Consistent n-phases Cahn-Hilliard systems and applications to multiphase flows

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1. Introduction
2. The two-phase Cahn-Hilliard equation revisited
3. The consistency issue for three-phase CH systems
4. Construction of consistent n-phase Cahn-Hilliard systems
5. Few words about numerics
6. Conclusion

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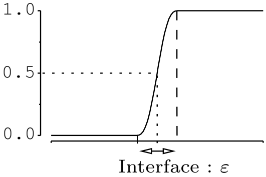
The two-phase Cahn-Hilliard equation

Principle of the diffuse interface modeling

- One unknown : the order parameter c (concentration of one phase)
- The surface tension $\sigma_{12} > 0$ is given.
- Interfaces have small but positive thickness $\varepsilon > 0$ which is fixed.

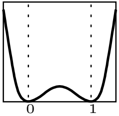
$$\begin{cases} c(x) = 1, & \text{for } x \in \text{phase 2}, \\ 0 < c(x) < 1, & \text{for } x \in \text{interface} \,, \\ c(x) = 0, & \text{for } x \in \text{phase 1}. \end{cases}$$



The two-phase total energy

$f(c) = c^2(1-c)^2$

$$\mathcal{F}_\varepsilon^{[\sigma_{12}]}(c) = \int_\Omega \left(12 \frac{\sigma_{12}}{\varepsilon} f(c) + \frac{3}{4} \varepsilon \sigma_{12} |\nabla c|^2 \right) dx.$$



1D Equilibrium : $c_{eq}(x) = \dfrac{1 + \tanh(2x/\varepsilon)}{2}$ and $\mathcal{F}_\varepsilon^{[\sigma_{12}]}(c_{eq}) = \sigma_{12}$.

$$\mathcal{F}_{\varepsilon}^{[\sigma_{12}]}(c) = \int_{\Omega} \left(12 \frac{\sigma_{12}}{\varepsilon} f(c) + \frac{3}{4} \varepsilon \sigma_{12} |\nabla c|^2 \right) dx.$$

EVOLUTION EQUATION (GRADIENT STRUCTURE)

$\frac{D.}{Dc}$=functional derivative

$$\begin{cases} \partial_t c = M_0 \, \Delta\mu, \\ \mu = \dfrac{D\mathcal{F}_{\varepsilon}^{[\sigma_{12}]}}{Dc}(c) = -\dfrac{3}{2}\varepsilon\sigma_{12}\Delta c + \dfrac{12\sigma_{12}}{\varepsilon} f'(c), \\ \dfrac{\partial c}{\partial n} = \dfrac{\partial \mu}{\partial n} = 0, \quad \text{on } \partial\Omega. \end{cases}$$

REMARKS

- $1 - c$ satisfies the same equation.
- The total energy is dissipated

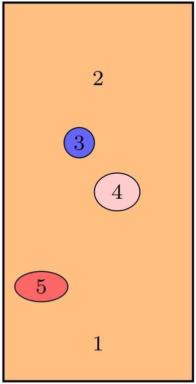
$$\frac{d}{dt}\mathcal{F}_{\varepsilon}^{[\sigma_{12}]}(c) + M_0 \int_{\Omega} |\nabla \mu|^2 \, dx = 0.$$

Build n-phase Cahn-Hilliard systems which are able to cope with two-phase situations

Notation

- Constant vector $\mathbf{1} = (1, \dots, 1)^t \in \mathbb{R}^n$,
- n order parameters $\mathbf{c} = (c_1, \dots, c_n)^t \in \mathbb{R}^n$
- We shall **require** that

$$1 = \sum_i c_i = \mathbf{c} \cdot \mathbf{1}.$$



Surface tensions are given

$$\boldsymbol{\sigma} = (\sigma_{ij})_{1 \le i,j \le n}, \quad \boldsymbol{\sigma}^t = \boldsymbol{\sigma},$$

with $\sigma_{ii} = 0, \quad \forall 1 \le i \le n.$

Applications to multiphase flows through the coupling with NS

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FORMULATION WITH TWO ORDER PARAMETERS $\mathbf{c} = (c_1, c_2)^t$, $\boldsymbol{\sigma} = \begin{pmatrix} 0 & \sigma_{12} \\ \sigma_{12} & 0 \end{pmatrix}$

$$\text{Total energy} \quad \mathcal{F}_\varepsilon^{[\boldsymbol{\sigma}]}(\mathbf{c}) = \int_\Omega \frac{12}{\varepsilon} F^{[\boldsymbol{\sigma}]}(\mathbf{c}) - \frac{3}{4}\varepsilon\sigma_{12}(\nabla c_1, \nabla c_2)\, dx,$$

$$\text{Potential} \quad F^{[\boldsymbol{\sigma}]}(\mathbf{c}) = \frac{\sigma_{12}}{2}\left(f(c_1) + f(c_2) - f(c_1 + c_2)\right).$$

N.B. : For any c we have, $\mathcal{F}_\varepsilon^{[\boldsymbol{\sigma}]}(c, 1-c) = \mathcal{F}_\varepsilon^{[\sigma_{12}]}(c)$.

Formulation with two order parameters $\mathbf{c} = (c_1, c_2)^t$, $\boldsymbol{\sigma} = \begin{pmatrix} 0 & \sigma_{12} \\ \sigma_{12} & 0 \end{pmatrix}$

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N.B. : For any c we have, $\mathcal{F}_\varepsilon^{[\boldsymbol{\sigma}]}(c, 1-c) = \mathcal{F}_\varepsilon^{[\sigma_{12}]}(c)$.

The evolution system

$$\begin{cases} \partial_t c_1 = M_0\, \Delta\left(\alpha_{11}\mu_1 + \alpha_{12}\mu_2\right), \\ \partial_t c_2 = M_0\, \Delta\left(\alpha_{12}\mu_1 + \alpha_{22}\mu_2\right), \\ \quad \mu_1 = \dfrac{D\mathcal{F}_\varepsilon^{[\boldsymbol{\sigma}]}}{Dc_1}(c_1, c_2) = \dfrac{3}{4}\varepsilon\sigma_{12}\Delta c_2 + \dfrac{12}{\varepsilon}\dfrac{\partial F^{[\boldsymbol{\sigma}]}}{\partial c_1}(c_1, c_2), \\ \quad \mu_2 = \dfrac{D\mathcal{F}_\varepsilon^{[\boldsymbol{\sigma}]}}{Dc_2}(c_1, c_2) = \dfrac{3}{4}\varepsilon\sigma_{12}\Delta c_1 + \dfrac{12}{\varepsilon}\dfrac{\partial F^{[\boldsymbol{\sigma}]}}{\partial c_2}(c_1, c_2). \end{cases}$$

First constraint :

