

Port Hamiltonian systems with moving interface: a phase field approach

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Abstract: In this paper, we give a formulation of distributed parameter systems with a moving diffuse interface using the Port Hamiltonian formalism. For this purpose, we suggest to use the phase field modeling approach. In the first part we recall the phase field models, in particular the Cahn–Hilliard and Allen–Cahn equations, and show that they may be expressed in terms of a dissipative Hamiltonian system. In the second part we show how this Hamiltonian model may be extended to a Boundary Port Hamiltonian System and illustrate the construction on the example of crystallization.

Keywords: Boundary control systems, Port Hamiltonian systems, Phase fields, Solidification

1. INTRODUCTION

In this paper we consider the modeling problem of distributed parameter systems with internal moving interface. The interface is the narrow region which separates two spatial regions of different material states (solid/liquid, liquid/gas, solid/solid, etc). One way to model such systems is to consider *sharp interfaces* and to divide the spatial domain into sub-systems. Each sub-system is governed by a set of conservation laws interconnected at the interfaces through boundary conditions resulting from flux conditions and constitutive relations. This implies an explicit tracking of the interface position, both in space and time. This representation of multi-phase distributed parameter systems increases the complexity of modeling, analysis, and numerical discretization schemes (Godlewski and Raviart, 2004; Boutin et al., 2008).

An alternative approach is to consider *diffuse interfaces* where phases are defined by continuous variables in space and time. This is the phase field approach. The dynamics of phase variable are governed by partial differential equations derived from thermodynamics potentials. Most models falling into the scope of phase field systems are then described by Cahn–Hilliard (Cahn and Hilliard, 1958) or Allen–Cahn (Allen and Cahn, 1979) equations which describe conservative and non-conservative processes, respectively. Sharp interface models can be recovered from phase field ones by considering infinitely small interface thickness (Elder et al., 2001). See the monograph (Emmerich, 2003) for more details on the develop-

ment, the analysis and the applications of this modeling tool. Allen–Cahn and Cahn–Hilliard equations are employed as boundary control models. Chehab et al. (2017) used a 1–D Allen–Cahn equation to model the interface formation in a lithium electric battery and to control the number of interface through a Neumann boundary control variable. Chen (1993) proposed a boundary optimal control law for the Allen–Cahn equation.

The boundary control port Hamiltonian formulation of infinite-dimensional systems is convenient to model systems governed by conservation laws (van der Schaft and Maschke, 2002). The port Hamiltonian formulation of sharp moving boundary in 1–D systems was addressed by Diagne and Maschke (2013). In this work we define phase field systems within the boundary control port Hamiltonian framework. Toward this end we introduce phase fields models. We define the potential of the interface and the conservative and non-conservative modeling approaches. The port Hamiltonian representations for phase field systems are obtained by prolongation of the systems on their jet spaces. This approach was already introduced in various examples Maschke and van der Schaft (2005, 2013); Schöberl and Siuka (2014). The contribution is concluded with a solidification example (Elder et al., 2001).

The paper is structured as follows. In Section 2 the phase field modeling is introduced and Stokes–Dirac structures are recalled in Section 3. The main contributions are presented in sections 4 and 5 where boundary port Hamiltonian formulations of non-conserved and conserved phase field models are stated, respectively. In Section 6 a solidification example illustrates the contribution.

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2. INTRODUCTION TO PHASE FIELD MODELS

Interfaces are implicitly represented through a continuous time-varying distributed parameter named the phase field variable. This parameter possesses its own dynamics and physical properties. Hence, a phase field model is defined by two elements. Firstly a functional representing a thermodynamical potential such as the energy or the entropy (or any other Legendre transformations). Secondly a state equation governing the phase field dynamics. Two phenomenological behaviors are distinguished depending on the phase field conservative properties. The state equations are conservation laws or gradient systems. For an overview of phase field models see the review article (Kobayashi, 2010) or the monograph (Emmerich, 2003).

Consider z to be the space variable defined in the spatial domain $\Omega \subset \mathbb{R}^3$ with boundary $\partial\Omega \subset \mathbb{R}^2$ and $t \in [0, +\infty)$ to be the time variable. The conserved phase field variable $c(t, z) \in [0, +\infty) \times \Omega \rightarrow [0, 1]$ is a scalar distributed parameter. Values 0 and 1 enable the representation of two phases. Intermediate values indicate the proximity with the dissipative interface. We have deliberately chosen the interval $[0, 1]$ for simplicity but any interval $[a, b]$ for any $a > b \in \mathbb{R}$ is adequate to represent two phases. Non-conserved phase field variables are labelled $\phi(t, z) \in [0, +\infty) \times \Omega \rightarrow [0, 1]$. Phase fields are initialized at time $t = 0$ as $\phi(0, z) = \phi_0(z) \in C^\infty(\Omega, [0, 1])$ and $c(0, z) = c_0(z) \in C^\infty(\Omega, [0, 1])$ for all $z \in \Omega$.

