2}\left[\Omega_i(\boldsymbol{x}, t) + \Omega_i(\boldsymbol{x}+\boldsymbol{c}_i\delta t, t+\delta t)\right]$$

Variable change $\overline{f}_i = f_i + (\delta t/2\lambda)(f_i - f_i^{eq})$ see next slide

- 1rst and 2nd order yield to

$$\begin{aligned} f_i(\boldsymbol{x}+\boldsymbol{c}_i\delta t, t+\delta t) &= f_i(\boldsymbol{x}, t) + \delta t \Omega\left(f_i(\boldsymbol{x}, t), f_i^{eq}(\boldsymbol{x}, t)\right) \\ &= f_i(\boldsymbol{x}, t) - \frac{\delta t}{\lambda}\left[f_i(\boldsymbol{x}, t), f_i^{eq}(\boldsymbol{x}, t)\right] \qquad \text{(Hyp. coll BGK)} \end{aligned}$$

LBE-BGK without source term

$$f_i(\boldsymbol{x}+\boldsymbol{c}_i\delta t, t+\delta t) = f_i(\boldsymbol{x}, t) - \frac{1}{\tau}\left[f_i(\boldsymbol{x}, t) - f_i^{eq}(\boldsymbol{x}, t)\right] \qquad \text{with } \tau = \lambda/\delta t$$

LB schemes 1/2: incompressible Navier-Stokes V1

Distrib function f_i for p and $\rho\boldsymbol{u}$

$$f_i(\boldsymbol{x}+\boldsymbol{c}_i\delta t,\, t+\delta t) = f_i(\boldsymbol{x},\, t) - \frac{1}{\tau_f+1/2}\left[f_i(\boldsymbol{x},\, t) - f_i^{eq}(\boldsymbol{x},\, t)\right] + \delta t\mathcal{F}_i(\boldsymbol{x},\, t)$$

$$f_i^{eq}(\boldsymbol{x},\, t) = w_i\left[p + \rho(\phi)c_s^2\left(\frac{\boldsymbol{c}_i\cdot\boldsymbol{u}}{c_s^2} + \frac{(\boldsymbol{c}_i\cdot\boldsymbol{u})^2}{2c_s^4} - \frac{\boldsymbol{u}\cdot\boldsymbol{u}}{2c_s^2}\right)\right] - \frac{\delta t}{2}\mathcal{F}_i(\boldsymbol{x},\, t)$$

Source term $\mathcal{F}_i$:

$$\mathcal{F}_i(\boldsymbol{x},\, t) = (\boldsymbol{c}_i - \boldsymbol{u})\cdot\left\{\boldsymbol{\nabla}\rho c_s^2\left[\Gamma_i - \Gamma_i(\boldsymbol{0})\right] + \Gamma_i\left(\mu_\phi\boldsymbol{\nabla}\phi + \rho\boldsymbol{g}\right)\right\} + w_i\rho c_s^2\dot{m}'''\left(\frac{1}{\rho_g} - \frac{1}{\rho_l}\right)$$

$$\Gamma_i(\boldsymbol{u}) = w_i\left[1 + \frac{\boldsymbol{c}_i\cdot\boldsymbol{u}}{c_s^2} + \frac{(\boldsymbol{c}_i\cdot\boldsymbol{u})^2}{c_s^4} - \frac{\boldsymbol{u}\cdot\boldsymbol{u}}{2c_s^2}\right]$$

Updating velocity and pressure

$$\rho\boldsymbol{u} = \frac{1}{c_s^2}\sum_i f_i\boldsymbol{c}_i + \frac{\delta t}{2}\left[\mu_\phi\boldsymbol{\nabla}\phi + \rho\boldsymbol{g}\right]$$

$$p = \sum_i f_i + \frac{\delta t}{2}\left[\boldsymbol{u}\cdot\boldsymbol{\nabla}\rho c_s^2 + \rho c_s^2\dot{m}'''\left(\frac{1}{\rho_g} - \frac{1}{\rho_l}\right)\right]$$

LB scheme 2/2: conservative Allen-Cahn

Distribution function g_i for ϕ

$$g_i(\boldsymbol{x}+\boldsymbol{c}_i\delta t,\, t+\delta t) = g_i(\boldsymbol{x},\, t) - \frac{1}{\tau_g + 1/2}\left[g_i(\boldsymbol{x},\, t) - g_i^{eq}(\boldsymbol{x},\, t)\right] + \delta t \mathcal{G}_i \qquad \mathcal{G}_i = w_i \frac{\dot{m}'''}{\rho g}$$

$$g_i^{eq}(\boldsymbol{x},\, t) = w_i\phi\left[1 + 3\frac{\boldsymbol{c}_i\cdot\boldsymbol{u}}{c^2}\right] + w_i M_\phi \left[\frac{4}{W}\phi(1-\phi)\right]\frac{(\boldsymbol{c}_i\cdot\boldsymbol{n})}{c_s^2} - \frac{\delta t}{2}\mathcal{G}_i$$

$$\phi = \sum_i g_i + \frac{\delta t}{2}\mathcal{G}_i \qquad \text{and} \qquad M_\phi = \frac{1}{3}\tau_g\frac{\delta x^2}{\delta t}$$

Normal vector computation $\boldsymbol{n} = \boldsymbol{\nabla}\phi/\left|\boldsymbol{\nabla}\phi\right|$

Directional derivatives:

$$\boldsymbol{e}_i\cdot\boldsymbol{\nabla}\phi\big|_{\boldsymbol{x}} = \frac{1}{2\delta x}\left[\phi(\boldsymbol{x}+\boldsymbol{e}_i\delta x) - \phi(\boldsymbol{x}-\boldsymbol{e}_i\delta x)\right]$$

$$\boldsymbol{\nabla}\phi = \frac{1}{e^2}\sum_{i=0}^{N_{pop}} w_i\boldsymbol{e}_i\left(\boldsymbol{e}_i\cdot\boldsymbol{\nabla}\phi\big|_{\boldsymbol{x}}\right)$$

Norm:

$$\left|\boldsymbol{\nabla}\phi\right| = \sqrt{(\partial_x\phi)^2 + (\partial_y\phi)^2 + (\partial_z\phi)^2}$$

LB schemes 3/3: temperature equation

Similar as ϕ-equation

Distribution function h_i for T:

$$h_i(\boldsymbol{x}+\boldsymbol{c}_i\delta t,\, t+\delta t) = h_i(\boldsymbol{x},\, t) - \frac{1}{\tau_h + 1/2}\left[h_i(\boldsymbol{x},\, t) - h_i^{eq}(\boldsymbol{x},\, t)\right] + \delta t \mathcal{H}_i$$

$$h_i^{eq}(\boldsymbol{x},\, t) = w_i T\left[1 + 3\frac{\boldsymbol{c}_i\cdot\boldsymbol{u}}{c}\right] - \frac{\delta t}{2}\mathcal{H}_i$$

$$\mathcal{H}_i = w_i\left[\boldsymbol{\nabla}\cdot(\boldsymbol{u}\phi) + \frac{\partial\phi}{\partial t}\right]\frac{\mathcal{L}}{\mathcal{C}_p}$$

Diffusivity:

$$\alpha = \frac{1}{3}\tau_h\frac{\delta x^2}{\delta t}$$

Updating temperature

$$T = \sum_i h_i + \mathcal{H}_i\frac{\delta t}{2}$$

+ BC «Dirichlet» or «zero flux» on all boundaries

END OF APPENDICES