Structure-preserving Discretization of the Cahn-Hilliard Equations Recast as a Port-Hamiltonian System

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Abstract. The structure-preserving discretization of the Cahn-Hillard equation, a phase field model describing phase separation with diffuse interface, is proposed using the Partitioned Finite Element Method. The discrete counter-part of the power balance is proved and a sufficient condition for the phase preservation is provided.

Keywords: Phase field · port-Hamiltonian system · Structure-preserving discretization

1 Introduction

Eutectic freeze crystallization is a promising process for desalinizing water for it requires fewer energy than other methods [1,11]. Due to the thermodynamic nature of this process, the port-Hamiltonian (pH) framework is an interesting approach for modelling this control system [9,10]. Indeed, pH systems are especially well-suited for modelling energy exchange through boundaries [13,14].

In this article, we will focus on the structure-preserving discretization of the phase separation problem using the Cahn-Hilliard equation [5,7]. The Partitioned Finite Element Method (PFEM) [6] is applied to the pH formulation of this problem, with the aim to achieve simulations of a separation process [7].

The PFEM has already been successfully applied to the Allen-Cahn equation [2,3], a model of solidification process. The Cahn-Hilliard equation is more challenging since a second order differential operator is to be found in its pH formulation [16]. Furthermore, in addition to the power balance satisfied by the Hamiltonian, the preservation of the phase at the discrete level would clearly provide more physically meaningful simulations.

The paper is organized as follows: in Sect. 2, the modelling of the phase field system is presented. The PFEM is applied in Sect. 3, and it is shown that the method is able to mimic the free energy balance and the phase preservation at the discrete level. Some perspectives are discussed in Sect. 5.

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2 Cahn-Hilliard Model as a Port-Hamiltonian System

2.1 Phase Field Modelling

The modelling of phase separation or transition can be tackle by considering a *phase field* representation with *diffuse interface*. Let us consider $\phi(x,t) : \Omega \times \mathbb{R} \to [0,1]$ the phase function, that represents *e.g.* the state of the phase field at a given point or the concentration of a solute in a solution. The dynamics of the system is then given by minimizing the Landau-Ginzburg free energy:

$$\mathcal{G}(\phi) := \int_\Omega g(\phi) + \frac{1}{2}\kappa\, \mathbf{grad}(\phi) \cdot \mathbf{grad}(\phi),$$

where g is the bulk free energy (often a double-well potential) and κ the coefficient corresponding to the interface energy, that prevents the system from having an infinitely thin interface between the two phases.

2.2 Cahn-Hilliard as a Port-Hamiltonian System

This section was made after the work of Benjamin Vincent on the Allen-Cahn and Cahn-Hilliard equations [5,16].

The Cahn-Hilliard model proposes the following dynamics for the phase:

$$\begin{cases} \partial_t \phi = -\mathrm{div}(\boldsymbol{j_\phi}), \\ \boldsymbol{j_\phi} = -\Gamma\, \mathbf{grad}(\frac{\delta \mathcal{G}}{\delta \phi}), \end{cases} \tag{1}$$

where $\Gamma > 0$ represents the interface mobility. The phase field ϕ is transported by the flux $\boldsymbol{j_\phi}$: thus, it is a conserved quantity.

In order to recast (1) in the pH formalism, the state is augmented by considering $\boldsymbol{\psi} := \mathbf{grad}(\phi)$. The potential is rewritten as:

$$\tilde{\mathcal{G}}(\phi, \boldsymbol{\psi}) = \int_\Omega g(\phi) + \frac{1}{2}\kappa \|\boldsymbol{\psi}\|^2.$$

Let us introduce the *flow* variable:

$$\boldsymbol{F_\phi} := -\mathbf{grad}\left(\frac{\delta \tilde{\mathcal{G}}}{\delta \phi} - \mathrm{div}(\frac{\boldsymbol{\delta \tilde{\mathcal{G}}}}{\boldsymbol{\delta \psi}})\right), \tag{2}$$

so that the system reads [16]:

$$\begin{pmatrix} \partial_t \phi \\ \partial_t \boldsymbol{\psi} \\ \boldsymbol{F_\phi} \end{pmatrix} = \begin{pmatrix} 0 & 0 & -\mathrm{div} \\ 0 & 0 & -\mathbf{grad}(\mathrm{div}(\cdot)) \\ -\mathbf{grad}\ \mathbf{grad}(\mathrm{div}(\cdot)) & & 0 \end{pmatrix} \begin{pmatrix} \frac{\delta \tilde{\mathcal{G}}}{\delta \phi} \\ \frac{\boldsymbol{\delta \tilde{\mathcal{G}}}}{\boldsymbol{\delta \psi}} \\ \boldsymbol{j_\phi} \end{pmatrix},$$

together with the constitutive relations:

$$\frac{\delta \tilde{\mathcal{G}}}{\delta \phi} = g'(\phi), \quad \frac{\boldsymbol{\delta \tilde{\mathcal{G}}}}{\boldsymbol{\delta \psi}} = \kappa \boldsymbol{\psi}, \quad \boldsymbol{j_\phi} = \Gamma \boldsymbol{F_\phi}.$$

Let us compute $\frac{d\tilde{\mathcal{G}}(\phi,\psi)}{dt}(t)$ in order to obtain the free energy balance equation, and identify physically relevant boundary terms.