2.1 The Landau–Ginzburg functional

The cornerstone of phase field modeling relies on the definition of the functional representing indifferently its entropy density, its energy density or other thermodynamical potentials. This function is a thermodynamic potential where a phase field variable is added to the thermodynamic variables present in the system (Emmerich, 2003). Consider any, conserved or non-conserved, phase field variable x . The Landau–Ginzburg model for interfaces is defined with the functional $\mathcal{G} : C^\infty(\Omega) \rightarrow \mathbb{R}$ (Emmerich, 2003):

$$\mathcal{G}(x) = \int_{\Omega} g(x) + \frac{1}{2} \kappa_x(z) (\text{grad } x)^2 dV, \quad (1)$$

where $\kappa_x(z) \in C^\infty(\Omega, \mathbb{R}^+)$ is the gradient entropy coefficient and relates the interface surface tension and width (Kobayashi, 2010). The functional (1) is the sum of a quadratic term that represents the cost for inhomogeneities and $g(x) \in C^\infty([0, 1], \mathbb{R})$ is an analytic potential function that generates the interface dynamics. This function exhibits two minima in the interval $[0, 1]$ enabling the thermodynamic consistency of each phase (Emmerich, 2003).

The dynamics of either a non-conserved phase field variable or a conserved one are generated by variations of the potential function (1).

2.2 Non-conserved phase field variable

A non-conserved phase field variable, $\phi(t, z)$, is governed by a gradient equation of the following form:

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

where $\Gamma_\phi(z) \in C^\infty(\Omega, \mathbb{R}^+)$ represents the isotropic interface mobility and $\delta \mathcal{G} / \delta \phi$ denotes the functional derivative of the functional \mathcal{G} with respect to the phase field variable $\phi(t, z)$. The variational differentiation of the functional (1) is given by:

$$\frac{\delta \mathcal{G}}{\delta \phi}(\phi) = \frac{\partial g}{\partial \phi}(\phi) - \text{div} \left(\kappa_\phi(z) \text{grad } \phi(t, z) \right). \quad (3)$$

According to the functional derivative (3), the phase field state equation (2) reads as follows:

$$\frac{\partial \phi}{\partial t} = -\Gamma_\phi \left(-\text{div} \left(\kappa_\phi \text{grad } \phi \right) + \frac{\partial g}{\partial \phi}(\phi) \right), \quad (4)$$

where time and space dependences on the state variable and coefficients are omitted for sake of clarity. Equation (4) is named the Allen–Cahn equation (Allen and Cahn, 1979). To define a Cauchy problem we include initial conditions at $t = 0$ with $\phi(0, z) = \phi_0(z)$ for all $z \in \Omega$, and boundary conditions, evaluated on $\partial\Omega$, that can be Dirichlet, Neumann or Danckwerts (Nauman and He, 2001).

Remark 1. The Allen–Cahn equation (4) is a parabolic equation (Duindam et al., 2009), e.g. a heat diffusion equation, and can be formulated as a Hamiltonian system. Nevertheless one has to use a different Hamiltonian function than the potential (1), defined as:

$$\mathcal{H}(\phi) = \int_{\Omega} \frac{1}{2} \phi^2 dV, \quad (5)$$

along with the conservation law:

$$\frac{\partial \phi}{\partial t} + \text{div } j_\phi = 0, \quad (6)$$

where j_ϕ denotes the non-conserved flux given by:

$$j_\phi = -\Gamma_\phi \text{grad } \frac{\delta \mathcal{H}}{\delta \phi}. \quad (7)$$

Then the Hamiltonian representation of the Allen–Cahn equation (4) is given by:

$$\begin{pmatrix} \frac{\partial \phi}{\partial t} + \frac{\partial g}{\partial \phi}(\phi) \\ F_\phi \end{pmatrix} = \begin{pmatrix} 0 & -\text{div} \\ -\text{grad} & 0 \end{pmatrix} \begin{pmatrix} \frac{\delta \mathcal{H}}{\delta \phi} \\ j_\phi \end{pmatrix}, \quad (8)$$

where F_ϕ denotes the thermodynamic phase flux. The Hamiltonian function (5) is not physically based as the potential function (1). Therefore, the contribution due to the density potential function $g(\phi)$ is not included as an effort term but arises in the left hand side of equation (8) as a distributed source term. This implies the definition of non-physical port variables and motivates the formulation of an extended port Hamiltonian representation of the Allen–Cahn equation (4).

