A hyperbolic approximation of the Cahn-Hilliard equation

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Cahn-Hilliard equations (1958)

The Cahn-Hilliard equation is postulated as a conservative diffusion equation which writes

$$\frac{\partial c}{\partial t} = \Delta\left(c^3 - c - \gamma \Delta c\right).$$

- $c \in [-1, 1]$ is the order parameter indicating the phases.
- $\gamma \ll 1$ is such that $\sqrt{\gamma}$ is the diffuse interface characterstic length.
- describes well the process of phase separation in binary systems: spinodal decomposition, Ostwald Ripening phenomena, etc
- Has applications for modeling binary alloys, sedimentation problems, etc ...

About the equation

$$\frac{\partial c}{\partial t} = \Delta \left(c^3 - c - \gamma \Delta c\right).$$

Cool features

- scalar PDE.
- Well-posed.
- diffuse-interface model (able to deal with strong topological changes).

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Not so cool features

- non-convex energy potential (Requires very careful treatment)
- 4th Order in space (Forget about explicit solvers)
- Violates principle of Causality (Laplace operator)

Plan of presentation

Conservative form and chemical potential

The Cahn-Hilliard equation can be cast into a conservation-law form which writes

$$\frac{\partial c}{\partial t} + \mathrm{div}\left(\mathbf{j}\right) = 0, \tag{1}$$

where the mass flux $\mathbf{j}$ is **assumed** to obey a generalized Fick's law such that

$$\mathbf{j} = -\nabla \mu,$$

and μ is the chemical potential of the system given by

$$\mu = \frac{\delta f}{\delta c} = \frac{\partial f}{\partial c} - \mathrm{div}\left(\frac{\partial f}{\partial \nabla c}\right) = c^3 - c - \gamma \Delta c,$$

where

$$f(c, \nabla c) = \frac{\left(c^2 - 1\right)^2}{4} + \frac{\gamma}{2}\left|\left|\nabla c\right|\right|^2,$$

Lyapunov functional

CH equation admits the Lyapunov functional

$$F(c, \nabla c) = \int_{\mathcal{D}} f(c, \nabla c)\ d\Omega$$

Indeed, we have

$$\frac{\partial f}{\partial t} + \mathrm{div}\,(\mu J) = -\left|\left|\nabla \mu\right|\right|^2,$$

which in integral form writes

$$\frac{\partial F}{\partial t} = -\int_{\mathcal{D}} \left|\left|\nabla \mu\right|\right|^2\ d\Omega \leq 0.$$

Hyperbolic reformulation

Modified action functional

Let us introduce the following action functional

$$a = \int_t \int_{\mathcal{D}} \mathcal{L} \; d\mathcal{D} dt$$

where

$$\mathcal{L}\left(c, \varphi, \nabla\varphi, \frac{\partial \varphi}{\partial t}\right) = -\frac{\left(c^2-1\right)^2}{4} - \frac{\gamma}{2}\left|\left|\nabla\varphi\right|\right|^2 - \frac{\alpha}{2}(c-\varphi)^2 + \frac{\beta}{2}\left(\frac{\partial \varphi}{\partial t}\right)^2 .$$

- φ is a new variable substituting c as the order parameter.
- $\alpha \gg 1$ so that $(c-\varphi)$ vanishes in the limit $\alpha \to +\infty$.
- $\beta \ll 1$ is a small parameter.