Proposition 1 ([16]). *The Landau-Ginzburg free energy satisfies:*

$$\frac{d\tilde{\mathcal{G}}(\phi,\boldsymbol{\psi})}{dt} = -\int_\Omega \boldsymbol{F_\phi}\cdot\boldsymbol{j_\phi} + \int_{\partial\Omega}\left[\frac{\delta\tilde{\mathcal{G}}}{\delta\phi}\boldsymbol{j_\phi}.\boldsymbol{n} + div(\boldsymbol{j_\phi})\frac{\boldsymbol{\delta\tilde{\mathcal{G}}}}{\boldsymbol{\delta\psi}}.\boldsymbol{n} - div\left(\frac{\boldsymbol{\delta\tilde{\mathcal{G}}}}{\boldsymbol{\delta\psi}}\right)\boldsymbol{j_\phi}.\boldsymbol{n}\right]. \tag{3}$$

The boundary ports (f^∂, e^∂) are then defined as follows:

$$f^\partial := \begin{pmatrix} \frac{\delta\tilde{\mathcal{G}}}{\delta\phi}_{|\partial\Omega} \\ \frac{\boldsymbol{\delta\tilde{\mathcal{G}}}}{\boldsymbol{\delta\psi}}_{|\Omega}\cdot\mathbf{n} \\ -\boldsymbol{j_\phi}_{|\partial\Omega}\cdot\mathbf{n} \end{pmatrix}, \qquad e^\partial := \begin{pmatrix} \boldsymbol{j_\phi}_{|\partial\Omega}\cdot\mathbf{n} \\ \mathrm{div}(\boldsymbol{j_\phi})_{|\partial\Omega} \\ \mathrm{div}\left(\frac{\boldsymbol{\delta\tilde{\mathcal{G}}}}{\boldsymbol{\delta\psi}}_{|\partial\Omega}\right) \end{pmatrix}.$$

Thanks to $\boldsymbol{j_\phi} = \Gamma\boldsymbol{F_\phi}$, the pH system is *lossy*: $\frac{d\tilde{\mathcal{G}}(\phi,\psi)}{dt}(t) \leq \int_{\partial\Omega} f^\partial\cdot e^\partial$.

3 Structure-preserving Discretization of Cahn-Hilliard Model

In order to spatially discretize the system, PFEM is used, which has already allowed for discretizing a various amount of pHs (see *e.g.* [2,6,15]). The method consists of 3 steps: (1) write a weak formulation of the problem, (2) select a *partition* of the variables, use Stokes theorem to perfom an integration by parts which makes appear the useful control in the boundary term (3) Choose a set of finite element families for the state and control variables. Thanks to this method, a finite-dimensional power balance is then satisfied at the discrete level. Note that a structure-preserving method has already been proposed in [8] for the Allen-Cahn equations.

Variational Problem. Let $\lambda \in C^\infty(\Omega,\mathbb{R})$ and $\boldsymbol{\mu},\boldsymbol{\xi} \in C^\infty(\Omega,\mathbb{R}^3)$ be three test functions corresponding to the flow variables: $\frac{\delta\tilde{\mathcal{G}}}{\delta\phi}, \frac{\boldsymbol{\delta\tilde{\mathcal{G}}}}{\boldsymbol{\delta\psi}}$ and $\boldsymbol{F_\phi}$. Then the variational problem is:

$$\begin{cases} \int_\Omega \lambda\partial_t\phi = -\int_\Omega \lambda\ \mathrm{div}(\boldsymbol{j_\phi})\,, \\ \int_\Omega \boldsymbol{\mu}\cdot\partial_t\boldsymbol{\psi} = -\int_\Omega \boldsymbol{\mu}\cdot\mathbf{grad}(\mathrm{div}(\boldsymbol{j_\phi}))\,, \\ \int_\Omega \boldsymbol{\xi}\cdot\boldsymbol{F_\phi} = -\int_\Omega \boldsymbol{\xi}\cdot\mathbf{grad}(\frac{\delta\tilde{\mathcal{G}}}{\delta\phi}) + \int_\Omega \boldsymbol{\xi}\cdot\mathbf{grad}(\mathrm{div}(\frac{\boldsymbol{\delta\tilde{\mathcal{G}}}}{\boldsymbol{\delta\psi}}))\,. \end{cases} \tag{4}$$

