Numerical methods for the simulation of a diffuse interface model for three-phase flows

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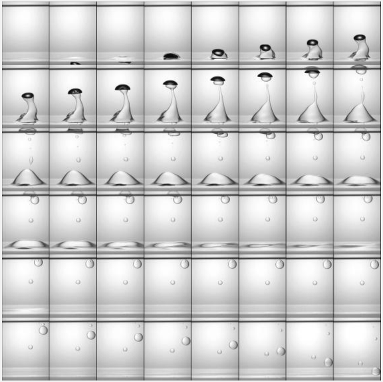
Regensburg, February 14, 2011

In the context of nuclear safety



Air bubble crossing a water/silicon interface.

Cranga, 02

- Three immiscible phases,
- No phase change,
- Compressibility of the phases can be neglected,
- Important densities ratio,
- Three different surface tensions,
- 3D flow without symmetry
- Topological changes of the interfaces.

1. A three-phase Cahn-Hilliard/Navier-Stokes model
2. Discretization of the Cahn-Hilliard system
3. Coupling with the Navier-Stokes system
4. Adaptive local refinement
5. Parameters influence - Benchmark - Numerical illustrations

1. A three-phase Cahn-Hilliard/Navier-Stokes model
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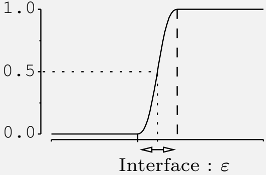
Principle

- Interfaces have small but positive thickness :

> The interface thickness $\varepsilon > 0$ is a parameter of the model.

- Order parameters (phase fields) :
  - Three **smooth** functions c_i, (volume fractions)
  - There are related through the relationship $c_1 + c_2 + c_3 = 1, \forall t, \forall x$.

$$\begin{cases} c_i(x) = 1, & \text{for } x \in \text{phase } i, \\ 0 < c_i(x) < 1, & \text{for } x \in \text{interface } i/j, \\ c_i(x) = 0, & \text{for } x \notin \text{phase } i. \end{cases}$$



The given physical parameters

- The densities ϱ_i and the viscosities η_i.
- The **three surface tensions** σ_{12}, σ_{13} and σ_{23}.

The two-phase case

$$\mathcal{F}^{\text{diph}}_{\sigma,\varepsilon}(c) = \int_\Omega \left(12\frac{\sigma}{\varepsilon} c^2(1-c)^2 + \frac{3}{4}\sigma\varepsilon\, |\nabla c|^2 \right) dx$$

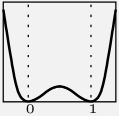
1D Equilibrium : $c_{eq}(x) = \dfrac{1+\tanh(2x/\varepsilon)}{2}$ and $\mathcal{F}^{\text{diph}}_{\sigma,\varepsilon}(c_{eq}) = \sigma$.

▶ Ansatz for the **free energy** functional :

$$\mathcal{F}^{\text{triph}}_{\mathbf{\Sigma},\varepsilon}(\mathbf{c}) = \int_\Omega \frac{12}{\varepsilon} F(\mathbf{c}) + \frac{3}{8}\varepsilon \sum_{i=1}^{3} \Sigma_i |\nabla c_i|^2 \, dx.$$

with $\mathbf{c} = (c_1, c_2, c_3)$.

- **Bulk contribution** $F(\mathbf{c}) \sim$ **triple-well structure** :
  - It accounts for the immiscibility of the phases,
  - The minimal value of this term is achieved when the interface thickness is 0.



- **Capillary terms** $|\nabla c_i|^2$:
  - They penalize the thickness of the interface.
  - An interface of thickness $\varepsilon > 0$ "costs" $1/\varepsilon$.
- **Competition between the two terms** :
  - Critical points of the energy are constituted of diffuse interfaces with typical thickness $\sim \varepsilon$.

▶ How to determine F and $\mathbf{\Sigma} = (\Sigma_i)_i$?

▶ What is the suitable gradient flow associated with $\mathcal{F}^{\text{triph}}_{\mathbf{\Sigma},\varepsilon}$?

(B.-Lapuerta, '06)

Ansatz for the energy :

$$\mathcal{F}^{\text{triph}}_{\mathbf{\Sigma},\varepsilon}(\mathbf{c}) = \int_\Omega \frac{12}{\varepsilon} F(\mathbf{c}) + \frac{3}{8}\varepsilon\Sigma_1|\nabla c_1|^2 + \frac{3}{8}\varepsilon\Sigma_2|\nabla c_2|^2 + \frac{3}{8}\varepsilon\Sigma_3|\nabla c_3|^2\,dx.$$

The potential F and the coefficients $(\Sigma_1, \Sigma_2, \Sigma_3)$ are undetermined yet.

We do not impose *a priori* that $\Sigma_i > 0, \forall i$

(B.-Lapuerta, '06)

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Evolution of the system = gradient flow in $(H^1)'$ of the energy

▶ Preserve the constraints : volume conservation and $c_1 + c_2 + c_3 \equiv 1$.

$$\begin{cases} \dfrac{\partial c_i}{\partial t} = \text{div}\,(M_i \nabla \mu_i)\,, \\[2ex] \mu_i = \dfrac{\delta \mathcal{F}^{\text{triph}}_{\mathbf{\Sigma},\varepsilon}}{\delta c_i} + \beta = -\dfrac{3}{4}\varepsilon\Sigma_i\Delta c_i + \dfrac{12}{\varepsilon}\partial_i F(\mathbf{c}) + \beta, \end{cases}$$

where β is a *Lagrange multiplier*, unknown for the moment.

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where β is a *Lagrange multiplier*, unknown for the moment.

▶ For the constraint $c_1 + c_2 + c_3 \equiv 1$ to hold, we need that :

$$M_1\Sigma_1 = M_2\Sigma_2 = M_3\Sigma_3 \equiv M_0 \implies \Sigma_i \neq 0, \forall i.$$

$$\beta = -\sum_{i=1}^{3} \frac{4\Sigma_T}{\varepsilon\Sigma_i}\partial_i F(\mathbf{c}), \text{ with } \frac{1}{\Sigma_T} = \frac{1}{3}\left(\frac{1}{\Sigma_1} + \frac{1}{\Sigma_2} + \frac{1}{\Sigma_3}\right).$$

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Evolution of the system = gradient flow in $(H^1)'$ of the energy

(CH)

$$\begin{cases} \dfrac{\partial c_i}{\partial t} = \operatorname{div}\left(\dfrac{M_0}{\Sigma_i}\nabla\mu_i\right), \ \forall i \in \{1,2,3\} \\ \mu_i = \dfrac{4\Sigma_T}{\varepsilon}\displaystyle\sum_{j\neq i}\left(\frac{1}{\Sigma_j}\left(\partial_i F(\mathbf{c}) - \partial_j F(\mathbf{c})\right)\right) - \frac{3}{4}\varepsilon\Sigma_i\Delta c_i. \end{cases}$$

with

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

and Neuman BC for $\mathbf{c}$ and $\boldsymbol{\mu}$.

(B.-Lapuerta, '06)

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First properties

- *A posteriori :* we can write a system for c_1 and c_2 only
- Formally, the energy satisfies the following equation

$$\frac{d}{dt}\mathcal{F}^{\text{triph}}_{\boldsymbol{\Sigma},\varepsilon}(\mathbf{c}) + \int_\Omega \sum_{i=1}^{3} \frac{M_0}{\Sigma_i}|\nabla\mu_i|^2 \, dx = 0.$$

Assumptions

1. $\Sigma_i + \Sigma_j > 0, \forall i \neq j$, and $\Sigma_1\Sigma_2 + \Sigma_1\Sigma_3 + \Sigma_2\Sigma_3 > 0$.
2. $F(\mathbf{c}) \geq 0$ for any $\mathbf{c} \in \mathcal{S}$.

$$\mathcal{F}^{\text{triph}}_{\boldsymbol{\Sigma},\varepsilon}(\mathbf{c}) = \int_\Omega \underbrace{\frac{12}{\varepsilon}F(\mathbf{c})}_{\geq 0 \;\Longleftarrow\; ❷} + \underbrace{\frac{3}{8}\varepsilon\Sigma_1|\nabla c_1|^2 + \frac{3}{8}\varepsilon\Sigma_2|\nabla c_2|^2 + \frac{3}{8}\varepsilon\Sigma_3|\nabla c_3|^2}_{\geq 0 \;\Longleftarrow\; ❶} dx$$

$$\frac{d}{dt}\mathcal{F}^{\text{triph}}_{\boldsymbol{\Sigma},\varepsilon}(\mathbf{c}) + \int_\Omega \underbrace{\sum_{i=1}^{3} \frac{M_0}{\Sigma_i}|\nabla \mu_i|^2}_{= \sum_{i=1}^{3} M_0\Sigma_i \left|\frac{\nabla \mu_i}{\Sigma_i}\right|^2 \geq 0 \;\Longleftarrow\; ❶} dx = 0,$$

ASSUMPTIONS

1. $\Sigma_i + \Sigma_j > 0, \forall i \neq j$, and $\Sigma_1\Sigma_2 + \Sigma_1\Sigma_3 + \Sigma_2\Sigma_3 > 0$.
2. $F(\mathbf{c}) \geq 0$ for any $\mathbf{c} \in \mathcal{S}$.
3. There exists $B > 0$ such that
$$|F''(\mathbf{c})| \quad \leq \quad B(1+|\mathbf{c}|^{p-2}), \quad \forall \mathbf{c} \in \mathcal{S},$$
with $p = 6$ in 3D, and $2 \leq p < +\infty$ in 2D.
4. There exists $D \geq 0$ such that
$$\big(F''(\mathbf{c})\xi, \xi\big) \geq -D\,(1 + |\mathbf{c}|^q)\,|\xi|^2, \quad \forall \mathbf{c} \in \mathcal{S}, \forall \xi \in \mathbb{R}^3,$$
where $1 \leq q < 4$ in 3D and $1 \leq q < +\infty$ in 2D.

THEOREM

Under assumptions 1 - 4, *for any* $\mathbf{c}^0 \in (\mathrm{H}^1(\Omega))^3$ *such that* $\sum_{i=1}^3 c_i^0(x) = 1$ *for a.e.* $x \in \Omega$, *there exists a unique global solution* $(\mathbf{c}, \boldsymbol{\mu})$ *of* (CH) *such that*

$$\sum_{i=1}^{3} c_i(t,x) = 1, \text{ for almost every } (t,x) \in [0,+\infty[\times\Omega,$$

$$\mathbf{c} \in \mathcal{C}_b^0([0,+\infty[;(\mathrm{H}^1(\Omega))^3) \cap \mathrm{L}^2_{loc}(0,+\infty;(\mathrm{H}^3(\Omega))^3),$$
$$\boldsymbol{\mu} \in \mathrm{L}^2(0,+\infty;(\mathrm{H}^1(\Omega))^3).$$

Principle

The three-phase model has to account suitably for two-phase situations.

