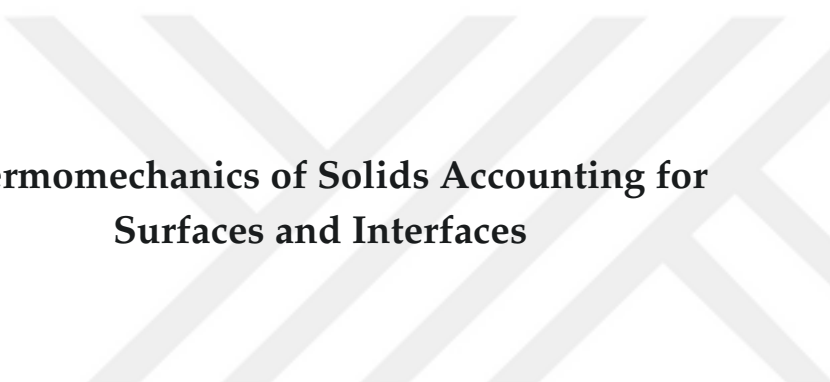




Thermomechanics of Solids Accounting for Surfaces and Interfaces

Thermomechanik von Festkörpern unter Berücksichtigung von Oberflächen und Grenzflächen

Der Technischen Fakultät der
Universität Erlangen-Nürnberg

zur Erlangung des Grades

DOKTOR-INGENIEUR

vorgelegt von

Ali Javili

Erlangen - 2012



Als Dissertation genehmigt von
der Technischen Fakultät der
Universität Erlangen-Nürnberg

Tag der Einreichung:	29.05.2012
Tag der Promotion:	02.11.2012
Dekan:	Prof. Dr.-Ing. habil. Marion Merklein
Berichterstatter:	Prof. Dr.-Ing. habil. Paul Steinmann
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Schriftenreihe Technische Mechanik
Band 7 · 2012

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**Thermomechanics of Solids Accounting for
Surfaces and Interfaces**

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Erlangen 2012

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ISSN 2190-023X

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Preface

The research work presented in this thesis was carried out during my employment as a teaching assistant (Wissenschaftlicher Assistent) at the Chair of Applied Mechanics (LTM), University of Erlangen–Nuremberg, Germany from October 2007 to April 2012.

I believe, it is impossible to express my gratitude by means of words, since this concept per se is complex and ambiguous. Nevertheless, as a customary practice and in order to show my appreciation in black and white, I would like to acknowledge a few people here.

First and foremost I wish to express my most sincere gratitude to my supervisor, Professor Paul Steinmann, whose broad view and deep understanding of the subject has formed the foundation of this work. I have been constantly enjoying his wise guidance and subtle suggestions as well as his cordial support.

I am highly indebted to Professor Samuel Forest and Professor B. Daya Reddy for accepting the review of this manuscript and providing me with helpful remarks. A special thanks to Andrew McBride for his significant input and close collaboration during the last two years.

I wish to use this occasion for expressing my gratitude to my teachers and several people, even though not necessarily connected directly with this project, whose comments and works had a profound influence on my research, to name a few:¹

- | | | |
|-------------------------|-------------------------|------------------|
| • Swantje Bargmann | • Ahmed Benallal | • Esteban Busso |
| • George Chatzigeorgiou | • Francesco dell’Isola | • Marc Geers |
| • Carolin Körner | • Detlef Kuhl | • Valery Levitas |
| • Gérard Maugin | • Julia Mergheim | • Jörn Mosler |
| • Ingo Müller | • Harold Park | • Franz Peters |
| • Kenneth Runesson | • Stanisław Stupkiewicz | • Julien Yvonnet |

Last but not least, I wish to express my gratitude to my family and friends who have supported me.

Erlangen, November 2012

Ali Javili

¹ The names are sorted in alphabetical order. The titles are omitted for the sake of space.

Zusammenfassung

Oberflächen und Grenzflächen können eine wichtige Rolle beim thermomechanischen Verhalten von Festkörpern spielen. Ihr Einfluss kann in der Kontinuumsmechanik gut durch Modelle beschrieben werden, die Ober- und Grenzflächen eigene energetische Strukturen zuordnen. Derartige Ansätze gewinnen insbesondere bei der Modellierung des thermomechanischen Verhaltens von Nanostrukturen zunehmend an Bedeutung. Diese Arbeit stellt eine systematische Herleitung der thermomechanischen Gleichungen des Körpers, seiner Oberfläche, einer inneren Grenzfläche und deren Schnittkurve auf Grundlage jeweils eigener energetischer Strukturen vor. Dabei werden die konstitutiven Beziehungen all dieser Komponenten in thermodynamisch konsistenter Weise entwickelt. Terme für Wärme- und Entropiefluss sowie die Nebenbedingungen an das Temperaturfeld werden aus der Nichtnegativitätsbedingung an die Dissipation abgeleitet. Schließlich wird die schwache Formulierung der Gleichungen hergeleitet, die als Grundlage für die numerische Approximation mit der Methode der finiten Elemente dient. Darüber hinaus werden verschiedene Formen der Helmholtz-Energie vorgestellt. Während sich der überwiegende Teil der Literatur zu Oberflächenelastizität auf infinitesimal kleine Deformationen beschränkt, werden in dieser Arbeit außerdem die Spannungsmaße für große Deformationen linearisiert und die Ergebnisse diskutiert. Zuletzt werden die entwickelten theoretischen Ergebnisse anhand numerischer Beispiele verdeutlicht.

Abstract

Surfaces and interfaces can play a significant role in the overall response of a solid body. Their behaviour is well described by continuum theories that endow the surface and interface with their own energetic structures. Such theories are becoming increasingly important when modelling the response of materials at the nanoscale. This work presents a systematic procedure to derive the equations governing a bulk material surrounded by a surface, containing an interface, the intersection of which with the surface is a curve, all of which possess their own energetic structures. The constitutive relations in the bulk, on the surface, interface and curve are derived in a thermodynamically consistent manner. Expressions for the heat and entropy flux vectors, and the constraints on the temperature field, all subject to the restriction of non-negative dissipation, are then explored. Thereafter, the weak formulation of the governing equations is presented which serves as the basis for their approximation using the finite element method. Various forms for a Helmholtz energy that describes the fully-coupled thermomechanical response of the system are given. The vast majority of the literature on surface elasticity is framed in the infinitesimal deformation setting. The finite deformation stress measures are thus linearised and the structure of the resulting stresses discussed. The final objective is to elucidate the theory using a series of numerical example problems.

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Chapter 1

Introduction

The surface of a solid body typically exhibits properties that differ from those of the enclosed bulk. These differences, caused by processes such as surface oxidation, ageing, coating, atomic rearrangement and the termination of atomic bonds, are present in comparatively thin boundary layers. Similarly, interfaces within the bulk can be viewed as two-sided internal surfaces. The mechanical and thermal properties of the interface can also differ significantly from the surrounding bulk. Surface and interface effects are especially significant for nanomaterials due to their large surface-to-volume ratio. These effects were appreciated already in the early 1900's by Pawlow [1], for example, who predicted the decrease in the melting temperature of a particle as its size reduces.

There exist two principal approaches to study the thermodynamics of surfaces and interfaces:

- The zero-thickness layer or Gibbs (geometrical) method wherein a mathematical surface with zero thickness is introduced to capture excess quantities on the surface [2].
- The finite-thickness layer method which dates back to Van der Waals wherein a layer of finite thickness can be imagined instead of the interface.

The reader is referred to Guggenheim [3] for further details and a comparison of the two approaches.

Following Gibbsian thermodynamics, various models have been proposed to endow the surface and interface with their own distinct properties, e.g. Adam [4], Shuttleworth

[5], Herring [6], Bikerman [7], Orowan [8], Cahn [9, 10]. The physical chemistry of surfaces and interfaces for liquids and solids is studied in [4, 11–15], among others.

The thermodynamic fundamentals of surface science was reviewed by Rusanov in [16, 17]. Müller and Saul [18] presented a review on the importance of stress and strain effects on surface physics. The role of stress at solid surfaces was critically examined by Ibach [19]. Leo and Sekerka [20] investigated the equilibrium conditions for interfaces using a variational approach wherein the excess energy associated with the interface is allowed to depend on both the deformation of the interface and the crystallographic normal to the interface. Cammarata [21–24] highlighted the surface and interface stress effects on thin films and nano-scaled structures. Fischer et al. [25] studied the role of surface energy and surface stress in phase-transforming nano-particles and reported on the thermodynamics of a moving surface.

Gutman [26] recognised an inconsistency between the notion of the surface stress defined by, e.g. Shuttleworth, and that of the continuum elasticity theory. Bottomley and Ogino [27] examined an alternative to the Shuttleworth formulation of surface stress in solids [see also 28]. Kramer and Weissmüller [29] criticised [26–28] and clarified various misleading statements in the literature. Fischer et al. [25] circumvented such issues by a careful handling of the actual and reference configurations. Furthermore, Fischer et al. utilised the concept of configurational forces [30, 31] as a convenient framework for distinguishing between surface energy, surface tension and surface stress.

A widely-adopted model, proposed by Gurtin and Murdoch [32, 33], gives the surface its own tensorial stress measures [see e.g. 22, 34–36, for applications in nano-materials]. Murdoch [37], Gurtin and Struthers [38], Gurtin et al. [39] extended this approach to consider interfaces within a solid. An important extension of the Gurtin and Murdoch model to account for the flexural resistance of the surface was developed by Steigmann and Ogden [40] and further studied in [41–43]. Moeckel [44] followed a different approach to Gurtin and Murdoch [32] for a moving interface within a thermomechanical solid. A master-balance equation is derived and applied to various key fields on the interface [see also 45]. The resulting equations are then restricted using the entropy principles of Müller [46] and constitutive relations for material interfaces derived. An alternative approach to develop general governing equations for the interface is to integrate the known equations for the bulk over the thickness of the interfacial layers [see e.g. 47]. Daher and Maugin [48] used the method of virtual power [49, 50] to derive the governing equations for an interface within a thermomechanical solid. This flexible approach is well suited to describing complex phenomena. For example, Daher and Maugin [51] applied the method to a model of deformable semiconductors with interfaces [see also 52]. Murdoch [53] addressed various aspects of surface modelling. Šilhavý [54] proved the existence of equilibrium of a two-phase state with an elastic solid bulk and deformation dependent interfacial energy.

Park et al. [55], Park and Klein [56] developed an alternative continuum framework based on the surface Cauchy–Born model, an extension of the classical Cauchy–Born model, to include surface stresses [see also 57, 58].

The effect of surface energetics for ellipsoidal inclusions and the size-dependent elastic state of embedded inhomogeneities was investigated by Sharma et al. [59], Sharma and Ganti [60], Sharma and Wheeler [61]. They utilised the classical formulation of Eshelby [62, 63] for embedded inclusions and modified it by incorporating surface energies. Duan et al. [64] extended the Eshelby formalism for inclusion/inhomogeneity problems to the nanoscale. Effective mechanical and thermal properties of heterogeneous materials containing nano-inhomogeneities based on the generalised Eshelby formalism is investigated in [64–66], see also related works [67–69].

Zöllner et al. [70] recently reported that to explore the biomechanical interaction during tissue expansion, one could model skin growth using a surface energy. The thermomechanical behaviour of low-dimensional systems was reviewed by Sun [71] together with a theoretical analysis elaborating on existing approximations in continuum mechanics and quantum computations. Johnson [72] studied the thermodynamics of a coherent interface separating two non-hydrostatically stressed crystals.

The objective of this presentation is to derive the equations governing the nonlinear coupled transient thermomechanical response of a body composed of a bulk, intersected by an interface, and encased by a surface, all of which are assumed to be energetic. Furthermore, an energetic curve that accounts for the interaction between the interface and the surface is also present. The importance of capturing such an interaction when modelling ionic nanowires was recently observed in [73].

A particular emphasis is placed here on the thermomechanical response of the interface. The governing equations for the various parts of the body are obtained from the balances of several key properties, namely linear and angular momentum, energy, and entropy. The corresponding constitutive relations then arise as thermodynamic restrictions on the dissipation. The diffusion of mass or chemical species is not accounted for in this contribution [see e.g. 74, 75, for the case of diffusion].

Interfaces can be classified as follows. A *material interface* is one that does not move independently of the surrounding bulk material. An *energetic interface* is understood here to imply that the interface possesses its own thermomechanical structure in the form of an internal energy, entropy, constitutive relations and dissipation. Such an interface is termed a *thermodynamical singular surface* by Daher and Maugin [48]. A *thermal interface* is defined as one which allows for heat conduction along the interface but possesses no energetic structure. Finally, a *standard interface* does not allow heat conduction along the interface and possesses no energetic structure. Daher and Maugin [48] term such an interface a *free singular surface*.

An interface can be classified further according to its *thermal* properties as follows.

- *Thermally perfect interface*: The jump in the temperature and in the normal heat flux across the interface is zero.
- *Generic imperfect interface*: In this general case neither the jump in the temperature nor the jump in the normal heat flux across the interface need be zero. A thermal interface is an example of a generic imperfect interface. Özdemir et al. [76], for example, developed a thermomechanical cohesive zone model for generic imperfect interfaces. The following two models are specialisations of the generic imperfect interface model [see 77–79, and references therein].
 - (i) *Weakly-conducting (Kapitza) interface*: This type of imperfect interface is modelled using Kapitza’s concept of thermal resistance.¹ The model allows for a temperature jump across the interface. The normal heat flux is, however, continuous across the interface. The Kapitza model for thermal interfaces has been widely investigated [see e.g. 81, and references therein].
 - (ii) *Highly-conducting (HC) interface*: This type of imperfect interface models the temperature as continuous across the interface, whilst allowing a jump in the normal component of the heat flux. Yvonnet et al. [82] have used the HC model to numerically investigate the effective conductivity of nano-composites containing interfaces. For non-energetic interfaces, a jump in the heat flux across the interface is only possible if there is an associated heat flux along the interface [see e.g. 83]. This restriction does not hold for energetic interfaces [84].

Mosler and Scheider [85] recently described the admissible assumptions for the motion of the interface for a class of damage-type cohesive models. In a similar spirit, the relation of the interface temperature to that in the surrounding bulk is discussed here in detail. In particular, it is shown that *the interface temperature is not, in general, equal to the average of the temperature across the interface*.

Steinmann and Häsner [86] considered an energetic interface (with zero dissipation across the interface) within a thermomechanical solid subject to the assumption of infinitesimal deformation. Steinmann [87] presented extensive details on energetic surfaces using both the deformational and configurational frameworks of continuum mechanics. That investigation did not consider thermal contributions, interfaces or numerical aspects. Javili and Steinmann [88–91] extended the work to account for the thermomechanics of

¹Pyotr Leonidovich Kapitza (1894–1984) was a physicist and Nobel laureate who first proposed the presence of thermal interface resistance corresponding to a discontinuous temperature field across an interface for liquid helium, see Kapitza [80].

energetic surfaces and the implementation of the model using the finite element method. The current manuscript includes an extension of these works to account for the role of the interface and curve. Related works by Yvonnet et al. [81, 82] focus on stationary heat conduction across thermal interfaces.

The focus of this work is on *energetic elasticity* as compared to *entropic elasticity*. For entropic elastic materials, e.g. polymers, the temperature increases due to stretching. On the contrary, energetic elastic materials, e.g. metals, cool down when stretched. The thermomechanical coupling, whether for energetic or entropic elasticity, is termed henceforth the Gough–Joule effect. The Gough–Joule effect is often used for entropic elastic materials as it was originally realised for rubbers (see Gough [92] and Joule [93]). It is noteworthy, that the Gough–Joule effect is not solely due to the deformation but, it is rather the rate of a deformation which induces a change in the temperature field.

In summary, the key objectives and contributions of this work are as follows:

- To systematically derive the equations governing the response of a thermomechanical body, intersected by a material interface and enclosed by a surface, undergoing finite deformations coupled to transient heat conduction. The procedure used to derive the equations is general and could be applied to a range of complex phenomena;
- To account for the interaction between the interface and the surface;
- To derive the thermodynamically consistent constitutive relations, dissipation inequalities and temperature evolution equations in the various parts of the body (bulk, surface, interface and curve);
- To briefly present the weak formulation of the governing equations for the general case of a thermomechanical solid possessing an energetic surface, interface and curve. Various other models are shown to arise as restrictions of this general case;
- To elaborate various aspects of material (constitutive) modelling and discuss the admissible range of material parameters;
- To elucidate the theory with numerical examples based on a finite element and finite difference approximations of the governing equations.

This manuscript is organised as follows. The theory is presented in Chapter 2. The notation and certain key concepts are introduced briefly in Section 2.1. The equations governing the response of the bulk, surface, interface and curve are derived from fundamental balance principles in Section 2.2. A thermodynamic framework is then utilised in Section 2.3 to determine the form of the thermodynamically consistent constitutive relations.

The nature of the coupling between the primary fields (i.e. the displacement and the temperature), and the various parts of the body is made clear. The dissipation inequality for the interface is analysed in detail to show the possible relations between the interface temperature and that of the surrounding bulk. The computational aspects are then detailed in Chapter 3. The weak formulation of the governing equations is given in Section 3.1 thereby the mechanical and thermal weak forms for their most general case are derived. Various important problems, which result as restrictions of this general weak formulation, are highlighted. The finite element implementation of the obtained weak forms are detailed in Section 3.2. Aspects of material modelling are elaborated in Chapter 4. A surface Helmholtz energy is introduced and the relationship between surface material parameters is discussed. The admissibility of surface negative material parameters is investigated. A series of numerical example problems, based on approximations of the weak formulation, is presented in Chapter 5 to elucidate the theory. Chapter 6 concludes this work.

Substantial portions of the work presented here are contained in the following publications [31, 74, 84, 88–91, 94–98]:

- A. Javili and P. Steinmann. A finite element framework for continua with boundary energies. Part I: The two-dimensional case. *Computer Methods in Applied Mechanics and Engineering*, 198(27-29):2198–2208, 2009.
- A. Javili and P. Steinmann. A finite element framework for continua with boundary energies. Part II: The three-dimensional case. *Computer Methods in Applied Mechanics and Engineering*, 199(9-12):755–765, 2010.
- A. Javili and P. Steinmann. On thermomechanical solids with boundary structures. *International Journal of Solids and Structures*, 47(24):3245–3253, 2010.
- A. Javili and P. Steinmann. A finite element framework for continua with boundary energies. Part III: The thermomechanical case. *Computer Methods in Applied Mechanics and Engineering*, 200(21-22):1963–1977, 2011.
- A. McBride, A. Javili, P. Steinmann, and S. Bargmann. Geometrically nonlinear continuum thermomechanics with surface energies coupled to diffusion. *Journal of the Mechanics and Physics of Solids*, 59(10):2116–2133, 2011.
- P. Steinmann, A. McBride, S. Bargmann, and A. Javili. A deformational and configurational framework for geometrically non-linear continuum thermomechanics coupled to diffusion. *International Journal of Non-Linear Mechanics*, 47(2):215–227, 2012

- A. McBride, J. Mergheim, A. Javili, P. Steinmann, and S. Bargmann. Micro-to-macro transitions for heterogeneous material layers accounting for in-plane stretch. *Journal of the Mechanics and Physics of Solids*, 60(6):1221–1239, 2012.
- A. Javili, A. McBride, P. Steinmann, and B. D. Reddy. Relationships between the admissible range of surface material parameters and stability of linearly elastic bodies. *Philosophical Magazine*, 92:3540–3563, 2012.
- A. Javili, A. McBride, and P. Steinmann. Numerical modelling of thermomechanical solids with mechanically energetic (generalised) Kapitza interfaces. *Computational Material Science*, 65:542–551, 2012.
- A. Javili, A. McBride, and P. Steinmann. Numerical modelling of thermomechanical solids with highly-conductive energetic interfaces. *International Journal for Numerical Methods in Engineering*, 2012. doi: 10.1002/nme.4402.
- A. Javili, A. McBride, and P. Steinmann. Thermomechanics of solids with lower-dimensional Energetics: On the importance of surface, interface and curve structures at the nanoscale. A unifying review. (in print).
- A. Javili, A. McBride, P. Steinmann, J. Mergheim, and U. Schmidt. Micro-to-macro transitions for continua with surface structure at the microscale. (in review).

Chapter 2

Theory

The objective of this section is to derive the governing equations in the various parts of the body, i.e. in the bulk, on the surface, on the interface and on the curve. The notation and key concepts which are used throughout are introduced in Section 2.1. Then the problem is defined and the corresponding theorems and identities are detailed. In Section 2.2 the governing equations are derived from fundamental balance principles. Thereafter, a thermodynamic framework is utilised in Section 2.3 to determine the form of the thermodynamically consistent constitutive relations. The nature of the coupling between the primary fields, i.e. the displacement and the temperature, in the various parts of the body is made clear. The dissipation inequality for the interface is analysed in detail to show the possible relations between the interface temperature and that of the surrounding bulk. Finally, the temperature evolution equations are derived which, together with the balance of linear momentum, serve as the basis for the weak form of the balance equations and the computational implementation using the finite element method.

2.1 PRELIMINARIES

The purpose of this section is to summarise certain key concepts in nonlinear continuum mechanics and to introduce the notation adopted here. Detailed expositions on nonlinear continuum mechanics can be found in Marsden and Hughes [99], Šilhavý [100], Gurtin et al. [102], Holzapfel [103], Besson et al. [104], among others. For further details concerning the continuum mechanics of deformable surfaces and interfaces the reader is referred

to Gurtin and Struthers [38], Moeckel [44], Daher and Maugin [48] and the references therein.

2.1.1 Notation and definitions

Direct notation is adopted throughout. Occasional use is made of index notation, the summation convention for repeated indices being implied. The three-dimensional Euclidean space is denoted $\mathbb{E}^3$. The scalar product of two vectors $\mathbf{a}$ and $\mathbf{b}$ is denoted $\mathbf{a} \cdot \mathbf{b} = [\mathbf{a}]_i [\mathbf{b}]_i$. The scalar product of two second-order tensors $\mathbf{A}$ and $\mathbf{B}$ is denoted $\mathbf{A} : \mathbf{B} = [\mathbf{A}]_{ij} [\mathbf{B}]_{ij}$. The composition of two second-order tensors $\mathbf{A}$ and $\mathbf{B}$, denoted $\mathbf{A} \cdot \mathbf{B}$, is a second-order tensor with components $[\mathbf{A} \cdot \mathbf{B}]_{ij} = [\mathbf{A}]_{im} [\mathbf{B}]_{mj}$. The vector product of two vectors $\mathbf{a}$ and $\mathbf{b}$ is denoted $\mathbf{a} \times \mathbf{b}$ with $[\mathbf{a} \times \mathbf{b}]_k = [\varepsilon]_{ijk} [\mathbf{a}]_i [\mathbf{b}]_j$, where ε denotes the third-order permutation (Levi-Civita) tensor. Analogously, the vector product of a vector $\mathbf{a}$ and a second-order tensor $\mathbf{B}$ is denoted $\mathbf{a} \times \mathbf{B}$ with $[\mathbf{a} \times \mathbf{B}]_{kl} = [\varepsilon]_{ijk} [\mathbf{a}]_i [\mathbf{B}]_{jl}$. The non-standard products of a fourth-order tensor $\mathbb{C}$ and a vector $\mathbf{b}$ are defined by $[\mathbf{b} \cdot \mathbb{C}]_{ikl} = [\mathbb{C}]_{ijkl} [\mathbf{b}]_j$ and $[\mathbb{C} \cdot \mathbf{b}]_{ijl} = [\mathbb{C}]_{ijkl} [\mathbf{b}]_k$. Other non-standard products of a fourth-order tensor $\mathbb{C}$ and a vector $\mathbf{b}$ are defined by $[\mathbf{b} \cdot \mathbb{C}]_{ijl} = [\mathbb{C}]_{ijkl} [\mathbf{b}]_k$ and $[\mathbb{C} \cdot \mathbf{b}]_{ikl} = [\mathbb{C}]_{ijkl} [\mathbf{b}]_j$. The non-standard product of a fourth-order tensor $\mathbb{C}$ and a second-order tensor $\mathbf{A}$ is defined by $[\mathbb{C} \cdot \mathbf{A}]_{ik} = [\mathbb{C}]_{ijkl} [\mathbf{A}]_{jl}$. The non-standard minor transposes of a fourth-order tensor $\mathbb{C}$ are defined by $[\mathbf{t}\mathbb{C}]_{ijkl} = [\mathbb{C}]_{jikl}$ and $[\mathbb{C}^t]_{ijkl} = [\mathbb{C}]_{ijlk}$. The action of a second-order tensor $\mathbf{A}$ on a vector $\mathbf{a}$ is given by $[\mathbf{A} \cdot \mathbf{a}]_i = [\mathbf{A}]_{ij} [\mathbf{a}]_j$. The tensor product of two vectors $\mathbf{a}$ and $\mathbf{b}$ is a second-order tensor $\mathbf{D} = \mathbf{a} \otimes \mathbf{b}$ with $[\mathbf{D}]_{ij} = [\mathbf{a}]_i [\mathbf{b}]_j$. The tensor product of two second-order tensors $\mathbf{A}$ and $\mathbf{B}$ is a fourth-order tensor $\mathbb{D} = \mathbf{A} \otimes \mathbf{B}$ with $[\mathbb{D}]_{ijkl} = [\mathbf{A}]_{ij} [\mathbf{B}]_{kl}$. The two non-standard tensor products of two second-order tensors $\mathbf{A}$ and $\mathbf{B}$ are the fourth-order tensors $[\mathbf{A} \bar{\otimes} \mathbf{B}]_{ijkl} = [\mathbf{A}]_{ik} [\mathbf{B}]_{jl}$ and $[\mathbf{A} \underline{\otimes} \mathbf{B}]_{ijkl} = [\mathbf{A}]_{il} [\mathbf{B}]_{jk}$.