Generalized Fick's law for c

$$\mathcal{L}\left(c, \varphi, \nabla\varphi, \frac{\partial\varphi}{\partial t}\right) = -\frac{\left(c^2-1\right)^2}{4} - \frac{\gamma}{2}\,||\nabla\varphi||^2 - \frac{\alpha}{2}(c-\varphi)^2 + \frac{\beta}{2}\left(\frac{\partial\varphi}{\partial t}\right)^2.$$

Generalized Fick's law now becomes

$$\frac{\partial c}{\partial t} + \operatorname{div}\left(-\nabla\mu\right) = 0, \quad \mu = -\frac{\delta\mathcal{L}}{\delta c} = -\frac{\partial\mathcal{L}}{\partial c} = c^3 - c + \alpha(c-\varphi),$$

$\Rightarrow$ 2nd-order PDE, no 4th-order terms

$$\frac{\partial c}{\partial t} - \Delta\left(c^3 - c + \alpha(c-\varphi)\right) = 0, \qquad (I)$$

Euler-Lagrange equation for φ

$$\mathcal{L}\left(c, \varphi, \nabla\varphi, \frac{\partial\varphi}{\partial t}\right) = -\frac{\left(c^2-1\right)^2}{4} - \frac{\gamma}{2}\left|\left|\nabla\varphi\right|\right|^2 - \frac{\alpha}{2}(c-\varphi)^2 + \frac{\beta}{2}\left(\frac{\partial\varphi}{\partial t}\right)^2.$$

For φ, we simply write the Euler-Lagrange equations.

$$\frac{\partial}{\partial t}\left(\frac{\partial\mathcal{L}}{\partial\varphi_t}\right) + \operatorname{div}\left(\frac{\partial\mathcal{L}}{\partial\nabla\varphi}\right) = \frac{\partial\mathcal{L}}{\partial\varphi}.$$

which gives

$$\beta\frac{\partial^2\varphi}{\partial t^2} - \operatorname{div}\left(\gamma\nabla\varphi\right) = \alpha(c-\varphi) \qquad (II)$$

2nd-order approximation of the Cahn-Hilliard equation

Thus so far we have obtained the following system of two 2nd order PDEs

$$\frac{\partial c}{\partial t} - \Delta\left(c^3 - c + \alpha(c-\varphi)\right) = 0, \qquad (I)$$

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- Equation (I) is reminiscent of heat equation.
  $\Rightarrow$ Cattaneo-type relaxation.

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- Equation (I) is reminiscent of heat equation. $\Rightarrow$ Cattaneo-type relaxation.
- Equation (II) is a hyperbolic wave equation with right-hand side. $\Rightarrow$ Order reduction.

Order reduction for (II)

$$\beta \frac{\partial^2 \varphi}{\partial t^2} - \operatorname{div}(\gamma \nabla \varphi) = \alpha(c - \varphi) \qquad (II)$$

Let us denote the independent variables

$$w = \beta \frac{\partial \varphi}{\partial t}, \qquad \mathbf{p} = \nabla \varphi.$$

Order reduction for (II)

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Let us denote the independent variables

$$w = \beta \frac{\partial \varphi}{\partial t}, \qquad \mathbf{p} = \nabla \varphi.$$

Therefore (II) becomes

$$\frac{\partial w}{\partial t} - \operatorname{div}(\gamma \mathbf{p}) = -\alpha(\varphi - c),$$
$$\frac{\partial \varphi}{\partial t} = \frac{1}{\beta} w,$$
$$\frac{\partial \mathbf{p}}{\partial t} - \frac{1}{\beta} \nabla w = 0.$$

Relaxation for equation (I)

$$
\begin{aligned}
\frac{\partial c}{\partial t} + \operatorname{div}\left(\frac{1}{\tau}\mathbf{q}\right) = 0, \\
\frac{\partial \mathbf{q}}{\partial t} + \nabla\mu = -\frac{1}{\tau}\mathbf{q},
\end{aligned}
$$

- $\tau \ll 1$ is a relaxation time.
- c is still a conserved quantity in this framework.

