Modélisation par Champ de Phase de la Solidification de l'eau : Une Approche Hamiltonienne à Port

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Phase Field Modeling of Water Solidification: A Port Hamiltonian Approach

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Abstract

This thesis presents a study on modeling, formulating, and discretizing solidification processes using the Port Hamiltonian framework combined with the phase field approach. The goal is to provide numerical models suitable for simulating, designing, and controlling such processes. It addresses the challenges of representing and controlling phase change phenomena in distributed parameter models with moving interfaces, with a particular focus on the solidification of pure water. The work has been motivated by the development of green processes for water purification technologies such as cyclic melt and crystallization of water, which offer a low-energy solution while minimizing the use of hazardous materials.

The first chapter recalls briefly the physical models of multiphase systems and the description of the interface between the phases, in terms of thin or diffuse interfaces. It presents the phase field theory and the associated thermodynamical models of the multiphase systems. Finally, it expresses the dynamics of solidification processes as a coupled system of evolution equations consisting of the Allen-Cahn equation and energy balance equations. A main contribution of this chapter consists in a comprehensive presentation of solidification using the entropy functional approach within the phase field framework.

In the second chapter, the Port Hamiltonian formulation of the dynamics of solidification processes using the phase field approach is developed. This chapter introduces Boundary Port Hamiltonian Systems and shows how an extension of the state space to the gradient of the phase field variable leads to a Port Hamiltonian formulation of the solidification model. The model is written in such a way that it utilizes the available thermodynamic data for liquid water and ice, allowing for a detailed and physically-based modeling, leading to an implicit Boundary Port Hamiltonian model.

The final chapter focuses on the structure-preserving discretization of the solidification process using the Partitioned Finite Element Method. This ensures that the discretized model retains the Port Hamiltonian structure and, in turn, the key properties such as energy conservation and passivity. The chapter covers weak formulations, projections, and discrete Hamiltonians for the heat equation and the Allen-Cahn equation, leading to the spatial discretization of the solidification model. The principal contribution of this chapter lies in the discretization methodology applied to the implicit Port Hamiltonian model of the solidification process using entropy as the generating function.

Overall, this thesis provides structured models of solidification processes using the Port Hamiltonian framework, providing a foundation for their physics-based simulation and control and for future research and development in distributed parameter systems with moving interfaces, particularly for environmental and chemical engineering applications.

Keywords: Distributed Parameter Systems, Port Hamiltonian systems, Boundary Port Hamiltonian Systems, Moving Interfaces, Solidification Processes, Diffuse Interfaces, Phase Field Approach, Allen-Cahn Equation, Heat Diffusion Equation, Structure-Preserving Discretization, Partitioned Finite Element Method

Résumé

Cette thèse présente une étude sur la modélisation, la formulation par le formalisme des Systèmes Hamiltoniens à ports et la discrétisation des processus de solidification dont l'interface est supposée diffuse et est modélisée par l'approche des champs de phase. Ses travaux traitent en détail de la solidification de l'eau dans le contexte de fournir des modèles numériques adaptés à la simulation, à la conception et au contrôle de procédés de purification de l'eau.

Le premier chapitre rappelle d'abord de manière synthétique les modèles physiques de systèmes biphasique et de leur interface. Il présente ensuite en détail l'approche des champs de phase pour la modélisation des interfaces diffuses ainsi que le modèle thermodynamique du système biphasique. Puis il rappelle le modèle dynamique de la solidification d'une espèce, en particulier de l'eau, comme un système de deux équations d'évolution, l'équation d'Allen-Cahn et l'équation de bilan d'énergie. Ces modèles sont basés sur les propriétés thermodynamiques employant l'entropie totale comme potentiel thermodynamique.

Dans le deuxième chapitre, après le rappel de la définition de systèmes hamiltoniens dissipatifs à port frontière, on rappelle que l'on peut formuler l'équation d'Allen-Cahn ainsi que le modèle de solidification complet sous cette forme, en augmentant les variables d'état avec le gradient de la variable de champ de phase. Puis l'on montre que les relations thermodynamiques issues des données sont exprimées en termes de variables intensives et mènent à une formulation hamiltonienne à port implicite.

Le dernier chapitre se concentre sur la discrétisation préservant la structure du processus de solidification en utilisant la Méthode des Éléments Finis Partitionnés. Cela garantit que le modèle discrétisé conserve des propriétés clés telles que la conservation de l'énergie et la passivité. Le chapitre développe les formulations faibles, les projections et les hamiltoniens discrets pour l'équation de la chaleur et l'équation d'Allen-Cahn, puis développe la discrétisation du modèle de solidification complet. La principale contribution de ce chapitre réside dans la méthodologie de discrétisation appliquée au modèle Port Hamiltonien implicite du processus de solidification en utilisant l'entropie comme fonction génératrice.

Globalement, cette thèse propose une approche pour la modélisation, la simulation et le contrôle des processus de solidification en utilisant le cadre Hamiltoniens à ports. Les résultats posent une base complète pour de futures recherches et développements dans les systèmes à paramètres distribués avec interfaces mobiles, en particulier pour les applications en ingénierie environnementale et chimique.

Mots-clés: Systèmes à Paramètres Distribués, Systèmes Hamiltoniens à Port frontière, Interfaces Mobiles, Processus de Solidification, Interfaces Diffuses, Approche par Champ de Phase, Équation d'Allen-Cahn, Équation de Diffusion Thermique, Méthode des Éléments Finis Partitionnés

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— John F. Kennedy

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Résumé étendu

Cette thèse traite des modèles de paramètres distribués de systèmes biphasiques interagissant à travers des interfaces mobiles. De tels systèmes apparaissent dans les procédés de cristallisation, les évaporateurs, les condensateurs, la séparation de phase par décomposition spinodale ou les procédés d'extrusion [23]. Leurs modèles dynamiques consistent en des systèmes d'équations aux dérivées partielles (EDP) résultant des équations de bilan de chaque phase, couplés à un système dynamique décrivant l'interface mobile. L'interface est une région étroite séparant deux régions spatiales d'états matériels différents. Il existe de nombreuses façons de modéliser l'interface comme le problème de Stefan à deux phases qui décrit les processus de changement de phase tels que la solidification et la fusion [79] ou les modèles d'interface mince [109]. Des études antérieures comme celles de [40], [21] et [52], ont discuté en détail de la modélisation et du contrôle de tels processus.

La représentation d'une interface mobile varie des interfaces nettes aux interfaces diffuses. Dans l'approche d'interface nette, certaines variables d'intérêt sont discontinues à l'interface en raison des conditions aux limites imposées, et l'interface doit être suivie [99]. En revanche, dans l'approche d'interface diffuse, suivant les idées de Gibbs, les variables varient rapidement mais de façon continue le long de l'épaisseur de l'interface. Les différentes phases sont différenciées par un paramètre d'ordre qui varie continument d'une valeur à une autre[1] le long de l'épaisseur de l'interface. La dynamique de cette variable de phase est régie par une équation aux dérivées partielles : l'équation d'Allen-Cahn dans le cas de la solidification.

L'approche de champ de phase est largement utilisée en physique et en science des matériaux [98]. À notre connaissance, elle est très peu utilisée en génie des procédés. Récemment, certaines applications ont émergé dans ce domaine, telles que le projet WATERSAFE [31], qui est une application motivant ce travail. Il traite d'un nouveau processus de purification de l'eau par congélation, visant spécifiquement à éliminer les polluants solubles à faible concentration des effluents liquides aqueux.

Le travail proposé concerne la modélisation de la solidification de l'eau en suivant l'approche d'interface diffuse par la méthode des champs de phase basée sur les travaux de [110].

En raison de la nature thermodynamique du processus de congélation et de la méthode de champ de phase, le cadre port-Hamiltonien semble utile dans ce contexte à des fins de modélisation, pour faciliter l'interconnexion avec un environnement macroscopique, pour la simulation ou même pour la synthèse de contrôle. En effet, cette approche encode directement les principes physiques sous-jacents, tels que les lois de conservation, dans la structure géométrique du modèle du système, ainsi que dans les conditions aux limites. De plus, la structure géométrique peut être facilement réduite spatialement pour obtenir des modèles hamiltoniens de dimension finie, qui sont ensuite facilement adaptables à la simulation. Enfin, la synthèse de commande basés sur la passivité peut être facilement appliquée aux systèmes port-Hamiltoniens, qui sont naturellement passifs [70]. Dans ce travail, nous développons une formulation port-Hamiltonienne, qui fournit un cadre théorique systémique pour la réduction d'ordre de modèle et le contrôle basé sur la passivité, en s'appuyant sur les méthodologies décrites par [70], [75], [7], et [93].

[1] par exemple de 0 à 1 où 0 et 1 représentent les deux phases

Les systèmes port-Hamiltoniens (PHS) sont utilisés pour modéliser et contrôler les systèmes physiques impliquant des échanges d'énergie [61], [63]. Ils combinent des éléments qui stockent l'énergie, dissipent l'énergie et acheminent l'énergie dans un cadre cohérent [84]. Les PHS sont définis par l'interaction entre une structure de Dirac et une fonction hamiltonienne [18]. La structure de Dirac définit comment l'énergie circule dans le système, tandis que la fonction hamiltonienne représente l'énergie totale du système [16, 86]. Au cours de la dernière décennie, ce cadre de modélisation puissant a été utilisé pour une large gamme de systèmes physiques de dimension infinie tels que les systèmes électriques, mécaniques, électromécaniques, hydrauliques et de génie chimique multiphasique où des phénomènes de transfert de chaleur et de masse se produisent. Il a également été appliqué pour représenter des systèmes à interface mobile [23, 24] ainsi que des systèmes port-Hamiltoniens implicites définis sur des sous-espaces de Lagrange dans des espaces de Hilbert [88, 105]. Les détails du cadre PHS et son application au processus de solidification sont largement discutés au chapitre 3 de cette thèse.

Le premier objectif de cette thèse est d'utiliser l'procha hamiltonienne à port pour modéliser les processus de solidification en combinant l'équation d'Allen-Cahn (pour les changements de phase) avec l'équation de la chaleur (pour la conduction thermique). Deux approches principales ont été explorées dans le cadre PH : le modèle d'interface mince et le modèle d'interface diffuse. Le modèle d'interface mince, étudié par [24], et [28], fournit une représentation simplifiée de la dynamique de l'interface. En revanche, le modèle d'interface diffuse, basé sur les travaux de [110], offre une description plus détaillée du comportement de l'interface. Cette thèse suit l'approche d'interface diffuse. Le modèle utilise la fonction de densité d'entropie comme fonction génératrice, qui dépend de la variable de phase ϕ et de l'énergie interne u, pour décrire la dynamique couplée des changements de phase et du transfert de chaleur [110]. Nous utilisons des systèmes port-Hamiltoniens implicites définis sur des sous-espaces de Lagrange pour exprimer la fonctionnelle de densité d'entropie en termes de température réciproque τ et de la variable de champ de phase ϕ comme donné dans les tables de [42, 43].

Le deuxième objectif est de formuler les systèmes PH des processus de solidification basés sur ces modèles thermodynamiques. Ces modèles affinés sont discrétisés en utilisant une formulation implicite. Cette approche, dérivée des modèles thermodynamiques non linéaires, vise à préserver la structure et les propriétés du système continu d'origine pendant les simulations numériques.

Ce travail met également en évidence l'importance de maintenir l'intégrité structurelle des systèmes PH pendant la discrétisation. Plusieurs techniques de discrétisation préservant la structure sont utilisées pour approcher les solutions tout en garantissant que les propriétés essentielles du système, telles que la conservation de l'énergie et la passivité, sont maintenues. Ces techniques incluent la méthode des éléments finis mixtes par [35, 36], les méthodes pseudo-spectrales explorées par [39, 66, 111], et l'approche du calcul extérieur discret étendue aux systèmes PH par [53, 97]. La méthode des éléments finis partitionnés (PFEM), développée par [9, 10], [15], et [96], est particulièrement mise en avant pour son efficacité à préserver la structure des systèmes PH pendant les simulations numériques, que nous utiliserons dans notre discrétisation du modèle de solidification.

L'objectif principal de ce manuscrit est de donner la représentation port-Hamiltonienne du processus de solidification de l'eau pure en utilisant le formalisme de champ de phase et l'entropie totale du système biphasique comme potentiel thermodynamique, ainsi que son équivalent discrétisé.

Modélisation du processus de solidification

Dans le premier chapitre, *Modélisation du processus de solidification*, nous présentons une synthèse raisonnée des modèles principaux du processus de solidification dans les substances pures et aboutissons au modèle dynamique qui sera utilisé dans la suite de la thèse.

Nous commençons donc par un aperçu des modèles de systèmes multiphasiques et de leurs propriétés thermodynamiques, en nous concentrant sur la compréhension du comportement des interfaces pendant les transitions de phase. Cela prépare le terrain pour discuter du problème de Stefan, un modèle classique à interface nette de la solidification. Nous introduisons ensuite la théorie du champ de phase, qui modélise les interfaces diffuses [28].

Cela est particulièrement pertinent pour le génie environnemental et les études de solidification. Nous présentons les modèles thermodynamiques et dynamiques de la solidification de l'eau, en nous concentrant spécifiquement sur la thermodynamique des systèmes biphasiques et en utilisant la notion de modèles de champ de phase. À cette fin, nous suivons de près l'approche thermodynamique de Wang et Boettinger [112, 8]. À travers l'exemple de la formulation de Stefan de la solidification [28, 81, 45], nous fournissons un examen détaillé du modèle dynamique de la solidification en utilisant à la fois l'approche classique, où l'énergie libre ou l'énergie libre de Gibbs est utilisée [32], et un modèle alternatif où l'entropie est utilisée comme potentiel thermodynamique pour le modèle de champ de phase [116].

Les principales contributions de ce chapitre incluent l'introduction d'un modèle détaillé de la solidification en utilisant l'approche de la fonctionnelle d'entropie dans le cadre du champ de phase, y compris une exploration de la dynamique entre les différentes phases et le rôle de l'entropie dans la modélisation des interfaces diffuses. En particulier, nous avons proposé d'écrire le modèle thermodynamique en termes d'une fonction d'entropie non linéaire dépendant de la variable de champ de phase ϕ et de la température T. Cette approche diffère de la plupart des méthodes classiques, qui utilisent l'énergie libre de Gibbs ou l'énergie libre de Helmholtz comme dans [112], [8] et [50].

Le chapitre est organisé comme suit:

1. **Présentation générale des systèmes multiphasiques:** Examine les connaissances fondamentales nécessaires pour comprendre les interactions au sein des systèmes multiphasiques, en se concentrant sur les approches de modélisation des interfaces mobiles à différentes échelles.
2. **Propriétés thermodynamiques des systèmes multiphasiques:** Souligne l'importance des interfaces dans l'analyse thermodynamique des systèmes multiphasiques, avec un accent particulier sur la solidification des liquides.
3. **Modélisation de la solidification d'un composant pur:** Présente le modèle de Stefan et l'approche de modélisation par champ de phase pour la solidification d'un composant pur, en mettant l'accent sur les aspects thermodynamiques.

4. **Modélisation par champ de phase de la solidification de l'eau pure en utilisant la fonctionnelle d'entropie:** Décrit l'application des fonctionnelles d'entropie dans la modélisation par champ de phase pour expliquer le processus de solidification de l'eau pure, en démontrant la signification théorique et pratique de la méthode.

Pour récapituler les équations d'évolution du modèle de solidification dans ce chapitre:

- **Variables d'état:**
  - ϕ: Variable de champ de phase
  - u: Énergie interne
- **Modèle thermodynamique:** Dans la modélisation par champ de phase, l'entropie est caractérisée par une fonction d'entropie spécifique, $s^*(\phi, T)$, qui décrit les interactions thermodynamiques entre les phases liquide et solide. Cette fonction inclut $s^*_{sol}(T)$ pour l'entropie spécifique du solide (glace) et $s^*_{liq}(T)$ pour le liquide (eau), utilisant des polynômes double puits et d'interpolation, $p_w(\phi)$ et $p_i(\phi)$, pour modéliser la transition de phase:
$$s^*(\phi, T) = s^*_{sol}(T) + p_i(\phi)[s^*_{liq}(T) - s^*_{sol}(T)] + wp_w(\phi). \tag{1}$$
- **Équations d'évolution:** L'évolution du champ de phase est régie par l'équation suivante, mettant en évidence le rôle intégral de l'entropie spécifique dans le modèle:
$$\frac{\partial \phi}{\partial t} = -\frac{1}{\eta}\frac{\partial s^*}{\partial \phi}(\phi, T) + \frac{\epsilon^2}{\eta}\text{div}(\text{grad}\phi) \tag{2}$$
De plus, l'équation de bilan énergétique est:
$$\frac{\partial u}{\partial t} = -\text{div}\,(q) \tag{3}$$
où u est l'énergie interne et q est le flux de chaleur.
- **Conditions aux limites:** Les conditions aux limites sont exprimées en termes de:
$$\phi_{\text{boundary}} = \text{tr}(\phi) \quad \text{on} \quad \partial\Omega \tag{4}$$
$$\text{grad}\phi \cdot \mathbf{n} = 0 \quad \text{on} \quad \partial\Omega \tag{5}$$
où $\text{tr}(\phi)$ est la trace de la variable de champ de phase et $\mathbf{n}$ est le vecteur normal à la surface limite $\partial\Omega$.

En conclusion, nous avons rappelé les modèles de systèmes bi-phasiques avec transitions de phase, en utilisant la variable de champ de phase pour représenter l'interface mobile entre les phases. Les propriétés thermodynamiques des systèmes biphasiques avec des modèles de champ de phase ont été présentées, l'entropie servant de potentiel thermodynamique [116, 31]. Nous avons ensuite présenté le modèle dynamique, qui comprend une dynamique de conduction thermique couplée et un système de gradient pour la dynamique de la variable de champ de phase.

En particulier, nous avons proposé d'écrire le modèle thermodynamique en termes d'une fonction d'entropie non linéaire dépendant de la variable de champ de phase ϕ et de la

température T. Cette approche diffère de la plupart des méthodes classiques, qui utilisent l'énergie libre de Gibbs ou l'énergie libre de Helmholtz. En utilisant la fonction d'entropie, nous préparons le modèle port-Hamiltonien qui utilise la fonctionnelle d'entropie comme fonction génératrice.

Formulation comme système Hamiltonien à ports

Dans le deuxième chapitre, *Formulation port-Hamiltonienne du processus de solidification*, nous discutons de l'approche des systèmes port-Hamiltoniens (PHS) pour modéliser les processus de solidification [61]. Cela commence par une introduction aux aspects fondamentaux des systèmes port-Hamiltoniens, en se concentrant sur les fondements conceptuels et mathématiques des structures de Dirac et leur rôle dans la modélisation des systèmes physiques. Les systèmes port-Hamiltoniens de frontière fournissent un cadre efficace pour lier les principes physiques à la théorie des systèmes et au contrôle. Ce chapitre s'appuie sur les travaux fondamentaux de [77] et [84], qui soulignent le rôle des systèmes de frontière dans la préservation des propriétés structurelles des systèmes physiques. La discussion couvre à la fois les systèmes de dimension finie et infinie, mettant en évidence le comportement dissipatif dans le contrôle de l'énergie. Le chapitre analyse l'application des PHS aux équations régissant les processus de solidification. Celles-ci incluent l'équation de diffusion et l'équation d'Allen-Cahn. Il démontre les avantages des PHS pour comprendre et gérer la dynamique énergétique des processus de solidification.

Nous rappelons d'abord les opérateurs hamiltoniens canoniques et la définition des structures de Stokes-Dirac [54, 94], car ils sont essentiels pour comprendre les principes sous-jacents des systèmes port-Hamiltoniens. De plus, le concept de systèmes port-Hamiltoniens de frontière sera introduit.

Ensuite, nous élaborons sur la formulation port-Hamiltonienne de frontière de l'équation de diffusion thermique et de l'équation d'Allen-Cahn. En appliquant les principes des PHS, nous démontrerons comment ces formulations peuvent être utilisées pour modéliser la dynamique des processus de solidification. Cela implique le couplage des équations de diffusion thermique et d'Allen-Cahn pour obtenir une formulation port-Hamiltonienne de frontière complète du processus de solidification.

Initialement, nous avons dérivé le modèle explicite du processus de solidification en utilisant l'entropie comme fonction génératrice, les variables d'état étant la variable de champ de phase ϕ et l'énergie interne u.

Système port-Hamiltonien dissipatif:

$$\begin{pmatrix} \frac{\partial \phi}{\partial t} \\ \frac{\partial \psi}{\partial t} \\ F_{\phi\psi} \\ \frac{\partial u}{\partial t} \\ F \end{pmatrix} = \mathcal{J}_S \begin{pmatrix} -\frac{\partial s}{\partial \phi}(\phi, u) \\ \epsilon^2 \psi \\ E_{\phi\psi} \\ -\tau \\ q \end{pmatrix} \tag{6}$$

L'opérateur hamiltonien $\mathcal{J}_S$ est défini comme suit:

$$\mathcal{J}_S = \begin{pmatrix} 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & -\text{grad} & 0 & 0 \\ 1 & -\text{div} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\text{div} \\ 0 & 0 & 0 & -\text{grad} & 0 \end{pmatrix} \tag{7}$$

Variables de port aux frontières : L'opérateur de frontière $\widetilde{\mathcal{W}}$ synthétise les interactions de frontière provenant à la fois de la diffusion thermique et de la dynamique d'Allen-Cahn:

$$\widetilde{\mathcal{W}} = \begin{pmatrix} 0 & -\gamma_\perp & 0 & 0 & 0 & 0 \\ 0 & 0 & \gamma_0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \gamma_0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\gamma_\perp \end{pmatrix} \tag{8}$$

Les variables de port aux frontières pour la dynamique de la chaleur et du champ de phase sont exprimées comme suit:

$$\begin{pmatrix} f_\partial^{\phi\psi} \\ e_\partial^{\phi\psi} \\ f_\partial \\ e_\partial \end{pmatrix} = \widetilde{\mathcal{W}} \begin{pmatrix} -\frac{\partial s}{\partial \phi}(\phi, u) \\ \epsilon^2 \psi \\ F_{\phi\psi} \\ -\tau \\ q \end{pmatrix} = \begin{pmatrix} -\gamma_\perp(\epsilon^2 \psi) \\ \gamma_0 \left(1/\eta E_{\phi\psi}\right) \\ \gamma_0 \tau \\ -\gamma_\perp M_\tau(-\text{grad}(\tau)) \end{pmatrix} \tag{9}$$

Afin de se rapprocher le plus possible des formulations existantes en génie des Procédés, nous avons décidé d'utiliser la température réciproque $\tau = 1/T$. Ce changement nous permet d'utiliser les données disponibles et les propriétés thermodynamiques de l'eau liquide et de la glace, telles que trouvées dans la littérature [42] et [43]. Le potentiel thermodynamique fourni est l'énergie de Gibbs, exprimée en fonction de la température et de la pression.

Nous avons ensuite défini les propriétés thermodynamiques du système biphasique eau-glace, conduisant aux expressions de la densité d'entropie dépendant de la température plutôt que de l'énergie interne. Cela nécessitait de changer l'espace de coordonnées de l'énergie interne u (une variable extensive) à la température T (une variable intensive).

Pour reformuler le modèle port-Hamiltonien explicite, nous avons introduit la formulation port-Hamiltonienne implicite utilisant des sous-variétés lagrangiennes, qui permettent la définition des équations constitutives réciproques de manière sans coordonnées [105], [88]. Cette approche peut être adaptée aux systèmes à paramètres distribués [60], [106]. Enfin, nous avons dérivé une formulation implicite du modèle de solidification en intégrant des équations différentielles-algébriques (DAE) et des équations aux dérivées partielles (PDE).

Modèle implicite:

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ \frac{\partial^2 s^*}{\partial \phi \partial \tau} & 0 & 0 & \frac{\partial^2 s^*}{\partial \tau^2} & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \frac{\partial \phi}{\partial t} \\ \frac{\partial \psi}{\partial t} \\ F_{\phi\psi} \\ \frac{\partial \tau}{\partial t} \\ F \end{pmatrix} = \mathcal{J}_S \begin{pmatrix} -\frac{\partial s^*}{\partial \phi}(\phi, \tau) \\ \epsilon^2 \psi \\ E_{\phi\psi} \\ -\tau \\ q \end{pmatrix}. \tag{10}$$

Ce cadre modélise la dynamique en termes de température réciproque, s'alignant avec les propriétés thermodynamiques empiriques de systèmes tels que l'eau et la glace.

Notre discussion fera référence au cadre thermodynamique de modélisation et de simulation [5] et [116] pour illustrer les applications pratiques de ces constructions théoriques.

Les principales contributions sont structurées autour du développement d'un cadre théorique et de son application aux phénomènes physiques, en s'appuyant sur la littérature existante:

1. **Dérivation de la dynamique d'Allen-Cahn:** En s'appuyant sur les travaux de Vincent et al. [110], ce chapitre présente la dérivation de la représentation port-Hamiltonienne de l'équation d'Allen-Cahn dans la représentation de l'entropie.
2. **Formulation implicite du modèle de solidification:** Afin d'utiliser les données empiriques des propriétés thermodynamiques des systèmes, données en termes de température réciproque, une formulation port-Hamiltonienne implicite est développée. Cette formulation est exprimée en termes d'un système d'équations différentielles-algébriques partielles (DA-PDE). Ces systèmes appartiennent à la classe récemment définie des systèmes port-Hamiltoniens sur des sous-variétés de Lagrange, tels que définis dans [105, 60, 106, 6].

En conclusion, ce chapitre présente une représentation dissipative port-Hamiltonienne de frontière pour les processus de solidification de l'eau et d'autres substances pures, en utilisant l'entropie comme fonction génératrice pour la dynamique. En s'appuyant sur les travaux fondamentaux, tels que ceux de [110], le chapitre étend le cadre port-Hamiltonien pour inclure l'équation d'Allen-Cahn, modélisant efficacement la dynamique des variables de champ de phase non conservées et l'équation de la chaleur.

Nous avons initialement développé le modèle explicite du processus de solidification en utilisant l'entropie comme fonction génératrice, les variables d'état étant la variable de champ de phase ϕ et l'énergie interne u. Nous avons ensuite reformulé le modèle port-Hamiltonien explicite en une formulation port-Hamiltonienne implicite utilisant des sous-variétés lagrangiennes. Cette approche, détaillée dans des travaux tels que [105] et [88], permet la définition des équations constitutives réciproques de manière sans coordonnées et peut être adaptée aux systèmes à paramètres distribués [60], [106]. Finalement, cela a conduit à une formulation implicite du modèle de solidification en intégrant des équations différentielles-algébriques (DAE) et des équations aux dérivées partielles (PDE). Ce cadre, modélisant la dynamique en termes de température réciproque, s'aligne bien avec les propriétés thermodynamiques empiriques des systèmes comme l'eau et la glace.

Discrétisation spatiale

Dans le troisième chapitre, *Discrétisation du processus de solidification*, nous nous concentrons sur la discrétisation préservant la structure du modèle port-Hamiltonien (PH) de frontière du processus de solidification. Une discrétisation préservant la structure garantit que le modèle discrétisé conserve la structure PH, en préservant les propriétés clés telles que la conservation de l'énergie et la passivité [17, 11]. Plusieurs techniques de discrétisation préservant la structure sont utilisées pour approcher les solutions tout en maintenant ces propriétés structurelles. Selon [77], les techniques suivantes sont notables:

- **Méthode des éléments finis mixtes** par Golo et al. [35, 36]: Cette méthode utilise des bases différentes pour les variables d'énergie et de co-énergie, les intégrant en fonction du degré de la forme différentielle les définissant.
- **Méthodes pseudo-spectrales** pour les systèmes PH explorées par Moulla et al. [66, 111, 39].
- **Approche du calcul extérieur discret** étendue aux systèmes PH par Seslija et al. [97, 53]: Cette méthode représente les systèmes discrets de lois de conservation sous forme matricielle, reflétant les formulations continues.
- **Méthode des éléments finis partitionnés (PFEM)** développée par Cardoso et al. [15], Serhani [96], et Brugnoli et al. [9, 10]: PFEM sera discuté en détail ci-après.

Dans ce chapitre, nous utilisons la méthode des éléments finis partitionnés (PFEM), basée sur les travaux de [38], pour assurer la discrétisation préservant la structure de l'équation de la chaleur et de l'équation d'Allen-Cahn. PFEM maintient les propriétés physiques et géométriques des systèmes port-Hamiltoniens (PH) pendant les simulations numériques, ce qui est crucial pour représenter et analyser avec précision les phénomènes de solidification.

La contribution principale de ce chapitre réside dans la méthodologie de discrétisation appliquée au modèle port-Hamiltonien (PH) de l'équation de la chaleur, en se concentrant sur deux innovations principales:

1. **Intégration de l'entropie comme fonction génératrice:** Nous avons appliqué la méthode des éléments finis partitionnés (PFEM) au modèle PH où nous utilisons des relations constitutives non linéaires, correspondant à des fonctions hamiltoniennes non quadratiques issues des modèles thermodynamiques présentés au chapitre 2, avec l'entropie s comme fonction génératrice.
2. **Formulation implicite avec température réciproque:** Nous avons introduit et discrétisé une formulation implicite de l'équation de la chaleur utilisant la température réciproque $\tau = \frac{1}{T}$ comme variable d'état. De plus, nous avons discrétisé l'équation d'Allen-Cahn, conduisant à la discrétisation de l'ensemble du modèle implicite du processus de solidification. Cette formulation s'aligne avec le cadre des systèmes hamiltoniens dissipatifs, incorporant des ports de frontière.

En utilisant les approximations par éléments finis et les matrices de masse et de rigidité définies dans ce chapitre, le système discret peut être représenté comme suit:

$$\underbrace{\begin{bmatrix} M_\phi & 0 & 0 & 0 & 0 \\ 0 & M_\psi & 0 & 0 & 0 \\ 0 & 0 & M_{F_{\phi\psi}} & 0 & 0 \\ M_{\phi\tau} & 0 & 0 & M_\tau & 0 \\ 0 & 0 & 0 & 0 & M_{\bar{F}} \end{bmatrix}}_{\tilde{M}} \begin{pmatrix} \frac{d\bar{\phi}}{dt}(t) \\ \frac{d\bar{\psi}}{dt}(t) \\ \bar{F}_{\phi\psi}(t) \\ \frac{d\bar{\tau}}{dt}(t) \\ \bar{F}(t) \end{pmatrix} = \underbrace{\begin{bmatrix} 0 & 0 & -M_\phi & 0 & 0 \\ 0 & 0 & G_\psi & 0 & -B_\psi \\ M_\phi & -D_\phi^\top & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -D_\tau \\ 0 & B_\psi^\top & 0 & D_\tau^\top & 0 \end{bmatrix}}_{\mathcal{J}_S} \begin{pmatrix} \bar{e}_\phi(t) \\ \epsilon^2\bar{\psi}(t) \\ \bar{E}_{\phi\psi}(t) \\ -\bar{\tau}(t) \\ \bar{q}(t) \end{pmatrix}, \tag{11}$$

où $\tilde{M}$ est la matrice de masse combinée, et $\mathcal{J}_S$ inclut la dynamique du système et les interactions de frontière.

Notre approche a consisté à dériver des formulations faibles, à projeter les variables sur des espaces d'éléments finis et à définir et calculer des matrices de masse. Ces étapes ont permis une discrétisation préservant la structure, préservant les propriétés physiques et géométriques du système continu d'origine. Les modèles discrétisés résultants ont des matrices de masse dépendant de l'état.

En conclusion, dans ce chapitre, nous avons présenté la discrétisation du phénomène de solidification en utilisant la méthode des éléments finis partitionnés (PFEM) dans le cadre port-Hamiltonien. Tout d'abord, nous avons discrétisé une formulation implicite de l'équation de la chaleur en utilisant la température réciproque $\tau = \frac{1}{T}$ comme variable d'état. De plus, nous avons discrétisé l'équation d'Allen-Cahn, conduisant à la discrétisation complète du modèle implicite du processus de solidification.

Conclusion

En conclusion, cette thèse a discuté et présenté la modélisation, la formulation et la discrétisation des processus de solidification en utilisant le cadre port-Hamiltonien (PH) combiné à l'approche de champ de phase.

Dans le chapitre 2, nous avons présenté une approche de modélisation détaillée des processus de solidification en utilisant la fonctionnelle d'entropie dans le cadre du champ de phase [112, 116]. Les contributions clés incluent une présentation complète de la solidification en utilisant l'approche de la fonctionnelle d'entropie et une analyse de la dynamique entre les différentes phases, en mettant l'accent sur le rôle de l'entropie dans la modélisation des interfaces diffuses.

Dans le chapitre 3, nous avons étendu le cadre PH au processus de solidification, en intégrant la méthode d'interface diffuse avec les variables de champ de phase. Cela impliquait de développer une formulation port-Hamiltonienne de frontière combinant l'équation de diffusion thermique et l'équation d'Allen-Cahn. La principale contribution de ce chapitre a été la reformulation du modèle port-Hamiltonien explicite en une formulation port-Hamiltonienne implicite utilisant des sous-variétés lagrangiennes. Cette approche, détaillée dans des travaux tels que [105] et [88], permet la définition des équations constitutives réciproques de manière sans coordonnées et peut être adaptée aux systèmes à paramètres distribués [60, 106]. Ce changement nous permet d'utiliser les données disponibles et les propriétés thermodynamiques de l'eau liquide et de la glace, telles que trouvées dans la littérature [42, 43]. Le potentiel thermodynamique fourni est l'énergie de Gibbs, exprimée en fonction de la température et de la pression. En définissant les propriétés thermodynamiques du système biphasique eau-glace, nous avons dérivé les expressions de la densité d'entropie basées sur la température plutôt que sur l'énergie interne. Cela nécessitait de changer l'espace de coordonnées de l'énergie interne u (une variable extensive) à la température T (une variable intensive).

Le chapitre 4 a mis l'accent sur la discrétisation préservant la structure du modèle PH de la solidification. En utilisant la méthode des éléments finis partitionnés (PFEM), nous avons veillé à ce que le modèle discrétisé conserve la structure PH, en préservant des propriétés clés telles que la conservation de l'énergie et la passivité. Ce chapitre a détaillé plusieurs techniques de discrétisation préservant la structure, en soulignant l'importance de maintenir les

propriétés physiques et géométriques du système continu d'origine. Les principales contributions incluent l'application de la PFEM au modèle PH utilisant des relations constitutives non linéaires avec l'entropie comme fonction génératrice [38], et l'introduction et la discrétisation d'une formulation implicite de l'équation de la chaleur en utilisant la température réciproque $\tau = \frac{1}{T}$ comme variable d'état. De plus, nous avons discrétisé l'équation d'Allen-Cahn, conduisant à la discrétisation complète du modèle implicite du processus de solidification, où les modèles discrétisés résultants ont des matrices de masse dépendant de l'état.