We require $\mathbf{c} \cdot \mathbf{1} = c_1 + c_2 = 1$, $\forall t, x$ as soon as $c_1(0, .) + c_2(0, .) = 1$

$$\frac{\partial(c_1 + c_2)}{\partial t} = M_0\Delta\big((\alpha_{11} + \alpha_{12})\mu_1 + (\alpha_{12} + \alpha_{22})\mu_2\big),$$

$$\Longrightarrow \begin{Bmatrix} \alpha_{11} + \alpha_{12} = 0 \\ \alpha_{12} + \alpha_{22} = 0 \end{Bmatrix} \Longrightarrow \boxed{-\alpha_{12} = \alpha_{11} = \alpha_{22}}.$$

FORMULATION WITH TWO ORDER PARAMETERS $\mathbf{c} = (c_1, c_2)^t$, $\boldsymbol{\sigma} = \begin{pmatrix} 0 & \sigma_{12} \\ \sigma_{12} & 0 \end{pmatrix}$

$$\text{Total energy} \quad \mathcal{F}_\varepsilon^{[\boldsymbol{\sigma}]}(\mathbf{c}) = \int_\Omega \frac{12}{\varepsilon} F^{[\boldsymbol{\sigma}]}(\mathbf{c}) - \frac{3}{4}\varepsilon\sigma_{12}(\nabla c_1, \nabla c_2)\, dx,$$

$$\text{Potential} \quad F^{[\boldsymbol{\sigma}]}(\mathbf{c}) = \frac{\sigma_{12}}{2}\left(f(c_1) + f(c_2) - f(c_1 + c_2)\right).$$

N.B. : For any c we have, $\mathcal{F}_\varepsilon^{[\boldsymbol{\sigma}]}(c, 1-c) = \mathcal{F}_\varepsilon^{[\sigma_{12}]}(c)$.

THE EVOLUTION SYSTEM

$$\begin{cases} \partial_t c_1 = M_0\, \Delta\left(\mu_1 - \mu_2\right), \\ \partial_t c_2 = M_0\, \Delta\left(\mu_2 - \mu_1\right), \\ \mu_1 = \dfrac{D\mathcal{F}_\varepsilon^{[\boldsymbol{\sigma}]}}{Dc_1}(c_1, c_2) = \dfrac{3}{4}\varepsilon\sigma_{12}\Delta c_2 + \dfrac{12}{\varepsilon}\dfrac{\partial F^{[\boldsymbol{\sigma}]}}{\partial c_1}(c_1, c_2), \\ \mu_2 = \dfrac{D\mathcal{F}_\varepsilon^{[\boldsymbol{\sigma}]}}{Dc_2}(c_1, c_2) = \dfrac{3}{4}\varepsilon\sigma_{12}\Delta c_1 + \dfrac{12}{\varepsilon}\dfrac{\partial F^{[\boldsymbol{\sigma}]}}{\partial c_2}(c_1, c_2). \end{cases}$$

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THE EVOLUTION SYSTEM

$$\begin{cases} \partial_t c_1 = M_0\, \Delta\left(\mu_1 - \mu_2\right), \\ c_2 = 1 - c_1, \\ \mu_1 = \dfrac{D\mathcal{F}_\varepsilon^{[\boldsymbol{\sigma}]}}{Dc_1}(c_1, c_2) = -\dfrac{3}{4}\varepsilon\sigma_{12}\Delta c_1 + \dfrac{12}{\varepsilon}\dfrac{\partial F^{[\boldsymbol{\sigma}]}}{\partial c_1}(c_1, 1 - c_1), \\ \mu_2 = \dfrac{D\mathcal{F}_\varepsilon^{[\boldsymbol{\sigma}]}}{Dc_2}(c_1, c_2) = +\dfrac{3}{4}\varepsilon\sigma_{12}\Delta c_1 + \dfrac{12}{\varepsilon}\dfrac{\partial F^{[\boldsymbol{\sigma}]}}{\partial c_2}(c_1, 1 - c_1). \end{cases}$$

FORMULATION WITH TWO ORDER PARAMETERS $\mathbf{c} = (c_1, c_2)^t$, $\boldsymbol{\sigma} = \begin{pmatrix} 0 & \sigma_{12} \\ \sigma_{12} & 0 \end{pmatrix}$

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$$\text{Potential} \quad F^{[\boldsymbol{\sigma}]}(\mathbf{c}) = \frac{\sigma_{12}}{2}(f(c_1) + f(c_2) - f(c_1 + c_2)).$$

N.B. : For any c we have, $\mathcal{F}_\varepsilon^{[\boldsymbol{\sigma}]}(c, 1-c) = \mathcal{F}_\varepsilon^{[\sigma_{12}]}(c)$.

THE EVOLUTION SYSTEM

$$\begin{cases} \partial_t c_1 = M_0\, \Delta\,(\mu_1 - \mu_2)\,, \\ c_2 = 1 - c_1, \\ \mu_1 = \dfrac{D\mathcal{F}_\varepsilon^{[\boldsymbol{\sigma}]}}{Dc_1}(c_1, c_2) = -\dfrac{3}{4}\varepsilon\sigma_{12}\Delta c_1 + \dfrac{6\sigma_{12}}{\varepsilon}(f'(c_1) - \underbrace{f'(1)}_{=0}), \\ \mu_2 = -\mu_1. \end{cases}$$

Formulation with two order parameters $\mathbf{c} = (c_1, c_2)^t$, $\boldsymbol{\sigma} = \begin{pmatrix} 0 & \sigma_{12} \\ \sigma_{12} & 0 \end{pmatrix}$

$$\text{Total energy} \quad \mathcal{F}_\varepsilon^{[\boldsymbol{\sigma}]}(\mathbf{c}) = \int_\Omega \frac{12}{\varepsilon} F^{[\boldsymbol{\sigma}]}(\mathbf{c}) - \frac{3}{4}\varepsilon\sigma_{12}(\nabla c_1, \nabla c_2)\, dx,$$

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N.B. : For any c we have, $\mathcal{F}_\varepsilon^{[\boldsymbol{\sigma}]}(c, 1-c) = \mathcal{F}_\varepsilon^{[\sigma_{12}]}(c)$.

The evolution system

$$\begin{cases} \partial_t c_1 = M_0 \, \Delta \left(2\mu_1\right), \\ c_2 = 1 - c_1, \\ 2\mu_1 = -\dfrac{3}{2}\varepsilon\sigma_{12}\Delta c_1 + \dfrac{12\sigma_{12}}{\varepsilon} f'(c_1), \\ \mu_2 = -\mu_1. \end{cases}$$

Conclusions

- We recover the usual CH equation (one single equation !).
- We can eliminate **a posteriori** and **arbitrarily** one of the order parameters without breaking symmetry.