Final system approximating the Cahn-Hilliard equations

$$
\begin{aligned}
&\frac{\partial c}{\partial t} + \operatorname{div}\left(\frac{1}{\tau}\mathbf{q}\right) = 0\\
&\frac{\partial \mathbf{q}}{\partial t} + \nabla\left(c^3 - c + \alpha(c-\varphi)\right) = -\frac{1}{\tau}\mathbf{q}\\
&\frac{\partial w}{\partial t} - \operatorname{div}\left(\gamma\mathbf{p}\right) = -\alpha(\varphi - c)\\
&\frac{\partial \mathbf{p}}{\partial t} - \frac{1}{\beta}\nabla w = 0\\
&\frac{\partial \varphi}{\partial t} = \frac{1}{\beta}w
\end{aligned}
$$

- System of hyperbolic equations with relaxations.
- Equations are conservative also in multiple dimensions.

Final system approximating the Cahn-Hilliard equations

$$
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&\frac{\partial w}{\partial t} - \operatorname{div}\left(\gamma \mathbf{p}\right) = -\alpha(\varphi - c) \\
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- System of hyperbolic equations with relaxations.
- Equations are conservative also in multiple dimensions.

(Has curl involutions on both $\mathbf{q}$ and $\mathbf{p}$ if you want to test curl-free schemes ...)

Hyperbolicity

System admits a full set of real eigenvalues $(\alpha > 1)$ given by

$$
\begin{aligned}
\lambda_1 &= -\frac{\sqrt{3c^2+\alpha-1}}{\sqrt{\tau}},\\
\lambda_2 &= -\frac{\sqrt{\gamma}}{\sqrt{\beta}},\\
\lambda_{3-7} &= 0,\\
\chi_8 &= \frac{\sqrt{\gamma}}{\sqrt{\beta}},\\
\lambda_9 &= \frac{\sqrt{3c^2+\alpha-1}}{\sqrt{\tau}}.
\end{aligned}
$$

and a corresponding set of linearly independent eigenvectors. (easily computed explicitly).

Lyapunov Functional

Proposition

The proposed hyperbolic Cahn-Hilliard system admits the following Lyapunov functional

$$E = \int_{\mathcal{D}} e(c, \varphi, \mathbf{q}, \mathbf{p}, w)\ d\Omega,$$

$$e(c, \varphi, \mathbf{p}, w) = \frac{\left(c^2 - 1\right)^2}{4} + \frac{\gamma}{2} \left|\left|\mathbf{p}\right|\right|^2 + \frac{\alpha}{2}(c - \varphi)^2 + \frac{1}{2\beta} w^2 + \frac{1}{2\tau} \left|\left|\mathbf{q}\right|\right|^2$$

Proof

We express the fluxes as a function of the conjugate variables

$$
\begin{aligned}
&\frac{\partial c}{\partial t} + \operatorname{div}\left(\frac{\partial e}{\partial \mathbf{q}}\right) = 0 \\
&\frac{\partial \mathbf{q}}{\partial t} + \nabla\left(\frac{\partial e}{\partial c}\right) = -\frac{\partial e}{\partial \mathbf{q}} \\
&\frac{\partial w}{\partial t} - \operatorname{div}\left(\frac{\partial e}{\partial \mathbf{p}}\right) = -\frac{\partial e}{\partial \varphi} \\
&\frac{\partial \mathbf{p}}{\partial t} - \nabla\left(\frac{\partial e}{\partial w}\right) = 0 \\
&\frac{\partial \varphi}{\partial t} = \frac{\partial e}{\partial w}
\end{aligned}
$$

Proof

We express the fluxes as a function of the conjugate variables

$$\frac{\partial e}{\partial c} \cdot \left\{ \frac{\partial c}{\partial t} + \operatorname{div}\left(\frac{\partial e}{\partial \mathbf{q}}\right) = 0 \right.$$

$$\frac{\partial e}{\partial \mathbf{q}} \cdot \left\{ \frac{\partial \mathbf{q}}{\partial t} + \nabla\left(\frac{\partial e}{\partial c}\right) = -\frac{\partial e}{\partial \mathbf{q}} \right.$$

$$\frac{\partial e}{\partial w} \cdot \left\{ \frac{\partial w}{\partial t} - \operatorname{div}\left(\frac{\partial e}{\partial \mathbf{p}}\right) = -\frac{\partial e}{\partial \varphi} \right.$$

$$\frac{\partial e}{\partial \mathbf{p}} \cdot \left\{ \frac{\partial \mathbf{p}}{\partial t} - \nabla\left(\frac{\partial e}{\partial w}\right) = 0 \right.$$

$$\frac{\partial e}{\partial \varphi} \cdot \left\{ \frac{\partial \varphi}{\partial t} = \frac{\partial e}{\partial w} \right.$$

