

Structure-preserving discretization of a coupled Allen-Cahn and heat equation system[★]

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Abstract: Eutectic freeze crystallisation is a promising way of purifying water for it may require less energy than other methods. In order to simulate such a process, phase field models such as Allen-Cahn and Cahn-Hilliard can be used. In this paper, a port-Hamiltonian formulation of the Allen-Cahn equations is used and coupled to heat conduction, which allows for a thermodynamically consistent system to be written with the help of the entropy functional. In a second part, the Partitioned Finite Element Method, a structure-preserving spatial discretization method, is applied to the Allen-Cahn equation; it gives rise to an exact free energy balance at the discrete level. Finally some numerical results are presented.

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1. INTRODUCTION

Water desalination is a critical process and can be achieved in different ways. One of them is eutectic freeze crystallisation, see van der Ham et al. (1998), Randall et al. (2011); this method seems more energy efficient due to the difference between the latent heat of fusion and the latent heat of vaporisation of water, see Beier et al. (2007), Yuan et al. (2020). In this work, we want to develop and implement a numerical model for simulation and control design of such a system (see Kobayashi (1993) and Church et al. (2019)).

Because of the thermodynamic nature of the freezing process, the port-Hamiltonian framework seems useful for modelling, since it preserves the structure of the system and the classification between intensive and extensive variables, see e.g. van der Schaft (2006). In this paper, following Kobayashi (2010) and Penrose and Fife (1990), we shall use the diffuse interface modelling framework as an alternative to the thin interface model.

In this work, the goal is to compute the solutions of the system of Allen-Cahn equations coupled with the heat equation, using the pHs formalism (see Vincent et al.

(2020) for Allen-Cahn), and by spatially discretizing it using the partitioned finite element method introduced in Cardoso-Ribeiro et al. (2021). More details about thermodynamics relations and the implicit pHs representation of the coupled system can be found in the companion paper Yaghi et al. (2022).

The paper is organized as follows: first in § 2 we will go through the phase field method and pHs formalism for the Allen-Cahn equation, then in § 3, a short reminder on heat equation will be given. After introducing these two systems their interconnection is presented in § 4 making use of the entropy as Hamiltonian functional, followed by the structure-preserving discretization in § 5. Finally some numerical simulations results are discussed in § 6.

2. PHASE FIELD MODELLING

Following Gibbs' diffuse interface approach, we shall use a phase field model (e.g. Allen-Cahn) in order to approximate the sharp interface by a diffuse one.

Let us define $\phi : \mathbb{R}^3 \times \mathbb{R} \rightarrow [0, 1]$ the phase function. It can be used to represent various quantities and the two boundaries of its range are purely *arbitrary*. For instance $\phi(x, t)$ can be the phase state of a solution at a given point or the concentration of a certain chemical specie in a solvent.

Assuming ϕ represents the phase of a solution (e.g. $\phi^{-1}(\{0\})$ is solid and $\phi^{-1}(\{1\})$ is liquid) it is immediate to

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observe that the regularity of ϕ induces in-between phase states (e.g. there exist x and t such that $\phi(x, t) = 0.5$) which are sometimes not physically exact, for instance the interface between solid water and liquid water is sharp and therefore the value 0.5 is questionable, see Boettinger et al. (2002).

Then the goal of the Allen-Cahn and Cahn-Hilliard model is to provide the dynamics of this function over time (e.g. solidification, phase separation). Both of them rely on the minimization of the Ginzburg-Landau functional, see e.g. Hohenberg and Krekhov (2015), Cahn and Hilliard (1958):

$$\mathcal{G}(\phi) := \int_{\Omega} f(\phi(z, t)) + \kappa(z) \|\mathbf{grad}(\phi)(z, t)\|^2 dz. \quad (1)$$

This functional represents the *free energy* of the system, where:

- $f : \mathbb{R} \rightarrow \mathbb{R}$ represents the bulk free energy linked to a certain phase state. Note that f is almost always a double-welled potential with its two local minima located at 0 and 1, and that f may vary with temperature as well¹. therefore, by minimizing the free energy of the system, the two phases will tend to separate in two distinct values (either 0 or 1)
- $\kappa(z)$ is a positive parameter which represents the *price to pay* for having an interface between two phases.