2.3 Conserved phase field variable

Dynamics of a conserved phase field variable $c(t, z) \in [0, 1]$, are governed by a balance equation of the following form:

$$\frac{\partial c}{\partial t}(t, z) + \text{div } j_c(t, z) = 0, \quad (9)$$

where the phase field flux $j_c(t, z) \in C^\infty(\Omega, \mathbb{R}^3)$ is closed by the following linear transport relation:

$$j_c = -\Gamma_c(z) \text{grad} \left(\frac{\delta \mathcal{G}}{\delta c}(c) \right), \quad (10)$$

where $\Gamma_c(z) \in C^\infty(\Omega, \mathbb{R}^+)$ represents the phase field diffusion coefficient. After injecting the phase field flux (10)

into the conservation law (9), with the variational derivative (3), one finds the Cahn–Hilliard equation (Cahn and Hilliard, 1958):

$$\frac{\partial c}{\partial t} = \operatorname{div} \left(\Gamma_c \operatorname{grad} \left(-\operatorname{div}(\kappa_c \operatorname{grad} c) + \frac{\partial g}{\partial c} \right) \right), \quad (11)$$

where time and space dependences on the state variable and coefficients are omitted. To define a Cauchy problem we add initial conditions $c(0, z) = c_0(z)$ for all $z \in \Omega$ and boundary conditions on $\partial\Omega$ to the phase field equation (11).

Remark 2. Similarly to the Allen–Cahn equation, the Cahn–Hilliard equation (11) can be represented as a Hamiltonian system. Indeed we have a conservation law (9) which can be formulated with the same operator as in equation (8):

$$\begin{pmatrix} \frac{\partial c}{\partial t} \\ F_c \end{pmatrix} = \begin{pmatrix} 0 & -\operatorname{div} \\ -\operatorname{grad} & 0 \end{pmatrix} \begin{pmatrix} \frac{\delta \mathcal{G}}{\delta c} \\ F_c \end{pmatrix}, \quad (12)$$

with the thermodynamic force F_c is defined as:

$$F_c = -\operatorname{grad} \frac{\delta \mathcal{G}}{\delta c}. \quad (13)$$

One should note the presence of differential operators in the functional derivative (3). This motivates the formulation of an alternative Hamiltonian formulation of the Cahn–Hilliard equation (11) where the extended representation includes all differential terms in the structure.

Both conserved and non-conserved phase field variables can be present in the same dynamical system. This will be illustrated with a solidification process in Section 6.

3. PORT HAMILTONIAN SYSTEMS AND STOKES–DIRAC STRUCTURES

The port Hamiltonian formulation of infinite-dimensional systems relies on the definition of a Stokes–Dirac structure (van der Schaft and Maschke, 2002). Hereby we recall the definition needed for the structured representation of the Cahn–Hilliard (11) and the Allen–Cahn (4) equations. Consider an n -dimensional space $\mathcal{F} \subset \mathbb{R}$ and $\mathcal{E} = \mathcal{F}'$ its dual, i.e. the space of linear operator $e : \mathcal{F} \rightarrow \mathbb{R}$. The elements of $f \in \mathcal{F}$ and of $e \in \mathcal{E}$ are called flows and efforts, respectively. The pair of boundary port variables (e^∂, f^∂) are defined in the boundary spaces \mathcal{E}^∂ and \mathcal{F}^∂ , respectively. Power is defined with the dual product between e and f as $\langle e, f \rangle = e(f)$. The space of power variables is given by:

$$\mathcal{B} = \{(f, f^\partial, e, e^\partial) \in \mathcal{F} \times \mathcal{F}^\partial \times \mathcal{E} \times \mathcal{E}^\partial\}, \quad (14)$$

such that the duality pairing between elements of \mathcal{B} is defined as:

$$\begin{aligned} \langle \langle (f_1, f_1^\partial, e_1, e_1^\partial), (f_2, f_2^\partial, e_2, e_2^\partial) \rangle \rangle = \\ \langle e_1, f_2 \rangle + \langle e_2, f_1 \rangle + \langle e_1^\partial, f_2^\partial \rangle_{\partial\Omega} + \langle e_2^\partial, f_1^\partial \rangle_{\partial\Omega}. \end{aligned} \quad (15)$$

Definition 1

Le Gorrec et al. (2005) A Stokes–Dirac structure \mathcal{D} on the bond space \mathcal{B} is a subspace of \mathcal{B} which is maximally isotropic with respect to the canonical symmetrical pairing (15), i.e. $\mathcal{D} = \mathcal{D}^\perp$, where \mathcal{D}^\perp denotes the orthogonal subspace of \mathcal{D} with respect to the pairing (15).