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The consistency issue for three-phase systems

In **(Kim-Lowengrub, IFB '05)** we find the following Cahn-Hilliard system

$$\begin{cases} \partial_t c_1 = M_0 \Delta \mu_1, \\ \partial_t c_2 = M_0 \Delta \mu_2, \\ c_3 = 1 - c_1 - c_2, \\ \mu_1 = \dfrac{1}{\varepsilon}\left(\dfrac{\partial \tilde{F}_0}{\partial c_1}(\mathbf{c}) - \dfrac{\partial \tilde{F}_0}{\partial c_3}(\mathbf{c})\right) - \varepsilon \Delta c_1 - \dfrac{\varepsilon}{2}\Delta c_2, \\ \mu_2 = \dfrac{1}{\varepsilon}\left(\dfrac{\partial \tilde{F}_0}{\partial c_2}(\mathbf{c}) - \dfrac{\partial \tilde{F}_0}{\partial c_3}(\mathbf{c})\right) - \dfrac{\varepsilon}{2}\Delta c_1 - \varepsilon \Delta c_2, \end{cases}$$

with the three-phase potential

$$\tilde{F}_0(\mathbf{c}) = \sigma_{12} c_1^2 c_2^2 + \sigma_{13} c_1^2 c_3^2 + \sigma_{23} c_2^2 c_3^2.$$

This model is not suitable for our purposes

Symmetry breaking

The equation satisfied by c_3 is not formally the same as the one for c_1 and c_2.

Non-consistency with two-phase situations

If $c_i \equiv 0$ at $t = 0$ then c_i is in general not 0 for $t > 0$.

We proposed in **(B.-Lapuerta, '06)** to consider

$$(\text{CH}) \qquad \begin{cases} \dfrac{\partial c_i}{\partial t} = M_0 \operatorname{div}\left(\dfrac{1}{\Sigma_i}\nabla \mu_i\right), \quad \forall i \\ \mu_i = \dfrac{4\Sigma_T}{\varepsilon}\displaystyle\sum_{j\neq i}\left(\dfrac{1}{\Sigma_j}\left(\partial_i F^{[\boldsymbol{\sigma}]}(\mathbf{c}) - \partial_j F^{[\boldsymbol{\sigma}]}(\mathbf{c})\right)\right) - \dfrac{3}{4}\varepsilon\Sigma_i\Delta c_i, \quad \forall i. \end{cases}$$

where

$$\text{Spreading parameters are given by} \quad \begin{cases} \Sigma_1 = \sigma_{12} + \sigma_{13} - \sigma_{23}, \\ \Sigma_2 = \sigma_{12} + \sigma_{23} - \sigma_{13}, \\ \Sigma_3 = \sigma_{13} + \sigma_{23} - \sigma_{12}, \end{cases}$$

$$\frac{1}{\Sigma_T} = \frac{1}{3}\left(\frac{1}{\Sigma_1} + \frac{1}{\Sigma_2} + \frac{1}{\Sigma_3}\right),$$

and our potential is defined by

$$F^{[\boldsymbol{\sigma}]}(\mathbf{c}) = \underbrace{\sigma_{12}c_1^2c_2^2 + \sigma_{13}c_1^2c_3^2 + \sigma_{23}c_2^2c_3^2}_{=\tilde{F}_0(\mathbf{c}),\text{non-consistent}} + c_1c_2c_3(\Sigma_1c_1 + \Sigma_2c_2 + \Sigma_3c_3).$$

We proposed in **(B.-Lapuerta, '06)** to consider

$$(\text{CH}) \qquad \begin{cases} \dfrac{\partial c_i}{\partial t} = M_0 \operatorname{div}\left(\dfrac{1}{\Sigma_i}\nabla \mu_i\right), \quad \forall i \\ \mu_i = \dfrac{4\Sigma_T}{\varepsilon}\displaystyle\sum_{j\neq i}\left(\dfrac{1}{\Sigma_j}\left(\partial_i F^{[\boldsymbol{\sigma}]}(\mathbf{c}) - \partial_j F^{[\boldsymbol{\sigma}]}(\mathbf{c})\right)\right) - \dfrac{3}{4}\varepsilon\Sigma_i\Delta c_i, \quad \forall i. \end{cases}$$

where

$$\text{Spreading parameters are given by} \quad \begin{cases} \Sigma_1 = \sigma_{12} + \sigma_{13} - \sigma_{23}, \\ \Sigma_2 = \sigma_{12} + \sigma_{23} - \sigma_{13}, \\ \Sigma_3 = \sigma_{13} + \sigma_{23} - \sigma_{12}, \end{cases}$$

$$\frac{1}{\Sigma_T} = \frac{1}{3}\left(\frac{1}{\Sigma_1} + \frac{1}{\Sigma_2} + \frac{1}{\Sigma_3}\right),$$

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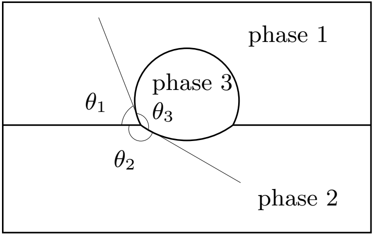
$$F^{[\boldsymbol{\sigma}]}(\mathbf{c}) = \underbrace{\sigma_{12}c_1^2c_2^2 + \sigma_{13}c_1^2c_3^2 + \sigma_{23}c_2^2c_3^2}_{=\tilde{F}_0(\mathbf{c}),\text{non-consistent}} + c_1c_2c_3(\Sigma_1c_1 + \Sigma_2c_2 + \Sigma_3c_3).$$

EQUIVALENT FORM OF THE POTENTIAL $\qquad f(c) = c^2(1-c)^2$

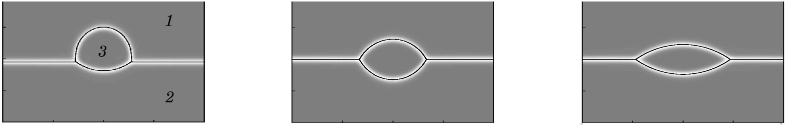
$$F^{[\boldsymbol{\sigma}]}(\mathbf{c}) = \frac{\sigma_{12}}{2}\left[f(c_1) + f(c_2) - f(c_1+c_2)\right] + \frac{\sigma_{13}}{2}\left[f(c_1) + f(c_3) - f(c_1+c_3)\right] + \frac{\sigma_{23}}{2}\left[f(c_2) + f(c_3) - f(c_2+c_3)\right].$$