Quantities or operators corresponding to the bulk, surface, interface and curve are denoted as $\{\bullet\}$, $\{\bullet\}$, $\{\bullet\}$ and $\{\bullet\}$, respectively, unless specified otherwise. Note, $\{\bullet\}$ denotes a surface-quantity which is not necessarily tangent to the surface. A bulk quantity $\{\bullet\}$ on the surface implies the evaluation of $\{\bullet\}$ on the surface and is not, in general, equivalent to the corresponding surface quantity $\{\bullet\}$.

The expression *the various parts of the body* implies *the bulk, the surface, the interface and the curve*.

Key definitions are given in Table 2.1 and Table 2.2. For the derivations thereof and extensive technical details see e.g. Steinmann [87]. Basic concepts and terminologies of surfaces and curves can be found in classical manuscripts on differential geometry [see 105–110, among others]. The fundamentals of differential geometry on surfaces and curves are briefly reviewed in Appendix A.

Table 2.1: Summary of the notation used to denote key quantities and operators in the various parts of the body. Quantities and operators corresponding to the material and spatial configurations are distinguished by a semicolon.

	Bulk	Surface	Interface	Curve
Domain	$\mathcal{B}_0; \mathcal{B}_t$	$\mathcal{S}_0; \mathcal{S}_t$	$\mathcal{S}_0; \mathcal{S}_t$	$\mathcal{C}_0; \mathcal{C}_t$
normal		$N; n$	$\bar{N}; \bar{N}^\mp; \bar{n}, \bar{n}^\mp$	$\bar{N}_c, \bar{N}_i, \bar{N}_s, \bar{N}_s^\pm; \tilde{n}_c, \tilde{n}_i, \tilde{n}_s, \tilde{n}_s^\pm$
tangent		$\bar{N}_s, \bar{N}; \tilde{n}_s, \tilde{n}$	$\bar{N}_i; \tilde{n}_i$	$\bar{N}; \tilde{n}$
Unit tensor	$I; i$	$\hat{I}; \hat{i}$	$\bar{I}; \bar{i}$	$\tilde{I}; \tilde{i}$
Differential element	$dV; dv$	$dA; da$	$dA; da$	$dL; dl$
Oriented element	–	$dA; da$	$dA; da$	$dL; dl$
Control regions	$\mathcal{B}_0; \mathcal{B}_t$	$S_0; S_t$	$\mathcal{I}_0; \mathcal{I}_t$	$\mathcal{C}_0; \mathcal{C}_t$
Curvature	–	$\hat{C}; \hat{c}$	$\bar{C}; \bar{c}$	$\tilde{C}; \tilde{c}$
Covariant basis	$G_1, G_2, G_3; g_1, g_2, g_3$	$\hat{G}_1, \hat{G}_2; \hat{g}_1, \hat{g}_2$	$\bar{G}_1, \bar{G}_2; \bar{g}_1, \bar{g}_2$	$\tilde{G}_1; \tilde{g}_1$
Contravariant basis	$G^1, G^2, G^3; g^1, g^2, g^3$	$\hat{G}^1, \hat{G}^2; \hat{g}^1, \hat{g}^2$	$\bar{G}^1, \bar{G}^2; \bar{g}^1, \bar{g}^2$	$\tilde{G}^1; \tilde{g}^1$
Placement	$X; x$	$\hat{X}; \hat{x}$	$\bar{X}; \bar{x}$	$\tilde{X}; \tilde{x}$
Tangent map	$F; f$	$\hat{F}; \hat{f}$	$\bar{F}; \bar{f}$	$\tilde{F}; \tilde{f}$
Normal map	$\text{Cof } F; \text{cof } f$	$\widehat{\text{Cof}} \hat{F}; \widehat{\text{cof}} \hat{f}$	$\overline{\text{Cof}} \bar{F}; \overline{\text{cof}} \bar{f}$	$\widetilde{\text{Cof}} \tilde{F}; \widetilde{\text{cof}} \tilde{f}$
Jacobian	$J; j$	$\hat{J}; \hat{j}$	$\bar{J}; \bar{j}$	$\tilde{J}; \tilde{j}$
Velocity	$V; v$	$\hat{V}; \hat{v}$	$\bar{V}; \bar{v}$	$\tilde{V}; \tilde{v}$
Divergence	$\text{Div}; \text{div}$	$\widehat{\text{Div}}; \widehat{\text{div}}$	$\overline{\text{Div}}; \overline{\text{div}}$	$\widetilde{\text{Div}}; \widetilde{\text{div}}$
Gradient	$\text{Grad}; \text{grad}$	$\widehat{\text{Grad}}; \widehat{\text{grad}}$	$\overline{\text{Grad}}; \overline{\text{grad}}$	$\widetilde{\text{Grad}}; \widetilde{\text{grad}}$
Determinant	$\text{Det}; \text{det}$	$\widehat{\text{Det}}; \widehat{\text{det}}$	$\overline{\text{Det}}; \overline{\text{det}}$	$\widetilde{\text{Det}}; \widetilde{\text{det}}$
Cofactor	$\text{Cof}; \text{cof}$	$\widehat{\text{Cof}}; \widehat{\text{cof}}$	$\overline{\text{Cof}}; \overline{\text{cof}}$	$\widetilde{\text{Cof}}; \widetilde{\text{cof}}$

Table 2.2: Summary of the notation used to denote key quantities and operators in the bulk, on the surface and interface and on the curve corresponding to the material and spatial configurations.

Material configuration	Spatial configuration
$I := G_1 \otimes G^1 + G_2 \otimes G^2 + G_3 \otimes G^3$ $\text{Grad}\{\bullet\} := \partial_x \{\bullet\} \quad \text{Div}\{\bullet\} := \text{Grad}\{\bullet\} : I$ $\text{Det}\{\bullet\} := [\{\bullet\} \cdot G_1] \cdot [\{\bullet\} \cdot G_2] \times [\{\bullet\} \cdot G_3] / [G_1 \cdot [G_2 \times G_3]]$ $\text{Cof}\{\bullet\} := \text{Det}\{\bullet\} \{\bullet\}^{-t} \quad dv = J dV \quad da = \text{Cof } F \cdot dA$	$i := g_1 \otimes g^1 + g_2 \otimes g^2 + g_3 \otimes g^3$ $\text{grad}\{\bullet\} := \partial_x \{\bullet\} \quad \text{div}\{\bullet\} := \text{grad}\{\bullet\} : i$ $\text{det}\{\bullet\} := [\{\bullet\} \cdot g_1] \cdot [\{\bullet\} \cdot g_2] \times [\{\bullet\} \cdot g_3] / [g_1 \cdot [g_2 \times g_3]]$ $\text{cof}\{\bullet\} := \text{det}\{\bullet\} \{\bullet\}^{-t} \quad dV = j dv \quad dA = \text{cof } f \cdot da$
$\hat{I} := \hat{G}_1 \otimes \hat{G}^1 + \hat{G}_2 \otimes \hat{G}^2 = I - N \otimes N$ $\widehat{\text{Grad}}\{\bullet\} := \text{Grad}\{\bullet\} \cdot \hat{I} \quad \widehat{\text{Div}}\{\bullet\} := \widehat{\text{Grad}}\{\bullet\} : \hat{I}$ $\widehat{\text{Det}}\{\bullet\} := [[\{\bullet\} \cdot \hat{G}_1] \times [\{\bullet\} \cdot \hat{G}_2]] / \hat{G}_1 \times \hat{G}_2 $ $\widehat{\text{Cof}}\{\bullet\} := \widehat{\text{Det}}\{\bullet\} \{\bullet\}^{-t} \quad da = \hat{J} dA \quad dL = \widehat{\text{Cof}} \hat{F} \cdot dL$	$\hat{i} := \hat{g}_1 \otimes \hat{g}^1 + \hat{g}_2 \otimes \hat{g}^2 = i - n \otimes n$ $\widehat{\text{grad}}\{\bullet\} := \text{grad}\{\bullet\} \cdot \hat{i} \quad \widehat{\text{div}}\{\bullet\} := \widehat{\text{grad}}\{\bullet\} : \hat{i}$ $\widehat{\text{det}}\{\bullet\} := [[\{\bullet\} \cdot \hat{g}_1] \times [\{\bullet\} \cdot \hat{g}_2]] / \hat{g}_1 \times \hat{g}_2 $ $\widehat{\text{cof}}\{\bullet\} := \widehat{\text{det}}\{\bullet\} \{\bullet\}^{-t} \quad dA = \hat{j} da \quad dL = \widehat{\text{cof}} \hat{f} \cdot dL$
$\bar{I} := \bar{G}_1 \otimes \bar{G}^1 + \bar{G}_2 \otimes \bar{G}^2 = I - \bar{N} \otimes \bar{N}$ $\overline{\text{Grad}}\{\bullet\} := \text{Grad}\{\bullet\} \cdot \bar{I} \quad \overline{\text{Div}}\{\bullet\} := \overline{\text{Grad}}\{\bullet\} : \bar{I}$ $\overline{\text{Det}}\{\bullet\} := [[\{\bullet\} \cdot \bar{G}_1] \times [\{\bullet\} \cdot \bar{G}_2]] / \bar{G}_1 \times \bar{G}_2 $ $\overline{\text{Cof}}\{\bullet\} := \overline{\text{Det}}\{\bullet\} \{\bullet\}^{-t} \quad da = \bar{J} dA \quad dL = \overline{\text{Cof}} \bar{F} \cdot dL$	$\bar{i} := \bar{g}_1 \otimes \bar{g}^1 + \bar{g}_2 \otimes \bar{g}^2 = i - \bar{n} \otimes \bar{n}$ $\overline{\text{grad}}\{\bullet\} := \text{grad}\{\bullet\} \cdot \bar{i} \quad \overline{\text{div}}\{\bullet\} := \overline{\text{grad}}\{\bullet\} : \bar{i}$ $\overline{\text{det}}\{\bullet\} := [[\{\bullet\} \cdot \bar{g}_1] \times [\{\bullet\} \cdot \bar{g}_2]] / \bar{g}_1 \times \bar{g}_2 $ $\overline{\text{cof}}\{\bullet\} := \overline{\text{det}}\{\bullet\} \{\bullet\}^{-t} \quad dA = \bar{j} da \quad dL = \overline{\text{cof}} \bar{f} \cdot dL$
$\tilde{I} := \tilde{G}_1 \otimes \tilde{G}^1 = \tilde{N} \otimes \tilde{N}$ $\widetilde{\text{Grad}}\{\bullet\} := \text{Grad}\{\bullet\} \cdot \tilde{I} \quad \widetilde{\text{Div}}\{\bullet\} := \widetilde{\text{Grad}}\{\bullet\} : \tilde{I}$ $\widetilde{\text{Det}}\{\bullet\} := [\{\bullet\} \cdot \tilde{G}_1] / \tilde{G}_1 $ $\widetilde{\text{Cof}}\{\bullet\} := \widetilde{\text{Det}}\{\bullet\} \{\bullet\}^{-t} \quad dL = \tilde{J} dL \quad \tilde{n} = \widetilde{\text{Cof}} \tilde{F} \cdot \tilde{N}$	$\tilde{i} := \tilde{g}_1 \otimes \tilde{g}^1 = \tilde{n} \otimes \tilde{n}$ $\widetilde{\text{grad}}\{\bullet\} := \text{grad}\{\bullet\} \cdot \tilde{i} \quad \widetilde{\text{div}}\{\bullet\} := \widetilde{\text{grad}}\{\bullet\} : \tilde{i}$ $\widetilde{\text{det}}\{\bullet\} := [\{\bullet\} \cdot \tilde{g}_1] / \tilde{g}_1 $ $\widetilde{\text{cof}}\{\bullet\} := \widetilde{\text{det}}\{\bullet\} \{\bullet\}^{-t} \quad dL = \tilde{j} dL \quad \tilde{N} = \widetilde{\text{cof}} \tilde{f} \cdot \tilde{n}$

2.1.2 Kinematics

Consider a continuum body that takes the open set $B_0 \subset \mathbb{E}^3$ at the time $t = 0$. The boundary of the body B_0 is denoted by $S_0 := \partial B_0$. The body B_0 is partitioned into two disjoint subdomains, denoted by the open sets B_0^+ and B_0^- , by a two-sided interface $\mathcal{I}_0$. The interface $\mathcal{I}_0$ is an open set, thus $B_0 = B_0^+ \cup \mathcal{I}_0 \cup B_0^-$. The boundary of the interface, a two-sided curve, is denoted as $\mathcal{C}_0 := \partial \mathcal{I}_0$. In a similar fashion to the interface, the curve $\mathcal{C}_0$ partitions the surface S_0 into two open sets $\mathcal{I}_0^+$ and $\mathcal{I}_0^-$ such that $\mathcal{I}_0^+ \cap \mathcal{I}_0^- = \emptyset$ and $S_0 = \mathcal{I}_0^+ \cup \mathcal{C}_0 \cup \mathcal{I}_0^-$.

Remark The boundary S_0 is closed and is assumed to be smooth. For the more general case where the boundary S_0 is non-smooth, the curve $\mathcal{C}_0$ can be understood as a geometrical entity. For the restricted case considered here where the boundary is smooth, the curve $\mathcal{C}_0$ accounts for the interaction between the interface and the surface and should be understood as a physical entity. The extension of this work to non-smooth boundaries is straightforward. Nevertheless, it involves introducing additional geometric concepts and further notation while providing little additional insight into the fundamental concepts. $\square$

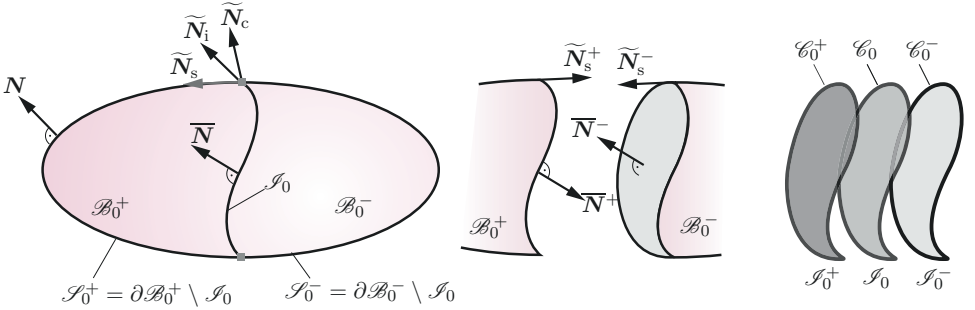


Figure 2.1: The domains B_0 , S_0 , $\mathcal{I}_0$ and $\mathcal{C}_0$ and the various unit normals.

The bulk is defined by $B_0 := B_0^+ \cup B_0^-$ and is the reference placement of material particles labelled $\mathbf{X} \in B_0$. The two sides of the interface $\mathcal{I}_0$ are denoted $\mathcal{I}_0^+ := \partial B_0^+ \cap \mathcal{I}_0$ and $\mathcal{I}_0^- := \partial B_0^- \cap \mathcal{I}_0$, with $\mathcal{I}_0 = \mathcal{I}_0^+ \cup \mathcal{I}_0^-$. Material particles on the interface are labelled $\bar{\mathbf{X}} \in \mathcal{I}_0$ and, by definition, $\bar{\mathbf{X}} := \mathbf{X}|_{\mathcal{I}_0}$. The outward unit normals to $\mathcal{I}_0^+$ and $\mathcal{I}_0^-$ are denoted $\bar{\mathbf{N}}^+$ and $\bar{\mathbf{N}}^-$, respectively, with $\bar{\mathbf{N}}^+(\bar{\mathbf{X}}) = -\bar{\mathbf{N}}^-(\bar{\mathbf{X}})$. The unit normal to $\mathcal{I}_0$, as depicted in Fig. 2.1, is denoted $\bar{\mathbf{N}}(\bar{\mathbf{X}}) := \bar{\mathbf{N}}^-(\bar{\mathbf{X}})$.

The surface is defined by $S_0 := \mathcal{I}_0^+ \cup \mathcal{I}_0^-$ with outward unit normal $\mathbf{N}$. Material particles on the surface are labelled $\hat{\mathbf{X}} \in S_0$ and, by definition, $\hat{\mathbf{X}} = \mathbf{X}|_{S_0}$. The two sides of the curve $\mathcal{C}_0$ are denoted $\mathcal{C}_0^+ := \partial \mathcal{I}_0^+$ and $\mathcal{C}_0^- := \partial \mathcal{I}_0^-$, with $\mathcal{C}_0 = \mathcal{C}_0^+ \cup \mathcal{C}_0^-$. Material

particles on the curve $\mathcal{C}_0$ are labelled $\tilde{\mathbf{X}} \in \mathcal{C}_0$, where $\tilde{\mathbf{X}} := \mathbf{X}|_{\mathcal{C}_0}$. The outward unit normals to $\mathcal{C}_0^+$ and $\mathcal{C}_0^-$, tangential to $\mathcal{I}_0$ and identical at a point $\tilde{\mathbf{X}}$, are denoted $\tilde{\mathbf{N}}_i$. The unit normals to $\mathcal{C}_0^+$ and $\mathcal{C}_0^-$, tangential to $\mathcal{S}_0$, are denoted $\tilde{\mathbf{N}}_s^+$ and $\tilde{\mathbf{N}}_s^-$, respectively, with $\tilde{\mathbf{N}}_s^+(\tilde{\mathbf{X}}) = -\tilde{\mathbf{N}}_s^-(\tilde{\mathbf{X}})$. The unit normal to $\mathcal{C}_0$, tangential to $\mathcal{S}_0$, is defined by $\tilde{\mathbf{N}}_s(\tilde{\mathbf{X}}) := \tilde{\mathbf{N}}_s^+(\tilde{\mathbf{X}})$. The unit normals to $\mathcal{C}_0$ in the sense of the Frénet–Serret formulae and identical at a point $\tilde{\mathbf{X}}$, are denoted $\tilde{\mathbf{N}}_c$. Note that $\tilde{\mathbf{N}}_c$ does not necessarily coincide with either $\tilde{\mathbf{N}}_i$ or $\tilde{\mathbf{N}}_s$.

Let $\mathcal{T} = [0, t_{\text{end}}] \subset \mathbb{R}_+$ denote the time domain. A motion of the reference placement for a time $t \in \mathcal{T}$ is denoted by the orientation-preserving map $\varphi : \mathcal{B}_0 \times \mathcal{T} \rightarrow \mathbb{E}^3$. The current placement of the bulk associated with the motion φ is denoted $\mathcal{B}_t = \varphi(\mathcal{B}_0(\mathbf{X}), t)$ with particles designated as $\mathbf{x} = \varphi(\mathbf{X}, t) \in \mathcal{B}_t$ (see Fig. 2.2).¹

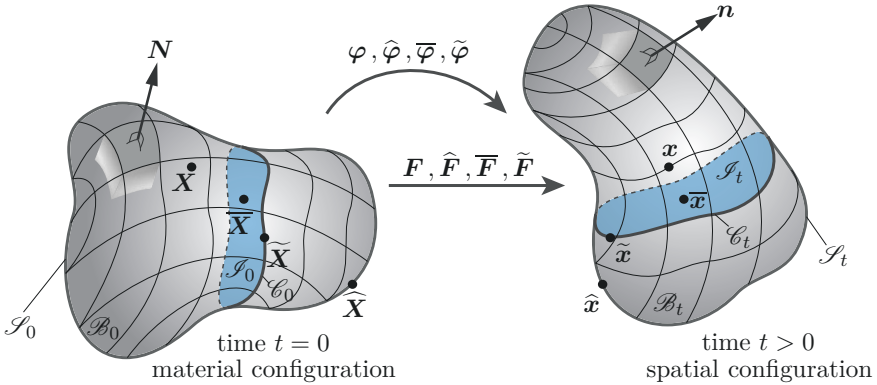


Figure 2.2: The material and spatial configurations of a continuum body, and the associated motions, deformation gradients and velocity measures in the various parts of the body.

The restriction of the motion φ to the surface $\mathcal{S}_0$ is denoted $\hat{\varphi}$. The current placement of the surface is denoted $\mathcal{S}_t = \hat{\varphi}(\mathcal{S}_0(\tilde{\mathbf{X}}), t)$ with particles $\hat{\mathbf{x}} = \hat{\varphi}(\tilde{\mathbf{X}}, t) \in \mathcal{S}_t$. It is assumed that particles on the surface of the body $\mathcal{S}_0$ constitute the surface for all times $t \in \mathcal{T}$ and $\hat{\varphi} = \varphi|_{\mathcal{S}_0}$, consequently $\hat{\mathbf{x}} = \mathbf{x}|_{\mathcal{S}_t}$. This assumption, referred to as kinematic slavery by Steinmann and Häsner [86], mimics coherence in interfaces.

The restriction of the motion φ to the positive and negative sides of the interface $\mathcal{I}_0$ is denoted $\bar{\varphi}^+$ and $\bar{\varphi}^-$, respectively. The placements of the positive and negative sides of the interface at time t are denoted $\mathcal{I}_t^+ = \bar{\varphi}^+(\mathcal{I}_0^+(\tilde{\mathbf{X}}), t)$ and $\mathcal{I}_t^- = \bar{\varphi}^-(\mathcal{I}_0^-(\tilde{\mathbf{X}}), t)$,

¹Here and henceforth, the subscripts t and 0 shall designate spatial and material quantities, respectively, unless specified otherwise.

respectively, with particles $\bar{x}^+ = \bar{\varphi}^+(\bar{X}, t) \in \mathcal{I}_t^+$ and $\bar{x}^- = \bar{\varphi}^-(\bar{X}, t) \in \mathcal{I}_t^-$. The material interface is assumed to be coherent: the motion is not necessarily smooth across the interface, however, it is continuous across the interface, smooth away from the interface and smooth up to the interface from either side [111]. Thus, $\bar{\varphi}^+ = \bar{\varphi}^- = \varphi|_{\mathcal{I}_0}$ and consequently $\bar{x}^+ = \bar{x}^- = x|_{\mathcal{I}_t}$. The restriction of the motion φ to the interface is defined by $\bar{\varphi} := \varphi|_{\mathcal{I}_0}$ with particles designated as $\bar{x} = \bar{\varphi}(\bar{X}, t) \in \mathcal{I}_t$.

Remark Given that this work focuses on coherent material interfaces it may seem superfluous to distinguish between $\mathcal{I}_t^+$ and $\mathcal{I}_t^-$. However coherence concerns only the continuity of the motion across the interface and jumps in other fields, e.g. temperature, are permitted. $\square$

Following from the aforementioned assumptions, the restriction of the motion φ to the curve $\mathcal{C}_0$ at the junction of the interface and the surface is denoted $\tilde{\varphi}$. The current placement of the curve is denoted $\mathcal{C}_t = \tilde{\varphi}(\mathcal{C}_0(\tilde{X}), t)$ with particles $\tilde{x} = \tilde{\varphi}(\tilde{X}, t) \in \mathcal{C}_t$. Finally, $\tilde{\varphi} = \varphi|_{\mathcal{C}_0}$ and $\tilde{x} = x|_{\mathcal{C}_t} = \bar{x}|_{\mathcal{C}_t} = \hat{x}|_{\mathcal{C}_t}$.

For the normal vectors to the surface, interface and curve in the spatial configuration the same convention as in the material configuration is used, however, with lower-case n instead of upper-case N (see Table 2.1).