Port Hamiltonian systems defined by the state variable $x(t) \in \mathcal{F}$, the potential function $\mathcal{H}(x(t)) \in \mathcal{E}$ with

boundary port variables $\zeta(t) \in \mathcal{Z}$. Then the port Hamiltonian system is defined by the Stokes–Dirac structure

$$\left(-\dot{x}(t), f^\partial, \frac{\delta \mathcal{H}}{\delta x}(x(t)), e^\partial \right) \in \mathcal{D}. \quad (16)$$

Dirac structures are defined for various physical applications. For details and properties concerning their composition one can refer to (Duindam et al., 2009). The case of a system with two conservations laws is discussed in (Kotyczka et al., 2018). Dirac structures are also defined on Hilbert spaces (Kurula et al., 2010).

4. PORT HAMILTONIAN FORMULATION OF NON-CONSERVED PHASE FIELDS

Consider the model of a non-conserved phase field variable $\phi(t, z) \in C^\infty(\Omega, [0, 1])$ defined with the storage function (1) and the gradient equation (2). To emphasize the linear structure behind the phase field model we augment the system. This is a modeling technique already used for port Hamiltonian systems (see example 4.3 in Maschke and van der Schaft (2005)). The state space representation (4) is augmented as:

$$\begin{pmatrix} \phi \\ \psi \end{pmatrix} \triangleq \begin{pmatrix} \phi \\ \operatorname{grad} \phi \end{pmatrix} \in C^\infty(\Omega, [0, 1]) \times C^\infty(\Omega, \mathbb{R}^3), \quad (17)$$

Hence the potential (1) is re-written as:

$$\bar{\mathcal{G}}(\phi, \psi) = \int_{\Omega} \frac{\kappa_\phi}{2} \psi^2 + g(\phi) dV. \quad (18)$$

Furthermore we introduce the new distributed parameter $E_\phi(t, z) \in C^\infty(\Omega, \mathbb{R})$ given by:

$$E_\phi(t, z) = \Gamma_\phi(z) F_\phi(t, z), \quad (19)$$

where $F_\phi(t, z) \in C^\infty(\Omega, \mathbb{R})$ denotes the variational derivative of the potential function (3) expressed in terms of the new pair of variables (17) as:

$$F_\phi = \frac{\delta \bar{\mathcal{G}}}{\delta \phi} - \operatorname{div} \left(\frac{\delta \bar{\mathcal{G}}}{\delta \psi} \right). \quad (20)$$

The gradient equation (2) is now:

$$\frac{\partial \phi}{\partial t}(t, z) = -E_\phi(t, z). \quad (21)$$

The time variation of the second variable $\psi(t, z) \in C^\infty(\Omega, \mathbb{R}^3)$ is given by

$$\frac{\partial \psi}{\partial t}(t, z) = \frac{\partial}{\partial t} \operatorname{grad} \phi(t, z). \quad (22)$$

The gradient operator and the time derivative commute since $\phi(t, z) \in C^\infty(\Omega, [0, 1])$, and plugging equation (21) in (22) one obtains:

$$\frac{\partial \psi}{\partial t}(t, z) = -\operatorname{grad} E_\phi(t, z). \quad (23)$$

The balance equation of the potential function (18) is given by:

$$\frac{d\bar{\mathcal{G}}}{dt} = - \int_{\Omega} E_\phi F_\phi dV - \int_{\partial\Omega} \vec{n} \frac{\delta \bar{\mathcal{G}}}{\delta \psi} E_\phi dS, \quad (24)$$

where we have used the state equations (21) and (23), and applied integration by parts and Stokes' theorem. The outward unit normal vector acting on the boundary $\partial\Omega$ is denoted \vec{n} . One identifies a distributed dissipative term, due to the interface diffusion in the all domain Ω , in the first integral term in equation (24). The second term in the right hand side of equation (24) denotes the potential

variation due to the exchanges through the boundary $\partial\Omega$. With the state equations (21) and (23), and the closure relation (19), one identifies the following implicit structured representation:

$$f_\phi = \mathcal{J}_\phi e_\phi, \quad (25)$$

where the flow variable f_ϕ and the effort variables e_ϕ are

$$f_\phi^\top = \left(\frac{\partial\phi}{\partial t}, \frac{\partial\psi}{\partial t}, F_\phi \right)^\top \in \mathcal{F}_\phi, \quad (26)$$

where $\mathcal{F}_\phi = C^\infty(\Omega, \mathbb{R}) \times C^\infty(\Omega, \mathbb{R}^3)^2$ and

$$e_\phi^\top = \left(\frac{\delta\bar{\mathcal{G}}}{\delta\phi}, \frac{\delta\bar{\mathcal{G}}}{\delta\psi}, E_\phi \right)^\top \in \mathcal{E}_\phi, \quad (27)$$

where $\mathcal{E}_\phi = C^\infty(\Omega, \mathbb{R}) \times C^\infty(\Omega, \mathbb{R}^3) \times C^\infty(\Omega, \mathbb{R})$, respectively. Furthermore the linear operator \mathcal{J}_ϕ takes the following form:

$$\mathcal{J}_\phi = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & -grad \\ 1 & -div & 0 \end{pmatrix}. \quad (28)$$