Cette thèse a jeté une base pour de futures recherches et développements dans le domaine des systèmes à paramètres distribués avec interfaces mobiles. Plusieurs directions pour les travaux futurs sont prometteuses:

- Effectuer des simulations numériques du processus de solidification. Un travail préliminaire sur les simulations, utilisant les relations constitutives non linéaires, a conduit à des résultats partiels qui ont montré un problème non linéaire assez difficile.
- Explorer son contrôle en utilisant des méthodes de contrôle optimal suivant, par exemple, [40]. Ces études initiales ont montré que les propriétés thermodynamiques non linéaires conduisent à un problème de contrôle optimal très difficile qui reste un problème ouvert intéressant.
- Ce modèle pourrait fournir un sous-modèle pour le processus de purification de l'eau tel que présenté dans le projet WATERSAFE et éventuellement aider à son contrôle.

Les résultats de cette thèse ont plusieurs implications pour la recherche théorique et les applications pratiques. En utilisant le cadre PH, nous avons fourni un moyen systématique d'incorporer les principes physiques dans la modélisation, la simulation et le contrôle des processus de solidification. Les recherches futures pourraient prolonger ce travail dans plusieurs directions, notamment l'amélioration des modèles thermodynamiques pour inclure des interactions plus complexes et des phases supplémentaires, le développement de stratégies de contrôle avancées utilisant le cadre PH, et l'application de ces méthodologies à d'autres processus de transition de phase et systèmes multiphasiques.

Les recherches futures peuvent s'appuyer sur ces résultats pour améliorer encore les processus de solidification. Les directions potentielles incluent l'extension des modèles à des dimensions supérieures et à des formes plus complexes pour mieux représenter la solidification réelle, l'application des modèles à d'autres types de transitions de phase et de systèmes multiphasiques, l'utilisation de méthodes numériques pour rendre les simulations plus efficaces et précises, la réalisation de davantage d'expériences pour valider et affiner les modèles, et le développement de stratégies de contrôle basées sur le cadre port-Hamiltonien pour gérer les processus de solidification dans les applications industrielles.

Contents

Nomenclature

z	Space variable
Ω	Spatial domain
t	Time variable
G	Functional representing thermodynamical potential
ϕ	Non–conserved phase field variable
κ_ϕ	Non–negative gradient coefficient related to the interface
$g(\phi)$	Analytic density potential function that generates the interface dynamics
Γ_ϕ	Isotropic interface mobility
$\delta G/\delta\phi$	Functional derivative
trace	Trace operator in boundary conditions
U	Internal energy
T	Temperature
p	Pressure
V	Volume
μ	Chemical potential
N	Number of moles
$g_{sol}(T,p)$	Specific Gibbs energy of the solid phase
$g_{liq}(T,p)$	Specific Gibbs energy of the liquid phase
f^*	Specific Helmholtz energy
$\mathcal{H}$	Hamiltonian function
s^*	Specific entropy
H_d	Discrete total energy
J_Q	Heat flux
u_∂	Boundary input variable
y_∂	Boundary output variable
M_φ	Mobility constant

$\delta F/\delta\varphi$ Functional derivative of free energy

F Total free energy

j_ϕ Non–conserved flux

$\pi(\varphi)$ Interpolation polynomial for phase transition

$w(\varphi)$ Weight function for phase transition

$\varphi_{boundary}$ Phase field variable at boundary

div Divergence operator

$\partial\Omega$ Boundary of the domain

n Normal vector to boundary surface

$\mathrm{tr}(\varphi)$ Trace of the phase field variable

ρ Density

c_p Specific heat capacity at constant pressure

div Divergence

λ Thermal conductivity

$grad$ Gradient

F Thermodynamic force

ψ State variable := gradϕ

E_ϕ Flux

F_ϕ Driving force

$\mathcal{J}$ Linear differential operator

$\mathcal{F}$ Space of flow variables

$\mathcal{E}$ Space of effort variables

$\mathcal{B}$ Bond space ($\mathcal{B} = \mathcal{F} \times \mathcal{E}$)

f_∂, e_∂ Boundary port variables

$\mathcal{W}$ Boundary operator

γ_0 Continuous unique extension of a boundary trace mapping

$\gamma_\perp$ Continuous unique extension of a normal trace mapping

f_{bulk} Flow variable

e_{bulk} Effort variable

s Entropy density

τ Reciprocal temperature

S Entropy functional

q Heat flux

$F_{\phi\psi}$ Driving force after the extension of the state space by ψ

$E_{\phi\psi}$ Flux after the extension of the state space by ψ

$\bar{S}$ Entropy functional after the extension of the state space by ψ

$f_{\phi\psi}$ Flow variable of the extended state space

$e_{\phi\psi}$ Effort variable of the extended state space

$\bar{F}$ Driving force

$\mathcal{J}_e$ Extended linear differential operator

$tr(\cdot)$ Boundary trace operator

$f_{\tilde{\partial}}$, $e_{\tilde{\partial}}$ Boundary port variables

$\mathcal{G}_R$ Differential operator

$\mathcal{G}_R^*$ Formal adjoint operator of $\mathcal{G}_R$

$\mathcal{S}$ Bounded coercive operator

J_{ext} Extended linear differential operator for boundary interactions

$\mathcal{R}$ Positive, coercive matrix operator for dissipation

$T(\zeta)$ Tensor describing material properties in the wave equation

$\rho(\zeta)$ Density of the medium at point ζ

$w(t, \zeta)$ Wave displacement variable

$\mathcal{D}$ Dirac structure

Γ_0, Γ_1 Disjoint parts of the boundary with different boundary conditions

$\frac{\partial H}{\partial x}$ Gradient of the Hamiltonian function

$\frac{d}{dt}H$ Time derivative of the Hamiltonian

$\dot{x}$ Rate of change of the state variable

Q Dissipative force

F Flux variable associated with dissipation

$\partial_t z(t, x)$ Partial derivative with respect to time of state variable z

$\delta_x H$ Functional derivative of Hamiltonian with respect to state variable x

f_S, e_S Flow and effort variables associated with energy-storing elements

f_R, e_R Flow and effort variables associated with resistive elements

f_P, e_P Flow and effort variables associated with external ports

$\mathcal{J}(x)$ Skew-symmetric differential operator for infinite-dimensional systems

$\mathcal{G}_R$ Differential operator for dissipative interactions

$\mathcal{G}_R^*$ Adjoint operator of $\mathcal{G}_R$ for dissipation

$\mathcal{R}$ Operator describing resistive interactions

$\mathcal{S}$ Bounded coercive operator in dissipative systems

$\mathcal{X}$ State space for energy-storing elements

$\mathcal{F}_R$ Space of flow variables for resistive elements

x, ζ State variables in the spatial domain

H Hamiltonian or total energy of the system

R Resistive structure in Port-Hamiltonian systems

$u(t)$ Control input in boundary conditions

I Identity matrix

$T(\zeta)$ Elasticity tensor in wave equation

$x(t, \zeta)$ State variable vector in wave equation

$\mathcal{J}_{\text{ext}}$ Extended skew-symmetric operator for dissipative systems

Q, F Dissipative force and flux variables

$\delta_{x_1}\mathcal{H}, \delta_{x_2}\mathcal{H}$ Functional derivatives of Hamiltonian in extended systems

$\mathcal{W}, \overline{\mathcal{W}}$ Boundary operators for port variables

Chapter 1

Introduction

This thesis deals with distributed parameter models of bi-phasic systems consisting of two phases interacting through moving interfaces. Such systems arise as models of multiphase systems like crystallization processes, evaporators, or condensers [23]. Their dynamical models comprise systems of Partial Differential Equations (PDEs) arising from balance equations of each phase, coupled with a dynamical system describing the moving interface. The interface is a narrow region separating two spatial regions of different material states. There are many ways to model the interface, including the Two-phase Stefan problem [79] and Thin interface models [109]. These interfaces separate domains filled with different phases (solid, liquid, or vapor), such as in solidification or crystallization processes [112]. A classical problem is the Stefan problem, which describes phase change processes like also solidification and melting. It is a fundamental issue in various scientific and engineering fields. Previous studies, including those by [40], [21], and [52], have extensively discussed the control and modeling of such processes. Many inhomogeneous systems involve well-defined phase domains separated by an interface. If the systems are not in equilibrium, the interface will move in a certain direction. Examples of moving interfaces include phase separation by spinodal decomposition, modeling microstructure evolution in materials science, or solidification with dendritic growth [102, 28].

The representation of a moving interface varies from sharp interfaces to diffuse ones. In the sharp interface approach, certain variables of interest are discontinuous at the interface due to imposed boundary conditions, and the interface must be tracked [99]. In contrast, in the diffuse interface approach, following Gibbs' ideas, the variables vary rapidly but smoothly along the interface thickness. The different phases are differentiated by an order parameter that changes continuously from one value to another along the interface thickness, with each phase corresponding to these values. The dynamics of this phase variable are driven by a partial differential equation. The sharp interface approach is not well adapted to describe complex patterns of the interface. In this case, the diffuse interface approach is preferred through the phase field approach. Therefore, in our work, we follow the diffuse interface approach based on the work by [110]. This approach uses a phase field variable ϕ describing the interface, which varies continuously between the values representing the solid and liquid phases and obeys various dynamical models such as the Allen-Cahn equation.

The phase field approach is extensively used in physics and material science [98]. Although it is not frequently used in chemical engineering, we discuss its thermodynamic properties and the phase field approach in detail in Chapter 2. Recently, some applications have emerged in this field, such as the WATERSAFE project, which is one application motivating this work. It deals with a new process of water purification by freezing, aiming specifically to remove soluble pollutants at low concentrations from aqueous liquid effluents. The WATERSAFE ANR project (WATERSAFE: Advancing Water Purification through Solidification-Melt Cycles) conducted by Aurélie Galfré from LAGEPP has two primary objectives: conducting an in-depth analysis of ice crystallization phenomena to prevent the incorporation of impurities, especially salts, into the ice, thus ensuring its purity; and developing an innovative ice layer crystallization (ILC) process for pollutant treatment that is optimized for continuous operation and liquid phase recycle modes. This project aims to bridge the gap between theoretical models and practical applications, focusing on the thermodynamics of phase transitions and the dynamics of multiphase systems. The use of the phase field model will permit better control of operating conditions by analyzing the dendritic growth during solidification.

Due to the thermodynamic nature of the freezing process and the phase field method, the Port-Hamiltonian framework seems useful in this context for modeling purposes, to facilitate interconnection with a macroscopic environment, for simulation, or even for control synthesis. Indeed, this approach encodes the underlying physical principles, such as conservation laws, directly into the geometric structure of the system model, as well as into the boundary conditions. Moreover, the geometric structure can be used in spatial reduction to derive finite-dimensional Hamiltonian models. These models share the same physical properties as their infinite-dimensional counterparts, including the representation of systems of balance equations and inherent passivity, making them particularly suitable for simulation. Finally, passivity-based control can easily be applied to Port-Hamiltonian systems, which are naturally passive systems [70]. In this work, we develop a port-Hamiltonian formulation, which provides a system-theoretic framework for model order reduction and passivity-based control, building on methodologies outlined by [70], [75], [7], and [93].

Port Hamiltonian Systems (PHS) are used to model and control physical systems involving energy exchange [63], [61]. They combine elements that store energy, dissipate energy, and route energy within a consistent framework [84]. PHS are defined by the interaction between a Dirac structure and a Hamiltonian function [18]. The Dirac structure defines how energy flows within the system, while the Hamiltonian function represents the total energy of the system [86, 16]. In the last decade, this powerful modeling framework has been used for a wide range of infinite-dimensional physical systems such as electrical, mechanical, electromechanical, hydraulic, and multiphase chemical engineering systems where heat and mass transfer phenomena occur. It has also been applied to represent moving interface systems [23, 24] as well as Implicit Port Hamiltonian Systems defined on Lagrange subspaces in Hilbert spaces [105, 88]. The details of the PHS framework and its application to the solidification process are thoroughly discussed in Chapter 3 of this thesis.

The first objective of this thesis is to use PHS to model solidification processes by combining the Allen-Cahn equation (for phase changes) with the heat equation (for heat conduction). Two primary approaches have been explored within the PH framework: the thin interface model and the diffuse interface model. The thin interface model, as studied by [28] and

[24], provides a simplified representation of the interface dynamics. In contrast, the diffuse interface model, based on the work by [110], offers a more detailed description of the interface behavior. This thesis follows the diffuse interface approach. The model uses the entropy density function as the generating function, which depends on the phase variable ϕ and internal energy u, to describe the coupled dynamics of phase changes and heat transfer [110]. We use Implicit Port Hamiltonian Systems defined on Lagrange subspaces to express the entropy density functional in terms of the reciprocal temperature τ and the phase field variable ϕ as given in the tables of [42, 43].

The second objective is to formulate the PH systems of solidification processes based on these thermodynamic models. These refined models are discretized using an implicit formulation. This approach, derived from nonlinear thermodynamic models, aims to preserve the structure and properties of the original continuous system during numerical simulations.

This work also emphasizes the importance of maintaining the structural integrity of the PH systems during discretization. Several structure-preserving discretization techniques are employed to approximate solutions while ensuring that essential system properties, such as energy conservation and passivity, are maintained. These techniques include the Mixed Finite-Elements Method by [35, 36], Pseudo-Spectral Methods explored by [66, 111, 39], and the Discrete Exterior Calculus approach extended to PH systems by [97, 53]. The Partitioned Finite Element Method (PFEM), developed by [15], [96], and [9, 10], is particularly highlighted for its effectiveness in preserving the structure of the PH systems during numerical simulations, which we will be using in our discretization of the solidification model.

We suggest a discretization of the implicit model using the Partitioned Finite Element Method (PFEM). The explicit model of the solidification process was developed using entropy as the generating function, with state variables being the phase field variable ϕ and the internal energy u based on the work by [112]. Due to the limited availability of data for the entropy density function $s = s(\phi, u)$, we transitioned to using the reciprocal temperature $\tau = 1/T$. This adjustment allowed us to utilize existing thermodynamic properties of liquid water and ice as mentioned earlier, as documented by sources such as the International Association for the Properties of Water and Steam [42, 43]. The Gibbs energy, expressed as a function of temperature and pressure, facilitated a practical definition of the thermodynamic properties of the bi-phasic water-ice system. Consequently, we derived expressions for the entropy density based on temperature rather than internal energy, necessitating a shift in the state space coordinate from internal energy u to temperature T.

We then reformulated the explicit Port Hamiltonian model into an implicit Port Hamiltonian formulation using Lagrangian submanifolds. This approach, detailed in works such as [89] and [105, 88], allows for the definition of reciprocal constitutive equations in a coordinate-free manner and can be adapted to distributed parameter systems. Ultimately, this led to an implicit formulation of the solidification model by integrating Differential-Algebraic Equations (DAE) and Partial Differential Equations (PDE). This framework, modeling the dynamics in terms of reciprocal temperature, aligns well with the empirical thermodynamic properties of systems like water and ice.

The main goal of this manuscript is to give the Port Hamiltonian representation of the solidification process of pure water using the phase field formalism and the total entropy of

the bi-phasic system as the thermodynamic potential, and its discretized counterpart.

1.1 Structuration of the Manuscript

The thesis is divided into three chapters, each addressing different aspects of the solidification process. Below is an overview of the manuscript's organization.

1.1.1 Chapter 2: Modeling of the Solidification Process

Chapter 2 delves into the modeling of solidification processes. It begins with an introduction to multiphase systems and their thermodynamic framework, highlighting the importance of interfaces and the role of entropy in phase transitions. The chapter presents both sharp interface and phase field models, providing a detailed examination of the dynamics and thermodynamics of solidification.

Key contributions of this chapter include:

- A comprehensive presentation of solidification using the entropy functional approach within the phase field framework.
- An analysis of the dynamics between different phases and the role of entropy in modeling diffuse interfaces.

1.1.2 Chapter 3: Port Hamiltonian Formulation of the Solidification Processes

Chapter 3 introduces the Port Hamiltonian Systems (PHS) approach to the mathematical modeling and control of solidification processes. The chapter covers the foundational concepts of PHS, including Dirac structures and their role in the geometric structuring of power dynamics within physical systems [91]. The application of PHS to fundamental equations governing solidification processes, such as the diffusion equation and the Allen-Cahn equation, is explored in detail.

Key contributions of this chapter include:

- Development of a Boundary Port Hamiltonian Framework integrating the diffuse interface method with phase field variables.
- Extension of Allen-Cahn dynamics within the PHS framework [110].
- Formulation of an integrated approach that combines Differential-Algebraic Equations (DAE) and Partial Differential Equations (PDE) for modeling dynamics in terms of reciprocal temperature [116].

1.1.3 Chapter 4: Discretization of the Solidification Process

Chapter 4 focuses on the discretization methods for the solidification process. It discusses advances in structure-preserving numerical analysis and control theory, particularly in the context of multi-physical systems. The chapter introduces the Partitioned Finite Element

Method (PFEM) and discusses the discretization of the heat equation and the Allen-Cahn equation, emphasizing the importance of structure-preservation in numerical methods [38, 94].

Key contributions of this chapter include:

- Application of the Partitioned Finite Element Method (PFEM) to the PH model using nonlinear constitutive relations, corresponding to non-quadratic Hamiltonian functions arising from the thermodynamic models presented in Chapter 2, with entropy s as the generating function.
- Introduction and discretization of an implicit formulation of the heat equation using the reciprocal temperature $\tau = \frac{1}{T}$ as the state variable. Additionally, the chapter discusses the discretization of the Allen-Cahn equation, leading to the complete discretization of the implicit model of the solidification process. This formulation aligns with the dissipative Hamiltonian systems framework, incorporating boundary ports.

Chapter 2

Modeling of the Solidification Process

Contents

Abstract

This chapter examines the dynamics of solidification processes, utilizing the Allen-Cahn equation and energy balance equations to model phase transitions essential for water purification technologies. The analysis begins with an examination of the behavior of thin and diffuse interfaces, which are important for understanding solidification phenomena. It then explores phase field theory, illustrating how this framework captures the complexities of multiphase systems and interfacial dynamics. This discussion covers the thermo-

dynamic foundations of the employed models and spans various scales, from macroscopic system behavior to microscopic interactions.

2.1 Introduction to the chapter

This chapter presents the thermodynamic and dynamical models of the solidification of water, focusing specifically on the thermodynamics of bi-phasic systems and introducing the notion of phase field models. For this purpose, we closely follow the thermodynamic approach of Wang and Boettinger [112, 8]. Through the example of the Stefan formulation of solidification [28, 81, 45], we provide a detailed examination of the dynamical model of solidification using both the classical approach, where the free energy or Gibbs free energy is used [32], and an alternative model where the entropy is used as the thermodynamic potential for the phase field model [116].

We begin with an overview of multiphase systems and their thermodynamic properties, focusing on understanding the behavior of interfaces during phase transitions. This sets the stage for discussing the Stefan problem, a classical sharp interface model of solidification. We then introduce phase field theory, which models diffuse interfaces [28].

In this chapter, we conclude with a thermodynamically consistent dynamical model of the solidification process using an entropy functional approach within the phase field framework. This approach enhances our understanding of the solidification process by emphasizing entropy as a key factor in phase transitions.

2.2 Overview and Contributions of the chapter

This chapter aims to provide a comprehensive understanding of the solidification process in pure substances, with a particular focus on the role of entropy in phase transitions. It is especially relevant to environmental engineering and solidification studies. The key contributions of this chapter include introducing a detailed model of solidification using the entropy functional approach within the phase field framework, including an exploration of the dynamics between different phases and the role of entropy in modeling diffuse interfaces. Specifically, we have proposed writing the thermodynamic model in terms of a non-linear entropy function depending on the phase field variable ϕ and the temperature T. This approach differs from most classical methods, which use the Gibbs free energy or Helmholtz free energy as in [112], [8] and [50].

The choice of the diffuse interface model in this study, rather than the classical sharp interface model (such as the Stefan model), is motivated by several key advantages. The diffuse interface approach offers a thermodynamically consistent way to describe phase transitions without explicitly tracking the interface position, making it better suited for capturing complex interfacial dynamics and multiphysics coupling. Additionally, this choice aligns with the goals of the Watersafe project, which also employs the diffuse interface framework due to its robustness in modeling complex solidification processes involving environmental conditions.

The chapter is organized as follows:

1. **General presentation of Multiphase Systems:** Examines the foundational knowledge required to understand interactions within multiphase systems, focusing on modeling approaches for moving interfaces at various scales.
2. **Thermodynamic Properties of Multiphase Systems:** Highlights the importance of interfaces in the thermodynamic analysis of multiphase systems, with a focus on liquid solidification.
3. **Solidification Modeling of a Pure Component:** Presents the Stefan model and phase field modeling approach for the solidification of a pure component, emphasizing the thermodynamic aspects.
4. **Phase Field Modeling of Solidification of Pure Water Using Entropy Functional:** Describes the application of entropy functionals within phase field modeling to explain the solidification process of pure water, demonstrating the method's theoretical and practical significance.

2.3 Multiphase Systems

A multiphase system is a physical system that contains more than one distinct phase of matter, such as gas, liquid, or solid. The thermodynamic state variables of each phase change smoothly and continuously within the system. At the boundary between different phases, discontinuities arise in the state variables, enabling a clear delineation between the different phases present. These boundaries between the phases are referred to as interfaces.

Interfaces can be of various types, such as:

- Liquid/Gas (e.g., cavitation) [1]
- Gas/Solid (e.g., deflagration, sublimation, deposition) [12]
- Solid/Liquid (e.g., melting, solidification) [101]
- Liquid/Liquid (e.g., emulsion, phase separation) [37]

In this thesis, we are concerned with the melting and solidification process.

Models of interfaces are important for the description of the dynamics of multiphase systems and are the object of numerous studies. Melting and solidification have been extensively studied in the context of metallurgy [46, 68], and in this thesis, we consider the context of chemical engineering, focusing on processes involving the melting and solidification of water [20, 29].

In the sequel, we shall briefly recall the two main approaches for macroscopic models: the sharp interface and diffuse interface models. Both models may be derived from microscopic models, which describe interactions at the molecular and atomic scales [107].

1. **Sharp Interface Models:** In sharp interface models, the interface is a spatial domain of zero measure, known as phase boundaries. These models use the principles of continuum mechanics and the conservation of mass, momentum, and energy in the bulk phases. An example of a sharp interface model is the Stefan problem, which can be used to model the melting of ice or the solidification of liquid [74].

2. **Diffuse Interface Models:** In diffuse interface models, the interface has a spatial domain of small but non-zero measure. The composition of the interfacial region varies continuously but rapidly from one phase to another. The phase field approach is an example where a sharp interface is replaced by a diffuse interface. The phase is represented by a phase field variable ϕ, which can represent a conserved quantity (e.g., a molar fraction) as in the Cahn-Hilliard model used for phase separation or a non-conserved quantity (a smoothened characteristic function of the spatial domains of the phases) as in the Allen-Cahn model used for solidification [13, 2]. An overview of phase field models is given in the articles [51] and the monography [28].

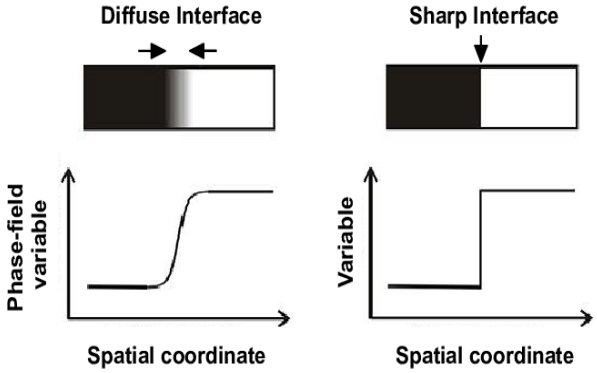

Figure 1: Diffuse and sharp interface

Figure 1 shows the two possible representations of interfaces [76].

The position of the interface is governed by thermodynamic and mechanical phenomena in the bulk phases as well as at the interface. Properties of the fluid differ from those of the bulk as we approach the solid phase. Complex geometric structures may arise at the interface, such as the formation of microstructures like dendrites, which may strongly influence the dynamics at the interface, such as the velocity of formation of the solid.

2.4 Thermodynamic Properties of Multiphase Systems

We present here briefly the thermodynamic model of a multiphase system with respect to the thermodynamic properties of each phase following [28].

Thermodynamics of Single Phases

The thermodynamic equilibrium properties of a single phase are described by the Gibbs equation [32], which relates the thermodynamic state variables: entropy, temperature, volume, pressure, number of moles, and chemical potential. For a simple thermodynamic system, the Gibbs equation can be expressed as:

$$dU = TdS - pdV + \mu dN \tag{2.1}$$

where U is the internal energy, T is the temperature, S is the entropy, p is the pressure, V is the volume, μ is the chemical potential, and N is the number of moles.

Stability of Equilibrium

Stability of a phase is characterized by properties of its internal energy or its entropy [14]. Considering a simple system with internal energy $U(S, V, N)$ as a function of entropy S, volume V, and mole number N, the system is in stable equilibrium if:

- $dU = 0$
- $d^2U > 0$

Similarly, if entropy $S(U, V, N)$ is considered as a function of U, V, and N, the system is in stable equilibrium if:

- $dS = 0$
- $d^2S < 0$

This implies that U must be convex with respect to its extensive variables S, V, and N, and S must be concave with respect to U, V, and N. These stability conditions, derived from the Maxwell relations, impose sign properties on thermodynamic parameters like heat capacity and compressibility.

These stability conditions can also be extended to other potentials such as free energy $F(T, V, N) = U - TS$ or the Gibbs free energy $G(T, P, N) = U - TS + PV$. These potentials must be convex with respect to their extensive variables V and N, respectively, at constant intensive variables. These stability conditions will be used in the phase field model to construct extended (since valid for a two phase system) adequate thermodynamic potential functional as we will see later on. In the case of solidification, phase diagrams are critical tools in thermodynamics for visualizing the stability regions of different bulk phases under varying conditions of temperature and pressure. These diagrams are crucial for predicting the conditions under which a substance may exist in either solid or liquid forms, or in a mixture of phases, providing a graphical representation of phase equilibria [28].

2.5 Thermodynamics of Interfaces

At the interface between two phases, such as liquid and solid, the interactions between the molecules of the different phases give rise to an additional thermodynamic model at the interface, considered as an interfacial phase. This model is defined by specific thermodynamic potentials, also called the surface energy.

Gibbs introduced a dividing surface between the two phases, considered as homogeneous up to this dividing surface. The thermodynamics of each phase is given by the fundamental equation of Gibbs without taking into account the interfaces:

$$\begin{aligned} dU^L &= TdS^L - p^L dV^L + \mu dN^L, \\ dU^S &= TdS^S - p^S dV^S + \mu dN^S. \end{aligned} \tag{2.2}$$

Considering a system containing two phases L and S separated by an interface, the total amounts are:

$$\begin{aligned} n &= n^L + n^S + n^{\text{int}}, \\ V &= V^L + V^S, \\ U &= U^L + U^S + U^{\text{int}}, \\ S &= S^L + S^S + S^{\text{int}}. \end{aligned} \tag{2.3}$$

The thermodynamic model of the interface is given by the following Gibbs equation, where the extensive variables associated with space have the dimension of an area A instead of a volume:

$$dU^{\text{int}} = TdS^{\text{int}} - \sigma dA + \mu dN^{\text{int}} \tag{2.4}$$

where σ is the interfacial energy (surface tension) between the two phases and A is the interfacial area. This accounts for the work done to modify the interface's surface.

The variation of the internal energy of the total system, consisting of the two phases including the interface, is then expressed as:

$$dU = TdS - p^L dV^L - p^S dV^S + \mu dN + \sigma dA \tag{2.5}$$

In nonequilibrium situations, these quantities are not constant, and thermodynamic relationships must be established in a local form using densities of the extensive properties and adopting the local equilibrium assumption. In this case, the interface possesses its own temperature T^{int} and chemical potential μ^{int}. In nonequilibrium situations, the interfacial excess densities of energy (u^{int}), entropy (s^{int}), and mole number (n^{int}), as well as excess pressure (p^{int}), can be defined [82].

Additionally, the role of interfacial energy becomes significant in determining the dynamics of phase boundaries and solidification kinetics. It impacts the development of microstructural features during solidification, such as dendrites, described by models and theories from [13], and further explored through stability analyses by [67].

Finally, the Gibbs-Thomson effect describes how surface energy affects the melting point of materials [28]. The Gibbs-Thomson equation describes the excess energy at the interface during solidification:

$$\Delta G = \sigma \Delta A \tag{2.6}$$

where: ΔG is the excess energy at the interface, σ is the interfacial energy, ΔA is the change in surface area of the solid-liquid interface.

2.6 Solidification Model of a Pure Substance

In this section, we present the modeling of the solidification process of a pure substance using both thin (sharp) and diffuse interface approaches. We begin by discussing the one-dimensional Stefan problem to illustrate the sharp interface model and then compare this with the diffuse interface model offered by the phase-field approach. These models provide fundamental insights into the dynamics and thermodynamics of the solidification process.

2.6.1 The One-Dimensional Two-phase Stefan Problem for Solidification

The Stefan problem is a classical mathematical formulation used to describe liquid-solid phase transitions such as solidification and melting [81, 45, 27]. It is particularly important in the study of heat transfer in systems undergoing a change from one phase to another. This section focuses on the one-dimensional, two-phase Stefan problem, which models the solidification of a pure substance.

- We consider constant density $\rho_s = \rho_l = \rho$, melt temperature T_m, phase-wise constant specific heats c_l, c_s, and thermal conductivities λ_l, λ_s. Heat is transferred only by conduction, through both the solid and the liquid phases.
- The moving interface between the solid and liquid phases is important for understanding the dynamics of the system [28]. The position of this interface, denoted as $l(t)$, changes over time due to the phase change process. The basic setup involves two regions: the solid phase $s(x < l(t))$ and the liquid phase $l(x > l(t))$.
- In each phase i, the energy balance is given by:

$$\rho_i \frac{\partial u_i}{\partial t} = \lambda_i \frac{\partial^2 T_i}{\partial x^2}, \quad \text{for } i = l, s \tag{2.7}$$

where $u_i(x,t)$ and $T_i(x,t)$ represent the energy field and temperature field respectively.

The Stefan Condition

The interface dynamics $l(t)$ is derived from the total energy balance and the first law of thermodynamics stating that the total energy is conserved.

At the interface, the power continuity equation is written:

$$\frac{dl}{dt}\left(u_l|_{x=l(t)+} - u_s|_{x=l(t)-}\right) = \lambda_s \frac{\partial T_s}{\partial x}\bigg|_{x=l(t)-} - \lambda_l \frac{\partial T_l}{\partial x}\bigg|_{x=l(t)+} \tag{2.8}$$

where the term $(u_l|_{x=l(t)+} - u_s|_{x=l(t)-})$ represents the latent heat.

Constitutive Relation: Thermodynamic Equilibrium at the Interface

To complete the system, the temperature at the interface must be specified. The simplest assumption is that the temperatures are at thermodynamic equilibrium. Therefore, at the interface position $l(t) \in (0, L)$, the temperature is equal to the melting temperature T_m:

$$T_l(t, l(t)) = T_s(t, l(t)) = T_m, \quad \forall t > 0. \tag{2.9}$$

This means that the temperature at the interface, for both the liquid state T_l and the solid state T_s, is equal to the melting temperature T_m [109].

However, this constitutive relation does not account for surface tension at the interface. In a more detailed model, the Gibbs-Thomson effect could be included to consider the influence of surface tension on the equilibrium temperature. The Gibbs-Thomson law, which takes into account surface effects, provides a more accurate description:

$$T_m = T_m^0 - \frac{\sigma \kappa}{L_f}, \tag{2.10}$$

where T_m^0 is the equilibrium melting temperature for a flat interface, σ is the surface tension, κ is the curvature of the interface, and L_f is the latent heat of fusion [78].

Finally, to solve the Stefan problem numerically, appropriate boundary conditions on the fixed boundaries and initial conditions for the temperature distribution and interface position must be specified. Typically, these boundary conditions include fixed temperatures or heat fluxes at the domain boundaries, and the initial temperature profile and interface position should reflect the initial state of the system.

In conclusion, the one-dimensional Stefan problem for solidification is a coupled system of partial differential equations (PDEs) for heat conduction in the solid and liquid phases, along with an ordinary differential equation (ODE) for the interface position. This model provides a fundamental framework for studying phase change processes in materials science and engineering [81, 45].

Numerical Methods and Front Tracking

A primary challenge of the Stefan problem is that the spatial domains of the fluid and the solid are time-varying, and the dynamics of the position of the interface is finite-dimensional. This gives rise to a coupled system of PDEs and ODEs, which must be solved together. The interface $l(t)$ is not given explicitly; it must be determined as part of the solution. This inherent characteristic poses significant challenges for both analytical and numerical treatments, as it requires solving for a moving boundary whose position is a priori unknown [47, 49].

To address these challenges, various numerical methods have been developed:

- **Finite Difference Method:** This method discretizes the domain into a grid and approximates derivatives at each grid point. The challenge with a moving interface is to ensure that the grid can accurately track the position of the interface over time, which may require adaptive meshing or re-meshing techniques [83].
- **Front Tracking Method:** This method explicitly tracks the solid-liquid interface as it advances in time, using the energy balance at the interface to determine the evolution of the front position and temperature [22], [115], [58].
- **Level Set Method:** This method represents the moving interface as the zero level set of a signed distance function, with the interface's evolution governed by the level set equation coupled with the heat equation [100].
- **Immersed Boundary Method:** This method models the solid-liquid phase change with the interface represented as an immersed boundary within the domain, enforcing

boundary conditions at the interface using methods like penalty or projection techniques [41].

- **Lattice Boltzmann Method:** This method handles the heat conduction problem with phase change by modeling the distribution functions of particle velocities, particularly useful in scenarios with complex boundary conditions and can naturally accommodate the moving interface problem [48].

The choice of method depends on the specific requirements of the problem, such as accuracy, computational efficiency, and ease of implementation.

2.6.2 Solidification of a Pure Substance Using Phase Field Approach

In this section, we present an alternative model for the solidification process using the diffuse interface approach. First, we recall the classical phase-field models using phase field variables [73, 112]. Then, we define an equivalent model using the entropy as the generating function instead of the energy.

As previously observed, methods with a sharp interface can necessitate significant computational resources, and reconstruction techniques can introduce numerical inaccuracies. It is well-documented that the phase field approach offers a more accurate and flexible means of modeling solidification processes compared to the traditional sharp interface method [8, 28].

In this thesis, we follow a thermodynamic approach to phase field models. The cornerstone of phase field modeling relies on the definition of a functional representing its entropy density, energy density, or other thermodynamic potentials. The thermodynamic basis of the phase-field approach was first discussed in the nineties by [73] and [112] for the solidification of a pure liquid. These foundations were essential for representing anisotropy-induced preferential growth and nonlinear transition kinetics [30].

In this section, we present the classical phase-field approach to solidification using an energy functional. The next section will tackle the same problem with the entropy functional.