The deformation gradient $F : T\mathcal{B}_0 \rightarrow T\mathcal{B}_t$, that is the (invertible) linear tangent map between spatial and material line elements $dx \in T\mathcal{B}_t$ (tangent space to $\mathcal{B}_t$) and $dX \in T\mathcal{B}_0$, and the associated (material) velocity V are defined by

$$F(X, t) := \text{Grad} \varphi(X, t) \quad \text{and} \quad V := D_t \varphi(X, t).$$

Similarly, the various deformation gradients and the (material) velocities for the remainder of the body are given by

$$\begin{aligned} \hat{F} : T\mathcal{S}_0 &\rightarrow T\mathcal{S}_t, & \hat{F}(\hat{X}, t) &:= \widehat{\text{Grad}} \hat{\varphi}(\hat{X}, t) & \text{and} & \quad \hat{V} := D_t \hat{\varphi}(\hat{X}, t), \\ \bar{F} : T\mathcal{I}_0 &\rightarrow T\mathcal{I}_t, & \bar{F}(\bar{X}, t) &:= \overline{\text{Grad}} \bar{\varphi}(\bar{X}, t) & \text{and} & \quad \bar{V} := D_t \bar{\varphi}(\bar{X}, t), \\ \tilde{F} : T\mathcal{C}_0 &\rightarrow T\mathcal{C}_t, & \tilde{F}(\tilde{X}, t) &:= \widetilde{\text{Grad}} \tilde{\varphi}(\tilde{X}, t) & \text{and} & \quad \tilde{V} := D_t \tilde{\varphi}(\tilde{X}, t). \end{aligned}$$

Here, $D_t \{\bullet\}$ denotes the material time derivative of a quantity. The material time derivative $D_t \{\bullet\}$ is related to the spatial time derivative $d_t \{\bullet\}$ according to

$$\begin{aligned} D_t \{\bullet\} &= d_t \{\bullet\} + \text{grad} \{\bullet\} \cdot V, & D_t \{\hat{\bullet}\} &= d_t \{\hat{\bullet}\} + \widehat{\text{grad}} \{\hat{\bullet}\} \cdot \hat{V}, \\ D_t \{\bar{\bullet}\} &= d_t \{\bar{\bullet}\} + \overline{\text{grad}} \{\bar{\bullet}\} \cdot \bar{V}, & D_t \{\tilde{\bullet}\} &= d_t \{\tilde{\bullet}\} + \widetilde{\text{grad}} \{\tilde{\bullet}\} \cdot \tilde{V}. \end{aligned}$$

Furthermore, a spatial description of the motion can be obtained from the material description by transforming the independent variables from the material coordinates to the

spatial coordinates. The spatial velocity fields in the various parts of the body are obtained from the material velocity fields via

$$v(\varphi(\mathbf{X}, t), t) = \mathbf{V}(\mathbf{X}, t), \quad \widehat{v}(\widehat{\varphi}(\widehat{\mathbf{X}}, t), t) = \widehat{\mathbf{V}}(\widehat{\mathbf{X}}, t), \quad (2.1)$$

$$\overline{v}(\overline{\varphi}(\overline{\mathbf{X}}, t), t) = \overline{\mathbf{V}}(\overline{\mathbf{X}}, t), \quad \widetilde{v}(\widetilde{\varphi}(\widetilde{\mathbf{X}}, t), t) = \widetilde{\mathbf{V}}(\widetilde{\mathbf{X}}, t). \quad (2.2)$$

The inverse deformation gradient $\mathbf{f} : T\mathcal{B}_t \rightarrow T\mathcal{B}_0$, i.e. the linear tangent map between material and spatial line elements $d\mathbf{X}$ and $d\mathbf{x}$, is defined by

$$\mathbf{f}(\mathbf{x}, t) := \text{grad}\varphi^{-1}(\mathbf{x}, t) \quad \text{with} \quad \mathbf{F} \cdot \mathbf{f} = \mathbf{i}, \quad \mathbf{f} \cdot \mathbf{F} = \mathbf{I}.$$

The surface, interface and curve deformation gradients ($\widehat{\mathbf{F}}$, $\overline{\mathbf{F}}$ and $\widetilde{\mathbf{F}}$) are non-invertible linear tangent maps between the respective spatial and material elements. Although these deformation gradients are non-invertible, due to rank deficiency, they each possess an inverse, denoted as $\widehat{\mathbf{f}}$, $\overline{\mathbf{f}}$ and $\widetilde{\mathbf{f}}$ respectively, in the following generalised sense:

$$\widehat{\mathbf{F}} \cdot \widehat{\mathbf{f}} = \widehat{\mathbf{i}}, \quad \widehat{\mathbf{f}} \cdot \widehat{\mathbf{F}} = \widehat{\mathbf{I}}, \quad \overline{\mathbf{F}} \cdot \overline{\mathbf{f}} = \overline{\mathbf{i}}, \quad \overline{\mathbf{f}} \cdot \overline{\mathbf{F}} = \overline{\mathbf{I}}, \quad \widetilde{\mathbf{F}} \cdot \widetilde{\mathbf{f}} = \widetilde{\mathbf{i}}, \quad \widetilde{\mathbf{f}} \cdot \widetilde{\mathbf{F}} = \widetilde{\mathbf{I}}.$$

The volume elements in the bulk, the area elements on the surface and interface and the line elements on the curve in the material and spatial configurations can be mapped into each other by means of the Jacobian determinants of their associated deformation gradients and their inverses in the various parts of the body as:

$$\begin{aligned} dv &= J dV \quad \text{with} \quad J := \text{Det } \mathbf{F}, & dV &= j dv \quad \text{with} \quad j := \det \mathbf{f}, \\ da &= \widehat{J} dA \quad \text{with} \quad \widehat{J} := \widehat{\text{Det}} \widehat{\mathbf{F}}, & dA &= \widehat{j} da \quad \text{with} \quad \widehat{j} := \widehat{\det} \widehat{\mathbf{f}}, \\ da &= \overline{J} dA \quad \text{with} \quad \overline{J} := \overline{\text{Det}} \overline{\mathbf{F}}, & dA &= \overline{j} da \quad \text{with} \quad \overline{j} := \overline{\det} \overline{\mathbf{f}}, \\ dl &= \widetilde{J} dL \quad \text{with} \quad \widetilde{J} := \widetilde{\text{Det}} \widetilde{\mathbf{F}}, & dL &= \widetilde{j} dl \quad \text{with} \quad \widetilde{j} := \widetilde{\det} \widetilde{\mathbf{f}}. \end{aligned}$$

2.1.3 Control regions

The equations governing the coupled response of the various parts of the body are obtained from the balances of linear and angular momentum, energy, and entropy performed over a control region. These balances are then localised at arbitrary points in the bulk $\mathcal{B}_0$, on the surface $\mathcal{S}_0$, on the interface $\mathcal{I}_0$ or on the curve $\mathcal{C}_0$.

The canonical control region is defined as one which possibly has as part of its boundary the surface $\mathcal{S}_0$ and is denoted $\mathcal{B}_0 \subset \mathcal{B}_0$ with boundary $\partial\mathcal{B}_0$ (see Fig. 2.3). The orientable external surface of the control region is defined by $S_0^{\text{ext}} := \partial\mathcal{B}_0 \cap \mathcal{S}_0$ while the interior surface is $S_0^{\text{int}} := \partial\mathcal{B}_0 \setminus S_0^{\text{ext}}$. The outward unit normals to S_0^{int} and S_0^{ext} are denoted $\mathbf{M}$ and $\mathbf{N}$, respectively. The surface of the control region is defined by $S_0 := S_0^{\text{ext}} \cup S_0^{\text{int}}$. The boundary of S_0^{ext} , a curve, is defined by $\mathcal{L}_0 := \partial S_0^{\text{ext}}$. The unit normal to the curve $\mathcal{L}_0$ is denoted $\widehat{\mathbf{N}}$ and is tangent to the surface S_0^{ext} .

The control region $\mathcal{B}_0$ can include a segment of the interface $\mathcal{I}_0$ defined by $\mathcal{I}_0 := \mathcal{B}_0 \cap \mathcal{I}_0$. Thus, $\mathcal{B}_0$ can be partitioned into two subdomains $\mathcal{B}_0^+$ and $\mathcal{B}_0^-$. The interface $\mathcal{I}_0$ has two sides $\mathcal{I}_0^+ := \mathcal{I}_0 \cap \partial\mathcal{B}_0^+$ and $\mathcal{I}_0^- := \mathcal{I}_0 \cap \partial\mathcal{B}_0^-$ with $\mathcal{I}_0 = \mathcal{I}_0^+ \cup \mathcal{I}_0^-$.

The boundary of the interface $\partial\mathcal{I}_0$ is a curve denoted as $\mathcal{C}_0$. The, possibly empty, intersection of the curves $\mathcal{C}_0$ and $\mathcal{C}_0$ is denoted as $\mathcal{C}_0^{\text{ext}} := \mathcal{C}_0 \cap \mathcal{C}_0$. The interior boundary of the interface $\mathcal{I}_0$ is $\mathcal{C}_0^{\text{int}} := \mathcal{C}_0 \setminus \mathcal{C}_0^{\text{ext}}$. The outward unit normal to the curve $\mathcal{C}_0^{\text{int}}$ is denoted $\overline{M}$ and is tangent to the interface $\mathcal{I}_0$. The unit normal to the curve $\mathcal{C}_0^{\text{ext}}$, tangent to the interface $\mathcal{I}_0$, is denoted $\widetilde{N}_i$. The unit normal to the curve $\mathcal{C}_0^{\text{ext}}$, in the sense of Frénet–Serret formulae, is denoted $\widetilde{N}_c$. The unit normal to the curve $\mathcal{C}_0^{\text{ext}}$, tangent to the surface $\mathcal{S}_0$, is denoted $\widetilde{N}_s$. The unit normal to the boundary of the curve $\partial\mathcal{C}_0^{\text{ext}}$, tangent to the curve $\mathcal{C}_0^{\text{ext}}$ is denoted $\widetilde{N}$. The curve $\mathcal{C}_0^{\text{ext}}$ has two sides $^+\mathcal{C}_0^{\text{ext}} := \mathcal{C}_0^{\text{ext}} \cap \partial\mathcal{I}_0^+$ and $^-\mathcal{C}_0^{\text{ext}} := \mathcal{C}_0^{\text{ext}} \cap \partial\mathcal{I}_0^-$ with $\mathcal{C}_0^{\text{ext}} = ^+\mathcal{C}_0^{\text{ext}} \cup ^-\mathcal{C}_0^{\text{ext}}$. Analogously, $^+\mathcal{C}_0^{\text{int}} := \mathcal{C}_0^{\text{int}} \cap \partial\mathcal{I}_0^+$ and $^-\mathcal{C}_0^{\text{int}} := \mathcal{C}_0^{\text{int}} \cap \partial\mathcal{I}_0^-$ with $\mathcal{C}_0^{\text{int}} = ^+\mathcal{C}_0^{\text{int}} \cup ^-\mathcal{C}_0^{\text{int}}$.

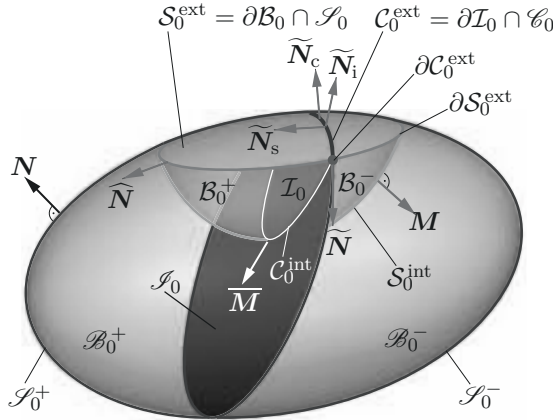


Figure 2.3: The bulk $\mathcal{B}_0$ and the canonical control region $\mathcal{B}_0$ and its representation in the bulk, and on the surface, interface and curve.

2.1.4 Key definitions and identities

Various key definitions and identities which are required in the remainder of the presentation are now introduced. Several other useful relations are recorded in Appendix B.1.

2.1.4.1 Jump and average relations

The following identity relates the jump of the product of two quantities (scalars or tensors, arbitrarily denoted $\mathbf{a}$ and $\mathbf{c}$) to the products of their jumps and averages:

$$\llbracket \mathbf{a} \star \mathbf{c} \rrbracket = \llbracket \mathbf{a} \rrbracket \star \langle \mathbf{c} \rangle + \langle \mathbf{c} \rangle \star \llbracket \mathbf{a} \rrbracket, \quad (2.3)$$

where the operator $\star$ denotes either scalar multiplication or a contraction. The average and the jump of a quantity over the interface $\mathcal{S}_0$ are defined as:

$$\langle \{\bullet\} \rangle := \frac{1}{2} [\{\bullet\}|_{\mathcal{S}_0^+} + \{\bullet\}|_{\mathcal{S}_0^-}] \quad \text{and} \quad \llbracket \{\bullet\} \rrbracket := \{\bullet\}|_{\mathcal{S}_0^+} - \{\bullet\}|_{\mathcal{S}_0^-}.$$

2.1.4.2 Integral relations

The extended form of the divergence theorem in the material configuration for the various parts of the body is now given. The (bulk) divergence theorem relates the material divergence of a quantity over the control volume $\mathcal{B}_0$ entirely within the bulk, possibly containing an interface $\mathcal{I}_0$, to the flux of the quantity over the boundary $\partial\mathcal{B}_0$, and the jump of the flux in the quantity over the interface $\mathcal{I}_0$ [see e.g. 99, for further details]. For a tensor field $\{\bullet\}$

$$\int_{\mathcal{B}_0} \text{Div} \{\bullet\} \, dV = \int_{\partial\mathcal{B}_0} \{\bullet\} \cdot \mathbf{M} \, dA - \int_{\mathcal{I}_0} \llbracket \{\bullet\} \rrbracket \cdot \bar{\mathbf{N}} \, dA. \quad (2.4)$$

Similarly, the corresponding surface, interface and curve divergence theorems for tensorial quantities on the surface $\{\bullet\}$, interface $\{\bullet\}$ and curve $\{\bullet\}$ are respectively given by

$$\int_{\mathcal{S}_0^{\text{ext}}} \widehat{\text{Div}} \{\bullet\} \, dA = \int_{\mathcal{L}_0} \{\bullet\} \cdot \widehat{\mathbf{N}} \, dL - \int_{\mathcal{S}_0^{\text{ext}}} \widehat{C} \{\bullet\} \cdot \mathbf{N} \, dA - \int_{\mathcal{C}_0^{\text{ext}}} \llbracket \{\bullet\} \rrbracket \cdot \widetilde{\mathbf{N}}_s \, dL, \quad (2.5)$$

$$\int_{\mathcal{I}_0} \overline{\text{Div}} \{\bullet\} \, dA = \int_{\mathcal{C}_0^{\text{int}}} \{\bullet\} \cdot \overline{\mathbf{M}} \, dL + \int_{\mathcal{C}_0^{\text{ext}}} \{\bullet\} \cdot \widetilde{\mathbf{N}}_i \, dL - \int_{\mathcal{I}_0} \overline{C} \{\bullet\} \cdot \bar{\mathbf{N}} \, dA, \quad (2.6)$$

$$\int_{\mathcal{C}_0^{\text{ext}}} \widetilde{\text{Div}} \{\bullet\} \, dL = \sum_{\partial\mathcal{C}_0^{\text{ext}}} \{\bullet\} \cdot \widetilde{\mathbf{N}} - \int_{\mathcal{C}_0^{\text{ext}}} \widetilde{C} \{\bullet\} \cdot \widetilde{\mathbf{N}}_c \, dL. \quad (2.7)$$

where the curvatures of the surface, interface and curve in the material configuration are denoted as $\widehat{C}$, $\overline{C}$ and $\widetilde{C}$, respectively, and are defined by:

$$\widehat{C} := -\widehat{\text{Div}} \mathbf{N} \quad \overline{C} := -\overline{\text{Div}} \bar{\mathbf{N}} \quad \widetilde{C} := -\widetilde{\text{Div}} \widetilde{\mathbf{N}}_c. \quad (2.8)$$

Remark The extended divergence theorems here correspond to the material configuration. The spatial forms of the divergence theorems in the spatial configuration can be obtained by integrating over the spatial domains and replacing the material quantities by their spatial counterparts. $\square$

2.1.4.3 Piola identity and Piola transform

The local balance equations expressed in spatial quantities can be obtained from the material versions using the standard (bulk) Piola identity:

$$\text{Div}(\text{Cof } \mathbf{F}) = \mathbf{0}. \quad (2.9)$$

The surface, interface and curve divergence theorems together with their corresponding Nanson's formulae result in the following surface, interface and curve Piola identities:

$$\widehat{\text{Div}}(\widehat{\text{Cof}} \hat{\mathbf{F}}) = \hat{J} \hat{\mathbf{c}} \mathbf{n}, \quad \overline{\text{Div}}(\overline{\text{Cof}} \bar{\mathbf{F}}) = \bar{J} \bar{\mathbf{c}} \bar{\mathbf{n}}, \quad \widetilde{\text{Div}}(\widetilde{\text{Cof}} \tilde{\mathbf{F}}) = \tilde{J} \tilde{\mathbf{c}} \tilde{\mathbf{n}}_c. \quad (2.10)$$

where the curvatures of the surface, interface and curve in the spatial configuration are denoted as $\hat{c}$, $\bar{c}$ and $\tilde{c}$, respectively, and are defined by:

$$\hat{c} := -\widehat{\text{div}} \mathbf{n} \quad \bar{c} := -\overline{\text{div}} \bar{\mathbf{n}} \quad \tilde{c} := -\widetilde{\text{div}} \tilde{\mathbf{n}}_c. \quad (2.11)$$

A bulk Cauchy stress, heat flux or entropy, collectively denoted as a Cauchy quantity γ , transforms into its corresponding Piola quantity Γ via the (bulk) Piola transform:

$$\Gamma = \gamma \cdot \text{Cof } \mathbf{F}. \quad (2.12)$$

Analogously, a surface, interface and curve Cauchy quantity denoted as $\hat{\gamma}$, $\bar{\gamma}$ and $\tilde{\gamma}$, respectively, transform into their corresponding Piola quantities $\hat{\Gamma}$, $\bar{\Gamma}$ and $\tilde{\Gamma}$ via the Piola transforms:

$$\hat{\Gamma} = \hat{\gamma} \cdot \widehat{\text{Cof}} \hat{\mathbf{F}}, \quad \bar{\Gamma} = \bar{\gamma} \cdot \overline{\text{Cof}} \bar{\mathbf{F}}, \quad \tilde{\Gamma} = \tilde{\gamma} \cdot \widetilde{\text{Cof}} \tilde{\mathbf{F}}. \quad (2.13)$$

2.1.4.4 Superficial and tangential tensor fields

Material second-order tensors and vectors on the surface, interface and curve can be respectively classified as superficial (in their tangent spaces) or tangential. Superficial material second-order tensors on the surface, interface and curve, respectively possess the orthogonality properties:

$$\{\bullet\} \cdot \mathbf{N} = \mathbf{0}, \quad \{\bullet\} \cdot \bar{\mathbf{N}} = \mathbf{0}, \quad \{\bullet\} \cdot \tilde{\mathbf{N}}_c = \mathbf{0}.$$

If the arbitrary quantities in the preceding relations are vectors, they are termed tangential. Tangential material second-order tensors on the surface, interface and curve, respectively possess the orthogonality properties:

$$\begin{aligned} \{\bullet\} \cdot \mathbf{N} = \mathbf{0} \quad \text{and} \quad \mathbf{N} \cdot \{\bullet\} = \mathbf{0}, \quad \{\bullet\} \cdot \bar{\mathbf{N}} = \mathbf{0} \quad \text{and} \quad \bar{\mathbf{N}} \cdot \{\bullet\} = \mathbf{0}, \\ \{\bullet\} \cdot \tilde{\mathbf{N}}_c = \mathbf{0} \quad \text{and} \quad \tilde{\mathbf{N}}_c \cdot \{\bullet\} = \mathbf{0}, \end{aligned}$$

or alternatively

$$\widehat{\mathbf{I}} \cdot \{\widehat{\bullet}\} \cdot \widehat{\mathbf{I}} = \{\widehat{\bullet}\} , \quad \overline{\mathbf{I}} \cdot \{\overline{\bullet}\} \cdot \overline{\mathbf{I}} = \{\overline{\bullet}\} , \quad \widetilde{\mathbf{I}} \cdot \{\widetilde{\bullet}\} \cdot \widetilde{\mathbf{I}} = \{\widetilde{\bullet}\} .$$

Spatial second-order tensors and vectors can be defined in the same fashion by replacing the material quantities with the spatial ones. Note that the set of all tangential second-order tensors is contained within the set of all superficial second-order tensors.

2.2 GOVERNING EQUATIONS

The coupled governing equations for the thermomechanical problem in the various parts of the body are now derived using an arbitrary (canonical) control region $\mathcal{B}_0 \subset \mathcal{B}_0$. Thereafter, the balances of momentum, energy and entropy, i.e. the governing equations in integral form, are given. Finally, these integral balance expressions are localised at arbitrary points in the bulk $\mathcal{B}_0$, on the surface $\mathcal{S}_0$ or interface $\mathcal{S}_0$, or on the curve $\mathcal{C}_0$ thereby giving the local (strong) form of the governing equations.²

The integral form of the governing equations over the control region, in their most general form, consists of eight terms which account for the contributions from the various parts of the body; that is:

$$\begin{aligned} \mathbf{0} \text{ (or } 0) = & \int_{\mathcal{B}_0} \{\bullet\} \, dV + \int_{\mathcal{S}_0^{\text{ext}}} \{\widehat{\bullet}\} \, dA + \int_{\mathcal{I}_0} \{\overline{\bullet}\} \, dA + \int_{\mathcal{C}_0^{\text{ext}}} \{\widetilde{\bullet}\} \, dL \\ & + \int_{\mathcal{S}_0^{\text{int}}} \{\circ\} \cdot \mathbf{M} \, dA + \int_{\mathcal{L}_0} \{\widehat{\circ}\} \cdot \widehat{\mathbf{N}} \, dL + \int_{\mathcal{C}_0^{\text{int}}} \{\overline{\circ}\} \cdot \overline{\mathbf{M}} \, dL + \sum_{\partial \mathcal{C}_0^{\text{ext}}} \{\widetilde{\circ}\} \cdot \widetilde{\mathbf{N}} , \end{aligned}$$

where $\{\bullet\}$ denotes a source-like term and $\{\circ\}$ is the corresponding flux. The corresponding integral expressions for the balance of linear and angular momentum are derived and subsequently localised in Section 2.2.1. The localisation process is explained in detail. In Section 2.2.2 the integral and resulting local forms of the energy balance are given. Finally, in Section 2.2.3 the process is repeated for the entropy balance.

²Note that inertial forces are omitted. Furthermore, in the absence of mass flux, mass is conserved (trivially) via the definition of the Jacobians.

2.2.1 Mechanical power

The global working, i.e. the mechanical power, in the material configuration is denoted $\mathcal{W}_0$ and given by

$$\begin{aligned} \mathcal{W}_0 &= \mathcal{W}_0 \left(\mathbf{V}, \widehat{\mathbf{V}}, \overline{\mathbf{V}}, \widetilde{\mathbf{V}} \right) \\ &:= \int_{\mathcal{B}_0} \mathbf{V} \cdot \mathbf{B}^p \, dV + \int_{S_0^{\text{ext}}} \widehat{\mathbf{V}} \cdot \widehat{\mathbf{B}}^p \, dA + \int_{\mathcal{I}_0} \overline{\mathbf{V}} \cdot \overline{\mathbf{B}}^p \, dA + \int_{C_0^{\text{ext}}} \widetilde{\mathbf{V}} \cdot \widetilde{\mathbf{B}}^p \, dL \\ &\quad + \int_{S_0^{\text{int}}} \mathbf{V} \cdot [\mathbf{P} \cdot \mathbf{M}] \, dA + \int_{\mathcal{L}_0} \widehat{\mathbf{V}} \cdot [\widehat{\mathbf{P}} \cdot \widehat{\mathbf{N}}] \, dL \\ &\quad + \int_{C_0^{\text{int}}} \overline{\mathbf{V}} \cdot [\overline{\mathbf{P}} \cdot \overline{\mathbf{M}}] \, dL + \sum_{\partial C_0^{\text{ext}}} \widetilde{\mathbf{V}} \cdot [\widetilde{\mathbf{P}} \cdot \widetilde{\mathbf{N}}] \, dL. \end{aligned} \quad (2.14)$$

The prescribed bulk (body) force per unit reference volume, dimensionally $[\text{N}/\text{m}^3]$, of $\mathcal{B}_0$ is denoted $\mathbf{B}^p$ where the superscript p indicates a prescribed quantity. The prescribed tractions per unit reference area of the surface S_0^{ext} and the interface $\mathcal{I}_0$ are denoted $\widehat{\mathbf{B}}^p$ $[\text{N}/\text{m}^2]$ and $\overline{\mathbf{B}}^p$ $[\text{N}/\text{m}^2]$, respectively. The prescribed traction per unit reference length of the curve C_0^{ext} is denoted $\widetilde{\mathbf{B}}^p$ $[\text{N}/\text{m}]$. As with the bulk force $\mathbf{B}^p$, the prescribed tractions on the surface, interface and curve can be understood as prescribed surface, interface and curve forces, respectively. The bulk, surface, interface and curve Piola stresses are denoted $\mathbf{P}$, $\widehat{\mathbf{P}}$, $\overline{\mathbf{P}}$ and $\widetilde{\mathbf{P}}$, respectively. The terms $\mathbf{P} \cdot \mathbf{M}$, $\widehat{\mathbf{P}} \cdot \widehat{\mathbf{N}}$, $\overline{\mathbf{P}} \cdot \overline{\mathbf{M}}$ and $\widetilde{\mathbf{P}} \cdot \widetilde{\mathbf{N}}$ denote the tractions acting on S_0^{int} , $\mathcal{L}_0$, C_0^{int} and $\partial C_0^{\text{ext}}$, respectively.

Remark It assumed that the Cauchy theorem holds for the bulk, surface, interface and curve Piola stresses. Furthermore, $\widehat{\mathbf{P}}$, $\overline{\mathbf{P}}$ and $\widetilde{\mathbf{P}}$ are superficial tensor fields in their tangent spaces. $\square$

Invoking arguments concerning the invariance of the working under superposed rigid-body motions [see 90, for details concerning the case of thermomechanical solids with surface energy only] yields the global balances of linear momentum:

$$\begin{aligned} &\int_{\mathcal{B}_0} \mathbf{B}^p \, dV + \int_{S_0^{\text{ext}}} \widehat{\mathbf{B}}^p \, dA + \int_{\mathcal{I}_0} \overline{\mathbf{B}}^p \, dA + \int_{C_0^{\text{ext}}} \widetilde{\mathbf{B}}^p \, dL \\ &\quad + \int_{S_0^{\text{int}}} \mathbf{P} \cdot \mathbf{M} \, dA + \int_{\mathcal{L}_0} \widehat{\mathbf{P}} \cdot \widehat{\mathbf{N}} \, dL + \int_{C_0^{\text{int}}} \overline{\mathbf{P}} \cdot \overline{\mathbf{M}} \, dL + \sum_{\partial C_0^{\text{ext}}} \widetilde{\mathbf{P}} \cdot \widetilde{\mathbf{N}} \, dL = \mathbf{0}, \end{aligned} \quad (2.15)$$

and the global balances of angular momentum:

$$\begin{aligned} &\int_{\mathcal{B}_0} \mathbf{R} \times \mathbf{B}^p \, dV + \int_{S_0^{\text{ext}}} \widehat{\mathbf{R}} \times \widehat{\mathbf{B}}^p \, dA + \int_{\mathcal{I}_0} \overline{\mathbf{R}} \times \overline{\mathbf{B}}^p \, dA + \int_{C_0^{\text{ext}}} \widetilde{\mathbf{R}} \times \widetilde{\mathbf{B}}^p \, dL \\ &\quad + \int_{S_0^{\text{int}}} \mathbf{R} \times [\mathbf{P} \cdot \mathbf{M}] \, dA + \int_{\mathcal{L}_0} \widehat{\mathbf{R}} \times [\widehat{\mathbf{P}} \cdot \widehat{\mathbf{N}}] \, dL \\ &\quad + \int_{C_0^{\text{int}}} \overline{\mathbf{R}} \times [\overline{\mathbf{P}} \cdot \overline{\mathbf{M}}] \, dL + \sum_{\partial C_0^{\text{ext}}} \widetilde{\mathbf{R}} \times [\widetilde{\mathbf{P}} \cdot \widetilde{\mathbf{N}}] \, dL = \mathbf{0}, \end{aligned} \quad (2.16)$$

where $\mathbf{R}$, $\widehat{\mathbf{R}}$, $\overline{\mathbf{R}}$ and $\widetilde{\mathbf{R}}$ are vectors to the points in the bulk, surface, interface and curve, respectively, relative to a fixed point in $\mathbb{E}^3$, e.g. the origin.