With the functional (24) we identify the following pair of boundary port variables

$$\begin{pmatrix} f_\phi^\partial \\ e_\phi^\partial \end{pmatrix} = \begin{pmatrix} 0 & -\vec{n} \cdot 0 \\ 0 & 0 & 1 \end{pmatrix} e_\phi|_{\partial\Omega} = \begin{pmatrix} -\vec{n} \frac{\delta\bar{\mathcal{G}}}{\delta\psi} \\ E_\phi \end{pmatrix}, \quad (29)$$

Boundary port variables f_ϕ^∂ and e_ϕ^∂ are defined in the linear spaces of boundary flows and efforts $\mathcal{F}_\phi^\partial = C^\infty(\partial\Omega, \mathbb{R}^3)$ and $\mathcal{E}_\phi^\partial = C^\infty(\partial\Omega, \mathbb{R})$, respectively. Finally, the space of power variables is the Cartesian product of the bulk and boundary efforts and flow variables:

$$\mathcal{B}_\phi = \{ (f_\phi, f_\phi^\partial, e_\phi, e_\phi^\partial) \in \mathcal{F}_\phi \times \mathcal{F}_\phi^\partial \times \mathcal{E}_\phi \times \mathcal{E}_\phi^\partial \}. \quad (30)$$

The duality pairing between elements of \mathcal{B}_ϕ is defined as:

$$\begin{aligned} & \langle \langle (f_\phi^1, f_\phi^{1\partial}, e_\phi^1, e_\phi^{1\partial}), (f_\phi^2, f_\phi^{2\partial}, e_\phi^2, e_\phi^{2\partial}) \rangle \rangle = \\ & \langle e_\phi^1, f_\phi^2 \rangle + \langle e_\phi^2, f_\phi^1 \rangle + \langle e_\phi^{1\partial}, f_\phi^{2\partial} \rangle_{\partial\Omega} + \langle e_\phi^{2\partial}, f_\phi^{1\partial} \rangle_{\partial\Omega}. \end{aligned} \quad (31)$$

Let us formally show that the non-conserved phase field model is equipped with a Stokes–Dirac structure.

Proposition 1

Consider the space of power variables \mathcal{B}_ϕ , the bilinear product $\langle \cdot, \cdot \rangle$, and the linear operator \mathcal{J}_ϕ defined in (30), (31), and (28), respectively. Then the following linear subspace $\mathcal{D}_\phi \subset \mathcal{B}_\phi$:

$$\mathcal{D}_\phi = \left\{ \begin{pmatrix} \left(\begin{pmatrix} f_\phi \\ f_\phi^\partial \end{pmatrix}, \begin{pmatrix} e_\phi \\ e_\phi^\partial \end{pmatrix} \right) \in \mathcal{B}_\phi \text{ s.t.} \\ f_\phi = \mathcal{J}_\phi e_\phi, \left(\begin{pmatrix} f_\phi^\partial \\ e_\phi^\partial \end{pmatrix} \right) = \mathcal{W}_\phi e_\phi|_{\partial\Omega} \end{pmatrix} \right\}, \quad (32)$$

is a Stokes–Dirac structure.

Proof 1. The linear operator \mathcal{J}_ϕ is skew-symmetric. Following (van der Schaft and Maschke, 2002) one shows that the subspace \mathcal{D}_ϕ is a Dirac structure, *i.e.* $\mathcal{D}_\phi = \mathcal{D}_\phi^\perp$ where \mathcal{D}_ϕ^\perp denotes the orthogonal complement with respect to the bilinear form (31).

Remark 3. Integrations over the domain Ω and its boundary $\partial\Omega$, *e.g.* the potential balance equation (24), are independent on the interface position. This is a major difference with the traditional way of modeling moving interface systems where the domain of integration moves with the interface (Diagne and Maschke, 2013). Hence

the Stokes–Dirac structure (32), and by extension the port Hamiltonian system is defined independently of the interface position.