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Definition

The model is said to be consistent *with the two-phase Cahn-Hilliard models if and only if*

(P1) *When there is no phase i in the system, the free energy should be the one of the two-phase model.*

$$\mathcal{F}^{triph}_{\mathbf{\Sigma},\varepsilon}(c, 1-c, 0) = \mathcal{F}^{diph}_{\sigma_{12},\varepsilon}(c), \quad \forall c \in \mathrm{H}^1(\Omega),$$
$$\mathcal{F}^{triph}_{\mathbf{\Sigma},\varepsilon}(c, 0, 1-c) = \mathcal{F}^{diph}_{\sigma_{13},\varepsilon}(c), \quad \forall c \in \mathrm{H}^1(\Omega),$$
$$\mathcal{F}^{triph}_{\mathbf{\Sigma},\varepsilon}(0, c, 1-c) = \mathcal{F}^{diph}_{\sigma_{23},\varepsilon}(c), \quad \forall c \in \mathrm{H}^1(\Omega).$$

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- **(P1)** *When there is no phase i in the system, the free energy should be the one of the two-phase model.*
- **(P2)** *Any solution $\mathbf{c}$ of* (CH) *should satisfy*

$$c_i(0) = 0 \Longrightarrow c_i(t) = 0, \ \forall t \geq 0.$$

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(P2) *Any solution* $\mathbf{c}$ *of* (CH) *should satisfy*

$$c_i(0) = 0 \Longrightarrow c_i(t) = 0, \ \forall t \geq 0.$$

Theorem

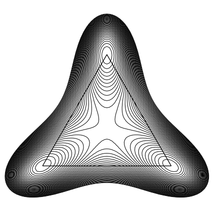
Let σ_{12}, σ_{13}, σ_{23} *be given. The three-phase model defined before is algebraically consistent if and only if*

$$\boxed{\Sigma_i = \sigma_{ij} + \sigma_{ik} - \sigma_{jk}, \ \forall i \in \{1, 2, 3\},}$$

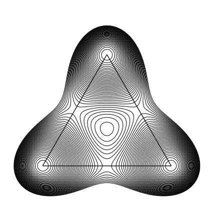
There exists a function $\Lambda : \mathbb{R}^3 \mapsto \mathbb{R}$ *such that*

$$F(\mathbf{c}) = \sigma_{12} c_1^2 c_2^2 + \sigma_{13} c_1^2 c_3^2 + \sigma_{23} c_2^2 c_3^2 + c_1 c_2 c_3 (\Sigma_1 c_1 + \Sigma_2 c_2 + \Sigma_3 c_3) + c_1^2 c_2^2 c_3^2 \, \Lambda(\mathbf{c}), \ \forall \mathbf{c} \in \mathbb{R}^3.$$

Contour lines of F on the Gibbs triangle



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



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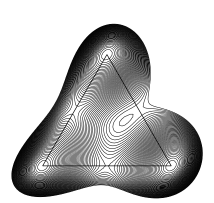
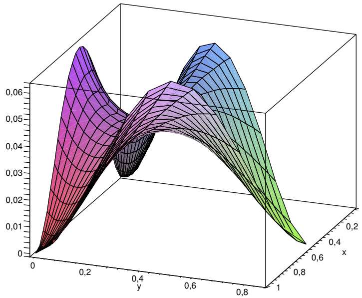


$\Sigma_1 = 6, \Sigma_2 = 8, \Sigma_3 = 4,$
$F = F_0$

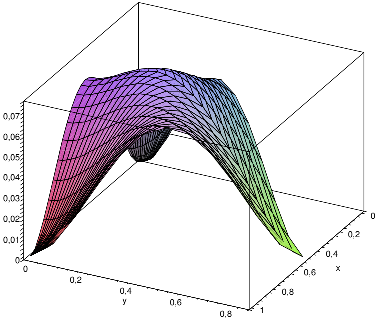
- $\tilde{F}_0(\mathbf{c}) \stackrel{\text{def}}{=} \sigma_{12}c_1^2c_2^2 + \sigma_{13}c_1^2c_3^2 + \sigma_{23}c_2^2c_3^2$ $\Longleftarrow$ Non-consistent
- $F_0(\mathbf{c}) \stackrel{\text{def}}{=} \tilde{F}_0(\mathbf{c}) + c_1c_2c_3(\Sigma_1 c_1 + \Sigma_2 c_2 + \Sigma_3 c_3)$ $\Longleftarrow$ Consistent

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



Non consistent model

$$F = \widetilde{F}_0$$



Consistent model

$$F = F_0$$

In **(Kim-Lowengrub '05, Kim-Kang '09)**, we can find the following model

$$\begin{cases} \dfrac{\partial c_1}{\partial t} = \operatorname{div}\left(M_0 \nabla \mu_1\right), \\ \dfrac{\partial c_2}{\partial t} = \operatorname{div}\left(M_0 \nabla \mu_2\right), \\ \mu_1 = \dfrac{1}{\varepsilon}\Big(\partial_1 \tilde{F}_0(\mathbf{c}) - \partial_3 \tilde{F}_0(\mathbf{c})\Big) - \varepsilon \Delta c_1 - \dfrac{\varepsilon}{2}\Delta c_2, \\ \mu_2 = \dfrac{1}{\varepsilon}\Big(\partial_2 \tilde{F}_0(\mathbf{c}) - \partial_3 \tilde{F}_0(\mathbf{c})\Big) - \dfrac{\varepsilon}{2}\Delta c_1 - \varepsilon \Delta c_2, \end{cases}$$

TWO DRAWBACKS OF THIS MODEL FOR OUR PURPOSES :

- Lack of symmetry
  The equation satisfied by the third component $c_3 = 1 - c_1 - c_2$ is not formally the same as the one for c_1, and c_2.

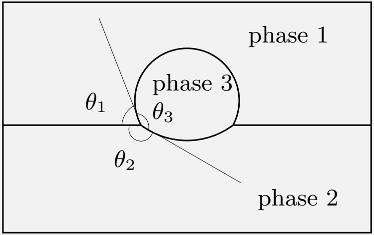
  The solution depends on the numbering of the phases.

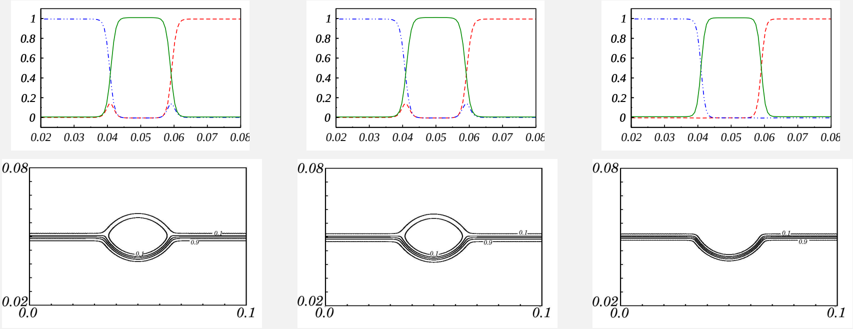
- Does not respect two-phase situations

  If $c_i \equiv 0$ at $t = 0$, then we may have $c_i(t) \neq 0$, for $t > 0$.

YOUNG'S LAW

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





(Kim et al.) | our model with $F = \widetilde{F}_0$ | our model with $F = F_0$

CAHN-HILLIARD SYSTEM

$$\begin{cases} \dfrac{\partial c_i}{\partial t} = \operatorname{div}\left(\dfrac{M_0}{\Sigma_i}\nabla \mu_i\right), \quad \forall i = 1,2,3, \\ \mu_i = \dfrac{4\Sigma_T}{\varepsilon}\displaystyle\sum_{j\neq i}\left(\dfrac{1}{\Sigma_j}\left(\partial_i F(\mathbf{c}) - \partial_j F(\mathbf{c})\right)\right) - \dfrac{3}{4}\varepsilon\Sigma_i\Delta c_i, \quad \forall i = 1,2,3, \end{cases}$$

INCOMPRESSIBLE NAVIER-STOKES SYSTEM

$$\begin{cases} \dfrac{\partial}{\partial t}(\varrho\mathbf{u}) + \operatorname{div}\left(\varrho\mathbf{u}\otimes\mathbf{u}\right) \\ \qquad - \operatorname{div}\left(2\eta D(\mathbf{u})\right) + \nabla p = \varrho\mathbf{g}, \\ \operatorname{div}\mathbf{u} = 0. \end{cases}$$

CAHN-HILLIARD SYSTEM

$$\begin{cases} \dfrac{\partial c_i}{\partial t} + \mathbf{u} \cdot \nabla c_i = \operatorname{div}\left(\dfrac{M_0}{\Sigma_i} \nabla \mu_i\right), \quad \forall i = 1,2,3, \\ \mu_i = \dfrac{4\Sigma_T}{\varepsilon} \displaystyle\sum_{j \neq i} \left(\dfrac{1}{\Sigma_j} \left(\partial_i F(\mathbf{c}) - \partial_j F(\mathbf{c})\right)\right) - \dfrac{3}{4} \varepsilon \Sigma_i \Delta c_i, \quad \forall i = 1,2,3, \end{cases}$$

INCOMPRESSIBLE NAVIER-STOKES SYSTEM

$$\begin{cases} \left(\varrho \dfrac{\partial \mathbf{u}}{\partial t} + \dfrac{1}{2} \mathbf{u} \dfrac{\partial \varrho}{\partial t}\right) + \left((\varrho \mathbf{u} \cdot \nabla)\mathbf{u} + \dfrac{\mathbf{u}}{2} \operatorname{div}(\varrho \mathbf{u})\right) \\ \qquad - \operatorname{div}\,(2\eta D(\mathbf{u})) + \nabla p = \varrho \mathbf{g} \; + \displaystyle\sum_{i=1}^{3} \mu_i \nabla c_i, \\ \operatorname{div} \mathbf{u} = 0. \end{cases}$$

$\mathbf{c} \mapsto \varrho(\mathbf{c})$ and $\mathbf{c} \mapsto \eta(\mathbf{c})$ are given *a priori.*

ALTERNATIVE STRATEGIES

(Lowengrub-Truskinovsky '98) (B. '02)

(Ding-Spelt-Shu '07) (Abels-Garcke-Grün '10)

▶ Kinetic energy evolution

$$\frac{d}{dt}\int_{\mathcal{B}_t}\frac{1}{2}\varrho|\mathbf{u}|^2\,dx=\int_{\mathcal{B}_t}\frac{\partial}{\partial t}\left(\frac{1}{2}\varrho|\mathbf{u}|^2\right)+\operatorname{div}\left(\frac{1}{2}\varrho|\mathbf{u}|^2\mathbf{u}\right)\,dx$$
$$=\int_{\mathcal{B}_t}\left[\left(\varrho\frac{\partial\mathbf{u}}{\partial t}+\frac{1}{2}\mathbf{u}\frac{\partial\varrho}{\partial t}\right)+\left((\varrho\mathbf{u}\cdot\nabla)\mathbf{u}+\frac{\mathbf{u}}{2}\operatorname{div}(\varrho\mathbf{u})\right)\right]\cdot\mathbf{u}\,dx,$$

where $\mathcal{B}_t$ is a material volume evolving with the flow $\mathbf{u}$.