2.2.1.1 Bulk

The global statements (2.15)–(2.16) are now localised at arbitrary $\mathbf{X} \in \mathcal{B}_0$ by considering a control region $\mathcal{B}_0$ such that $\partial\mathcal{B}_0$ *does not contain* any portion of the surface or interface, i.e. $\partial\mathcal{B}_0 \cap \mathcal{S}_0 = \partial\mathcal{B}_0 \cap \mathcal{I}_0 = \emptyset$. Under such restrictions the limits of the integrals in Eq. (2.15)–(2.16) are

$$\begin{aligned} \mathcal{B}_0 &\neq \emptyset, & \mathcal{S}_0^{\text{ext}} &= \emptyset, & \mathcal{I}_0 &= \emptyset, & \mathcal{C}_0^{\text{ext}} &= \emptyset, \\ \mathcal{S}_0^{\text{int}} = \partial\mathcal{B}_0 &\neq \emptyset, & \mathcal{L}_0 &= \emptyset, & \mathcal{C}_0^{\text{int}} &= \emptyset, & \partial\mathcal{C}_0^{\text{ext}} &= \emptyset. \end{aligned}$$

From the arbitrariness of the control region $\mathcal{B}_0$, and taking into account the corresponding extended (bulk) divergence theorem (2.4) together with Eq. (B.1)₁, one obtains the familiar local balances of linear and angular momentum in the bulk $\mathcal{B}_0$:

$$\text{Div } \mathbf{P} + \mathbf{B}^{\text{p}} = \mathbf{0}, \quad (2.17)$$

$$\mathbf{F} \cdot \mathbf{P}^{\text{t}} = \mathbf{P} \cdot \mathbf{F}^{\text{t}}. \quad (2.18)$$

2.2.1.2 Surface

The global statements (2.15)–(2.16) are now localised at arbitrary $\widehat{\mathbf{X}} \in \mathcal{S}_0$ by considering a control region $\mathcal{B}_0$ where $\partial\mathcal{B}_0$ *contains* a portion of the surface, i.e. $\partial\mathcal{B}_0 \cap \mathcal{S}_0 \neq \emptyset$, but *does not contain* any portion of the interface, i.e. $\partial\mathcal{B}_0 \cap \mathcal{I}_0 = \emptyset$. Under such restrictions the limits of the integrals in Eq. (2.15)–(2.16) are

$$\begin{aligned} \mathcal{B}_0 &\neq \emptyset, & \mathcal{S}_0^{\text{ext}} &\neq \emptyset, & \mathcal{I}_0 &= \emptyset, & \mathcal{C}_0^{\text{ext}} &= \emptyset, \\ \mathcal{S}_0^{\text{int}} = \partial\mathcal{B}_0 / \mathcal{S}_0^{\text{ext}} &\neq \emptyset, & \mathcal{L}_0 &\neq \emptyset, & \mathcal{C}_0^{\text{int}} &= \emptyset, & \partial\mathcal{C}_0^{\text{ext}} &= \emptyset. \end{aligned}$$

The volume of the control region is then decreased to zero, i.e. the limit $\mathcal{B}_0 \rightarrow \emptyset$ is taken and, consequently, $\mathcal{S}_0^{\text{int}} = \mathcal{S}_0^{\text{ext}}$ with $\mathbf{M} = -\mathbf{N}$ and $\mathbf{R} = \widehat{\mathbf{R}}$. From the arbitrariness of the control region $\mathcal{B}_0$, and taking into account the corresponding extended surface divergence theorem (2.5) together with Eq. (B.1)₂, one obtains the local balances of linear and angular momentum on the surface $\mathcal{S}_0$ as

$$\widehat{\text{Div}} \widehat{\mathbf{P}} + \widehat{\mathbf{B}}^{\text{p}} - \mathbf{P} \cdot \mathbf{N} = \mathbf{0}, \quad (2.19)$$

$$\widehat{\mathbf{F}} \cdot \widehat{\mathbf{P}}^{\text{t}} = \widehat{\mathbf{P}} \cdot \widehat{\mathbf{F}}^{\text{t}}. \quad (2.20)$$

2.2.1.3 Interface

Following the general approach outlined for the bulk and the surface, the global statements (2.15)–(2.16) are now localised at arbitrary $\overline{\mathbf{X}} \in \mathcal{I}_0$. Thus, a control region $\mathcal{B}_0$ is

considered such that $\partial\mathcal{B}_0$ contains a portion of the interface, i.e. $\partial\mathcal{B}_0 \cap \mathcal{I}_0 \neq \emptyset$, but $\partial\mathcal{B}_0$ does not contain any portion of the surface, i.e. $\partial\mathcal{B}_0 \cap \mathcal{S}_0 = \emptyset$. Under such restrictions the limits of the integrals in Eq. (2.15)–(2.16) are

$$\begin{aligned} \mathcal{B}_0 &\neq \emptyset, & \mathcal{S}_0^{\text{ext}} &= \emptyset, & \mathcal{I}_0 &\neq \emptyset, & \mathcal{C}_0^{\text{ext}} &= \emptyset, \\ \mathcal{S}_0^{\text{int}} &= \partial\mathcal{B}_0/\mathcal{I}_0 \neq \emptyset, & \mathcal{L}_0 &= \emptyset, & \mathcal{C}_0^{\text{int}} &= \partial\mathcal{I}_0 \neq \emptyset, & \partial\mathcal{C}_0^{\text{ext}} &= \emptyset. \end{aligned}$$

The volume of the control region is then decreased to zero, i.e. the limit $\mathcal{B}_0 \rightarrow \emptyset$ is taken and consequently, $\mathcal{S}_0^{\text{int}} = \mathcal{I}_0$ with $\mathbf{M} = \overline{\mathbf{N}}$ on $\mathcal{I}_0^+$, $\mathbf{M} = -\overline{\mathbf{N}}$ on $\mathcal{I}_0^-$ and $\mathbf{R} = \overline{\mathbf{R}}$. Once again, from the arbitrariness of the control region $\mathcal{B}_0$, and taking into account the corresponding extended interface divergence theorem (2.6) together with Eq. (B.1)₃, one obtains the local balance of linear and angular momentum on the interface $\mathcal{I}_0$ as

$$\overline{\text{Div}} \overline{\mathbf{P}} + \overline{\mathbf{B}}^{\text{p}} + \llbracket \mathbf{P} \rrbracket \cdot \overline{\mathbf{N}} = \mathbf{0}, \quad (2.21)$$

$$\overline{\mathbf{F}} \cdot \overline{\mathbf{P}}^{\text{t}} = \overline{\mathbf{P}} \cdot \overline{\mathbf{F}}^{\text{t}}. \quad (2.22)$$

2.2.1.4 Curve

Finally, the global statements (2.15)–(2.16) are localised at arbitrary $\widetilde{\mathbf{X}} \in \mathcal{C}_0$. Thus, a control region $\mathcal{S}_0^{\text{ext}}$ is considered such that $\mathcal{S}_0^{\text{ext}}$ contains a portion of the curve, i.e. $\mathcal{S}_0^{\text{ext}} \cap \mathcal{C}_0 \neq \emptyset$. Under such restrictions the limits of the integrals in Eq. (2.15)–(2.16) are

$$\begin{aligned} \mathcal{B}_0 &= \emptyset, & \mathcal{S}_0^{\text{ext}} &\neq \emptyset, & \mathcal{I}_0 &= \emptyset, & \mathcal{C}_0^{\text{ext}} &\neq \emptyset, \\ \mathcal{S}_0^{\text{int}} &= \mathcal{S}_0^{\text{ext}} \neq \emptyset, & \mathcal{L}_0 &\neq \emptyset, & \mathcal{C}_0^{\text{int}} &= \mathcal{C}_0^{\text{ext}} \neq \emptyset, & \partial\mathcal{C}_0^{\text{ext}} &\neq \emptyset. \end{aligned}$$

The limit $\mathcal{S}_0^{\text{ext}} \rightarrow \emptyset$ is then taken such that $\partial\mathcal{S}_0^{\text{ext}} = \mathcal{C}_0^{\text{ext}}$ with $\widehat{\mathbf{N}} = \widetilde{\mathbf{N}}_{\text{s}}$ on ${}^+\mathcal{C}_0^{\text{ext}}$, $\widehat{\mathbf{N}} = -\widetilde{\mathbf{N}}_{\text{s}}$ on ${}^-\mathcal{C}_0^{\text{ext}}$ and $\widehat{\mathbf{R}} = \widetilde{\mathbf{R}}$. From the arbitrariness of the control region $\mathcal{S}_0^{\text{ext}}$, and taking into account the corresponding extended divergence theorem (2.7) together with Eq. (B.1)₄, one obtains the local balance of linear and angular momentum on the curve $\mathcal{C}_0$ as

$$\widetilde{\text{Div}} \widetilde{\mathbf{P}} + \widetilde{\mathbf{B}}^{\text{p}} - \overline{\mathbf{P}} \cdot \widetilde{\mathbf{N}}_{\text{i}} + \llbracket \widehat{\mathbf{P}} \rrbracket \cdot \widetilde{\mathbf{N}}_{\text{s}} = \mathbf{0}, \quad (2.23)$$

$$\widetilde{\mathbf{F}} \cdot \widetilde{\mathbf{P}}^{\text{t}} = \widetilde{\mathbf{P}} \cdot \widetilde{\mathbf{F}}^{\text{t}}. \quad (2.24)$$

Remark The local balance of momentum on the interface Eq. (2.21) relates the interface Piola stress to the jump of the bulk Piola stress across the interface. The curve Piola stress, however, is coupled not only to the jump of the surface Piola stress across the curve but also to a contribution from the interface Piola stress according to Eq. (2.23). $\square$

2.2.1.5 Material and spatial formulations

In summary, the local balances of linear and angular momentum for the various parts of the body in material quantities read:

$$\begin{aligned}
 \text{Div } \mathbf{P} + \mathbf{B} &= \mathbf{0} & \text{and } \mathbf{F} \cdot \mathbf{P}^t &= \mathbf{P} \cdot \mathbf{F}^t \text{ in } \mathcal{B}_0 \\
 \text{where } \mathbf{B} &= \mathbf{B}^p, \\
 \widehat{\text{Div}} \widehat{\mathbf{P}} + \widehat{\mathbf{B}} &= \mathbf{0} & \text{and } \widehat{\mathbf{F}} \cdot \widehat{\mathbf{P}}^t &= \widehat{\mathbf{P}} \cdot \widehat{\mathbf{F}}^t \text{ in } \mathcal{S}_0 \\
 \text{where } \widehat{\mathbf{B}} &= \widehat{\mathbf{B}}^p - \mathbf{P} \cdot \mathbf{N}, \\
 \overline{\text{Div}} \overline{\mathbf{P}} + \overline{\mathbf{B}} &= \mathbf{0} & \text{and } \overline{\mathbf{F}} \cdot \overline{\mathbf{P}}^t &= \overline{\mathbf{P}} \cdot \overline{\mathbf{F}}^t \text{ in } \mathcal{S}_0 \\
 \text{where } \overline{\mathbf{B}} &= \overline{\mathbf{B}}^p + \llbracket \mathbf{P} \rrbracket \cdot \overline{\mathbf{N}}, \\
 \widetilde{\text{Div}} \widetilde{\mathbf{P}} + \widetilde{\mathbf{B}} &= \mathbf{0} & \text{and } \widetilde{\mathbf{F}} \cdot \widetilde{\mathbf{P}}^t &= \widetilde{\mathbf{P}} \cdot \widetilde{\mathbf{F}}^t \text{ in } \mathcal{C}_0 \\
 \text{where } \widetilde{\mathbf{B}} &= \widetilde{\mathbf{B}}^p - \overline{\mathbf{P}} \cdot \widetilde{\mathbf{N}}_i + \llbracket \widehat{\mathbf{P}} \rrbracket \cdot \widetilde{\mathbf{N}}_s.
 \end{aligned} \tag{2.25}$$

Using the Piola identities (2.9)–(2.10), the local momentum balance equations (2.25) can be expressed in terms of spatial quantities as:

$$\begin{aligned}
 \text{div } \boldsymbol{\sigma} + \mathbf{b} &= \mathbf{0} & \text{and } \boldsymbol{\sigma} &= \boldsymbol{\sigma}^t \text{ in } \mathcal{B}_t \\
 \text{where } \mathbf{b} &= \mathbf{b}^p, \\
 \widehat{\text{div}} \widehat{\boldsymbol{\sigma}} + \widehat{\mathbf{b}} &= \mathbf{0} & \text{and } \widehat{\boldsymbol{\sigma}} &= \widehat{\boldsymbol{\sigma}}^t \text{ in } \mathcal{S}_t \\
 \text{where } \widehat{\mathbf{b}} &= \widehat{\mathbf{b}}^p - \boldsymbol{\sigma} \cdot \mathbf{n}, \\
 \overline{\text{div}} \overline{\boldsymbol{\sigma}} + \overline{\mathbf{b}} &= \mathbf{0} & \text{and } \overline{\boldsymbol{\sigma}} &= \overline{\boldsymbol{\sigma}}^t \text{ in } \mathcal{S}_t \\
 \text{where } \overline{\mathbf{b}} &= \overline{\mathbf{b}}^p + \llbracket \boldsymbol{\sigma} \rrbracket \cdot \overline{\mathbf{n}}, \\
 \widetilde{\text{div}} \widetilde{\boldsymbol{\sigma}} + \widetilde{\mathbf{b}} &= \mathbf{0} & \text{and } \widetilde{\boldsymbol{\sigma}} &= \widetilde{\boldsymbol{\sigma}}^t \text{ in } \mathcal{C}_t \\
 \text{where } \widetilde{\mathbf{b}} &= \widetilde{\mathbf{b}}^p - \overline{\boldsymbol{\sigma}} \cdot \widetilde{\mathbf{n}}_i + \llbracket \widehat{\boldsymbol{\sigma}} \rrbracket \cdot \widetilde{\mathbf{n}}_s,
 \end{aligned} \tag{2.26}$$

where the prescribed bulk force per unit current volume of $\mathcal{B}_t$ is denoted $\mathbf{b}^p := j \mathbf{B}^p$. In an identical fashion, the prescribed surface, interface and curve forces are denoted $\widehat{\mathbf{b}}^p := \widehat{j} \widehat{\mathbf{B}}^p$, $\overline{\mathbf{b}}^p := \overline{j} \overline{\mathbf{B}}^p$ and $\widetilde{\mathbf{b}}^p := \widetilde{j} \widetilde{\mathbf{B}}^p$, respectively.

2.2.1.6 Reformulation of mechanical power in terms of stresses

Invoking the balances of momentum in the various parts of the body (2.25), the expression (2.14) for the mechanical power can be reformulated in terms of the stresses (the proof is given in Appendix B.2) as

$$\begin{aligned} \mathcal{W}_0 = & \int_{\mathcal{B}_0} \mathbf{P} : \text{Grad } \mathbf{V} \, dV + \int_{\mathcal{I}_0} \overline{\mathbf{P}} : \overline{\text{Grad}} \, \overline{\mathbf{V}} \, dA \\ & + \int_{S_0^{\text{ext}}} \widehat{\mathbf{P}} : \widehat{\text{Grad}} \, \widehat{\mathbf{V}} \, dA + \int_{C_0^{\text{ext}}} \widetilde{\mathbf{P}} : \widetilde{\text{Grad}} \, \widetilde{\mathbf{V}} \, dL. \end{aligned} \quad (2.27)$$

The (bulk) Cauchy stress $\boldsymbol{\sigma}$ and the surface, interface and curve tangential Cauchy stresses, denoted $\widehat{\boldsymbol{\sigma}}$, $\overline{\boldsymbol{\sigma}}$ and $\widetilde{\boldsymbol{\sigma}}$, respectively, are related to their corresponding Piola stresses via the Piola transforms (2.12)–(2.13). The working in Eq. (2.27) can thus be reformulated in terms of spatial quantities as

$$\begin{aligned} \mathcal{W}_t = & \int_{\mathcal{B}_t} \boldsymbol{\sigma} : \text{grad } \mathbf{v} \, dv + \int_{\mathcal{I}_t} \overline{\boldsymbol{\sigma}} : \overline{\text{grad}} \, \overline{\mathbf{v}} \, da \\ & + \int_{S_t^{\text{ext}}} \widehat{\boldsymbol{\sigma}} : \widehat{\text{grad}} \, \widehat{\mathbf{v}} \, da + \int_{C_t^{\text{ext}}} \widetilde{\boldsymbol{\sigma}} : \widetilde{\text{grad}} \, \widetilde{\mathbf{v}} \, dl. \end{aligned}$$

2.2.2 Thermal power

In order to derive the internal energy balance equation one needs a relation for the global heating. The global heating, i.e. the global external thermal power, expressed in the material configuration is denoted $\mathcal{Q}_0$ and takes the form

$$\begin{aligned} \mathcal{Q}_0 := & \int_{\mathcal{B}_0} Q^{\text{P}} \, dV + \int_{S_0^{\text{ext}}} \widehat{Q}^{\text{P}} \, dA + \int_{\mathcal{I}_0} \overline{Q}^{\text{P}} \, dA + \int_{C_0^{\text{ext}}} \widetilde{Q}^{\text{P}} \, dL \\ & + \int_{S_0^{\text{int}}} [-\mathbf{Q} \cdot \mathbf{M}] \, dA + \int_{\mathcal{L}_0} [-\widehat{\mathbf{Q}} \cdot \widehat{\mathbf{N}}] \, dL \\ & + \int_{C_0^{\text{int}}} [-\overline{\mathbf{Q}} \cdot \overline{\mathbf{M}}] \, dL + \sum_{\partial C_0^{\text{ext}}} [-\widetilde{\mathbf{Q}} \cdot \widetilde{\mathbf{N}}] \, dL. \end{aligned} \quad (2.28)$$

The prescribed bulk (body) heat source per unit reference volume (and per unit time) in $\mathcal{B}_0$ is denoted Q^{P} [N/s m²]. The prescribed heat sources per unit reference area (and per unit time) of the surface S_0^{ext} and the interface $\mathcal{I}_0$ are denoted $\widehat{Q}^{\text{P}}$ [N/s m] and $\overline{Q}^{\text{P}}$ [N/s m], respectively. The prescribed heat source per unit length (and per unit time) of the curve C_0^{ext} is denoted $\widetilde{Q}^{\text{P}}$ [N/s]. The bulk, surface, interface and curve Piola heat flux vectors are denoted $\mathbf{Q}$, $\widehat{\mathbf{Q}}$, $\overline{\mathbf{Q}}$ and $\widetilde{\mathbf{Q}}$, respectively. The terms $\mathbf{Q} \cdot \mathbf{M}$, $\widehat{\mathbf{Q}} \cdot \widehat{\mathbf{N}}$, $\overline{\mathbf{Q}} \cdot \overline{\mathbf{M}}$ and $\widetilde{\mathbf{Q}} \cdot \widetilde{\mathbf{N}}$ denote the heat fluxes on S_0^{int} , $\mathcal{L}_0$, C_0^{int} and $\partial C_0^{\text{ext}}$, respectively. It is assumed that the Cauchy theorem holds for the heat flux vectors in all parts of the body. Note that $\widehat{\mathbf{Q}}$, $\overline{\mathbf{Q}}$ and $\widetilde{\mathbf{Q}}$ are tangential vectors fields.

The rate of change of total internal energy expressed in the material configuration $\mathcal{E}_0$ is given by

$$\mathcal{E}_0 := \int_{\mathcal{B}_0} D_t E \, dV + \int_{S_0} D_t \widehat{E} \, dA + \int_{\mathcal{I}_0} D_t \overline{E} \, dA + \int_{C_0} D_t \widetilde{E} \, dL,$$

where the bulk internal energy per unit reference volume, the surface and interface internal energies per unit reference area and the curve internal energy per unit reference length are denoted E [N/m²], $\widehat{E}$ [N/m], $\overline{E}$ [N/m] and $\widetilde{E}$ [N], respectively.

The internal energy balance states that working and heating cause a change in the internal energy, that is:

$$\mathcal{W}_0 + \mathcal{Q}_0 = \mathcal{E}_0. \quad (2.29)$$

The global statement (2.29) is now localised at arbitrary $\mathbf{X} \in \mathcal{B}_0$, $\widehat{\mathbf{X}} \in \mathcal{S}_0$, $\overline{\mathbf{X}} \in \mathcal{I}_0$ and $\widetilde{\mathbf{X}} \in \mathcal{C}_0$. The resulting local balances of energy for the various parts of the body expressed in material quantities are:

$$\begin{array}{ll} \mathbf{P} : \text{Grad } \mathbf{V} - \text{Div } \mathbf{Q} + Q = D_t E & \text{in } \mathcal{B}_0 \\ \text{where } Q = Q^P, & \\ \widehat{\mathbf{P}} : \widehat{\text{Grad}} \widehat{\mathbf{V}} - \widehat{\text{Div}} \widehat{\mathbf{Q}} + \widehat{Q} = D_t \widehat{E} & \text{in } \mathcal{S}_0 \\ \text{where } \widehat{Q} = \widehat{Q}^P + \mathbf{Q} \cdot \mathbf{N}, & \\ \overline{\mathbf{P}} : \overline{\text{Grad}} \overline{\mathbf{V}} - \overline{\text{Div}} \overline{\mathbf{Q}} + \overline{Q} = D_t \overline{E} & \text{in } \mathcal{I}_0 \\ \text{where } \overline{Q} = \overline{Q}^P - \llbracket \mathbf{Q} \rrbracket \cdot \overline{\mathbf{N}}, & \\ \widetilde{\mathbf{P}} : \widetilde{\text{Grad}} \widetilde{\mathbf{V}} - \widetilde{\text{Div}} \widetilde{\mathbf{Q}} + \widetilde{Q} = D_t \widetilde{E} & \text{in } \mathcal{C}_0 \\ \text{where } \widetilde{Q} = \widetilde{Q}^P + \overline{\mathbf{Q}} \cdot \widetilde{\mathbf{N}}_i - \llbracket \widehat{\mathbf{Q}} \rrbracket \cdot \widetilde{\mathbf{N}}_s. & \end{array} \quad (2.30)$$

The Piola identities for the various parts of the body allow Eq. (2.30) to be expressed solely in terms of spatial quantities. The (bulk) Cauchy heat flux vector $\mathbf{q}$ and the surface, interface and curve tangential Cauchy heat flux vectors, denoted $\widehat{\mathbf{q}}$, $\overline{\mathbf{q}}$ and $\widetilde{\mathbf{q}}$, respectively, are related to their corresponding Piola heat flux vectors via the Piola transforms (2.12)–(2.13).

Thus, the local balances of energy for the various parts of the body in terms of spatial

quantities are:

$$\begin{aligned}
 & \boldsymbol{\sigma} : \text{grad } \mathbf{v} - \text{div}(\mathbf{q} + e\mathbf{v}) + q = \text{d}_t e && \text{in } \mathcal{B}_t \\
 & \quad \text{where } q = q^P, \\
 & \widehat{\boldsymbol{\sigma}} : \widehat{\text{grad}} \widehat{\mathbf{v}} - \widehat{\text{div}}(\widehat{\mathbf{q}} + \widehat{e}\widehat{\mathbf{v}}) + \widehat{q} = \text{d}_t \widehat{e} && \text{in } \mathcal{S}_t \\
 & \quad \text{where } \widehat{q} = \widehat{q}^P + \mathbf{q} \cdot \mathbf{n}, \\
 & \overline{\boldsymbol{\sigma}} : \overline{\text{grad}} \overline{\mathbf{v}} - \overline{\text{div}}(\overline{\mathbf{q}} + \overline{e}\overline{\mathbf{v}}) + \overline{q} = \text{d}_t \overline{e} && \text{in } \mathcal{I}_t \\
 & \quad \text{where } \overline{q} = \overline{q}^P - [\![\mathbf{q}]\!] \cdot \overline{\mathbf{n}}, \\
 & \widetilde{\boldsymbol{\sigma}} : \widetilde{\text{grad}} \widetilde{\mathbf{v}} - \widetilde{\text{div}}(\widetilde{\mathbf{q}} + \widetilde{e}\widetilde{\mathbf{v}}) + \widetilde{q} = \text{d}_t \widetilde{e} && \text{in } \mathcal{C}_t \\
 & \quad \text{where } \widetilde{q} = \widetilde{q}^P + \overline{\mathbf{q}} \cdot \widetilde{\mathbf{n}}_i - [\![\widehat{\mathbf{q}}]\!] \cdot \widetilde{\mathbf{n}}_s,
 \end{aligned} \tag{2.31}$$

where the prescribed heat source per unit current volume (and unit time) in $\mathcal{B}_t$ is denoted $q^P := jQ^P$. The bulk internal energy per unit current volume is denoted $e := jE$. In an identical fashion to the bulk, the prescribed surface, interface and curve heat sources are denoted $\widehat{q}^P := \widehat{j}\widehat{Q}^P$, $\overline{q}^P := \overline{j}\overline{Q}^P$ and $\widetilde{q}^P := \widetilde{j}\widetilde{Q}^P$, respectively. Similarly, $\widehat{e} := \widehat{j}\widehat{E}$, $\overline{e} := \overline{j}\overline{E}$ and $\widetilde{e} := \widetilde{j}\widetilde{E}$ denote the surface, interface and curve internal energies, respectively. Recall that d_t denotes the spatial time derivative.