And for the constitutive relations:

$$\begin{cases} \int_\Omega \lambda\frac{\delta\tilde{\mathcal{G}}}{\delta\phi} = \int_\Omega \lambda\, g'(\phi)\,, \\ \int_\Omega \boldsymbol{\mu}\cdot\frac{\boldsymbol{\delta\tilde{\mathcal{G}}}}{\boldsymbol{\delta\psi}} = \int_\Omega \boldsymbol{\mu}\cdot(\kappa\boldsymbol{\psi})\,, \\ \int_\Omega \boldsymbol{\xi}\cdot\boldsymbol{j_\phi} = \int_\Omega \boldsymbol{\xi}\cdot(\Gamma\boldsymbol{F_\phi})\,. \end{cases} \tag{5}$$

Choice of Causality. In order to make the boundary control (i.e. choose a causality), one needs to integrate by parts the previous equations. Here, choosing the integration by parts have to be made carefully, indeed the formal adjoint of $\mathrm{div}(\cdot)$ is $-\mathbf{grad}(\cdot)$, and only one integration by parts on the first or third line is required. But $\mathbf{grad}(\mathrm{div}(\cdot))$ is formally *symmetric*, and we will need to integrate by parts twice to make a skew symmetric matrix appear. Therefore we can choose between integrating the second or third line two times or both lines one time. In our case the idea is the following: integrating by parts on the first line makes the $\boldsymbol{j_\phi}$ (the flux of ϕ at the boundary) control appear, which is physically meaningful. Finally integrating by parts the second term of the third line as well as the second line allows us to use divergence conforming first order Finite Elements (FE), e.g. Raviart-Thomas elements, instead of second order ones.

Let us integrate by parts on the first, second and third line:

$$\begin{aligned}
-\int_\Omega \lambda \mathrm{div}(\boldsymbol{j_\phi}) &= \int_\Omega \mathbf{grad}(\lambda)\cdot \boldsymbol{j_\phi} - \int_{\partial\Omega} \lambda \boldsymbol{j_\phi}\cdot\boldsymbol{n}\,,\\
-\int_\Omega \boldsymbol{\mu}\cdot\mathbf{grad}(\mathrm{div}(\boldsymbol{j_\phi})) &= \int_\Omega \mathrm{div}(\boldsymbol{\mu})\mathrm{div}(\boldsymbol{j_\phi}) - \int_{\partial\Omega}\mathrm{div}(\boldsymbol{j_\phi})\boldsymbol{\mu}\cdot\boldsymbol{n}\,,\\
\int_\Omega \boldsymbol{\xi}\cdot\mathbf{grad}(\mathrm{div}(\frac{\boldsymbol{\delta}\tilde{\boldsymbol{\mathcal{G}}}}{\boldsymbol{\delta\psi}})) &= -\int_\Omega \mathrm{div}(\boldsymbol{\xi})\mathrm{div}(\frac{\boldsymbol{\delta}\tilde{\boldsymbol{\mathcal{G}}}}{\boldsymbol{\delta\psi}}) + \int_{\partial\Omega}\mathrm{div}(\frac{\boldsymbol{\delta}\tilde{\boldsymbol{\mathcal{G}}}}{\boldsymbol{\delta\psi}})\,\boldsymbol{\xi}\cdot\boldsymbol{n}\,.
\end{aligned}$$

From this result, we deduce that 3 different scalar boundary controls are required: $e_{\boldsymbol{j_\phi}} := \boldsymbol{j_\phi}\cdot\boldsymbol{n}_{|\partial\Omega}$, $e_d := \mathrm{div}(\boldsymbol{j_\phi})_{|\partial\Omega}$ and $e_\psi := \mathrm{div}(\frac{\boldsymbol{\delta}\tilde{\boldsymbol{\mathcal{G}}}}{\boldsymbol{\delta\psi}})_{|\partial\Omega}$.

Finite Elements Families. Now let us choose, 6 finite elements families: 3 for the flow and effort variables, and 3 for the control. Let $(\lambda_i)_{i\in[1,n]} \in L^2(\Omega,\mathbb{R})$, $(\boldsymbol{\mu}_i)_{i\in[1,m]} \in L^2(\Omega,\mathbb{R}^3)$ and $(\boldsymbol{\xi}_i)_{i\in[1,k]} \in H^2(\Omega,\mathbb{R}^3)$ be the families corresponding to the flow variables $\phi, \boldsymbol{\psi}$ and $\boldsymbol{F_\phi}$ of cardinal $n, m, k \in \mathbb{N}$ respectively . And let $(\gamma_i)_{i\in[1,n_\phi]}, (\eta_i)_{i\in[1,n_d]}, (\nu_i)_{i\in[1,n_\psi]} \in L^2(\partial\Omega,\mathbb{R})$ be the families corresponding to the control variables $e_{\boldsymbol{j_\phi}} := \boldsymbol{j_\phi}\cdot\boldsymbol{n}_{|\partial\Omega}$, $e_d := \mathrm{div}(\boldsymbol{j_\phi})_{|\partial\Omega}$ and $e_\psi := \mathrm{div}(\frac{\boldsymbol{\delta}\tilde{\boldsymbol{\mathcal{G}}}}{\boldsymbol{\delta\psi}})_{|\partial\Omega}$.,of cardinal n_ϕ, n_d and n_ψ respectively. Then by decomposing the flow, effort and control variables over these families, it yields:

$$\begin{cases}\text{for the flow variables:}\\ \phi^d(x,t) = \sum_1^n \phi_i(t)\lambda_i(x)\\ \boldsymbol{\psi}^d(x,t) = \sum_1^m \psi_i(t)\boldsymbol{\mu}_i(x)\\ \boldsymbol{F_\phi}^d(x,t) = \sum_1^k F_\phi^i(t)\boldsymbol{\xi}_i(x)\end{cases}
\quad
\begin{cases}\text{for the effort variables:}\\ \frac{\delta\tilde{\mathcal{G}}}{\delta\phi}^d(x,t) = \sum_1^n \partial_\phi\mathcal{G}^i(t)\lambda_i(x)\\ \frac{\boldsymbol{\delta}\tilde{\boldsymbol{\mathcal{G}}}}{\boldsymbol{\delta\psi}}^d(x,t) = \sum_1^m \partial_{\boldsymbol{\phi}}\mathcal{G}^i(t)\boldsymbol{\mu}_i(x)\\ \boldsymbol{j_\phi}^d(x,t) = \sum_1^k j_\phi^i(t)\boldsymbol{\xi}_i(x)\end{cases} \tag{6}$$

$$\begin{cases}\text{and for the boundary control variables:}\\ e_{\boldsymbol{j_\phi}} = \sum_1^{n_{j_\phi}} e^i_{\boldsymbol{j_\phi}}(t)\gamma_i(x)\\ e_d = \sum_1^{n_d} e^i_d(t)\eta_i(x)\\ e_{\boldsymbol{\psi}} = \sum_1^{n_\psi} e^i_\psi(t)\nu_i(x)\end{cases}$$

Let us note:

$$\begin{cases} \overline{\phi}(t) := (\phi_i)_{i\in[1,n]} \\ \overline{\psi}(t) := (\psi_i)_{i\in[1,m]} \\ \overline{F_\phi}(t) := (F_\phi^i)_{i\in[1,k]} \end{cases}, \begin{cases} \overline{\partial_\phi \mathcal{G}}(t) := (\partial_\phi \mathcal{G}^i)_{i\in[1,n]} \\ \overline{\partial_\psi \mathcal{G}}(t) := (\partial_\psi \mathcal{G}^i)_{i\in[1,m]} \\ \overline{j_\phi}(t) := (j_\phi^i)_{i\in[1,k]} \end{cases}, \begin{cases} \overline{e_{\boldsymbol{j}_\phi}} := (e^i_{\boldsymbol{j}_\phi})_{i\in[1,n_\phi]} \\ \overline{e_d} := (e_d^i)_{i\in[1,n_d]} \\ \overline{e_\psi} := (e_\psi^i)_{i\in[1,n_\psi]} \\ u_\partial := \left[\overline{e_{\boldsymbol{j}_\phi}}^\top \ \overline{e_d}^\top \ \overline{e_\psi}^\top\right]^\top \end{cases} \tag{7}$$

The variational problem then becomes:

$$\begin{cases} \forall j \in [1,n], \sum_i^n \phi_i(t) \int_\Omega \lambda_j\lambda_i = \sum_i^k j_\phi^i(t) \int_\Omega \mathbf{grad}(\lambda_j)\cdot\boldsymbol{\xi}_i - \sum_i^{n_{j_\phi}} e^i_{\boldsymbol{j}_\phi}(t) \int_{\partial\Omega} \lambda_j\gamma_i \,, \\ \forall j \in [1,m], \sum_i^m \psi_i(t) \int_\Omega \boldsymbol{\mu}_j\cdot\boldsymbol{\mu}_i = \sum_i^k j_\phi^i(t) \int_\Omega \mathrm{div}(\boldsymbol{\mu}_j)\,\mathrm{div}(\boldsymbol{\xi}_i) - \sum_i^{n_d} e_d^i \int_{\partial\Omega} \lambda_j\eta_i \,, \\ \forall j \in [1,k], \displaystyle\sum_i^k F_\phi^i(y) \int_\Omega \boldsymbol{\xi}_i\cdot\boldsymbol{\xi}_j = -\sum_i^n \partial_\phi\mathcal{G}^i \int_\Omega \mathbf{grad}(\lambda_i)\cdot\boldsymbol{\xi}_j \\ \qquad\qquad - \displaystyle\sum_i^m \partial_\psi\mathcal{G}^i(t) \int_\Omega \mathrm{div}(\boldsymbol{\mu}_i)\,\mathrm{div}(\boldsymbol{\xi}_j) \\ \qquad\qquad + \displaystyle\sum_i^{n_\psi} e_\psi^i \int_{\partial\Omega} \mathrm{div}(\boldsymbol{\xi_j})\nu_i \,. \\ \text{And for the constitutive relations:} \\ \forall j \in [1,n], \sum_i^n \partial_\phi\mathcal{G}^i(t) \int_\Omega \lambda_i\lambda_j = \int_\Omega \lambda_j\, g'(\sum_i^m \phi_i\lambda_i) \,, \\ \forall j \in [1,m], \sum_i^m \partial_\psi\mathcal{G}^i(t) \int_\Omega \boldsymbol{\mu}_i\cdot\boldsymbol{\mu}_j = \sum_i^m \psi_i(t) \int \boldsymbol{\mu}_j\cdot(\kappa\boldsymbol{\mu}_i) \,, \\ \forall j \in [1,k], \sum_i^k j_\phi^i(t) \int_\Omega \boldsymbol{\xi_i}\cdot\boldsymbol{\xi_j} = \sum_i^k F_\phi^i(t) \int_\Omega \Gamma\boldsymbol{\xi_i}\cdot\boldsymbol{\xi_j} \,. \end{cases} \tag{8}$$