▶ Inertia terms

$$\left(\varrho\frac{\partial\mathbf{u}}{\partial t}+\frac{1}{2}\mathbf{u}\frac{\partial\varrho}{\partial t}\right)+\left((\varrho\mathbf{u}\cdot\nabla)\mathbf{u}+\frac{\mathbf{u}}{2}\operatorname{div}(\varrho\mathbf{u})\right)$$
$$=\frac{\partial}{\partial t}(\varrho\mathbf{u})+\operatorname{div}(\varrho\mathbf{u}\otimes\mathbf{u})\qquad\underbrace{-\frac{1}{2}\left[\frac{\partial\varrho}{\partial t}+\operatorname{div}(\varrho\mathbf{u})\right]\mathbf{u}}_{\sim C(\sum_i\Delta\mu_i)}$$

⇝ The momentum equation is thus modified inside interfaces.

(Guermond-Quartapelle, ’00) (Shen et al., ’10)

Boundary conditions

- $\nabla c_i \cdot n = 0$ on $\partial\Omega$
- $\nabla \mu_i \cdot n = 0$ on $\partial\Omega$ (no diffusion across the boundary of the domain)
- no-slip conditions $\mathbf{u} = 0$ on $\partial\Omega$

Properties

- **Capillary forces** are naturally given by a volumic approximation

$$\sum_{i=1}^{3} \mu_i \nabla c_i \underset{\varepsilon \to 0}{\sim} \sum_{ij} \sigma_{ij} \kappa_{ij} \mathbf{n}_{ij} \delta_{ij}$$

- Formal evolution of the total energy :

$$\frac{d}{dt}\left[\int_\Omega \frac{1}{2} \varrho |\mathbf{u}|^2 \, dx + \mathcal{F}^{\text{triph}}_{\mathbf{\Sigma},\varepsilon}(\mathbf{c}) \right] + \int_\Omega 2\eta |D\mathbf{u}|^2 \, dx + \int_\Omega M_0 |\nabla \mu|^2 \, dx = \int_\Omega \varrho \mathbf{g} \cdot \mathbf{u} \, dx.$$

- **Volume conservation** of each phase :

$$\int_\Omega c_i(t,\cdot)\, dx = \int_\Omega c_i(0,\cdot)\, dx, \quad \forall t, \quad \forall i \in \{1,2,3\}.$$

- Conforming finite element $\mathbb{P}_1$ or $\mathbb{Q}_1$ for $\mathbf{c}$ and $\boldsymbol{\mu}$,
- LBB stable finite elements $\mathbb{P}_2/\mathbb{P}_1$ or $\mathbb{Q}_2/\mathbb{Q}_1$ for $(\mathbf{u}, p)$,
- **Semi-implicit** time discretization for (CH), **(Part 2)**
- **Unconditionally stable uncoupled** resolution of (CH/NS),
- **Incremental projection method** for (NS), **(Part 3)**
- **Adaptive local refinement conforming** method **(Part 4)**
- **Benchmarking - Parameters influence ...** **(Part 5)**

The numerical platform **PELICANS**

Plate-forme Evolutive de LIbrairies de Composants pour l'Analyse Numérique et la Simulation

- **Numerical kernel** for industrial codes at IRSN,
- C++ Library for developing scientific computation softwares.
- Free OpenSource project

licence	CeCILL-C, French version of LGPL (`http://www.cecill.info`)
	`https://gforge.irsn.fr/gf/project/pelicans`

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(B.-Minjeaud, '11)

Time discretization

$$\begin{cases} \dfrac{c_i^{n+1}-c_i^n}{\Delta t} = \operatorname{div}\left(\dfrac{M_0(c_i^n)}{\Sigma_i}\nabla\mu_i^{n+1}\right), \\ \mu_i^{n+1} = \dfrac{4\Sigma_T}{\varepsilon}\displaystyle\sum_{j\neq i}\left(\dfrac{1}{\Sigma_j}\left(d_i^F(\mathbf{c}^{n+1},\mathbf{c}^n) - d_j^F(\mathbf{c}^{n+1},\mathbf{c}^n)\right)\right) - \dfrac{3}{4}\varepsilon\Sigma_i\Delta c_i^{n+\beta}, \end{cases}$$

with $d_i^F \sim \partial_i F$, $\quad c_i^{n+\beta} = (1-\beta)c_i^n + \beta c_i^{n+1}$ $\quad$ and $\quad \frac{1}{2} \leqslant \beta \leqslant 1.$

Conforming Lagrange finite elements in space

Find $(\mathbf{c}_h^{n+1}, \boldsymbol{\mu}_h^{n+1}) \in (\mathcal{V}_h^c)^3 \times (\mathcal{V}_h^\mu)^3$ such that $\forall \nu_h^\mu \in \mathcal{V}_h^\mu, \forall \nu_h^c \in \mathcal{V}_h^c,$

$$\begin{cases} \displaystyle\int_\Omega \frac{c_{ih}^{n+1}-c_{ih}^n}{\Delta t}\nu_h^\mu\,dx = -\int_\Omega \frac{M_0(c_{ih}^n)}{\Sigma_i}\nabla\mu_{ih}^{n+1}\cdot\nabla\nu_h^\mu\,dx, \\ \displaystyle\int_\Omega \mu_{ih}^{n+1}\nu_h^c\,dx = \int_\Omega \frac{4\Sigma_T}{\varepsilon}\sum_{j\neq i}\left(\frac{1}{\Sigma_j}\left(d_i^F(\mathbf{c}_h^{n+1},\mathbf{c}_h^n) - d_j^F(\mathbf{c}_h^{n+1},\mathbf{c}_h^n)\right)\right)\nu_h^c\,dx \\ \displaystyle\qquad\qquad + \int_\Omega \frac{3}{4}\Sigma_i\varepsilon\nabla c_{ih}^{n+\beta}\cdot\nabla\nu_h^c\,dx. \end{cases}$$

- For any $(\mathbf{c}_h^{n+1}, \mu_h^{n+1})$ solution of the discrete problem, we have :

$$\mathcal{F}_{\mathbf{\Sigma},\varepsilon}^{\text{triph}}(\mathbf{c}_h^{n+1}) - \mathcal{F}_{\mathbf{\Sigma},\varepsilon}^{\text{triph}}(\mathbf{c}_h^{n}) + \Delta t \int_\Omega \sum_{i=1}^{3} \frac{M_0(c_{ih}^n)}{\Sigma_i} \left|\nabla \mu_{ih}^{n+1}\right|^2 dx$$
$$+ (2\beta - 1) \int_\Omega \frac{3}{8}\varepsilon \sum_{i=1}^{3} \Sigma_i \left|\nabla (c_{ih}^{n+1} - c_{ih}^n)\right|^2 dx$$
$$= \frac{12}{\varepsilon} \int_\Omega \left[F(\mathbf{c}_h^{n+1}) - F(\mathbf{c}_h^n) - \mathbf{d}^F(\mathbf{c}_h^{n+1}, \mathbf{c}_h^n) \cdot \left(\mathbf{c}_h^{n+1} - \mathbf{c}_h^n\right)\right] dx,$$

where $\mathbf{d}^F(x,y)$ stands for $(d_i^F(x,y))_{i=1,2,3}$.

- The last two terms of the left-hand side are non-negative, provided that

$$\beta \geq 1/2,$$

$$\Sigma_1 + \Sigma_2 > 0,\ \Sigma_1 + \Sigma_3 > 0,\ \Sigma_2 + \Sigma_3 > 0,$$
$$\Sigma_1\Sigma_2 + \Sigma_1\Sigma_3 + \Sigma_2\Sigma_3 > 0.$$

Theorem (Existence and convergence)

We assume that the following inequality holds

$$F(\mathbf{c}_h^{n+1}) - F(\mathbf{c}_h^n) - \mathbf{d}^F(\mathbf{c}_h^{n+1}, \mathbf{c}_h^n) \cdot \left(\mathbf{c}_h^{n+1} - \mathbf{c}_h^n\right) \leqslant 0.$$

Then,

- *There exists at least one solution to the discrete problem.*
- *The sequence of approximate solutions converge towards a weak solution of the problem.*

- **Existence** : Brouwer degree theory.
- **Convergence** : Compactness results.

QUESTION : Are there discretizations satisfying

$$F(\mathbf{c}_h^{n+1}) - F(\mathbf{c}_h^n) - \mathbf{d}^F(\mathbf{c}_h^{n+1}, \mathbf{c}_h^n) \cdot \left(\mathbf{c}_h^{n+1} - \mathbf{c}_h^n\right) \leqslant 0 \quad ?$$

- Let us concentrate on

$$F(\mathbf{c}) = F_0(\mathbf{c}) = \sigma_{12} c_1^2 c_2^2 + \sigma_{13} c_1^2 c_3^2 + \sigma_{23} c_2^2 c_3^2 + c_1 c_2 c_3 (\Sigma_1 c_1 + \Sigma_2 c_2 + \Sigma_3 c_3)$$

- Three possible methods
  - Implicit discretization
  - Convex-concave discretization
  - Semi-implicit discretization

$$d_i^{F_0}(\mathbf{c}^{n+1}, \mathbf{c}^n) = \partial_i F_0(\mathbf{c}^{n+1})$$

- Since F_0 is not convex, we **do not have** the property

$$F_0(\mathbf{c}_h^{n+1}) - F_0(\mathbf{c}_h^n) - \mathbf{d}^{F_0}(\mathbf{c}_h^{n+1}, \mathbf{c}_h^n) \cdot \left(\mathbf{c}_h^{n+1} - \mathbf{c}_h^n\right) \leqslant 0.$$

- Nevertheless, it can be shown that

- **In the case when** $\forall i,\ \Sigma_i > 0$ **:**
  - ⇝ We have existence for any Δt, since the concave part of F_0 is low degree,
  - ⇝ We have convergence, thanks to numerical diffusion

$$F_0(\mathbf{c}_h^{n+1}) - F_0(\mathbf{c}_h^n) - \mathbf{d}^{F_0}(\mathbf{c}_h^{n+1}, \mathbf{c}_h^n) \cdot \left(\mathbf{c}_h^{n+1} - \mathbf{c}_h^n\right) \leqslant \sum_{i=1}^{3} \frac{\Sigma_i}{4} \left|c_{hi}^{n+1} - c_{hi}^n\right|^2.$$

- **In the case when** $\exists i,\ \Sigma_i < 0$ **:**
  - ⇝ We do not know if the approximate solution exists.
  - ⇝ **Serious convergence problems** of the Newton algorithm.