Proof

We express the fluxes as a function of the conjugate variables

$$\frac{\partial e}{\partial c} \cdot \begin{cases} \dfrac{\partial c}{\partial t} + \operatorname{div}\left(\dfrac{\partial e}{\partial \mathbf{q}}\right) = 0 \end{cases}$$

$$\frac{\partial e}{\partial \mathbf{q}} \cdot \begin{cases} \dfrac{\partial \mathbf{q}}{\partial t} + \nabla\left(\dfrac{\partial e}{\partial c}\right) = -\dfrac{\partial e}{\partial \mathbf{q}} \end{cases}$$

$$\frac{\partial e}{\partial w} \cdot \begin{cases} \dfrac{\partial w}{\partial t} - \operatorname{div}\left(\dfrac{\partial e}{\partial \mathbf{p}}\right) = -\dfrac{\partial e}{\partial \varphi} \end{cases}$$

$$\frac{\partial e}{\partial \mathbf{p}} \cdot \begin{cases} \dfrac{\partial \mathbf{p}}{\partial t} - \nabla\left(\dfrac{\partial e}{\partial w}\right) = 0 \end{cases}$$

$$\frac{\partial e}{\partial \varphi} \cdot \begin{cases} \dfrac{\partial \varphi}{\partial t} = \dfrac{\partial e}{\partial w} \end{cases}$$

$$\implies \quad \frac{\partial e}{\partial t} + \operatorname{div}\left(\frac{\partial e}{\partial c}\frac{\partial e}{\partial \mathbf{q}} - \frac{\partial e}{\partial \mathbf{p}}\frac{\partial e}{\partial w}\right) = -\left\|\frac{\partial e}{\partial \mathbf{q}}\right\|^2 \leq 0,$$

Numerical methods

In order to solve the model numerically and also compare it with reference solutions, we propose here:

1. A numerical scheme for the original Cahn-Hilliard equation based on 4th order semi-implicit conservative finite differences
2. Explicit MUSCL-Hancock for the hyperbolic approximation.

Implicit conservative finite differences for CH

We propose here a semi-implicit conservative in order to solve numerically the original Cahn-Hilliard equations. We rewrite the latter as follows

$$\frac{\partial c}{\partial t} - \operatorname{div}(\mathbf{F}) + \gamma \Delta^2 c = 0$$

where $\mathbf{F}$ is the flux given by

$$\mathbf{F} = \chi(c)\, \nabla c, \quad \chi(c) = 3c^2 - 1$$

The scheme writes

$$c_{i,j}^{n+1} = c_{i,j}^{n} + \frac{\Delta t}{\Delta x}\left(\mathcal{F}_{i+\frac{1}{2},j}^{n+1} - \mathcal{F}_{i-\frac{1}{2},j}^{n+1}\right) + \frac{\Delta t}{\Delta y}\left(\mathcal{G}_{i,j+\frac{1}{2}}^{n+1} - \mathcal{G}_{i,j-\frac{1}{2}}^{n+1}\right) - \gamma \Delta \Delta_h c_{i,j}^{n+1}.$$