Note that g' is *non linear*, this means that the integral in the first constitutive relation has to be computed at each time step, which increases the computational time. However, if g' is *polynomial*, which happens to be the case for the double-well potential [4], one can take advantage of off-line computations if required, as proposed in [6], allowing for a possible trade-off between computation time and memory usage.

Matrices Definition. Finally let us define the matrices of the finite-dimensional system. Let $M_\lambda := (\int_\Omega \lambda_i\lambda_j)_{i,j\in[1,n]}$, $M_{\boldsymbol{\mu}} := (\int_\Omega \boldsymbol{\mu}_i\cdot\boldsymbol{\mu}_j)_{i,j\in[1,m]}$ and $M_{\boldsymbol{\xi}} := (\int_\Omega \boldsymbol{\xi}_i\boldsymbol{\xi}_j)_{i,j\in[1,k]}$ be the mass matrices. Let us define two rectangular matrices $D_\nabla := \left(\int_\Omega \mathbf{grad}(\lambda_i)\cdot\boldsymbol{\xi_j}\right)_{i,j}$ of size $n\times k$ and $D_{\mathrm{divdiv}} := \left(\int_\Omega \mathrm{div}(\boldsymbol{\mu}_i)\mathrm{div}(\boldsymbol{\xi}_j)\right)_{i,j}$ of size $m\times k$ as the structure matrices. Let $C_\kappa := (\int_\Omega \cdot\boldsymbol{\mu}_i.(\kappa\boldsymbol{\mu}_j))_{i,j\in[1,m]}$ and $C_\Gamma := (\int_\Omega \boldsymbol{\xi}_i.(\Gamma\boldsymbol{\xi}_j))_{i,j\in[1,k]}$ be the two constitutive relations matrices, and let $\overline{h}(\overline{\phi}) := (h_i(\overline{\phi}))_{i\in[\![1,n]\!]}$ be the $n\times 1$ vector corresponding to the non-linear constitutive relation:

$$h_i(\overline{\phi}) = \int_\Omega \lambda_i(x)\, g'(\sum_j^n \phi_j(t)\lambda_j(x)) \,.$$

Finally let $B_{\boldsymbol{j}_\phi} := (\int_{\partial\Omega}\gamma_j\boldsymbol{\xi}_i\cdot\boldsymbol{n})_{(i,j)\in[1,k],[1,n_{j_\phi}]}$, $B_d := (\int_{\partial\Omega}\eta_j\boldsymbol{\xi}_i\cdot\boldsymbol{n})_{(i,j)\in[1,k],[1,n_d]}$ and $B_\psi := (\int_{\partial\Omega}\nu_j\mathrm{div}(\boldsymbol{\xi}_i))_{(i,j)\in[1,k],[1,n_\phi]}$ be the partial control matrices. Let us note $B := \left[-B_{\boldsymbol{j}_\phi}\ B_d\ B_\psi\right]^\top$ the control matrix.

Fully Spatially Discretized System. With finite-dimensional vectors, the fully discretized system then reads:

$$\begin{cases} \begin{bmatrix} M_\lambda & 0 & 0 \\ 0 & M_{\boldsymbol{\mu}} & 0 \\ 0 & 0 & M_{\boldsymbol{\xi}} \end{bmatrix} \begin{pmatrix} \partial_t \overline{\phi} \\ \partial_t \overline{\psi} \\ \overline{F_\phi} \end{pmatrix} = \begin{bmatrix} 0 & 0 & D_\nabla \\ 0 & 0 & D_{\text{divdiv}} \\ -D_\nabla^T & -D_{\text{divdiv}}^T & 0 \end{bmatrix} \begin{pmatrix} \overline{\partial_\phi \mathcal{G}} \\ \overline{\partial_\psi \mathcal{G}} \\ \overline{j_\phi} \end{pmatrix} + B u_\partial \,, \\ \text{With the collocated observations:} \\ M_\partial y_\partial = B^\top \begin{pmatrix} \overline{\partial_\phi \mathcal{G}} \\ \overline{\partial_\psi \mathcal{G}} \\ \overline{j_\phi} \end{pmatrix} \,, \\ \text{and the constitutive relations:} \\ M_\lambda \overline{\partial_\phi \mathcal{G}} = \overline{h}(\overline{\phi}) \,, \\ M_{\boldsymbol{\mu}} \overline{\partial_\psi \mathcal{G}} = M_\kappa \overline{\psi} \,, \\ M_{\boldsymbol{\xi}} \overline{j_\phi} = M_\Gamma \overline{F_\phi} \,. \end{cases} \tag{9}$$