To summarize, the structured model of a non-conserved phase field is defined by the states (ϕ, ψ) , with the Hamiltonian function (18) and the Stokes–Dirac structure:

$$\left(\frac{\partial\phi}{\partial t}, \frac{\partial\psi}{\partial t}, F_\phi, f_\phi^\partial, \frac{\delta\bar{\mathcal{G}}}{\delta\phi}, \frac{\delta\bar{\mathcal{G}}}{\delta\psi}, E_\phi, e_\phi^\partial \right) \in \mathcal{D}_\phi \quad (33)$$

where F_ϕ and E_ϕ are closed by the algebraic equation (19). Boundary conditions f_ϕ^∂ and e_ϕ^∂ are defined by the relation (29). They physically represent the gradient of the phase field variable passing through the boundary $\partial\Omega$ and the functional derivative of the potential function.

5. PORT HAMILTONIAN FORMULATION OF CONSERVED PHASE FIELDS

Consider now the case of conserved phase field variables as introduced in Section 2.3. The same methodology as for the non-conserved case is followed. Let us introduce the augmented state variables:

$$\begin{pmatrix} c \\ \gamma \end{pmatrix} \triangleq \begin{pmatrix} c \\ grad c \end{pmatrix} \in C^\infty(\Omega, \mathbb{R}) \times C^\infty(\Omega, \mathbb{R}^3), \quad (34)$$

such that the potential (1) is now given by:

$$\bar{\mathcal{G}}(c, \gamma) = \int_\Omega g(c) + \frac{\kappa_c}{2} \gamma^2 dV. \quad (35)$$

The phase field variable c is governed by the following balance equation (9):

$$\frac{\partial c}{\partial t} = -div j_c, \quad (36)$$

and the state equation associated to the variable γ is given by:

$$\frac{\partial \gamma}{\partial t} = -grad (div j_c), \quad (37)$$

where we have used the definition of γ , and the balance equation (36). The gradient operator and the time derivative commute since $c(t, z) \in C^\infty(\Omega, [0, 1])$. The phase field flux $j_c \in C^\infty(\Omega, \mathbb{R}^3)$ is closed by a linear transport relation (10),

$$j_c = \Gamma_c F_c, \quad (38)$$

where $F_c \in C^\infty(\Omega, \mathbb{R}^3)$ denotes the phase field thermodynamic force:

$$F_c = -grad \left(\frac{\delta\bar{\mathcal{G}}}{\delta c} - div \frac{\delta\bar{\mathcal{G}}}{\delta \gamma} \right). \quad (39)$$

Remark 4. With the structure representation of conserved phase field variables the constitutive relation (38) is an algebraic equation. The differential part of the closure equation is gathered in the thermodynamic force (39) which will be included in the Stokes–Dirac Structure.

The balance equation of the potential function (35) enables us to identify the boundary port variables and is given by:

$$\begin{aligned} \frac{d\bar{\mathcal{G}}}{dt} = & - \int_{\partial\Omega} \vec{n} \left(-j_c div \frac{\delta\bar{\mathcal{G}}}{\delta \gamma} + \frac{\delta\bar{\mathcal{G}}}{\delta \gamma} div j_c + \frac{\delta\bar{\mathcal{G}}}{\delta c} j_c \right) dS \\ & - \int_\Omega j_c F_c dV, \end{aligned} \quad (40)$$

where we have derived $\bar{\mathcal{G}}$ along the states trajectories defined by the state equations (36) and (37), and applied

two integrations by parts. The balance equation (36), the state equation (37) and the closure relation (38) are gathered in the following unique equation:

$$f_c = \mathcal{J}_c e_c. \quad (41)$$

Let us define the linear operator \mathcal{J}_c :

$$\mathcal{J}_c = \begin{pmatrix} 0 & 0 & -\text{div}(\cdot) \\ 0 & 0 & -\text{grad}(\text{div}(\cdot)) \\ -\text{grad}(\cdot) & \text{grad}(\text{div}(\cdot)) & 0 \end{pmatrix}. \quad (42)$$

The vector of flows f_c and effort e_c variables are defined as:

$$f_c^\top = \left(\frac{\partial c}{\partial t}, \frac{\partial \gamma}{\partial t}, F_c \right)^\top \in \mathcal{F}^c, \quad (43)$$

with $\mathcal{F}^c = C^\infty(\Omega, \mathbb{R}) \times C^\infty(\Omega, \mathbb{R}^3)^2$, and

$$e_c^\top = \left(\frac{\delta \bar{\mathcal{G}}}{\delta c}, \frac{\delta \bar{\mathcal{G}}}{\delta \gamma}, j_c \right)^\top \in \mathcal{E}_c, \quad (44)$$

with $\mathcal{E}_c = C^\infty(\Omega, \mathbb{R}) \times C^\infty(\Omega, \mathbb{R}^3)^2$, respectively. One identifies in the balance equation (40) the following boundary port variables:

$$\begin{pmatrix} f_c^\partial \\ e_c^\partial \end{pmatrix} = \begin{pmatrix} 0 & \text{div} & 0 \\ 0 & 0 & -\text{div} \\ -1 & 0 & 0 \\ 0 & 0 & \vec{n} \\ 0 & \vec{n} & 0 \\ 0 & 0 & \vec{n} \end{pmatrix} e_c|_{\partial\Omega}, \quad (45)$$

where $\mathcal{E}_c^\partial \in C^\infty(\partial\Omega, \mathbb{R}^3)^2 \times C^\infty(\partial\Omega, \mathbb{R})$ and $\mathcal{F}_c^\partial \in C^\infty(\partial\Omega, \mathbb{R}^3)^3$.

Remark 5. The choice of boundary port variable is consistent with the balance equation (40), but other boundary port variables are possible (Le Gorrec et al., 2005).

The space of power variables is given by the:

$$\mathcal{B}_c = \{ (f_c, f_c^\partial, e_c, e_c^\partial) \in \mathcal{F}_c \times \mathcal{F}_c^\partial \times \mathcal{E}_c \times \mathcal{E}_c^\partial \}. \quad (46)$$

The duality pairing between elements of \mathcal{B}_c is defined as:

$$\begin{aligned} \langle \langle (f_c^1, f_c^{1\partial}, e_c^1, e_c^{1\partial}), (f_c^2, f_c^{2\partial}, e_c^2, e_c^{2\partial}) \rangle \rangle = \\ \langle e_c^1, f_c^2 \rangle + \langle e_c^2, f_c^1 \rangle + \langle e_c^{1\partial}, f_c^{2\partial} \rangle_{\partial\Omega} + \langle e_c^{2\partial}, f_c^{1\partial} \rangle_{\partial\Omega}. \end{aligned} \quad (47)$$

Let us show that the conserved phase field model has a Stokes–Dirac structure.

Proposition 2

Consider the space of power variables \mathcal{B}_c , the bilinear product $\langle \langle \cdot, \cdot \rangle \rangle$, and the linear operator \mathcal{J}_c defined in (46), (47), and (42), respectively. The following linear subspace $\mathcal{D}_c \subset \mathcal{B}_c$:

$$\mathcal{D}_c = \left\{ \begin{pmatrix} \left(\begin{pmatrix} f_c \\ f_c^\partial \end{pmatrix}, \begin{pmatrix} e_c \\ e_c^\partial \end{pmatrix} \right) \in \mathcal{B}_c \text{ s. t.} \\ f_c = \mathcal{J}_c e_c, \left(\begin{pmatrix} f_c^\partial \\ e_c^\partial \end{pmatrix} = \mathcal{W}_c e_c|_{\partial\Omega} \end{pmatrix} \right\} \quad (48)$$

is a Stokes–Dirac structure.

Proof 2. The sketch of the proof follows the following two steps. Firstly, one can easily show the skew-symmetry of the second order linear operator \mathcal{J}_c defined at equation (42). Secondly, following (van der Schaft and Maschke, 2002), one can prove that the subspace \mathcal{D}_c is a Dirac structure, i.e. $\mathcal{D}_c = \mathcal{D}_c^\perp$ where \mathcal{D}_c^\perp denotes the orthogonal complement with respect to the bilinear form (47). The first step consists of verifying $\mathcal{D}_c \subset \mathcal{D}_c^\perp$. The second step aims at showing that $\mathcal{D}_c^\perp \subset \mathcal{D}_c$.

To summarize the structured model of a conserved phase field is defined by the state variables (c, γ) , the Hamiltonian function (1), and the following Stokes–Dirac structure:

$$\left(\frac{\partial c}{\partial t}, \frac{\partial \gamma}{\partial t}, F_c, f_c^\partial, \frac{\delta \bar{\mathcal{G}}}{\delta c}, \frac{\delta \bar{\mathcal{G}}}{\delta \gamma}, j_c, e_c^\partial \right) \in \mathcal{D}_c, \quad (49)$$

where F_c and j_c are closed by equation (38). Boundary terms are defined at equation (45).