A Brief Introduction to the Phase Field Model for Solidification-Melting Processes

The Phase Field Variable and the Domain

The phase field approach is based on the phase field variable ϕ. This variable is a continuous function defined over the entire domain of the system, representing the local phase composition at each point in space and time. Values range from ϕ_{min} (e.g., solid phase) to ϕ_{max} (e.g., liquid phase), with intermediate values depicting the diffuse interface. The evolution of ϕ is governed by partial differential equations describing the kinetics and energetics of phase transitions within the material.

Kinetic Transitions: The Allen-Cahn Equation and the Ginzburg-Landau Functional

The Allen-Cahn equation is a partial differential equation on the phase field variable ϕ derived from the Ginzburg-Landau theory of phase transitions, primarily based on thermodynamics. During the process of solidification, this equation models the evolution of the interface between the two phases that minimizes the Ginzburg-Landau functional. This functional represents most of the time the total free energy of the system, which comprises the bulk free energy and the interfacial free energy. The bulk free energy addresses the energy associated with the crystal structure of the solid phase and with the liquid phase. Meanwhile, the interfacial free energy considers the energy at the interface between these phases. The generic form of the Allen-Cahn equation is given by (2.11):

$$\frac{\partial \phi}{\partial t} = -M_\phi \frac{\delta F}{\delta \phi} \tag{2.11}$$

where F represents the total free energy of the system, $\frac{\delta F}{\delta \phi}$ the functional derivative with respect to ϕ and M_ϕ the mobility constant.

The free energy functional

This paragraph examines the thermodynamic treatment that is essential to phase-field modeling [28, 8] and gives the thermodynamic concepts that link the phase field variable and energy.

For this purpose, we consider the case of the solidification of a pure substance in non-isothermal conditions. We also assume that density is unchanged in the phase transition.

The free energy functional, F, is defined as:

$$F = \int_V \left[f(\phi, T) + \frac{\epsilon_\phi^2}{2} |\nabla \phi|^2 \right] dV, \tag{2.12}$$

where ϵ_ϕ^2 is the gradient energy coefficient and T is the temperature field. $f(\phi, T)$ represents the free energy density on the domain, and $\frac{\epsilon_\phi^2}{2}|\nabla \phi|^2$ is the gradient energy density.

In a two-phase system, $f(\phi, T)$ is commonly expressed as the free energy expressions of the coexisting phases ($f_l(\ T)$, $f_s(\phi, T)$ for liquid and solid respectively) combined by an interpolation function $h(\phi)$ and a double-well function $g(\phi)$. we have :

$$f(\phi, T) = h(\phi) f_l(T) + \big(1 - h(\phi)\big) f_s(T) + g(\phi) \tag{2.13}$$

$h(\phi)$ expresses the continuous passage to the liquid phase to the solid one (so from ϕ_{min} to ϕ_{max}. In order to satisfy the intrinsic stability of the solid and liquid pure phase since f has to verify [14]:

$$\frac{\partial f}{\partial \phi}|_{\phi=\phi_{min}} = \frac{\partial f}{\partial \phi}|_{\phi=\phi_{max}} \tag{2.14}$$

$$\frac{\partial f}{\partial \phi^2}^2 |_{\phi=\phi_{min},\phi_{max}} > 0 \tag{2.15}$$

So $g(\phi)$ must be a double-well function. Details of thermodynamics and function calculation will be given in the next section in the case where the Ginzburg-Landau function is entropy.

We finally obtain the following form for the Allen-Cahn equation:

$$\frac{\partial \phi}{\partial t} = -M_\phi \left[\frac{\partial f}{\partial \phi} + \epsilon_\phi^2 \nabla^2 \phi \right], \tag{2.16}$$

The energy balance

Let us consider that molar volume of liquid and solid phase are the same and pressure remains constant. The energy balance over the domain is given by:

$$\frac{\partial u(\phi, T)}{\partial t} = \nabla \cdot (\lambda(\phi) \nabla T) \tag{2.17}$$

where $u(\phi, T)$ is the internal energy field, $\lambda(\phi)$ is the thermal conductivity, and Q is a source term. The thermal conductivity is a function of the phase field, and it is chosen to ensure the correct behavior of the temperature field [114].

To proceed further, let us give the expression of the internal energy. From the free energy (2.13), the internal energy can be written as (see [42]):

$$\begin{aligned} u(\phi, T) &= u_s(T) + h(\phi) L(T) \\ &= u_l(T) + \big(h(\phi) - 1\big) L(T) \end{aligned} \tag{2.18}$$

where $L(T) = u_l(T) - u_s(T)$ is the heat of fusion.

So the energy balance can be finally written as [112]:

$$\Big(c_l(T) + \big(h(\phi) - 1\big) \frac{\partial L}{\partial T} \Big) \frac{\partial T(\phi, T)}{\partial t} + \frac{\partial h}{\partial \phi} L(T) = \nabla \cdot (\lambda(\phi) \nabla T) \tag{2.19}$$

where $c_l(T)$ is the specific heat constant of liquid phase.

The Model for Solidification of a Pure Substance in the Case of Constant Heat of Fusion

The mathematical model for the solidification process combines the Allen-Cahn equation with the energy balance over the domain. In the case of water, the heat of fusion is assumed to be constant in the temperature range $[-20°C, 0°C]$, conforming to the revised standards by IAPWS [42]. The difference in free energy between the liquid and solid at the melting point T_m is given by:

$$f_l(T_m) - f_s(T_m) = \frac{L\big(T - T_m\big)}{T_m}, \tag{2.20}$$

where L represents the heat of fusion at T_m. The dynamics of the phase field variable ϕ and temperature field T are described by the following coupled differential equations:

$$\frac{\partial \phi}{\partial t} = -M_\phi \left[\frac{L\big(T - T_m\big)}{T_m} \frac{\partial h}{\partial \phi} + \epsilon_\phi^2 \nabla^2 \phi \right], \tag{2.21}$$

$$\frac{\partial T}{\partial t} = \frac{1}{c_l(T)} \nabla \cdot (\lambda(\phi) \nabla T) - \frac{1}{c_l(T)} \frac{\partial h}{\partial \phi} L. \tag{2.22}$$

Boundary and Initial Conditions To solve this model, specific boundary conditions (BCs) and initial conditions (ICs) must be defined. Here, z represents the spatial coordinate along the length of the domain.

Boundary Conditions: The boundaries of the domain are maintained to represent the solid and liquid phases. At the left boundary ($z = 0$), the system is in the liquid phase with $\phi = 1$ and $T = 274.15\,K$. At the right boundary ($z = L$), the system is in the solid phase with $\phi = 0$ and $T = 272.15\,K$.

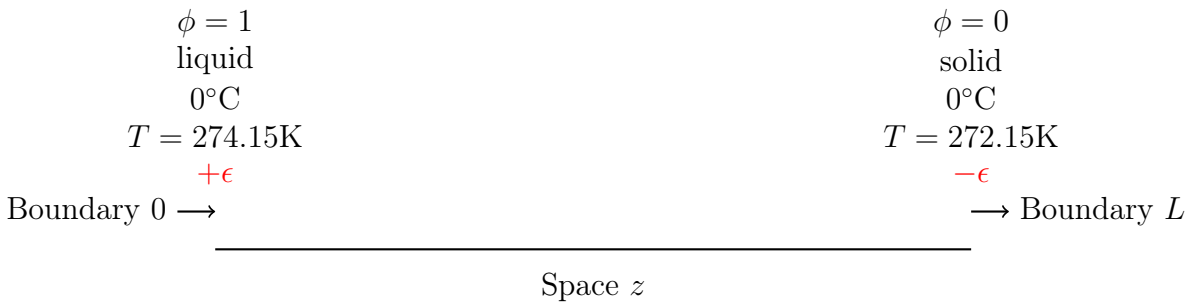

Figure 2: Boundary conditions for the phase field variable ϕ and temperature T.

Initial Conditions: At $t = 0$, the temperature throughout the domain is assumed uniform, $T(t = 0, z) = 273.15\,K$, and $\phi(t = 0, z)$ is initialized based on the distribution of phases, typically $\phi = 1$ in liquid regions and $\phi = 0$ in solid regions.

This setup, with clearly defined boundary and initial conditions, allows for the modeling of the solidification process, capturing the transition between liquid and solid phases.

2.7 Phase Field Model for Solidification of Water Using the Entropy Functional

This section presents the phase field model for the solidification of pure water, using the entropy functional as the thermodynamical potential. This representation will be used in later chapters to formulate the solidification process model in detail.

2.7.1 The Entropy Functional

Following the approach of [112], we shall present a model that uses the entropy as the thermodynamic potential. Its expression is analogous to the expression of the energy in equation (2.12):

$$S = \int_V \left[s(\phi) - \frac{\epsilon_\phi^2}{2} |\text{grad}\, \phi|^2 \right] dV, \tag{2.23}$$

where s represents the entropy density, ϕ the phase-field variable, and ϵ_ϕ the entropy coefficient associated with the phase-field gradient in this entropy representation.

Thermodynamic Model

To derive the thermodynamic properties of the phase-field variable ϕ, the entropy balance and Gibbs' equations are employed in entropy form:

$$ds = \left(\frac{\partial s}{\partial \phi} \right) d\phi + \tau du, \tag{2.24}$$

where s represents the entropy density, u the internal energy density, and τ is defined as the reciprocal temperature ($\tau = (\frac{\partial s}{\partial u})_\phi = \frac{1}{T}$). This reciprocal form is used to simplify the differential treatment of temperature effects in the system, assumed to have uniform mass density as per [112].

The thermodynamic potential of the phase field system, the total entropy of the biphasic system, is formulated using the Landau-Ginzburg entropy functional:

$$S(\phi, u) = \int_V \left(s(\phi, u) - \frac{1}{2} \epsilon^2 (\text{grad}\, \phi)^2 \right) dv, \tag{2.25}$$

where ϵ is a parameter indicative of the interface thickness. The quadratic term models the energy cost of variations in ϕ, helping to simulate the interface behaviors.

2.7.2 Dynamic Model Equation

The dynamic model consists of the phase-field dynamics governed by the Allen-Cahn equation, which describes the evolution of the phase-field variable ϕ based on entropy considerations and interface mobility:

$$\frac{\partial \phi}{\partial t} = -\frac{1}{\eta} \left(\frac{\partial s}{\partial \phi}(\phi) - \epsilon^2 \text{div}(\text{grad}\, \phi) \right) = -\frac{1}{\eta} \frac{\delta S}{\delta \phi}, \tag{2.26}$$

where η is the positive interface mobility, enhancing the model's ability to simulate the rapid changes at the interface. The variational derivative $\frac{\delta S}{\delta \phi}$ ensures that the phase-field evolution adheres to the thermodynamic driving forces, effectively coupling material properties with phase dynamics.

The theoretical framework and equations presented here are based on solid thermodynamic principles, as outlined in foundational works [112, 8].

This phase-field model provides a thermodynamically consistent description of the solidification process, using entropy as the generating function.

2.8 Thermodynamic Properties of Water and Ice

Thermodynamic properties of liquid water and ice can be found in the literature, such as in [42] and [43]. These sources provide thermodynamic potentials, specifically the Gibbs energy, expressed as functions of temperature and pressure. The specific Gibbs energy of the liquid phase is given by:

$$g_{liq}(T,p)/g^* = \sum_{j=0}^{7}\sum_{k=0}^{6} g_{jk}\tau^j\pi^k, \tag{2.27}$$

Here, the reduced temperature $\tau = (T - T_0)/T^*$ and the reduced pressure $\pi = (p - p_0)/p^*$. Constants T_0, p_0, T^*, p^*, g^*, and g_{jk} can be found in [43]. Similarly, the specific Gibbs energy of the solid phase is expressed as:

$$\begin{aligned} g_{sol}(T,p) = g_0(p) - s_0 T_t \tau + T_t Re\Bigg(\sum_{k=1}^{2} r_k \Big[(t_k - \tau) \\ \ln(t_k - \tau) + (t_k + \tau)\ln(t_k + \tau) - 2t_k \ln(t_k) \\ - \frac{\tau^2}{t_k} \Big] \Bigg) \end{aligned} \tag{2.28}$$

In this case, $g_0(p) = \sum_{k=0}^{4} g_{0k}(\pi - \pi_0)^k$ and $r_2(p) = \sum_{k=0}^{2} r_{2k}(\pi - \pi_0)^k$, $\tau = T/T_t$, $\pi = p/p_t$, and $\pi_0 = p_0/p_t$. Constants $T_t, p_t, p_0, s_0, g_0, r_1$, as well as g_{ok}, r_{2k}, and t_k are given in [42].

Other specific thermodynamic quantities, such as entropy, Helmholtz energy, and density for each phase, can be derived from standard thermodynamic computations (see [42, 43], and [**callen1998thermodynamics**]. For instance, the specific Helmholtz energy $f_\star$, specific entropy $s_\star$ as a function of temperature and pressure, density $\rho_\star$, and heat capacity $c_{p_\star}$ can be deduced from $g_\star$ for $\star = sol, liq$ using the formulas:

$$f_\star(T,p) = g_\star - p\frac{\partial g_\star}{\partial p}, \tag{2.29}$$

$$s_\star(T,p) = -\frac{\partial g_\star}{\partial T}, \tag{2.30}$$

$$\rho_\star(T,p) = \left(\frac{\partial g_\star}{\partial p}\right)^{-1}, \tag{2.31}$$

$$c_{p_\star}(T,p) = -T\frac{\partial^2 g_\star}{\partial T^2}. \tag{2.32}$$

Table 2.1 shows some thermodynamic property values at the melting temperature (273.15 K) and atmospheric pressure.

Table 2.1: Values of some thermodynamic properties at the melting temperature

$\star$	$g_\star$	$f_\star$	$s_\star$	$\rho_\star$	$c_{p_\star}$
liq	101.343	0.0018	–0.1476	999.843	4219.41
sol	101.343	– 9.1870	– 1220.769	916.721	2096.71

The Extended Equation of State

For brevity, we focus on the extended specific entropy s while assuming constant density. This assumption simplifies the mathematical treatment and is reasonable for many practical applications where density variations are negligible compared to other effects. The thermodynamic stability principle, when two phases are present, requires (see Section 2.4 on thermodynamics and [14]):

$$\left.\frac{\partial s}{\partial \phi}\right|_{\phi=0} = \left.\frac{\partial s}{\partial \phi}\right|_{\phi=1} = 0, \quad \left.\frac{\partial^2 s}{\partial \phi^2}\right|_{\phi=0,1} < 0, \tag{2.33}$$

These conditions, essential for phase stability at the boundaries, ensure that the entropy function does not promote non-physical behaviors at the extremes of the phase field variable ϕ. At equilibrium, the variational derivative of the Landau-Ginzburg entropy functional must vanish, ensuring consistency with physical laws of thermodynamics [112, 50, 8]:

$$\left.\frac{\partial s}{\partial \phi}\right|_{\phi=0,1} = 0 \text{ and } \left.\frac{\partial^2 s}{\partial \phi^2}\right|_{\phi=0,1} < 0. \tag{2.34}$$

Following the general approach discussed in [112], we derive the extended specific entropy function:

$$s(\phi, T) = s_{sol}(T) + p_i(\phi)[s_{liq}(T) - s_{sol}(T)] + w p_w(\phi), \tag{2.35}$$

$$p_i(\phi) = \phi^3(6\phi^2 - 15\phi + 10), \quad p_w(\phi) = -\phi^2(1-\phi)^2, \tag{2.36}$$

where s_{liq} and s_{sol} represent the specific entropies of pure water and ice, respectively, and w is a parameter that adjusts the energy barrier between these phases. Figure 3 provides a visual representation of the entropy landscape shaped by these polynomials, illustrating how the choice of p_i and p_w affects the model's ability to simulate the phase transition.

This extended entropy function ensures that our model adheres to the fundamental principles of thermodynamics, as delineated by [14], providing a robust and physically accurate description of phase transitions in water and ice systems.

2.9 Recap: Evolution Equations for the Solidification Model

We recall the model presented before in the form of a system of evolution equations:

- **State Variables:**

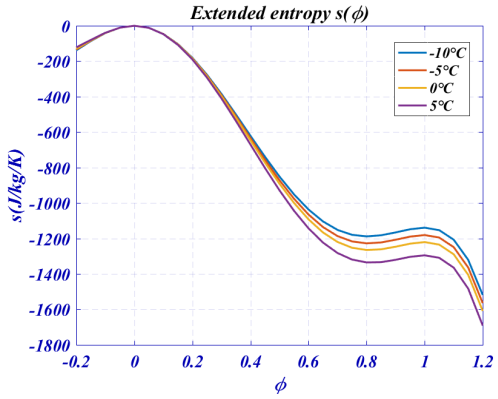

Figure 3: Extended specific entropy with $w = 18 \times 10^3$; this graph shows how entropy varies as a function of ϕ, highlighting the stability at phase boundaries.

  - ϕ: Phase field variable
  - u: Internal energy

- **Thermodynamic Model:** In phase field modeling, entropy is characterized by a specific entropy function, $s^*(\phi, T)$, which describes the thermodynamic interactions between liquid and solid phases. This function includes $s^*_{sol}(T)$ for the specific entropy of the solid (ice) and $s^*_{liq}(T)$ for the liquid (water), using double-well and interpolating polynomials, $p_w(\phi)$ and $p_i(\phi)$, to model the phase transition:

$$s^*(\phi, T) = s^*_{sol}(T) + p_i(\phi)[s^*_{liq}(T) - s^*_{sol}(T)] + wp_w(\phi) \tag{2.37}$$

  where:
  - $p_i(\phi) = \phi^3(6\phi^2 - 15\phi + 10)$
  - $p_w(\phi) = -\phi^2(1-\phi)^2$

- **Evolution Equations:** The phase field's evolution is governed by the following equation, highlighting the integral role of specific entropy in the model:

$$\frac{\partial \phi}{\partial t} = -\frac{1}{\eta}\frac{\partial s^*}{\partial \phi}(\phi, T) + \frac{\epsilon^2}{\eta}\text{div}(\text{grad}\phi) \tag{2.38}$$

  where:
  - $\frac{\partial s^*}{\partial \phi}(\phi, T) = (30\phi^4 - 60\phi^3 + 30\phi^2)g + w(-4\phi^3 + 6\phi^2 + 2\phi)$
  - $p_i'(\phi) = 30\phi^4 - 60\phi^3 + 30\phi^2$
  - $p_w'(\phi) = -4\phi^3 + 6\phi^2 + 2\phi$

  Additionally, the energy balance equation is:

$$\frac{\partial u}{\partial t} = -\text{div}\,(q) \tag{2.39}$$

  where u is the internal energy and q is the heat flux.

- **Boundary Conditions:** The boundary conditions are expressed in terms of:

$$\phi_{\text{boundary}} = \text{tr}(\phi) \quad \text{on} \quad \partial\Omega \tag{2.40}$$

$$\text{grad}\phi \cdot \mathbf{n} = 0 \quad \text{on} \quad \partial\Omega \tag{2.41}$$

  where $\mathbf{n}$ is the normal vector to the boundary surface $\partial\Omega$.

2.10 Conclusion

We have recalled the models of bi-phasic systems with phase transitions using the phase field variable representing the moving interface between the phases. We have presented the thermodynamic properties of biphasic systems with phase field models using entropy as the thermodynamic potential [116, 31]. We concluded with the dynamical model consisting of coupled heat conduction dynamics and a gradient system for the dynamics of the phase field variable.

Specifically, we have proposed writing the thermodynamic model in terms of a non-linear entropy function depending on the phase field variable ϕ and the temperature T. This approach differs from most classical methods, which use the Gibbs free energy or Helmholtz free energy.

By using the entropy function, we prepare the Port Hamiltonian model which uses the entropy functional as the generating function.

Chapter 3

Port Hamiltonian Formulation of the Solidification Process

Contents

Abstract

This chapter discusses the application of Port Hamiltonian Systems (PHS) to the mathematical modeling and control of solidification processes. It introduces the foundational concepts of PHS, including Dirac structures and their role in the geometric structuring of power dynamics within physical systems. By examining both finite and infinite-dimensional systems, the chapter applies these concepts to the diffusion equation, Allen-Cahn Equation, and solidification processes, emphasizing energy dissipating behaviors and their mathematical representations.

3.1 Introduction to the chapter

Boundary Port Hamiltonian systems (PHS) provide an efficient framework to link physical principles with systems theory and control. This chapter builds on the review paper and lecture notes of [77] and [84], for the presentation of the definition, the properties of Boundary Port Hamiltonian Systems.

We first recall the canonical Hamiltonian operators and the definition of Stokes-Dirac structures [54, 94], as these are essential in understanding the underlying principles of Port Hamiltonian systems. Besides, the concept of Boundary Port Hamiltonian systems will be introduced.

Next, we elaborate on the Boundary Port Hamiltonian formulation of the heat diffusion equation and the Allen-Cahn equation. By applying the principles of PHS, we will demonstrate how these formulations can be used to model the dynamics of solidification processes. This involves coupling the heat diffusion and Allen-Cahn equations to obtain a comprehensive Boundary Port Hamiltonian formulation of the solidification process.

Initially, we derived the explicit model of the solidification process using the entropy as the generating function, with the state variables being the phase field variable ϕ and the internal energy u. However, due to the lack of data concerning the expression of the entropy density function (2.25) $s = s(\phi, u)$, we switched to using the reciprocal temperature $\tau = 1/T$. This change allows us to utilize available data and thermodynamic properties of liquid water and ice, as found in the literature [42] and [43]. The provided thermodynamic potential is the Gibbs energy, expressed as a function of temperature and pressure.

We then defined the thermodynamic properties of the bi-phasic water-ice system, leading to the expressions of the entropy density (2.35) depending on the temperature rather than the internal energy. This required changing the state space coordinate from the internal energy u (an extensive variable) to the temperature T (an intensive variable).

To reformulate the explicit Port Hamiltonian model, we introduced the Implicit Port Hamiltonian formulation using Lagrangian submanifolds, which allow the definition of reciprocal constitutive equations in a coordinate-free way [105], [88]. This approach can be adapted to distributed parameter systems [60], [106]. Finally, we derived an implicit formulation of the solidification model by integrating Differential-Algebraic Equations (DAE) and Partial Differential Equations (PDE). This framework models the dynamics in terms of reciprocal temperature, aligning with empirical thermodynamic properties of systems like water and ice.

Our discussion will refer to the Thermodynamic Framework for Modeling and Simulation [5] and [116] to illustrate the practical applications of these theoretical constructs.

3.2 Overview of the chapter

This chapter discusses the Port Hamiltonian Systems (PHS) approach to modeling solidification processes [61]. It starts with an introduction to the fundamental aspects of PHS, focusing on the conceptual and mathematical foundations of Dirac structures and their role in modeling physical systems. The discussion covers both finite and infinite-dimensional systems, highlighting dissipative behavior in energy control. The chapter analyzes the application of PHS to the equations governing solidification processes. These include the diffusion equation and the Allen-Cahn equation. It demonstrates the advantages of PHS in understanding and managing the energy dynamics of solidification processes.

3.3 Contributions and Structure of the chapter

The main contributions are structured around the development of a theoretical framework and its application to physical phenomena, building on existing literature:

1. **Derivation of the Allen-Cahn Dynamics:** Building on the work of Vincent et al. ([110]), this chapter presents the derivation of the Port Hamiltonian representation of the Allen-Cahn equation in the entropy representation.
2. **Implicit Formulation of the Solidification Model:** In order to use the empirical data of thermodynamic properties systems, given in terms of the reciprocal temperature, an implicit port-Hamiltonian formulation is developed. This formulation is expressed in terms of a system of Differential-Algebraic Partial Differential Equations (DA-PDE). These systems belong to the recently defined class of port Hamiltonian systems on Lagrange submanifolds, as defined in [105, 60, 106, 6].

3.4 Introduction to Port Hamiltonian Systems

Port-Hamiltonian systems (PHS) provide a framework for analyzing and controlling open physical systems, originally developed for finite-dimensional applications [63, 61]. At the core of this methodology is the concept of power-conjugated variable pairings and the associated geometric structure known as the Dirac structure [18]. This structure highlights the geometric properties of physical systems and their relationships with the external environment [62]. These insights include topological features, port connectivity, and constraints across different domains [19].

The geometric framework of PHS has been useful in developing implicit Hamiltonian systems and those incorporating port variables, leading to stable control strategies [19, 59]. Recent advancements have extended PHS to infinite-dimensional settings, which is beneficial for systems with boundary-focused energy distributions [65].

A basic property of a Dirac structure is power conservation: the Dirac structure links the various port (flow and effort) variables f and e so that the total power $e^\intercal f$ is zero.

In infinite-dimensional settings, the state space is characterized by differential forms, and the defining characteristic of such systems revolves around the Stokes-Dirac structure dictated by external derivatives and differential form rankings [64]. This structure has been adapted to include fluid dynamics and beam models [86]. Moreover, the Hamiltonian formulation of distributed parameter systems in a bounded spatial domain, especially when energy transfer takes place across the boundary, has led to the definition of a specific Dirac structure called *Stokes-Dirac structure* [86, 9, 56].

Complementing this discussion with linear skew-symmetric differential operators, we clarify the nature of Dirac structures and the core essence of PHS, emphasizing singular degree differential operators. Additionally, alternative Dirac structures in Hilbert spaces, as discussed in [71], are explored, particularly in scattering contexts.

Port-Hamiltonian systems theory integrates principles from various classical physical systems modeling and analysis approaches:

- **Port-based modeling**: Initiated by Henry Paynter in the late 1950s [72], this methodology emphasizes energy as the unifying metric, typically represented using bond graphs [33].
- **Geometric Mechanics**: Building on foundational work such as [3], this perspective enriches the Hamiltonian view of classical mechanics through geometry, offering deeper insights [69].
- **Systems and Control Theory**: Based on the theory of electrical network synthesis [85], the introduction of the Dirac structure [113] helped manage interconnected systems.

PHS are characterized by their flexible geometric framework and their ability to account for energy dissipation, making them adaptable to various engineering contexts. Serving as a common language, energy connects different physical domains in these systems, forming the basis for control strategies that leverage the inherent properties of physical systems.

Infinite Port Hamiltonian systems extend the energy-based modeling approach inherent in PHS to systems defined over infinite-dimensional spaces, often encountered in distributed parameter systems such as flexible beams, fluid flow, or heat conduction in continuous media [92].

Throughout this chapter, we will discuss in more details the Port-Hamiltonian formulation, highlighting its effectiveness for processes such as solidification.

3.5 Introduction to Dirac Structures

Dirac structures arise in constrained Hamiltonian systems and port Hamiltonian systems. In systems theory, especially for systems with constraints or connections, the concept of Dirac structures provides a unifying geometric framework. Rooted in differential geometry, Dirac structures offer a systematic approach to capturing power-preserving connections in dynamical systems [56, 108, 84].

3.5.1 Dirac Structures in Finite Dimensional Vector Spaces

For the formal definition of a Dirac structure, we start with an abstract finite-dimensional linear space of flows $\mathcal{F}$. The elements of $\mathcal{F}$ are denoted by $f \in \mathcal{F}$ and are called flow vectors. The space of efforts is given by the *dual*[1] linear space $\mathcal{E} := \mathcal{F}^*$, and its elements are denoted by $e \in \mathcal{E}$ [104]. The total space of flow and effort variables is $\mathcal{F} \times \mathcal{E}$, and will be called the space of port variables. The power on the total space of port variables is defined by

$$P = \langle e|f\rangle, \quad (f, e) \in \mathcal{F} \times \mathcal{E}, \tag{3.1}$$

where $\langle e|f\rangle$ denotes the duality product, that is, the linear functional $e \in \mathcal{E} = \mathcal{F}^*$ acting on $f \in \mathcal{F}$. In the usual case of $\mathcal{F} = \mathbb{R}^k$ this amounts to

[1]The definition $\mathcal{E} = \mathcal{F}^*$ for the effort space is in some sense the minimal required structure. All definitions and results directly extend to the case that $\mathcal{F}$ has an inner-product structure. In this case, we may take $\mathcal{E} = \mathcal{F}$ with the duality product $\langle e|f\rangle$ replaced by the inner product $\langle e, f\rangle$.

$$\langle e|f\rangle = e^{\intercal} f, \tag{3.2}$$

where both $f \in \mathbb{R}^k$ and $e \in (\mathbb{R}^k)^*$ are represented as column vectors.

Definition 3.5.1

[104] Consider a finite-dimensional linear space $\mathcal{F}$ with $\mathcal{E} = \mathcal{F}^*$. A subspace $D \subset \mathcal{F} \times \mathcal{E}$ is a Dirac structure if:

1. $\langle e|f\rangle = 0$, *for all* $(f, e) \in D$,
2. $\dim D = \dim \mathcal{F}$.

Property 1. corresponds to power conservation, and expresses the fact that the total power entering (or leaving) a Dirac structure is zero. It can be shown that the maximal dimension of any subspace $D \subset \mathcal{F} \times \mathcal{E}$ satisfying Property 1. is equal to dim $\mathcal{F}$; for the proof see [104].

To further characterize a Dirac structure, we look more closely at the geometric structure of the total space of flow and effort variables $\mathcal{F} \times \mathcal{E}$. Related to the definition of power, there exists a canonically defined bilinear form $\langle \cdot, \cdot \rangle$ on the space $\mathcal{F} \times \mathcal{E}$, defined as:

$$\langle (f^a, e^a), (f^b, e^b) \rangle = \langle e^a | f^b \rangle + \langle e^b | f^a \rangle, \quad (f^a, e^a), (f^b, e^b) \in \mathcal{F} \times \mathcal{E}. \tag{3.3}$$

Note that this bilinear form is indefinite, that is, $\langle (f, e), (f, e) \rangle$ may be positive or negative. It is non-degenerate in the sense that $\langle (f^a, e^a), (f^b, e^b) \rangle = 0$ for all (f^b, e^b) implies that $(f^a, e^a) = 0$ ([104]).

Proposition 3.5.1

[18, 25] A Dirac structure on $\mathcal{F} \times \mathcal{E}$ is a subspace $D \subset \mathcal{F} \times \mathcal{E}$ such that

$$D = D^{\perp\perp}, \tag{3.4}$$

where $\perp\perp$ denotes the orthogonal companion with respect to the bilinear form $\langle \cdot, \cdot \rangle$.

Alternatively, $D \subset \mathcal{F} \times \mathcal{E}$, with $\mathcal{F}$ and $\mathcal{E}$ finite-dimensional, is a Dirac structure if and only if it satisfies Property 1 in Definition 3.5.1 and has maximal dimension with respect to this property, that is, if the subspace D' also satisfies Property 1 then dim $D' \leq$ dim D. This maximal dimension is equal to dim $\mathcal{F}$ = dim $\mathcal{E}$.

For the proof we refer to [104].

Kernel Representation [94] Let $\mathcal{B} := \mathcal{F} \times \mathcal{E}$ equipped with an inner product $(\cdot, \cdot)_{\mathcal{B}}$, and $E, F \in \mathbb{R}^{N \times N}$. Then,

$$D := \{(f, e) \in \mathcal{F} \times \mathcal{E} \mid Ff + Ee = 0\} \tag{3.5}$$

is a Dirac structure for the pairing $\langle\langle \cdot, \cdot \rangle\rangle$ defined from the inner product $(\cdot, \cdot)_{\mathcal{B}}$ as in (3.3), if and only if:

- The matrix $EF^{\top}$ is anti-symmetric for the inner product $(\cdot, \cdot)_{\mathcal{B}}$.

- The rank of $[F : E]$ equals $\dim\mathcal{F}$, where the notation $[F : E]$ represents the horizontal concatenation of the matrices F and E.

Image Representation

Let $\mathcal{B} := \mathcal{F} \times \mathcal{E}$ equipped with an inner product $(\cdot, \cdot)_{\mathcal{B}}$, and $E, F \in \mathbb{R}^{N\times N}$. Then,

$$D := \{(f, e) \in \mathcal{F} \times \mathcal{E} \mid \exists\lambda \in \mathbb{R}^N \text{ such that } f = F^\top\lambda, e = E^\top\lambda\} \tag{3.6}$$

is a Dirac structure for the pairing $\langle\langle\cdot, \cdot\rangle\rangle$ defined from the inner product $(\cdot, \cdot)_{\mathcal{B}}$ as in (3.3), if and only if:

- The matrix $EF^\top$ is anti-symmetric for the inner product $(\cdot, \cdot)_{\mathcal{B}}$.
- The rank of $[F : E]$ equals $\dim\mathcal{F}$.

There are a number of direct examples of Dirac structures $D \subset \mathcal{F} \times \mathcal{E}$:

1. Let $J : \mathcal{E} \to \mathcal{F}$ be a skew-symmetric linear mapping, that is, $J = -J^*$, where $J^* : \mathcal{E} \to \mathcal{E}^* = \mathcal{F}$ is the adjoint mapping. Then graph $J := \{(f, e) \in \mathcal{F} \times \mathcal{E} \mid f = Je\}$ is a Dirac structure.
2. Let $\omega : \mathcal{F} \to \mathcal{E}$ be a skew-symmetric linear mapping, then graph $\omega := \{(f, e) \in \mathcal{F} \times \mathcal{E} \mid e = \omega f\}$ is a Dirac structure.
3. Let $K \subset \mathcal{F}$ be any subspace. Define $K^\perp = \{e \in \mathcal{E} \mid \langle e, f\rangle = 0 \text{ for all } f \in K\}$. Then $K \times K^\perp \subset \mathcal{F} \times \mathcal{E}$ is a Dirac structure.

3.5.2 Dirac Structures in Hilbert Spaces

Two primary methods have been used to extend Dirac structures to infinite-dimensional spaces.

The first method, elaborated in [86], focuses on the Hamiltonian formulation of systems with two conservation laws, such as the wave equation or Maxwell's equations. It uses exterior differential forms as spaces of flow and effort variables, denoted by $\mathcal{F}$ and $\mathcal{E}$, respectively.

The second approach, elaborated in [34], defines Dirac structures on Hilbert spaces. In this thesis, we use Hilbert spaces as flow and effort spaces and briefly recall the definition given in [34].

Let $\mathcal{F}$ and $\mathcal{E}$ be real Hilbert spaces (in the sequel the word real will be omitted for brevity) with inner products $\langle\cdot, \cdot\rangle_{\mathcal{F}}$ and $\langle\cdot, \cdot\rangle_{\mathcal{E}}$, respectively. We make the following assumption throughout.

In practice, we often use L_2 spaces for both flow and effort variables, with the map $r_{\mathcal{F},\mathcal{E}}$ being the identity.