Denote J the $(n+m+k) \times (n+m+k)$ skew-symmetric structure matrix and M the $(n+m+k) \times (n+m+k)$ symmetric mass matrix on the first line of (9).

Discrete Free Energy Balance Equation: Let us define the discrete free energy functional:

$$\overline{G}(\overline{\phi}, \overline{\psi}) := \int_\Omega g(\phi^d) + \frac{1}{2} \boldsymbol{\psi}^d \cdot \kappa \boldsymbol{\psi}^d = \int_\Omega g(\sum \phi_i \lambda_i) + \frac{1}{2} \overline{\psi} \cdot C_\kappa \overline{\psi} \,.$$

The following theorem can then be proved:

Theorem 1 *The discrete free energy balance is given by:*

$$\boxed{\frac{d}{dt} \overline{G}(\overline{\phi}, \overline{\psi}) = -\overline{F_\phi} M_\gamma \overline{F_\phi} + y_\partial^T M_\partial u_\partial \quad \leq y_\partial^T M_\partial u_\partial \,.}$$

Proof: Let us compute the discrete free energy balance:

$$\begin{aligned} \left(\overline{\partial_\phi \mathcal{G}}^T \ \overline{\partial_\psi \mathcal{G}}^T \ \overline{j_\phi}^T \right) M \begin{pmatrix} \partial_t \overline{\phi} \\ \partial_t \overline{\psi} \\ \overline{F_\phi} \end{pmatrix} &= \left(\overline{\partial_\phi \mathcal{G}}^T \ \overline{\partial_\psi \mathcal{G}}^T \ \overline{j_\phi}^T \right) \left(J \begin{pmatrix} \overline{\partial_\phi \mathcal{G}} \\ \overline{\partial_\psi \mathcal{G}} \\ \overline{j_\phi} \end{pmatrix} + B \begin{bmatrix} \overline{e_{\boldsymbol{j}_\phi}} \\ \overline{e_d} \\ \overline{e_\psi} \end{bmatrix} \right) \,, \\ &= 0 + \left(\overline{\partial_\phi \mathcal{G}}^T \ \overline{\partial_\psi \mathcal{G}}^T \ \overline{j_\phi}^T \right) B \begin{pmatrix} \overline{e_{\boldsymbol{j}_\phi}} \\ \overline{e_d} \\ \overline{e_\psi} \end{pmatrix} \,; \end{aligned} \tag{10}$$

and therefore:

$$y_\partial^T M_\partial u_\partial = \overline{\partial_\phi \mathcal{G}}^T M_\lambda \partial_t \overline{\phi} + \overline{\partial_\psi \mathcal{G}}^T M_{\boldsymbol{\mu}} \partial_t \overline{\psi} + \overline{j_\phi}^T M_{\boldsymbol{\xi}} \overline{F_\phi} \,. \tag{11}$$

Also we can compute more precisely:

$$\frac{d}{dt}\int_\Omega g(\sum \phi_i\lambda_i) = \sum_j \int_\Omega g'(\sum \phi_i\lambda_i)\lambda_j\phi_j'(t) = \overline{h}(\overline{\phi})\cdot\frac{d}{dt}\overline{\phi} = \overline{\partial_\phi \mathcal{G}}^T M_\lambda \partial_t\overline{\phi}\,,$$

which gives:

$$\frac{d}{dt}\overline{G}(\overline{\phi},\overline{\psi}) = \overline{\partial_\phi \mathcal{G}}^T M_\lambda \partial_t\overline{\phi} + \overline{\partial_\psi \mathcal{G}}^T M_{\boldsymbol{\mu}} \partial_t\overline{\psi}\,,$$

which yields the *exact* free energy balance:

$$\begin{aligned}\frac{d}{dt}\overline{G}(\overline{\phi},\overline{\psi}) &= -\overline{j_\phi}^T M_\xi \overline{F_\phi} + y_\partial^T M_\partial u_\partial\,,\\ &= -\overline{F_\phi} M_\gamma \overline{F_\phi} + y_\partial^T M_\partial u_\partial\,,\\ &\leq y_\partial^T M_\partial u_\partial\,.\end{aligned}$$

Note that this discrete free energy balance mimics the previous one (3) obtained in the continuous setting.