- **Idea :** **(Eyre, '98)**
  - We write F_0 as a **sum** of a **convex part** and a **concave part**,
  - **Implicit discretization** for the **convex** part of F_0,
  - **Explicit discretization** of the **concave** part of F_0.
- If we have $F_0 = F_0^+ + F_0^-$ we take

$$\mathbf{d}^{F_0}(\mathbf{c}_h^{n+1}, \mathbf{c}_h^n) = \nabla F_0^+(\mathbf{c}_h^{n+1}) + \nabla F_0^-(\mathbf{c}_h^n)$$

- For any $(\Sigma_i)_i$ such that $\Sigma_1\Sigma_2 + \Sigma_1\Sigma_3 + \Sigma_2\Sigma_3 > 0$, we have $\forall \Delta t > 0$,

$$F_0(\mathbf{c}_h^{n+1}) - F_0(\mathbf{c}_h^n) - \mathbf{d}^{F_0}(\mathbf{c}_h^{n+1}, \mathbf{c}_h^n) \cdot \left(\mathbf{c}_h^{n+1} - \mathbf{c}_h^n\right) \leqslant 0.$$

$\Longrightarrow$ **Existence and convergence** of approximate solutions.

(Kim-Kang-Lowengrub, '04)

▶ **Idea :** Build an approximation satisfying

$$F_0(\mathbf{c}^{n+1}) - F_0(\mathbf{c}^n) - \mathbf{d}^{F_0}(\mathbf{c}^{n+1},\mathbf{c}^n)\cdot(\mathbf{c}^{n+1}-\mathbf{c}^n) = 0$$

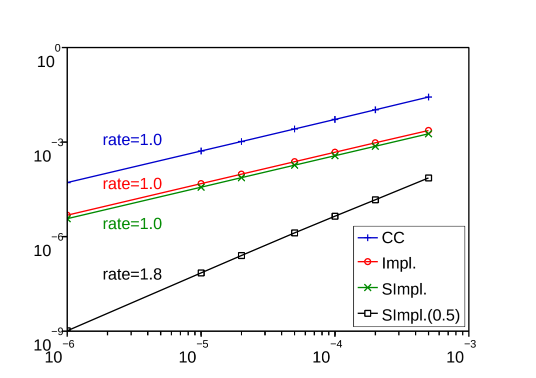
$$\begin{aligned} d_i^{F_0}(\mathbf{c}^{n+1},\mathbf{c}^n) = \quad & \frac{\Sigma_i}{4}\left[c_i^{n+1}+c_i^n\right]\left[(c_j^{n+1}+c_k^{n+1})^2+(c_j^n+c_k^n)^2\right] \\ & +\frac{\Sigma_j}{4}\left((c_j^{n+1})^2+(c_j^n)^2\right)\left(c_i^{n+1}+c_k^{n+1}+c_i^n+c_k^n\right) \\ & +\frac{\Sigma_k}{4}\left((c_k^{n+1})^2+(c_k^n)^2\right)\left(c_i^{n+1}+c_j^{n+1}+c_i^n+c_j^n\right) \end{aligned}$$

▶ **Existence ($\forall\Delta t$) and convergence** for any $(\Sigma_i)_i$ such that $\Sigma_1\Sigma_2+\Sigma_1\Sigma_3+\Sigma_2\Sigma_3>0$.

▶ The scheme is symmetric in $\mathbf{c}^n$ and $\mathbf{c}^{n+1}$ and thus is formally second order.

NOTATION : SImpl.(β) and SImpl.=SImpl.(1)

Convergence rate

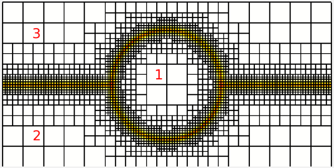


Norm of the error as a function of Δt.

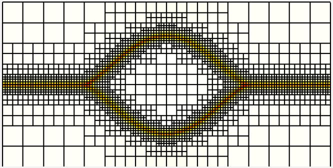
- ▶ Schemes CC, Impl. et SImpl. : first order
- ▶ Scheme SImpl.(0.5) : **second order**

$\Sigma_1 = 0.2,\ \Sigma_2 = \Sigma_3 = 1,\ \Lambda = 0.$

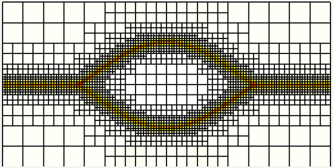
Evolution of the interface position



$t = 0$

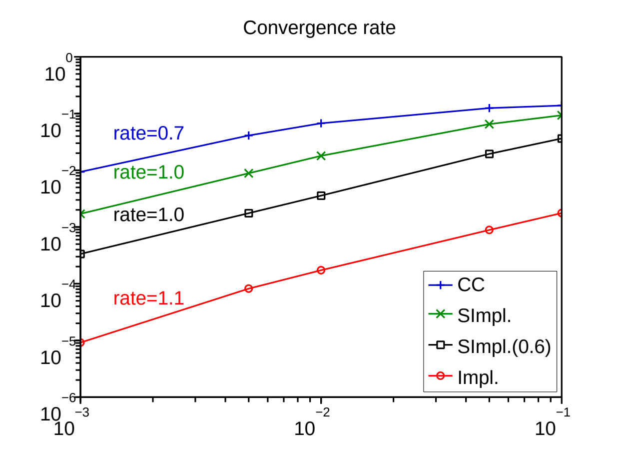


$t = 0.8$



$t = 1.8$

Reference solution $\overline{\mathbf{c}_h}$ computed with the Impl. scheme and $\Delta t = 5.10^{-4}$.



Norm of the error $|\mathbf{c}_h(t,\cdot) - \overline{\mathbf{c}_h}(t,\cdot)|_{L^2(\Omega)}$ at t=3.8 as a function of Δt.

▶ All the schemes are asymptotically first order but with different accuracies at a given time step.

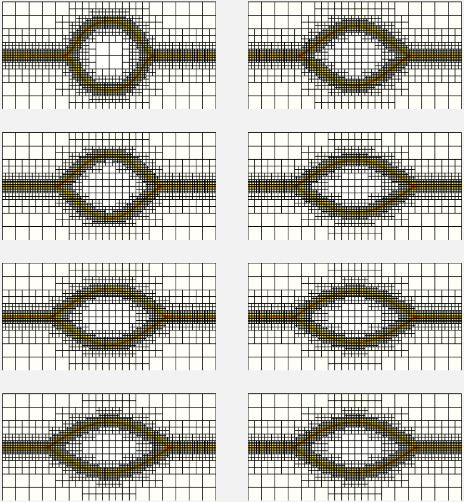
Influence of the scheme on the interface position

CC

SImpl.

SImpl.(0.6)

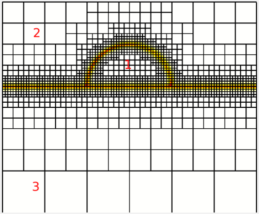
Impl.



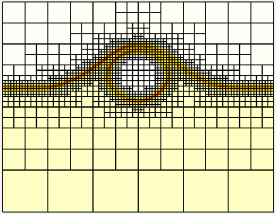
$\Delta t = 10^{-1}$ $\Delta t = 10^{-2}$

$\Sigma_1 = \Sigma_2 = 3,\ \Sigma_3 = -1,\ \Lambda = 7/3.$

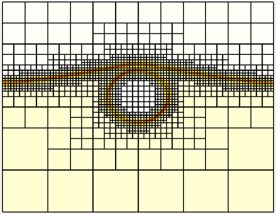
Evolution of the interface positions



$t = 0$



$t = 2$



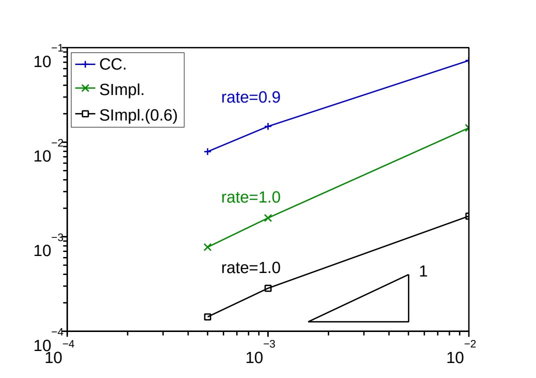
$t = 3$

Reference solution $\overline{\mathbf{c}_h}$ computed with SImpl. and $\Delta t = 10^{-3}$.

Iteration count for the Newton solver

Scheme \ Δt	10^{-1}	5.10^{-2}	10^{-2}	5.10^{-3}	10^{-3}	5.10^{-4}	10^{-4}
CC.	5	5	5	5	5	5	4
SImpl.	-	-	9	9	6	6	5
SImpl.(0.6)	-	-	29	-	7	6	5
Impl.	-	-	-	-	-	-	7

Convergence rate



Norm of the error $|\mathbf{c}_h(t,\cdot) - \overline{\mathbf{c}_h}(t,\cdot)|_{L^2(\Omega)}$ at t=3.8 as a function of Δt.

- First order for all the schemes but here also we observe very poor performance of the CC scheme.