2.1 Recasting Allen-Cahn model into a pHs

In the Allen-Cahn model, we do not seek to keep $\int_{\Omega} \phi$ constant. Therefore, the simplest law ensuring the decrease over time of $\mathcal{G}(\phi)$ is to set a gradient relaxation dynamics:

$$\frac{\partial \phi}{\partial t} = -\Gamma \frac{\delta \mathcal{G}}{\delta \phi}, \quad (2)$$

where $\frac{\delta \mathcal{G}}{\delta \phi} := f'(\phi) - \text{div}(\kappa \mathbf{grad}(\phi))$ is the functional derivative of \mathcal{G} with respect to ϕ and $\Gamma(z) > 0$ the interface mobility.

To recast the equations into the pHs formalism, following the work of Vincent et al. (2020), we use an augmented state representation by considering ψ :

$$\begin{pmatrix} \phi \\ \psi \end{pmatrix} := \begin{pmatrix} \phi \\ \mathbf{grad}(\phi) \end{pmatrix}. \quad (3)$$

Therefore the free energy can be rewritten as:

$$\mathcal{G}(\phi) = \bar{\mathcal{G}}(\phi, \psi) = \int_{\Omega} f(\phi) + \kappa \|\psi\|^2.$$

We then introduce two new *flow* and *effort* variables:

$$\begin{cases} F_{\phi} := \frac{\delta \bar{\mathcal{G}}}{\delta \phi} - \text{div}(\frac{\delta \bar{\mathcal{G}}}{\delta \psi}), \\ E_{\phi} := \Gamma F_{\phi}. \end{cases} \quad (4)$$

Let us note $f := \begin{pmatrix} \partial_t \phi \\ \psi \\ F_{\phi} \end{pmatrix}$ and $e := \begin{pmatrix} \frac{\delta \bar{\mathcal{G}}}{\delta \phi} \\ \frac{\delta \bar{\mathcal{G}}}{\delta \psi} \\ \frac{\delta \psi}{E_{\phi}} \end{pmatrix}$ the flow and effort variables, and $\mathcal{J} = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & -\mathbf{grad} \\ 1 & -\text{div} & 0 \end{pmatrix}$ the structure operator.

In Vincent et al. (2020) it is shown that (2) and (1) can be written as a pHs:

$$\begin{cases} \begin{pmatrix} \partial_t \phi \\ \partial_t \psi \\ F_{\phi} \end{pmatrix} = \mathcal{J} \begin{pmatrix} \frac{\delta \bar{\mathcal{G}}}{\delta \phi} \\ \frac{\delta \bar{\mathcal{G}}}{\delta \psi} \\ \frac{\delta \psi}{E_{\phi}} \end{pmatrix}, \\ \text{with constitutive relations:} \\ \frac{\delta \bar{\mathcal{G}}}{\delta \phi} = f'(\phi), \quad \frac{\delta \bar{\mathcal{G}}}{\delta \psi} = \kappa \psi, E_{\phi} = \Gamma F_{\phi}, \\ \text{and boundary ports: } \begin{pmatrix} f^{\partial} \\ e^{\partial} \end{pmatrix} = \begin{pmatrix} \frac{\delta \bar{\mathcal{G}}}{\delta \psi} \cdot \mathbf{n} \\ \frac{\delta \psi}{E_{\phi}|\partial\Omega} \end{pmatrix}, \end{cases} \quad (5)$$

where the boundary ports define the interaction between the environment and the model.

3. REMINDER ON THE HEAT EQUATION

The goal now is to describe the heat equation in a pHs formalism. Following the work of Serhani et al. (2019a), let us recall the entropy of a thermodynamic system :

$$S(u) = \int_{\Omega} s(u) dv$$

Let us choose u the internal energy density as the energy variable. Then the co-energy variable is $\beta := \delta_u S = \frac{\partial s}{\partial u} = \frac{1}{T}$, the reciprocal temperature.

The full heat equation then reads :

$$\begin{cases} \begin{pmatrix} \partial_t u \\ -\mathbf{grad}(\frac{1}{T}) \end{pmatrix} = \begin{pmatrix} 0 & -\text{div} \\ -\mathbf{grad} & 0 \end{pmatrix} \begin{pmatrix} \beta \\ j_Q \end{pmatrix}, \\ \beta^{-1} = T = \frac{u}{\rho C_p}, \\ j_Q = -\lambda \mathbf{grad}(T), \end{cases} \quad (6)$$

where we have used Fourier's law for the heat flux with thermal conductivity λ , and Dulong-Petit relation for the internal energy.