YOUNG'S LAW

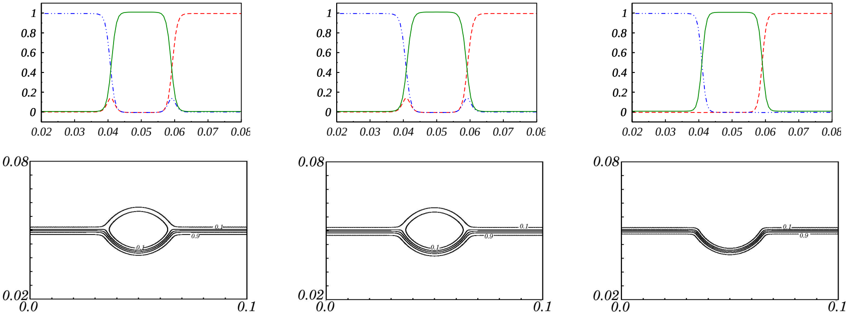
$$\frac{\sin\theta_1}{\sigma_{23}} = \frac{\sin\theta_2}{\sigma_{13}} = \frac{\sin\theta_3}{\sigma_{12}}$$



EXAMPLES FOR VARIOUS VALUES OF $(\sigma_{12};\sigma_{13};\sigma_{23})$



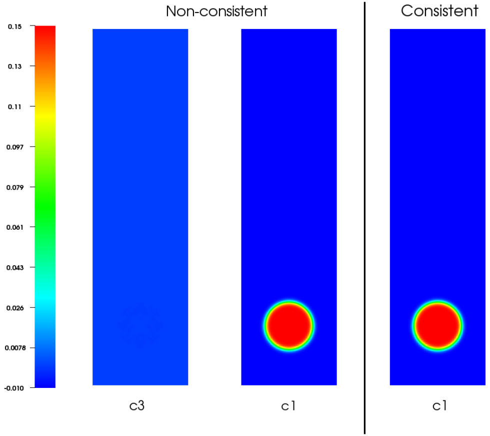
(1 ; 0.8 ; 1.4) (1 ; 1 ; 1) (1 ; 0.6 ; 0.6)



(Kim–Lowengrub, '05) — Our model using $\widetilde{F}_0$ — Our model using $F^{[\boldsymbol{\sigma}]}$

In each case, numerical convergence is achieved

A two-phase CH/NS computation with a three-phase model



phase 1 = bubble

phase 2 = liquid

phase 3 = virtual ...

$\sigma_{12} = 0.07$

$\sigma_{13} = 0.07$

$\sigma_{23} = 0.05$

$$\frac{\rho_2}{\rho_1} = 10^3$$

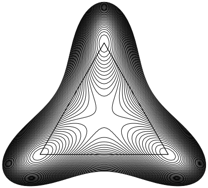
$$\frac{\rho_3}{\rho_1} = 10^4$$

$$\frac{\mu_2}{\mu_1} = 10^{-3}$$

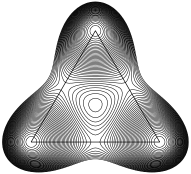
$$\frac{\mu_3}{\mu_1} = 5.10^{-3},$$

$\rightsquigarrow$ Using a non-consistent potential leads to $c_3 \approx 15\%$ instead of $c_3 = 0$!

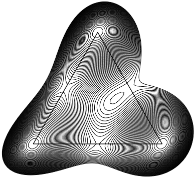
Isolines of the potential F on the Gibbs triangle



$\Sigma_1 = \Sigma_2 = \Sigma_3 = 4$,
non-consistent $\tilde{F}_0$

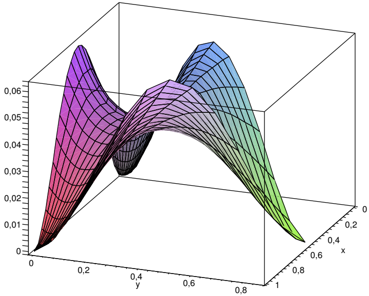


$\Sigma_1 = \Sigma_2 = \Sigma_3 = 4$,
consistent $F^{[\boldsymbol{\sigma}]}$

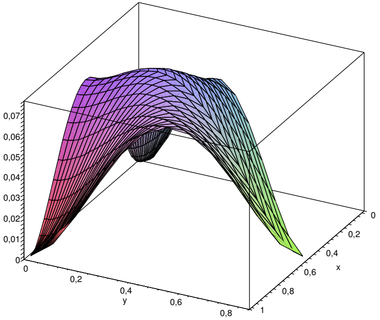


$\Sigma_1 = 6, \Sigma_2 = 8, \Sigma_3 = 4$,
consistent $F^{[\boldsymbol{\sigma}]}$

$$\Sigma_1 = \Sigma_2 = \Sigma_3 = 4,$$



non-consistent $\widetilde{F}_0$



consistent $F^{[\boldsymbol{\sigma}]}$

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(B.-Minjeaud, '12)

Cahn-Hilliard Potential ansatz

$$F^{[\boldsymbol{\sigma}]}(\mathbf{c}) = \frac{1}{4}\sum_{i,j}\sigma_{ij}(f(c_i)+f(c_j)-f(c_i+c_j)) + \sum_{s<t<u<v} c_s c_t c_u c_v H_{stuv}(\mathbf{c}).$$

- For $n=2$: we recover the usual Cahn-Hilliard potential (no term in $H_\bullet$)
- For $n=3$: we recover the 3-phase potential proposed in (B.-Lapuerta, '06) (no term $H_\bullet$)
- For $n \geq 4$: we will see that the terms $H_\bullet$ are necessary for consistency to hold.

First consistency property

For any l, we have $\quad F^{[\boldsymbol{\sigma}]}(\mathbf{c}) = F^{[\widetilde{\boldsymbol{\sigma}}^l]}(\widetilde{\mathbf{c}}^l),\quad$ as soon as $c_l = 0$.

NOTATION : Removing the phase number l from the system

$$\widetilde{\boldsymbol{\sigma}}^l = (\sigma_{ij})_{\substack{1\leq i,j,\leq n\\ i\neq l, j\neq l}} \in M_{n-1}(\mathbb{R}),$$

$$\widetilde{\mathbf{c}}^l = (c_1, ..., c_{l-1}, c_{l+1}, ..., c_n)^t \in \mathbb{R}^{n-1}.$$

Ansatz for the Cahn-Hilliard total energy

$$\mathcal{F}_{\varepsilon}^{[\boldsymbol{\sigma}]}(\mathbf{c}) = \int_{\Omega} \frac{12}{\varepsilon} F^{[\boldsymbol{\sigma}]}(\mathbf{c}) - \frac{3}{8}\varepsilon \left(\sum_{i,j} \sigma_{ij} (\nabla c_i, \nabla c_j) \right) dx.$$

Coercivity condition for capillary terms

We assume that the matrix $-\boldsymbol{\sigma}$ is definite positive in $\{\mathbf{1}\}^{\perp}$ that is

$$\text{(C1)} \qquad \sum_{ij} (-\sigma_{ij}) \xi_i \xi_j > 0, \quad \forall \xi \in \mathbb{R}^n \setminus \{0\}, \text{such that } \xi \cdot \mathbf{1} = 0.$$