1. A three-phase Cahn-Hilliard/Navier-Stokes model
2. Discretization of the Cahn-Hilliard system
3. Coupling with the Navier-Stokes system
4. Adaptive local refinement
5. Parameters influence - Benchmark - Numerical illustrations

(Minjeaud, '11)

CAHN-HILLIARD SYSTEM

$$\begin{cases} \dfrac{c_i^{n+1} - c_i^n}{\Delta t} + \begin{matrix}\textit{Transport} \\ \textit{term}\end{matrix} = \text{div}\left(\dfrac{M_0^n}{\Sigma_i} \nabla \mu_i^{n+1}\right), \\ \mu_i^{n+1} = D_i^F(\mathbf{c}^n, \mathbf{c}^{n+1}) - \dfrac{3}{4}\varepsilon \Sigma_i \Delta c_i^{n+\beta}. \end{cases}$$

NAVIER-STOKES SYSTEM

$$\begin{cases} \varrho^n \dfrac{\mathbf{u}^{n+1} - \mathbf{u}^n}{\Delta t} + \dfrac{1}{2} \dfrac{\varrho^{n+1} - \varrho^n}{\Delta t} \mathbf{u}^{n+1} + (\varrho^{n+1}\mathbf{u}^n \cdot \nabla)\mathbf{u}^{n+1} + \dfrac{\mathbf{u}^{n+1}}{2} \text{div}\,(\varrho^{n+1}\mathbf{u}^n) \\ \qquad - \text{div}\left(\eta^{n+1} D\mathbf{u}^{n+1}\right) + \nabla p^{n+1} = \begin{matrix}\textit{Capillary} \\ \textit{forces}\end{matrix} + \varrho^{n+1}\mathbf{g}, \\ \text{div}\,(\mathbf{u}^{n+1}) = 0. \end{cases}$$

At the continuous level : $\displaystyle\sum_{i=1}^{3}\big(\mathbf{u}\cdot\nabla c_i\big)\mu_i = \Big(\sum_{i=1}^{3}\mu_i\nabla c_i\Big)\cdot\mathbf{u}$

Discrete case : $\displaystyle\sum_{i=1}^{3}\begin{pmatrix}\textit{Transport}\\ \textit{term}\\ \text{CH}\end{pmatrix}\mu_i^{n+1} = \begin{pmatrix}\textit{Capillary}\\ \textit{forces}\\ \text{NS}\end{pmatrix}\cdot\mathbf{u}^{n+1}$?

IMPLICIT DISCRETIZATION :

$$\begin{matrix}\textit{Transport}\\ \textit{terms}\\ \text{CH}\end{matrix} = \mathbf{u}^{n+1}\cdot\nabla c_i^{n+1}, \qquad \begin{matrix}\textit{Capillary}\\ \textit{forces}\\ \text{NS}\end{matrix} = \sum_{i=1}^{3}\mu_i^{n+1}\nabla c_i^{n+1}$$

- **Advantage :** No contribution to the energy evolution :

$$\sum_{i=1}^{3}\big(\mathbf{u}^{n+1}\cdot\nabla c_i^{n+1}\big)\mu_i^{n+1} = \Big(\sum_{i=1}^{3}\mu_i^{n+1}\nabla c_i^{n+1}\Big)\cdot\mathbf{u}^{n+1}$$

- **Drawbacks :** Strong coupling between the two systems (CH) and (NS)

At the continuous level : $\displaystyle\sum_{i=1}^{3}\Big(\mathbf{u}\cdot\nabla c_i\Big)\mu_i = \Big(\sum_{i=1}^{3}\mu_i\nabla c_i\Big)\cdot\mathbf{u}$

Discrete case : $\displaystyle\sum_{i=1}^{3}\left(\begin{array}{c}\textit{Transport}\\ \textit{term}\\ \text{CH}\end{array}\right)\mu_i^{n+1} = \left(\begin{array}{c}\textit{Capillary}\\ \textit{forces}\\ \text{NS}\end{array}\right)\cdot\mathbf{u}^{n+1}$?

FIRST TRY TO OBTAIN AN UNCOUPLED SYSTEM :

$$\begin{array}{c}\textit{Transport}\\ \textit{terms}\\ \text{CH}\end{array} = \mathbf{u}^n\cdot\nabla c_i^{n+1}, \qquad \begin{array}{c}\textit{Capillary}\\ \textit{forces}\\ \text{NS}\end{array} = \sum_{i=1}^{3}\mu_i^{n+1}\nabla c_i^{n+1}$$

- Contribution to the total energy evolution :

$$\Delta t\sum_{i=1}^{3}\Big((\mathbf{u}^{n+1}-\mathbf{u}^n)\cdot\nabla c_i^{n+1}\Big)\mu_i^{n+1}$$

- Conditional stability : $\Delta t \leqslant Ch$.

(Kay-Styles-Welford, '08)

(Minjeaud, '11)

First idea : separation of the capillary forces term from the (NS) system

Let us first take into account the capillary forces

$$\varrho^n \frac{\mathbf{u}^* - \mathbf{u}^n}{\Delta t} + \nabla p^* = \sum_{i=1}^{3} \mu_i^{n+1} \nabla c_i^{n+1}, \qquad \mathrm{div}\,(\mathbf{u}^*) = 0.$$

Cahn-Hilliard system

$$\begin{cases} \dfrac{c_i^{n+1} - c_i^n}{\Delta t} + \mathbf{u}^* \cdot \nabla c_i^{n+1} = \mathrm{div}\left(\dfrac{M_0^n}{\Sigma_i} \nabla \mu_i^{n+1}\right), \\ \mu_i^{n+1} = D_i^F(\mathbf{c}^n, \mathbf{c}^{n+1}) - \dfrac{3}{4}\varepsilon \Sigma_i \Delta c_i^{n+\beta}. \end{cases}$$

Navier-Stokes equations

$$\begin{cases} \varrho^n \dfrac{\mathbf{u}^{n+1} - \mathbf{u}^*}{\Delta t} + \dfrac{1}{2}\dfrac{\varrho^{n+1} - \varrho^n}{\Delta t}\mathbf{u}^{n+1} + (\varrho^{n+1}\mathbf{u}^n \cdot \nabla)\mathbf{u}^{n+1} + \dfrac{\mathbf{u}^{n+1}}{2}\mathrm{div}\,(\varrho^{n+1}\mathbf{u}^n) \\ \qquad - \mathrm{div}\left(\eta^{n+1} D\mathbf{u}^{n+1}\right) + \nabla(p^{n+1} - p^*) = \varrho^{n+1}\mathbf{g}, \\ \mathrm{div}\,(\mathbf{u}^{n+1}) = 0. \end{cases}$$

Unfortunately, the first two steps are still strongly coupled.

(Minjeaud, '11)

Second idea : Forget about the divergence-free condition in the first step.

$$\mathbf{u}^* = \mathbf{u}^n - \frac{\Delta t}{\varrho^n} \sum_{i=1}^{3} (c_i^n - \alpha_i) \nabla \mu_i^{n+1}, \qquad \alpha_i = \frac{1}{|\Omega|} \int_\Omega c_i^0 \, dx$$

▶ Advection velocity $\mathbf{u}^*$ in (CH) is no more divergence-free but we still have

$$\mathbf{u}^* \cdot \mathbf{n} = 0, \quad \text{on } \partial\Omega.$$

CAHN-HILLIARD SYSTEM

$$\begin{cases} \dfrac{c_i^{n+1} - c_i^n}{\Delta t} + \operatorname{div}\left((c_i^n - \alpha_i)\mathbf{u}^*\right) = \operatorname{div}\left(\dfrac{M_0^n}{\Sigma_i} \nabla \mu_i^{n+1}\right), \\ \mu_i^{n+1} = D_i^F(\mathbf{c}^n, \mathbf{c}^{n+1}) - \dfrac{3}{4}\varepsilon \Sigma_i \Delta c_i^{n+\beta}. \end{cases}$$

▶ We use the conservative form of the transport term ⇒ volume conservation is ensured.

▶ Since $\sum_{i=1}^{3} \alpha_i = 1 \Rightarrow$

The sum of the three order parameters remains equal to 1.

Navier-Stokes system

$$
\begin{cases}
\varrho^n \dfrac{\mathbf{u}^{n+1} - \mathbf{u}^*}{\Delta t} + \dfrac{1}{2} \dfrac{\varrho^{n+1} - \varrho^n}{\Delta t} \mathbf{u}^{n+1} + (\varrho^{n+1}\mathbf{u}^n \cdot \nabla)\mathbf{u}^{n+1} + \dfrac{\mathbf{u}^{n+1}}{2} \mathrm{div}\,(\varrho^{n+1}\mathbf{u}^n) \\
\qquad\qquad - \mathrm{div}\left(\eta^{n+1} D\mathbf{u}^{n+1}\right) + \nabla p^{n+1} = \varrho^{n+1}\mathbf{g}, \\
\mathrm{div}\,(\mathbf{u}^{n+1}) = 0,
\end{cases}
$$

Properties of the scheme

- Systems (CH) and (NS) are fully uncoupled
- Volume conservation still holds
- The property $\sum_{i=1}^{3} c_i = 1$ still holds
- **Unconditional stability**

(Minjeaud, '11)

Theorem (Existence and convergence)

- *The fully discrete scheme has a solution.*
- *Stability :*

$$\forall \Delta t > 0, \textit{the sequence } \mathcal{F}^{triph}_{\mathbf{\Sigma},\varepsilon}(\mathbf{c}_h^n) + \int_\Omega \frac{1}{2}\varrho_h^n |\mathbf{u}_h^n|^2 \, dx \textit{ is decreasing (for } \mathbf{g} = 0).$$

- *In the homogeneous case ($\rho_1 = \rho_2 = \rho_3$), we can prove convergence of the approximate solution.*

(Chorin, '68) ; (Temam, '68) ; (Guermond-Minev-Shen, '06)

Suppose we are given $(\mathbf{u}^n, p^n) \in \mathcal{V}_0^{\mathbf{u}} \times \mathcal{V}^p$.