Moreover, this system is completed with a pair of boundary port variables: the normal component of the heat flux at the boundary $j_Q \cdot \mathbf{n}$, and the Dirichlet trace of β the reciprocal temperature.

4. INTERCONNECTION

In order to interconnect the two systems using the pHs formalism, we will choose another Hamiltonian which will facilitate the process: S , the entropy of the system; this functional is the same as in Yaghi et al. (2022), and has

¹ e.g. fusion of a solid when temperature rises.

already been used in Wang et al. (1993), but without resorting to the pHs formalism.

The free energy of the system is defined as (Boettinger et al., 2002):

$$f(\phi, T) := Wg(\phi) + L\frac{T_0 - T}{T_0}p(\phi),$$

With $W \geq 0$, L some thermodynamic parameters that control the speed of the process, T_0 the temperature of fusion, g a double well potential, and p an increasing function going smoothly from 0 to 1. For instance one can use : $p(\phi) = \phi^3(6\phi^2 - 15\phi + 10)$ and $g(\phi) = \phi^2(1 - \phi^2)$.

Remark : This definition of the free energy is well explained in (Boettinger et al., 2002) and a justification of this approximation is provided in the Appendix.

By the thermodynamical definition of free energy, $F = U - TS$, therefore, we have that: $S = \frac{U}{T} - \frac{F}{T}$.

Let us now define:

$$\mathcal{S} := \int_{\Omega} s(\phi, u) = \int_{\Omega} \left(\frac{u}{T} - \frac{f(\phi, T) + \frac{1}{2}\kappa \mathbf{grad}(\phi) \cdot \mathbf{grad}(\phi)}{T} \right)$$

Extending the state space to the new energy variables,

$$\begin{pmatrix} u \\ \phi \\ \psi := \mathbf{grad}(\phi) \end{pmatrix}, \mathcal{S} \text{ can then be rewritten as } \bar{\mathcal{S}}:$$

$$\bar{\mathcal{S}}(u, \phi, \psi) = \int_{\Omega} \left(\frac{u}{T} - \frac{f(\phi, T) + \frac{1}{2}\kappa \psi \cdot \psi}{T} \right),$$

$$\text{and the co-energy variables are: } \begin{pmatrix} \delta_u \bar{\mathcal{S}} = \frac{1}{T} \\ \delta_{\phi} \bar{\mathcal{S}} = -\frac{1}{T} \partial_{\phi} f \\ \delta_{\psi} \bar{\mathcal{S}} = -\frac{1}{T} \kappa \psi \end{pmatrix}.$$

From the previous formulation, we had that : $\partial_t \phi = -\Gamma \frac{\delta \mathcal{G}}{\delta \phi}$, from that we can deduce that the dynamic is given by :

$$\begin{cases} \partial_t u = -\operatorname{div}(\mathbf{j}_Q), \\ \partial_t \phi = +\Gamma T (\partial_{\phi} s), \\ \partial_t \psi = \mathbf{grad}(\Gamma T (\partial_{\psi} s)). \end{cases}$$

Let us define $F := -\frac{\delta \bar{\mathcal{S}}}{\delta \phi} + \operatorname{div}(\frac{\delta \bar{\mathcal{S}}}{\delta \psi})$ and $E := -T \Gamma F$. The full system is then found to be:

$$\begin{pmatrix} \partial_t u \\ \partial_t \phi \\ \partial_t \psi \\ -\mathbf{grad}(\beta) \\ F \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & -\operatorname{div} & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & \mathbf{grad} \\ -\mathbf{grad} & 0 & 0 & 0 & 0 \\ 0 & -1 & \operatorname{div} & 0 & 0 \end{pmatrix} \begin{pmatrix} \beta \\ \frac{\delta \bar{\mathcal{S}}}{\delta \phi} \\ \frac{\delta \bar{\mathcal{S}}}{\delta \psi} \\ \frac{\delta \bar{\mathcal{S}}}{\delta \psi} \\ \mathbf{j}_Q \\ E \end{pmatrix}$$

$$\begin{cases} \beta = ((u/\rho - L\phi)/C_v(\phi))^{-1} \text{ (First principle),} \\ \frac{\delta \bar{\mathcal{S}}}{\delta \phi} = -\frac{W}{T} g'(\phi) - L \frac{T_0 - T}{T_0 T} p'(\phi), \\ \frac{\delta \bar{\mathcal{S}}}{\delta \psi} = -\frac{\kappa \psi}{T}, \\ \mathbf{j}_Q = -\lambda(\phi) \mathbf{grad}(T), \\ E = -\Gamma T F. \end{cases}$$