Discrete Phase Balance Equation: Let us first recall the phase balance equation in the *continuous* setting:

$$\frac{d}{dt}\int_\Omega \phi = -\int_{\partial\Omega} \boldsymbol{j_\phi}\cdot\boldsymbol{n} = -\int_{\partial\Omega} e_{\boldsymbol{j_\phi}}\,.$$

Let us note $c : x \mapsto 1$ the constant function equal to 1 over Ω, and let us note $V^h = Vect(\lambda_1, ..., \lambda_n)$. Let us note p_λ the orthogonal projection of $H^1(\Omega)$ on V^h, and for any $f \in H^1(\Omega)$, $\overline{p_\lambda}(f)$ the vector of size n corresponding to the coefficients of this projection over $\lambda_1, ..., \lambda_n$.

Theorem 2. *Let us assume $c \in V^h$, then:*

$$\boxed{\frac{d}{dt}\int_\Omega \phi^d = -\mathbf{1}_\lambda^T B_{\boldsymbol{j_\phi}}\,\overline{e_{\boldsymbol{j_\phi}}}.} \tag{12}$$

Proof: Firstly, let us compute the following :

$$0 = \mathbf{grad}(c) = \mathbf{grad}(p_\lambda(c)) = \mathbf{grad}(\sum_i \alpha_i\lambda_i) = \sum_i \alpha_i \mathbf{grad}(\lambda_i)$$

Then,

$$\begin{aligned}\forall i \in [\![1,k]\!], \quad (D_\nabla^T\,\overline{p_\lambda}(c))_i &= \sum_j^n \int_\Omega \xi_i\cdot\mathbf{grad}(\lambda_j)\alpha_j\\ &= \int_\Omega \xi_i\cdot(\sum_j \alpha_j\mathbf{grad}(\lambda_j))\\ &= 0\end{aligned} \tag{13}$$

Therefore, $\mathbf{1}_\lambda := \overline{p_\lambda}(c) \in \ker(D_\nabla^T)$. Then, let us compute $\frac{d}{dt}\int_\Omega \phi^d$:

$$\frac{d}{dt}\int_\Omega \phi^d = \frac{d}{dt}\int_\Omega 1 \sum_i \lambda_i \phi_i = \mathbf{1}_\lambda^T M_\lambda \frac{d}{dt}\overline{\phi} = \mathbf{1}_\lambda^T (D_\nabla \overline{j_\phi} - B_{j_\phi}\overline{e_{j_\phi}}) = -\mathbf{1}_\lambda^T B_{j_\phi}\overline{e_{j_\phi}}.$$

Remark: Note that the hypothesis of Theorem 2 is really a very weak hypothesis. Indeed, the constant function 1 does belong to most finite element approximation spaces. Thus, the phase balance equation is preserved at the discrete level.

4 Numerical Experiment

In order to show the efficiency of the approach, we consider a square of length π and a given smooth distribution of ϕ at initial time. Parameters are chosen as follows: $\kappa = 0.0004$, $\Gamma = 10$, and $g(\phi) = 0.25\,\phi^2(1-\phi)^2$. Note that κ is taken to correspond to the square of the parameter ε $(= 0.02)$ appearing in the *classical* statement of the Cahn-Hilliard equations [7]. Futhermore, Γ is taken large enough to observe a displacement of the interface in a relatively small time. For the sake of simplicity, controls are taken equal to zero in this first example.

Regarding the discretization in space, the mesh size is $\Delta x = \Delta y = 0.1$, and we use Lagrange finite element of order 1 for all variables (both scalar and vector fields). The final system has about 13,000 °C of freedom. The SCRIMP[1] simulation environment has been used.

For the time discretization of the obtained port-Hamiltonian Differential Algebraic Equation (pH-DAE), following e.g. [12] and references therein, a Backward Differentiation Formula (BDF) of order 4 has been chosen, and the nonlinearity induced by $h(\phi) = g'(\phi)$ has been treated explicitly as a right-hand side, making use of the previous time step.

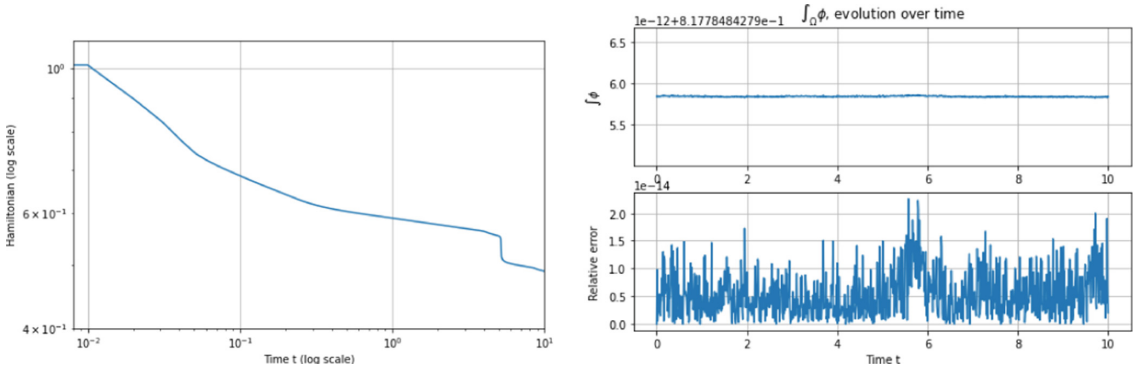

Fig. 1. Evolution of the Hamiltonian over time (left), visualisation of the phase preservation with relative error at machine precision (right).