Assumption 1. *$\mathcal{F}$ and $\mathcal{E}$ are isometrically isomorphic.*

Assumption 1 entails the existence of a bijective isometry $r_{\mathcal{F},\mathcal{E}} : \mathcal{F} \to \mathcal{E}$. That is, $r_{\mathcal{F},\mathcal{E}}$ is an invertible linear transformation satisfying

$$\langle r_{\mathcal{F},\mathcal{E}} f_1, r_{\mathcal{F},\mathcal{E}} f_2\rangle_{\mathcal{E}} = \langle f_1, f_2\rangle_{\mathcal{F}}, \quad \forall f_1, f_2 \in \mathcal{F}. \tag{3.7}$$

Let $r_{\mathcal{E},\mathcal{F}} : \mathcal{E} \to \mathcal{F}$ be the inverse of $r_{\mathcal{F},\mathcal{E}}$. Then for any e_1 and e_2,

$$\langle r_{\mathcal{E},\mathcal{F}} e_1, r_{\mathcal{E},\mathcal{F}} e_2 \rangle_{\mathcal{F}} = \langle e_1, e_2 \rangle_{\mathcal{E}}, \quad \forall e_1, e_2 \in \mathcal{E}. \tag{3.8}$$

We can now introduce a pairing $\langle \cdot | \cdot \rangle : \mathcal{F} \times \mathcal{E} \to \mathbb{R}$ as follows:

$$\langle e | f \rangle = \langle f, r_{\mathcal{E},\mathcal{F}} e \rangle_{\mathcal{F}}, \quad \forall f \in \mathcal{F}, \forall e \in \mathcal{E}. \tag{3.9}$$

Since $r_{\mathcal{F},\mathcal{E}}$ is an isometry, this pairing may also be represented by:

$$\langle e | f \rangle = \langle e, r_{\mathcal{F},\mathcal{E}} f \rangle_{\mathcal{E}}, \quad \forall f \in \mathcal{F}, \forall e \in \mathcal{E}. \tag{3.10}$$

Remark 1. *If the term $\langle e|f \rangle$ has the dimension of power, then the pairing described by (3.9) or (3.10) is a power product. Indeed,*

$$\begin{aligned} \langle e | \alpha f^1 + \beta f^2 \rangle &= \langle \alpha f^1 + \beta f^2, r_{\mathcal{E},\mathcal{F}} e \rangle_{\mathcal{F}} \\ &= \alpha \langle f^1, r_{\mathcal{E},\mathcal{F}} e \rangle_{\mathcal{F}} + \beta \langle f^2, r_{\mathcal{E},\mathcal{F}} e \rangle_{\mathcal{F}} \\ &= \alpha \langle e | f^1 \rangle + \beta \langle e | f^2 \rangle, \end{aligned}$$

for all $f^1, f^2 \in \mathcal{F}$, $e \in \mathcal{E}$, and $\alpha, \beta \in \mathbb{R}$.

Thus, the map described by (3.9) and (3.10) is linear in the first argument. Similarly, it is linear in the second argument. Moreover, $\langle e|f \rangle = 0$ for all $e \in \mathcal{E}$ implies $r_{\mathcal{F},\mathcal{E}} f = 0$ and consequently $f = 0$. Similarly, $\langle e|f \rangle = 0$ for all $f \in \mathcal{F}$ means $e = 0$.

Furthermore, the bond space $\mathcal{B} = \mathcal{F} \times \mathcal{E}$ is also a Hilbert space. The inner product for this space is defined as:

$$\langle b^1, b^2 \rangle_{\mathcal{B}} = \langle f^1, f^2 \rangle_{\mathcal{F}} + \langle e^1, e^2 \rangle_{\mathcal{E}}, \tag{3.11}$$

for all $b^1, b^2 \in \mathcal{B}$, where $b^1 = (f^1, e^1)$ and $b^2 = (f^2, e^2)$.

The bilinear form associated with this inner product is:

$$\langle\langle b^1, b^2 \rangle\rangle = \langle b^1, \mathcal{R} b^2 \rangle_{\mathcal{B}}, \tag{3.12}$$

for all $b^1, b^2 \in \mathcal{B}$, where the linear operator $\mathcal{R} : \mathcal{B} \to \mathcal{B}$ is defined by:

$$\mathcal{R} = \begin{bmatrix} 0 & r_{\mathcal{E},\mathcal{F}} \\ r_{\mathcal{F},\mathcal{E}} & 0 \end{bmatrix}. \tag{3.13}$$

Given that $r_{\mathcal{F},\mathcal{E}}$ is an isometry, $\mathcal{R}$ is a bounded linear operator that satisfies $\mathcal{R}^2 = I_{\mathcal{B}}$ (where $I_{\mathcal{B}}$ is the identity operator on $\mathcal{B}$). It's evident that $\mathcal{R}$ is invertible, and its inverse is $\mathcal{R}^{-1} = \mathcal{R}$ [34].

For any subspace $\mathcal{Z} \subset \mathcal{B}$, $\mathcal{Z}^c$ represents the orthogonal complement of $\mathcal{Z}$ with respect to $\langle \cdot, \cdot \rangle_{\mathcal{B}}$. Formally, we can represent $\mathcal{Z}^c$ as:

$$\mathcal{Z}^c = \{ b \in \mathcal{B} : \langle b, \tilde{b} \rangle_{\mathcal{B}} = 0, \forall \tilde{b} \in \mathcal{Z} \}. \tag{3.14}$$

Similarly, we use $\mathcal{Z}^\perp$ to denote the subspace defined by:

$$\mathcal{Z}^\perp = \{ b \in \mathcal{B} : \langle\langle b, \tilde{b} \rangle\rangle = 0, \forall \tilde{b} \in \mathcal{Z} \}. \tag{3.15}$$

Proposition 3.5.2

[34] Let $\mathcal{Z}$ be a subspace of $\mathcal{B}$. Then, $\mathcal{Z}^{\perp} = \mathcal{R}\mathcal{Z}^{c}$.

Remark 2. *Given that $\mathcal{Z}^{c}$ is a closed subspace and $\mathcal{R}$ is a bounded operator, we can infer that $\mathcal{Z}^{\perp}$ is also a closed subspace.*

Let the symbol $\oplus^{\perp}$ represent the orthogonal direct sum with respect to $\langle \cdot, \cdot \rangle_{\mathcal{B}}$. Thus, $\mathcal{Z}_1 \oplus^{\perp} \mathcal{Z}_2 = \mathcal{B}$ implies that $\mathcal{Z}_1 \oplus \mathcal{Z}_2 = \mathcal{B}$ and $\mathcal{Z}_1$ is orthogonal to $\mathcal{Z}_2$ concerning $\langle \cdot, \cdot \rangle_{\mathcal{B}}$.

Proposition 3.5.3

[34] Consider $\mathcal{D}$ as a subspace of $\mathcal{B}$. The subsequent statements are equivalent:

1. *$\mathcal{D}$ is a Dirac structure on $\mathcal{B}$.*
2. *$\mathcal{D}^{c} = \mathcal{R}\mathcal{D}$.*
3. *$\mathcal{D} \oplus^{\perp} \mathcal{R}\mathcal{D} = \mathcal{B}$.*
4. *$\mathcal{D}^{c} \oplus^{\perp} \mathcal{R}\mathcal{D}^{c} = \mathcal{B}$ and $\mathcal{D}$ is a closed subspace.*

Remark 3. *Statement (4) implies that if $\mathcal{D}$ is a Dirac structure on $\mathcal{B}$, then $\mathcal{D}^{c}$ is also a Dirac structure on $\mathcal{B}$.*

3.6 A Canonical Stokes-Dirac Structure Arising from the Adjoint Operators Gradient and Divergence

The Stokes-Dirac structure, which we present here, is constructed from the two fundamental operators: the gradient (grad) and the divergence (div).

3.6.1 Adjoint Relationships Between Gradient and Divergence Operators on Bounded Domains

It is well-established that the formal adjoint of the gradient operator on an n-dimensional domain is the negative of the divergence operator. The duality between these operators has been extensively investigated, as we shall recall, following [54].

This work deals with the computation of the adjoint of the gradient operator defined on a connected, open, and bounded subset Ω of $\mathbb{R}^n$, with a Lipschitz-continuous boundary $\partial\Omega$. Assume that the gradient's domain is an arbitrary vector space G such that $H_0^1(\Omega) \subset G \subset H^1(\Omega)$. Subsequently, we construct a subspace D with $H_0^{\mathrm{div}}(\Omega) \subset D \subset H^{\mathrm{div}}(\Omega)$.

The main result establishes the adjoint relationship: $\mathrm{grad}|_G^* = -\mathrm{div}|_D$. For clarity, we provide a brief overview of the key concepts and terminology related to Dirichlet and normal trace mappings before proceeding further.

Theorem 3.6.1

[54] Let's consider a bounded Lipschitz domain, Ω. The following properties are important:

1. *The boundary trace mapping, $g \to g|_{\partial\Omega} : C^1(\bar{\Omega}) \to C(\partial\Omega)$, has a unique continuous extension, γ_0, that acts on $H^1(\Omega)$ and maps to $H^{1/2}(\partial\Omega)$. Hence, the space can be expressed as:*
$$H_0^1(\Omega) = \{g \in H^1(\Omega) \mid \gamma_0 g = 0\}. \tag{3.16}$$

2. *The normal trace mapping defined as $u \to v \cdot \gamma_0 u : H^1(\Omega)^n \to L^2(\partial\Omega)$ has its own unique continuous extension, $\gamma_\perp$. This extension acts on $H^{div}(\Omega)$ and maps to $H^{-1/2}(\partial\Omega)$. The dot, $\cdot$, represents the inner product in $\mathbb{R}^n$, as given by $p \cdot q = q^\top p$. Moreover, the space is:*
$$H_0^{div}(\Omega) = \{f \in H^{div}(\Omega) \mid \gamma_\perp f = 0\}. \tag{3.17}$$

We denote the term γ_0 as the Dirichlet trace and $\gamma_\perp$ as the normal trace map. More on these can be found in [54], specifically in (Definition 3.3 on page 5 and Theorem 5.5 on page 11).

Theorem 3.6.2

[54] Let Ω be a bounded Lipschitz domain in $\mathbb{R}^n$. For all $f \in H^{div}(\Omega)$ and $g \in H^1(\Omega)$ it holds that
$$\langle div\, f, g\rangle_{L^2(\Omega)} + \langle f, grad\, g\rangle_{L^2(\Omega)} = (\gamma_\perp f, \gamma_0 g)_{H^{-1/2}(\partial\Omega), H^{1/2}(\partial\Omega)}. \tag{3.18}$$

This defines a Stokes-Dirac structure for closed systems.

Theorem 3.6.3

[54] Let Ω be a bounded Lipschitz domain in $\mathbb{R}^n$ and let $H_0^1(\Omega) \subset G \subset H^1(\Omega)$. Setting
$$D := \left\{f \in H^{div}(\Omega) \mid (\gamma_\perp f, \gamma_0 g)_{H^{-1/2}(\partial\Omega), H^{1/2}(\partial\Omega)} = 0 \ \ \forall g \in G\right\}, \tag{3.19}$$

we obtain the following [54]:

1. *The set D is a closed subspace of $H^{div}(\Omega)$ that contains $H_0^{div}(\Omega)$, i.e.,*
$$H_0^{div}(\Omega) \subset D \subset H^{div}(\Omega). \tag{3.20}$$

2. *When we identify $L^2(\Omega)$ and $L^2(\Omega)^n$ with their own duals, and we consider $grad|_G$ as an unbounded operator mapping the dense subspace G of $L^2(\Omega)$ into $L^2(\Omega)^n$, we have*
$$grad^*|_G = -div|_D. \tag{3.21}$$

3. *Let G be closed in $H^1(\Omega)$. Then $D = H^{div}(\Omega)$ if and only if $G = H_0^1(\Omega)$, and $D = H_0^{div}(\Omega)$ if and only if $G = H^1(\Omega)$.*

3.6.2 Definition of Some Spaces

Definition 3.6.1

(Spaces $H^{1/2}(\partial\Omega)$ and $H^{-1/2}(\partial\Omega)$). We define the space $H^{1/2}(\partial\Omega)$ as the image of the

Dirichlet trace,

$$H^{1/2}(\partial\Omega) := \gamma_0(H^1(\Omega)) \tag{3.22}$$

equipped with the norm

$$\|v\|_{H^{1/2}(\partial\Omega)} := \inf\left\{\|\tilde{v}\|_{H^1(\Omega)}, \quad \tilde{v} \in H^1(\Omega) \text{ such that } \gamma_0(\tilde{v}) = v\right\}. \tag{3.23}$$

In particular, the operator γ_0 is continuous from $H^1(\Omega)$ to $H^{1/2}(\partial\Omega)$.

The space $H^{-1/2}(\partial\Omega)$ is defined as the dual of $H^{1/2}(\partial\Omega)$ with respect to the pivot space $L^2(\partial\Omega)$.

These are Hilbert spaces equipped with the norms defined above and the dual norm, respectively.

3.6.3 Canonical Stokes-Dirac Structure Associated with the Dual Operators Gradient and Divergence

We begin by presenting a canonical operator that appears in physical models like the wave equation or diffusion equation and demonstrate its skew-adjoint property. Subsequently, we recall the associated Stokes-Dirac structure.

Proposition 3.6.1

Let $\Omega \subset \mathbb{R}^n$ and $\partial\Omega$ be as described previously. Consider the gradient operator grad defined on $G = H_0^1(\Omega)$. By the main result presented in Theorem 3.6.3, the adjoint of the gradient operator with this specific domain is $-$div, with domain $D = H^{div}(\Omega)$. This leads us to the implication that the operator

$$\mathcal{J} := \begin{bmatrix} 0 & div \\ grad & 0 \end{bmatrix} \tag{3.24}$$

with domain

$$dom(\mathcal{J}) := \begin{bmatrix} H_0^1(\Omega) \\ H^{div}(\Omega)^n \end{bmatrix} \tag{3.25}$$

is skew-adjoint on

$$\begin{bmatrix} L^2(\Omega) \\ L^2(\Omega)^n \end{bmatrix}.$$

3.7 $\mathcal{J}$ as a Hamiltonian Operator

Building on the foundational work of Kurula and colleagues [54, 55], this section aims to enhance the conventional understanding of the Hamiltonian operator, specifically within the bounded Lipschitz domain Ω.

3.7.1 Properties of $\mathcal{J}$

The Hamiltonian operator $\mathcal{J}$ encapsulates significant physical insights and governs the system dynamics with its unique properties:

- **Skew-Symmetry:** Central to energy conservation within the system, the skew-symmetry of $\mathcal{J}$ ensures that energy within the domain is neither created nor destroyed, only transformed or relocated. Mathematically, this property is expressed as:

$$\langle f, \mathcal{J}e\rangle = -\langle \mathcal{J}f, e\rangle, \tag{3.26}$$

  where f and e represent the energy and co-energy variables respectively.

- **Jacobi Identity:** The Jacobi identity, as an integrability property of $\mathcal{J}$, indicates the existence of canonical coordinates and ensures that fundamental properties of Hamiltonian systems such as conservation laws and symplectic structures are preserved:

$$\{\{F, G\}, H\} + \{\{G, H\}, F\} + \{\{H, F\}, G\} = 0, \tag{3.27}$$

  for any functions F, G, and H in the Hamiltonian system.

- **Boundary Conditions:** The effectiveness of $\mathcal{J}$ in managing boundary interactions is crucial, particularly in bounded Lipschitz domains where boundary dynamics can significantly influence the system's behavior. The implementation of Dirichlet or Neumann boundary conditions affects how $\mathcal{J}$ manages energy distribution and transformation at the boundaries.

By recalling the definition of a Hamiltonian operator and referencing Olver's work [69], we further establish that $\mathcal{J}$, being a constant coefficient matrix differential operator, inherently satisfies the Jacobi identities.

3.7.2 Hamiltonian Operator: Domain Definition

To check the formal skew-symmetry of $\mathcal{J}$ as a Hamiltonian operator, it's important to define its domain appropriately. Using the results from Theorems 3.6.2 and Theorem 3.6.3, the domain of $\mathcal{J}$ is given by:

$$\mathcal{F} = \text{dom } \mathcal{J} = L^2(\Omega) \times D \times G \subset \mathcal{E}, \tag{3.28}$$

where $\mathcal{F}$ represents the space of flow variables, and $\mathcal{E}$ represents the space of effort variables.

We shall denote also elements of the domain as

$$e_{bulk} = (e_0, e_d, e_g)^\top \in \mathcal{F} \; and \;\; f_{bulk} = (f_0, f_d, f_g)^\top \in \mathcal{E}, \tag{3.29}$$

to delve deeper into the domain specifics and to proceed further in the coming section (3.10). Consider the elements $e_d \in H^{\text{div}}(\Omega)$ and $e_g \in H^1(\Omega)$. Assuming $H_0^1(\Omega) \subset G \subset H^1(\Omega)$, the domain can be explicitly formulated as:

$$D = \{e_d \in H^{\text{div}}(\Omega) \mid (\gamma_\perp e_d, \gamma_0 e_g)_{H^{-1/2}(\partial\Omega), H^{1/2}(\partial\Omega)} = 0 \; \forall g \in G\}. \tag{3.30}$$

Additionally, $H^{\text{div}}(\Omega)$ is defined as:

$$H^{\text{div}}(\Omega) = \{v \in L^2(\Omega)^n \mid \operatorname{div} v \in L^2(\Omega)\}, \tag{3.31}$$

and $H^{1/2}(\Omega)$ is defined as the space consisting of all $f \in L^2(\Omega)$ such that:

$$\|f\|^2_{H^{1/2}(\Omega)} = \|f\|^2_{L^2(\Omega)} + \int_\Omega \int_\Omega \frac{|f(x) - f(y)|^2}{\|x - y\|^{n+1}_{\mathbb{R}^n}} \, dx \, dy < \infty. \tag{3.32}$$

The space $H^{1/2}(\Omega)$ is a Hilbert space and the inner product on $H^{1/2}(\Omega)$ is found by polarization of (3.32), see [54] and [103].

3.7.3 Boundary Port Variables and Stokes-Dirac Structure of the Operator $\mathcal{J}$

When the operator $\mathcal{J}$ is defined on a domain where it is no longer skew-symmetric, it is important to understand the integration of boundary port variables within the Stokes-Dirac structure associated with $\mathcal{J}$. So we now consider the operator $\mathcal{J}$ in equation (3.24) on a larger functional domain where the skew-symmetry property is no longer satisfied.

Theorem 3.7.1

[94](Stokes-Dirac Structure) The geometric structure D defined by,

$$(f_q, f_p, f_\partial, e_q, e_p, e_\partial) \in \mathcal{F} \times \mathcal{E} \tag{3.33}$$

$$D := \begin{cases} \text{such that, } \mathcal{F} := L^2(\Omega) \times L^2(\Omega) \times H^{1/2}(\partial\Omega), \mathcal{E} := L^2(\Omega) \times L^2(\Omega) \times H^{-1/2}(\partial\Omega), \\ \begin{bmatrix} f_q \\ f_p \end{bmatrix} = \begin{bmatrix} 0 & \text{grad} \\ \text{div} & 0 \end{bmatrix} \begin{bmatrix} e_q \\ e_p \end{bmatrix}, f_\partial(x) = -\gamma_\perp(e_p(x)), \quad e_\partial(x) = \gamma_0(e_q(x)), \\ \text{div } e_q \in L^2(\Omega), \quad \text{grad } e_p \in L^2(\Omega). \end{cases} \tag{3.34}$$

is a Stokes-Dirac structure for the pairing,

$$\begin{aligned} &\langle\langle (f_q^1, f_p^1, f_\partial^1, e_q^1, e_p^1, e_\partial^1), (f_q^2, f_p^2, f_\partial^2, e_q^2, e_p^2, e_\partial^2) \rangle\rangle_D \\ &:= (e_q^1, f_q^2)_{L^2(\Omega)} + (e_p^1, f_p^2)_{L^2(\Omega)} + (e_q^2, f_q^1)_{L^2(\Omega)} + (e_p^2, f_p^1)_{L^2(\Omega)} \\ &\quad + \langle e_\partial^1, f_\partial^2 \rangle_{H^{-1/2}(\partial\Omega), H^{1/2}(\partial\Omega)} + \langle e_\partial^2, f_\partial^1 \rangle_{H^{-1/2}(\partial\Omega), H^{1/2}(\partial\Omega)}. \end{aligned} \tag{3.35}$$

For the detailed proof see [94].

Note: To conduct a geometric study of the PHS later on, we will adopt the flows-efforts representation based on the above Theorem (3.7.1).

Defining the flows as:

$$f = \begin{bmatrix} f_q \\ f_p \\ f_\partial \end{bmatrix}. \tag{3.36}$$

And the efforts as:

$$e = \begin{bmatrix} e_q \\ e_p \\ e_\partial \end{bmatrix}, \tag{3.37}$$

where the ports (f_q, e_q) and (f_p, e_p) are associated with the energy and co-energy variables and (f_∂, e_∂) is the port associated with the boundary.

Following the work of [94], we define the two boundary variables

$$\begin{cases} f(x) = -\gamma_\perp(e_p(x)), \\ e(x) = \gamma_0(e_q(x)), \end{cases} \tag{3.38}$$

referred to as Port boundary variables, and extend the operator to a Stokes-Dirac structure. We denote the term γ_0 as the Dirichlet trace and $\gamma_\perp$ as the normal trace map.

The boundary port variables (f, e) are defined within the linear spaces of boundary flows $\mathcal{F} = H^{-1/2}(\partial\Omega)$ and efforts $\mathcal{E} = H^{1/2}(\partial\Omega)$, respectively. Their relationship is explicitly given by:

$$\begin{pmatrix} f \\ e \end{pmatrix} = \mathcal{W} \begin{pmatrix} e_d \\ e_g \end{pmatrix}. \tag{3.39}$$

Where the boundary operator $\mathcal{W}$ is specifically defined by:

$$\mathcal{W} = \begin{pmatrix} -\gamma_\perp & 0 \\ 0 & \gamma_0 \end{pmatrix}. \tag{3.40}$$

This defines a Stokes-Dirac structure for open systems with boundary port variables.

3.8 Port-Hamiltonian Systems on Dirac Structures

In port-based modeling, physical systems are perceived as interconnected assemblies of three principal kinds of ideal components:

1. Energy-storing components,
2. Energy-dissipating (or resistive) components,
3. Energy-routing components.

The essence of a port Hamiltonian system is captured by the idea of a Dirac structure, visualized in Figure 1 below as D [84]. This Dirac structure can be compared to the blueprint of an electrical circuit, analogous to a 'circuit board layout,' excluding elements that either store or dissipate energy. It serves as the basic 'connectivity' for the whole system.

Common examples of energy-storing elements include ideal inductors, capacitors, masses, and springs [84]. Energy-dissipating components typically include resistors and dampers, while energy-directing elements can include transformers, gyrators, and ideal constraints. It is important to note that energy-routing components neither store nor dissipate energy; they simply redirect the flow of power within the system [104].

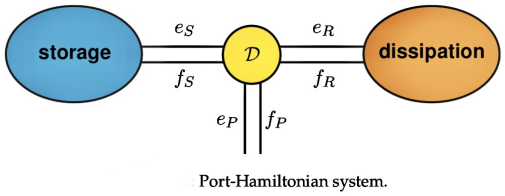

Figure 1: PHS Modeling [104]

In the context of the port Hamiltonian framework [33], energy-storing elements are grouped under an entity labeled S (indicating 'storage'), while energy-dissipating elements are grouped under R ('resistance'). The interconnections of all energy conducting elements are abstracted into a structure called D, which is formalized using the concept of a Dirac structure.

A central idea in the modeling of port-Hamiltonian systems is the representation of these components by ports defined by pairs (f, e) of flow and effort variables. These ports connect the elements S, R, and D. The interaction of the system with its external environment, including control actions, is also through such ports.

3.8.1 Energy-storing elements

The energy-storing multi-port element S corresponds to the union of all the energy-storing elements of the system. The port variables of the Dirac structure associated with the energy-storing multi-port element are denoted by (f_S, e_S), where f_S and e_S are vectors of equal dimension with their product $e_S^\top f_S$ denoting the total power flowing into the Dirac structure from the energy-storing elements (or, equivalently, minus the total power flowing into the storage elements). The total energy storage of the system is defined by a state space $\mathcal{X}$, together with a Hamiltonian function $H : \mathcal{X} \to \mathbb{R}$ denoting the energy. For now, we will assume that the state space $\mathcal{X}$ is finite-dimensional and is a linear space [84].

The vector of flow variables of the energy-storing multi-port element is given by the rate $\dot{x}$ of the state $x \in \mathcal{X}$. Thus for any current state $x \in \mathcal{X}$, the flow vector $\dot{x}$ will be an element of the linear space $T_x\mathcal{X}$, the tangent space of $\mathcal{X}$ at x. By choosing local coordinates $x = (x_1, \ldots, x_n)^\top$ for $\mathcal{X}$, this means that the vector of flow variables is given by the vector $\dot{x} = (\dot{x}_1, \ldots, \dot{x}_n)^\top$. In the case of a linear state space $\mathcal{X}$, the tangent space $T_x\mathcal{X}$ can be identified with $\mathcal{X}$, and we can take (global) linear coordinates for $\mathcal{X}$, thus identifying $\mathcal{X}$ with $\mathbb{R}^n$.

Furthermore, the vector of effort variables of the energy-storing multi-port element is given by the gradient vector $\frac{\partial \mathcal{H}}{\partial x}(x) \in T_x^*\mathcal{X}$, the dual space of the tangent space $T_x\mathcal{X}$. In coordinates $x = (x_1, \ldots, x_n)^\top$ for $\mathcal{X}$, this means that the vector of effort variables is given by the vector $\frac{\partial \mathcal{H}}{\partial x}(x)$ of partial derivatives of $\mathcal{H}$ with respect to $x_1, \ldots, x_n$ (which we throughout write as a column vector).

We obtain the following computation of the time derivative of the Hamiltonian:

$$\frac{d}{dt}H = \langle \frac{\partial H}{\partial x}(x) \,|\, \dot{x} \rangle = \frac{\partial^\top H}{\partial x}(x)\dot{x}. \tag{3.41}$$

The interconnection of the energy-storing elements to the storage port (f_S, e_S) of the Dirac structure is accomplished by setting:

$$f_S = -\dot{x} \quad \text{and} \quad e_S = \frac{\partial H}{\partial x}(x). \tag{3.42}$$

Hence, the computation of the time derivative of the Hamiltonian (3.41) can also be written as:

$$\frac{d}{dt}H = \frac{\partial^\top H}{\partial x}(x)\dot{x} = -e_S^\top f_S. \tag{3.43}$$

Remark 4. *The minus sign in* (3.42) *is inserted in order to have a consistent power flow convention:* $\frac{\partial H^\top}{\partial x}(x)\dot{x}$ *is the power flowing into the energy-storing elements, whereas* $e_S^\top f_S$ *is the power flowing into the Dirac structure.*

3.8.2 Energy-dissipating (resistive) elements

The second multi-port element R corresponds to internal energy dissipation (due to friction, resistance, etc.), and its port variables are denoted by (f_R, e_R). These port variables are terminated on a static energy-dissipating (resistive) relation R [84]. In general, a resistive relation will be a subset $R \subset \mathcal{F}_R \times \mathcal{E}_R$, with the property that:

$$\langle e_R | f_R \rangle = e_R^\top f_R \leq 0, \quad \text{for all } (f_R, e_R) \in R. \tag{3.44}$$

We call the subset R an energy-dissipating relation, or a resistive structure.

Recall the basic property of Dirac structures, as in Definition (3.5.1), since the Dirac structure of a port-Hamiltonian system (without external port) satisfies the power-balance:

$$e_S^\top f_S + e_R^\top f_R = 0, \tag{3.45}$$

this leads by substitution of the equations (3.43) and (3.44) to:

$$\frac{d}{dt}H = -e_S^\top f_S = e_R^\top f_R \leq 0. \tag{3.46}$$

The resistive structure R, combined with the energy-dissipating port (f_R, e_R), models the mechanisms by which the system loses energy. This is often an important component in real systems where energy losses due to factors like friction or resistance are involved.

3.8.3 Dirac Structure and External Ports

The Dirac structure D integrates energy-storing elements, dissipative elements, and open ports, ensuring conservation of energy throughout the system and its environment. It incorporates port variables $f_P(t)$ and $e_P(t)$, which facilitate interactions with external systems, enabling the transfer of power [84].

External ports (f_P, e_P) represent the system's interface with its environment, accommodating various scenarios. These port variables are acausal, allowing them to be completed with

additional elements like sources or through interconnections with other Port Hamiltonian systems. This might involve another Dirac structure, known as an interconnection Dirac structure, which connects our system to another subsystem [16].

Types of external port variables include:

- *Controller action* ports, which are directly manipulable to influence system behavior.
- *Interaction ports*, exemplified by a controlled robotic system interacting with its environment.
- *Source ports* in an electrical circuit, where the voltage source specifies the input, and the current through the source becomes the output.

Incorporating external ports, the power balance equation extends to:

$$e_S^\top f_S + e_R^\top f_R + e_P^\top f_P = 0, \tag{3.47}$$

This leads to the extended Hamiltonian dynamics:

$$\frac{d}{dt}H = e_R^\top f_R + e_P^\top f_P \leq e_P^\top f_P, \tag{3.48}$$

indicating that any increase in internally stored energy (the Hamiltonian) is always less than or equal to the power supplied externally, since $e_R^\top f_R \leq 0$. This framework effectively captures both the internal dynamics and the interactions at the boundaries of the system.

3.8.4 Finite Dimensional Port-Hamiltonian Systems

Port-Hamiltonian systems (PHS) in finite dimensions are defined through the interaction between a Dirac structure, which specifies the interconnection relations, and a Hamiltonian function that describes the system's total energy.

System Configuration

Consider a physical system characterized by a power-conserving interconnection described by a Dirac structure $\mathcal{D}$, and a set of energy-storing elements represented by a vector of energy variables x within a linear state space $\mathcal{X}$. The system dynamics are derived from the energies stored in these elements, described collectively by the Hamiltonian $H(x)$.

Integration of System Dynamics

The system dynamics integrate the resistive and energy transfer interactions among all elements. These interactions, as described previously in sections 3.8.1 and 3.8.2, include flow (f_R, f_S) and effort (e_R, e_S) variables managed by the Dirac structure $\mathcal{D}$. This integration effectively captures the energy exchange within the system, leading to a well-defined Port-Hamiltonian system structure [87].

Definition 3.8.1

[16] Consider a state space $\mathcal{X}$ and a Hamiltonian $H : \mathcal{X} \to \mathbb{R}$, defining energy storage. A Port-Hamiltonian system on $\mathcal{X}$ is defined by a Dirac structure as:

$$\mathcal{D} \subset T_x\mathcal{X} \times T_x^*\mathcal{X} \times \mathcal{F}_R \times \mathcal{E}_R \times \mathcal{F}_P \times \mathcal{E}_P, \tag{3.49}$$

featuring an energy-storing port (f_S, e_S) *and a resistive structure* R*, corresponding to an energy-dissipating port* (f_R, e_R)*. The dynamics are specified by:*

$$\begin{aligned} &\big(-\dot{x}(t), \frac{\partial H}{\partial x}(x(t)), f_R(t), e_R(t), f_P(t), e_P(t)\big) \in \mathcal{D}(x(t)), \\ &(f_R(t), e_R(t)) \in R(x(t)), \quad t \in \mathbb{R}, \end{aligned} \tag{3.50}$$

thus defining the Port-Hamiltonian system dynamics.

Furthermore, the operational relationships and the kernel representation (3.5) within the system adhere to:

$$\mathcal{F}\begin{pmatrix} -\dot{x} \\ f_R \\ f_P \end{pmatrix} + \mathcal{E}\begin{pmatrix} \frac{\partial H}{\partial x} \\ e_R \\ e_P \end{pmatrix} = 0, \quad \text{with ports, and} \quad R(f_R(t), e_R(t)) = 0. \tag{3.51}$$

3.9 Infinite-dimensional Port Hamiltonian Systems

Infinite-dimensional Port-Hamiltonian systems (IPHS) are important for modeling systems that extend over spatial domains and involve dynamics governed by partial differential equations (PDEs) [92]. The transition from finite to infinite-dimensional systems represents not merely an extension in dimensionality but a fundamental change in the nature of the system's dynamic operators.

Mathematical Formulation: An IPHS typically involves the state variable $z(t, x)$, defined over a spatial domain where x represents spatial coordinates and t time. The dynamics are governed by differential operators reflecting the system's spatial structure, encapsulated in a Hamiltonian framework:

$$\partial_t z(t, x) = \mathcal{J}(x)\delta_x H(z(t, x)) - \mathcal{R}(x)\delta_x H(z(t, x)), \tag{3.52}$$

where:

- $\mathcal{J}(x)$, a skew-symmetric differential operator, represents the energy-conserving dynamics, extending beyond simple matrix representations to handle spatially dependent interactions.
- $\mathcal{R}(x)$, a symmetric positive differential operator, models the system's damping or resistive effects, reflecting energy dissipation across the spatial domain.
- H is the Hamiltonian functional, representing the system's total energy.
- $\delta_x H$ denotes the functional derivative of H, indicating how the Hamiltonian changes with variations in the state variable.

This formulation shows how infinite-dimensional systems, through the use of differential operators, naturally give rise to the necessity for boundary port variables. These variables emerge due to the spatial extent of the operators and the boundary conditions that must be managed to maintain system integrity and functionality [26].

Dirac Structures and Boundary Control

Infinite-dimensional Dirac structures are essential for accurately modeling the interactions at the system boundaries and across its distributed parameters. They ensure that the system adheres to energy conservation laws and effectively manages energy flow, which is crucial for systems extending over spatial domains.

Boundary Port Variables: Boundary port variables in IPHS help manage interactions at the boundaries, making it easier to implement control strategies and observe system responses:

$$f_\partial(t,x) = \text{boundary flow variable}, \tag{3.53}$$
$$e_\partial(t,x) = \text{boundary effort variable}. \tag{3.54}$$

These variables are formulated according to the canonical Stokes-Dirac structure, enabling detailed control and analysis of boundary interactions and ensuring that the system's dynamics are consistent with physical laws of energy conservation and dissipation.

IPHS are applicable in various scientific and engineering fields, where their capability to handle complex boundary conditions and distributed parameters is invaluable [57]. Examples include modeling wave phenomena, thermal processes, and fluid dynamics within a structured Hamiltonian framework, which enhances the ability to control and monitor these processes effectively.

3.9.1 Wave Equation

Introduction to the Wave Equation in Port-Hamiltonian Systems

The wave equation is a fundamental PDE that models the propagation of various types of waves, such as sound, light, or mechanical vibrations, through different media. It is traditionally expressed as a second-order PDE in both time and space variables.

We consider the wave equation in a bounded domain $\Omega \subseteq \mathbb{R}^n$ with a Lipschitz boundary $\partial\Omega$, divided into two disjoint parts: Γ_0 and Γ_1. Here, Γ_0 and Γ_1 represent parts of the boundary where different types of boundary conditions are applied, and they do not overlap ($\Gamma_0 \cap \Gamma_1 = \emptyset$).

The tensor $T(\zeta)$ in the domain Ω describes the material properties affecting wave propagation, such as tension or density variations, and is assumed to be positive definite and smoothly varying.