Finally, the following entropy balance can be computed :

$$\frac{d\bar{\mathcal{S}}}{dt} = \int_{\Omega} \beta^2 \lambda \mathbf{grad}(T) \cdot \mathbf{grad}(T) + \int_{\Omega} -\frac{1}{T} E F - \int_{\partial\Omega} \frac{1}{T} \mathbf{j}_Q \cdot \mathbf{n} - \int_{\partial\Omega} E \frac{\kappa}{T} \psi \cdot \mathbf{n} \quad (7)$$

And by using the constitutive relations, we get:

$$\frac{d\bar{\mathcal{S}}}{dt} = \int_{\Omega} \beta^2 \lambda^{-1} \|\mathbf{j}_Q\|^2 + \int_{\Omega} \beta^2 \Gamma^{-1} E^2 - \int_{\partial\Omega} \beta \mathbf{j}_Q \cdot \mathbf{n} + \int_{\partial\Omega} E \left(-\frac{\kappa}{T} \psi \right) \cdot \mathbf{n} \quad (8)$$

This shows that the entropy of the system is indeed increasing and that the boundary control is the sum of the boundary control of the Heat equation and the Allen-Cahn equation.

Moreover, the global structure matrix is a compound version of the previous ones, and an additional non-linear constitutive relation is present ($E = -\Gamma T F$).

Properly defining the boundary ports and expressing the Stokes-Dirac structure associated with this system is possible, and is fully detailed in Yaghi et al. (2022).

5. STRUCTURE-PRESERVING DISCRETIZATION

In this section we shall apply a spatial discretization which preserves the structure: the exterior derivative, skew-symmetry of the Hamiltonian operator, the port variables and the balance equation. The Partitioned Finite Element Method (PFEM) is such a compatible numerical method for spatially discretizing various pHs, see e.g. Cardoso-Ribeiro et al. (2021). It proceeds in 3 main steps:

- (1) write a weak formulation of the problem,
- (2) select a Partition of the variables, use Stokes theorem to perform an integration by parts which makes appear the useful control in the boundary term,
- (3) choose conforming families of Finite Elements to compute the associated matrix representation.

Following this Method, we end up with a finite-dimensional pHs, for which the power balance is automatically satisfied at the discrete level.

Because of the way the two systems were coupled at the continuous level, the discretization of both systems does not introduce extra difficulty and is presented separately in § 5.1 and § 5.2; moreover, in order to illustrate the flexibility of the approach, it is formulated here with the Gibbs free energy instead of entropy functional as Hamiltonian; further details and other choices of Hamiltonian can be found in Bendimerad-Hohl et al. (2022).

5.1 Allen-Cahn Discretization

Variational problem To apply PFEM, we first need to formulate the variational problem: Let $\lambda, \xi \in C^\infty(\Omega, \mathbb{R})$ and $\mu \in C^\infty(\Omega, \mathbb{R}^3)$ three test functions (either scalar- or vector-valued) over Ω . Let us multiply each line of the full system with the corresponding test function and integrate over Ω :

$$\left\{ \begin{array}{l} \int_{\Omega} \lambda \partial_t \phi = - \int_{\Omega} \lambda E_{\phi} \\ \int_{\Omega} \boldsymbol{\mu} \cdot \partial_t \boldsymbol{\psi} = - \int_{\Omega} \boldsymbol{\mu} \cdot \mathbf{grad}(E_{\phi}) \\ \int_{\Omega} \xi F_{\phi} = \int_{\Omega} \xi \left(\frac{\delta \bar{\mathcal{G}}}{\delta \phi} - \operatorname{div} \left(\frac{\delta \bar{\mathcal{G}}}{\delta \boldsymbol{\psi}} \right) \right) \\ \text{and for the constitutive relations:} \\ \int_{\Omega} \lambda \frac{\delta \bar{\mathcal{G}}}{\delta \phi} = \int_{\Omega} \lambda f'(\phi) \\ \int_{\Omega} \boldsymbol{\mu} \cdot \frac{\delta \bar{\mathcal{G}}}{\delta \boldsymbol{\psi}} = \int_{\Omega} \boldsymbol{\mu} \cdot (\kappa \boldsymbol{\psi}) \\ \int_{\Omega} \xi E_{\phi} = \int_{\Omega} \xi \Gamma F_{\phi} \end{array} \right. \quad (9)$$