First step : Velocity prediction $\rightsquigarrow \tilde{\mathbf{u}}^{n+1} \in \mathcal{V}_0^{\mathbf{u}}$

- **Principle :**
  - Forget about the constraint $\operatorname{div}(\mathbf{u}) = 0$,
  - Explicit approximation of the pressure.
- Find $\tilde{\mathbf{u}}^{n+1} \in \mathcal{V}_0^{\mathbf{u}}$ such that

$$\int_\Omega \varrho^n \frac{\tilde{\mathbf{u}}^{n+1} - \mathbf{u}^n}{\Delta t} \cdot \mathbf{v}\, dx + \int_\Omega \frac{1}{2} \frac{\varrho^{n+1} - \varrho^n}{\Delta t} \tilde{\mathbf{u}}^{n+1} \cdot \mathbf{v}\, dx + \frac{1}{2} \int_\Omega \varrho^{n+1} [(\mathbf{u}^n \cdot \nabla)\tilde{\mathbf{u}}^{n+1} \cdot \mathbf{v} - (\mathbf{u}^n \cdot \nabla)\mathbf{v} \cdot \tilde{\mathbf{u}}^{n+1}]\, dx$$

$$+ \int_\Omega 2\eta^{n+1} \mathrm{D}\tilde{\mathbf{u}}^{n+1} : \mathrm{D}\mathbf{v}\, dx - \int_\Omega p^n \operatorname{div} \mathbf{v}\, dx = \int_\Omega \varrho^{n+1} \mathbf{g} \cdot \mathbf{v}\, dx, \quad \forall \mathbf{v} \in \mathcal{V}_0^{\mathbf{u}}$$

- Skew-symmetric form of the advection term

$$\int_\Omega (\varrho \mathbf{u} \cdot \nabla)\mathbf{u} \cdot \mathbf{v} + \frac{\mathbf{u}}{2} \operatorname{div}(\varrho \mathbf{u}) \cdot \mathbf{v}\, dx$$

Second step : velocity projection $\rightsquigarrow \mathbf{u}^{n+1} \in \mathcal{V}_0^{\mathbf{u}}, p^{n+1} \in \mathcal{V}^p$

- **Principle :** projection on the space of divergence free vector fields :

$$\begin{cases} \varrho^{n+1} \dfrac{\mathbf{u}^{n+1} - \tilde{\mathbf{u}}^{n+1}}{\Delta t} + \nabla \Phi^{n+1} = 0, \\ \operatorname{div} \mathbf{u}^{n+1} = 0. \end{cases}$$

- **Substeps :**
  - Compute the pressure increment
    Find $\Phi^{n+1} \in \mathcal{V}^p$ such that

$$\int_\Omega \frac{1}{\varrho^{n+1}} \nabla \Phi^{n+1} \cdot \nabla \pi \, dx = - \int_\Omega \frac{1}{\Delta t} \pi \operatorname{div} \tilde{\mathbf{u}}^{n+1} \, dx, \quad \forall \pi \in \mathcal{V}^p$$

  - Velocity correction
    Find $\mathbf{u}^{n+1} \in \mathcal{V}_0^{\mathbf{u}}$ such that

$$\int_\Omega \frac{\varrho^{n+1}}{\Delta t} \mathbf{u}^{n+1} \cdot \mathbf{v} \, dx = \int_\Omega \frac{\varrho^{n+1}}{\Delta t} \tilde{\mathbf{u}}^{n+1} \cdot \mathbf{v} \, dx + \int_\Omega \Phi^{n+1} \operatorname{div} \mathbf{v} \, dx, \quad \forall \mathbf{v} \in \mathcal{V}_0^{\mathbf{u}}$$

  - Pressure correction

$$p^{n+1} = p^n + \Phi^{n+1}, \quad p^{n+1} \in \mathcal{V}^p$$

1. Compute the velocity prediction $\mathbf{u}^*$ taking into account capillary forces.
2. Solve the Cahn-Hilliard system :
   1. using $\mathbf{u}^*$ as a transport field *in conservative form*
   2. using a suitable semi-implicit time discretization of the potential term.
3. Solve the Navier-Stokes system starting from $\mathbf{u}^*$ without capillary forces by the projection method
   1. Compute the velocity prediction.
   2. Compute the pressure increment.
   3. Correction of the velocity.
   4. Correction of the pressure.

1 A three-phase Cahn-Hilliard/Navier-Stokes model

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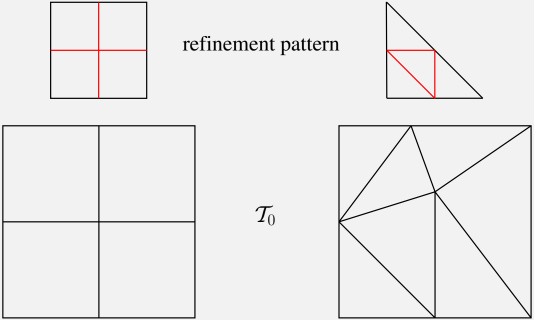
To refine basis functions instead of elements/cells

(Bank-Dupont-Yserentant, '88) (Yserentant, '92)
(Krysl-Grinspun-Schröder, '03) (B.-Lapuerta-Minjeaud-Piar, '09)

- The cells are divided by applying a given refinement pattern
- **Conforming approximation :** No need to modify the numerical scheme because of the adaptation
- Non conforming cells are implicitly taken into account without any treatment of hanging nodes
- The overall approach is independent of the Lagrange element we consider ($\mathbb{P}_1, \mathbb{P}_2, \mathbb{Q}_1, \mathbb{Q}_2$, ...)
- Same strategy in 2D and 3D.

Recursive construction

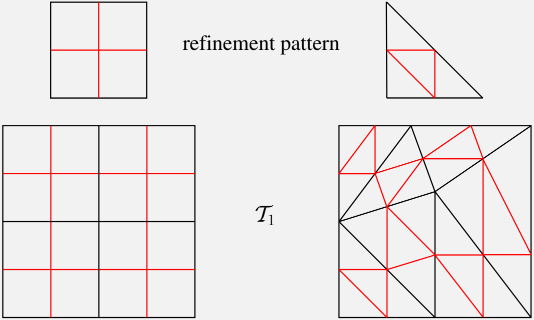
- Initial mesh : $\mathcal{T}_0$ geometrically conforming generated using $\widehat{K}$.



- Necessary compatibility conditions on the refinement pattern :
  - Compatibility between the faces of $\widehat{K}$.
  - The nodes of level [0] are also nodes of level [1].

Recursive construction

- Initial mesh : $\mathcal{T}_0$ geometrically conforming generated using $\widehat{K}$.

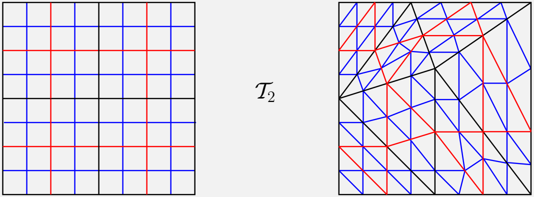


$\mathcal{T}_1$ is a conforming mesh generated using $\widehat{K}$.

- Necessary compatibility conditions on the refinement pattern :
  - Compatibility between the faces of $\widehat{K}$.
  - The nodes of level [0] are also nodes of level [1].

Recursive construction

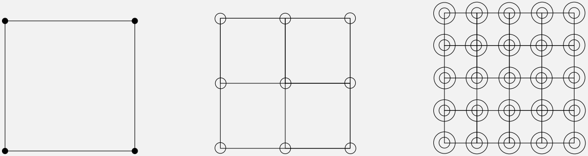
▶ Initial mesh : $\mathcal{T}_0$ geometrically conforming generated using $\widehat{K}$.



$\mathcal{T}_2$ is a conforming mesh generated using $\widehat{K}$.

▶ Necessary compatibility conditions on the refinement pattern :

- Compatibility between the faces of $\widehat{K}$.
- The nodes of level [0] are also nodes of level [1].



level 0 level 1 level 2

	Mesh	FE space			FE Basis
level 0	$\mathcal{T}_0$	X_0	$=$	span B_0	$\mathrm{B}_0 = \{\varphi_k^{[0]}; k = 1, \ldots, N_{\mathrm{dof}}^{[0]}\}$
		$\cap$			
level 1	$\mathcal{T}_1$	X_1	$=$	span B_1	$\mathrm{B}_1 = \{\varphi_k^{[1]}; k = 1, \ldots, N_{\mathrm{dof}}^{[1]}\}$
		$\cap$			
$\vdots$	$\vdots$	$\vdots$		$\vdots$	
		$\cap$			
level J	$\mathcal{T}_J$	X_J	$=$	span B_J	$\mathrm{B}_J = \{\varphi_k^{[J]}; k = 1, \ldots, N_{\mathrm{dof}}^{[J]}\}$

REFINEMENT EQUATIONS

$$X_j \subset X_{j+1} \quad \Rightarrow \quad \varphi_k^{[j]}(\boldsymbol{x}) = \sum_{\ell} \beta_{k\ell}^{[j+1]} \varphi_\ell^{[j+1]}(\boldsymbol{x}), \qquad \forall \boldsymbol{x} \in \Omega$$

- This formula can be obtained on the **reference element**
  $\Longrightarrow$ pre-computed coefficients, no need for storage.

PARENT/CHILD RELATIONSHIP

When $\beta_{k\ell}^{[j+1]} \neq 0$: $\varphi_k^{[j]}$ is a parent of $\varphi_\ell^{[j+1]}$,
$\varphi_\ell^{[j+1]}$ is a child of $\varphi_k^{[j]}$.

Multilevel FE approximation spaces

- **Multilevel FE basis** : a linearly independent subset $\mathcal{B}$ of $\bigcup_{j=0}^{J} \mathrm{B}_j$
- **Multilevel FE space** :

$$\mathcal{V}_h = \text{span } \mathcal{B} \subset \mathrm{H}^1(\Omega)$$

A natural way to ensure linear independence

The geometric nodes associated to two different basis functions in $\mathcal{B}$ are different.

Refinement/Unrefinement (quasi-hierarchical)

Let $\mathcal{B}^\star$ a multilevel basis.

(Un)refinement $\Longleftrightarrow$ to build a new multilevel basis $\mathcal{B}$.

- Refinement of $\varphi \in \mathcal{B}^\star$
  - Remove φ
  - Add all its children which are not refined in $\mathcal{B}^\star$.
- Unrefinement of φ which is refined in $\mathcal{B}^\star$ **without any child refined in $\mathcal{B}^\star$**
  - Add φ
  - Remove all the children of φ with no other parent refined in $\mathcal{B}^\star$.

Refinement criterion for the CH/NS system :

Refine basis functions until the diameter of the cells in the interfaces are at most equal to a given $h_i > 0$.

1. **Linear independence :**
   The refinement procedure preserves linear independence of multilevel basis.
2. **Conservation of information :**
   Let $\mathcal{B}$ which is obtained from $\mathcal{B}^\star$ through the refinement of a basis function then
   $$\text{span } \mathcal{B}^\star \subset \text{span } \mathcal{B}.$$
3. **Refinement order :**
   The approximation spaces obtained by refinement (resp. unrefinement) do not depend on the order we perform successive refinements (resp. unrefinements).

The Cahn-Hilliard equation

No need to modify the discretization scheme for the CH system (the integrals in the Galerkin formulation are computed exactly).