Port-Hamiltonian Formulation of the Wave Equation To cast the wave equation into a Port-Hamiltonian framework, we consider the state variable w representing the wave's displacement and its temporal derivative as the momentum. The spatial derivative $\operatorname{grad} w$ corresponds to the system's effort variables, encapsulating the wave's spatial dynamics. The system is then described by:

$$\frac{\partial^2 w}{\partial t^2} = \frac{1}{\rho(\zeta)} \operatorname{div}(T(\zeta) \operatorname{grad} w), \tag{3.55}$$

where $\rho(\zeta)$ represents the density of the medium at point ζ in Ω and $T(\zeta)$ the elasticity tensor.

For a controlled system, consider the following boundary conditions:

Dirichlet: $w(t,\xi) = 0 \quad \xi \in \Gamma_0$

Neumann: $T\text{grad}w(t,\xi) = u(t) \quad \xi \in \Gamma_1$

Robin: $w(t,\xi) + K(t,\xi) = u(t) \quad \xi \in \Gamma_1$

Mathematical Formulation and Analysis The system dynamics, in terms of energy variables, are well-posed as shown in [44]:

$$x(t,\zeta) = \begin{bmatrix} \rho(\zeta)\frac{\partial w}{\partial t}(t,\zeta) \\ \text{grad}\, w(t,\zeta) \end{bmatrix}, \tag{3.56}$$

leading to:

$$\frac{d}{dt}x(t) = \mathcal{J}\delta_x\mathcal{H}(x(t)), \tag{3.57}$$

where $\mathcal{J}$ is the skew-symmetric operator defined before (3.24), representing the system's inherent energy-conserving properties.

To explicitly connect this system to its Stokes-Dirac structure in open systems as defined before (3.7.1), we incorporate the following relation:

$$\left(\frac{\partial}{\partial t}x_1, \frac{\partial}{\partial t}x_2, f_\partial, \delta_{x_1}\mathcal{H}, \delta_{x_2}\mathcal{H}, e_\partial\right) \in \mathcal{D}, \tag{3.58}$$

The integration of the dynamics of the wave equation with its boundary port variables for an open system, but not a controlled one (control system), is a key aspect of this approach. In the open system, the control has yet to be defined. Nevertheless, two variables have been specified. As previously stated, we will recall the definition of boundary port variables from the open system, which are derived from a Hamiltonian operator $\mathcal{J}$ (3.24). Furthermore, we provide an acausal definition of the open system, which does not include the definition of input or output, and which allows the definition of any physical boundary conditions that can be realized in practice (controlled or not).

$$\mathcal{J} = \begin{bmatrix} 0 & -\text{div} \\ -\text{grad} & 0 \end{bmatrix}, \tag{3.59}$$

$$\frac{\partial}{\partial t}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \mathcal{J}\begin{bmatrix} \delta_{x_1}\mathcal{H} \\ \delta_{x_2}\mathcal{H} \end{bmatrix}, \tag{3.60}$$

Boundary port variables in terms of:

$$\begin{pmatrix} f_\partial \\ e_\partial \end{pmatrix} = \overline{\mathcal{W}}\begin{pmatrix} \delta_{x_1}\mathcal{H} \\ \delta_{x_2}\mathcal{H} \end{pmatrix}, \tag{3.61}$$

$$\overline{\mathcal{W}} = \begin{pmatrix} \gamma_0 & 0 \\ 0 & -\gamma_\perp \end{pmatrix}. \tag{3.62}$$

Instead of traditional boundary conditions, we define acausal boundary port variables:

$$f_\partial(t,\xi) = 0, \quad \text{(Dirichlet)} \tag{3.63}$$
$$e_\partial(t,\xi) = u(t), \quad \text{(Neumann)} \tag{3.64}$$

Interpreting these conditions through the Stokes-Dirac structure (3.7.1) derived from the Hamiltonian operator (3.24), provides a robust framework for handling boundary interactions and system dynamics within an IPHS context. References and further details on the derivation and implications of this formulation can be found in [44, 55].

3.9.2 Dissipative Port Hamiltonian Systems

In this section, we explain how to extend the Port Hamiltonian framework to include dissipative systems [118, 26]. We use the formalism for infinite-dimensional Port Hamiltonian systems discussed earlier and focus on a specific way to include the dissipative operator, revealing a hidden Hamiltonian structure that facilitates the inclusion of dissipation.

The system dynamics are given by this differential equation:

$$\frac{\partial x}{\partial t}(t,z) = (\mathcal{J} - \mathcal{G}_R \mathcal{R} \mathcal{G}_R^*)\frac{\delta H}{\delta x}, \tag{3.65}$$

where:

- $\mathcal{J}$ is a skew-symmetric operator representing the conservative part of the dynamics.
- $\mathcal{G}_R$ and its adjoint $\mathcal{G}_R^*$ model the interaction with dissipative effects.
- $\mathcal{R}$ is a positive semi-definite operator, responsible for dissipation (damping).
- H is the Hamiltonian functional, representing the total energy of the system.

The system dynamics can also be expressed as:

$$\begin{pmatrix} \frac{\partial x}{\partial t} \\ F \end{pmatrix} = \begin{pmatrix} 0 & \mathcal{G}_R \\ -\mathcal{G}_R^* & 0 \end{pmatrix} \begin{pmatrix} \frac{\delta H}{\delta x} \\ Q \end{pmatrix}, \tag{3.66}$$

Here, the relationship between the dissipative forces (Q) and the flux variables (F) is:

$$Q = \mathcal{R}F. \tag{3.67}$$

The boundary port variables, which describe the interface at the system's boundaries, are connected to the Stokes-Dirac structure, governed by the Hamiltonian operator:

$$\mathcal{J}_{\text{ext}} = \begin{bmatrix} 0 & \mathcal{G}_R \\ -\mathcal{G}_R^* & 0 \end{bmatrix}. \tag{3.68}$$

These boundary port variables are linear functions of the trace of the vector:

$$\begin{pmatrix} \frac{\delta H}{\delta x} & Q \end{pmatrix}^\perp. \tag{3.69}$$

Particular Case: When $\mathcal{J} = 0$, the system simplifies to:

$$\frac{\partial x}{\partial t}(t, z) = -\mathcal{G}_R \mathcal{R} \mathcal{G}_R^* \frac{\delta H}{\delta x}. \tag{3.70}$$

This simplified case still represents the main structure of the dissipative Port Hamiltonian system, focusing on the roles of $\mathcal{G}_R$ and $\mathcal{R}$.

3.9.3 Heat Equation With Entropy as Generating Function

The energy balance equation, which is important to the understanding of heat transfer during solidification, is:

$$\frac{\partial u}{\partial t} = -\text{div}\, q, \tag{3.71}$$

where u signifies the internal energy and q represents the heat flux.

Based on the above section (3.9.2), the work of [95], and our discussion in Chapter 2, we approach the heat equation with entropy s as the generating function:

$$\begin{pmatrix} \frac{\partial u}{\partial t} \\ F \end{pmatrix} = \begin{pmatrix} 0 & -\text{div} \\ -\text{grad} & 0 \end{pmatrix} \begin{pmatrix} \frac{\partial s}{\partial u} \\ q \end{pmatrix}, \tag{3.72}$$

the heat flux is given by :

$$q = M_\tau \bar{F}, \tag{3.73}$$

where $\bar{F}$ is the driving force for the heat flux, given by:

$$\bar{F} = -\text{grad}(\tau). \tag{3.74}$$

and the mobility coefficient $M_\tau = \frac{\lambda(\frac{1}{\tau}, \phi)}{\tau^2}$ integrates the effects of thermal conductivity (λ) and the reciprocal temperature (τ) on the heat transfer dynamics. The values for λ are detailed for both ice ($\phi = 0$) and water ($\phi = 1$) in references [43, 117].

The operator on the right

$$\mathcal{J}_u = \begin{pmatrix} 0 & -\text{div} \\ -\text{grad} & 0 \end{pmatrix} \tag{3.75}$$

represents the interaction dynamics within the system via the gradient and divergence operators, which is indeed the Hamiltonian operator defined before as $\mathcal{J}$ (3.24).

The boundary port variables are defined by:

$$\begin{pmatrix} f_\partial \\ e_\partial \end{pmatrix} = \overline{\mathcal{W}}\, e = \begin{pmatrix} \gamma_0 \frac{\delta s}{\delta u} \\ -\gamma_\perp q \end{pmatrix}, \tag{3.76}$$

where $e = \begin{pmatrix} \frac{\partial s}{\partial u} \\ q \end{pmatrix}$ and the boundary operator $\overline{\mathcal{W}}$ is defined as:

$$\overline{\mathcal{W}} = \begin{pmatrix} \gamma_0 & 0 \\ 0 & -\gamma_\perp \end{pmatrix}. \tag{3.77}$$

Here, γ_0 and $\gamma_\perp$ are the Dirichlet and normal trace maps, respectively, as mentioned before based on [54].

Physically, the boundary port variables represent the interaction of the system with its environment at the boundary $\partial\Omega$:

- $f_\partial = \gamma_0 \frac{\delta s}{\delta u}$ represents the reciprocal temperature at the boundary.
- $e_\partial = -\gamma_\perp q$ represents the heat flux at the boundary.

3.10 Port Hamiltonian formulation of the Allen-Cahn equation

In this section, we refer to the model established in the preceding chapter, section (2.6.2), focusing on its reformulation in a dissipative Port Hamiltonian framework. For convenience, we briefly recall the relevant equations before proceeding with their transformation [110].

Recall of Phase Field Model

The phase field modeling framework uses a phase field variable $\phi(t, z)$ to represent different phases within a material. This variable transitions smoothly across the interface, with values of 0 and 1 corresponding to distinct phases and intermediate values representing the interface [28].

The dynamics of the phase field variable ϕ are driven by the Landau–Ginzburg functional:

$$G(\phi) = \int_\Omega \left(g(\phi) + \frac{1}{2}\kappa_\phi(z)(\mathrm{grad}\phi)^2 \right) dV, \tag{3.78}$$

where $\kappa_\phi(z)$ is the gradient coefficient influencing the interface's surface tension and width, and $g(\phi)$ is a potential function with minima at 0 and 1.

Gradient Equation and Interface Mobility

The temporal evolution of the phase field variable $\phi(t, z)$ is governed by relaxation dynamics, described by the gradient equation:

$$\frac{\partial \phi}{\partial t}(t, z) = -\Gamma_\phi(z) \frac{\delta G}{\delta \phi}(\phi), \tag{3.79}$$

where $\Gamma_\phi(z)$ denotes the isotropic interface mobility, assumed to be a smoothly varying positive function across Ω, and $\frac{\delta G}{\delta \phi}$ is the functional derivative of the Landau–Ginzburg functional G with respect to ϕ.

The variational derivative of G is:

$$\frac{\delta G}{\delta \phi}(\phi) = \frac{\partial g}{\partial \phi}(\phi) - \mathrm{div}\left(\kappa_\phi(z)\,\mathrm{grad}\,\phi(t, z)\right), \tag{3.80}$$

leading to the state equation:

$$\frac{\partial \phi}{\partial t} = -\Gamma_\phi \left(-\operatorname{div}\left(\kappa_\phi \operatorname{grad} \phi\right) + \frac{\partial g}{\partial \phi}(\phi) \right), \tag{3.81}$$

commonly known as the Allen-Cahn equation.

Hamiltonian Formulation of the Allen-Cahn Equation

In the Hamiltonian formulation of phase field modeling, the Allen-Cahn equation describes interface dynamics within a framework that emphasizes energy conservation and dissipative dynamics. This approach helps in understanding the equation's ability to describe resistive diffusion-like processes in interfacial phenomena.

State Space Augmentation [110]

To better capture the system's dynamics, we introduce an auxiliary state variable, ψ, linked to the gradient of the phase field variable ϕ. This expands the state space for a more detailed analysis of the interfacial dynamics:

$$\begin{pmatrix} \phi \\ \psi \end{pmatrix} \triangleq \begin{pmatrix} \phi \\ \operatorname{grad} \phi \end{pmatrix} \in L^2(\Omega) \times L^2(\Omega). \tag{3.82}$$

The Landau–Ginzburg functional (3.78) can now be expressed in terms of ϕ and ψ as follows:

$$\mathcal{G}(\phi, \psi) = \int_\Omega \left(g(\phi) + \frac{1}{2}\kappa_\phi \psi^2 \right) dV. \tag{3.83}$$

Dissipative Constitutive Relations

We express the gradient dynamics' relaxation term by introducing $E_\phi(t, z)$ as a new variable within $L^2(\Omega)^2$, establishing the following relation:

$$E_\phi(t, z) = \Gamma_\phi(z) F_\phi(t, z), \tag{3.84}$$

where $F_\phi(t, z)$ is the driving force behind the relaxation dissipation, derived from the variational derivative of the potential function:

$$F_\phi = \frac{\delta \mathcal{G}}{\delta \phi} - \operatorname{div}\left(\frac{\delta \mathcal{G}}{\delta \psi} \right). \tag{3.85}$$

Evolution Equations

The evolution of ϕ and ψ is governed by:

$$\frac{\partial \phi}{\partial t}(t, z) = -E_\phi(t, z), \tag{3.86}$$

$$\frac{\partial \psi}{\partial t}(t, z) = \frac{\partial}{\partial t} \operatorname{grad} \phi(t, z), \tag{3.87}$$

where the gradient operator and the time derivative commute, leading to:

$$\frac{\partial \psi}{\partial t}(t,z) = -\text{grad}\, E_\phi(t,z). \tag{3.88}$$

Hamiltonian Representation

The system, governed by Eqs. (3.85), (3.88), and (3.86), can be represented by the Hamiltonian operator $\mathcal{J}_A$, detailed below:

$$\begin{pmatrix} \frac{\partial \phi}{\partial t} \\ \frac{\partial \psi}{\partial t} \\ F_\phi \end{pmatrix} = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & -\text{grad} \\ 1 & -\text{div} & 0 \end{pmatrix} \begin{pmatrix} \frac{\delta \mathcal{G}}{\delta \phi} \\ \frac{\delta \mathcal{G}}{\delta \psi} \\ E_\phi \end{pmatrix}, \tag{3.89}$$

where the linear differential operator $\mathcal{J}_A$ is defined as:

$$\mathcal{J}_A = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & -\text{grad} \\ 1 & -\text{div} & 0 \end{pmatrix} \tag{3.90}$$

This representation of $\mathcal{J}_A$ captures the essential dynamics of the Allen-Cahn equation augmented with the state variable ψ. Unlike the operator for heat diffusion (3.127), here the grad operator appears in the dynamical equation defining $\frac{\partial \psi}{\partial t}$. This highlights that the Allen-Cahn equation is derived from a gradient dynamics, not from a conservation law, emphasizing the dissipative nature of the process.

Port Hamiltonian Formulation of Allen-Cahn Equation

Having established the domain's structure before (3.28), our next objective is to ascertain the skew-symmetry of $\mathcal{J}_A$. This property is proven by evaluating the integral:

$$\int_\Omega \left(\overline{e}_{bulk}^\top \mathcal{J}_A e_{bulk} + e_{bulk}^\top \mathcal{J}_A \overline{e}_{bulk} \right) dV, \tag{3.91}$$

where an element of the domain is detailed as follows based on section (3.7.3):

$$e_{bulk} = (e_0, e_d, e_g)^\top \in \mathcal{F} \quad \text{and} \quad f_{bulk} = (f_0, f_d, f_g)^\top \in \mathcal{E}. \tag{3.92}$$

The detailed computation of (3.91) is delineated below (in what follows $\nabla := \text{grad}$):

$$\int_\Omega \left(\overline{e}_{bulk}^\top \mathcal{J}_A e_{bulk} + e_{bulk}^\top \mathcal{J}_A \overline{e}_{bulk} \right) dV = \int_\Omega \left[\overline{e}_d(-\nabla e_g) + \overline{e}_g(-\text{div } e_d) + e_d(-\nabla \overline{e}_g) + e_g(-\text{div } \overline{e}_d) \right] dV \tag{3.93a}$$

$$= \underbrace{\int_\Omega \left(\overline{e}_d(-\nabla e_g) + e_g(-\text{div } \overline{e}_d) \right) dV}_{\int_{\partial\Omega}(-\gamma_0 e_g)(\gamma_\perp \overline{e}_d)\, dS} + \underbrace{\int_\Omega \left(\overline{e}_g(-\text{div } e_d) + e_d(-\nabla \overline{e}_g) \right) dV}_{\int_{\partial\Omega}(-\gamma_0 \overline{e}_g)(-\gamma_\perp e_d)\, dS} \tag{3.93b}$$

From the above and by referring to Theorem (3.6.1), we infer:

$$\int_{\Omega} \left(\overline{e}_{bulk}^{\top} \mathcal{J}_A e_{bulk} + e_{bulk}^{\top} \mathcal{J}_A \overline{e}_{bulk} \right) dV = 0, \quad \forall \overline{e}_d \in H_0^{\text{div}}(\Omega) \text{ and } \overline{e}_g \in H_0^1(\Omega). \tag{3.94}$$

It's evident from the equations above, especially (3.94), that the boundary terms are nullified in the stipulated domain of $\mathcal{J}_A$, which is $\text{dom}\mathcal{J}_A = L^2 \times D \times G$, confirming its skew-symmetry and suitability as a Hamiltonian operator within the bounded Lipschitz domain Ω.

Boundary Port Variables

The relationship between boundary port variables and the operator $\mathcal{J}_A$ (3.90), as defined in section (3.7.3), is structured as follows:

$$\begin{pmatrix} f_\partial \\ e_\partial \end{pmatrix} = \mathcal{W}\, e_{bulk}, \tag{3.95}$$

where the boundary operator $\mathcal{W}$ is specified by:

$$\mathcal{W} = \begin{pmatrix} 0 & -\gamma_\perp & 0 \\ 0 & 0 & \gamma_0 \end{pmatrix}. \tag{3.96}$$

Their relationship is explicitly given by:

$$\begin{pmatrix} f_\partial \\ e_\partial \end{pmatrix} = \begin{pmatrix} -\gamma_\perp\, e_d \\ \gamma_0\, e_g \end{pmatrix}, \tag{3.97}$$

by referring to the Theorem (3.7.1).

Proof. The defining characteristic of a Dirac structure is that it is self-orthogonal, i.e., $\mathcal{D} = \mathcal{D}^\perp$.

Step 1. We aim to demonstrate that $\mathcal{D} \subset \mathcal{D}^\perp$.

For a space to be orthogonal to itself, the pairing of any element from the space with itself should be zero. In symbols, this condition can be written as:

$$\langle b, b \rangle_+ = 0 \quad \forall\, b \in \mathcal{D}. \tag{3.98}$$

Given that

$$f = (f_{\text{bulk}}, f_\partial) \in \mathcal{F} = L^2(\Omega)^3 \times H^{-1/2}(\partial\Omega) \tag{3.99}$$

and

$$e = (e_{\text{bulk}}, e_\partial) \in \mathcal{E} = L^2(\Omega) \times H^{\text{div}}(\Omega) \times H^1(\Omega) \times H^{1/2}(\partial\Omega), \tag{3.100}$$

where

$$e_{bulk} = \begin{pmatrix} e_0 \\ e_d \\ e_g \end{pmatrix} = \begin{pmatrix} \frac{\delta \mathcal{G}}{\delta \phi} \\ \frac{\delta \mathcal{G}}{\delta \psi} \\ E_\phi \end{pmatrix} \quad \text{and} \quad f_{bulk} = \begin{pmatrix} f_0 \\ f_d \\ f_g \end{pmatrix} = \begin{pmatrix} \frac{\partial \phi}{\partial t} \\ \frac{\partial \psi}{\partial t} \\ F_\phi \end{pmatrix}, \tag{3.101}$$

alongside the specific forms of e_{bulk} and f_{bulk} we've provided, the duality pairing, based on Eq. (3.34), is:

$$\langle b, b\rangle_+ = \langle (f_{\text{bulk}}, f_\partial, e_{\text{bulk}}, e_\partial), (\overline{f}_{\text{bulk}}, \overline{f}_\partial, \overline{e}_{\text{bulk}}, \overline{e}_\partial)\rangle_+ \tag{3.102}$$

we have:

$$\begin{aligned}
\langle b, b\rangle_+ &= 2\left(\langle e_{\text{bulk}}, f_{\text{bulk}}\rangle_{L^2(\Omega)} + \langle e_\partial, f_\partial\rangle_{\partial\Omega}\right) \\
&= 2\left(\int_\Omega e_{\text{bulk}}^\top f_{\text{bulk}}\, dV + \int_{\partial\Omega} e_\partial f_\partial\, dS\right) \\
&= 2\left(\int_\Omega e_{\text{bulk}}^\top \mathcal{J}_A e_{\text{bulk}}\, dV + \int_{\partial\Omega} (\gamma_0 e_g)(-\gamma_\perp e_d)\, dS\right) \\
&= 2\int_\Omega \left(e_0(-e_g) + e_d(-\operatorname{grad} e_g) + e_g(e_0 - \operatorname{div} e_d)\right)\, dV \\
&\quad + 2\int_{\partial\Omega} (\gamma_0 e_g)(-\gamma_\perp e_d)\, dS \\
&= 2\int_\Omega \left(e_d(-\operatorname{grad} e_g) + e_g(-\operatorname{div} e_d)\right)\, dV \\
&\quad + 2\int_{\partial\Omega} (\gamma_0 e_g)(-\gamma_\perp e_d)\, dS.
\end{aligned}$$

Using Theorem (3.6.2), given that,

$$\int_\Omega \left(e_d(-\operatorname{grad} e_g) + e_g(-\operatorname{div} e_d)\right)\, dV = \int_{\partial\Omega} (-\gamma_0 e_g)(-\gamma_\perp e_d)\, dS, \tag{3.103}$$

we have:

$$\langle b, b\rangle_+ = 2\int_{\partial\Omega} (\gamma_0 e_g)(\gamma_\perp e_d)\, dS - 2\int_{\partial\Omega} (\gamma_0 e_g)(\gamma_\perp e_d)\, dS = 0. \tag{3.104}$$

This leads to the result that $\langle b, b\rangle_+ = 0$, which concludes the proof of $\mathcal{D} \subset \mathcal{D}^\perp$.

Step 2. We aim to prove $\mathcal{D}^\perp \subset \mathcal{D}$. Formally, given $b \in \mathcal{D}^\perp$ in $\mathcal{B}$, we want to show that $b \in \mathcal{D}$.

Let

$$b = (f, e) = \left((f_{\text{bulk}}, f_\partial), (e_{\text{bulk}}, e_\partial)\right) \in \mathcal{B} \tag{3.105}$$

such that $b \in \mathcal{D}^\perp$. This means that for all $\overline{b} \in \mathcal{D}$, the pairing $\langle b, \overline{b}\rangle_+ = 0$.

Consider an arbitrary $\overline{b}$ given by:

$$\overline{b} = \left(\overline{f}, \overline{e}\right) = \left(\left(\overline{f}_{\text{bulk}}, \overline{f}_\partial\right), (\overline{e}_{\text{bulk}}, \overline{e}_\partial)\right), \tag{3.106}$$

where:

$$\overline{f}_{\text{bulk}} = \mathcal{J}_A \overline{e}_{\text{bulk}} = \begin{pmatrix} -\overline{e}_g \\ -\operatorname{grad} \overline{e}_g \\ \overline{e}_0 - \operatorname{div} \overline{e}_d \end{pmatrix}, \tag{3.107}$$

and:

$$\left(\overline{f}_{\partial}, \overline{e}_{\partial}\right) = \mathcal{W}\overline{e}_{\text{bulk}} = \begin{pmatrix} -\gamma_{\perp}\ \overline{e}_d \\ \gamma_0\ \overline{e}_g \end{pmatrix}. \tag{3.108}$$

Given $\overline{e}_{\text{bulk}} = \begin{pmatrix} \overline{e}_0 \\ \overline{e}_d \\ \overline{e}_g \end{pmatrix}$, we are free to choose in $\mathcal{E}$.

Using the definition of the duality pairing, we have:

$$\begin{aligned}
\langle b, \overline{b}\rangle_+ &= \langle (f_{\text{bulk}}, f_{\partial}, e_{\text{bulk}}, e_{\partial}), (\overline{f}_{\text{bulk}}, \overline{f}_{\partial}, \overline{e}_{\text{bulk}}, \overline{e}_{\partial})\rangle_+ \\
&= \int_{\Omega} e_{\text{bulk}} \mathcal{J}_A \overline{e}_{\text{bulk}}\, dV + \int_{\Omega} \overline{e}_{\text{bulk}} f_{\text{bulk}}\, dV \\
&\quad + \int_{\partial\Omega} e_{\partial} \mathcal{J}_A \overline{e}_{\partial}\, dS + \int_{\partial\Omega} \overline{e}_{\partial} f_{\partial}\, dS \\
&= \int_{\Omega} \left(e_0(-\overline{e}_g) + e_d(-\text{grad}\overline{e}_g) + e_g(\overline{e}_0 - \text{div}\overline{e}_d)\right)\, dV \\
&\quad + \int_{\Omega} \left(\overline{e}_0 f_0 + \overline{e}_d f_d + \overline{e}_g f_g\right)\, dV \\
&\quad + \int_{\partial\Omega} e_{\partial}(-\gamma_{\perp}\overline{e}_d)\, dS + \int_{\partial\Omega} (\gamma_0 \overline{e}_g) f_{\partial}\, dS.
\end{aligned}$$

To prove that $b \in \mathcal{D}$ when $b \in \mathcal{D}^{\perp}$, consider the following:

First Case: Choose

$$\overline{e}_0 \in L^2(\Omega), \overline{e}_d = 0, \text{ and } \overline{e}_g = 0. \tag{3.109}$$

We then have:

$$\begin{aligned}
\langle b, \overline{b}\rangle_+ &= \int_{\Omega} \left(e_g \overline{e}_0 + \overline{e}_0 f_0\right)\, d\Omega \\
&= \int_{\Omega} \overline{e}_0 \left(e_g + f_0\right)\, d\Omega \\
&= 0 \quad \forall \overline{e}_0 \in L^2(\Omega),
\end{aligned}$$

which implies:

$$f_0 + e_g = 0. \tag{3.110}$$

Second Case: Choose

$$\overline{e}_0 = 0, \overline{e}_d \in H_0^{\text{div}}(\Omega), \text{ and } \overline{e}_g = 0. \tag{3.111}$$

This yields:

$$\begin{aligned}
\langle b, \overline{b}\rangle_+ &= \int_{\Omega} \left(e_g(-\text{div}\overline{e}_d) + \overline{e}_d f_d\right)\, d\Omega \\
&= \int_{\Omega} \overline{e}_d \left(\text{grad} e_g\right)\, d\Omega \\
&= 0 \quad \forall \overline{e}_d \in H_0^{\text{div}}(\Omega),
\end{aligned}$$

leading to:

$$f_d + \text{grad} e_g = 0. \tag{3.112}$$

Third Case: Choose

$$\overline{e}_0 = 0, \overline{e}_d = 0, \text{ and } \overline{e}_g \in H_0^1(\Omega). \tag{3.113}$$

From this, we derive:

$$\begin{aligned} \langle b, \overline{b} \rangle_+ &= \int_\Omega (e_0(-\overline{e}_g) + e_d(-\text{grad}\overline{e}_g) + \overline{e}_g f_g) \, d\Omega \\ &= 0 \quad \forall \overline{e}_g \in H_0^1(\Omega), \end{aligned}$$

which implies:

$$f_g - e_0 + \text{div} e_d = 0. \tag{3.114}$$

Thus, our conclusion is:

$$f_{\text{bulk}} = \mathcal{J}_A e_{\text{bulk}} = \begin{pmatrix} -e_g \\ -\text{grad} e_g \\ e_0 - \text{div} e_d \end{pmatrix}.$$

By substituting the components of f_{bulk} into our equation and simplifying, we obtain our desired relations:

$$\overline{f}_{\text{bulk}} = \mathcal{J}_A \overline{e}_{\text{bulk}} = \begin{pmatrix} -\overline{e}_g \\ -\text{grad}\, \overline{e}_g \\ \overline{e}_0 - \text{div}\, \overline{e}_d \end{pmatrix} \tag{3.115}$$

and the orthogonality condition, we can expand the inner product as follows:

$$\begin{aligned} \langle b, \overline{b} \rangle_+ &= \int_\Omega (e_0(-\overline{e}_g) + e_d(-\text{grad}\, \overline{e}_g) + e_g(\overline{e}_0 - \text{div}\, \overline{e}_d)) \, dV \\ &\quad + \int_\Omega (\overline{e}_0 f_0 + \overline{e}_d f_d + \overline{e}_g f_g) \, dV \\ &\quad + \int_{\partial\Omega} e_\partial(-\gamma_\perp \overline{e}_d) \, dS + \int_{\partial\Omega} (\gamma_0 \overline{e}_g) f_\partial \, dS \\ &= \int_{\partial\Omega} (-\gamma_0 \overline{e}_g)(-\gamma_\perp e_d - f_\partial) \, dS \\ &\quad + \int_{\partial\Omega} (-\gamma_\perp \overline{e}_d)(-\gamma_0 e_g + e_\partial) \, dS \\ &= 0 \quad \forall \quad \overline{e}_d \in H_0^{\text{div}}(\Omega), \quad \overline{e}_g \in H_0^1(\Omega). \end{aligned}$$

This implies:

$$-\gamma_\perp e_d - f_\partial = 0 \quad \text{and} \quad -\gamma_0 e_g + e_\partial = 0. \tag{3.116}$$

Thus, $b \in \mathcal{D}$.

□

In this subsection, we have examined the boundary port variables, the space of power variables, and the associated Stokes-Dirac structure. We have highlighted the definitions and propositions associated with the operator $\mathcal{J}_A$ and its applications in the context of the non-conserved phase field model.

3.11 Port Hamiltonian Formulation of the Allen-Cahn Equation using the Entropy as Potential

The Allen-Cahn equation, as presented in Chapter 2, is used for modeling phase transitions in certain materials. It can be formulated using the Port-Hamiltonian framework, which provides insights into the system's energy dynamics. Building upon the work of [110] and [112], our contribution delves into a systematic study of this model, particularly emphasizing entropy as a potential.

3.11.1 State Space Augmentation

To effectively capture the dissipative dynamics within the Allen-Cahn framework, we shall proceed by augmenting the state space as we did in the above section 3.10. This extension allows for a more detailed representation of the system's thermodynamic properties:

$$\psi = \operatorname{grad} \phi \tag{3.117}$$

Here, ψ represents the gradient of the phase field variable ϕ, enriching the state space to include (ϕ, ψ, u).

Entropy Functional and Constitutive Relation

The dynamics of the Allen-Cahn equation are intrinsically linked to the thermodynamic potentials, encapsulated by the Landau-Ginzburg entropy functional $\bar{S}$ [112]:

$$\bar{S}(\phi, \psi, u) = \int_\Omega s(\phi, u) - \frac{1}{2}\epsilon^2 \psi^2 \, dV \tag{3.118}$$

The functional $\bar{S}$ is used to derive the system dynamics through variational principles:

$$\frac{\delta S}{\delta \phi} = \frac{\delta \bar{S}}{\delta \phi} - \operatorname{div}\left(\frac{\partial \bar{S}}{\partial \psi}\right) := F_{\phi\psi} \tag{3.119}$$

where and $F_{\phi\psi}$ denotes the driving force.

Dissipative Constitutive Relation

The gradient dynamics elucidate the dissipative nature of the system, essential for understanding the phase transitions:

$$E_{\phi\psi} = \frac{1}{\eta} F_{\phi\psi} \tag{3.120}$$

where $E_{\phi\psi}$ denotes the phase field flux.

Dynamics of the Added State Variable ψ

$$\frac{\partial \psi}{\partial t} = \frac{\partial}{\partial t}\text{grad}\phi = \text{grad}\frac{\partial \phi}{\partial t} = -\text{grad}\, E_{\phi\psi} \tag{3.121}$$

This equation reinforces the connection between the microscopic gradient changes in ϕ and the macroscopic system evolution.

3.11.2 Dissipative Port Hamiltonian Formulation of the Allen-Cahn Equation

The Allen-Cahn equation, when augmented by the dynamics of the additional state variable ψ, can be effectively described within the Port Hamiltonian framework using the entropy functional as the generating function (3.118). This framework captures both the system's Hamiltonian dynamics (inherent dynamics described by the Hamiltonian operator) and its dissipative characteristics (described by the algebraic constitutive relations), as demonstrated by the following representation:

$$\begin{pmatrix} \frac{\partial \phi}{\partial t} \\ \frac{\partial \psi}{\partial t} \\ F_{\phi\psi} \end{pmatrix} = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & -\text{grad} \\ 1 & -\text{div} & 0 \end{pmatrix} \begin{pmatrix} \frac{\delta(-\bar{S})}{\delta \phi} \\ \frac{\delta(-\bar{S})}{\delta \psi} \\ E_{\phi\psi} \end{pmatrix}, \tag{3.122}$$

where the neg-entropy $-\bar{S}$ is chosen as the generating functional, leading to a dissipative system. Note that one obtains the same differential operator $\mathcal{J}_A$ defined before (3.90) as for the Port Hamiltonian formulation using the energy as generating function.

Boundary Port Variables

Utilizing the same differential operator $\mathcal{J}_A$, the system adheres to the Stokes-Dirac structure established earlier in Theorem (3.7.1). The boundary port variables are defined as follows:

$$\begin{pmatrix} f_\partial^{\phi\psi} \\ e_\partial^{\phi\psi} \end{pmatrix} = \mathcal{W}\, e_{\phi\psi} = \begin{pmatrix} -\gamma_\perp \frac{\delta(-\bar{S})}{\delta \psi} \\ \gamma_0\, E_{\phi\psi} \end{pmatrix}, \tag{3.123}$$

$$\mathcal{W} = \begin{pmatrix} 0 & -\gamma_\perp & 0 \\ 0 & 0 & \gamma_0 \end{pmatrix}, \tag{3.124}$$

Physically, the variable $\gamma_\perp \frac{\delta(-\bar{S})}{\delta \psi}$ represents the flux, while $\gamma_0\, E_{\phi\psi}$ represents the conjugated intensive variable. This setup enables the system to interact with its external environment.

The choice of $-\bar{S}$ as a generating function is justified by the entropy balance equation:

$$\frac{d(-\bar{S})}{dt} = -\int_V \eta F_{\phi\psi}^2 dV + \int_{\partial V} e_\partial f_\partial \, dS, \tag{3.125}$$

which ensures that the system adheres to the second law of thermodynamics by accounting for entropy production within the volume V and entropy flux across the boundary ∂V. This equation highlights the dissipative nature of the system, where the internal dissipation is balanced by the entropy flux at the boundaries.

3.12 Port Hamiltonian Formulation of the Solidification Process

The process of solidification is the result of coupled phenomena: the phase field dynamics and the heat transfer. This process is modeled using the Port Hamiltonian framework by coupling the Port Hamiltonian representation of the Allen-Cahn equation for the phase field and the heat conduction equation.

The coupling occurs in two ways. First, the entropy becomes a function of both the phase field variable ϕ and the internal energy u according to the expressions derived in Chapter 2, Section (2.7), Equation (2.25). Second, the Hamiltonian operator of the coupled system consists of the product of the canonical Hamiltonian operator $\mathcal{J}_u$ in (3.75) and the Hamiltonian operator associated with the Allen-Cahn equation $\mathcal{J}_A$ in (3.90).