- Condition (C1) depends only on physical parameters.
- Moreover, if $\boldsymbol{\sigma}$ satisfies this condition, so does $\widetilde{\boldsymbol{\sigma}}^l$ for any l.
- For $n = 2$,

$$\text{(C1)} \Leftrightarrow \sigma_{12} > 0.$$

ANSATZ FOR THE CAHN-HILLIARD TOTAL ENERGY

$$\mathcal{F}_\varepsilon^{[\boldsymbol{\sigma}]}(\mathbf{c}) = \int_\Omega \frac{12}{\varepsilon} F^{[\boldsymbol{\sigma}]}(\mathbf{c}) - \frac{3}{8}\varepsilon \left(\sum_{i,j} \sigma_{ij} (\nabla c_i, \nabla c_j) \right) dx.$$

COERCIVITY CONDITION FOR CAPILLARY TERMS

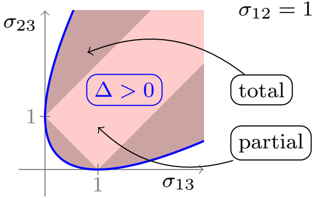
We assume that the matrix $-\boldsymbol{\sigma}$ is definite positive in $\{\mathbf{1}\}^\perp$ that is

(C1) $$\sum_{ij} (-\sigma_{ij})\xi_i\xi_j > 0, \quad \forall \xi \in \mathbb{R}^n \setminus \{0\}, \text{such that } \ \xi \cdot \mathbf{1} = 0.$$

- For $n = 3$, we have

$$\text{(C1)} \Leftrightarrow \begin{cases} \sigma_{12} > 0, \sigma_{13} > 0, \sigma_{23} > 0, \\ \Delta = \Sigma_1\Sigma_2 + \Sigma_1\Sigma_3 + \Sigma_2\Sigma_3 > 0, \end{cases}$$

where $\Sigma_i = \sigma_{ij} + \sigma_{ik} - \sigma_{jk}$ is the spreading parameter of phase i.



ANSATZ FOR THE CAHN-HILLIARD TOTAL ENERGY

$$\mathcal{F}_\varepsilon^{[\boldsymbol{\sigma}]}(\mathbf{c}) = \int_\Omega \frac{12}{\varepsilon} F^{[\boldsymbol{\sigma}]}(\mathbf{c}) - \frac{3}{8}\varepsilon \left(\sum_{i,j} \sigma_{ij} (\nabla c_i, \nabla c_j) \right) dx.$$

COERCIVITY CONDITION FOR CAPILLARY TERMS

We assume that the matrix $-\boldsymbol{\sigma}$ is definite positive in $\{\mathbf{1}\}^\perp$ that is

(C1) $$\sum_{ij} (-\sigma_{ij}) \xi_i \xi_j > 0, \quad \forall \xi \in \mathbb{R}^n \setminus \{0\}, \text{such that } \ \xi \cdot \mathbf{1} = 0.$$

- For $n = 4$, we introduce

$$\Sigma_i^l = \sigma_{ij} + \sigma_{ik} - \sigma_{jk}, \quad \text{the spreading coefficient of } i \text{ among } \{i,j,k\} \not\ni l,$$

$$\Delta^l = \Sigma_i^l \Sigma_j^l + \Sigma_i^l \Sigma_k^l + \Sigma_j^l \Sigma_k^l, \quad \forall l \in \{1, ..., 4\}.$$

Then, we have

$$(\text{C1}) \Leftrightarrow \begin{cases} \sigma_{ij} > 0, & \forall i \neq j, \\ \Delta^l > 0, & \forall l, \\ \Delta^k \Delta^l > (2\sigma_{ij}\Sigma_i^j - \Sigma_i^k \Sigma_j^k)^2, & \forall k, \forall l. \end{cases}$$

ANSATZ FOR THE CAHN-HILLIARD TOTAL ENERGY

$$\mathcal{F}_\varepsilon^{[\boldsymbol{\sigma}]}(\mathbf{c}) = \int_\Omega \frac{12}{\varepsilon} F^{[\boldsymbol{\sigma}]}(\mathbf{c}) - \frac{3}{8}\varepsilon \left(\sum_{i,j} \sigma_{ij} (\nabla c_i, \nabla c_j) \right) dx.$$

EVOLUTION SYSTEM TAKING INTO ACCOUNT $\mathbf{c} \cdot \mathbf{1} = \sum_i c_i = 1$

$$(\mathrm{CH}^{[\boldsymbol{\sigma}]}) \qquad \begin{cases} \partial_t c_i = M_0\, \Delta \left(\sum_{j \neq i} \alpha_{ij}^{[\boldsymbol{\sigma}]} (\mu_i - \mu_j) \right), \\ \mu_i = \dfrac{12}{\varepsilon} \dfrac{\partial F^{[\boldsymbol{\sigma}]}}{\partial c_i}(\mathbf{c}) + \dfrac{3}{4}\varepsilon \sum_{j \neq i} \sigma_{ij} \Delta c_j. \end{cases}$$

We assume that $\boldsymbol{\alpha}^{[\boldsymbol{\sigma}]}$ is symmetric and we set $\alpha_{ii}^{[\boldsymbol{\sigma}]} = -\sum_{j \neq i} \alpha_{ij}^{[\boldsymbol{\sigma}]}$ so that

$$\left(\sum_{j=1}^{n} \alpha_{ij}^{[\boldsymbol{\sigma}]} = 0, \ \forall i \right), \text{ that is } \boldsymbol{\alpha}^{[\boldsymbol{\sigma}]}.\mathbf{1} = 0.$$

HOW TO DETERMINE THE MATRIX $\boldsymbol{\alpha}^{[\boldsymbol{\sigma}]} = (\alpha_{ij}^{[\boldsymbol{\sigma}]})_{i,j}$?

ANSATZ FOR THE CAHN-HILLIARD TOTAL ENERGY

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$$(\mathrm{CH}^{[\boldsymbol{\sigma}]}) \qquad \begin{cases} \partial_t c_i = - M_0 \, \Delta \left(\sum_j \alpha_{ij}^{[\boldsymbol{\sigma}]} \mu_j \right), \\ \mu_i = \dfrac{12}{\varepsilon} \dfrac{\partial F^{[\boldsymbol{\sigma}]}}{\partial c_i}(\mathbf{c}) + \dfrac{3}{4}\varepsilon \sum_{j \neq i} \sigma_{ij} \Delta c_j. \end{cases}$$

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DEFINITION (SECOND CONSISTENCY ASSUMPTION)

Solutions of System $(\mathrm{CH}^{[\boldsymbol{\sigma}]})$ should satisfy for any l

$$c_l(t=0,.) \equiv 0 \Rightarrow c_l(t,.) \equiv 0, \quad \forall t > 0.$$

- For any l we need $\displaystyle\sum_k \alpha_{lk}^{[\boldsymbol{\sigma}]} \mu_k = 0$ as soon as $c_l \equiv 0$.