[1] https://github.com/g-haine/scrimp.

On the left of Fig. 1, one may appreciate the evolution of the Hamiltonian, which indeed shows the expected decaying behavior of Theorem 1. On the right of the same figure, the phase preservation is verified, in accordance with Theorem 2. More precisely, the relative error is at machine precision.

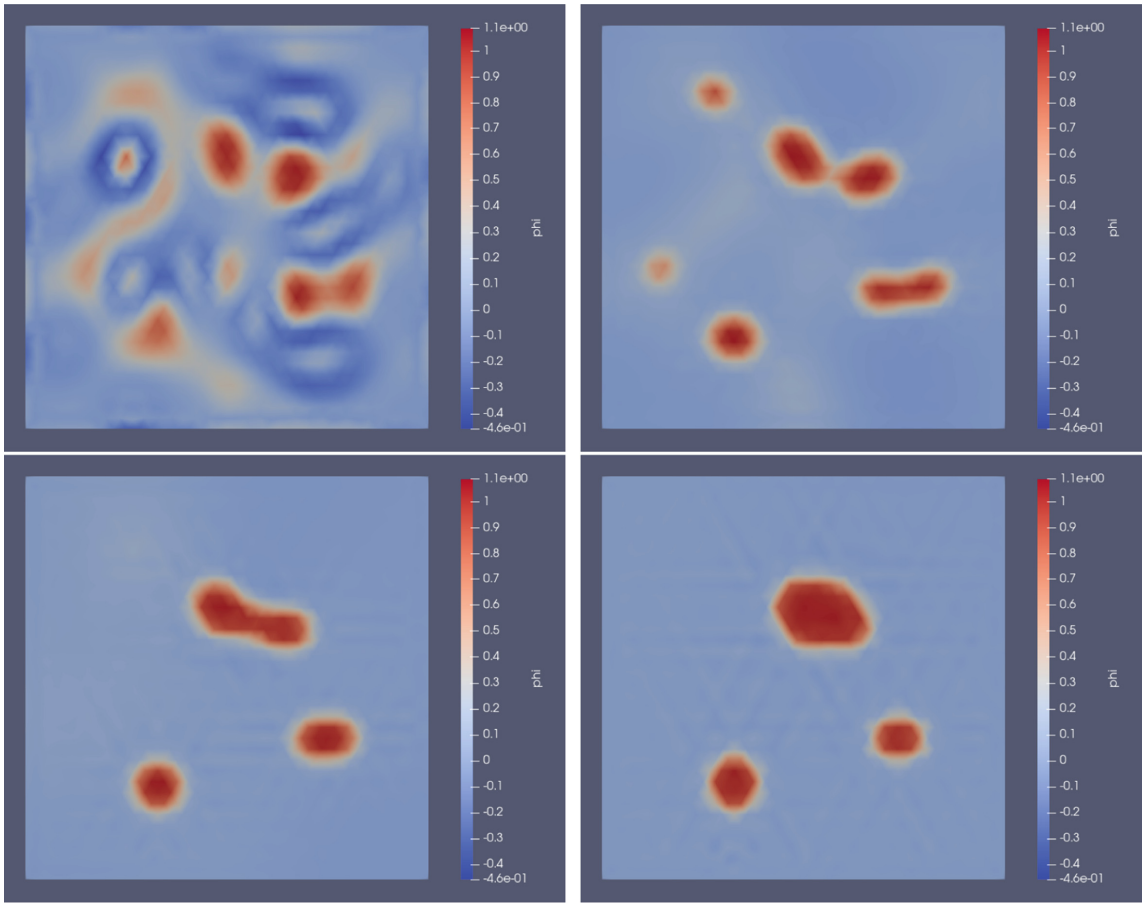

Fig. 2. Evolution of the phase at different times: $t = 0$, $t = 0.005$, $t = 0.05$ and $t = 0.3$.

On Fig. 2, four snapshots of the evolution of the phase distribution are presented, and one may observe the phase separation process as described by the Cahn-Hilliard equations. These results have been obtained at a relatively low numerical cost, showing that the PFEM is indeed able to capture the relevant physical properties of the continuous model, even at low resolution.

5 Conclusion

At the discrete level, the PFEM is able to mimic both the free energy balance, and the conservation of the phase of the Cahn-Hilliard equations. Moreover, making use of the SCRIMP software, simulation results have been obtained, showing the relevance of the port-Hamiltonian framework together with structure-preserving discretization.

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