Choice of causality The next step is to choose a causality. By using an integration by part on the right hand side of the second or third line, the control term will appear. For instance, let us integrate by part the third line:

$$\begin{aligned} \int_{\Omega} \xi F_{\phi} &= \int_{\Omega} \xi \left(\frac{\delta \bar{\mathcal{G}}}{\delta \phi} - \operatorname{div} \left(\frac{\delta \bar{\mathcal{G}}}{\delta \boldsymbol{\psi}} \right) \right) \\ &= \int_{\Omega} \xi \frac{\delta \bar{\mathcal{G}}}{\delta \phi} - \int_{\Omega} \xi \operatorname{div} \left(\frac{\delta \bar{\mathcal{G}}}{\delta \boldsymbol{\psi}} \right) \\ &= \int_{\Omega} \xi \frac{\delta \bar{\mathcal{G}}}{\delta \phi} + \int_{\Omega} \mathbf{grad}(\xi) \cdot \frac{\delta \bar{\mathcal{G}}}{\delta \boldsymbol{\psi}} - \int_{\partial \Omega} \xi \frac{\delta \bar{\mathcal{G}}}{\delta \boldsymbol{\psi}} \cdot \mathbf{n} \end{aligned}$$

In this case, our control is the value of $u_{\partial} := \frac{\delta \bar{\mathcal{G}}}{\delta \boldsymbol{\psi}} \cdot \mathbf{n}$ at the boundary.²

Finite elements families Now, let us choose three families of finite elements $(\lambda_i)_{i \in [1, n]} \in L^2(\Omega, \mathbb{R})^n$, $(\boldsymbol{\mu}_i)_{i \in [1, m]} \in L^2(\Omega, \mathbb{R}^3)^m$ and $(\xi_i)_{i \in [1, k]} \in H^1(\Omega, \mathbb{R})^k$ of size n, m and k respectively for the state. And a family $(\gamma_i)_{i \in [1, p]} \in L^2(\partial \Omega, \mathbb{R})^p$ for the control.

Then, let us decompose the flow f and effort e variables on these functions:

$$\left\{ \begin{array}{l} \text{for the flow variables} \\ \phi(z, t) = \sum_{i=1}^n \phi_i(t) \lambda_i(z) \\ \boldsymbol{\psi}(z, t) = \sum_{i=1}^m \psi_i(t) \boldsymbol{\mu}_i(z) \\ F_{\phi}(z, t) = \sum_{i=1}^k F_{\phi}^i(t) \xi_i(z) \end{array} \right. \left\{ \begin{array}{l} \text{for the effort variables} \\ \frac{\delta \bar{\mathcal{G}}}{\delta \phi} = \sum_{i=1}^n \partial_{\phi} \mathcal{G}^i(t) \lambda_i(z) \\ \frac{\delta \bar{\mathcal{G}}}{\delta \boldsymbol{\psi}}(z, t) = \sum_{i=1}^m \partial_{\boldsymbol{\psi}} \mathcal{G}^i(t) \boldsymbol{\mu}_i(z) \\ E_{\phi}(z, t) = \sum_{i=1}^k E_{\phi}^i(t) \xi_i(z) \\ \text{and the control:} \\ u_{\partial}(s, t) = \sum_{i=1}^p u_i(t) \gamma_i(s) \end{array} \right.$$

The variational formulation then becomes:

$$\left\{ \begin{array}{l} \forall j \in [1, n], \sum_{i=1}^n \phi_i(t) \int_{\Omega} \lambda_j \lambda_i = - \sum_{i=1}^k E_{\phi}^i(t) \int_{\Omega} \lambda_j \xi_i \\ \forall j \in [1, m], \sum_{i=1}^m \psi_i(t) \int_{\Omega} \boldsymbol{\mu}_j \cdot \boldsymbol{\mu}_i = - \sum_{i=1}^k E_{\phi}^i(t) \int_{\Omega} \boldsymbol{\mu}_j \cdot \mathbf{grad}(\xi_i) \\ \forall j \in [1, k], \sum_{i=1}^k F_{\phi}^i(t) \int_{\Omega} \xi_i \xi_j = \sum_{i=1}^n \partial_{\phi} \mathcal{G}^i(t) \int_{\Omega} \lambda_i \xi_j \\ + \sum_{i=1}^m \partial_{\boldsymbol{\psi}} \mathcal{G}^i(t) \int_{\Omega} \boldsymbol{\mu}_i \cdot \mathbf{grad}(\xi_j) - \sum_{i=1}^p u_i(t) \int_{\partial \Omega} \xi_j \gamma_i \\ \text{And for the constitutive relations:} \\ \forall j \in [1, n], \sum_{i=1}^n \partial_{\phi} \mathcal{G}^i(t) \int_{\Omega} \lambda_i \lambda_j = \int_{\Omega} \lambda_j f'(\phi) \\ \forall j \in [1, m], \sum_{i=1}^m \partial_{\boldsymbol{\psi}} \mathcal{G}^i(t) \int_{\Omega} \boldsymbol{\mu}_i \cdot \boldsymbol{\mu}_j = \sum_{i=1}^m \psi_i(t) \int_{\Omega} \boldsymbol{\mu}_j \cdot (\kappa \boldsymbol{\mu}_i) \\ \forall j \in [1, k], \sum_{i=1}^k E_{\phi}^i(t) \int_{\Omega} \xi_i \xi_j = \sum_{i=1}^k F_{\phi}^i(t) \int_{\Omega} \Gamma \xi_i \xi_j \end{array} \right. \quad (10)$$

Matrices definition Let us note: $M_{\lambda} := (\int_{\Omega} \lambda_i \lambda_j)_{i, j \in [1, n]}$, $M_{\boldsymbol{\mu}} := (\int_{\Omega} \boldsymbol{\mu}_i \cdot \boldsymbol{\mu}_j)_{i, j \in [1, m]}$ and $M_{\xi} := (\int_{\Omega} \xi_i \xi_j)_{i, j \in [1, k]}$ the mass matrices.

Also let us note:

$$D_{\phi} := (\int_{\Omega} \lambda_i \xi_j)_{i \in [1, n], j \in [1, k]}$$

the first structure matrix,

$$D_{\nabla} := (\int_{\Omega} \boldsymbol{\mu}_i \cdot \mathbf{grad} \xi_j)_{i \in [1, m], j \in [1, k]}$$

the second structure matrix.

$$C_{\kappa} := (\int_{\Omega} \kappa \boldsymbol{\mu}_i \cdot \boldsymbol{\mu}_j)_{i, j \in [1, m]}$$

the first constitutive relation matrix,

$$C_{\Gamma} := (\int_{\Omega} \Gamma \xi_i \xi_j)_{i, j \in [1, k]}$$

The second constitutive relation matrix.

Let $\bar{f}(\bar{\phi}(t)) = (\int_{\Omega} f'(\sum_j \phi_j(t) \lambda_j(x)) \lambda_i)_{i \in [1, n]}$ be the discrete vector corresponding to the non-linear constitutive relation.

And finally, let:

$$B_E = (\int_{\Omega} \Gamma \xi_i \gamma_j)_{i \in [1, k], j \in [1, p]}$$

be the partial control matrix, and

$$B = (\mathbf{0}_{n \times k}^T \quad \mathbf{0}_{m \times k}^T \quad B_E^T)^T$$

be the control matrix.

Fully spatially discretized system Let us note

$$\left\{ \begin{array}{l} \bar{\phi}(t) := (\phi_i)_{i \in [1, n]} \\ \bar{\psi}(t) := (\psi_i)_{i \in [1, m]} \\ \bar{F}_{\phi}(t) := (F_{\phi}^i)_{i \in [1, k]} \\ \bar{\partial}_{\phi} \mathcal{G}(t) := (\partial_{\phi} \mathcal{G}^i)_{i \in [1, n]} \\ \bar{\partial}_{\boldsymbol{\psi}} \mathcal{G}(t) := (\partial_{\boldsymbol{\psi}} \mathcal{G}^i)_{i \in [1, m]} \\ \bar{E}_{\phi}(t) := (E_{\phi}^i)_{i \in [1, k]} \\ \bar{u}_{\partial} := (u_i)_{i \in [1, p]} \end{array} \right. \quad (11)$$

² $\frac{\delta \bar{\mathcal{G}}}{\delta \boldsymbol{\psi}} = \kappa \mathbf{grad}(\phi)$ which means the control is the gradient of phase at the boundary, it could be seen as adding solid phase at the boundary to start the solidification of a supercooled solution.

the finite-dimensional vectors corresponding to the spatially discretized flow and effort variables.