6. EXAMPLE OF A SOLIDIFICATION PROCESS

Let us consider the solidification process proposed in Elder et al. (2001), where the spatial domain is labelled $\Omega \subset \mathbb{R}^3$ with its boundary $\partial\Omega \subset \mathbb{R}^2$. This binary concentration solidification process is achieved at uniform and constant temperature denoted T . This system possesses two phases: a solid phase and a liquid one. Two fields are used to represent the dynamics of this system: $\phi \in C^\infty(\Omega, [0, 1])$ a non-conserved phase-field, and $c \in C^\infty(\Omega, [0, 1])$ a conserved phase-field. The phase field c can be seen as a concentration. The potential used to drive the system's dynamics, here the Gibb's free energy is given by the integral

$$\mathcal{G}(\phi, c) = \int_{\Omega} G(\phi, c) dz, \quad (50)$$

with the density function:

$$G(\phi, c) = \frac{1}{2} \kappa_\phi (\text{grad } \phi)^2 + \frac{1}{2} \kappa_c (\text{grad } c)^2 + g(\phi, c). \quad (51)$$

The local bulk potential density $g(\phi, c)$ is defined as:

$$g(\phi, c) = -a \frac{T}{T_m} h(c) + k(\phi, c), \quad (52)$$

where the first term is function of the conserved field c and is pre-multiplied to the scalar coefficient $a \in \mathbb{R}$ and the ratio between the uniform temperature T and the melting temperature T_m . The second term on the right hand side of equation (52) denotes the free entropy associated to the diffusive interface. The function $h(c)$ defines the entropy of a random mixing for binary solutions, and is defined as $h(c) = -Rn [c \ln c + (1-c) \ln(1-c)]$, where R is the ideal gas constant, and n denotes the total moles number in the system. The mixing function $k(\phi, c)$ is given by:

$$k(\phi, c) = \left(\alpha \Delta T - \beta \left(c - \frac{1}{2} \right)^2 \right) \Phi(\phi) - \frac{1}{2} \phi^2 + \frac{1}{4} \phi^4, \quad (53)$$

where $\Phi(\phi) = 2\phi - \frac{4}{3}\phi^3 + \frac{2}{5}\phi^5$, $\Delta T = (T - T_m)/T_m$ denotes the normalized temperature, and parameters α, β and $u \in \mathbb{R}$ are empiric scalar parameters. With the potential function (50) one associates the Allen–Cahn equation (4) and the Cahn–Hilliard equation (11). Both phase field variables are initialized at time $t = 0$ as $c(0, z) = c_0(z) \in C^\infty(\Omega)$ and $\phi(0, z) = \phi_0(z) \in C^\infty(\Omega)$. The port Hamiltonian formulation naturally follows from the development of Sections 4 and 5 where one considers the augmented state variable: $(\phi, \psi, c, \gamma) \triangleq (\phi, \text{grad } \psi, c, \text{grad } c)$, with the reformulated potential (50):

$$\bar{\mathcal{G}}(\phi, \psi, c, \gamma) = \int_{\Omega} \frac{\kappa_\phi}{2} \psi^2 + \frac{\kappa_c}{2} \gamma^2 + g(\phi, c) dz. \quad (54)$$

Then the system under its structured representation is expressed as

$$f_s = \begin{pmatrix} \mathcal{J}_\phi & 0 \\ 0 & \mathcal{J}_c \end{pmatrix} e_s, \quad (55)$$

where flow and effort are defined as:

$$f_s^\top = \left(\frac{\partial \phi}{\partial t}, \frac{\partial \psi}{\partial t}, F_\phi, \frac{\partial c}{\partial t}, \frac{\partial \gamma}{\partial t}, F_c \right)^\top \quad (56)$$

and

$$e_s^\top = \left(\frac{\delta \bar{\mathcal{G}}}{\delta \phi}, \frac{\delta \bar{\mathcal{G}}}{\delta \psi}, E_\phi, \frac{\delta \bar{\mathcal{G}}}{\delta c}, \frac{\delta \bar{\mathcal{G}}}{\delta \gamma}, j_c \right)^\top, \quad (57)$$

respectively. From Proposition 1 and 2 it follows that the solidification example is a port Hamiltonian system with the boundary port variables defined for each sub-systems, see equations (29) and (45).

Remark 6. The coupling is intrinsically defined in the potential function (52). Thus there is no shared (boundary) port variables between the conserved and non-conserved sub-systems. This is where the phase field modeling approach differs from sharp interface models (Diagne and Maschke, 2013).

7. CONCLUSION

In this contribution we have introduced the formulation of phase field models as boundary control port Hamiltonian systems. The originality of this work resides in the presence of an underlying structure within the thermodynamic fluxes. The idea is to extend the system's state on their jet spaces (Maschke and van der Schaft, 2005) such that the port Hamiltonian systems of phase field models are defined along side algebraic constitutive relations. The conserved and non-conserved structured representation can be applied to multi-phase problems with moving interfaces. In Section 6 the problem of solidification was addressed.

Outgoing work includes the boundary control (Duindam et al., 2009) of the interface position in a pure substance solidification process (Wang et al., 1993).

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