The projection method

- The pressure correction step is not variational but purely algebraic.

$$p^{n+1} = p^n + \Phi^{n+1}$$

- After adaptation of the approximation space :

$$p^n \in \mathcal{V}^{p,n}, \Phi^{n+1} \in \mathcal{V}^{p,n+1} \not\Rightarrow p^n + \Phi^{n+1} \in \mathcal{V}^{p,n+1}$$

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- We need a new **pressure prediction step** : Find $\widetilde{p}^{n+1} \in \mathcal{V}^{p,n+1}$

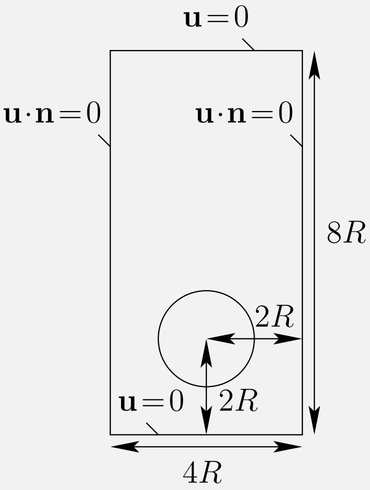
$$\int_\Omega \frac{\nabla \widetilde{p}^{n+1}}{\sqrt{\varrho^{n+1}}} \cdot \frac{\nabla \pi}{\sqrt{\varrho^{n+1}}}\, dx = \int_\Omega \frac{\nabla p^n}{\sqrt{\varrho^n}} \cdot \frac{\nabla \pi}{\sqrt{\varrho^{n+1}}}\, dx, \quad \forall \pi \in \mathcal{V}^{p,n+1}$$

- Then we use $\widetilde{p}^{n+1}$ in the **velocity prediction**, and in the **pressure correction**
- Similar ideas as in **(Guermond-Quartapelle, '00)** lead to stability.

1. A three-phase Cahn-Hilliard/Navier-Stokes model
2. Discretization of the Cahn-Hilliard system
3. Coupling with the Navier-Stokes system
4. Adaptive local refinement
5. Parameters influence - Benchmark - Numerical illustrations

- One single 2D gas bubble rising inside a liquid under the effect of gravity.
- GOALS : compare different models and numerical methods

ϱ_1	1000
ϱ_2	1
η_1	1
η_2	10
σ	24.5
T	3



THE MACROSCOPIC QUANTITIES OF INTEREST

- The bubble mass center position

$$x_{\mathcal{B}}^n = \frac{\sum_{K \in \mathcal{B}^n} |K| x_K}{\sum_{K \in \mathcal{B}^n} |K|},$$

where the "bubble" at time t^n is defined by

$$\mathcal{B}^n = \left\{ K, \quad \frac{1}{|K|} \int_K c^n \, dx \geq 1/2 \right\}.$$

- Mean velocity of the bubble at time t^n

$$\mathbf{u}_{\mathcal{B}}^n = \frac{\sum_{K \in \mathcal{B}^n} \int_K u^n}{\sum_{K \in \mathcal{B}^n} |K|},$$

- Circularity at time t^n

$$\phi_{\mathcal{B}}^n = \frac{\sqrt{V/\pi}}{\text{perimeter of the bubble}},$$

where

$$\text{perimeter of the bubble} \sim \int_\Omega |\nabla c| \, dx.$$

- We choose a degenerate mobility $M_0(\mathbf{c}) = M_{\text{deg}}(1-c_1)^2(1-c_2)^2(1-c_3)^2$.
- R is the initial radius of the bubble

Maximum mean-value velocity

M_{deg} \ ε	$\frac{R}{20}$	$\frac{R}{16}$	$\frac{R}{12}$
10	0.2973	0.3020	0.3082
1	0.2481	0.2490	0.2514
10^{-1}	0.2419	0.2413	0.2412
10^{-2}	0.2417	0.2403	0.2404
10^{-3}	0.2414	0.2400	0.2390
10^{-4}	0.2389	0.2361	0.2326
10^{-5}	0.2289	0.2215	0.2135
10^{-6}	0.2127	0.2050	0.1982
reference value : 0.2419 ± 0.0002			

- We choose a degenerate mobility $M_0(\mathbf{c}) = M_{\text{deg}}(1-c_1)^2(1-c_2)^2(1-c_3)^2$.
- R is the initial radius of the bubble

MASS CENTER POSITION AT TIME $T = 3$

M_{deg} \ ε	$\frac{R}{20}$	$\frac{R}{16}$	$\frac{R}{12}$
10	1.201	1.210	1.225
1	1.129	1.139	1.152
10^{-1}	1.089	1.088	1.090
10^{-2}	1.084	1.082	1.082
10^{-3}	1.084	1.081	1.080
10^{-4}	1.081	1.076	1.069
10^{-5}	1.059	1.043	1.022
10^{-6}	1.010	1.000	0.9806
reference value : 1.081 ± 0.001			

- We choose a degenerate mobility $M_0(\mathbf{c}) = M_{\text{deg}}(1-c_1)^2(1-c_2)^2(1-c_3)^2$.
- R is the initial radius of the bubble

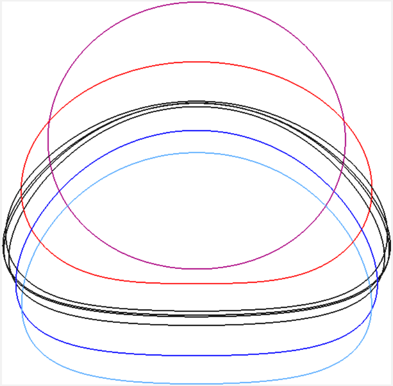
Minimal circularity

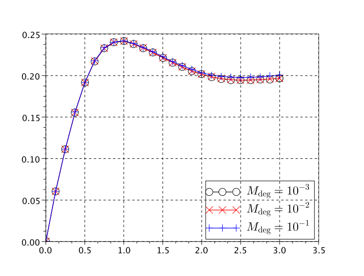
M_{deg} \ ε	$\frac{R}{20}$	$\frac{R}{16}$	$\frac{R}{12}$
10	0.9927	0.9915	0.9900
1	0.9491	0.9527	0.9578
10^{-1}	0.9197	0.9183	0.9165
10^{-2}	0.9097	0.9056	0.8991
10^{-3}	0.8989	0.8911	0.8786
10^{-4}	0.8815	0.8716	0.8626
10^{-5}	0.8882	0.8855	0.8928
10^{-6}	0.9094	0.9180	0.9358

reference value : 0.9012 ± 0.0001

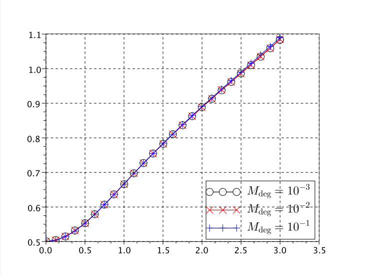
- We choose a degenerate mobility $M_0(\mathbf{c}) = M_{\text{deg}}(1-c_1)^2(1-c_2)^2(1-c_3)^2$.
- R is the initial radius of the bubble

SHAPE OF THE BUBBLE FOR DIFFERENCE VALUES OF M_{DEG}

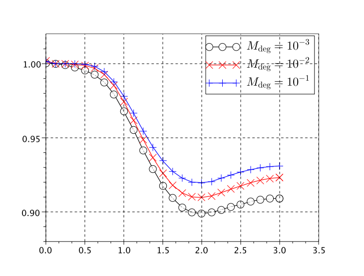




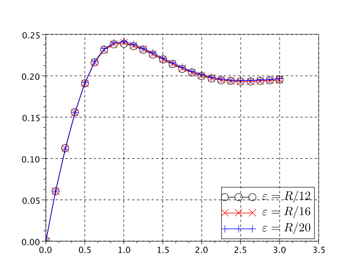
Mean velocity



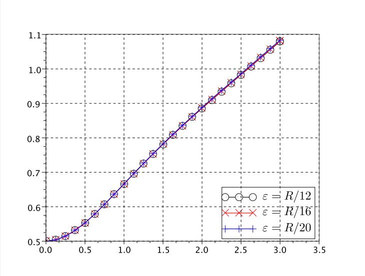
Mass center position



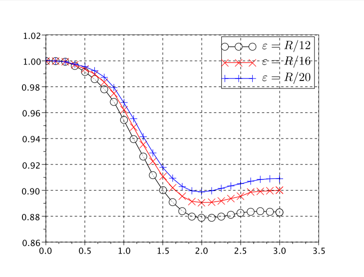
Circularity



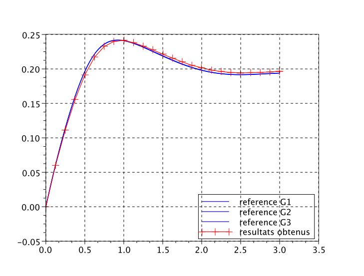
Mean velocity



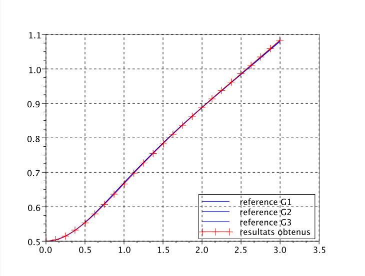
Mass center position



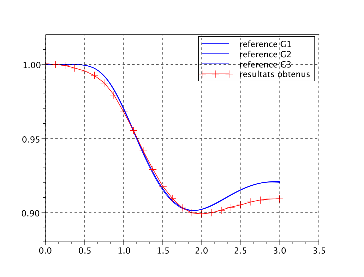
Circularity



Mean velocity

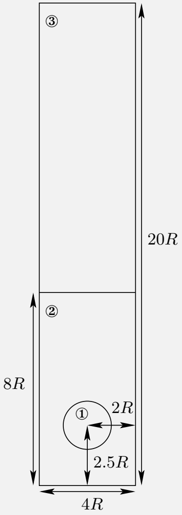


Mass center position

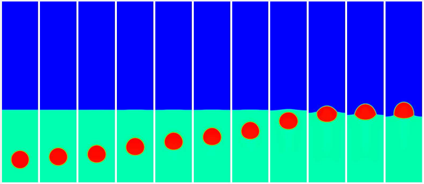


Circularity

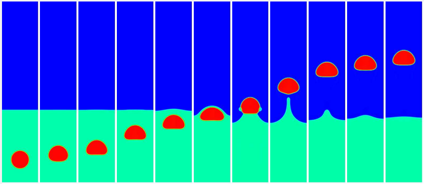
R	T	
0.006	0.8	
σ_{12}	σ_{13}	σ_{23}
0.07	0.07	0.05
ϱ_1	ϱ_2	ϱ_3
1	1200	1000
η_1	η_2	η_3
10^{-4}	0.15	0.1