We can now rewrite the dynamical system as:

$$\begin{cases} \begin{pmatrix} M_\lambda & 0 & 0 \\ 0 & M_\mu & 0 \\ 0 & 0 & M_\xi \end{pmatrix} \begin{pmatrix} \partial_t \bar{\phi} \\ \partial_t \bar{\psi} \\ \bar{F}_\phi \end{pmatrix} = \begin{pmatrix} 0 & 0 & -D_\phi \\ 0 & 0 & -D_\nabla \\ D_\phi^T & D_\nabla^T & 0 \end{pmatrix} \begin{pmatrix} \partial_\phi \bar{\mathcal{G}} \\ \partial_\psi \bar{\mathcal{G}} \\ \bar{E}_\phi \end{pmatrix} + B u_\partial \\ \text{with collocated observation:} \\ y_\partial := B^T \begin{pmatrix} \partial_\phi \bar{\mathcal{G}} \\ \partial_\psi \bar{\mathcal{G}} \\ \bar{E}_\phi \end{pmatrix} = B_E^T M_\xi^{-1} C_\Gamma \bar{F}_\phi \\ \text{and constitutive relations:} \\ M_\lambda \partial_\phi \bar{\mathcal{G}}(t) = \bar{f}(\bar{\phi}(t)), \quad M_\mu \partial_\psi \bar{\mathcal{G}}(t) = C_\kappa \bar{\psi}(t), \\ M_\xi \bar{E}_\phi(t) = C_\Gamma \bar{F}_\phi(t), \end{cases} \quad (12)$$

which is a finite-dimensional port-Hamiltonian system.

Note that because $\partial_\phi f(\phi)$ is a priori non-linear, \bar{f} has to be recomputed at each time step, which might increase the computational cost; but tackling the polynomial non-linearity more explicitly could enable off-line computations. However, one important point must be made here: because the non-linearity is only present in the *constitutive relations*, the algorithm complexity is less affected than if it were in the *structure matrix*.

Free energy balance equation Let us define the discrete free energy associated to the phase state :

$$F(\bar{\phi}) = \int_{\Omega} f(\sum_i \phi_i \lambda_i),$$

for which we can prove the following

Theorem 1. The discrete free energy balance equation is:

$$\frac{d}{dt}(\bar{G}(\bar{\phi}, \bar{\psi})) = \frac{d}{dt} \left[F(\bar{\phi}) + \frac{1}{2} \bar{\psi}^T C_\kappa \bar{\psi} \right] = -\bar{F}_\phi^T C_\Gamma \bar{F}_\phi + y_\partial^T u_\partial \quad (13)$$

The most technical point is the precise computation of the time derivative of $F(\bar{\phi}(t))$, the full proof can be found in Bendimerad-Hohl et al. (2022).

Theorem 1 shows that the free energy balance equation remains consistent throughout discretization whatever the mesh size, contrarily to other numerical method which are not structure-preserving.

5.2 Heat equation discretization

The discretization of (6) is performed in a similar way; following Serhani et al. (2019b), one can easily discretize the system as :

$$\begin{cases} \begin{pmatrix} M_u & 0 \\ 0 & M_{\nabla T} \end{pmatrix} \begin{pmatrix} \partial_t \bar{u} \\ \mathbf{grad}(T) \end{pmatrix} = \begin{pmatrix} 0 & -D_\nabla^T \\ D_\nabla & 0 \end{pmatrix} \begin{pmatrix} \bar{T} \\ \bar{j}_Q \end{pmatrix} + B_T u_T \\ \text{And for the constitutive relations :} \\ M_u \bar{T} = M_{\frac{1}{\rho C_v}} \bar{u}, \quad M_{\nabla T} \bar{j}_Q = -M_\lambda \mathbf{grad}(T) \\ y_T = B_T^T \begin{pmatrix} \bar{T} \\ \bar{j}_Q \end{pmatrix} \end{cases}$$

The balance equation of this system reads :

$$\frac{d}{dt} \left(\frac{1}{2} \bar{u}^T M_{\frac{1}{\rho C_v}} \bar{u} \right) = -\mathbf{grad}(T)^T M_\lambda \mathbf{grad}(T) + (y_T)^T u_T$$

Note that this system uses the Lyapunov functional which has no physical meaning, but other thermodynamical functional can be used as well (see Serhani et al. (2019b)).