Computation of the intercell fluxes

The intercell fluxes $\mathcal{F}^{n+1}_{i+\frac{1}{2},j}$ and $\mathcal{G}^{n+1}_{i,j+\frac{1}{2}}$, in the x and y directions respectively, are computed using conservative finite-differences as follows

$$\mathcal{F}^{n+1}_{i+\frac{1}{2},j} = \chi^n_{i+\frac{1}{2},j} \, (\nabla_x c)^{n+1}_{i+\frac{1}{2},j} \, ,$$

$$\begin{cases} \chi^n_{i+\frac{1}{2},j} \simeq \dfrac{1}{12} \left(7\,\chi^n_{i,j} - \chi^n_{i-1,j} + 7\,\chi^n_{i+1,j} - \chi^n_{i+2,j}\right) \\ (\nabla_x c)^{n+1}_{i+\frac{1}{2},j} \simeq -\dfrac{1}{12\,\Delta x} \left(15\,c^{n+1}_{i,j} - 15\,c^{n+1}_{i+1,j} + c^{n+1}_{i+2,j} - c^{n+1}_{i-1,j}\right) \end{cases}$$

(similarly for $\mathcal{G}^{n+1}_{i,j+\frac{1}{2}}$)

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(similarly for $\mathcal{G}^{n+1}_{i,j+\frac{1}{2}}$)

These are 4th order approximations.

Discretization of the bi-Laplacian operator

$\Delta\Delta_h c_{i,j}^{n+1}$ is a discretization of the bi-Laplacian operator in the cell-centers as follows

$$\begin{aligned}
\Delta\Delta_h c_{i,j}^{n+1} = &- \frac{1}{\Delta x^4}\left(c_{i-2,j}^{n+1} - 4c_{i-1,j}^{n+1} + 6c_{i,j}^{n+1} - 4c_{i+1,j}^{n+1} + c_{i+2,j}^{n+1}\right) \\
&- \frac{1}{\Delta y^4}\left(c_{i,j-2}^{n+1} - 4c_{i,j-1}^{n+1} + 6c_{i,j}^{n+1} - 4c_{i,j+1}^{n+1} + c_{i,j+2}^{n+1}\right) \\
&- \frac{2}{\Delta x^2 \Delta y^2}\big(c_{i-1,j-1}^{n+1} - 2c_{i,j-1}^{n+1} + c_{i+1,j-1}^{n+1} - 2c_{i-1,j}^{n+1} \\
&\qquad + 4c_{i,j}^{n+1} - 2c_{i+1,j}^{n+1} + c_{i-1,j+1}^{n+1} - 2c_{i,j+1}^{n+1} + c_{i+1,j+1}^{n+1}\big)
\end{aligned}$$

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&-\frac{1}{\Delta y^4}\left(c_{i,j-2}^{n+1} - 4c_{i,j-1}^{n+1} + 6c_{i,j}^{n+1} - 4c_{i,j+1}^{n+1} + c_{i,j+2}^{n+1}\right) \\
&-\frac{2}{\Delta x^2 \Delta y^2}\big(c_{i-1,j-1}^{n+1} - 2c_{i,j-1}^{n+1} + c_{i+1,j-1}^{n+1} - 2c_{i-1,j}^{n+1} \\
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\end{aligned}
$$

$$
c_{i,j}^{n+1} = c_{i,j}^{n} + \frac{\Delta t}{\Delta x}\left(\mathcal{F}_{i+\frac{1}{2},j}^{n+1} - \mathcal{F}_{i-\frac{1}{2},j}^{n+1}\right) + \frac{\Delta t}{\Delta y}\left(\mathcal{G}_{i,j+\frac{1}{2}}^{n+1} - \mathcal{G}_{i,j-\frac{1}{2}}^{n+1}\right) - \gamma\Delta\Delta_h c_{i,j}^{n+1}.
$$

is then solved using GMRES (Matrix is not symmetric ...)