3.12.1 Dissipative Port Hamiltonian Structure

The dissipative Port Hamiltonian model for solidification includes the phase field variables ϕ, ψ (where $\psi = \operatorname{grad}\phi$), and the internal energy variable u. The entropy relation is given by:

$$\frac{\delta \bar{S}}{\delta u} = \frac{\partial s}{\partial u} = \tau \tag{3.126}$$

where τ is the reciprocal of the temperature.

By combining the phase field and heat diffusion dynamics:

$$\begin{pmatrix} \frac{\partial u}{\partial t} \\ F \end{pmatrix} = \begin{pmatrix} 0 & -\operatorname{div} \\ -\operatorname{grad} & 0 \end{pmatrix} \begin{pmatrix} \frac{\partial(-\bar{S})}{\partial u} \\ q \end{pmatrix}, \tag{3.127}$$

and

$$\begin{pmatrix} \frac{\partial \phi}{\partial t} \\ \frac{\partial \psi}{\partial t} \\ F_{\phi\psi} \end{pmatrix} = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & -\operatorname{grad} \\ 1 & -\operatorname{div} & 0 \end{pmatrix} \begin{pmatrix} \frac{\delta(-\bar{S})}{\delta \phi} \\ \frac{\delta(-\bar{S})}{\delta \psi} \\ E_{\phi\psi} \end{pmatrix}, \tag{3.128}$$

we form a dissipative Port Hamiltonian system:

$$\begin{pmatrix} \frac{\partial \phi}{\partial t} \\ \frac{\partial \psi}{\partial t} \\ F_{\phi\psi} \\ \frac{\partial u}{\partial t} \\ F \end{pmatrix} = \mathcal{J}_S \begin{pmatrix} -\frac{\partial s}{\partial \phi}(\phi, u) \\ \epsilon^2 \psi \\ E_{\phi\psi} \\ -\tau \\ q \end{pmatrix} \tag{3.129}$$

The Hamiltonian operator $\mathcal{J}_S$ is defined as:

$$\mathcal{J}_S = \begin{pmatrix} 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & -\operatorname{grad} & 0 & 0 \\ 1 & -\operatorname{div} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\operatorname{div} \\ 0 & 0 & 0 & -\operatorname{grad} & 0 \end{pmatrix} \tag{3.130}$$

Boundary Port Variables

The boundary operator $\widetilde{\mathcal{W}}$ synthesizes the boundary interactions from both the heat diffusion and the Allen-Cahn dynamics:

$$\widetilde{\mathcal{W}} = \begin{pmatrix} 0 & -\gamma_\perp & 0 & 0 & 0 & 0 \\ 0 & 0 & \gamma_0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \gamma_0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\gamma_\perp \end{pmatrix} \tag{3.131}$$

The boundary port variables for both the heat and phase field dynamics are expressed as:

$$\begin{pmatrix} f_\partial^{\phi\psi} \\ e_\partial^{\phi\psi} \\ f_\partial \\ e_\partial \end{pmatrix} = \widetilde{\mathcal{W}} \begin{pmatrix} -\frac{\partial s}{\partial \phi}(\phi, u) \\ \epsilon^2 \psi \\ F_{\phi\psi} \\ -\tau \\ q \end{pmatrix} = \begin{pmatrix} -\gamma_\perp(\epsilon^2 \psi) \\ \gamma_0 \left(1/\eta E_{\phi\psi}\right) \\ \gamma_0 \tau \\ -\gamma_\perp M_\tau(-\mathrm{grad}(\tau)) \end{pmatrix} \tag{3.132}$$

Interpretation of Boundary Port Variables

In this solidification model:

- $f_\partial^{\phi\psi}$ represents the flux of the phase field across the boundary.
- $e_\partial^{\phi\psi}$ is an effort variable associated with the interface, specifically the trace of $(1/\eta E_{\phi\psi} = F_{\phi\psi}) = \frac{\delta S}{\delta \phi}$.
- f_∂ represents the reciprocal temperature at the boundary.
- e_∂ is the heat flux at the boundary.

These variables are fundamental for implementing control strategies and observing the system's responses at the boundaries.

3.12.2 Entropy Balance

The neg-entropy balance consists of three terms:

$$\frac{d(-\bar{S})}{dt} = -\int_V E_{\phi\psi} F_{\phi\psi} dV - \int_V q \bar{F} dV - \int_{\partial V} \tilde{e}_\partial \tilde{f}_\partial \, dS \tag{3.133}$$

or

$$\frac{d(-\bar{S})}{dt} = -\int_V \eta F_{\phi\psi}^2 dV - \int_V M_\tau \bar{F}^2 dV + \int_{\partial V} \tilde{e}_\partial \tilde{f}_\partial \, dS \tag{3.134}$$

The first two terms correspond to the irreversible entropy production in the bulk, due to the two dissipative phenomena, the gradient relaxation dynamics of the phase field and the heat conduction. The third term corresponds to the entropy flux through the boundary of the system.

3.13 Implicit Port Hamiltonian Models

The Port Hamiltonian formulation described in section (3.8) uses the Hamiltonian function as the entropy functional, as shown in equation (2.25). This functional relates the internal energy u, the phase field variable ϕ and its gradient ψ. In section (2.8) of the preceding chapter, we introduced a practical definition of the thermodynamic properties for the biphasic water-ice system, which resulted in an expression for the entropy density that depends on temperature rather than internal energy, as shown in equation (2.35). This dependence requires a transition from the internal energy u (an extensive variable) to the temperature T (an intensive variable) in the state space.

This section aims to reformulate the Port Hamiltonian model introduced in (3.129) by adopting the Implicit Port Hamiltonian formulation.

In this formulation, the energy function is defined indirectly by a set of constitutive relations between extensive and intensive variables, obeying Maxwell's reciprocity conditions. Geometrically, these relations can be interpreted as Lagrangian submanifolds, facilitating the definition of reciprocal constitutive equations in a coordinate-free manner. This approach, in line with discussions in [105, 88], is extendable to distributed parameter systems as shown in [60, 106].

To ensure clarity and completeness, we now recall the definition of a Port Hamiltonian system defined on a Lagrangian submanifold.

3.13.1 Port Hamiltonian Systems on Lagrangian Submanifolds

A Port Hamiltonian system can be defined on a Lagrangian submanifold of the cotangent manifold of the energy variables instead of using a Hamiltonian function as a generating function. According to [89], the standard definition of a Port Hamiltonian system involves a Dirac structure on a finite-dimensional manifold.

A Lagrangian submanifold L of the cotangent bundle T^*X is an n-dimensional submanifold where the canonical symplectic form is zero. In the linear case, a submanifold $L \subset T^*X$ is Lagrangian if the canonical symplectic form vanishes on L, i.e., $\omega|_L = 0$. In the nonlinear case, L is Lagrangian if for every $x \in L$, there exists a local chart in which L is given by $\{(q,p) \in T^*X \mid p = dS(q)\}$ for some function S on X [105, 88].

For a given Lagrangian submanifold $L \subset T^*X$, the dynamics of the system are described implicitly by the relations defining L [89].

Definition 3.13.1

A generalized Port Hamiltonian system with space of energy variables X with implicit energy storage is defined by the triple (D, L, R), where: D is a Dirac structure on the manifold X, L is a Lagrangian submanifold of T^*X, and R represents the energy dissipation.

The dynamics are given by:

$$(-\dot{x}(t), f_R(t), f_P(t), e_S(t), e_R(t), e_P(t)) \in D(x(t)), \tag{3.135}$$

$$(f_R(t), e_R(t)) \in R, \tag{3.136}$$

$$(x(t), e_S(t)) \in L, \tag{3.137}$$

where x are the state variables, f_R and e_R are the flow and effort variables related to energy dissipation, and f_P and e_P are the external port variables.

3.13.2 Lagrangian Submanifold and Implicit System for Heat Dynamics

In this section, we aim to derive the implicit Port Hamiltonian system for heat dynamics, starting from the given system (3.127):

$$\begin{pmatrix} \frac{\partial u}{\partial t} \\ \bar{F} \end{pmatrix} = \begin{pmatrix} 0 & -\text{div} \\ -\text{grad} & 0 \end{pmatrix} \begin{pmatrix} \frac{\partial s}{\partial u} \\ q \end{pmatrix}, \tag{3.138}$$

Lagrangian Submanifold for the Thermodynamic Properties of Incompressible Fluid Heat Dynamics

Consider the entropy density function $s(u)$. The Gibbs equation (2.24) associated with the entropy density function $s(u)$ gives rise to the following Lagrangian submanifold defined by the graph of $s(u)$:

$$L_s = \left\{ (u, \tau) \in \mathbb{R}^2 \times \mathbb{R}^2 : \tau = \frac{\partial s}{\partial u}(u); u \in \mathbb{R} \right\}. \tag{3.139}$$

To change the coordinates from the internal energy u to the reciprocal temperature τ, consider the Legendre transform of the entropy density $s(u)$ with respect to u:

$$s^*(\tau) = \tau u - s(u), \tag{3.140}$$

where the internal energy u is considered to be a function of the reciprocal temperature τ, obtained by inverting $\tau = \frac{\partial s}{\partial u}(u)$.

Then, the Legendre submanifold (3.139) can be defined as follows:

$$L_s = \left\{ (u, \tau) \in \mathbb{R}^2 \times \mathbb{R}^2 : u = \frac{\partial s^*}{\partial \tau}(\tau); \tau \in \mathbb{R} \right\}. \tag{3.141}$$

Implicit Heat Model

To derive the implicit heat model, we start with the given explicit energy balance equation and reformulate it using the Legendre transform. The system can be written as:

$$\begin{pmatrix} \frac{\partial u}{\partial t} \\ \bar{F} \end{pmatrix} = \begin{pmatrix} 0 & -\text{div} \\ -\text{grad} & 0 \end{pmatrix} \begin{pmatrix} \frac{\partial s}{\partial u}(u) \\ q \end{pmatrix}. \tag{3.142}$$

Next, we transform the coordinates from u to τ. Using the chain rule and the definition of the Legendre submanifold (3.141), we have:

$$\begin{aligned} \frac{\partial}{\partial t} \begin{pmatrix} u \\ \bar{F} \end{pmatrix} &= \frac{\partial}{\partial t} \begin{pmatrix} \frac{\partial s^*}{\partial \tau}(\tau) \\ \bar{F} \end{pmatrix} \\ &= \begin{pmatrix} \frac{\partial^2 s^*}{\partial \tau^2} & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \frac{\partial \tau}{\partial t} \\ \bar{F} \end{pmatrix}. \end{aligned} \tag{3.143}$$

Substituting (3.143) into the explicit model (3.142), we get:

$$\begin{pmatrix} \frac{\partial^2 s^*}{\partial \tau^2} & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \frac{\partial \tau}{\partial t} \\ F \end{pmatrix} = \begin{pmatrix} 0 & -\text{div} \\ -\text{grad} & 0 \end{pmatrix} \begin{pmatrix} \tau \\ q \end{pmatrix}. \tag{3.144}$$

3.13.3 Implicit Model of Solidification Process

Based on the above section (3.13.1), the implicit model for the solidification process can be expressed as follows: Given Gibbs' equation (2.24) associated with the entropy density function $s(\phi, u)$, we can delineate the following Lagrangian submanifold represented by the graph of $s(\phi, u)$:

$$L_s = \left\{ (x, e) \in \mathbb{R}^2 \times \mathbb{R}^2 : e = \begin{pmatrix} \frac{\partial s}{\partial \phi}(\phi, u) \\ \frac{\partial s}{\partial u}(\phi, u) \end{pmatrix}; x = \begin{pmatrix} \phi \\ u \end{pmatrix} \right\}. \tag{3.145}$$

For transitioning the coordinates, consider the Legendre transform of the entropy density $s(\phi, u)$ with respect to u:

$$s^*(\phi, \tau) = \tau u - s(\phi, u), \tag{3.146}$$

Here, u is expressed as a function of ϕ and the reciprocal temperature, derived by inverting $\tau = \frac{\partial s}{\partial u}(\phi, u)$ in terms of u[2].

Subsequently, we define the submanifold in equation (3.145) as:

$$L_s = \left\{ (x, e) \in \mathbb{R}^2 \times \mathbb{R}^2 : x = \begin{pmatrix} \phi \\ \frac{\partial s^*}{\partial \tau}(\phi, \tau) \end{pmatrix}; e = \begin{pmatrix} \frac{\partial s^*}{\partial \phi}(\phi, \tau) \\ \tau \end{pmatrix}; (\phi, \tau) \in \mathbb{R}^2 \right\}. \tag{3.147}$$

The dynamics of the solidification process can then be expressed as follows. First, considering the extended entropy functional (3.118), we have the associated Legendre submanifold:

$$\begin{aligned} L_{(-\bar{S})} = \Bigg\{ \left(\begin{pmatrix} x \\ \psi \end{pmatrix}, \begin{pmatrix} e \\ e_\psi \end{pmatrix} \right) \in \mathbb{R}^3 \times \mathbb{R}^3 \Bigg/ \\ (x, -e) \in L_s;\ e_\psi = \epsilon^2 \psi;\ \psi \in \mathbb{R} \Big\} \end{aligned} \tag{3.148}$$

First, we compute the time derivative of the vector x, with its expression in the definition (3.147) of the Lagrange submanifold L_s:

$$\begin{aligned} \frac{\partial}{\partial t} \begin{pmatrix} \phi \\ u \end{pmatrix} &= \frac{\partial}{\partial t} \begin{pmatrix} \phi \\ \frac{\partial s^*}{\partial u}(\phi, \tau) \end{pmatrix} \\ &= \begin{pmatrix} 1 & 0 \\ \frac{\partial s^*}{\partial \phi \partial \tau}(\phi, \tau) & \frac{\partial^2 s^*}{\partial \tau^2}(\phi, \tau) \end{pmatrix} \frac{\partial}{\partial t} \begin{pmatrix} \phi \\ \tau \end{pmatrix} \end{aligned} \tag{3.149}$$

[2]The invertibility stems from the strict concavity of $s(\phi, u)$, a direct consequence of the strict concavity of the entropy functions s_{sol} and s_{liq} for solid and liquid phases, and its formulation in equation (2.35).

with $\frac{\partial^2 s^*}{\partial \tau^2} = -c_p - \tau \frac{\partial c_p}{\partial \tau}$ where $c_p(\phi, \tau)$ is the extended heat capacity and $\frac{\partial s^*}{\partial \phi \partial \tau} = -\tau \frac{\partial c_p}{\partial \phi}$.
The thermal conductivity becomes:

$$\lambda = \lambda_{sol} + p_i(\phi)\Big[\lambda_{liq} - \lambda_{sol}\Big]. \tag{3.150}$$

Implicit Port Hamiltonian System of Solidification Process

The Port Hamiltonian System, using the expression in the definition (3.149) and the parametrization of the extensive variables e in (3.147), leads to the following implicit PDE:

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ \frac{\partial s^*}{\partial \phi \partial \tau} & 0 & 0 & \frac{\partial^2 s^*}{\partial \tau^2} & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \frac{\partial \phi}{\partial t} \\ \frac{\partial \psi}{\partial t} \\ F_{\phi\psi} \\ \frac{\partial \tau}{\partial t} \\ \bar{F} \end{pmatrix} = \mathcal{J}_S \begin{pmatrix} -\frac{\partial s^*}{\partial \phi}(\phi, \tau) \\ \epsilon^2 \psi \\ E_{\phi\psi} \\ -\tau \\ q \end{pmatrix}. \tag{3.151}$$

Since the matrix on the left is invertible, this system can be considered a regular Algebraic-Differential system. This PDE, augmented with the dissipative relations and the boundary port variables, defines a Dissipative Boundary Port Hamiltonian System.

It is remarkable that the dynamics of phase field models of solidification processes often lead to implicit formulations of the dynamics. For instance, [112] and [8] begin their work using the entropy as a thermodynamic potential to ensure the irreversible entropy creation of the phase field dynamics. However, they use the Helmholtz free energy density $f(\phi, T)$ as a generating function for the thermodynamic properties of the bi-phasic system. Yet, even with f, these authors finally obtain an implicit dynamic system.

3.14 Conclusion

This chapter presents a Dissipative Boundary Port Hamiltonian representation for the solidification processes of water and other pure substances, utilizing entropy as a generating function for the dynamics. Building on foundational work, such as that by [110], the chapter extends the Port Hamiltonian framework to include the Allen-Cahn equation, effectively modeling the dynamics of non-conserved phase field variables and the heat equation.

We initially developed the explicit model of the solidification process using entropy as the generating function, with state variables being the phase field variable ϕ and the internal energy u. However, due to the limited availability of data for the entropy density function $s = s(\phi, u)$, we transitioned to using the reciprocal temperature $\tau = 1/T$. This adjustment allowed us to utilize existing thermodynamic properties of liquid water and ice, as documented in the literature [42] and [43]. The Gibbs energy, expressed as a function of temperature and pressure, facilitated a practical definition of the thermodynamic properties of the bi-phasic water-ice system. Consequently, we derived expressions for the entropy density based on temperature rather than internal energy. This necessitated a shift in the state space coordinate from internal energy u to temperature T.

We then reformulated the explicit Port Hamiltonian model into an implicit Port Hamiltonian formulation using Lagrangian submanifolds. This approach, detailed in works such as [105] and [88], allows for the definition of reciprocal constitutive equations in a coordinate-free manner and can be adapted to distributed parameter systems [60], [106]. Ultimately, this led to an implicit formulation of the solidification model by integrating Differential-Algebraic Equations (DAE) and Partial Differential Equations (PDE). This framework, modeling the dynamics in terms of reciprocal temperature, aligns well with the empirical thermodynamic properties of systems like water and ice.

Chapter 4

Discretization of the Solidification Process

Contents

Abstract

This chapter focuses on numerical analysis within the Port Hamiltonian framework, focusing on the discretization of solidification processes using the Partitioned Finite Element Method (PFEM). It demonstrates structure-preserving numerical simulations of the heat equation and the Allen-Cahn equation. The chapter covers weak formulations, projections, and discrete Hamiltonians for these equations, finishing with a discretization of the complete model of the solidification process.

4.1 Introduction and Overview of the chapter

This chapter focuses on the structure-preserving discretization of the Boundary Port Hamiltonian (PH) model of the solidification process. A structure-preserving discretization ensures that the discretized model retains the PH structure, preserving key properties such as energy conservation and passivity [11, 17]. Several structure-preserving discretization techniques are employed to approximate solutions while maintaining these structural properties. According to [77], the following techniques are notable:

- **Mixed Finite-Elements Method** by Golo et al. [35, 36]: This method uses different bases for energy and co-energy variables, integrating them based on the degree of the differential form defining them.
- **Pseudo-Spectral Methods** for pH Systems explored by Moulla et al. [39, 66, 111].
- **Discrete Exterior Calculus** approach extended to pH systems by Seslija et al. [53, 97]: This method represents discrete systems of conservation laws in a matrix form that mirrors continuous formulations.
- **Partitioned Finite Element Method (PFEM)** developed by Cardoso et al. [15], Serhani [96], and Brugnoli et al. [9, 10]: PFEM will be discussed in detail hereafter.

In this chapter, we utilize the Partitioned Finite Element Method (PFEM), based on the work of [38], to ensure structure-preserving discretization of the heat equation and the Allen-Cahn equation. PFEM maintains the physical and geometrical properties of Port Hamiltonian (pH) systems during numerical simulations, which is crucial for accurately representing and

analyzing solidification phenomena.

4.2 Contributions of the chapter

The principal contribution of this chapter lies in the discretization methodology applied to the Port Hamiltonian (PH) model of the heat equation, focusing on two main innovations:

1. **Integration of Entropy as the Generating Function:** We applied the Partitioned Finite Element Method (PFEM) to the PH model where we use nonlinear constitutive relations, corresponding to non-quadratic Hamiltonian functions arising from the thermodynamic models presented in Chapter (2), with entropy s as the generating function.
2. **Implicit Formulation with Reciprocal Temperature:** We introduced and discretized an implicit formulation of the heat equation using the reciprocal temperature $\tau = \frac{1}{T}$ as the state variable. In addition, we discretized the Allen-Cahn equation, leading to the discretization of the entire implicit model of the solidification process.This formulation aligns with the dissipative Hamiltonian systems framework, incorporating boundary ports.

4.3 Introduction to the Partitioned Finite Element Method

The Partitioned Finite Element Method (PFEM), as proposed by Haine et al. [38], is a systematic approach designed to preserve the port-Hamiltonian structure of physical systems during numerical simulations. This section discusses the principles of PFEM, in particular its application to the heat equation and the Allen Cahn equa tion in the context of solidification processes.

PFEM maintains the structural identity of the Port Hamiltonian systems, ensuring that the energy conservation and dissipation properties of the continuous systems are preserved in the discrete model. This preservation is important for achieving accurate and efficient simulation results.

The method aligns with the principles of Port Hamiltonian systems, which provide a modular and comprehensive framework for modeling and controlling complex multi-physics systems. Over the past two decades, Port Hamiltonian frameworks have been instrumental in accurately describing interconnected systems with a strong emphasis on physical phenomena and geometric structures.

PFEM has been effectively applied to various systems, including wave-like systems where boundary conditions play a significant role. By employing structure-preserving discretization techniques, PFEM accurately approximates boundary terms, ensuring the precision of simulations even under complex boundary conditions. This is particularly important for solidification processes, where interactions at the boundaries significantly influence the system's behavior.

Several studies have demonstrated the effectiveness of PFEM in different applications:

- Haine et al. [38] illustrated the application of PFEM in simulating the dynamics of the heat equation within a Port Hamiltonian framework.
- PFEM has been utilized to model wave equations, demonstrating its ability to handle wave propagation and boundary interactions accurately [77].
- The method has been extended to control theory applications, showcasing its flexibility and robustness in managing energy-storing and dissipative elements in electrical, mechanical, and electro-mechanical systems [90].

This section delves into the application of PFEM for discretizing the heat equation and Allen-Cahn equation within the Port Hamiltonian framework, highlighting its advantages in maintaining structural integrity and ensuring accurate simulations in solidification processes.

4.4 Discretization of the Heat Equation - The Model

Introduction

This section discusses the use of the heat equation to model thermal energy distribution during solidification. We first recall the work by Cardoso-Ribeiro, Matignon, Lefèvre, and Serhani [95] on discretizing the heat equation using the classical Partitioned Finite Element Method (PFEM) within the Port Hamiltonian framework. In their work, Matignon et al. [5] used temperature T as a state variable, based on a linear model, and a linearity assumption leading to a quadratic function of temperature as the Hamiltonian function. Our approach builds on this by employing a thermodynamic nonlinear model with the total entropy as the Hamiltonian function, providing a more comprehensive and physically meaningful representation. We recall their work to illustrate the method of obtaining the weak formulation and computing the mass matrices.

Consider the temperature T of a 2D domain $\Omega \subset \mathbb{R}^2$. Let C_v denote the heat capacity at constant volume, ρ the mass density, and λ the heat conductivity (a positive definite tensor).

Assume that:

- The domain Ω does not change over time; i.e., we work at constant volume in a solid.
- No chemical reactions occur in the domain.
- The Dulong-Petit's model assumptions are valid: the internal energy is proportional to temperature.

Let us denote:

- u as the internal energy density,
- J_Q as the heat flux,
- T as the local temperature,
- $C_V := \left(\frac{du}{dT}\right)_V$ as the isochoric heat capacity.

The first law of thermodynamics, stating that in an isolated system, energy is preserved, reads:

$$\rho(x)\partial_t u(t,x) = -\mathrm{div}(J_Q(t,x)), \quad \forall t \geq 0,\, x \in \Omega.$$

Under Dulong-Petit's model, one has $u = C_V T$, which leads to:

$$\rho(x)C_V(x)\partial_t T(t,x) = -\mathrm{div}(J_Q(t,x)), \quad \forall t \geq 0,\, x \in \Omega.$$

As a constitutive relation, the classical Fourier's law is considered:

$$J_Q(t,x) = -\lambda(x) \cdot \mathrm{grad}(T(t,x)), \quad \forall t \geq 0,\, x \in \Omega,$$

where λ is the tensor-valued heat conductivity of the medium.

The well-known heat equation, subject to Neumann boundary control, governing the temperature distribution is given by:

$$\rho(x)C_v(x)\frac{\partial}{\partial t}T(t,x) - \mathrm{div}(\lambda(x) \cdot \mathrm{grad}(T(t,x))) = 0, \quad t \geq 0,\, x \in \Omega, \tag{4.1}$$

$$-(\lambda(x) \cdot \mathrm{grad}(T(t,x))) \cdot \mathbf{n} = u_\partial(t,x), \quad t \geq 0,\, x \in \partial\Omega, \tag{4.2}$$

where $\mathbf{n}$ is the outward normal to Ω.

Port Hamiltonian Framework

The **Hamiltonian** is the usual L^2 functional, which is chosen as the quadratic form for a parabolic equation, despite its lack of thermodynamic meaning:

$$\mathcal{H}(t) := \frac{1}{2}\int_\Omega \rho(x)C_v(x)(T(t,x))^2\,dx, \quad t \geq 0. \tag{4.3}$$

Taking the internal energy density $\alpha_u := u = C_v T$ as the **energy variable** (using the Dulong-Petit model), the Hamiltonian can be expressed as:

$$\mathcal{H}(t) = \mathcal{H}(\alpha_u(t,\cdot)) = \frac{1}{2}\int_\Omega \rho(x)\frac{\alpha_u^2(t,x)}{C_v(x)}\,dx. \tag{4.4}$$

The **co-energy variable**, denoted by e_u, is defined as the variational derivative of the Hamiltonian with respect to the weighted L^2-product with weight ρ:

$$e_u := \delta^\rho_{\alpha_u}\mathcal{H} = \frac{\alpha_u}{C_v} = T, \tag{4.5}$$

representing the temperature. This equality serves as the first **constitutive relation**.

Denoting J_Q as the heat flux, the first principle of thermodynamics is given by:

$$\frac{\partial}{\partial t}\rho u + \mathrm{div}(J_Q) = 0. \tag{4.6}$$

Fourier's law provides the second constitutive relation:

$$J_Q = -\lambda \cdot \mathrm{grad}(T). \tag{4.7}$$

To ensure a formally skew-symmetric operator for port-Hamiltonian systems (3.24), we augment the system with $-\text{grad}$, obtaining the heat equation as a port-Hamiltonian system:

$$\begin{pmatrix} \rho \frac{\partial}{\partial t} \alpha_u \\ f_Q \end{pmatrix} = \begin{bmatrix} 0 & -\text{div} \\ -\text{grad} & 0 \end{bmatrix} \begin{pmatrix} e_u \\ J_Q \end{pmatrix}, \quad \begin{cases} e_u = \frac{\alpha_u}{C_v}, \\ J_Q = \lambda \cdot f_Q. \end{cases} \tag{4.8}$$

To eliminate the first algebraic constraint resulting from the constitutive relation $e_u = \frac{\alpha_u}{C_v}$, we rewrite $\rho C_v \frac{\partial}{\partial t} T$. Additionally, Fourier's law is incorporated as $\lambda^{-1} \cdot J_Q = f_Q$ inside the Dirac structure. The resulting port-Hamiltonian system is expressed as:

$$\begin{pmatrix} \rho C_v \frac{\partial}{\partial t} T \\ \lambda^{-1} \cdot J_Q \end{pmatrix} = \begin{bmatrix} 0 & -\text{div} \\ -\text{grad} & 0 \end{bmatrix} \begin{pmatrix} T \\ J_Q \end{pmatrix}, \quad \begin{cases} \overline{u_\partial} = T|_{\partial\Omega} \\ \overline{y_\partial} = J_Q \cdot \mathbf{n} \end{cases} \tag{4.9}$$

Note: In our case, the change was in the choice of the **input** $\overline{u_\partial}$ and the **output** $\overline{y_\partial}$. As it appears above in eq. (4.9), our choices were:

$$\begin{cases} \overline{u_\partial} = T|_{\partial\Omega} \\ \overline{y_\partial} = J_Q \cdot \mathbf{n} \end{cases}$$

We desired to control the temperature as the input, whereas [94] choses $\overline{u_\partial} = J_Q \cdot \mathbf{n}$ and $\overline{y_\partial} = T$.

4.4.1 Weak Formulation

A weak formulation is a way of reformulating differential equations such that the solution space is broadened to include more generalized functions, allowing the use of test functions to derive integral equations that are easier to handle numerically [80]. It is especially useful in finite element methods for solving partial differential equations.

To establish a weak formulation, we use test functions ϕ_T, ϕ_Q, and ψ for the temperature, flux, and boundary conditions, respectively:

- ϕ_T: A scalar-valued test function, ϕ_T is used in the context of scalar differential equations, particularly those involving temperature. It tests the equation related to T (temperature) in the problem. The basis of ϕ_T comprises scalar functions within the solution space for the temperature equation in the weak formulation.
- ϕ_Q: As a vector-valued test function, ϕ_Q is employed for vector differential equations, such as those involving flux, denoted by J_Q. The basis for ϕ_Q includes vector functions that approximate the solution space for the flux-related part of the equation.
- ψ: This boundary scalar-valued test function is utilized for testing boundary conditions. It is applied to the boundary terms of the weak formulation, usually involving boundary fluxes or related variables. The basis of ψ consists of scalar functions defined on the domain's boundary ($\partial\Omega$), aiding in approximating the boundary conditions of the problem.

The weak formulation is expressed as follows:

$$\begin{cases} \int_\Omega \phi_T \rho C_v \frac{\partial}{\partial t} T = -\int_\Omega \phi_T \mathrm{div}(J_Q), \\ \int_\Omega \phi_Q \cdot \lambda^{-1} \cdot J_Q = -\int_\Omega \phi_Q \cdot \mathrm{grad}(T), \\ \int_{\partial\Omega} \psi y_\partial = \int_{\partial\Omega} \psi (J_Q \cdot n). \end{cases} \tag{4.10}$$

This formulation represents the weak version of the original system of equations, incorporating test functions to establish a variational framework for the problem.

As our aim is to discretize the div operator, performing integration by parts on the **second line** reveals the appearance of $\overline{u_\partial} = T$, which will be chosen in our case to be the input:

$$\begin{cases} \int_\Omega \phi_T \rho C_v \frac{\partial}{\partial t} T = -\int_\Omega \phi_T \mathrm{div}(J_Q), \\ \int_\Omega \phi_Q \cdot \lambda^{-1} \cdot J_Q = \int_\Omega \mathrm{div}(\phi_Q) T - \int_{\partial\Omega} \phi_Q \underbrace{T}_{\overline{u_\partial}}, \\ \int_{\partial\Omega} \psi y_\partial = \int_{\partial\Omega} \psi (J_Q \cdot n). \end{cases} \tag{4.11}$$

With this choice, the temperature appears as the induced choice of input, emphasizing the presence of $\overline{u_\partial} = T$ in the resulting equation.

4.4.2 Projection

Projection involves approximating the variables onto finite element spaces. A finite element space is a discretized function space used to approximate the solution of differential equations by dividing the domain into smaller, simpler parts (elements) and constructing polynomial functions over these elements [4].

Denoting $\underline{\star}$ as the (time-varying) vector of coordinates of $\star^d$ in its respective finite element family, we use this notation in what follows. Let $(\phi_T^i)_{1\leq i\leq N_T}$, $(\phi_Q^j)_{1\leq j\leq N_Q}$, and $(\psi^k)_{1\leq k\leq N_\partial}$ represent the finite element families for temperature-type, flux-type, and boundary-type variables, respectively. The variables are approximated as follows:

$$T^d(t,x) := \sum_{i=1}^{N_T} T^i(t)\phi_T^i(x), \quad J_Q^d(t,x) := \sum_{j=1}^{N_Q} J_Q^j(t)\phi_Q^j(x),$$

$$u_\partial^d(t,x) := \sum_{k=1}^{N_\partial} u_\partial^k(t)\psi^k(x), \quad y_\partial^d(t,x) := \sum_{k=1}^{N_\partial} y_\partial^k(t)\psi^k(x).$$

Matrix Definitions: The matrices M_T, M_Q, and M_∂ represent mass matrices corresponding to temperature, heat flux, and boundary variables, respectively:

$$(M_T)_{ij} := \int_\Omega \phi_T^i \rho C_v \phi_T^j, \tag{4.12}$$

$$(M_Q)_{ij} := \int_\Omega \phi_Q^i \cdot \lambda^{-1} \cdot \phi_Q^j, \tag{4.13}$$

$$(M_\partial)_{ij} := \int_{\partial\Omega} \psi^i \psi^j. \tag{4.14}$$

where ρ is the density, C_v the specific heat at constant volume, and λ the thermal conductivity. The matrices D and $\bar{B}$ are:

$$(D)_{ij} := \int_\Omega \operatorname{div}(\phi_Q^i) \cdot \phi_T^j, \tag{4.15}$$

$$(\bar{B})_{jk} := \int_{\partial\Omega} \phi_Q^j \psi^k. \tag{4.16}$$

The matrix D represents the discretization of the divergence operator, mapping fluxes to their divergences in the finite element space. The matrix $\bar{B}$ represents the boundary interaction terms, mapping the boundary temperature (the input) to the flux in the finite element space.

Discrete System Equations: Utilizing these matrices, the discrete system can be clearly represented. Let $\underline{T}(t)$, $J_Q(t)$, and $\underline{u_\partial}(t)$ denote the time-varying vectors of coordinates for the temperature, heat flux, and boundary input in their respective finite element families. The discrete system is then expressed as:

$$\underbrace{\begin{bmatrix} M_T & 0 & 0 \\ 0 & M_Q & 0 \\ 0 & 0 & M_\partial \end{bmatrix}}_{M} \begin{pmatrix} \frac{d}{dt}\underline{T}(t) \\ J_Q(t) \\ -\underline{y_\partial}(t) \end{pmatrix} = \underbrace{\begin{bmatrix} 0 & -D & 0 \\ D^\top & 0 & -\bar{B} \\ 0 & \bar{B}^\top & 0 \end{bmatrix}}_{J} \begin{pmatrix} \underline{T}(t) \\ J_Q(t) \\ \underline{u_\partial}(t) \end{pmatrix} \tag{4.17}$$

Here, M is the combined mass matrix and J encapsulates the system's dynamics and boundary interactions.

4.4.3 Discrete Hamiltonian and its balance equation

The discretized system satisfies an energy balance equation, where the energy is an approximation of the distributed energy. The discrete Hamiltonian is derived from the continuous Hamiltonian but is evaluated using approximated variables. Consider the continuous Hamiltonian $\mathcal{H}$, defined as:

$$\mathcal{H} = \frac{1}{2} \int_\Omega \rho C_v (T)^2 \, dx, \tag{4.18}$$

where ρ denotes density, C_v is the specific heat at constant volume, and T represents the temperature.

In a discrete framework, the Hamiltonian, now represented as $\mathcal{H}^d$, employs the discretized temperature field T^d:

$$\mathcal{H}^d := \frac{1}{2} \int_\Omega \rho C_v (T^d)^2 \, dx. \tag{4.19}$$

Here, T^d symbolizes the discretized temperature profile, a combination of nodal temperature values and their corresponding basis functions.