6. NUMERICAL SIMULATIONS

Simulations were conducted using Python as programming language, and different modules were used for the Finite Element Method and time integration, namely: **FEniCS** (Finite elements library), **PETSc** (Time integration library), and **SCRIMP** (a wrapper to speed up the coding process), as well as usual modules such as **NumPy** and **Matplotlib**.

Hereafter is the simulation of the coupled Allen-Cahn and thermal system

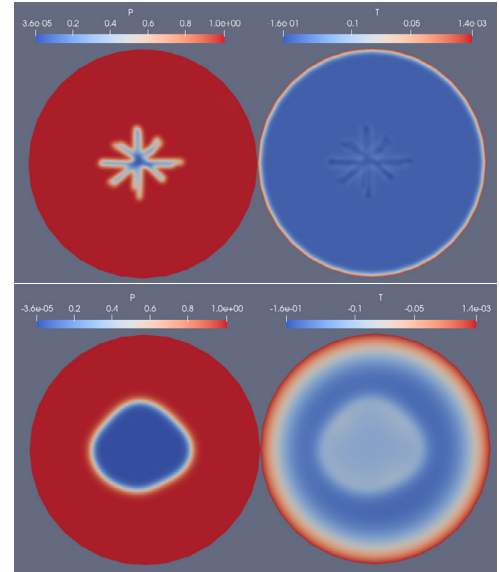


Figure 1. Simulation at step=1 and step=33. On the left is the phase field and on the right the temperature

In this simulation, the coupling is seen as the local heating of the domain where the phase went from 1 to 0 ; meaning that energy was released during the crystallization.

7. CONCLUSION AND FURTHER WORKS

The pHs framework along with PFEM allows to model such a coupled thermodynamical system and to simulate it, while keeping the port-Hamiltonian structure. Moreover, the ports highlight the different methods of controlling the system and the pHs structure gives the entropy balance associated with such boundary controls.

For more details about Cahn-Hilliard, Allen-Cahn as well as the binary solution case and more complete proofs of the present work, see Bendimerad-Hohl et al. (2022).

Note that another energy-preserving discretization of the Cahn-Hilliard equation which doesn't rely on the pHs framework exists and can be found in Egger et al. (2021)

8. SPECIAL THANKS

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APPENDIX

Thermodynamical properties: In order to justify the choice of $C_p(\phi)$ constant across each phase and $f = Wg(\phi) + p(\phi)L\frac{T_0-T}{T_0}$ let us consider these two graphs :

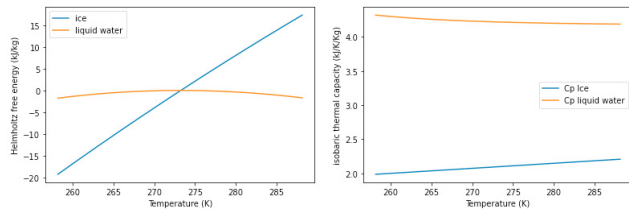


Figure 2. (Left): plot of the free energy of ice and liquid water at $P = 0.1\text{MPa}$. (Right): plot of C_p of ice and liquid water at $P = 0.1\text{MPa}$

These come from Wagner and Pruß (2002) and the associated Python module called *iapws* which allows for an accurate approximation of water's thermodynamical properties.

From these graphs, choosing $C_p \approx (1-p(\phi))C_p^S + p(\phi)C_p^L$ is validated, considering the fact that they are almost constant near 0°C .

Also, it is clear that f^L is almost constant and that f^S can be approximated by a linear function.

Moreover, given that we wrote $f(\phi, T) = Wg(\phi) + (1 - p(\phi))f^S(T) + p(\phi)f^L(T)$ and that only the derivatives of f matters in the kinematics, constants can be removed and we can rewrite f as $f = Wg(\phi) + p(\phi)L\frac{T_0-T}{T_0}$.

Dynamical properties: The value of the thermal conductivity of liquid water is already precisely known. But the question of the thermal conductivity of ice is a bit more complex for it involves the speed of the freezing process, as shown in Bonales et al. (2017).

Therefore, in order to find the thermal conductivity of ice, some coarse assumptions have to be made.

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