Numerical method for hyperbolic approximation

- Explicit second-order MUSCL-Hancock scheme
- We use either FORCE or Rusanov approximate Riemann solvers (One could also implement a Roe solver)

Exact solution for the original equation

One can find a family of exact one-dimensional stationary periodic solutions to the Cahn-Hilliard system expressed as

$$c_\epsilon(x) = \sqrt{1-\epsilon}\ \mathrm{sn}\left(\sqrt{\frac{\epsilon+1}{2\gamma}}(x-x_0),\ \sqrt{\frac{1-\epsilon}{1+\epsilon}}\right)$$

Here, $\mathrm{sn}(x,s)$ is the Jacobi elliptic sine function, and s is the elliptic modulus. $\epsilon \in [0,1]$.
It is worthy of note that in the limit $\epsilon \to 0$ corresponding to $s \to 1$, one recovers the well-known solution

$$c(x) = \tanh\left(\frac{x-x_0}{\sqrt{2\gamma}}\right)$$

as a particular case.

Exact elliptic function solution

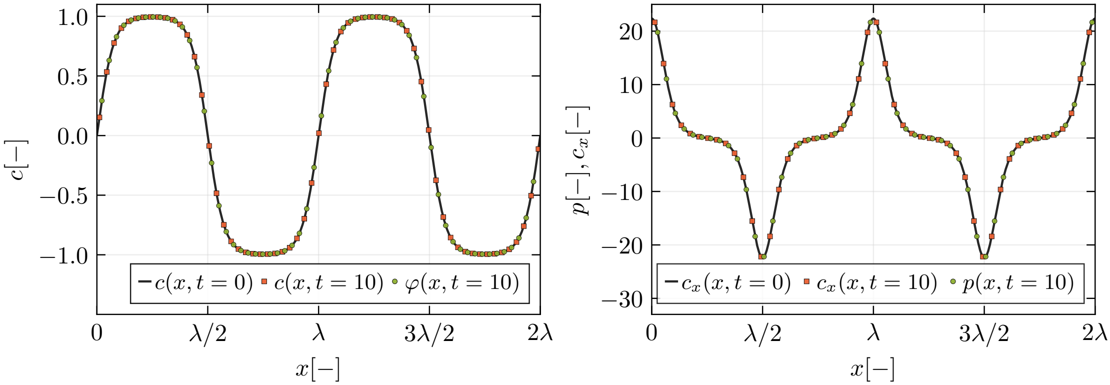


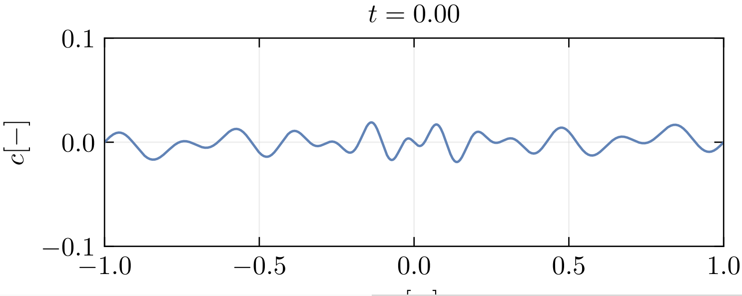
Figure 1: $\gamma = 0.001$. Computational domain is $[0, 2\lambda]$, discretized over $N = 2000$ cells. $\beta = 10^{-6}$, $\alpha = 500$ and $\tau = 8.10^{-4}$. $\mathrm{CFL} = 0.95$ and final simulation time is $t = 10$.

Spinodal decomposition

We suggest the following initial data

$$c(x) = \begin{cases} 0.01\left((\sin(10\pi(1+x)) - \sin\left(10\pi(1+x)^2\right)\right), & \text{if } x \in [-1,0] \\ -0.01\left((\sin(10\pi(1-x)) - \sin\left(10\pi(1-x)^2\right)\right), & \text{if } x \in [0,1]. \end{cases}$$

This function is built in such a way that it is C^∞ over $[-1,1]$ as well as over $\mathbb{R}$ by periodic prolongation.