2.2.3 Entropy power

The global entropy input rate in the material configuration, denoted $\mathcal{H}_0$, is given by

$$\begin{aligned}
 \mathcal{H}_0 := & \int_{\mathcal{B}_0} H^P \text{d}V + \int_{S_0^{\text{ext}}} \widehat{H}^P \text{d}A + \int_{\mathcal{I}_0} \overline{H}^P \text{d}A + \int_{\mathcal{C}_0^{\text{ext}}} \widetilde{H}^P \text{d}L \\
 & + \int_{S_0^{\text{int}}} [-\mathbf{H} \cdot \mathbf{M}] \text{d}A + \int_{\mathcal{L}_0} [-\widehat{\mathbf{H}} \cdot \widehat{\mathbf{N}}] \text{d}L \\
 & + \int_{\mathcal{C}_0^{\text{int}}} [-\overline{\mathbf{H}} \cdot \overline{\mathbf{M}}] \text{d}L + \sum_{\partial\mathcal{C}_0^{\text{ext}}} [-\widetilde{\mathbf{H}} \cdot \widetilde{\mathbf{N}}].
 \end{aligned} \tag{2.32}$$

The prescribed bulk (body) entropy source per unit reference volume (and unit time) in $\mathcal{B}_0$ is denoted H^P [N/sKm²]. The prescribed entropy sources on the surface S_0^{ext} and the interface $\mathcal{I}_0$ are denoted $\widehat{H}^P$ [N/sKm] and $\overline{H}^P$ [N/sKm], respectively. The prescribed entropy source on the curve $\mathcal{C}_0^{\text{ext}}$ is denoted $\widetilde{H}^P$ [N/sK]. In the global entropy input (2.32) the terms $\mathbf{H} \cdot \mathbf{M}$, $\widehat{\mathbf{H}} \cdot \widehat{\mathbf{N}}$, $\overline{\mathbf{H}} \cdot \overline{\mathbf{M}}$ and $\widetilde{\mathbf{H}} \cdot \widetilde{\mathbf{N}}$ denote the entropy fluxes on S_0^{int} , $\mathcal{L}_0$, $\mathcal{C}_0^{\text{int}}$ and $\partial\mathcal{C}_0^{\text{ext}}$, respectively. The vectors $\mathbf{H}$, $\widehat{\mathbf{H}}$, $\overline{\mathbf{H}}$ and $\widetilde{\mathbf{H}}$ are the bulk, surface, interface and curve Piola entropy flux vectors, respectively. The vectors $\widehat{\mathbf{H}}$, $\overline{\mathbf{H}}$ and $\widetilde{\mathbf{H}}$ are tangential tensor fields in their tangential spaces.

The total entropy production rate in the material configuration, denoted $\mathcal{P}_0$, is defined by

$$\mathcal{P}_0 := \int_{B_0} \Pi \, dV + \int_{S_0^{\text{ext}}} \widehat{\Pi} \, dA + \int_{\mathcal{I}_0} \overline{\Pi} \, dA + \int_{C_0^{\text{ext}}} \widetilde{\Pi} \, dL \geq 0,$$

where $\Pi \geq 0$, $\widehat{\Pi} \geq 0$, $\overline{\Pi} \geq 0$ and $\widetilde{\Pi} \geq 0$ are the entropy production rates per unit reference volume of the bulk, per unit reference area of the surface and interface, and per unit reference length of the curve, respectively, all constrained to be positive.

The rate of the change of total entropy in the material configuration, denoted $\mathcal{N}_0$, is defined by

$$\mathcal{N}_0 := \int_{B_0} D_t \Xi \, dV + \int_{S_0^{\text{ext}}} D_t \widehat{\Xi} \, dA + \int_{\mathcal{I}_0} D_t \overline{\Xi} \, dA + \int_{C_0^{\text{ext}}} D_t \widetilde{\Xi} \, dL,$$

where the bulk entropy per unit reference volume is denoted Ξ [N/Km²]. The surface and interface entropies per unit reference area are denoted $\overline{\Xi}$ [N/Km] and $\widehat{\Xi}$ [N/Km], respectively. The curve entropy is denoted $\widetilde{\Xi}$ [N/K].

The second law of thermodynamics imposes the physical restriction that the rate of increase of entropy in a body is not less than the total entropy supplied to the body, or equivalently that the entropy increase is due to positive entropy production and entropy input, that is

$$\mathcal{N}_0 = \mathcal{P}_0 + \mathcal{H}_0 \quad \text{with} \quad \mathcal{N}_0 \geq \mathcal{H}_0 \quad \text{since} \quad \mathcal{P}_0 \geq 0. \quad (2.33)$$

The global statement of balance of entropy (2.33) is then localised at arbitrary $\mathbf{X} \in \mathcal{B}_0$, $\widehat{\mathbf{X}} \in \mathcal{S}_0$, $\overline{\mathbf{X}} \in \mathcal{I}_0$ and $\widetilde{\mathbf{X}} \in \mathcal{C}_0$. The resulting local balances of entropy for the various parts of the body in material quantities are

$-\text{Div } \mathbf{H} + \Pi + H = D_t \Xi$ where $H = H^P$,	$\text{and } \Pi \geq 0 \quad \text{in } \mathcal{B}_0$	(2.34)
$-\widehat{\text{Div}} \widehat{\mathbf{H}} + \widehat{\Pi} + \widehat{H} = D_t \widehat{\Xi}$ where $\widehat{H} = \widehat{H}^P + \mathbf{H} \cdot \mathbf{N}$,	$\text{and } \widehat{\Pi} \geq 0 \quad \text{in } \mathcal{S}_0$	
$-\overline{\text{Div}} \overline{\mathbf{H}} + \overline{\Pi} + \overline{H} = D_t \overline{\Xi}$ where $\overline{H} = \overline{H}^P - \llbracket \mathbf{H} \rrbracket \cdot \overline{\mathbf{N}}$,	$\text{and } \overline{\Pi} \geq 0 \quad \text{in } \mathcal{I}_0$	
$-\widetilde{\text{Div}} \widetilde{\mathbf{H}} + \widetilde{\Pi} + \widetilde{H} = D_t \widetilde{\Xi}$ where $\widetilde{H} = \widetilde{H}^P + \overline{\mathbf{H}} \cdot \widetilde{\mathbf{N}}_i - \llbracket \widehat{\mathbf{H}} \rrbracket \cdot \widetilde{\mathbf{N}}_s$.	$\text{and } \widetilde{\Pi} \geq 0 \quad \text{in } \mathcal{C}_0$	

The (bulk) Cauchy entropy flux vector $\mathbf{h}$ and the surface, interface and curve tangential Cauchy entropy flux vectors, denoted $\widehat{\mathbf{h}}$, $\overline{\mathbf{h}}$ and $\widetilde{\mathbf{h}}$, respectively, are related to their corresponding Piola entropy flux vectors via the Piola transforms (2.12)–(2.13).

Following the same procedures employed in the previous sections, the local balances of entropy for the various parts of the body in terms of spatial quantities are

$$\begin{aligned}
 & -\operatorname{div}(\mathbf{h} + \xi \mathbf{v}) + \pi + h = d_t \xi & \text{and } \pi \geq 0 & \text{ in } \mathcal{B}_t \\
 & \quad \text{where } h = h^P, \\
 & -\widehat{\operatorname{div}}(\widehat{\mathbf{h}} + \widehat{\xi} \widehat{\mathbf{v}}) + \widehat{\pi} + \widehat{h} = d_t \widehat{\xi} & \text{and } \widehat{\pi} \geq 0 & \text{ in } \mathcal{S}_t \\
 & \quad \text{where } \widehat{h} = \widehat{h}^P + \mathbf{h} \cdot \mathbf{n}, \\
 & -\overline{\operatorname{div}}(\overline{\mathbf{h}} + \overline{\xi} \overline{\mathbf{v}}) + \overline{\pi} + \overline{h} = d_t \overline{\xi} & \text{and } \overline{\pi} \geq 0 & \text{ in } \mathcal{I}_t \\
 & \quad \text{where } \overline{h} = \overline{h}^P - \llbracket \mathbf{h} \rrbracket \cdot \overline{\mathbf{n}}, \\
 & -\widetilde{\operatorname{div}}(\widetilde{\mathbf{h}} + \widetilde{\xi} \widetilde{\mathbf{v}}) + \widetilde{\pi} + \widetilde{h} = d_t \widetilde{\xi} & \text{and } \widetilde{\pi} \geq 0 & \text{ in } \mathcal{C}_t \\
 & \quad \text{where } \widetilde{h} = \widetilde{h}^P + \overline{\mathbf{h}} \cdot \widetilde{\mathbf{n}}_i - \llbracket \widehat{\mathbf{h}} \rrbracket \cdot \widetilde{\mathbf{n}}_s,
 \end{aligned} \tag{2.35}$$

where the bulk prescribed entropy source, entropy and entropy production per unit current volume in $\mathcal{B}_t$ are denoted $h^P := j H^P$, $\xi := j \Xi$ and $\pi := j \Pi$, respectively. In an identical fashion to the bulk, the prescribed surface, interface and curve entropy sources are denoted $\widehat{h}^P := \widehat{j} \widehat{H}^P$, $\widehat{h}^P := \widehat{j} \widehat{H}^P$ and $\widehat{h}^P := \widehat{j} \widehat{H}^P$, respectively. Similarly, $\widehat{\xi} := \widehat{j} \widehat{\Xi}$, $\widehat{\xi} := \widehat{j} \widehat{\Xi}$ and $\widehat{\xi} := \widehat{j} \widehat{\Xi}$ denote the surface, interface and curve entropies, respectively. Finally, the prescribed surface, interface and curve entropy productions are denoted $\widehat{\pi} := \widehat{j} \widehat{\Pi}$, $\overline{\pi} := \overline{j} \overline{\Pi}$ and $\widetilde{\pi} := \widetilde{j} \widetilde{\Pi}$, respectively.

To proceed, the commonly made assumption that the entropy fluxes are the corresponding heat fluxes divided by the corresponding absolute temperatures is used, that is:

$$\begin{aligned}
 \mathbf{H} &:= \mathbf{Q} \Theta^{-1}, & \widehat{\mathbf{H}} &:= \widehat{\mathbf{Q}} \widehat{\Theta}^{-1}, & \overline{\mathbf{H}} &:= \overline{\mathbf{Q}} \overline{\Theta}^{-1}, & \widetilde{\mathbf{H}} &:= \widetilde{\mathbf{Q}} \widetilde{\Theta}^{-1}, \\
 H^P &:= Q^P \Theta^{-1}, & \widehat{H}^P &:= \widehat{Q}^P \widehat{\Theta}^{-1}, & \overline{H}^P &:= \overline{Q}^P \overline{\Theta}^{-1}, & \widetilde{H}^P &:= \widetilde{Q}^P \widetilde{\Theta}^{-1}.
 \end{aligned} \tag{2.36}$$

The variables $\Theta > 0$, $\widehat{\Theta} > 0$, $\overline{\Theta} > 0$ and $\widetilde{\Theta} > 0$ denote the absolute temperatures in the bulk, on the surface, interface and curve, respectively. Note that the assumption (2.36) is not true in general but holds for simple thermodynamic processes [see e.g. 30, 112, 113].

The dissipation power for the various parts of the body are denoted $\mathcal{D}$, $\widehat{\mathcal{D}}$, $\overline{\mathcal{D}}$ and $\widetilde{\mathcal{D}}$ and are defined by

$$\mathcal{D} := \Theta \Pi \geq 0, \quad \widehat{\mathcal{D}} := \widehat{\Theta} \widehat{\Pi} \geq 0, \quad \overline{\mathcal{D}} := \overline{\Theta} \overline{\Pi} \geq 0, \quad \widetilde{\mathcal{D}} := \widetilde{\Theta} \widetilde{\Pi} \geq 0.$$

Substituting these relations into the balances of entropy for the various parts of the body

(2.34) yields the localised dissipation inequalities:

$$\begin{aligned}
 \mathcal{D} &= \Theta D_t \Xi + \text{Div } \mathbf{Q} - \mathbf{Q} \cdot \text{Grad } \ln \Theta - Q^P \geq 0 \quad \text{in } \mathcal{B}_0, \\
 \widehat{\mathcal{D}} &= \widehat{\Theta} D_t \widehat{\Xi} + \widehat{\text{Div}} \widehat{\mathbf{Q}} - \widehat{\mathbf{Q}} \cdot \widehat{\text{Grad}} \ln \widehat{\Theta} \\
 &\quad - \left[\widehat{Q}^P + \frac{\widehat{\Theta}}{\Theta} \mathbf{Q} \cdot \mathbf{N} \right] \geq 0 \quad \text{in } \mathcal{S}_0, \\
 \overline{\mathcal{D}} &= \overline{\Theta} D_t \overline{\Xi} + \overline{\text{Div}} \overline{\mathbf{Q}} - \overline{\mathbf{Q}} \cdot \overline{\text{Grad}} \ln \overline{\Theta} \\
 &\quad - \left[\overline{Q}^P - \overline{\Theta} \left[\frac{\mathbf{Q}}{\Theta} \right] \cdot \overline{\mathbf{N}} \right] \geq 0 \quad \text{in } \mathcal{I}_0, \\
 \widetilde{\mathcal{D}} &= \widetilde{\Theta} D_t \widetilde{\Xi} + \widetilde{\text{Div}} \widetilde{\mathbf{Q}} - \widetilde{\mathbf{Q}} \cdot \widetilde{\text{Grad}} \ln \widetilde{\Theta} \\
 &\quad - \left[\widetilde{Q}^P + \frac{\widetilde{\Theta}}{\Theta} \mathbf{Q} \cdot \widetilde{\mathbf{N}}_i - \widetilde{\Theta} \left[\frac{\mathbf{Q}}{\Theta} \right] \cdot \widetilde{\mathbf{N}}_s \right] \geq 0 \quad \text{in } \mathcal{C}_0.
 \end{aligned} \tag{2.37}$$

The localised dissipation inequalities (2.37) can be reformulated using the energy balance equations (2.30) as

$$\begin{aligned}
 \mathcal{D} &= \Theta D_t \Xi - D_t E + \mathbf{P} : \text{Grad } \mathbf{V} - \mathbf{Q} \cdot \text{Grad } \ln \Theta \geq 0 \quad \text{in } \mathcal{B}_0, \\
 \widehat{\mathcal{D}} &= \widehat{\Theta} D_t \widehat{\Xi} - D_t \widehat{E} + \widehat{\mathbf{P}} : \widehat{\text{Grad}} \widehat{\mathbf{V}} - \widehat{\mathbf{Q}} \cdot \widehat{\text{Grad}} \ln \widehat{\Theta} \\
 &\quad + \left[1 - \frac{\widehat{\Theta}}{\Theta} \right] \mathbf{Q} \cdot \mathbf{N} \geq 0 \quad \text{in } \mathcal{S}_0, \\
 \overline{\mathcal{D}} &= \overline{\Theta} D_t \overline{\Xi} - D_t \overline{E} + \overline{\mathbf{P}} : \overline{\text{Grad}} \overline{\mathbf{V}} - \overline{\mathbf{Q}} \cdot \overline{\text{Grad}} \ln \overline{\Theta} \\
 &\quad + \left[\overline{\Theta} \left[\frac{\mathbf{Q}}{\Theta} \right] - [\mathbf{Q}] \right] \cdot \overline{\mathbf{N}} \geq 0 \quad \text{in } \mathcal{I}_0, \\
 \widetilde{\mathcal{D}} &= \widetilde{\Theta} D_t \widetilde{\Xi} - D_t \widetilde{E} + \widetilde{\mathbf{P}} : \widetilde{\text{Grad}} \widetilde{\mathbf{V}} - \widetilde{\mathbf{Q}} \cdot \widetilde{\text{Grad}} \ln \widetilde{\Theta} \\
 &\quad + \left[\widetilde{\Theta} \left[\frac{\mathbf{Q}}{\Theta} \right] - [\mathbf{Q}] \right] \cdot \widetilde{\mathbf{N}}_s + \left[1 - \frac{\widetilde{\Theta}}{\Theta} \right] \mathbf{Q} \cdot \widetilde{\mathbf{N}}_i \geq 0 \quad \text{in } \mathcal{C}_0.
 \end{aligned} \tag{2.38}$$

Next, the Helmholtz energy, obtained as a Legendre transformation of the internal energy in terms of entropy and temperature, is introduced. Separate Helmholtz energies in the bulk, on the surface, interface and curve, denoted Ψ , $\widehat{\Psi}$, $\overline{\Psi}$ and $\widetilde{\Psi}$, respectively, are permitted and are defined by

$$\Psi := E - \Theta \Xi, \quad \widehat{\Psi} := \widehat{E} - \widehat{\Theta} \widehat{\Xi}, \quad \overline{\Psi} := \overline{E} - \overline{\Theta} \overline{\Xi}, \quad \widetilde{\Psi} := \widetilde{E} - \widetilde{\Theta} \widetilde{\Xi}. \tag{2.39}$$

From the definitions of the Helmholtz energies, the extended Clausius–Duhem dissipation inequalities can be obtained as:

$$\begin{aligned}
 \mathcal{D} &= \mathbf{P} : \text{Grad } \mathbf{V} - D_t \Psi - \Xi D_t \Theta - \mathbf{Q} \cdot \text{Grad } \ln \Theta \geq 0 \quad \text{in } \mathcal{B}_0, \\
 \widehat{\mathcal{D}} &= \widehat{\mathbf{P}} : \widehat{\text{Grad}} \widehat{\mathbf{V}} - D_t \widehat{\Psi} - \widehat{\Xi} D_t \widehat{\Theta} - \widehat{\mathbf{Q}} \cdot \widehat{\text{Grad}} \ln \widehat{\Theta} \\
 &\quad + \left[1 - \frac{\widehat{\Theta}}{\Theta} \right] \mathbf{Q} \cdot \mathbf{N} \geq 0 \quad \text{in } \mathcal{S}_0, \\
 \overline{\mathcal{D}} &= \overline{\mathbf{P}} : \overline{\text{Grad}} \overline{\mathbf{V}} - D_t \overline{\Psi} - \overline{\Xi} D_t \overline{\Theta} - \overline{\mathbf{Q}} \cdot \overline{\text{Grad}} \ln \overline{\Theta} \\
 &\quad + \left[\overline{\Theta} \left[\frac{\overline{\mathbf{Q}}}{\overline{\Theta}} \right] - [\mathbf{Q}] \right] \cdot \overline{\mathbf{N}} \geq 0 \quad \text{in } \mathcal{S}_0, \\
 \widetilde{\mathcal{D}} &= \widetilde{\mathbf{P}} : \widetilde{\text{Grad}} \widetilde{\mathbf{V}} - D_t \widetilde{\Psi} - \widetilde{\Xi} D_t \widetilde{\Theta} - \widetilde{\mathbf{Q}} \cdot \widetilde{\text{Grad}} \ln \widetilde{\Theta} \\
 &\quad + \left[\widetilde{\Theta} \left[\frac{\widetilde{\mathbf{Q}}}{\widetilde{\Theta}} \right] - [\mathbf{Q}] \right] \cdot \widetilde{\mathbf{N}}_s + \left[1 - \frac{\widetilde{\Theta}}{\Theta} \right] \overline{\mathbf{Q}} \cdot \widetilde{\mathbf{N}}_i \geq 0 \quad \text{in } \mathcal{C}_0.
 \end{aligned} \tag{2.40}$$

2.3 THERMOHYPERELASTIC HELMHOLTZ ENERGY

To exploit the dissipation inequalities further, a thermohyperelastic constitutive model is specified by selecting a particular list of arguments for the Helmholtz energies. For the case of thermohyperelastic behaviour, the arguments of the Helmholtz energies are chosen as follows:

$$\begin{aligned}
 \Psi &:= \Psi(\mathbf{F}, \Theta), & \widehat{\Psi} &:= \widehat{\Psi}(\widehat{\mathbf{F}}, \widehat{\Theta}, \mathbf{n}), \\
 \overline{\Psi} &:= \overline{\Psi}(\overline{\mathbf{F}}, \overline{\Theta}, \overline{\mathbf{n}}), & \widetilde{\Psi} &:= \widetilde{\Psi}(\widetilde{\mathbf{F}}, \widetilde{\Theta}, \widetilde{\mathbf{n}}).
 \end{aligned} \tag{2.41}$$

Note that the surface and interface Helmholtz energies are allowed to depend on their corresponding normals in the spatial configuration to capture possible anisotropic behaviour. The anisotropy of the curve, however, is modelled by dependence of the curve Helmholtz energy on its tangent in the spatial configuration. It should be emphasised that in deriving the balance equations in Section 2.2, no isotropy assumptions were made.

2.3.1 Constitutive equations

Exploiting the dissipation inequalities in the various parts of the body (2.40) using a Coleman–Noll-like procedure yields the constitutive laws:

$$\begin{aligned}
 \mathbf{P} &= \partial_{\mathbf{F}} \Psi, & \Xi &= -\partial_{\Theta} \Psi, \\
 \hat{\mathbf{P}} &= \partial_{\hat{\mathbf{F}}} \hat{\Psi} - \mathbf{n} \otimes \hat{\mathbf{J}} \quad \text{with} \quad \hat{\mathbf{J}} := \partial_{\hat{\mathbf{n}}} \hat{\psi} \cdot \hat{\mathbf{i}} \cdot \widehat{\text{cof}} \hat{\mathbf{F}}, & \hat{\Xi} &= -\partial_{\hat{\Theta}} \hat{\Psi}, \\
 \bar{\mathbf{P}} &= \partial_{\bar{\mathbf{F}}} \bar{\Psi} - \bar{\mathbf{n}} \otimes \bar{\mathbf{J}} \quad \text{with} \quad \bar{\mathbf{J}} := \partial_{\bar{\mathbf{n}}} \bar{\psi} \cdot \bar{\mathbf{i}} \cdot \widehat{\text{cof}} \bar{\mathbf{F}}, & \bar{\Xi} &= -\partial_{\bar{\Theta}} \bar{\Psi}, \\
 \tilde{\mathbf{P}} &= \partial_{\tilde{\mathbf{F}}} \tilde{\Psi} - \tilde{\mathbf{j}} \otimes \tilde{\mathbf{N}} \quad \text{with} \quad \tilde{\mathbf{j}} := \partial_{\tilde{\mathbf{n}}} \tilde{\psi} \cdot [\mathbf{i} - \tilde{\mathbf{i}}], & \tilde{\Xi} &= -\partial_{\tilde{\Theta}} \tilde{\Psi},
 \end{aligned} \tag{2.42}$$

where the Helmholtz energies in the spatial configuration, i.e. per unit deformed area for the surface and interface, and per unit deformed length for the curve, are defined by $\hat{\psi} := \hat{j} \hat{\Psi}$, $\bar{\psi} := \bar{j} \bar{\Psi}$ and $\tilde{\psi} := \tilde{j} \tilde{\Psi}$, respectively. The quantities $\hat{\mathbf{J}}$, $\bar{\mathbf{J}}$ and $\tilde{\mathbf{j}}$ denote, respectively, the surface shear, interface shear and curve shear, see also Gurtin [111] and Simha and Bhattacharya [114]. Note that the terms $\mathbf{n} \otimes \hat{\mathbf{J}}$, $\bar{\mathbf{n}} \otimes \bar{\mathbf{J}}$ and $\tilde{\mathbf{j}} \otimes \tilde{\mathbf{N}}$ map from the tangent spaces to the material surface, interface and curve, to the normals to the spatial surface, interface and curve, respectively.

2.3.2 Reduced dissipation inequalities

Inserting the constitutive relations derived in Section 2.3.1 in the dissipation inequalities (2.40), results in the following reduced dissipation inequalities:

$$\begin{aligned}
 \mathcal{D} &= -\mathbf{Q} \cdot \text{Grad} \ln \Theta & \geq 0, \\
 \hat{\mathcal{D}} &= \underbrace{-\hat{\mathbf{Q}} \cdot \widehat{\text{Grad}} \ln \hat{\Theta}}_{\hat{\mathcal{D}}_{\parallel}} + \underbrace{\left[1 - \frac{\hat{\Theta}}{\Theta}\right] \mathbf{Q} \cdot \mathbf{N}}_{\hat{\mathcal{D}}_{\perp}} & \geq 0, \\
 \bar{\mathcal{D}} &= \underbrace{-\bar{\mathbf{Q}} \cdot \overline{\text{Grad}} \ln \bar{\Theta}}_{\bar{\mathcal{D}}_{\parallel}} + \underbrace{\left[\bar{\Theta} \left[\frac{\bar{\mathbf{Q}}}{\bar{\Theta}}\right] - [\mathbf{Q}]\right] \cdot \bar{\mathbf{N}}}_{\bar{\mathcal{D}}_{\perp}} & \geq 0, \\
 \tilde{\mathcal{D}} &= \underbrace{-\tilde{\mathbf{Q}} \cdot \widetilde{\text{Grad}} \ln \tilde{\Theta}}_{\tilde{\mathcal{D}}_{\parallel}} + \underbrace{\left[\tilde{\Theta} \left[\frac{\tilde{\mathbf{Q}}}{\tilde{\Theta}}\right] - [\mathbf{Q}]\right] \cdot \tilde{\mathbf{N}}_s + \left[1 - \frac{\tilde{\Theta}}{\Theta}\right] \bar{\mathbf{Q}} \cdot \tilde{\mathbf{N}}_i}_{\tilde{\mathcal{D}}_{\perp}} & \geq 0.
 \end{aligned} \tag{2.43}$$

Note that the first terms in Eq. (2.43)_{2–4} represent the dissipation along the surface, interface and curve, and are denoted $\hat{\mathcal{D}}_{\parallel}$, $\bar{\mathcal{D}}_{\parallel}$ and $\tilde{\mathcal{D}}_{\parallel}$, respectively. In contrast, the remaining terms represent the dissipation across the surface, interface and curve, and are denoted as $\hat{\mathcal{D}}_{\perp}$, $\bar{\mathcal{D}}_{\perp}$ and $\tilde{\mathcal{D}}_{\perp}$, respectively.