Expanding on this, we can express $\mathcal{H}^d$ in terms of the mass matrix M_T and the discrete temperature vector $\underline{T}(t)$:

$$\mathcal{H}^d(t) = \frac{1}{2}\underline{T}(t)^\top M_T \underline{T}(t). \tag{4.20}$$

This form effectively encapsulates the total energy within the system at a given time t in its discretized state.

It has been proven that a discrete energy balance is satisfied [96]. Moreover, the discrete power balance is crucial for understanding the energy dynamics within the system. The change rate of $\mathcal{H}^d$ is described by the following equation:

$$\frac{d}{dt}\mathcal{H}^d(t) = -\underline{J_Q}(t)^\top M_Q \underline{J_Q}(t) + \underline{\overline{u_\partial}}(t)^\top M_\partial \underline{\overline{y_\partial}}(t). \tag{4.21}$$

Here, the first term on the right side signifies energy dissipation due to heat flux ($\underline{J_Q}(t)$), and the second term represents the energy exchange at the system boundaries, where $\underline{\overline{u_\partial}}(t)$ and $\underline{\overline{y_\partial}}(t)$ are the discretized boundary input and output variables, respectively.

4.5 Discretization of the Implicit Heat Equation with Entropy as Generating Function

This section details the discretization of the implicit system of the heat equation using entropy as the generating function and reciprocal temperature $\tau = \frac{1}{T}$ as the state variable. We follow a strategy similar to the one outlined in the SCRIMP document by [10], including the weak formulation, mass matrices, and projection.

4.5.1 Mathematical Formulation

The implicit system is given by:

$$\begin{pmatrix} \frac{\partial^2 s^*}{\partial \tau^2} & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \frac{\partial \tau}{\partial t} \\ \bar{F} \end{pmatrix} = \begin{pmatrix} 0 & -\mathrm{div} \\ -\mathrm{grad} & 0 \end{pmatrix} \begin{pmatrix} \frac{\partial s}{\partial \tau} \\ q \end{pmatrix}, \tag{4.22}$$

where τ is the reciprocal temperature, s is the entropy, q is the heat flux vector, and $\bar{F}$ is the driving force for the heat flux.

4.5.2 Weak Formulation

Introduce test functions ϕ_τ for τ and ϕ_q for q. The weak formulation involves integrating against these test functions.

For the first equation:

$$\int_\Omega \phi_\tau \frac{\partial^2 s^*}{\partial \tau^2} \frac{\partial \tau}{\partial t}\, dx = \int_\Omega \phi_\tau \left(-\mathrm{div}(q)\right) dx. \tag{4.23}$$

For the second equation:

$$\int_\Omega \phi_q \cdot \bar{F}\, dx = \int_\Omega \phi_q \cdot \left(-\text{grad}\left(\frac{\partial s}{\partial \tau}\right)\right) dx. \tag{4.24}$$

4.5.3 Integration by Parts

Apply integration by parts to handle the divergence and gradient terms. This introduces boundary terms.

For the first equation:

$$\int_\Omega \phi_\tau \frac{\partial^2 s^*}{\partial \tau^2}\frac{\partial \tau}{\partial t}\, dx = \int_\Omega -\text{div}(\phi_\tau q)\, dx + \int_\Omega (\text{grad}(\phi_\tau)\cdot q)\, dx. \tag{4.25}$$

By Gauss's theorem:

$$\int_\Omega \phi_\tau \frac{\partial^2 s^*}{\partial \tau^2}\frac{\partial \tau}{\partial t}\, dx = \int_{\partial\Omega} (\phi_\tau q \cdot n)\, ds - \int_\Omega (\text{grad}(\phi_\tau)\cdot q)\, dx. \tag{4.26}$$

For the second equation:

$$\int_\Omega \phi_q \cdot \bar{F}\, dx = \int_\Omega \phi_q \cdot \left(-\text{grad}\left(\frac{\partial s}{\partial \tau}\right)\right) dx. \tag{4.27}$$

Integration by Parts:

As we aim to discretize the div operator, we the apply integration by parts to the second equation (4.27):

$$\int_\Omega \phi_q \cdot \bar{F}\, dx = -\int_\Omega \text{div}(\phi_q)\tau\, dx + \int_{\partial\Omega} \phi_q\, \tau\, ds. \tag{4.28}$$

4.5.4 Finite Element Discretization

We choose finite element spaces for approximating the reciprocal temperature τ, the heat flux q, and the boundary values. Let $(\phi_\tau^i)_{1\le i\le N_\tau}$, $(\phi_q^j)_{1\le j\le N_q}$, and $(\psi^k)_{1\le k\le N_\partial}$ be basis functions for these spaces.

Approximate τ, q, and u_∂ as:

$$\tau^d(t,x) = \sum_{i=1}^{N_\tau} \tau^i(t)\phi_\tau^i(x), \quad q^d(t,x) = \sum_{j=1}^{N_q} q^j(t)\phi_q^j(x), \quad u_\partial^d(t,x) = \sum_{k=1}^{N_\partial} u_\partial^k(t)\psi^k(x). \tag{4.29}$$

4.5.5 Mass and Stiffness Matrices

Define the mass matrices M_τ, M_q, and M_∂, as well as the stiffness matrices K_τ and $\bar{B}$:

$$(M_\tau)_{ij} = \int_\Omega \phi_\tau^i \frac{\partial^2 s^*}{\partial \tau^2}\phi_\tau^j\, dx, \quad (M_q)_{ij} = \int_\Omega \phi_q^i \cdot \phi_q^j\, dx, \quad (M_\partial)_{kl} = \int_{\partial\Omega} \psi^k\psi^l\, ds, \tag{4.30}$$

$$(K_\tau)_{ij} = \int_\Omega \text{div}(\phi_q^i)\phi_\tau^j\, dx, \quad (\bar{B})_{jk} = \int_{\partial\Omega} \phi_q^j\psi^k\, ds. \tag{4.31}$$

4.5.6 Assembly of the Discrete System

Using the defined mass and stiffness matrices, assemble the discrete system of equations:

$$M_\tau \frac{d}{dt}\underline{\tau} + K_\tau \underline{q} = 0, \tag{4.32}$$

$$M_q \underline{F} + \bar{B}\underline{u}_\partial = 0, \tag{4.33}$$

where $\underline{\tau}$, $\underline{q}$, and $\underline{u}_\partial$ are the coefficient vectors for τ^d, q^d, and u_∂^d, respectively.

Discrete Port-Hamiltonian System Representation

We now proceed to represent the discrete port-Hamiltonian formulation for the heat diffusion problem based on the mass and stiffness matrices introduced earlier. The resulting system can be expressed using a discrete port-Hamiltonian approach, highlighting the structure-preserving properties of the model.

The discrete system representation is given by:

$$\underbrace{\begin{bmatrix} M_\tau(\tau) & 0 & 0 \\ 0 & M_q & 0 \\ 0 & 0 & M_\partial \end{bmatrix}}_{M} \begin{pmatrix} \frac{d}{dt}\underline{\tau} \\ \underline{F} \\ \underline{y}_\partial \end{pmatrix} = \underbrace{\begin{bmatrix} 0 & -K_\tau & 0 \\ K_\tau^T & 0 & -\bar{B} \\ 0 & \bar{B}^T & 0 \end{bmatrix}}_{J} \begin{pmatrix} \underline{\tau} \\ \underline{q} \\ \underline{u}_\partial \end{pmatrix} \tag{4.34}$$

Where:

- M is the global mass matrix that combines all mass matrices defined for the system:
  - $M_\tau(\tau)$: Mass matrix for reciprocal temperature, depending on the state variable τ.
  - M_q: Mass matrix for the flux variable.
  - M_∂: Mass matrix for the boundary input/output values.
- J is the structure matrix that encapsulates the energy exchange and coupling between internal and boundary states:
  - K_τ: Stiffness matrix representing the discretization of the divergence operator.
  - $\bar{B}$: Stiffness matrix representing the coupling between boundary and internal states.
- $\underline{\tau}$, $\underline{F}$, $\underline{y}_\partial$, $\underline{q}$, and $\underline{u}_\partial$ are coefficient vectors:
  - $\underline{\tau}$: Coefficient vector for reciprocal temperature.
  - $\underline{F}$: Coefficient vector for the driving force.
  - $\underline{y}_\partial$: Coefficient vector for boundary output values, such as the flux at the boundary.
  - $\underline{q}$: Coefficient vector for the heat flux in the domain.
  - $\underline{u}_\partial$: Coefficient vector for boundary input values.

Notes on the Mass and Stiffness Matrices

The mass matrices M_τ, M_q, and M_∂ are associated with the finite element discretization of the state variables, flux, and boundary values. Specifically, M_τ depends on the second derivative of the entropy function s^* with respect to τ, making it a state-dependent matrix. The stiffness matrices K_τ and $\bar{B}$ are related to the gradient and divergence operators, capturing the coupling between the temperature field and flux.

In particular, the mass matrix $(M_\tau)_{ij}$ includes the entropy term $\frac{\partial^2 s^*}{\partial \tau^2}$, which differentiates it from the classical linear case, thereby accounting for the nonlinear nature of the thermodynamic relations in this model.

4.6 Discretization of the Allen-Cahn Equation

This section focuses on the discretization of the port Hamiltonian formulation of the Allen-Cahn equation presented earlier (see section 3.11).

Adapting Discretization from the Heat Equation to the Allen-Cahn Equation

This section focuses on adapting the discretization approach from the heat equation to the Allen-Cahn equation, which models physical phenomena during the solidification process.

While both equations model diffusion processes, they differ in their treatment of nonlinear terms, which are important for simulating phase transitions in the Allen-Cahn equation. The heat equation deals with linear diffusion, whereas the Allen-Cahn equation incorporates nonlinear dynamics necessary for describing phase boundaries.

We adapted the discretization approach based on the mathematical properties of the Allen-Cahn equation. This phase-field model includes nonlinear dynamics necessary for describing phase boundaries.

A key difference between the heat equation and the Allen-Cahn equation lies in the operators involved in their formulations. The heat equation is governed by the following system (3.127):

$$\begin{pmatrix} \frac{\partial u}{\partial t} \\ F \end{pmatrix} = \begin{pmatrix} 0 & -\mathrm{div} \\ -\mathrm{grad} & 0 \end{pmatrix} \begin{pmatrix} \frac{\partial s}{\partial u} \\ q \end{pmatrix}, \tag{4.35}$$

where u signifies the internal energy, and q represents the heat flux vector.

In contrast, the Allen-Cahn equation involves the following system (3.128):

$$\begin{pmatrix} \frac{\partial \phi}{\partial t} \\ \frac{\partial \psi}{\partial t} \\ F_{\phi\psi} \end{pmatrix} = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & -\mathrm{grad} \\ 1 & -\mathrm{div} & 0 \end{pmatrix} \begin{pmatrix} \frac{\delta(-\bar{S})}{\delta \phi} \\ \frac{\delta(-\bar{S})}{\delta \psi} \\ E_{\phi\psi} \end{pmatrix}, \tag{4.36}$$

where ψ represents the gradient of the phase field variable ϕ, the state space variables, $F_{\phi\psi}$ represents the driving force, and $E_{\phi\psi}$ represents the phase field flux.

In the Allen-Cahn equation, the grad operator appears in the dynamic equation, corresponding to the gradient dynamics that define the Allen-Cahn formulation. This difference in the

operators highlights the unique characteristics of the Allen-Cahn equation and the necessity for adapting the discretization strategy accordingly.

4.7 The Phase Field Model

We now describe the dynamic behavior of the system through a comprehensive set of equations that encapsulate the intricate interactions within a bi-phasic system. This system involves phase field variables and entropy considerations, leading to a detailed mathematical representation.

4.7.1 Dynamic System Representation

Recall that the dynamics of our bi-phasic system is described by the following port-Hamiltonian system:

$$\begin{pmatrix} \frac{\partial \phi}{\partial t} \\ \frac{\partial \psi}{\partial t} \\ F_{\phi\psi} \end{pmatrix} = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & -\text{grad} \\ 1 & -\text{div} & 0 \end{pmatrix} \begin{pmatrix} -\frac{\partial s^*}{\partial \phi}(\phi, \tau) \\ \epsilon^2 \psi \\ E_{\phi\psi} \end{pmatrix}. \tag{4.37}$$

Here, ϕ and ψ represent the phase field variable and its gradient, while $F_{\phi\psi}$ denotes the driving force and $E_{\phi\psi}$ the phase field flux.

4.7.2 Weak Formulation [5]

The weak formulation, a cornerstone in the numerical analysis of partial differential equations, is obtained by introducing test functions for each variable. Let v_ψ, v_F, v_ϕ, and v_b be the test functions for ψ, $F_{\phi\psi}$, ϕ, and the boundary, respectively. It's necessary to note that $v_F = v_\phi$ for consistency in the formulation. The weak formulation is then articulated as:

$$\begin{cases} \int_\Omega v_F^\top \frac{\partial \phi}{\partial t} dz = -\int_\Omega v_F^\top (E_{\phi\psi}) dz, \\ \int_\Omega v_\psi^\top \frac{\partial \psi}{\partial t} dz = -\int_\Omega v_\psi^\top \text{grad}(E_{\phi\psi}) dz, \\ \int_\Omega v_F^\top F_{\phi\psi} dz = \int_\Omega v_F^\top \left(-\frac{\partial s^*}{\partial \phi}(\phi, \tau) \right) dz - \int_\Omega v_F^\top \text{div}(\epsilon^2 \psi), \\ \int_{\partial\Omega} v_b y_\partial = \int_{\partial\Omega} v_b (\epsilon^2 \psi \cdot n). \end{cases} \tag{4.38}$$

An integration by parts on the **second line** of this weak formulation reveals the boundary term $u_\partial(t) = E_{\phi\psi}$, simplifying the expression:

$$\begin{cases} \int_\Omega v_F^\top \frac{\partial \phi}{\partial t} dz = -\int_\Omega v_F^\top (E_{\phi\psi}) dz, \\ \int_\Omega v_\psi^\top \frac{\partial \psi}{\partial t} dz = \int_\Omega \text{div}\, v_\psi^\top E_{\phi\psi} dz - \left[v_\psi^\top E_{\phi\psi} \right]_{\partial\Omega}, \\ \int_\Omega v_F^\top F_{\phi\psi} dz = \int_\Omega v_F^\top \left(-\frac{\partial s^*}{\partial \phi}(\phi, \tau) \right) dz - \int_\Omega v_F^\top \text{div}(\epsilon^2 \psi), \\ \int_{\partial\Omega} v_b y_\partial = \int_{\partial\Omega} v_b (\epsilon^2 \psi \cdot n). \end{cases} \tag{4.39}$$

4.7.3 Projection

Projection onto finite element spaces involves approximating the variables in their respective finite element families. The discrete representations of the variables are thus formulated as:

$$\begin{aligned}
\phi(t,z) &:= \sum \bar{\phi}(t) v_F(z), \\
\psi(t,z) &:= \sum \bar{\psi}(t) v_\psi(z), \\
F_{\phi\psi}(t,z) &:= \sum \bar{F}_{\phi\psi}(t) v_F(z), \\
E_{\phi\psi}(t,z) &:= \sum \bar{E}_{\phi\psi}(t) v_F(z), \\
u_\partial(t,z) &:= \sum \bar{u}_\partial(t) v_b(z), \\
y_\partial(t,z) &:= \sum \bar{y}_\partial(t) v_b(z), \\
e_\phi(t,z) &:= \sum \bar{e}_\phi(t) v_F(z).
\end{aligned}$$

The discrete system is then expressed as:

$$\underbrace{\begin{bmatrix} M_\phi & 0 & 0 & 0 \\ 0 & M_\psi & 0 & 0 \\ 0 & 0 & M_\phi & 0 \\ 0 & 0 & 0 & M_\partial \end{bmatrix}}_{M} \begin{pmatrix} \frac{d\bar{\phi}}{dt}(t) \\ \frac{d\bar{\psi}}{dt}(t) \\ \bar{F}_{\phi\psi}(t) \\ \bar{y}_\partial(t) \end{pmatrix} = \underbrace{\begin{bmatrix} 0 & 0 & -M_\phi & 0 \\ 0 & 0 & D & -B \\ M_\phi & -D^\top & 0 & 0 \\ 0 & B^\top & 0 & 0 \end{bmatrix}}_{J} \begin{pmatrix} \bar{e}_\phi(t) \\ \epsilon^2 \bar{\psi}(t) \\ \bar{E}_{\phi\psi}(t) \\ \bar{u}_\partial(t) \end{pmatrix} \tag{4.40}$$

where

M_ϕ: This matrix represents the mass matrix for the phase field variable ϕ. It is defined as:

$$(M_\phi)_{ij} := \int_\Omega v_F^i v_F^j \, dz \tag{4.41}$$

where v_F^i and v_F^j are the basis functions for ϕ.

M_ψ: This matrix represents the mass matrix for the auxiliary variable ψ. It is defined as:

$$(M_\psi)_{ij} := \int_\Omega v_\psi^i v_\psi^j \, dz \tag{4.42}$$

where v_ψ^i and v_ψ^j are the basis functions for ψ.

M_∂: This matrix represents the mass matrix for the boundary variable u_∂. It is defined as:

$$(M_\partial)_{ij} := \int_{\partial\Omega} v_b^i v_b^j \, dz \tag{4.43}$$

where v_b^i and v_b^j are the basis functions for the boundary variables.

D: This matrix represents the discretization of the divergence operator applied to ψ. It is defined as:

$$(D)_{ij} := \int_\Omega \operatorname{div} v_\psi^i v_F^j \, dz \tag{4.44}$$

where v_ψ^i is the basis function for ψ and v_F^j is the basis function for ϕ.

$-D^\top$: This matrix represents the transpose of the discretization of the divergence operator applied to ϕ. It is defined as:

$$(-D^\top)_{ij} := -\int_\Omega v_F^i \operatorname{div} v_\psi^j \, dz \tag{4.45}$$

where v_F^i is the basis function for ϕ and v_ψ^j is the basis function for ψ.

B: This matrix represents the boundary interaction terms. It is defined as:

$$(B)_{ij} := \int_{\partial\Omega} v_\psi^i v_F^j \, dz \tag{4.46}$$

where v_ψ^i is the basis function for ψ and v_F^j is the basis function for ϕ.

The discrete co-energy variable $\bar{e}_\phi$ is given by:

$$\bar{e}_\phi = M_\phi^{-1} \int_\Omega v_F^\top \left(-\frac{\partial s^*}{\partial \phi} \right) (\phi, \tau) dz. \tag{4.47}$$

with

$$\frac{\partial s^*}{\partial \phi}(\phi, T) = p_i'(\phi)[s_{liq}^*(T) - s_{sol}^*(T)] + w p_w'(\phi) \tag{4.48}$$

where $T = \frac{1}{\tau}$ and

- $p_i'(\phi) = 30\phi^4 - 60\phi^3 + 30\phi^2$
- $p_w'(\phi) = -4\phi^3 + 6\phi^2 + 2\phi$

according to the constitutive relations presented in section (2.9).

4.8 Discretization of the Solidification Process

This section details the discretization of the solidification process, combining the Allen-Cahn equation with the implicit heat equation model. We will utilize the Partitioned Finite Element Method (PFEM) within the Port Hamiltonian framework to ensure structure-preserving properties.

Recall that the combined system can be expressed as follows (3.151):

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ \frac{\partial^2 s^*}{\partial\phi\partial\tau} & 0 & 0 & \frac{\partial^2 s^*}{\partial\tau^2} & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \frac{\partial\phi}{\partial t} \\ \frac{\partial\psi}{\partial t} \\ F_{\phi\psi} \\ \frac{\partial\tau}{\partial t} \\ \bar{F} \end{pmatrix} = \mathcal{J}_S \begin{pmatrix} -\frac{\partial s^*}{\partial\phi}(\phi,\tau) \\ \epsilon^2\psi \\ E_{\phi\psi} \\ -\tau \\ q \end{pmatrix}, \tag{4.49}$$

where

$$\mathcal{J}_S = \begin{pmatrix} 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & -\text{grad} & 0 & 0 \\ 1 & -\text{div} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\text{div} \\ 0 & 0 & 0 & -\text{grad} & 0 \end{pmatrix} \tag{4.50}$$

is the combined skew-symmetric operator matrix representing the coupled system dynamics.

4.8.1 Weak Formulation

To obtain the weak formulation of the coupled system, we introduce appropriate test functions for each variable. Let v_ϕ, v_ψ, $v_{F_{\phi\psi}}$, v_τ, and $v_{\bar{F}}$ be the test functions for ϕ, ψ, $F_{\phi\psi}$, τ, and $\bar{F}$, respectively. The weak formulation is then given by:

$$\begin{cases} \int_\Omega v_\phi^\top \frac{\partial\phi}{\partial t}\, dz = -\int_\Omega v_\phi^\top E_{\phi\psi}\, dz, \\ \int_\Omega v_\psi^\top \frac{\partial\psi}{\partial t}\, dz = -\int_\Omega v_\psi^\top \text{grad}(E_{\phi\psi})\, dz, \\ \int_\Omega v_{F_{\phi\psi}}^\top F_{\phi\psi}\, dz = \int_\Omega v_{F_{\phi\psi}}^\top \left(-\frac{\partial s^*}{\partial\phi}(\phi,\tau)\right) dz - \int_\Omega v_{F_{\phi\psi}}^\top \text{div}(\epsilon^2\psi)\, dz, \\ \int_\Omega v_\tau^\top \left(\frac{\partial^2 s^*}{\partial\phi\partial\tau}\frac{\partial\phi}{\partial t} + \frac{\partial^2 s^*}{\partial\tau^2}\frac{\partial\tau}{\partial t}\right) dz = -\int_\Omega v_\tau^\top \text{div}(q)\, dz, \\ \int_\Omega v_{\bar{F}}^\top \bar{F}\, dz = \int_\Omega v_{\bar{F}}^\top \left(-\text{grad}(\tau)\right)\, dz. \end{cases} \tag{4.51}$$

By integrating by parts and applying the boundary conditions, the weak formulation is modified to:

$$\begin{cases} \int_\Omega v_\phi^\top \frac{\partial\phi}{\partial t}\, dz = -\int_\Omega v_\phi^\top E_{\phi\psi}\, dz, \\ \int_\Omega v_\psi^\top \frac{\partial\psi}{\partial t}\, dz = \int_\Omega \text{div}\left(v_\psi^\top E_{\phi\psi}\right)\, dz - \int_{\partial\Omega} v_\psi^\top E_{\phi\psi}\, d\sigma, \\ \int_\Omega v_{F_{\phi\psi}}^\top F_{\phi\psi}\, dz = \int_\Omega v_{F_{\phi\psi}}^\top \left(-\frac{\partial s^*}{\partial\phi}(\phi,\tau) - \text{div}(\epsilon^2\psi)\right) dz, \\ \int_\Omega v_\tau^\top \left(\frac{\partial^2 s^*}{\partial\phi\partial\tau}\frac{\partial\phi}{\partial t} + \frac{\partial^2 s^*}{\partial\tau^2}\frac{\partial\tau}{\partial t}\right) dz = \int_\Omega \text{div}\left(v_\tau^\top q\right)\, dz - \int_{\partial\Omega} v_\tau^\top q\, d\sigma, \\ \int_\Omega v_{\bar{F}}^\top \bar{F}\, dz = \int_\Omega v_{\bar{F}}^\top \left(-\text{grad}(\tau)\right)\, dz. \end{cases} \tag{4.52}$$

4.8.2 Finite Element Discretization

We choose finite element spaces to approximate ϕ, ψ, $F_{\phi\psi}$, τ, and $\bar{F}$. Let $(\phi_\phi^i)_{1\le i\le N_\phi}$, $(\phi_\psi^j)_{1\le j\le N_\psi}$, $(\phi_{F_{\phi\psi}}^k)_{1\le k\le N_{F_{\phi\psi}}}$, $(\phi_\tau^l)_{1\le l\le N_\tau}$, and $(\phi_{\bar{F}}^m)_{1\le m\le N_{\bar{F}}}$ represent the finite element basis functions for each variable, respectively. The approximations are given by:

$$\phi^d(t,x) := \sum_{i=1}^{N_\phi} \phi^i(t)\phi_\phi^i(x), \quad \psi^d(t,x) := \sum_{j=1}^{N_\psi} \psi^j(t)\phi_\psi^j(x),$$

$$F_{\phi\psi}^d(t,x) := \sum_{k=1}^{N_{F_{\phi\psi}}} F_{\phi\psi}^k(t)\phi_{F_{\phi\psi}}^k(x), \quad \tau^d(t,x) := \sum_{l=1}^{N_\tau} \tau^l(t)\phi_\tau^l(x),$$

$$\bar{F}^d(t,x) := \sum_{m=1}^{N_{\bar{F}}} \bar{F}^m(t)\phi_{\bar{F}}^m(x).$$

4.8.3 Forming Mass Matrices

Define the mass and stiffness matrices for each variable as follows:

$$(M_\phi)_{ij} := \int_\Omega \phi_\phi^i \phi_\phi^j \, dz, \tag{4.53}$$

$$(M_\psi)_{ij} := \int_\Omega \phi_\psi^i \phi_\psi^j \, dz, \tag{4.54}$$

$$(M_{F_{\phi\psi}})_{ij} := \int_\Omega \phi_{F_{\phi\psi}}^i \phi_{F_{\phi\psi}}^j \, dz, \tag{4.55}$$

$$(M_{\bar{F}})_{ij} := \int_\Omega \phi_{\bar{F}}^i \phi_{\bar{F}}^j \, dz. \tag{4.56}$$

Additionally, define the matrices involving the partial derivatives of s^* as follows:

$$(M_\tau)_{ij} := \int_\Omega \frac{\partial^2 s^*}{\partial \tau^2} \phi_\tau^i \phi_\tau^j \, dz, \tag{4.57}$$

$$(M_{\phi\tau})_{ij} := \int_\Omega \frac{\partial^2 s^*}{\partial \phi \partial \tau} \phi_\phi^i \phi_\tau^j \, dz. \tag{4.58}$$

The stiffness matrices for the divergence and gradient operators are defined as:

$$(D_\phi)_{ij} := \int_\Omega \operatorname{div}(\phi_\phi^i) \cdot \phi_{F_{\phi\psi}}^j \, dz, \tag{4.59}$$

$$(D_\tau)_{ij} := \int_\Omega \operatorname{div}(\phi_\tau^i) \cdot \phi_{\bar{F}}^j \, dz, \tag{4.60}$$

$$(G_\psi)_{ij} := \int_\Omega \operatorname{grad}(\phi_\psi^i) \cdot \phi_{F_{\phi\psi}}^j \, dz, \tag{4.61}$$

$$(G_{\bar{F}})_{ij} := \int_\Omega \operatorname{grad}(\phi_{\bar{F}}^i) \cdot \phi_\tau^j \, dz. \tag{4.62}$$

It is important to note that matrices D_ϕ and G_ψ are related by an antisymmetric property, as follows:

$$(D_\phi)_{ij} = -(G_\psi)_{ji}$$

This antisymmetry ensures that energy flow between these components is balanced, in line with the structure-preserving nature of port Hamiltonian systems (inspired by [5]). This property is crucial for maintaining the conservation properties intrinsic to Hamiltonian dynamics, ensuring that there is no net creation or destruction of energy within these components.

Additionally, to ensure a proper discrete negentropy balance for matrix $\tilde{M}$, the contributions involving M_τ and $M_{\phi\tau}$ are derived in alignment with the proof provided in [5], ensuring that the discretized dynamics respects the laws of thermodynamics, particularly the entropy balance equation.

4.8.4 Assembling the Discrete System

Using the finite element approximations and the defined mass and stiffness matrices, the discrete system can be represented as:

$$\underbrace{\begin{bmatrix} M_\phi & 0 & 0 & 0 & 0 \\ 0 & M_\psi & 0 & 0 & 0 \\ 0 & 0 & M_{F_{\phi\psi}} & 0 & 0 \\ M_{\phi\tau} & 0 & 0 & M_\tau & 0 \\ 0 & 0 & 0 & 0 & M_{\bar{F}} \end{bmatrix}}_{\tilde{M}} \begin{pmatrix} \frac{d\bar{\phi}}{dt}(t) \\ \frac{d\bar{\psi}}{dt}(t) \\ \bar{F}_{\phi\psi}(t) \\ \frac{d\bar{\tau}}{dt}(t) \\ \bar{F}(t) \end{pmatrix} = \underbrace{\begin{bmatrix} 0 & 0 & -M_\phi & 0 & 0 \\ 0 & 0 & G_\psi & 0 & -B_\psi \\ M_\phi & -D_\phi^\top & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -D_\tau \\ 0 & B_\psi^\top & 0 & D_\tau^\top & 0 \end{bmatrix}}_{\mathcal{J}_S} \begin{pmatrix} \bar{e}_\phi(t) \\ \epsilon^2\bar{\psi}(t) \\ \bar{E}_{\phi\psi}(t) \\ -\bar{\tau}(t) \\ \bar{q}(t) \end{pmatrix}, \tag{4.63}$$

where $\tilde{M}$ is the combined mass matrix, and $\mathcal{J}_S$ includes the system dynamics and boundary interactions.

It is important to note that among the mass matrices, M_ϕ, M_ψ, $M_{F_{\phi\psi}}$, and $M_{\bar{F}}$ depend only on the finite-element bases and are thus constant for a given discretization. On the other hand, M_τ and $M_{\phi\tau}$ are state-dependent, as they involve the partial derivatives of the entropy function s^*.

Additionally, the entropy function s^* is often given as a finite series expansion, making the resulting expressions for the mass matrices M_τ and $M_{\phi\tau}$ polynomial in nature.

Negentropy Balance: In line with the proof provided in [5], one may derive the discrete negentropy balance equation for the discretized system, ensuring that the discretized dynamics respects the laws of thermodynamics, here the entropy balance equation.

4.8.5 Preliminary 1D Numerical Simulations

To corroborate the claim that the geometric structure of the solidification process can be reduced spatially, we performed a series of preliminary 1D numerical simulations using the SCRIMP environment. The SCRIMP environment provides a numerical framework for simulating port-Hamiltonian systems, allowing for the integration of both thermal and phase field dynamics. This section discusses the results obtained from these simulations, focusing on the melting and solidification processes.

Melting Process

The melting process was simulated using simplified thermodynamic laws, omitting nonlinear interactions to focus on the basic dynamics of interface movement. The initial condition was set as a fully solid phase ($\phi = 0$) throughout the domain, and heat was applied to initiate the transition to the liquid phase. The evolution of the phase field variable ϕ is depicted in Figure 1.

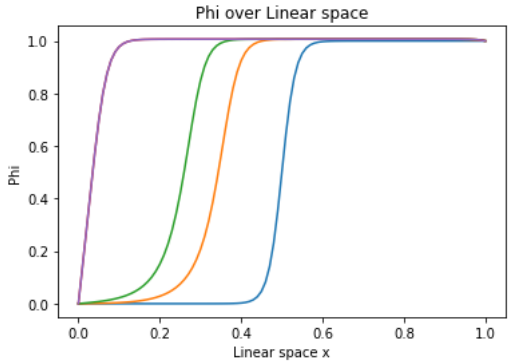

Figure 1: Melting process: The interface evolution is shown from the initial state ($t = 0$) to $t = 5.5$, demonstrating the transition from solid to liquid.

The simulation results show a clear movement of the interface as the solid phase transitions into the liquid phase. Due to the simplified thermodynamics, the interface evolves smoothly, demonstrating the efficacy of this approach in capturing basic melting dynamics. The results illustrate how the 1D domain can effectively represent the progression of the phase field, thereby supporting the claim of spatial reduction of the geometric structure.

Solidification Process

In contrast to the melting process, the solidification process presented additional challenges. Specifically, the lack of appropriate dimensionless parameters and thermodynamic properties led to a broader interface during the solidification process, as depicted in Figure 2.

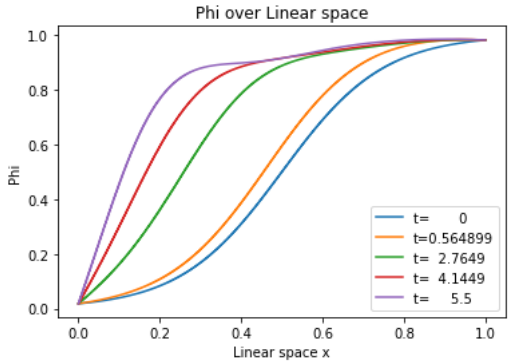

Figure 2: Solidification process: Interface evolution from the liquid phase to the solid phase. The broadening of the interface is evident, highlighting the need for more precise thermodynamic properties.

The challenge encountered during the solidification process was due to the use of linear thermodynamic properties, which resulted in a large interface thickness and an incomplete transition from the liquid to the solid phase. This underscores the need for incorporating more accurate thermodynamic models that can capture the nuances of phase transitions, such as anisotropic effects and non-isothermal conditions.

Connection to Geometric Structure Reduction

The presented simulations serve as preliminary evidence of the potential to reduce the geometric structure spatially while still capturing the essential dynamics of the solidification process. The 1D representation allows for a simplified yet informative study of phase field evolution and heat transfer, showcasing the capabilities of the port-Hamiltonian framework in modeling complex thermodynamic systems.

The simulation results presented here, while simplified, indicate that the overall dynamics can be effectively represented in a lower-dimensional space, thus validating our theoretical claims. In future work, a more refined parameter space exploration, including non-linear thermodynamic properties, is planned to further validate these findings and enhance the accuracy of the model.

Future Work

To improve the fidelity of the simulation results, the following improvements are suggested:

- Implement the full nonlinear thermodynamic laws to better predict phase behavior.
- Adjust dimensionless variables and physical parameters to align with established standards in the phase field modeling community.
- Perform detailed parameter space exploration to identify optimal settings for interface thickness and overall model accuracy.

4.9 Conclusion

In this chapter, we presented the discretization of the solidification process using the Partitioned Finite Element Method (PFEM) within the Port Hamiltonian framework. Our focus was on achieving a structure-preserving discretization that retains the physical and geometric properties of the original continuous system.

We began by discretizing the implicit formulation of the heat equation, where the reciprocal temperature $\tau = \frac{1}{T}$ was employed as the state variable. This involved deriving a weak formulation that accounted for entropy as the generating function, followed by the discretization of both the heat flux and the driving force for the flux. The discretized system naturally introduced state-dependent mass matrices M_τ and $M_{\phi\tau}$ due to the presence of partial derivatives of the entropy function s^*.

Next, we addressed the discretization of the Allen-Cahn equation, which models the evolution of the phase field during solidification. We adapted the PFEM to account for the nonlinearities specific to the Allen-Cahn equation. This required the careful handling of gradient and divergence operators within the weak formulation, ensuring that the discrete operators captured the dynamics of phase transitions accurately.