Spinodal decomposition ($\gamma = 10^{-3}, \beta = 10^{-7}, \alpha = 500, \tau = 10^{-5}$)

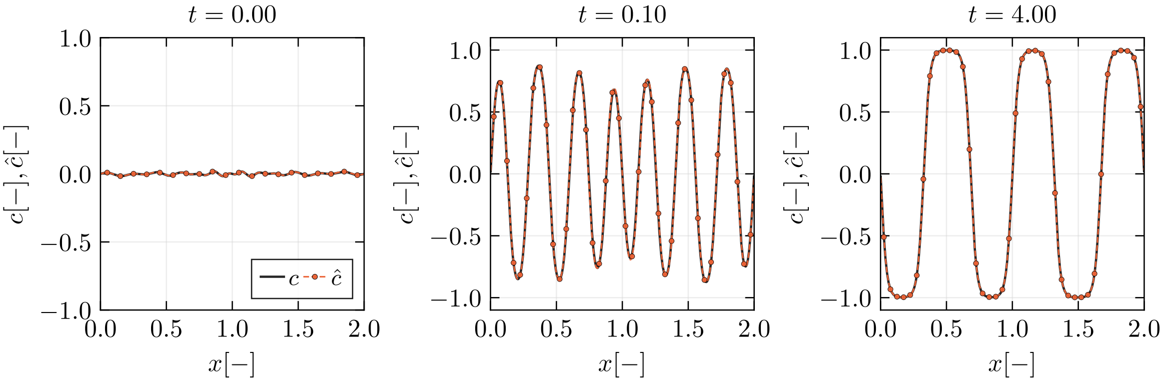


Figure 2: Comparison of the numerical results between the original model (orange) and its hyperbolic counterpart (black). $N = 2000$ computational cells.

Ostwald Ripening in 1D ($\gamma = 10^{-3}, \beta = 10^{-7}, \alpha = 500, \tau = 10^{-4}$)

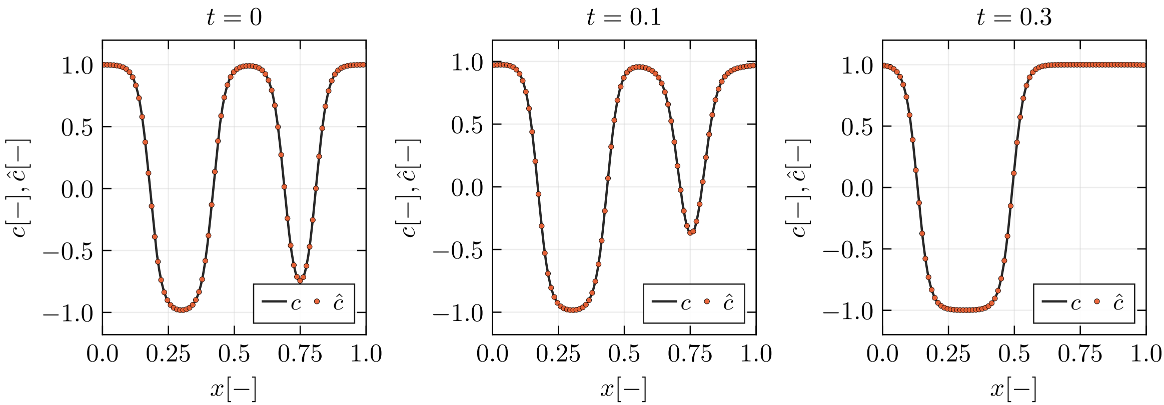
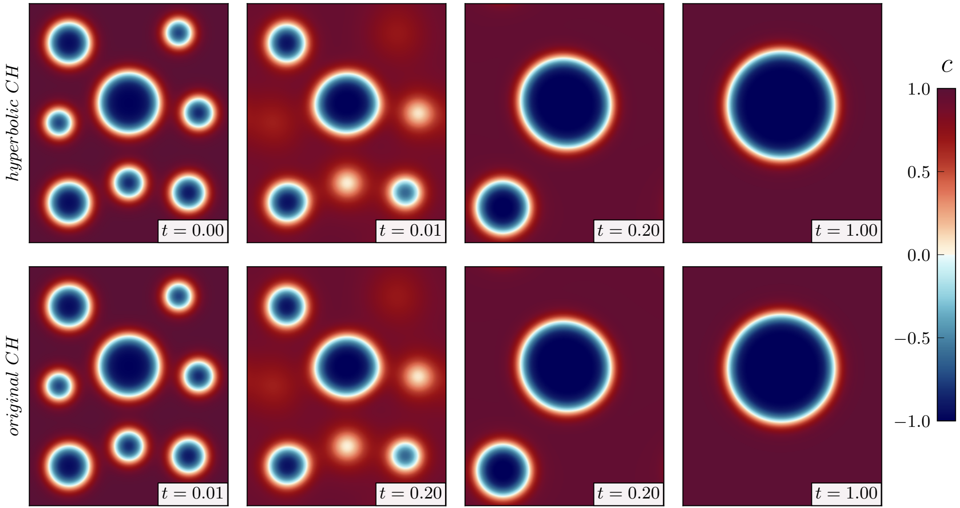