2.3.2.1 Dissipation inequalities in the bulk and along the surface, interface and curve

In order to partially ensure thermodynamic consistency by satisfying the dissipation inequalities along the surface, interface and curve, and in the spirit of Fourier's law, the heat flux vectors are assumed to be of the form:

$$\begin{aligned} \mathbf{Q} &= -J \mathbf{f} \cdot \mathbf{k} \cdot \mathbf{f}^t \cdot \text{Grad } \Theta, & \widehat{\mathbf{Q}} &= -\widehat{J} \widehat{\mathbf{f}} \cdot \widehat{\mathbf{k}} \cdot \widehat{\mathbf{f}}^t \cdot \widehat{\text{Grad}} \widehat{\Theta}, \\ \overline{\mathbf{Q}} &= -\overline{J} \overline{\mathbf{f}} \cdot \overline{\mathbf{k}} \cdot \overline{\mathbf{f}}^t \cdot \overline{\text{Grad}} \overline{\Theta}, & \widetilde{\mathbf{Q}} &= -\widetilde{J} \widetilde{\mathbf{f}} \cdot \widetilde{\mathbf{k}} \cdot \widetilde{\mathbf{f}}^t \cdot \widetilde{\text{Grad}} \widetilde{\Theta}, \end{aligned} \quad (2.44)$$

where $\mathbf{k}$, $\widehat{\mathbf{k}}$, $\overline{\mathbf{k}}$ and $\widetilde{\mathbf{k}}$ denote the bulk, surface, interface and curve positive semi-definite spatial thermal conductivity tensors, respectively.

Remark In view of Eq. (2.44), it is of particular interest to study thermally isotropic materials. Thermally isotropic materials can be classified as *materially* or *spatially* isotropic, depending on in which configuration they demonstrate isotropic behaviour. For such materials, the spatial thermal conductivity tensors $\mathbf{k}$ and $\widehat{\mathbf{k}}$ simplify to

$$\begin{aligned} \text{materially isotropic:} \quad \mathbf{k} &= k \mathbf{F} \cdot \mathbf{F}^t, & \widehat{\mathbf{k}} &= \widehat{k} \widehat{\mathbf{F}} \cdot \widehat{\mathbf{F}}^t, & \overline{\mathbf{k}} &= \overline{k} \overline{\mathbf{F}} \cdot \overline{\mathbf{F}}^t, & \widetilde{\mathbf{k}} &= \widetilde{k} \widetilde{\mathbf{F}} \cdot \widetilde{\mathbf{F}}^t \\ \text{spatially isotropic:} \quad \mathbf{k} &= k \mathbf{i} & \widehat{\mathbf{k}} &= \widehat{k} \widehat{\mathbf{i}}, & \overline{\mathbf{k}} &= \overline{k} \overline{\mathbf{i}}, & \widetilde{\mathbf{k}} &= \widetilde{k} \widetilde{\mathbf{i}}, \end{aligned}$$

where the scalars $k \geq 0$, $\widehat{k} \geq 0$, $\overline{k} \geq 0$ and $\widetilde{k} \geq 0$ denote the thermal conductivity coefficients in the various parts of the body. $\square$

2.3.2.2 Dissipation inequalities across the surface, interface and curve

Assuming that the dissipation inequalities in the bulk and along the surface, interface and curve are satisfied, the further reduced dissipation inequalities across the surface, interface and curve are given by:

$$\begin{aligned} \widehat{\mathcal{D}}_{\perp} &= \widehat{\Theta} \left[\frac{1}{\widehat{\Theta}} - \frac{1}{\Theta} \right] \mathbf{Q} \cdot \mathbf{N} & \geq 0, \\ \overline{\mathcal{D}}_{\perp} &= \overline{\Theta} \left[\left[\frac{\mathbf{Q}}{\widehat{\Theta}} \right] - \left[\frac{\mathbf{Q}}{\overline{\Theta}} \right] \right] \cdot \overline{\mathbf{N}} & \geq 0, \\ \widetilde{\mathcal{D}}_{\perp} &= \widetilde{\Theta} \left[\left[\frac{\widehat{\mathbf{Q}}}{\widehat{\Theta}} \right] - \left[\frac{\widehat{\mathbf{Q}}}{\widetilde{\Theta}} \right] \right] \cdot \widetilde{\mathbf{N}}_s + \widetilde{\Theta} \left[\frac{1}{\widetilde{\Theta}} - \frac{1}{\Theta} \right] \overline{\mathbf{Q}} \cdot \widetilde{\mathbf{N}}_i & \geq 0. \end{aligned} \quad (2.45)$$

The requirements for these inequalities to be satisfied are now discussed.

Surface

The most obvious choice to *sufficiently* satisfy the further reduced dissipation inequality on the surface (2.45)₁ is

$$\widehat{\Theta} = \Theta|_{\mathcal{S}_0}, \quad (2.46)$$

that is, to impose so-called thermal slavery on the surface. It should be emphasised that the thermal slavery condition on the surface is not an a priori assumption but arises, rather, as a natural consequence of the thermodynamics. Alternatively McBride et al. [74] propose a Robin-type boundary condition between the bulk and surface.

Interface

The conditions to satisfy the further reduced dissipation inequality on the interface (2.45)₂ are now presented. Equation (2.45)₂ can be reformulated³ using either of the two identities

$$\begin{aligned}\llbracket \frac{\mathbf{Q}}{\Theta} \rrbracket &= \llbracket \mathbf{Q} \rrbracket \llbracket \frac{1}{\Theta} \rrbracket + \{\{\mathbf{Q}\}\} \llbracket \frac{1}{\Theta} \rrbracket, \\ \frac{\llbracket \mathbf{Q} \rrbracket}{\Theta} &= \llbracket \frac{\mathbf{Q}}{\Theta} \rrbracket \frac{\{\{\Theta\}\}}{\Theta} + \{\{\frac{\mathbf{Q}}{\Theta}\}\} \frac{\llbracket \Theta \rrbracket}{\Theta},\end{aligned}\tag{2.47}$$

as

$$\begin{aligned}\Rightarrow \bar{\mathcal{D}}_{\perp} &= \bar{\Theta} \left[\llbracket \frac{1}{\Theta} \rrbracket - \frac{1}{\bar{\Theta}} \right] \llbracket \mathbf{Q} \rrbracket \cdot \bar{\mathbf{N}} + \bar{\Theta} \llbracket \frac{1}{\Theta} \rrbracket \{\{\mathbf{Q}\}\} \cdot \bar{\mathbf{N}} \geq 0 \quad (\text{using Eq. (2.47)}_1), \\ \Rightarrow \bar{\mathcal{D}}_{\perp} &= \left[\bar{\Theta} - \{\{\Theta\}\} \right] \llbracket \frac{\mathbf{Q}}{\Theta} \rrbracket \cdot \bar{\mathbf{N}} - \llbracket \Theta \rrbracket \{\{\frac{\mathbf{Q}}{\Theta}\}\} \cdot \bar{\mathbf{N}} \geq 0 \quad (\text{using Eq. (2.47)}_2).\end{aligned}\tag{2.48}$$

The further reduced dissipation inequality on the interface (2.45)₂ is satisfied if either of the two *equivalent* forms in Eq. (2.48) is satisfied.

By defining the coldness ϑ as the temperature inverse, i.e. $\vartheta := 1/\Theta$, Eq. (2.48) can be expressed in an alternative form as

$$\begin{aligned}\text{Eq. (2.48)}_1 &\Rightarrow -\bar{\mathcal{D}}_{\perp} = \left[\bar{\vartheta} - \{\{\vartheta\}\} \right] \llbracket \frac{\mathbf{Q}}{\vartheta} \rrbracket \cdot \bar{\mathbf{N}} - \llbracket \vartheta \rrbracket \frac{\{\{\mathbf{Q}\}\}}{\bar{\vartheta}} \cdot \bar{\mathbf{N}} \leq 0, \\ \text{Eq. (2.48)}_2 &\Rightarrow \bar{\mathcal{D}}_{\perp} = \left[\bar{\Theta} - \{\{\Theta\}\} \right] \llbracket \frac{\mathbf{Q}}{\Theta} \rrbracket \cdot \bar{\mathbf{N}} - \llbracket \Theta \rrbracket \{\{\frac{\mathbf{Q}}{\Theta}\}\} \cdot \bar{\mathbf{N}} \geq 0.\end{aligned}\tag{2.49}$$

Coldness-based discussion: The *sufficient* conditions to satisfy Eq. (2.49)₁ are examined first. The inequality is satisfied if the following conditions hold:

$$\left[\bar{\vartheta} - \{\{\vartheta\}\} \right] \llbracket \mathbf{Q} \rrbracket \cdot \bar{\mathbf{N}} \leq 0 \quad \text{and} \quad \llbracket \vartheta \rrbracket \{\{\mathbf{Q}\}\} \cdot \bar{\mathbf{N}} \geq 0.\tag{2.50}$$

A natural choice to satisfy the first relation (2.50)₁ is a Fourier-type law for the jump of the heat flux across the interface, that is:

$$\bar{\vartheta} - \{\{\vartheta\}\} = -\bar{\alpha}_{\vartheta} \llbracket \mathbf{Q} \rrbracket \cdot \bar{\mathbf{N}},\tag{2.51}$$

³ The reduced dissipation inequality on the interface is alternatively expressed in the literature [see e.g. 48] in one of the following forms

$$\bar{\mathcal{D}}_{\perp} = \bar{\Theta} \llbracket \mathbf{Q} \rrbracket \cdot \left[\frac{1}{\bar{\Theta}} - \frac{1}{\bar{\Theta}} \right] \cdot \bar{\mathbf{N}} = \bar{\Theta} \llbracket \frac{\mathbf{Q}}{\Theta} \rrbracket \cdot \left[1 - \frac{\Theta}{\bar{\Theta}} \right] \cdot \bar{\mathbf{N}} = \llbracket \frac{\mathbf{Q}}{\Theta} \rrbracket \cdot [\bar{\Theta} - \Theta] \cdot \bar{\mathbf{N}} \geq 0.$$

where $\bar{\alpha}_\vartheta \geq 0$ is a coldness sensitivity coefficient across the interface. To satisfy the second condition (2.50)₂ a Fourier-type law for the average heat flux across the interface can be chosen, that is

$$[\![\vartheta]\!] = \bar{r}_\vartheta \{ \![Q]\! \} \cdot \bar{N}, \quad (2.52)$$

where $\bar{r}_\vartheta \geq 0$ is a heat flux resistance coefficient across the interface.

Remark For a *thermal interface*, the jump in the normal component of the heat flux is given by Eq. (2.30)₃ as:

$$[\![Q]\!] \cdot \bar{N} = -\overline{\text{Div } Q}, \quad (2.53)$$

which is the thermal Young–Laplace equation on the interface. Equation (2.53) states that the normal jump of heat flux is equal to the negative of the divergence of the heat flux along the interface. In particular, in the absence of heat flux along the thermal interface the normal jump of the heat flux, i.e. the left-hand side of the Eq. (2.53) vanishes, i.e. the *standard interface*, and therefore Eq. (2.50)₁ is trivially satisfied. $\square$

Remark A *sufficient* condition for a thermal interface to satisfy Eq. (2.50)₁ is to choose the interface coldness equal to the average of the coldness across the interface. This conclusion shall be compared with Daher and Maugin [48] who viewed it as a necessity. $\square$

Remark Using the relation $[\![\vartheta]\!] = -\{ \![\vartheta]\! \} [\![\Theta]\!] / \{ \![\Theta]\! \}$, the condition (2.50)₂ can be reformulated as $[\![\Theta]\!] \{ \![Q]\! \} \cdot \bar{N} \leq 0$ which can be satisfied by a Fourier-type law for the average heat flux across the interface $[\![\Theta]\!] = -\bar{r}_Q \{ \![Q]\! \} \cdot \bar{N}$ where $\bar{r}_Q \geq 0$ denotes the Kapitza heat flux resistance coefficient. $\square$

Temperature-based discussion: The *sufficient* conditions to satisfy Eq. (2.49)₂ are now examined. The inequality is satisfied if the following conditions hold:

$$[\bar{\Theta} - \{ \![\Theta]\! \}] [\![\frac{Q}{\Theta}]\!] \cdot \bar{N} \geq 0 \quad \text{and} \quad [\![\Theta]\!] \{ \![\frac{Q}{\Theta}]\! \} \cdot \bar{N} \leq 0. \quad (2.54)$$

A natural choice to satisfy condition (2.54)₁ is a Fourier-type law for the jump in the entropy flux across the interface, that is

$$\bar{\Theta} - \{ \![\Theta]\! \} = \bar{\alpha}_\Theta [\![H]\!] \cdot \bar{N}, \quad (2.55)$$

where $\bar{\alpha}_\Theta \geq 0$ is a temperature sensitivity coefficient across the interface. Likewise, to satisfy the condition (2.54)₂ a Fourier-type law for the average entropy flux across the interface can be chosen, that is

$$[\![\Theta]\!] = -\bar{r}_\Theta \{ \![H]\! \} \cdot \bar{N}, \quad (2.56)$$

where $\bar{r}_\Theta \geq 0$ is the entropy flux resistance coefficient across the interface.

Remark For a *standard interface*, the jump of the entropy flux, in contrast to the jump of the heat flux, does not necessarily vanish according to Eq. (2.34)₃. That is, for a *standard*

interface Eq. (2.54)₁ is not trivially satisfied. Thus, a *sufficient* condition to satisfy Eq. (2.54)₁ is to choose the interface temperature equal to the average of the temperature across the interface. $\square$

Remark For a *highly-conducting interface* the jump of the temperature across the interface vanishes which corresponds to zero normal dissipation across the interface, i.e. $\widehat{D}_\perp = 0$. For this case $\bar{\Theta} := \llbracket \Theta \rrbracket$ or $1/\bar{\Theta} := \llbracket 1/\Theta \rrbracket$. Therefore, for a *highly-conducting interface*, the interface temperature (resp. coldness) is *trivially* the average of the temperature (resp. coldness) across the interface since $\Theta|_{\mathcal{S}_0^+} = \Theta|_{\mathcal{S}_0^-} = \bar{\Theta}$. $\square$

Remark Using the relation $\llbracket \Theta \rrbracket = -\llbracket \Theta \rrbracket \llbracket \vartheta \rrbracket / \llbracket \vartheta \rrbracket$, the condition (2.54)₂ can be reformulated as $\llbracket \vartheta \rrbracket \llbracket \mathbf{H} \rrbracket \cdot \bar{\mathbf{N}} \geq 0$ which can be satisfied by a Fourier-type law for the average entropy flux across the interface $\llbracket \vartheta \rrbracket = \bar{r}_H \llbracket \mathbf{H} \rrbracket \cdot \bar{\mathbf{N}}$ where $\bar{r}_H \geq 0$ denotes an entropy flux resistance coefficient. $\square$

Summary: Thus, in summary, the *sufficient* conditions to satisfy the further reduced dissipation inequality on the interface (2.45)₂ are

$$\bar{\vartheta} - \llbracket \vartheta \rrbracket = -\bar{\alpha}_\vartheta \llbracket \mathbf{Q} \rrbracket \cdot \bar{\mathbf{N}} \quad \text{and} \quad \left(\llbracket \vartheta \rrbracket = \bar{r}_\vartheta \llbracket \mathbf{Q} \rrbracket \cdot \bar{\mathbf{N}} \quad \text{or} \quad \llbracket \Theta \rrbracket = -\bar{r}_Q \llbracket \mathbf{Q} \rrbracket \cdot \bar{\mathbf{N}} \right),$$

or

$$\bar{\Theta} - \llbracket \Theta \rrbracket = \bar{\alpha}_\Theta \llbracket \mathbf{H} \rrbracket \cdot \bar{\mathbf{N}} \quad \text{and} \quad \left(\llbracket \Theta \rrbracket = -\bar{r}_\Theta \llbracket \mathbf{H} \rrbracket \cdot \bar{\mathbf{N}} \quad \text{or} \quad \llbracket \vartheta \rrbracket = \bar{r}_H \llbracket \mathbf{H} \rrbracket \cdot \bar{\mathbf{N}} \right).$$

Curve

The further reduced dissipation inequality on the curve (2.45)₃ has two parts. The first term involves jumps and formally resembles the further reduced dissipation inequality on the interface (2.45)₂. The second term formally resembles the further reduced dissipation inequality on the surface (2.45)₁. The *sufficient* condition to satisfy the further reduced dissipation inequality on the curve is to ensure that each of these two terms are non-negative. Analogous to the interface, one has two sets of conditions and one of them has to be satisfied to ensure that the first term in Eq. (2.45)₃ is non-negative, that is

$$\frac{1}{\bar{\Theta}} = \llbracket \frac{1}{\Theta} \rrbracket \quad \text{and} \quad \llbracket \widehat{\Theta} \rrbracket = -\tilde{r}_Q \llbracket \widehat{\mathbf{Q}} \rrbracket \cdot \widetilde{\mathbf{N}}_s, \quad (2.57)$$

or

$$\widetilde{\Theta} = \llbracket \widehat{\Theta} \rrbracket \quad \text{and} \quad \llbracket \frac{1}{\widetilde{\Theta}} \rrbracket = \tilde{r}_H \llbracket \widehat{\mathbf{H}} \rrbracket \cdot \widetilde{\mathbf{N}}_s, \quad (2.58)$$

where $\tilde{r}_Q \geq 0$ and $\tilde{r}_H \geq 0$ are the heat flux and entropy flux resistance coefficients, respectively. Analogous to the surface, thermal slavery on the curve can be imposed, i.e. $\bar{\Theta} = \bar{\Theta}|_{\mathcal{C}_0}$, as the most obvious way to guarantee that the second term in Eq. (2.45)₃ is non-negative. A second novel option is to impose a constraint between the temperatures on the curve $\bar{\Theta}$ and interface $\bar{\Theta}$ and the heat flux $\bar{\mathbf{Q}} \cdot \bar{\mathbf{N}}_i$ that resembles a Robin-type boundary condition between the curve and the interface.

2.3.3 Temperature evolution equations

The thermohyperelastic constitutive equations together with the local energy balance equations give the temperature evolution equations in the bulk, on the surface, interface and curve as:

$$\begin{aligned}
 c_F D_t \Theta &= -\text{Div } \mathbf{Q} + \Theta \partial_{\Theta} \mathbf{P} : D_t \mathbf{F} + Q^p && \text{in } \mathcal{B}_0, \\
 \widehat{c}_F D_t \widehat{\Theta} &= -\widehat{\text{Div}} \widehat{\mathbf{Q}} + \widehat{\Theta} \partial_{\widehat{\Theta}} \widehat{\mathbf{P}} : D_t \widehat{\mathbf{F}} + \widehat{Q}^p + \mathbf{Q} \cdot \mathbf{N} && \text{in } \mathcal{S}_0, \\
 \bar{c}_F D_t \bar{\Theta} &= -\bar{\text{Div}} \bar{\mathbf{Q}} + \bar{\Theta} \partial_{\bar{\Theta}} \bar{\mathbf{P}} : D_t \bar{\mathbf{F}} + \bar{Q}^p - \llbracket \mathbf{Q} \rrbracket \cdot \bar{\mathbf{N}} && \text{in } \mathcal{I}_0, \\
 \widetilde{c}_F D_t \widetilde{\Theta} &= -\widetilde{\text{Div}} \widetilde{\mathbf{Q}} + \widetilde{\Theta} \partial_{\widetilde{\Theta}} \widetilde{\mathbf{P}} : D_t \widetilde{\mathbf{F}} + \widetilde{Q}^p + \bar{\mathbf{Q}} \cdot \widetilde{\mathbf{N}}_i - \llbracket \widehat{\mathbf{Q}} \rrbracket \cdot \widetilde{\mathbf{N}}_s && \text{in } \mathcal{C}_0,
 \end{aligned} \tag{2.59}$$

whereby, c_F , $\widehat{c}_F$, $\bar{c}_F$ and $\widetilde{c}_F$ denote the heat capacity coefficients in the bulk, on the surface, interface and curve, respectively, defined as

$$c_F := -\Theta \partial_{\Theta} \Psi, \quad \widehat{c}_F := -\widehat{\Theta} \partial_{\widehat{\Theta}} \widehat{\Psi}, \tag{2.60}$$

$$\bar{c}_F := -\bar{\Theta} \partial_{\bar{\Theta}} \bar{\Psi}, \quad \widetilde{c}_F := -\widetilde{\Theta} \partial_{\widetilde{\Theta}} \widetilde{\Psi}. \tag{2.61}$$

The derivation of the interface temperature evolution equation (2.59)₃ is given in Appendix B.3.

Chapter 3

Computational aspects

The objective of this section is to study the computational aspects of modelling thermo-mechanical solids containing energetic surfaces, interfaces and curves. The finite element method is used to discretise the problem in space (spatially). In order to discretise the problem in time (temporally), the finite difference method is used. As a prerequisite for the finite element implementation, the weak form of the governing equation is derived in Section 3.1. The finite element implementation is detailed in Section 3.2.

3.1 WEAK FORMULATION

In order to establish a principle of virtual work like statement and as a prerequisite for the finite element method approximations, the mechanical weak form, i.e. the weak form of the linear momentum balance equations (2.25), and the thermal weak form, i.e. the weak form of the temperature evolution equations (2.60), are required.

3.1.1 Mechanical weak form

To derive the mechanical weak form, the local linear momentum balance equations for the various parts of the body (2.25)_{1–4} are tested from left with vector-valued test functions $\delta\varphi \in \mathcal{H}_0^1(\mathcal{B}_0)$, $\delta\hat{\varphi} \in \mathcal{H}_0^1(\mathcal{S}_0)$, $\delta\bar{\varphi} \in \mathcal{H}_0^1(\mathcal{I}_0)$ and $\delta\tilde{\varphi} \in \mathcal{H}_0^1(\mathcal{C}_0)$, respectively. The result is integrated over the corresponding domains in the material configuration to give the global weak form of the balance of linear momentum as:

Find $\varphi \in \mathcal{H}^1(\mathcal{B}_0)$, $\widehat{\varphi} \in \mathcal{H}^1(\mathcal{S}_0)$, $\overline{\varphi} \in \mathcal{H}^1(\mathcal{I}_0)$ and $\widetilde{\varphi} \in \mathcal{H}^1(\mathcal{C}_0)$ such that

$$\begin{aligned} & \int_{\mathcal{B}_0} \delta\varphi \cdot [\text{Div } \mathbf{P} + \mathbf{B}^{\text{P}}] \, dV + \int_{\mathcal{S}_0} \delta\widehat{\varphi} \cdot [\widehat{\text{Div}} \widehat{\mathbf{P}} + [\widehat{\mathbf{B}}^{\text{P}} - \mathbf{P} \cdot \mathbf{N}]] \, dA \\ & + \int_{\mathcal{S}_0} \delta\overline{\varphi} \cdot [\overline{\text{Div}} \overline{\mathbf{P}} + [\overline{\mathbf{B}}^{\text{P}} + [\mathbf{P}] \cdot \overline{\mathbf{N}}]] \, dA \\ & + \int_{\mathcal{C}_0} \delta\widetilde{\varphi} \cdot [\widetilde{\text{Div}} \widetilde{\mathbf{P}} + [\widetilde{\mathbf{B}}^{\text{P}} - \overline{\mathbf{P}} \cdot \widetilde{\mathbf{N}}_i + [[\widehat{\mathbf{P}}] \cdot \widetilde{\mathbf{N}}_s]] \, dL = 0, \\ & \forall \delta\varphi \in \mathcal{H}_0^1(\mathcal{B}_0), \quad \forall \delta\widehat{\varphi} \in \mathcal{H}_0^1(\mathcal{S}_0), \quad \forall \delta\overline{\varphi} \in \mathcal{H}_0^1(\mathcal{I}_0), \quad \forall \delta\widetilde{\varphi} \in \mathcal{H}_0^1(\mathcal{C}_0). \end{aligned}$$

Using Eq. (B.3)_{1–4} and the extended divergence theorems (2.4), the orthogonality properties of the Piola stress measures in the various parts of the body (which cause the integrals containing the curvature terms to vanish), and from the kinematic slavery condition:

$$\{\{\delta\varphi\}\}_{|\mathcal{S}_0} = \delta\overline{\varphi}, \quad \{\{\delta\widehat{\varphi}\}\}_{|\mathcal{C}_0} = \delta\widetilde{\varphi}, \quad \delta\varphi|_{\mathcal{S}_0} = \delta\widehat{\varphi}, \quad \delta\overline{\varphi}|_{\mathcal{C}_0} = \delta\widetilde{\varphi}, \quad (3.1)$$

the weak form of the balance of linear momentum becomes:

$$\begin{aligned} & \int_{\mathcal{B}_0} \mathbf{P} : \text{Grad} \delta\varphi \, dV + \int_{\mathcal{S}_0} \widehat{\mathbf{P}} : \widehat{\text{Grad}} \delta\widehat{\varphi} \, dA + \int_{\mathcal{S}_0} \overline{\mathbf{P}} : \overline{\text{Grad}} \delta\overline{\varphi} \, dA \\ & + \int_{\mathcal{C}_0} \widetilde{\mathbf{P}} : \widetilde{\text{Grad}} \delta\widetilde{\varphi} \, dL - \int_{\mathcal{B}_0} \delta\varphi \cdot \mathbf{B}^{\text{P}} \, dV - \int_{\mathcal{S}_0} \delta\widehat{\varphi} \cdot \widehat{\mathbf{B}}^{\text{P}} \, dA \\ & - \int_{\mathcal{S}_0} \delta\overline{\varphi} \cdot \overline{\mathbf{B}}^{\text{P}} \, dA - \int_{\mathcal{C}_0} \delta\widetilde{\varphi} \cdot \widetilde{\mathbf{B}}^{\text{P}} \, dL = 0, \end{aligned} \quad (3.2)$$

where the test functions satisfy the conditions given in Eq. (3.1).