$$(\mathrm{CH}^{[\boldsymbol{\sigma}]}) \quad \partial_t c_i = -M_0\,\Delta\left(\sum_j \alpha_{ij}^{[\boldsymbol{\sigma}]}\mu_j\right), \quad \mu_i = \frac{12}{\varepsilon}\frac{\partial F^{[\boldsymbol{\sigma}]}}{\partial c_i}(\mathbf{c}) \boxed{+\frac{3}{4}\varepsilon\sum_{j\neq i}\sigma_{ij}\Delta c_j}$$

Definition (Second consistency assumption)

Solutions of System $(\mathrm{CH}^{[\boldsymbol{\sigma}]})$ should satisfy for any l

$$c_l(t=0,.) \equiv 0 \Rightarrow c_l(t,.) \equiv 0, \quad \forall t > 0.$$

- For any l we need $\boxed{\sum_k \alpha_{lk}^{[\boldsymbol{\sigma}]}\mu_k = 0}$ as soon as $c_l \equiv 0$.
- Let us first look at capillary terms

$$\boxed{\mathcal{C}} = \sum_j \left(\sum_k \alpha_{lk}^{[\boldsymbol{\sigma}]}\sigma_{kj}\right)\Delta c_j = 0, \quad \text{as soon as } c_l \equiv 0$$

If the red coefficient does not depend on $j(\neq l)$ then $\mathcal{C}$ is proportional to Δc_l

$$c_1 + \ldots + c_n = 1 \Rightarrow \left(\sum_{j\neq l}\Delta c_j\right) = -\Delta c_l.$$

$$(\mathrm{CH}^{[\boldsymbol{\sigma}]}) \quad \partial_t c_i = -M_0\,\Delta\left(\sum_j \alpha_{ij}^{[\boldsymbol{\sigma}]}\mu_j\right), \quad \mu_i = \frac{12}{\varepsilon}\frac{\partial F^{[\boldsymbol{\sigma}]}}{\partial c_i}(\mathbf{c}) \boxed{+\frac{3}{4}\varepsilon\sum_{j\neq i}\sigma_{ij}\Delta c_j}$$

DEFINITION (SECOND CONSISTENCY ASSUMPTION)

Solutions of System $(\mathrm{CH}^{[\boldsymbol{\sigma}]})$ should satisfy for any l

$$c_l(t=0,.) \equiv 0 \Rightarrow c_l(t,.) \equiv 0, \quad \forall t > 0.$$

- For any l we need $\boxed{\sum_k \alpha_{lk}^{[\boldsymbol{\sigma}]}\mu_k = 0}$ as soon as $c_l \equiv 0$.
- Let us first look at capillary terms

$$\boxed{\mathcal{C}} = \sum_j \left(\sum_k \alpha_{lk}^{[\boldsymbol{\sigma}]}\sigma_{kj}\right)\Delta c_j = 0, \quad \text{as soon as } c_l \equiv 0$$

$\rightsquigarrow$ The problem is then to find a **symmetric** matrix $\boldsymbol{\alpha}^{[\boldsymbol{\sigma}]}$ such that

$$\begin{cases} \boldsymbol{\alpha}^{[\boldsymbol{\sigma}]}.\mathbf{1} = 0, \\ \boldsymbol{\alpha}^{[\boldsymbol{\sigma}]}.\boldsymbol{\sigma} = -I + \boldsymbol{\gamma}\otimes\mathbf{1}, \end{cases}$$

for some $\boldsymbol{\gamma} \in \mathbb{R}^n$. Assuming that the coercivity condition (C1) holds, we can show that **there is a unique solution** $(\boldsymbol{\alpha}^{[\boldsymbol{\sigma}]},\boldsymbol{\gamma})$.

$$(\mathrm{CH}^{[\boldsymbol{\sigma}]}) \quad \partial_t c_i = -M_0 \Delta \left(\sum_j \alpha_{ij}^{[\boldsymbol{\sigma}]} \mu_j \right), \quad \mu_i = \boxed{\frac{12}{\varepsilon} \frac{\partial F^{[\boldsymbol{\sigma}]}}{\partial c_i}(\mathbf{c})} + \frac{3}{4}\varepsilon \sum_{j \neq i} \sigma_{ij} \Delta c_j$$

DEFINITION (SECOND CONSISTENCY ASSUMPTION)

Solutions of System $(\mathrm{CH}^{[\boldsymbol{\sigma}]})$ should satisfy for any l

$$c_l(t=0,.) \equiv 0 \Rightarrow c_l(t,.) \equiv 0, \quad \forall t > 0.$$

- For any l we need $\boxed{\sum_k \alpha_{lk}^{[\boldsymbol{\sigma}]} \mu_k = 0}$ as soon as $c_l \equiv 0$.
- Let us look now at potential (nonlinear) terms

$$\boxed{\mathcal{N}} = \sum_k \alpha_{lk}^{[\boldsymbol{\sigma}]} \frac{\partial F^{[\boldsymbol{\sigma}]}}{\partial c_k}(\mathbf{c}) = 0, \quad \text{as soon as } c_l \equiv 0$$

Using that $\boldsymbol{\alpha}^{[\boldsymbol{\sigma}]}.\boldsymbol{\sigma} = -I + \boldsymbol{\gamma} \otimes \mathbf{1}$ and $\sum_i f'(c_i) = 12 \sum_{j<k<l} c_j c_k c_l$, we get

$$\sum_k \alpha_{lk}^{[\boldsymbol{\sigma}]} \frac{\partial F^{[\boldsymbol{\sigma}]}}{\partial c_k}(\mathbf{c}) = \frac{1}{2} \underbrace{f'(c_l)}_{=0, \text{ for } c_l = 0} + \sum_{i<j<k} \underbrace{\Lambda_{ijk}^l}_{\substack{\text{explicit}\\ \text{formula}}} c_i c_j c_k + \text{terms in } H_\bullet.$$

$$(\mathrm{CH}^{[\boldsymbol{\sigma}]}) \quad \partial_t c_i = -M_0\,\Delta\left(\sum_j \alpha_{ij}^{[\boldsymbol{\sigma}]}\mu_j\right), \quad \mu_i = \boxed{\frac{12}{\varepsilon}\frac{\partial F^{[\boldsymbol{\sigma}]}}{\partial c_i}(\mathbf{c})} + \frac{3}{4}\varepsilon\sum_{j\neq i}\sigma_{ij}\Delta c_j$$

DEFINITION (SECOND CONSISTENCY ASSUMPTION)