Figure 3: Comaprison of the numerical solutions for hyperbolic Cahn-Hilliard model (black line) and the original model (red dots)for the Ostwald Ripening test case at times $t = \{0, 0.1, 0.3\}$.

Ostwald Ripening in 2D($\gamma = 10^{-3}, \beta = 10^{-7}, \alpha = 500, \tau = 10^{-5}$)



Ostwald Ripening in 2D : horizontal Cuts

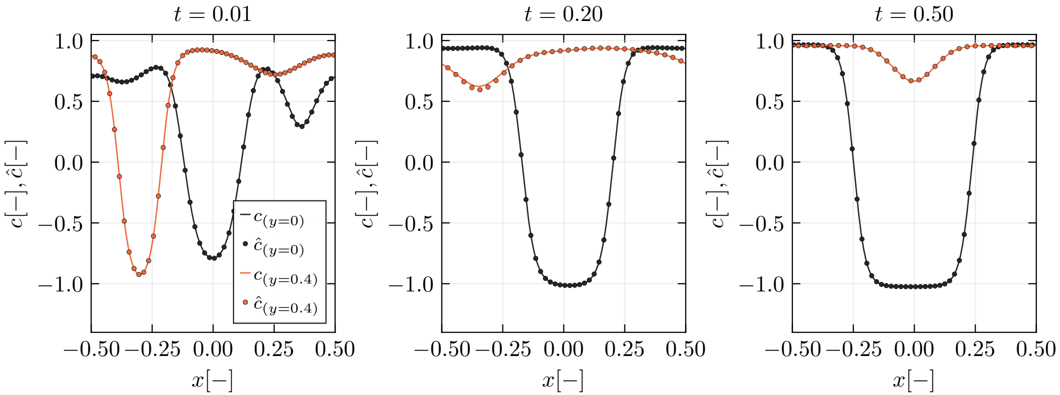


Figure 4: Horizontal cuts over the lines $y = 0$ (red) and $y = 0.4$ (black). Domain is 600×720

Conclusion and Perspective

- We presented a new formulation for an approximate hyperbolic Cahn-Hilliard system.
- An original scheme was conceived to solve the original equation using conservative finite differences.
- Comparison of results showed excellent agreement between the results in one and two dimensions.

Perspectives

- Better formulation fully from variational principles if possible.
- Extension to Navier-Stokes Cahn-Hilliard systems.
- Investigation of bound-preserving properties.
- Semi-implicit discretization, asymptotic preserving schemes, time-step optimization, etc ...

Thank you for your attention !

[1] Dhaouadi, Firas, Michael Dumbser, and Sergey Gavrilyuk. "A first-order hyperbolic reformulation of the Cahn-Hilliard equation." arXiv preprint arXiv:2408.03862 (2024).

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