3.1.2 Thermal weak form

In order to derive the thermal weak form we proceed formally. The local temperature evolution equations for the various parts of the body (2.59)_{1–4} are tested from left with scalar test functions $\delta\Theta \in \mathcal{H}_0^1(\mathcal{B}_0)$, $\delta\widehat{\Theta} \in \mathcal{H}_0^1(\mathcal{S}_0)$, $\delta\overline{\Theta} \in \mathcal{H}_0^1(\mathcal{I}_0)$ and $\delta\widetilde{\Theta} \in \mathcal{H}_0^1(\mathcal{C}_0)$, respectively. The result is integrated over the corresponding domains in the material configuration to give the global weak form of the temperature evolution equation as:

Find $\Theta \in \mathcal{H}^1(\mathcal{B}_0)$, $\widehat{\Theta} \in \mathcal{H}^1(\mathcal{S}_0)$, $\overline{\Theta} \in \mathcal{H}^1(\mathcal{I}_0)$ and $\widetilde{\Theta} \in \mathcal{H}^1(\mathcal{C}_0)$ such that

$$\begin{aligned} & \int_{\mathcal{B}_0} \delta\Theta [c_{\mathbf{F}} D_t \Theta + \text{Div } \mathbf{Q} - Q^{\text{P}} - \Theta \partial_{\Theta} \mathbf{P} : D_t \mathbf{F}] \, dV \\ & + \int_{\mathcal{S}_0} \delta\widehat{\Theta} [\widehat{c}_{\widehat{\mathbf{F}}} D_t \widehat{\Theta} + \widehat{\text{Div}} \widehat{\mathbf{Q}} - [\widehat{Q}^{\text{P}} + \mathbf{Q} \cdot \mathbf{N}] - \widehat{\Theta} \partial_{\widehat{\Theta}} \widehat{\mathbf{P}} : D_t \widehat{\mathbf{F}}] \, dA \\ & + \int_{\mathcal{S}_0} \delta\overline{\Theta} [\overline{c}_{\overline{\mathbf{F}}} D_t \overline{\Theta} + \overline{\text{Div}} \overline{\mathbf{Q}} - [\overline{Q}^{\text{P}} - [[\mathbf{Q}] \cdot \overline{\mathbf{N}}] - \overline{\Theta} \partial_{\overline{\Theta}} \overline{\mathbf{P}} : D_t \overline{\mathbf{F}}] \, dA \\ & + \int_{\mathcal{C}_0} \delta\widetilde{\Theta} [\widetilde{c}_{\widetilde{\mathbf{F}}} D_t \widetilde{\Theta} + \widetilde{\text{Div}} \widetilde{\mathbf{Q}} - [\widetilde{Q}^{\text{P}} + \overline{\mathbf{Q}} \cdot \widetilde{\mathbf{N}}_i - [[\widehat{\mathbf{Q}}] \cdot \widetilde{\mathbf{N}}_s] - \widetilde{\Theta} \partial_{\widetilde{\Theta}} \widetilde{\mathbf{P}} : D_t \widetilde{\mathbf{F}}] \, dL = 0, \\ & \forall \delta\Theta \in \mathcal{H}_0^1(\mathcal{B}_0), \quad \forall \delta\widehat{\Theta} \in \mathcal{H}_0^1(\mathcal{S}_0), \quad \forall \delta\overline{\Theta} \in \mathcal{H}_0^1(\mathcal{I}_0), \quad \forall \delta\widetilde{\Theta} \in \mathcal{H}_0^1(\mathcal{C}_0). \end{aligned} \quad (3.3)$$

Using Eq. (B.2)_{1–4} and the extended divergence theorems given in Eq. (2.4)–(2.7), the orthogonality properties of the heat flux vectors for the various parts of the body (which cause the integrals containing the curvatures to vanish), Eq. (2.3), and the assumption of thermal slavery for the surface and the curve, i.e. $\hat{\Theta} = \Theta|_{\mathcal{S}_0}$ and $\tilde{\Theta} = \bar{\Theta}|_{\mathcal{C}_0}$ so that

$$\delta\Theta|_{\mathcal{S}_0} = \delta\hat{\Theta}, \quad \delta\bar{\Theta}|_{\mathcal{C}_0} = \delta\tilde{\Theta}, \quad (3.4)$$

the global weak form of the temperature evolution equation becomes

$$\begin{aligned} & - \int_{\mathcal{S}_0} [\delta\Theta] \{ \{ \mathbf{Q} \} \cdot \bar{\mathbf{N}} + [\{ \delta\Theta \} - \delta\bar{\Theta}] \{ \mathbf{Q} \} \cdot \bar{\mathbf{N}} \, dA \\ & - \int_{\mathcal{C}_0} [\delta\hat{\Theta}] \{ \{ \hat{\mathbf{Q}} \} \cdot \tilde{\mathbf{N}}_s + [\{ \delta\hat{\Theta} \} - \delta\tilde{\Theta}] \{ \hat{\mathbf{Q}} \} \cdot \tilde{\mathbf{N}}_s \, dL \\ & = \int_{\mathcal{B}_0} \mathbf{Q} \cdot \text{Grad} \delta\Theta - \delta\Theta c_F D_t \Theta + \delta\Theta Q^P + \delta\Theta \Theta \partial_{\Theta} \mathbf{P} : D_t \mathbf{F} \, dV \\ & \quad + \int_{\mathcal{S}_0} \hat{\mathbf{Q}} \cdot \widehat{\text{Grad}} \delta\hat{\Theta} - \delta\hat{\Theta} \hat{c}_F D_t \hat{\Theta} + \delta\hat{\Theta} \hat{Q}^P + \delta\hat{\Theta} \hat{\Theta} \partial_{\hat{\Theta}} \hat{\mathbf{P}} : D_t \hat{\mathbf{F}} \, dA \\ & \quad + \int_{\mathcal{S}_0} \bar{\mathbf{Q}} \cdot \overline{\text{Grad}} \delta\bar{\Theta} - \delta\bar{\Theta} \bar{c}_F D_t \bar{\Theta} + \delta\bar{\Theta} \bar{Q}^P + \delta\bar{\Theta} \bar{\Theta} \partial_{\bar{\Theta}} \bar{\mathbf{P}} : D_t \bar{\mathbf{F}} \, dA \\ & \quad + \int_{\mathcal{C}_0} \tilde{\mathbf{Q}} \cdot \widetilde{\text{Grad}} \delta\tilde{\Theta} - \delta\tilde{\Theta} \tilde{c}_F D_t \tilde{\Theta} + \delta\tilde{\Theta} \tilde{Q}^P + \delta\tilde{\Theta} \tilde{\Theta} \partial_{\tilde{\Theta}} \tilde{\mathbf{P}} : D_t \tilde{\mathbf{F}} \, dL, \end{aligned} \quad (3.5)$$

where the test functions satisfy the conditions given in Eq. (3.4).

3.1.3 Comparison with several other models

The objective of this section is to briefly derive several models given in the literature by simplifying the weak forms (3.2) and (3.5). In particular, the focus is on the thermal weak form (3.5). The following cases are examined:

- standard thermomechanical solids [115];
- highly-conducting interfaces [82];
- Kapitza interfaces [81];
- thermomechanical surfaces [91];
- thermomechanical HC interfaces [84];
- generalised Kapitza interfaces [95].

Note that none of the aforementioned models account for the contributions from the curve and therefore all the corresponding integrals vanish identically.

3.1.3.1 Standard thermomechanical solids

For standard thermomechanical solids with neither energetic nor thermal interfaces, surfaces or curves, the left-hand side of Eq. (3.5) and the integrals over the interface, surface and curve vanish. Therefore, the thermal weak form is simply that of finite strain thermoelasticity and reads

$$\int_{\mathcal{B}_0} \mathbf{Q} \cdot \text{Grad} \delta \Theta - \delta \Theta c_F D_t \Theta + \delta \Theta Q^P + \delta \Theta \Theta \partial_{\Theta} \mathbf{P} : D_t \mathbf{F} \, dV = - \int_{\mathcal{S}_0} \delta \hat{\Theta} \hat{Q}^P \, dA.$$

The numerical implementation of finite strain thermo-elasticity is well documented in the literature [see e.g. 115, and references therein].

3.1.3.2 Stationary highly-conducting thermal interfaces

Thermal solids with highly-conducting interfaces do not allow for a jump in the temperature field across the interface, i.e. $\llbracket \Theta \rrbracket = 0$ and $\llbracket \delta \Theta \rrbracket = 0$. Thus, $\llbracket \Theta \rrbracket = \bar{\Theta}$ and $\llbracket \delta \Theta \rrbracket = \delta \bar{\Theta}$. Therefore, the stationary thermal weak form in the absence of (bulk) heat sources reads

$$\int_{\mathcal{B}_0} \mathbf{Q} \cdot \text{Grad} \delta \Theta \, dV + \int_{\mathcal{S}_0} \bar{\mathbf{Q}} \cdot \overline{\text{Grad} \delta \Theta} \, dA = - \int_{\mathcal{S}_0} \delta \hat{\Theta} \hat{Q}^P \, dA. \quad (3.6)$$

For details of the numerical implementation see e.g. Yvonnet et al. [82] and the references therein.

3.1.3.3 Stationary Kapitza thermal interfaces

For the case of thermal solids containing Kapitza interfaces, the normal heat flux is continuous across the interface, i.e. $\llbracket \mathbf{Q} \rrbracket \cdot \bar{\mathbf{N}} = 0$, but a jump in the temperature field is admissible via the relation $\llbracket \Theta \rrbracket = -\bar{r}_Q \llbracket \mathbf{Q} \rrbracket \cdot \bar{\mathbf{N}}$. Therefore, the stationary thermal weak form reads

$$\int_{\mathcal{B}_0} \mathbf{Q} \cdot \text{Grad} \delta \Theta \, dV - \int_{\mathcal{S}_0} \frac{1}{\bar{r}_Q} \llbracket \delta \Theta \rrbracket \llbracket \Theta \rrbracket \, dA = - \int_{\mathcal{B}_0} \delta \Theta Q^P \, dV. \quad (3.7)$$

This model has been studied by Yvonnet et al. [81].

3.1.3.4 Thermomechanical surfaces

For thermomechanical solids with energetic surfaces, the left-hand side of Eq. (3.5) and the integrals over the interface and curve vanish. Thus, the thermal weak form reads

$$\begin{aligned} & \int_{\mathcal{B}_0} \mathbf{Q} \cdot \text{Grad} \delta \Theta - \delta \Theta c_F D_t \Theta + \delta \Theta Q^P + \delta \Theta \Theta \partial_{\Theta} \mathbf{P} : D_t \mathbf{F} \, dV \\ & + \int_{\mathcal{S}_0} \hat{\mathbf{Q}} \cdot \widehat{\text{Grad} \delta \Theta} - \delta \hat{\Theta} \hat{c}_{\hat{\mathbf{F}}} D_t \hat{\Theta} + \delta \hat{\Theta} \hat{Q}^P + \delta \hat{\Theta} \hat{\Theta} \partial_{\hat{\Theta}} \hat{\mathbf{P}} : D_t \hat{\mathbf{F}} \, dA = 0, \end{aligned}$$

which is identical to the one given in Javili and Steinmann [91] and Section 5.1.2.

3.1.3.5 Thermomechanical highly-conducting interfaces

For thermomechanical solids with HC energetic interfaces, the left-hand side of Eq. (3.5) vanish since $[\![\Theta]\!] = 0$, $[\![\delta\Theta]\!] = 0$, $\{\!\{\Theta\}\!\} = \bar{\Theta}$ and $\{\!\{\delta\Theta\}\!\} = \delta\bar{\Theta}$. Thus, the thermal weak form reads

$$\begin{aligned} \int_{\mathcal{B}_0} \mathbf{Q} \cdot \text{Grad} \delta\Theta - \delta\Theta c_F D_t \Theta + \delta\Theta Q^P + \delta\Theta \Theta \partial_\Theta \mathbf{P} : D_t \mathbf{F} \, dV + \int_{\mathcal{I}_0} \delta\hat{\Theta} \hat{Q}^P \, dA \\ + \int_{\mathcal{I}_0} \bar{\mathbf{Q}} \cdot \overline{\text{Grad}} \delta\bar{\Theta} - \delta\bar{\Theta} \bar{c}_F D_t \bar{\Theta} + \delta\bar{\Theta} \bar{Q}^P + \delta\bar{\Theta} \bar{\Theta} \partial_{\bar{\Theta}} \bar{\mathbf{P}} : D_t \bar{\mathbf{F}} \, dA = 0. \end{aligned}$$

This model, as compared to Eq. (3.6), accounts for thermomechanical coupling in the bulk and on the interface and is not limited to the stationary case, see Javili et al. [84] and Section 5.2.1 for further details.

3.1.3.6 Generalised Kapitza interfaces

The Kapitza interface is termed *generalised* in the sense that the interface is mechanically energetic in contrast to classical Kapitza interfaces. For the case of thermomechanical solids containing generalised Kapitza interfaces, a jump in the temperature field is admissible via the relation $[\![\Theta]\!] = -\bar{r}_Q \{\!\{\mathbf{Q}\}\!\} \cdot \bar{\mathbf{N}}$ while $[\![\mathbf{Q}]\!] \cdot \bar{\mathbf{N}} = 0$. Therefore, the thermal weak form reads

$$\begin{aligned} \int_{\mathcal{B}_0} \mathbf{Q} \cdot \text{Grad} \delta\Theta - \delta\Theta c_F D_t \Theta + \delta\Theta Q^P + \delta\Theta \Theta \partial_\Theta \mathbf{P} : D_t \mathbf{F} \, dV + \int_{\mathcal{I}_0} \delta\hat{\Theta} \hat{Q}^P \, dA \\ - \int_{\mathcal{I}_0} \frac{1}{\bar{r}_Q} [\![\delta\Theta]\!] [\![\Theta]\!] \, dA = 0. \end{aligned}$$

This model, as compared to Eq. (3.7), not only endows the interface with its own mechanically energetic structure, but also accounts for thermomechanical coupling in the bulk and is not limited to the stationary case, see Javili et al. [95] and Section 5.2.2 for further details.

3.2 FINITE ELEMENT IMPLEMENTATION

Numerical solutions of problems in finite thermoelasticity date back to Oden [116]. These problems can be solved using either a staggered or a monolithic strategy [see e.g. 115, 117–119, for further details].

The finite element implementation of a model for interfaces bears certain similarities to that for surfaces and curves. Computational aspects of HC interfaces are formally identical to surfaces. Therefore, in this section the finite element implementations of the HC and Kapitza interfaces are studied. In doing so, all the energetic contributions from the surface and the curve are omitted henceforth in this section.

3.2.1 Thermomechanical highly-conducting interfaces

The point of departure for the numerical implementation is the weak form of the governing equations. The mechanical and thermal weak forms for a thermomechanical solid containing a HC interface are next obtained by simplifying the general weak forms Eq. (3.2) and (3.5) to the current case.

The weak form of the balance of linear momentum becomes:

$$\begin{aligned} \int_{\mathcal{B}_0} \mathbf{P} : \text{Grad} \delta \boldsymbol{\varphi} \, dV + \int_{\mathcal{I}_0} \overline{\mathbf{P}} : \overline{\text{Grad}} \delta \overline{\boldsymbol{\varphi}} \, dA \\ - \int_{\mathcal{B}_0} \delta \boldsymbol{\varphi} \cdot \mathbf{B}^P \, dV - \int_{\partial \mathcal{B}_0^{\text{NB}}} \delta \boldsymbol{\varphi} \cdot \widehat{\mathbf{B}}^P \, dA - \int_{\mathcal{I}_0} \delta \overline{\boldsymbol{\varphi}} \cdot \overline{\mathbf{B}}^P \, dA = 0, \end{aligned} \quad (3.8)$$

$$\forall \delta \boldsymbol{\varphi} \in \mathcal{H}_0^1(\mathcal{B}_0), \forall \delta \overline{\boldsymbol{\varphi}} \in \mathcal{H}_0^1(\mathcal{I}_0) \quad \text{with} \quad \delta \overline{\boldsymbol{\varphi}} = \llbracket \delta \boldsymbol{\varphi} \rrbracket, \llbracket \boldsymbol{\varphi} \rrbracket = \mathbf{0},$$

where $\widehat{\mathbf{B}}^P = \mathbf{P} \cdot \mathbf{N}$ denotes the prescribed traction (Neumann boundary condition) on a portion of the surface $\partial \mathcal{B}_0^{\text{NB}} \subset \partial \mathcal{B}_0$ upon which the traction, and not the motion, is prescribed.

In a near-identical fashion the thermal weak form can be derived. The global weak form of the temperature evolution equation reads

$$\begin{aligned} \int_{\mathcal{B}_0} \mathbf{Q} \cdot \text{Grad} \delta \Theta - \delta \Theta c_F D_t \Theta + \delta \Theta Q^P + \delta \Theta \Theta \partial_{\Theta} \mathbf{P} : D_t \mathbf{F} \, dV + \int_{\partial \mathcal{B}_0^{\text{NQ}}} \delta \Theta \widehat{Q}^P \, dA \\ + \int_{\mathcal{I}_0} \overline{\mathbf{Q}} \cdot \overline{\text{Grad}} \delta \overline{\Theta} - \delta \overline{\Theta} \overline{c}_F D_t \overline{\Theta} + \delta \overline{\Theta} \overline{Q}^P + \delta \overline{\Theta} \overline{\Theta} \partial_{\overline{\Theta}} \overline{\mathbf{P}} : D_t \overline{\mathbf{F}} \, dA = 0, \end{aligned} \quad (3.9)$$

$$\forall \delta \Theta \in \mathcal{H}_0^1(\mathcal{B}_0), \forall \delta \overline{\Theta} \in \mathcal{H}_0^1(\mathcal{I}_0) \quad \text{with} \quad \delta \overline{\Theta} = \llbracket \delta \Theta \rrbracket, \llbracket \Theta \rrbracket = 0,$$

where $\widehat{Q}^P = -\mathbf{Q} \cdot \mathbf{N}$ denotes the prescribed heat source (Neumann boundary condition) on a portion of the surface $\partial \mathcal{B}_0^{\text{NQ}} \subset \partial \mathcal{B}_0$ upon which the heat source, and not temperature, is prescribed.

Next the weak forms Eq. (3.8)–(3.9) are discretised. The discretisation is carried out first in time using a finite difference scheme and subsequently in space by means of the finite element method.

The time interval $\mathcal{T}$ is subdivided into a set of intervals Δt with

$$\mathcal{T} = \bigcup_{\tau=0}^{\text{n-ts}} [t_{\tau}, t_{\tau+1}],$$

where n-ts denotes the number of time steps and the time increment is defined by $\Delta t := t_{\tau+1} - t_{\tau}$. The unknown fields at the current time $t_{\tau+1}$ are obtained from the known results at the previous time t_{τ} . The various time derivatives are approximated as follows:

$$D_t \{\bullet\} \approx \frac{1}{\Delta t} [\{\bullet\}_{\tau+1} - \{\bullet\}_{\tau}].$$

In what follows, a classical Euler-backward integration scheme is employed. Thus the governing equations of the initial boundary value problem Eq. (3.8)–(3.9) are evaluated at $t_{\tau+1}$. That is,

$$\begin{aligned} & \int_{\mathcal{B}_0} \mathbf{P}_{\tau+1} : \text{Grad} \delta \varphi \, dV + \int_{\mathcal{I}_0} \overline{\mathbf{P}}_{\tau+1} : \overline{\text{Grad}} \delta \overline{\varphi} \, dA \\ & - \int_{\mathcal{B}_0} \delta \varphi \cdot \mathbf{B}_{\tau+1}^p \, dV - \int_{\partial \mathcal{B}_0^{\text{NB}}} \delta \varphi \cdot \widehat{\mathbf{B}}_{\tau+1}^p \, dA - \int_{\mathcal{I}_0} \delta \overline{\varphi} \cdot \overline{\mathbf{B}}_{\tau+1}^p \, dA = 0, \end{aligned} \quad (3.10)$$

and

$$\begin{aligned} & \int_{\mathcal{B}_0} \mathbf{Q}_{\tau+1} \cdot \text{Grad} \delta \Theta \, dV + \int_{\mathcal{I}_0} \overline{\mathbf{Q}}_{\tau+1} \cdot \overline{\text{Grad}} \delta \overline{\Theta} \, dA \\ & - \int_{\mathcal{B}_0} c_F \frac{1}{\Delta t} [\Theta_{\tau+1} - \Theta_{\tau}] \delta \Theta \, dV - \int_{\mathcal{I}_0} \overline{c}_F \frac{1}{\Delta t} [\overline{\Theta}_{\tau+1} - \overline{\Theta}_{\tau}] \delta \overline{\Theta} \, dA \\ & + \int_{\mathcal{B}_0} \Theta_{\tau+1} [\partial_{\Theta} \mathbf{P}]_{\tau+1} : \frac{1}{\Delta t} [\mathbf{F}_{\tau+1} - \mathbf{F}_{\tau}] \delta \Theta \, dV \\ & + \int_{\mathcal{I}_0} \overline{\Theta}_{\tau+1} [\partial_{\overline{\Theta}} \overline{\mathbf{P}}]_{\tau+1} : \frac{1}{\Delta t} [\overline{\mathbf{F}}_{\tau+1} - \overline{\mathbf{F}}_{\tau}] \delta \overline{\Theta} \, dA \\ & + \int_{\mathcal{B}_0} Q_{\tau+1}^p \delta \Theta \, dV + \int_{\mathcal{I}_0} \overline{Q}_{\tau+1}^p \delta \overline{\Theta} \, dA + \int_{\partial \mathcal{B}_0^{\text{NQ}}} \delta \Theta \widehat{Q}_{\tau+1}^p \, dA = 0. \end{aligned} \quad (3.11)$$

Next, the spatial discretisation of the problem domain is performed using the Bubnov-Galerkin finite element method. In order to have a straightforward and efficient finite element scheme, the interface elements are chosen to be consistent with the bulk elements. For example, if the bulk is discretised using triquadratic elements, then biquadratic interface elements are used. This choice has the advantage that the common facet of two adjacent bulk elements can be regarded as an interface element.

The reference domains $\mathcal{B}_0$ and $\mathcal{I}_0$ are discretised into a set of bulk and interface elements

$$\mathcal{B}_0^h \approx \bigcup_{\beta=1}^{\text{n-Bel}} \mathcal{B}_0^{\beta} \quad \text{and} \quad \mathcal{I}_0^h \approx \bigcup_{\gamma=1}^{\text{n-Iel}} \mathcal{I}_0^{\gamma},$$

where n-Bel and n-Iel denote the number of bulk and interface elements, respectively.

The geometry and temperature of the bulk and the interface are approximated as a function of the natural coordinates $\boldsymbol{\xi} \in [-1, 1]^3$ and $\overline{\boldsymbol{\xi}} \in [-1, 1]^2$ assigned to the bulk and the interface, respectively, using standard interpolations according to the isoparametric

concept as follows:

$$\begin{aligned} \mathbf{X}|_{\mathcal{B}_0^\beta} &\approx \mathbf{X}^h(\boldsymbol{\xi}) = \sum_{i=1}^{\text{nn-B}} N^i(\boldsymbol{\xi}) \mathbf{X}^i, & \bar{\mathbf{X}}|_{\mathcal{J}_0^\gamma} &\approx \bar{\mathbf{X}}^h(\bar{\boldsymbol{\xi}}) = \sum_{i=1}^{\text{nn-I}} \bar{N}^i(\bar{\boldsymbol{\xi}}) \bar{\mathbf{X}}^i, \\ \Theta|_{\mathcal{B}_0^\beta} &\approx \Theta^h(\boldsymbol{\xi}) = \sum_{i=1}^{\text{nn-B}} N^i(\boldsymbol{\xi}) \Theta^i, & \bar{\Theta}|_{\mathcal{J}_0^\gamma} &\approx \bar{\Theta}^h(\bar{\boldsymbol{\xi}}) = \sum_{i=1}^{\text{nn-I}} \bar{N}^i(\bar{\boldsymbol{\xi}}) \bar{\Theta}^i, \\ \varphi|_{\mathcal{B}_0^\beta} &\approx \varphi^h(\boldsymbol{\xi}) = \sum_{i=1}^{\text{nn-B}} N^i(\boldsymbol{\xi}) \varphi^i, & \bar{\varphi}|_{\mathcal{J}_0^\gamma} &\approx \bar{\varphi}^h(\bar{\boldsymbol{\xi}}) = \sum_{i=1}^{\text{nn-I}} \bar{N}^i(\bar{\boldsymbol{\xi}}) \bar{\varphi}^i, \end{aligned}$$

where the shape functions of the bulk and interface elements at their local node i are denoted as N^i and $\bar{N}^i$, respectively. The bulk elements consist of nn-B nodes and nn-I denotes the number of nodes per interface element.