The combined discretized system, representing the solidification process, involved several key operators and matrices:

- **Discretized Operators:** The divergence operator div was discretized to handle the spatial derivatives in the system, leading to the matrices D and G, respectively.
- **Boundary Inputs:** The discretization included the boundary interaction terms, represented by the matrices B and $\bar{B}$, which map the boundary temperatures and fluxes into the system.
- **Mass Matrices:** The mass matrices M_ϕ, M_ψ, $M_{F_{\phi\psi}}$, and $M_{\bar{F}}$ were derived based on the finite element basis functions and were constant for a given discretization. In contrast, the mass matrices M_τ and $M_{\phi\tau}$ were state-dependent, reflecting the thermodynamic relations through the entropy function.

Our approach involved deriving weak formulations, projecting variables onto finite element spaces, and defining and computing mass matrices. These steps ensured a structure-preserving discretization that retains the physical and geometric properties of the original continuous system. The resulting discretized models have state-dependent mass matrices. Overall, the chapter demonstrated how the PFEM can be effectively utilized to discretize complex, nonlinear phenomena in a structure-preserving manner.

Chapter 5

Conclusion

This thesis has discussed and presented the modeling, formulation, and discretization of solidification processes using the Port Hamiltonian (PH) framework combined with the phase field approach. By focusing on distributed parameter models with moving interfaces, we have addressed challenges in representing and controlling phase change phenomena. Throughout this work, we aimed to develop a comprehensive approach to understanding and managing the dynamics of solidification processes, particularly for pure water.

In Chapter 2, we presented a detailed modeling approach for solidification processes using the entropy functional within the phase field framework [112, 116]. This chapter began with an introduction to multiphase systems and their thermodynamic properties, highlighting the importance of interfaces and the role of entropy in phase transitions. By employing both sharp interface and phase field models, we provided a thorough examination of the dynamics and thermodynamics involved in solidification. Key contributions included a comprehensive presentation of solidification using the entropy functional approach and an analysis of the dynamics between different phases, focusing on the role of entropy in modeling diffuse interfaces.

In Chapter 3, we extended the PH framework to the solidification process, integrating the diffuse interface method with phase field variables. This involved developing a Boundary Port Hamiltonian formulation that combines the heat diffusion equation and the Allen-Cahn equation. The main contribution of this chapter we reformulated the explicit Port Hamiltonian model into an implicit Port Hamiltonian formulation using Lagrangian submanifolds. This approach, detailed in works such as [105] and [88], allows for the definition of reciprocal constitutive equations in a coordinate-free manner and can be adapted to distributed parameter systems [60, 106]. This change enables us to utilize available data and thermodynamic properties of liquid water and ice, as found in the literature [42, 43]. The provided thermodynamic potential is the Gibbs energy, expressed as a function of temperature and pressure. By defining the thermodynamic properties of the bi-phasic water-ice system, we derived the expressions of the entropy density based on temperature rather than internal energy. This required changing the state space coordinate from internal energy u (an extensive) to the temperature T (an intensive variable).

Chapter 4 focused on the structure-preserving discretization of the PH model of the solid-

ification process. Using the Partitioned Finite Element Method (PFEM), we ensured that the discretized model retained the PH structure, preserving key properties such as energy conservation and passivity. This chapter detailed several structure-preserving discretization techniques, emphasizing the importance of maintaining the physical and geometric properties of the original continuous system. The main contributions included the application of PFEM to the PH model using nonlinear constitutive relations with entropy as the generating function [38], and the introduction and discretization of an implicit formulation of the heat equation using the reciprocal temperature $\tau = \frac{1}{T}$ as the state variable. Additionally, we discretized the Allen-Cahn equation, leading to the complete discretization of the implicit model of the solidification process, where the resulting discretized models have state-dependent mass matrices.

This thesis has laid a strong foundation for future research and development in the area of distributed parameter systems with moving interfaces. Several directions for future work are promising:

Performing numerical simulations of the solidification process. Preliminary work on the simulations, using the nonlinear constitutive relations, led to partial results which have shown a quite difficult nonlinear problem. Exploring its control using optimal control methods following, for example, [40]. These initial studies have shown that the nonlinear thermodynamic properties lead to a highly challenging optimal control problem which remains an interesting open problem. This model could provide a submodel for the water purification process as presented in the WATERSAFE project and eventually help in its control.

The findings of this thesis have several implications for both theoretical research and practical applications. By utilizing the PH framework, we have provided a systematic way to incorporate physical principles into the modeling, simulation, and control of solidification processes. Future research could extend this work in several directions, including the enhancement of thermodynamic models to include more complex interactions and additional phases, the development of advanced control strategies using the PH framework, and the application of these methodologies to other phase transition processes and multiphase systems.

Future research can build on these findings to further improve solidification processes. Potential directions include extending the models to higher dimensions and more complex shapes to better represent real-world solidification, applying the models to other types of phase transitions and multiphase systems, using numerical methods to make the simulations more efficient and accurate, conducting more experiments to validate and refine the models, and developing control strategies based on the Port Hamiltonian framework to manage solidification processes in industrial applications.

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Appendix A

Publications Presented in This Thesis

The contributions presented in this thesis appear in the following publication:

A.1 Peer-Reviewed International Conference

- **Yaghi**, **Mohammed**, Françoise Couenne, Aurélie Galfré, Laurent Lefèvre, and Bernhard Maschke. "Port Hamiltonian formulation of the solidification process for a pure substance: A phase field approach." IFAC-PapersOnLine 55, no. 18 (2022): 93-98.

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Port Hamiltonian formulation of the solidification process for a pure substance: A phase field approach ⋆

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Abstract: In this paper we suggest a Port Hamiltonian model of the solidification process of water, using the phase field approach. Firstly, the Port Hamiltonian formulation of the dynamics of the phase field variable, governed by the Allen-Cahn equation, is recalled. It is based on adding to the phase field variable, its gradient, and extending the system with its dynamics. Secondly, the model is completed by the energy balance equation for the heat conduction and the complete Port Hamiltonian model is derived. Thirdly an Algebro-differential Port Hamiltonian representation is suggested, where the Port Hamiltonian system is defined on a Lagrangian submanifold, allowing to use directly the variables defining the thermodynamical data.

Keywords: Port Hamiltonian systems on Lagrange subspaces, Phase Field, Diffuse interface, Solidification process, Thermodynamical properties

1. INTRODUCTION

The deterioration of the environment through the discharge of wastewater, harmful to the flora and the fauna, leads also to the shortage of clean water ressources. In this context, the green processes development like melt crystallization of water may provide a low energy solution and simultaneously enables the minimization of use of hazardous material (Yin et al. (2017)). In this paper, we suggest a structured Port Hamiltonian model of the solidification process in order to provide numerical models suitable for the simulation, design and control of such a processes. The companion paper of (Bendimerad-Hohl et al. (2022)) gives the procedure to derive a finite-dimensional discretized model preserving the Port Hamiltonian structure. The main challenge to establish this solidification model is the moving interface between the solid and the liquid phases.

Two approaches are possible. The first one, called *thin interface approach*, consists in describing the interface as the boundary of the spatial domains of each phase, using for instance their characteristic functions. The second one called *diffuse interface approach*, consists in introducing a function called *phase field* that is a smooth approximation of the characteristic function of the domain. The boundary is replaced by a narrow interface layer corresponding to intermediate values of the phase field variable.

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In this paper we suggest a Dissipative Port-Hamiltonian formulation of a solidification process. Port-Hamiltonian systems are a modelling framework, allowing the thermodynamically consistent representation of open physical systems (Duindam et al. (2009); van der Schaft and Jeltsema (2014)) and well-suited for representing open thermodynamical processes (Ramirez et al. (2013b,a); Favache et al. (2010)).

The Port-Hamiltonian formulation of systems with moving interface has been proposed following both approaches, considering sharp interfaces in (Diagne and Maschke (2013)) and diffuse interfaces (Vincent et al. (2020)). In this paper we shall elaborate on the phase field approach and extend the model Port Hamiltonian formulation of the Allen-Cahn equation formulated by Vincent et al. (2020) by coupling it to the heat diffusion to an extended Port Hamiltonian system. In section 2, we shall recall the definition of Port Hamiltonian systems and recall the Port Hamiltonian formulation of the phase field variable dynamics described by the Allen-Cahn equation (Vincent et al. (2020)) and finish with its extension to the complete process of solidification. In section 3, we shall recall the thermodynamical properties of the water and ice and their extension to a bi-phasic model with diffuse interface, including the phase field variable. In section 4, we shall reformulate the Port Hamiltonian model of section 2, using the entropy as generating function, but using an formulation as a Differential-Algebraic Port Hamiltonian system, or an Implicit Port Hamiltonian System (Maschke and van der Schaft (2020); van der Schaft and Maschke (2021)), thereby expressing the dynamics in terms of intensive rather than extensive variables.

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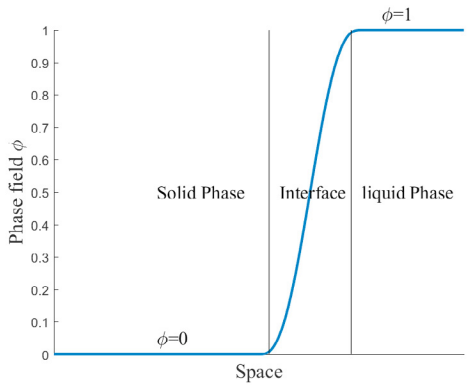

Fig. 1. Liquid/Solid interface : Phase field representation

2. PORT HAMILTONIAN FORMULATION OF SOLIDIFICATION PROCESS

In this section, we present a Port Hamiltonian formulation of the phase field model of a solidification process, following the thermodynamic approach of (Wang et al. (1993)). This model consists in coupling the energy balance equation with the Allen-Cahn equation, taking the entropic form of the Gibbs' equation. This leads to extend the Port Hamiltonian formulation of the Allen Cahn equation of (Vincent et al. (2020)) by coupling it to the Port Hamiltonian model of heat diffusion model.

2.1 Reminder of the solidification model

Following the phase field approach, (Wang et al. (1993)) present a model of a solidification process, consisting in a closed system of volume V in which a pure material undergoes a phase transition between solid and liquid.

Thermodynamic model This model corresponds to the diffuse interface model of bi-phasic systems where the spatial localization of the two phases is represented by the continuous *phase field variable* ϕ. ϕ takes values in the interval [0, 1], taking value 0 for the solid state, 1 for the liquid state and intermediate value at the diffuse interface (see figure∼1). The authors write the entropy balance equation and use *Gibbs' equation in the entropy form* [1] :

$$ds = \left(\frac{\partial s}{\partial \phi}\right) d\phi + \tau du \tag{1}$$

where s denotes the entropy density, u the internal energy density and τ the reciprocal temperature $\tau = (\frac{\partial s}{\partial u})_\phi = (\frac{1}{T})$.

The total entropy functional of the bi-phasic system is expressed by the *Landau-Ginzburg* entropy functional:

$$S(\phi, u) = \int_V \left(s(\phi, u) - \frac{1}{2}\epsilon^2 (grad\,\phi)^2 \right) dv, \tag{2}$$

where the quadratic term in the integral accounts for the entropy of the diffuse interface, ϵ is a constant related to the thickness of the interface (see Boettinger et al. (2002); Kobayashi (1993)) and $s(\phi, u)$ is the entropy density function associated with Gibbs' equation (1).

Dynamic equations The dynamical model consists first in the energy balance equation:

$$\frac{\partial u}{\partial t} = -div\, q \tag{3}$$

where q denotes the heat flux

$$q = M_\tau \bar{F} \tag{4}$$

and $\bar{F}$ the driving force

$$\bar{F} = -grad(\tau) \tag{5}$$

where $M_\tau = -\frac{\lambda(\frac{1}{\tau},\phi)}{\tau^2}$, λ being the thermal conductivity of the bi-phasic system [2]. It is coupled to the relaxation dynamics of the phase field variable ϕ, the gradient system called *Allen Cahn equation*:

$$\eta \frac{\partial \phi}{\partial t} = \frac{\partial s}{\partial \phi}(\phi) + div(\epsilon^2 grad\,\phi) = -\frac{\delta(-S)}{\delta \phi}, \tag{7}$$

where η is the positive interface mobility and $\frac{\delta S}{\delta \phi}$ denotes the variational derivative of the functional S with respect to ϕ.

2.2 Reminder on dissipative Port Hamiltonian Systems

Consider the following dissipative systems :

$$\frac{\partial x}{\partial t}(t, z) = (-\mathcal{G}_R \mathcal{R} \mathcal{G}_R^*)\, \frac{\delta \mathcal{H}}{\delta x}, \tag{8}$$

where $x(t, z) \in \mathbb{R}^n$ is the state variable defined on the spatial domain V and a time interval in $\mathbb{R}_+$, $\mathcal{H}$ is the Hamiltonian functional, $\mathcal{R}$ is a positive, coercive matrix operator and $\mathcal{G}_R$ is a matrix differential operator ($\mathcal{G}_R^*$ denoting its formal adjoint).

Its Port Hamiltonian formulation is defined by considering the Hamiltonian matrix differential operator

$$\mathcal{J}_e = \begin{bmatrix} 0 & \mathcal{G}_R \\ -\mathcal{G}_R^* & 0 \end{bmatrix}, \tag{9}$$

and decomposing the system (8) into

$$\begin{pmatrix} \frac{\partial x}{\partial t} \\ F \end{pmatrix} = \mathcal{J}_e \begin{pmatrix} \frac{\delta \mathcal{H}}{\delta x} \\ Q \end{pmatrix} \tag{10}$$

where the driving force F and the flux variable Q are related by the *dissipative closure relation* :

$$Q = \mathcal{R}\, F \tag{11}$$

The Port Hamiltonian system is then obtained by augmenting the system with *boundary port variables* (the

[1] In this paper, we make the usual assumption that the mass density is uniform Wang et al. (1993).

[2] The thermal conductivity is defined by interpolation by a polynomial $p_i(\phi)$ taking values in $[0, 1]$ for $\phi \in [0, 1]$:

$$\lambda = \lambda_{sol} + p_i(\phi)\left[\lambda_{liq} - \lambda_{sol}\right]. \tag{6}$$

where the thermal conductivity of the ice λ_{sol} and the water λ_{liq} can be found in Yen (1981); IAPWS (2009b)

interface variables of the system at its boundary) associated with the *Stokes-Dirac structure* defined by the Hamiltonian operator $\mathcal{J}_e$ (van der Schaft and Maschke (2002)). These boundary port variables are defined by linear combinations of the *trace* of the vector $\begin{pmatrix} \frac{\delta \mathcal{H}}{\delta x} & Q \end{pmatrix}^{\perp}$.

Example: the heat conduction The energy balance equation (3) and the definition of the driving force (5) leads to the Dissipative Port Hamiltonian formulation (10) (11) with $\mathcal{G}_R = -div$ and $\mathcal{R} = M_\tau$:

$$\begin{pmatrix} \frac{\partial u}{\partial t} \\ \bar{F} \end{pmatrix} = \begin{pmatrix} 0 & -div \\ -grad & 0 \end{pmatrix} \begin{pmatrix} \frac{\delta s}{\delta u} \\ q \end{pmatrix} \tag{12}$$

The associated pair of boundary port variables is :

$$\begin{pmatrix} f_\partial \\ e_\partial \end{pmatrix} = \overline{\mathcal{W}}\, e = \begin{pmatrix} \gamma_0 \frac{\delta s}{\delta u} \\ -\gamma_\perp q \end{pmatrix} \tag{13}$$

where the boundary operator $\overline{\mathcal{W}}$ is defined as:

$$\overline{\mathcal{W}} = \begin{pmatrix} \gamma_0 & 0 \\ 0 & -\gamma_\perp \end{pmatrix} \tag{14}$$

and γ_0 is the *Dirichlet trace map* and $\gamma_\perp$ is the *normal trace map*, (Kurula and Zwart (2012)).

2.3 Port Hamiltonian formulation of the Allen-Cahn equation

We briefly recall now the dissipative Hamiltonian formulation of the Allen-Cahn equation as suggested by (Vincent et al. (2020)). The state space representation is augmented with the new state :

$$\psi := grad\, \phi \tag{15}$$

leading to define the extended state vector : (ϕ, ψ, u). The Landau-Ginzburg entropy functional (2) is then written :

$$\bar{S}(\phi, \psi, u) = \int_\Omega s(\phi, u) - \frac{1}{2}\epsilon^2 \psi^2 \, dV \tag{16}$$

Let us now compute the variational derivative $\frac{\delta S}{\delta \phi}$ in (7) in terms of $\bar{S}(\phi, \psi, u)$:

$$\frac{\delta S}{\delta \phi} = \frac{\delta \bar{S}}{\delta \phi} - div \frac{\partial \bar{S}}{\partial \psi} := F_{\phi\psi} \tag{17}$$

Defining

$$E_{\phi\psi} = -\frac{\partial \phi}{\partial t} \tag{18}$$

the gradient dynamics (7) is expressed by the following dissipative constitutive relation

$$E_{\phi\psi} = 1/\eta F_{\phi\psi} \tag{19}$$

The dynamics of the added state variable ψ is then easily obtained by permutation of the spatial and time derivatives :

$$\frac{\partial \psi}{\partial t} = \frac{\partial}{\partial t} grad \phi = grad \frac{\partial \phi}{\partial t} = -grad\, E_{\phi\psi} \tag{20}$$

Hence the Allen-Cahn equation augmented with the dynamics of the added variable ψ admits the Dissipative Port Hamiltonian formulation (10) (11):

$$\begin{pmatrix} \frac{\partial \phi}{\partial t} \\ \frac{\partial \psi}{\partial t} \\ F_{\phi\psi} \end{pmatrix} = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & -grad \\ 1 & -div & 0 \end{pmatrix} \begin{pmatrix} \frac{\delta(-\bar{S})}{\delta \phi} \\ \frac{\delta(-\bar{S})}{\delta \psi} \\ E_{\phi\psi} \end{pmatrix} \tag{21}$$

with $\mathcal{G}_R = \begin{pmatrix} -1 \\ -grad \end{pmatrix}$ and $\mathcal{R} = \eta$.

Once again with the aid of (Kurula and Zwart (2012)), the boundary port variables of the Port Hamiltonian formulation of the Allen-Cahn equation are :

$$\begin{pmatrix} f_\partial^{\phi\psi} \\ e_\partial^{\phi\psi} \end{pmatrix} = \mathcal{W}\, e_{\phi\psi} = \begin{pmatrix} -\gamma_\perp \frac{\delta(-\bar{S})}{\delta \psi} \\ \gamma_0\, E_{\phi\psi} \end{pmatrix} \tag{22}$$

with the boundary operator $\mathcal{W}$:

$$\mathcal{W} = \begin{pmatrix} 0 & -\gamma_\perp & 0 \\ 0 & 0 & \gamma_0 \end{pmatrix} \tag{23}$$

2.4 Port Hamiltonian formulation of the solidification process

Recalling that $\frac{\delta \bar{S}}{\delta u} = \frac{\partial s}{\partial u} = \tau$, the Dissipative Port Hamiltonian formulation of solidification process is obtained by assembling (12) and (21)

$$\begin{pmatrix} \frac{\partial \phi}{\partial t} \\ \frac{\partial \psi}{\partial t} \\ F_{\phi\psi} \\ \frac{\partial u}{\partial t} \\ \bar{F} \end{pmatrix} = \mathcal{J} \begin{pmatrix} -\frac{\partial s}{\partial \phi}(\phi, u) \\ \epsilon^2 \psi \\ E_{\phi\psi} \\ -\tau \\ q \end{pmatrix} = \mathcal{J}\mathcal{E} \tag{24}$$

with Hamiltonian matrix differential operator

$$\mathcal{J} = \begin{pmatrix} 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & -grad & 0 & 0 \\ 1 & -div & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -div \\ 0 & 0 & 0 & -grad & 0 \end{pmatrix} \tag{25}$$

and Hamiltonian functional $-\bar{S}$ defined in (16), completed with the two dissipative closure relations (4) and (19).

The associated boundary operator $\widetilde{\mathcal{W}}$ are also obtained by assembling the boundary operators of the heat conduction and the augmented Allen-Cahn equation :

$$\widetilde{\mathcal{W}} = \begin{pmatrix} 0 & -\gamma_\perp & 0 & 0 & 0 & 0 \\ 0 & 0 & \gamma_0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \gamma_0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\gamma_\perp \end{pmatrix} \tag{26}$$

and the extended pair of boundary port variables is :

$$\begin{pmatrix} f_\partial^{\phi\psi} \\ e_\partial^{\phi\psi} \\ f_\partial \\ e_\partial \end{pmatrix} = \widetilde{\mathcal{W}}\mathcal{E} = \begin{pmatrix} -\gamma_\perp(\epsilon^2 \psi) \\ \gamma_0\,(1/\eta F_{\phi\psi}) \\ \gamma_0 \tau \\ -\gamma_\perp M_\tau(-grad(\tau)) \end{pmatrix} \tag{27}$$

It may be shown, from (Vincent et al. (2020); Kurula and Zwart (2012)), that the operator $\mathcal{J}$ in (25) and the boundary operator $\widetilde{\mathcal{W}}$ in (26) define a Stokes-Dirac structure (van der Schaft and Maschke (2002)).

From the properties of a Stokes-Dirac structure, one may deduce the neg-entropy balance equation :

$$\frac{d(-\bar{S})}{dt} = -\int_V E_{\phi\psi}F_{\phi\psi}dV - \int_V q\bar{F}dV - \int_{\partial V}\tilde{e}_\partial \tilde{f}_\partial \, dS \quad (28)$$

which becomes, by means of the dissipation relations (4) and (19)

$$\frac{d(-\bar{S})}{dt} = -\int_V \eta E_{\phi\psi}^2 dV - \int_V M_\tau \bar{F}^2 dV + \int_{\partial V}\tilde{e}_\partial \tilde{f}_\partial \, dS \quad (29)$$

where the two first terms correspond to the irreversible entropy production due to the gradient dynamics of the phase field and the heat conduction and the third one corresponds to the external entropy flow flowing into the system.

3. THERMODYNAMIC PROPERTIES USING PHASE FIELD

The objective of this section is to recall how to derive the thermodynamic properties of the bi-phasic systems from the thermodynamic properties of the liquid water and ice.

3.1 Thermodynamic properties of liquid water and ice

Thermodynamics properties of the liquid water and ice are practically found in literature (IAPWS (2009a)) and (IAPWS (2009b)). The provided thermodynamic potential is Gibbs' energy expressed as a function of temperature and pressure. The expression of the specific Gibbs energy of the liquid phase is given as:

$$g_{liq}(T,p)/g^* = \sum_{j=0}^{7}\sum_{k=0}^{6} g_{jk}T_r^i\pi^k \quad (30)$$

with the reduced temperature $T_r = (T - T_0)/T^*$ and the reduced pressure $\pi = (p - p_0)/p^*$. The constants T_0, p_0, T^*, p^*, g^* and the g_{jk} are given in (IAPWS (2009b)). In a same way the expression of the specific Gibbs energy of the solid phase is given as:

$$g_{sol}\ (T,p) = g_0(p) - s_0T_tT_r + T_tRe\Bigg(\sum_{k=1}^{2} r_k\Big[(t_k - T_r)\ln(t_k - T_r) + (t_k + T_r)\ln(t_k + T_r) - 2t_k\ln(t_k) - \frac{T_r^2}{t_k}\Big]\Bigg) \quad (31)$$

with $g_0(p) = \sum_{k=0}^{4} g_{0k}(\pi - \pi_0)^k$ and $r_2(p) = \sum_{k=0}^{2} r_{2k}(\pi - \pi_0)^k$, $T_r = T/T_t$, $\pi = p/p_t$, and $\pi_0 = p_0/p_t$. All The constants T_t, p_t, p_0, s_0, g_0, r_1 as well as the g_{ok}, r_{2k}, t_k are given in (IAPWS (2009a)). From the expression of these state equations, other specific thermodynamic quantities as entropy, Helmholtz energy and volumic density for each phase may be derived using standard thermodynamic computations (see IAPWS (2009a), IAPWS (2009b) and Callen (1991)). As an example, the specific Helmholtz energy f_δ, the specific entropy s_δ^* as a function of temperature and pressure and the density ρ_δ as well as the heat capacity c_{p_δ} can be deduced from g_δ for $\delta = sol, liq$ by the formulas:

$$f_\delta(T,p) = g - p\frac{\partial g_\delta}{\partial p} \quad (32)$$

$$s_\delta^*(T,p) = -\frac{\partial g_\delta}{\partial T} \quad (33)$$

$$\rho_\delta(T,p) = \Big(\frac{\partial g_\delta}{\partial p}\Big)^{-1} \quad (34)$$

$$c_{p_\delta}(T,p) = -T\frac{\partial^2 g_\delta}{\partial T^2} \quad (35)$$

Finally, we give some values of these properties at the melting temperature (273.15K) at atmospheric pressure.

Table 1. Values of some thermodynamic properties at the melting temperature

δ	g_δ	f_δ	s_δ^*	ρ_δ	c_{p_δ}
liq	101.343	0.0018	–0.1476	999.843	4219.41
sol	101.343	– 9.1870	– 1220.769	916.721	2096.71

3.2 The Equation of State of bi-phasic system

For the sake of brevity, we restrict our attention to the specific entropy function of the bi-phasic system s^* assuming constant density. The stability principle of thermodynamics when two phases are present requires (see Callen (1991)):

$$\left.\frac{\partial s^*}{\partial\phi}\right|_{\phi=0} = \left.\frac{\partial s^*}{\partial\phi}\right|_{\phi=1} \text{ and } \left.\frac{\partial^2 s^*}{\partial\phi^2}\right|_{\phi=0,1} < 0. \quad (36)$$

From the constraint that, at equilibrium, the variational derivative of the Landau-Ginzburg entropy functional must be equal to 0 in each phase , we have (see Wang et al. (1993); Boettinger et al. (2002)):

$$\left.\frac{\partial s^*}{\partial\phi}\right|_{\phi=0,1} = 0 \text{ and } \left.\frac{\partial^2 s^*}{\partial\phi^2}\right|_{\phi=0,1} < 0. \quad (37)$$

Following the method proposed in Boettinger et al. (2002), the specific entropy function of bi-phasic system becomes:

$$s^*(\phi,T) = s_{sol}^*(T) + p_i(\phi)[s_{liq}^*(T) - s_{sol}^*(T)] + wp_w(\phi) \quad (38)$$

with $p_i(\phi) = \phi^3(6\phi^2 - 15\phi + 10)$, $p_w(\phi) = -\phi^2(1-\phi)^2$ where s_{liq}^*, s_{sol}^* represent the specific entropy of pure water and of pure ice respectively. $p_w(\phi)$ is the double-well polynomial and $p_i(\phi)$ is the interpolating polynomial. This choice of p_i ensures that $\left.\frac{\partial s^*}{\partial\phi}\right|_{\phi=0,1} = 0$. The parameter w allows to tune of the hollow between the two local maxima (see Boettinger et al. (2002))and w must be positive in order to ensure that $\frac{\partial^2 s^*}{\partial\phi^2}\frac{\partial^2 s^*}{\partial u^2} - \Big(\frac{\partial^2 s^*}{\partial\phi\partial u}\Big)^2 > 0$ (see Callen (1991)). Figure 2 shows the specific entropy of bi-phasic system for water and ice.

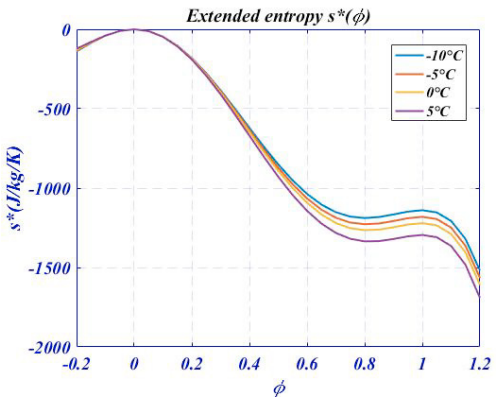

Fig. 2. specific entropy of bi-phasic system with $w = 18\ 10^3$

4. IMPLICIT PORT HAMILTONIAN SYSTEM

In the Port Hamiltonian formulation of section 2, the Hamiltonian function is the entropy functional (2) which depends on the internal energy u and the phase field variable ϕ and its gradient ψ. In the section 3, the practical definition of the thermodynamic properties of the bi-phasic water-ice system has been given in terms of the entropy density function (38), depending on the temperature rather than the internal energy.

In this section, we reformulate the Port Hamiltonian model of Section 2, using an Implicit Port Hamiltonian formulation where the energy function is not defined explicitly but rather by a set of constitutive relations between the extensive and intensive variables. As these relations satisfy Maxwell's reciprocity conditions (Callen (1991), chapter 7), the graph of these relations has a geometrical interpretation as a Lagrangian submanifold on which these Port Hamiltonian Systems are defined (van der Schaft and Maschke (2018); van der Schaft and Maschke (2020)) (Maschke and van der Schaft (2020); van der Schaft and Maschke (2021)).

Consider Gibbs' equation (1) associated with the entropy density function $s(\phi, u)$; the graph of its differential gives rise to the following Lagrangian submanifold

$$L_s = \left\{ (x,e) \in \mathbb{R}^2 \times \mathbb{R}^2 :\ e = \begin{pmatrix} \frac{\partial s}{\partial \phi}(\phi,u) \\ \frac{\partial s}{\partial u}(\phi,u) \end{pmatrix};\ x = \begin{pmatrix} \phi \\ u \end{pmatrix} \right\} \tag{39}$$

In order to perform the change of coordinates, let us consider the Legendre transform of the entropy density $s(\phi, u)$ with respect to u, that we call *co-entropy*

$$s^*(\phi, \tau) = \tau\, u - s(\phi, u) \tag{40}$$

where the internal energy u is considered to be a function of the phase field variable ϕ and the reciprocal temperature obtained by partial inversion of $\tau = \frac{\partial s}{\partial u}(\phi, u)$with respect to u [3] . Then the Legendre submanifold (39) can be defined as follows

$$L_s = \left\{ (x,e) \in \mathbb{R}^2 \times \mathbb{R}^2 \,/\, x = \begin{pmatrix} \phi \\ \frac{\partial s^*}{\partial \tau}(\phi,\tau) \end{pmatrix};\ e = \begin{pmatrix} -\frac{\partial s^*}{\partial \phi}(\phi,\tau) \\ \tau \end{pmatrix};\ \begin{pmatrix} \phi \\ \tau \end{pmatrix} \in \mathbb{R}^2 \right\} \tag{41}$$

The dynamics of the solidification process can then be expressed as follows. First, considering the entropy functional of the bi-phasic system (16), one has the associated Legendre submanifold:

$$L = \left\{ \left(\begin{pmatrix} x \\ \psi \end{pmatrix}, \begin{pmatrix} e \\ e_\psi \end{pmatrix} \right) \in \mathbb{R}^3 \times \mathbb{R}^3 \,\Big/\, (x, -e) \in L_s;\ e_\psi = \epsilon^2 \psi;\ \psi \in \mathbb{R} \right\} \tag{42}$$

Now let us write the Port Hamiltonian system, *in the new coordinates*. First compute the time derivative of the vector x, with its expression in the definition (41) of the Lagrange submanifold L_s:

$$\begin{aligned} \frac{\partial}{\partial t}\begin{pmatrix} \phi \\ u \end{pmatrix} &= \frac{\partial}{\partial t}\begin{pmatrix} \phi \\ \frac{\partial s^*}{\partial u}(\phi,\tau) \end{pmatrix} \\ &= \begin{pmatrix} 1 & 0 \\ \frac{\partial s^*}{\partial \phi \partial \tau}(\phi,\tau) & \frac{\partial^2 s^*}{\partial \tau^2}(\phi,\tau) \end{pmatrix} \frac{\partial}{\partial t}\begin{pmatrix} \phi \\ \tau \end{pmatrix} \end{aligned} \tag{43}$$

The Port Hamiltonian System (24), using (43) in the right-hand side term and the parametrization of the extensive variables e in (41), leads to the following implicit PDE:

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ \frac{\partial s^*}{\partial \phi \partial \tau} & 0 & 0 & \frac{\partial^2 s^*}{\partial \tau^2} & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \frac{\partial \phi}{\partial t} \\ \frac{\partial \psi}{\partial t} \\ F_{\phi\psi} \\ \frac{\partial \tau}{\partial t} \\ F \end{pmatrix} = \mathcal{J} \begin{pmatrix} -\frac{\partial s^*}{\partial \phi}(\phi,\tau) \\ \epsilon^2 \psi \\ E_{\phi\psi} \\ -\tau \\ q \end{pmatrix}. \tag{44}$$

This PDE, augmented with the dissipative relations (19) and (4) and with the boundary port variables (27), defines a Dissipative Boundary Port Hamiltonian System.

Note that this Differential-Algebraic Partial Differential System is regular as the matrix on the left hand side is full rank for any state. Indeed for each phase $\delta = sol, liq$ $\frac{\partial^2 s^*_\delta}{\partial \tau^2}(\tau) = -\frac{c_\delta}{\tau^2} < 0$ as its heat capacitance $c_\delta > 0$ according to the thermodynamic stability condition ((Callen, 1991, chap.8)). As the interpolation polynomial p_i maps $[0,1]$ into itself (Boettinger et al. (2002)), the co-entropy function s^* (38) of the bi-phasic system is a convex combination of the co-entropy functions of each phase, hence it satisfies also $\frac{\partial^2 s^*}{\partial \tau^2} < 0$.

It is remarkable that the dynamics of phase field models of solidification processes often lead to implicit formulations of the dynamics. For instance (Wang et al. (1993)) and (Boettinger et al. (2002)) begin their paper using the entropy as thermodynamical potential, in order to ensure the irreversible entropy creation of the phase field dynamics. However, they use Helmholtz free energy density $f(\phi, T)$ as

[3] The invertibility is actually ensured by the strict concavity of $s(\phi, u)$ due to the strict concavity of the entropy functions s_{sol} and s_{liq} of the solid and liquid phases and its definition (38).

a generating function of Thermodynamic properties of the bi-phasic system and finally obtain an implicit dynamic system (see for instance equations (54) to (58) in Wang et al. (1993)).

5. CONCLUSION

In this contribution, we have proposed a Boundary Port Hamiltonian representation of the solidification of water or any other pure substance using the diffuse interface approach and using a phase field variable. Therefore, we have augmented the Port Hamiltonian representation suggested by (Vincent et al. (2020)) of the Allen-Cahn equation, representing the dynamics of a non-conserved phase field variable, to a Port Hamiltonian system including the heat transport. Finally we have suggested a DAE-PDE Port Hamiltonian formulation of the system, that allow to change in a consistent way the coordinates on which the dynamics is expressed. In the given case, we have expressed the energy balance equation in terms of the reciprocal temperature instead of the internal energy, enabling the use the experimental datas of thermodynamic properties of water and ice.

Forthcoming work will consist in modifying this model by adding the pollutant in the thermodynamics functional and in the conservation equations in order to provide a model of the melt crystallisation process as well as relaxing the assumption of uniform mass density. Furthermore the control of the process will be considered, using passivity-based control methods, taking account of the energy balance and entropy balance equations (Ramirez et al. (2016)).

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