Solutions of System $(\mathrm{CH}^{[\boldsymbol{\sigma}]})$ should satisfy for any l

$$c_l(t=0,.)\equiv 0 \Rightarrow c_l(t,.)\equiv 0, \quad \forall t>0.$$

- For any l we need $\boxed{\sum_k \alpha_{lk}^{[\boldsymbol{\sigma}]}\mu_k = 0}$ as soon as $c_l \equiv 0$.
- Let us look now at potential (nonlinear) terms

$$\boxed{\mathcal{N}} = \sum_k \alpha_{lk}^{[\boldsymbol{\sigma}]}\frac{\partial F^{[\boldsymbol{\sigma}]}}{\partial c_k}(\mathbf{c}) = 0, \quad \text{as soon as } c_l \equiv 0$$

For $n \geq 4$, we need to compensate (as soon as $c_l \equiv 0$!)

$$\sum_{\substack{i<j<k\\ \neq l}} \underbrace{\Lambda_{ijk}^{l}}_{\text{explicit formula}} c_i c_j c_k + \sum_{\substack{i<j<k\\ \neq l}} c_i c_j c_k \left(\sum_{s\notin\{i,j,k\}} \alpha_{ls}^{[\boldsymbol{\sigma}]} H_{sijk}(\mathbf{c})\right) + \ldots$$

GOAL

Find functions $H_\bullet$ such that, for any l and any $i < j < k$ different from l, we have

$$\sum_{s \notin \{i,j,k\}} \alpha_{ls}^{[\boldsymbol{\sigma}]} H_{sijk}(\mathbf{c}) = \Lambda_{ijk}^{l}, \quad \text{as soon as } c_l = 0.$$

CASE 1 : FOR ANY $n \geq 4$ AND $\sigma_{ij} = \sigma$

We can show that the value Λ_{ijk}^{l} is independent of i, j, k, l and we find that

$$H_{s,i,k,l}(\mathbf{c}) = 14\sigma,$$

fulfills the conditions, and System $(\mathrm{CH}^{[\boldsymbol{\sigma}]})$ then reads

$$\begin{cases} \partial_t c_i = M_0 \, \Delta \underbrace{\left(-\sum_j \alpha_{ij}^{[\boldsymbol{\sigma}]} \mu_j \right)}_{=\tilde{\mu}_i}, \\ \tilde{\mu}_i = n\sigma^2 \left(-\dfrac{3\varepsilon}{4} \Delta c_i + \dfrac{6}{\varepsilon} f'(c_i) - \dfrac{24}{\varepsilon} \sum_{\substack{j<k \\ \neq i}} c_i c_j c_k \right). \end{cases}$$

GOAL

Find functions $H_\bullet$ such that, for any l and any $i < j < k$ different from l, we have

$$\sum_{s \notin \{i,j,k\}} \alpha_{ls}^{[\boldsymbol{\sigma}]} H_{sijk}(\mathbf{c}) = \Lambda_{ijk}^{l}, \quad \text{as soon as } c_l = 0.$$

CASE 2 : FOR $n = 4$ AND $\boldsymbol{\sigma}$ GENERIC :

Only one function H_{1234} to determine

$$\begin{cases} H_{1234}(\mathbf{c}) = \dfrac{\Lambda_{234}^{1}}{\alpha_{11}^{[\boldsymbol{\sigma}]}}, & \text{for } c_1 = 0, \\ H_{1234}(\mathbf{c}) = \dfrac{\Lambda_{134}^{2}}{\alpha_{22}^{[\boldsymbol{\sigma}]}}, & \text{for } c_2 = 0, \\ H_{1234}(\mathbf{c}) = \dfrac{\Lambda_{124}^{3}}{\alpha_{33}^{[\boldsymbol{\sigma}]}}, & \text{for } c_3 = 0, \\ H_{1234}(\mathbf{c}) = \dfrac{\Lambda_{123}^{4}}{\alpha_{44}^{[\boldsymbol{\sigma}]}}, & \text{for } c_4 = 0. \end{cases}$$

Such a function **cannot be continuous** but we can choose for instance

$$H_{1234}(\mathbf{c}) = \left(\sum_{i=1}^{4} \frac{\Lambda_{jkl}^{i}}{\alpha_{ii}^{[\boldsymbol{\sigma}]}} \phi(c_i, c_j c_k c_l) \right) \Big/ \left(\sum_{i=1}^{4} \phi(c_i, c_j c_k c_l) \right), \text{ with } \phi(a,b) = \frac{|b|}{|a| + |b|}.$$

NB : The function $\mathbf{c} \mapsto c_1 c_2 c_3 c_4 H_{1234}(\mathbf{c})$ is $\mathcal{C}^1$!

$$(\mathrm{CH}^{[\boldsymbol{\sigma}]}) \qquad \begin{cases} \partial_t c_i = M_0\, \Delta \left(-\sum_j \alpha_{ij}^{[\boldsymbol{\sigma}]} \mu_j \right), \\ \mu_i = \dfrac{12}{\varepsilon} \dfrac{\partial F^{[\boldsymbol{\sigma}]}}{\partial c_i}(\mathbf{c}) + \dfrac{3}{4} \varepsilon \sum_{j \neq i} \sigma_{ij} \Delta c_j. \end{cases}$$

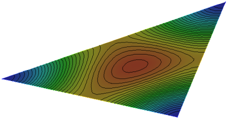
PROPOSITION

Assuming the coercivity condition (C1), *the system satisfies the energy dissipation equality*

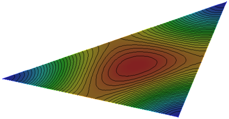
$$\frac{d}{dt} \mathcal{F}_\varepsilon^{[\boldsymbol{\sigma}]} + M_0 \underbrace{\sum_{i,j} -\alpha_{ij}^{[\boldsymbol{\sigma}]} \left(\nabla \mu_i, \nabla \mu_j \right)}_{\geq 0} = 0.$$

Isolines of potentials on the Gibbs simplex

Consistent



Non-consistent (with $H_\bullet = 0$)

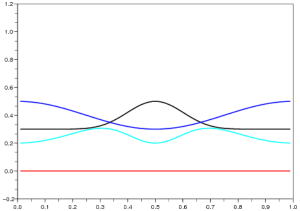


1D numerical simulations

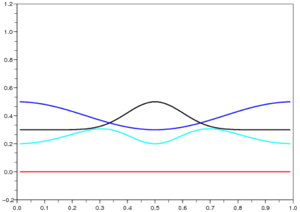
We choose $c_4 \equiv 0$ at the initial time.