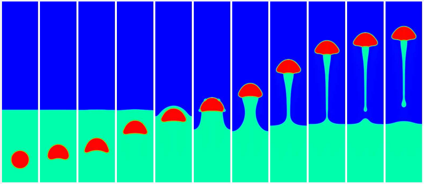
CC scheme



SImpl scheme



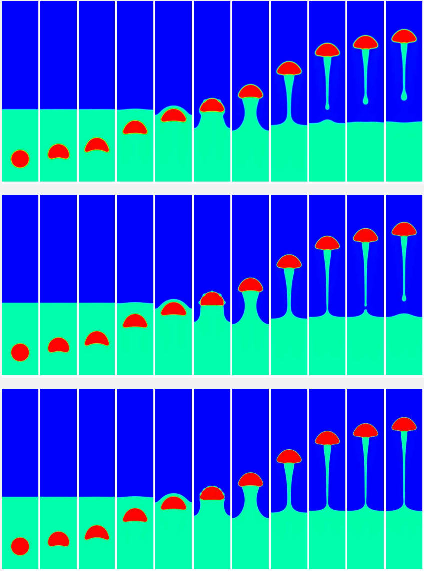
SImpl(0.5) scheme



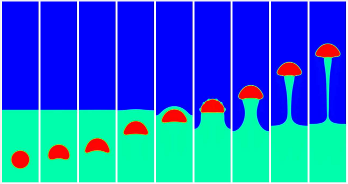
$\varepsilon = R/10$

$\varepsilon = R/15$

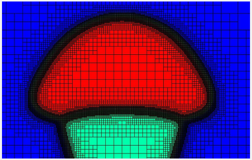
$\varepsilon = R/20$



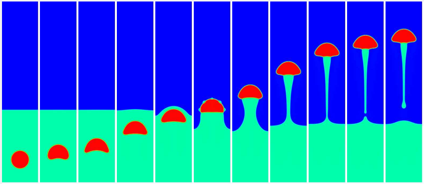
$h_i = \frac{\varepsilon}{4}$

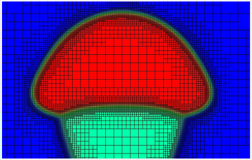


N/A

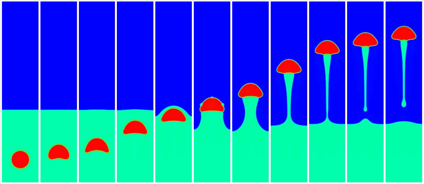


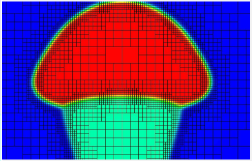
$h_i = \frac{\varepsilon}{2}$





$h_i = \varepsilon$





Outflow BC for the Navier-Stokes equations

(Bruneau-Fabrie '94, '96) (B.-Fabrie '07)

Given a reference flow $(\mathbf{u}_{\text{ref}}, p_{\text{ref}})$ we consider the following outflow BC

$$(\star) \qquad (2\eta D\mathbf{u} - p\text{Id}) \cdot \mathbf{n} = (2\eta D\mathbf{u}_{\text{ref}} - p_{\text{ref}}\text{Id}) \cdot \mathbf{n} - \frac{1}{2}\rho(\mathbf{u} \cdot \mathbf{n})^{-}(\mathbf{u} - \mathbf{u}_{\text{ref}}).$$

Outflow BC for the Cahn-Hilliard equation

(B.-Duval-Introïni-Latché-Piar, '09)

For a **fixed** advection field $\mathbf{u}$ we propose to use

$$(\star\star) \qquad \nabla c \cdot \mathbf{n} = -\frac{1}{(\mathbf{u} \cdot \mathbf{n})^{+}} \frac{\partial c}{\partial t},$$

the BC condition on μ being unchanged.

Outflow BC for the CH / NS system

We combine $(\star)$-$(\star\star)$ but with a precomputation of a capillary pressure

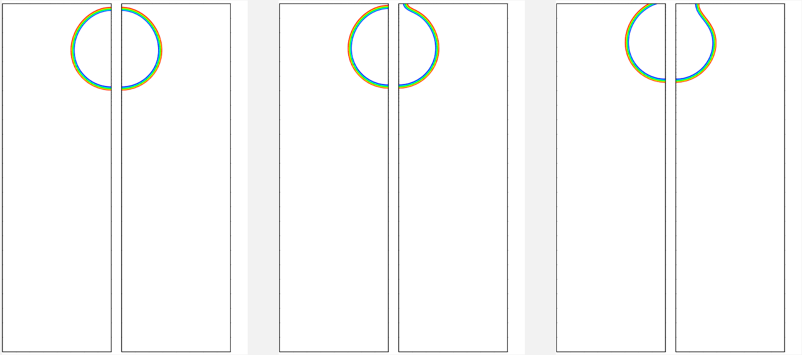
$$\sqrt{\rho^{n+1}\rho^{n}} \frac{\tilde{\mathbf{u}} - \mathbf{u}^{n}}{\Delta t} + \nabla p_{\text{cap}}^{n+1} = \mathcal{F}_{\text{cap}}^{n+1},$$

$$\text{div}\, \tilde{\mathbf{u}} = \text{div}\, \mathbf{u}^{n},$$

Thus, the open BC $(\star)$ is applied only on the dynamic part of the pressure.

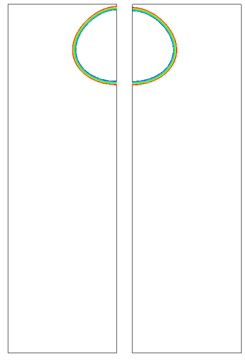
- **Left plot** : Improved outflow BC ($\star$)-($\star\star$)
- **Right plot** : Standard outflow BC

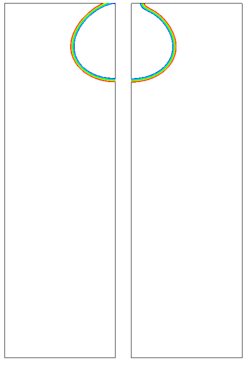
CONVECTED CH EQUATION

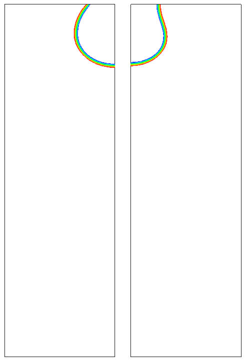


- **Left plot** : Improved outflow BC ($\star$)-($\star\star$)
- **Right plot** : Standard outflow BC

Full NS/CH system







- **Left plot** : Improved outflow BC $(\star)$-$(\star\star)$
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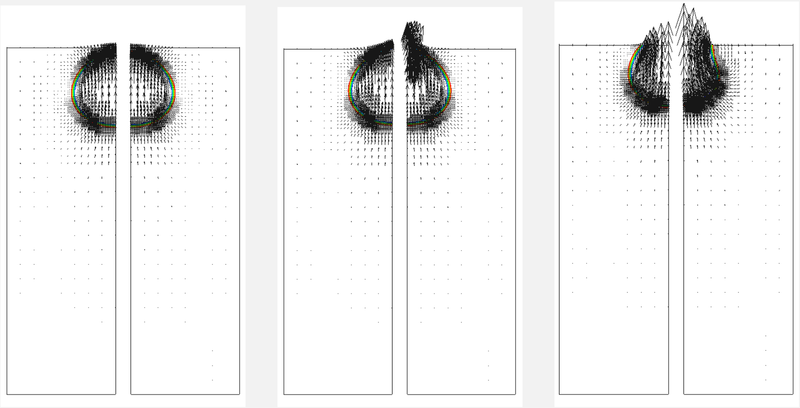
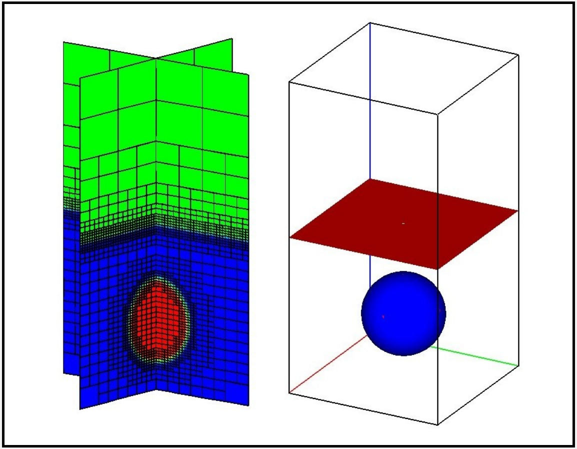
FULL NS/CH SYSTEM





$\sigma_{12} = \sigma_{13} = 0.07$

$\sigma_{23} = 0.05$

$\varrho_1 = 1$

$\eta_1 = 10^{-4}$

$\varrho_2 = 1200$

$\eta_2 = 0.15$

$\varrho_3 = 1000$

$\eta_3 = 0.1$

$R = 8 \times 10^{-3}$

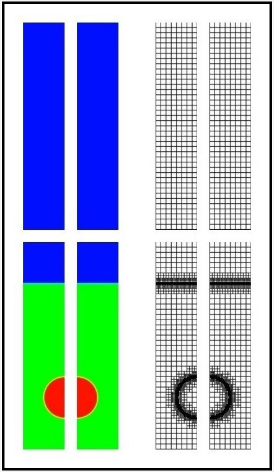
$\varepsilon = 1.6 \times 10^{-3} = \frac{R}{5}$

Number of DOFs associated with one $\mathbb{Q}_1$ scalar unknown :

- Local refinement $\sim$ 120 000.
- Global refinement $\sim$ 550 000.

Summary

- Consistent three phase Cahn-Hilliard systems.
- Study of the time discretization schemes.
- Coupling schemes with the Navier-Stokes system.
- Incremental projection method.
- Conforming local adaptive refinement method.
- Multigrid preconditioning.
- Benchmarking and study of the influence of numerical/modeling parameters.
- Outflow boundary conditions
- Parallel implementation.
- Parasitic currents elimination **(Minjeaud-Piar, '11)**



Perspectives

- Using a $\mathbb{Q}_2$ discretization for $\mathbf{c}$ and $\boldsymbol{\mu}$ (leads to volume conservation problems).
- Using a lower order discretization for $(\mathbf{u}, p)$.
- Convergence proofs in the non-matched densities case.