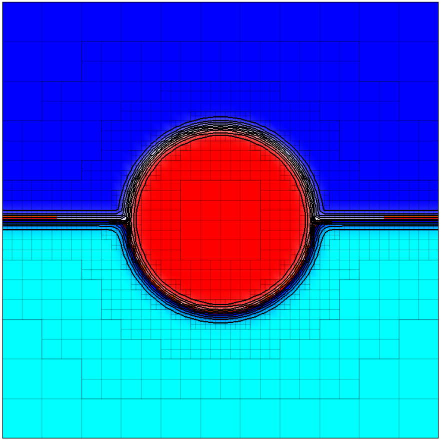
$$\boldsymbol{\sigma} = \begin{pmatrix} 0 & 1 & 0.9 & 1.4 \\ 1 & 0 & 0.6 & 1 \\ 0.9 & 0.6 & 0 & 1 \\ 1.4 & 1 & 1 & 0 \end{pmatrix}.$$

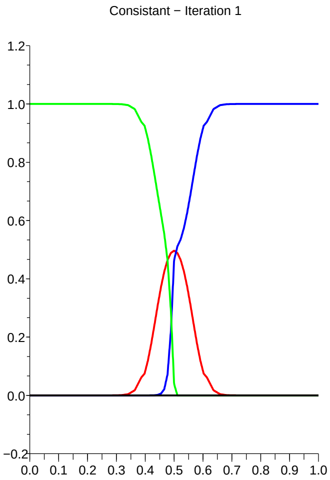
Consistent potential



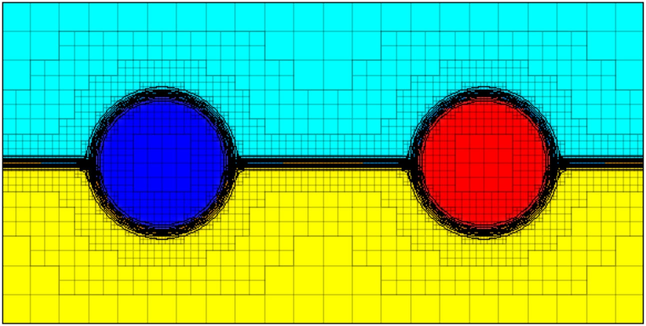
Non-consistent potential (that is $H_\bullet = 0$)







At a given Δt, the computation blows up for a non-consistent potential



$\sigma_{ij} = 0.05$

$\rho_1 = 1$

$\rho_2 = 1000$

$\rho_3 = 1100$

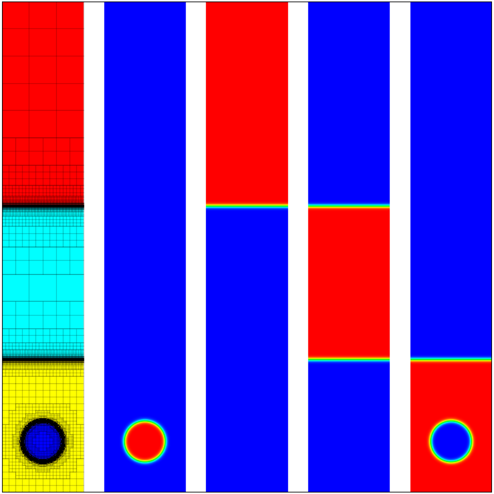
$\rho_4 = 1200$

$\mu_1 = 10^{-4}$

$\mu_2 = 0.1$

$\mu_3 = 0.01$

$\mu_4 = 10^{-3}$



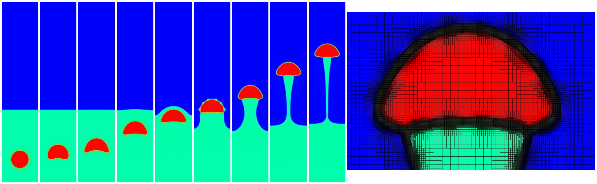
1. Introduction
2. The two-phase Cahn-Hilliard equation revisited
3. The consistency issue for three-phase CH systems
4. Construction of consistent n-phase Cahn-Hilliard systems
5. Few words about numerics
6. Conclusion

- COUPLING WITH THE NAVIER-STOKES SYSTEM
  We mainly use $\mathbb{P}^2/\mathbb{P}^1$ or $\mathbb{Q}^2/\mathbb{Q}^1$ element for (u, p) and $\mathbb{P}^1$ or $\mathbb{Q}^1$ for (c_i, μ_i).
  - Projection method (velocity prediction, pressure correction) to solve the Navier-Stokes system.
  - An unconditionally stable and fully uncoupled CH / NS method.
    (Minjeaud, '12)

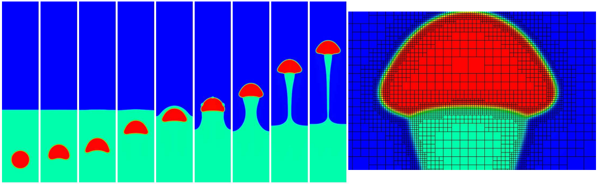
- COUPLING WITH THE NAVIER-STOKES SYSTEM
- ADAPTIVE LOCAL REFINEMENT

based on **conforming** approximation spaces : CHARMS method.

$$h_{int} = \frac{\varepsilon}{4}$$



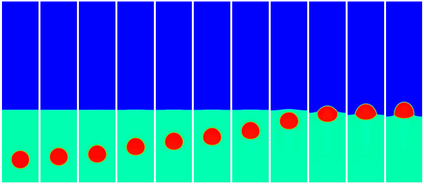
$$h_{int} = \varepsilon$$



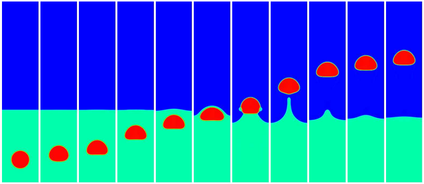
- COUPLING WITH THE NAVIER-STOKES SYSTEM
- ADAPTIVE LOCAL REFINEMENT
- SUITABLE TIME DISCRETISATION FOR CAHN-HILLIARD SYSTEMS
  - Explicit or convex-concave schemes are very robust but inaccurate.
  - Implicit schemes are much more accurate but lead to instabilities.
  - $\rightsquigarrow$ Development and analysis of adapted semi-implicit schemes.

(B.-Minjeaud, '08)

CC scheme



SImpl scheme



- Coupling with the Navier-Stokes system
- Adaptive local refinement
- Suitable time discretisation for Cahn-Hilliard systems
- But also ...
  - Multigrid solvers.
  - Outflow boundary conditions.

1 Introduction

2 The two-phase Cahn-Hilliard equation revisited

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5 Few words about numerics

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SUMMARY AND COMMENTS

- We build n-phase CH systems which are consistent with 2-phase systems.
- Suitable for phase-field modelling through a coupling with the NS equations.

- Well-posedness of such systems can be shown with suitable assumptions (for the three-phase case, see **(B.-Lapuerta '06)**)
- The overall strategy can be extended to two-phase potentials other than $f(c) = c^2(1-c)^2$ provided that

$$f(c) = f(1-c), \quad \forall c,$$

$$f'(0) = 0.$$

OPEN PROBLEMS

- What to do when the coercivity condition is not satisfied (even for $n = 3$) ?
- Numerics : how to solve efficiently the system with the singular terms $H_\bullet$?