The fully-discrete form of the semi-discrete balance equations (3.10)–(3.11) are now obtained by applying the spatial approximation.¹ The fully-discrete form of mechanical and thermal residuals at time $t_{\tau+1}$ associated with the global node I are defined by

$$\begin{aligned} [\text{tot} \mathbf{R}_\varphi^I]_{\tau+1} &:= \int_{\mathcal{B}_0} \mathbf{P}_{\tau+1} \cdot \text{Grad} N^I \, dV + \int_{\mathcal{J}_0} \bar{\mathbf{P}}_{\tau+1} \cdot \overline{\text{Grad}} \bar{N}^I \, dA \\ &\quad - \int_{\mathcal{B}_0} N^I \mathbf{B}_{\tau+1}^p \, dV - \int_{\mathcal{J}_0} \bar{N}^I \bar{\mathbf{B}}_{\tau+1}^p \, dA, \end{aligned} \quad (3.12)$$

and

$$\begin{aligned} [\text{tot} \mathbf{R}_\Theta^I]_{\tau+1} &:= - \int_{\mathcal{B}_0} \mathbf{Q}_{\tau+1} \cdot \text{Grad} N^I \, dV - \int_{\mathcal{J}_0} \bar{\mathbf{Q}}_{\tau+1} \cdot \overline{\text{Grad}} \bar{N}^I \, dA \\ &\quad + \int_{\mathcal{B}_0} c_F \frac{1}{\Delta t} [\Theta_{\tau+1} - \Theta_\tau] N^I \, dV + \int_{\mathcal{J}_0} \bar{c}_F \frac{1}{\Delta t} [\bar{\Theta}_{\tau+1} - \bar{\Theta}_\tau] \bar{N}^I \, dA \\ &\quad - \int_{\mathcal{B}_0} \Theta_{\tau+1} [\partial_\Theta \mathbf{P}]_{\tau+1} : \frac{1}{\Delta t} [\mathbf{F}_{\tau+1} - \mathbf{F}_\tau] N^I \, dV \\ &\quad - \int_{\mathcal{J}_0} \bar{\Theta}_{\tau+1} [\partial_{\bar{\Theta}} \bar{\mathbf{P}}]_{\tau+1} : \frac{1}{\Delta t} [\bar{\mathbf{F}}_{\tau+1} - \bar{\mathbf{F}}_\tau] \bar{N}^I \, dA \\ &\quad - \int_{\mathcal{B}_0} Q_{\tau+1}^p N^I \, dV - \int_{\mathcal{J}_0} \bar{Q}_{\tau+1}^p \bar{N}^I \, dA. \end{aligned} \quad (3.13)$$

The total global residuals Eq. (3.12)–(3.13) must vanish at the time $t_{\tau+1}$.²

¹In what follows, for the sake of brevity, homogeneous Neumann boundary conditions are assumed. Thus the integrals over $\partial \mathcal{B}_0^{\text{NB}}$ and $\partial \mathcal{B}_0^{\text{NQ}}$ vanish identically. Even if one were not to make this assumption, the integrals are standard. Furthermore they are not influenced by the energetic interface which is the focus of this section.

²The subscript $\tau+1$ is dropped in the remainder of this section for the sake of readability.

Note that the total nodal mechanical (momentum) residual ${}^{\text{tot}}\mathbf{R}_\varphi^I$ and the total nodal thermal (energy) residual ${}^{\text{tot}}\mathbf{R}_\Theta^I$ consist of contributions from both the bulk and the interface, i.e.

$${}^{\text{tot}}\mathbf{R}_\varphi^I = \mathbf{R}_\varphi^I + \bar{\mathbf{R}}_\varphi^I \quad \text{and} \quad {}^{\text{tot}}\mathbf{R}_\Theta^I = \mathbf{R}_\Theta^I + \bar{\mathbf{R}}_\Theta^I.$$

The global momentum and energy residual vectors take the form

$${}^{\text{tot}}\mathbf{R} = \begin{bmatrix} {}^{\text{tot}}\mathbf{R}_\varphi \\ {}^{\text{tot}}\mathbf{R}_\Theta \end{bmatrix} \quad \text{with} \quad {}^{\text{tot}}\mathbf{R}_\varphi = \begin{bmatrix} {}^{\text{tot}}\mathbf{R}_\varphi^1 \\ {}^{\text{tot}}\mathbf{R}_\varphi^2 \\ \vdots \\ {}^{\text{tot}}\mathbf{R}_\varphi^I \\ \vdots \\ {}^{\text{tot}}\mathbf{R}_\varphi^{\text{nn}} \end{bmatrix}, \quad {}^{\text{tot}}\mathbf{R}_\Theta = \begin{bmatrix} {}^{\text{tot}}\mathbf{R}_\Theta^1 \\ {}^{\text{tot}}\mathbf{R}_\Theta^2 \\ \vdots \\ {}^{\text{tot}}\mathbf{R}_\Theta^I \\ \vdots \\ {}^{\text{tot}}\mathbf{R}_\Theta^{\text{nn}} \end{bmatrix}, \quad (3.14)$$

where nn denotes the total number of nodes.

The fully-discrete coupled nonlinear system of governing equations can be stated as follows:

$${}^{\text{tot}}\mathbf{R} = {}^{\text{tot}}\mathbf{R}({}^{\text{tot}}\mathbf{d}) \stackrel{!}{=} \mathbf{0}, \quad (3.15)$$

where ${}^{\text{tot}}\mathbf{d}$ is the unknown global vector of spatial coordinates and temperatures defined by

$${}^{\text{tot}}\mathbf{d} = \begin{bmatrix} {}^{\text{tot}}\mathbf{d}_\varphi \\ {}^{\text{tot}}\mathbf{d}_\Theta \end{bmatrix} \quad \text{with} \quad {}^{\text{tot}}\mathbf{d}_\varphi = \begin{bmatrix} \varphi^1 \\ \varphi^2 \\ \vdots \\ \varphi^I \\ \vdots \\ \varphi^{\text{nn}} \end{bmatrix}, \quad {}^{\text{tot}}\mathbf{d}_\Theta = \begin{bmatrix} \Theta^1 \\ \Theta^2 \\ \vdots \\ \Theta^I \\ \vdots \\ \Theta^{\text{nn}} \end{bmatrix}.$$

In order to solve Eq. (3.15), i.e. to find ${}^{\text{tot}}\mathbf{d}$ such that ${}^{\text{tot}}\mathbf{R}$ vanishes, a Newton–Raphson scheme is utilised. The consistent linearisation of the resulting system of equations yields

$${}^{\text{tot}}\mathbf{R}({}^{\text{tot}}\mathbf{d}) + \frac{\partial {}^{\text{tot}}\mathbf{R}}{\partial {}^{\text{tot}}\mathbf{d}} \Big|_\zeta \Delta {}^{\text{tot}}\mathbf{d}_\zeta \stackrel{!}{=} \mathbf{0} \quad \text{and} \quad {}^{\text{tot}}\mathbf{d}_{\zeta+1} = {}^{\text{tot}}\mathbf{d}_\zeta + \Delta {}^{\text{tot}}\mathbf{d}_\zeta, \quad (3.16)$$

Table 3.1: Consistent linearisation of the residual and the components of the algorithmic tangent.

$\mathbf{K}_{\varphi\varphi}^{IJ} = \frac{\partial \mathbf{R}_{\varphi}^I}{\partial \varphi^J} = \int_{\mathcal{B}_0} \text{Grad} N^I : \left[\frac{\partial \mathbf{P}}{\partial \mathbf{F}} \right] \cdot \text{Grad} N^J \, dV$
$\mathbf{K}_{\varphi\Theta}^{IJ} = \frac{\partial \mathbf{R}_{\varphi}^I}{\partial \Theta^J} = \int_{\mathcal{B}_0} N^J \left[\frac{\partial \mathbf{P}}{\partial \Theta} \right] \cdot \text{Grad} N^I \, dV$
$\mathbf{K}_{\Theta\varphi}^{IJ} = \frac{\partial \mathbf{R}_{\Theta}^I}{\partial \varphi^J} = \int_{\mathcal{B}_0} -N^I \left[\frac{\partial (\Theta \mathbf{P}_{,\Theta} : \mathbf{D}_t \mathbf{F})}{\partial \mathbf{F}} \right] \cdot \text{Grad} N^J - \text{Grad} N^I \cdot \left[\frac{\partial \mathbf{Q}}{\partial \mathbf{F}} \right] \cdot \text{Grad} N^J \, dV$
$\mathbf{K}_{\Theta\Theta}^{IJ} = \frac{\partial \mathbf{R}_{\Theta}^I}{\partial \Theta^J} = \int_{\mathcal{B}_0} -\text{Grad} N^I \cdot \left[\frac{\partial \mathbf{Q}}{\partial \text{Grad} \Theta} \right] \cdot \text{Grad} N^J + N^I \left[\frac{c_F}{\Delta t} - \left[\frac{\partial (\Theta \mathbf{P}_{,\Theta} : \mathbf{D}_t \mathbf{F})}{\partial \Theta} \right] \right] N^J \, dV$
$\overline{\mathbf{K}}_{\varphi\varphi}^{IJ} = \frac{\partial \overline{\mathbf{R}}_{\varphi}^I}{\partial \overline{\varphi}^J} = \int_{\mathcal{S}_0} \overline{\text{Grad}} \overline{N}^I : \left[\frac{\partial \overline{\mathbf{P}}}{\partial \overline{\mathbf{F}}} \right] \cdot \overline{\text{Grad}} \overline{N}^J \, dA$
$\overline{\mathbf{K}}_{\varphi\Theta}^{IJ} = \frac{\partial \overline{\mathbf{R}}_{\varphi}^I}{\partial \Theta^J} = \int_{\mathcal{S}_0} \overline{N}^J \left[\frac{\partial \overline{\mathbf{P}}}{\partial \Theta} \right] \cdot \overline{\text{Grad}} \overline{N}^I \, dA$
$\overline{\mathbf{K}}_{\Theta\varphi}^{IJ} = \frac{\partial \overline{\mathbf{R}}_{\Theta}^I}{\partial \overline{\varphi}^J} = \int_{\mathcal{S}_0} -\overline{N}^I \left[\frac{\partial (\Theta \overline{\mathbf{P}}_{,\Theta} : \mathbf{D}_t \overline{\mathbf{F}})}{\partial \overline{\mathbf{F}}} \right] \cdot \overline{\text{Grad}} \overline{N}^J - \overline{\text{Grad}} \overline{N}^I \cdot \left[\frac{\partial \overline{\mathbf{Q}}}{\partial \overline{\mathbf{F}}} \right] \cdot \overline{\text{Grad}} \overline{N}^J \, dA$
$\overline{\mathbf{K}}_{\Theta\Theta}^{IJ} = \frac{\partial \overline{\mathbf{R}}_{\Theta}^I}{\partial \Theta^J} = \int_{\mathcal{S}_0} -\overline{\text{Grad}} \overline{N}^I \cdot \left[\frac{\partial \overline{\mathbf{Q}}}{\partial \overline{\text{Grad}} \Theta} \right] \cdot \overline{\text{Grad}} \overline{N}^J + \overline{N}^I \left[\frac{\overline{c}_F}{\Delta t} - \left[\frac{\partial (\Theta \overline{\mathbf{P}}_{,\Theta} : \mathbf{D}_t \overline{\mathbf{F}})}{\partial \Theta} \right] \right] \overline{N}^J \, dA$

where ζ is the iteration. Solving (3.16) yields the iterative increment $\Delta^{\text{tot}} \mathbf{d}_{\zeta}$ and consequently $^{\text{tot}} \mathbf{d}_{\zeta+1}$. The corresponding total (algorithmic) tangent matrix is defined by

$$^{\text{tot}} \mathbf{K} := \frac{\partial^{\text{tot}} \mathbf{R}}{\partial^{\text{tot}} \mathbf{d}},$$

which can be decomposed into mechanical and thermal contributions from the bulk and the interface as follows

$$^{\text{tot}} \mathbf{K} = \begin{bmatrix} ^{\text{tot}} \mathbf{K}_{\varphi\varphi} & ^{\text{tot}} \mathbf{K}_{\varphi\Theta} \\ ^{\text{tot}} \mathbf{K}_{\Theta\varphi} & ^{\text{tot}} \mathbf{K}_{\Theta\Theta} \end{bmatrix} = \begin{bmatrix} \mathbf{K}_{\varphi\varphi} & \mathbf{K}_{\varphi\Theta} \\ \mathbf{K}_{\Theta\varphi} & \mathbf{K}_{\Theta\Theta} \end{bmatrix} + \begin{bmatrix} \overline{\mathbf{K}}_{\varphi\varphi} & \overline{\mathbf{K}}_{\varphi\Theta} \\ \overline{\mathbf{K}}_{\Theta\varphi} & \overline{\mathbf{K}}_{\Theta\Theta} \end{bmatrix},$$

where

$$\begin{aligned} \mathbf{K}_{\varphi\varphi}^{IJ} &= \frac{\partial \mathbf{R}_{\varphi}^I}{\partial \varphi^J}, & \mathbf{K}_{\varphi\Theta}^{IJ} &= \frac{\partial \mathbf{R}_{\varphi}^I}{\partial \Theta^J}, & \mathbf{K}_{\Theta\varphi}^{IJ} &= \frac{\partial \mathbf{R}_{\Theta}^I}{\partial \varphi^J}, & \mathbf{K}_{\Theta\Theta}^{IJ} &= \frac{\partial \mathbf{R}_{\Theta}^I}{\partial \Theta^J}, \\ \overline{\mathbf{K}}_{\varphi\varphi}^{IJ} &= \frac{\partial \overline{\mathbf{R}}_{\varphi}^I}{\partial \overline{\varphi}^J}, & \overline{\mathbf{K}}_{\varphi\Theta}^{IJ} &= \frac{\partial \overline{\mathbf{R}}_{\varphi}^I}{\partial \Theta^J}, & \overline{\mathbf{K}}_{\Theta\varphi}^{IJ} &= \frac{\partial \overline{\mathbf{R}}_{\Theta}^I}{\partial \overline{\varphi}^J}, & \overline{\mathbf{K}}_{\Theta\Theta}^{IJ} &= \frac{\partial \overline{\mathbf{R}}_{\Theta}^I}{\partial \Theta^J}. \end{aligned} \quad (3.17)$$

These sub-matrices are computed according to the results summarised in Table 3.1.

3.2.2 Generalised Kapitza interfaces

In this section, computational aspects of generalised Kapitza interfaces are briefly reviewed. The contents of this section rely heavily on Section 3.2.1 and the repetition, unless necessary, is avoided. The generalised Kapitza interface is mechanically energetic and the mechanical weak form is identical to the mechanical weak form for HC interfaces (3.8). Therefore, the weak form and subsequent derivations are skipped.

Remark Due to the assumption of the interface being Kapitza, the jump of the normal heat flux across the interface vanishes, that is $\llbracket \mathbf{Q} \rrbracket \cdot \bar{\mathbf{N}} = 0$. Note that, to the best of author's knowledge, no study of Kapitza interfaces endows the interface with its own energetic structure [see e.g. 81, and references therein]. A key feature of this work is to generalise the Kapitza interface model to interfaces with their own mechanically energetic structure. It seems natural to extend this to thermomechanically energetic interfaces. However, endowing the interface with its own thermally energetic structure leads to a jump of the heat flux across the interface. Hence such a formulation can not be described by a Kapitza interface model. This extension requires a generic imperfect interface model which is out of the scope of this manuscript. $\square$

The global weak form of the temperature evolution equation of a generalised Kapitza interface reads

$$\begin{aligned} \int_{\mathcal{B}_0} \mathbf{Q} \cdot \text{Grad} \delta \Theta - \delta \Theta c_F D_t \Theta + \delta \Theta Q^P + \delta \Theta \Theta \partial_\Theta \mathbf{P} : D_t \mathbf{F} \, dV \\ + \int_{\mathcal{S}_0} \llbracket \delta \Theta \rrbracket \llbracket \mathbf{Q} \rrbracket \cdot \bar{\mathbf{N}} \, dA + \int_{\partial \mathcal{B}_0^{\text{NQ}}} \delta \Theta \hat{Q}^P \, dA = 0, \quad \forall \delta \Theta \in \mathcal{H}_0^1(\mathcal{B}_0). \end{aligned} \quad (3.18)$$

Note that for a Kapitza interface the relation $\llbracket \Theta \rrbracket = -\bar{r}_Q \llbracket \mathbf{Q} \rrbracket \cdot \bar{\mathbf{N}}$ holds between the average normal heat flux and the temperature jump across the interface.

Next the weak forms (3.8) and (3.18) are discretised in time and space in a similar manner to the HC interface. In contrast to the HC interface, the temperature, or rather the temperature jump, on the Kapitza interface is approximated as a function of the natural coordinates $\bar{\xi}$ according to:

$$\llbracket \Theta \rrbracket \Big|_{\mathcal{S}_0^\gamma} \approx \llbracket \Theta \rrbracket^h(\bar{\xi}) = \sum_{i=1}^{nn-1} \bar{N}^i(\bar{\xi}) \llbracket \Theta^i \rrbracket,$$

The fully-discrete form of the mechanical residual is identical to that of the HC interface given in Eq. (3.12). The fully-discrete form of the thermal residuals at time $t_{\tau+1}$

associated with the global node I is

$$\begin{aligned}
 [\text{tot} \mathbf{R}_\Theta^I]_{\tau+1} = & - \int_{\mathcal{B}_0} \mathbf{Q}_{\tau+1} \cdot \text{Grad} N^I \, dV - \int_{\mathcal{B}_0} Q_{\tau+1}^p N^I \, dV \\
 & - \int_{\mathcal{B}_0} \Theta_{\tau+1} [\partial_\Theta \mathbf{P}]_{\tau+1} : \frac{1}{\Delta t} [\mathbf{F}_{\tau+1} - \mathbf{F}_\tau] N^I \, dV \\
 & + \int_{\mathcal{B}_0} c_F \frac{1}{\Delta t} [\Theta_{\tau+1} - \Theta_\tau] N^I \, dV \\
 & + \int_{\mathcal{S}_0^+} \frac{1}{\bar{r}_Q} \bar{N}^I [\Theta] \, dA - \int_{\mathcal{S}_0^-} \frac{1}{\bar{r}_Q} \bar{N}^I [\Theta] \, dA.
 \end{aligned} \tag{3.19}$$

The total global residuals in Eq. (3.12) and (3.19) must vanish at the time $t_{\tau+1}$. In view of the last two terms in Eq. (3.13), it is important to bear in mind that the global node I on the positive side of the interface is the same as the global node I on the negative side and assumes the same geometrical degrees of freedom on both sides. However, the thermal degree of freedom of the global node I on the positive side of the interface is different from that of the negative side. Therefore, the last two terms in Eq. (3.13) refer to different degrees of freedom and do not vanish together although they look identical.

The rest of the computational procedure is formally very similar to that given in Section 3.2.1 and is not repeated. Note that the structure of the corresponding total (algorithmic) tangent stiffness matrix is slightly different from that of HC interfaces since the thermomechanical contributions on the interface vanish for the generalised Kapitza interface. For this case, the tangent stiffness matrix is

$$\text{tot} \mathbf{K} = \begin{bmatrix} \text{tot} \mathbf{K}_{\varphi\varphi} & \text{tot} \mathbf{K}_{\varphi\Theta} \\ \text{tot} \mathbf{K}_{\Theta\varphi} & \text{tot} \mathbf{K}_{\Theta\Theta} \end{bmatrix} = \begin{bmatrix} \mathbf{K}_{\varphi\varphi} & \mathbf{K}_{\varphi\Theta} \\ \mathbf{K}_{\Theta\varphi} & \mathbf{K}_{\Theta\Theta} \end{bmatrix} + \begin{bmatrix} \bar{\mathbf{K}}_{\varphi\varphi} & \mathbf{0} \\ \mathbf{0} & \bar{\mathbf{K}}_{\Theta\Theta} \end{bmatrix}.$$

For a classical Kapitza interface not only the thermomechanical contributions, but also the mechanical contributions of the interface vanish, i.e. $\bar{\mathbf{K}}_{\varphi\varphi} = \mathbf{0}$.

Chapter 4

Material modelling

The objective of this section is to elaborate on aspects of material modelling for the elasticity theory in the various parts of the body. From the material modelling point of view, the surface and the material coherent interface are formally identical. The Helmholtz energy of a HC interface simplifies for a Kapitza interface. Furthermore, most of the derivations for the surfaces either hold or simplify in case of the curves. Finally, this work has particular relevance to applications in nano-mechanics in which (mechanical) surfaces are widely studied. Therefore, without any loss of generality, only the material modelling of the surface is elaborated in this section keeping that in mind that the extension of the discussion here to the interfaces and curves is straightforward.

The material model on the surface possesses additional complexity when compared to the well-known one of the bulk due to several reasons:

- The surface deformation gradient $\hat{\mathbf{F}}$ is rank deficient. Thus the derivations and linearisations are more complicated and not nearly as well-established as their counterparts in the bulk.
- Due to the two-dimensional nature of the surfaces, the relationship between the surface material parameters and their admissible ranges differ from those of the bulk.
- The surface tension, which corresponds to a constant energy per unit area of the spatial configuration, introduces non-standard terms in the Helmholtz energy. The Helmholtz energy for the strain-free configuration no longer vanishes and the classical (bulk) growth conditions [120, 121] are no longer valid.

- The notions of the surface energy, surface tension and surface stress are often used inappropriately in the literature [for a detailed discussion see 25, and references therein].
- The definition of the surface elasticity theory in the seminal work of Gurtin and Murdoch [32] has a serious defect. This error was reported by the authors in [122], but has often been overlooked by others.
- Gurtin and Murdoch used the letter S to denote the Piola stress and called it the Piola–Kirchhoff stress. The letter S is widely used in the literature to denote the (second) Piola–Kirchhoff stress.
- The infinitesimal surface strain tensor is tangential. In general, in contrast to the bulk, it is not equal to the symmetric surface gradient of the displacement at the surface. This issue is carefully studied here and the given definitions are consistent.

For these reasons, there exists considerable confusion and inconsistency in the literature on surface elasticity [see 26, 29, 123, and references therein]. In order to clarify the theory and to present a self-contained and consistent framework, a Helmholtz energy for the surface is introduced based on finite-strain measures, and the stresses derived. The vast majority of the literature on surface elasticity theory is based on the small-strain setting. Therefore, the stress measures are linearised at the material configuration to obtain the small-strain version of the surface constitutive laws. It is shown here that the linearisation of the surface Piola stress $\hat{P}$ at the material configuration is different from that of the surface Piola–Kirchhoff stress $\hat{S}$. Recall that for the bulk the linearisations of the Piola stress P and the Piola–Kirchhoff stress S at the material configuration are identical.

First a hyperelastic material model for the bulk is introduced and corresponding Piola and Piola–Kirchhoff stresses given. Next, in Section 4.2, the derivations of the surface Piola and Piola–Kirchhoff stresses corresponding to an introduced hyperelastic material model for the surface are carried out. Also, the surface material parameters and their admissible ranges are discussed for the linear elastic case. Furthermore, in order to elucidate the role of surface tension and the dependence of the surface operators upon the curvature within a simplified setting, an example involving the Young–Laplace equation is detailed. Finally, the hyperelastic material models are extended to the case of thermohyperelasticity in Section 4.3.

Remark The form of the Helmholtz energy on the interface, and indeed in the bulk, can be obtained from fundamental reasoning or from atomistic modelling [see e.g. 25, 124]. Dingreville and Qu [125] developed a semi-analytic method to compute the surface elastic properties of crystalline materials. Moreover, an interface energy can be constructed using the surface Cauchy–Born hypothesis [57]. In [126] the surface elastic parameters are

extracted from ab-initio calculations. Similar strategies can be employed to extract the interface parameters. Thus, in general, thermal and mechanical constants can be obtained using inverse parameter identification. $\square$

4.1 HYPERELASTIC MATERIAL IN THE BULK

Assuming that the bulk response is hyperelastic, a neo-Hookean type Helmholtz energy Ψ of the following form can be chosen

$$\Psi(\mathbf{F}) = \frac{1}{2}\lambda \ln^2 J + \frac{1}{2}\mu[\mathbf{F} : \mathbf{F} - 3 - 2 \ln J] \quad \text{with} \quad J = \text{Det } \mathbf{F} > 0,$$

where the Helmholtz energy is characterised by the two Lamé constants μ and λ . Alternatively, and in order to assure objectivity, the Helmholtz energy is expressed in terms of the right Cauchy–Green stretch tensor $\mathbf{C} := \mathbf{F}^t \cdot \mathbf{F}$ as

$$\Psi(\mathbf{C}) = \frac{1}{2}\lambda \ln^2 J + \frac{1}{2}\mu[\text{Tr } \mathbf{C} - 3 - 2 \ln J] \quad \text{with} \quad J = \text{Det } \mathbf{F} = [\text{Det } \mathbf{C}]^{\frac{1}{2}},$$

where $\text{Tr } \{\bullet\} = \{\bullet\} : \mathbf{I}$ denotes the trace operator.

The Piola stress $\mathbf{P}$ and Piola–Kirchhoff stress $\mathbf{S}$ follow from Eq. (2.42) as

$$\mathbf{P}(\mathbf{F}) = \partial_{\mathbf{F}} \Psi(\mathbf{F}) = \lambda \ln J \mathbf{f}^t + \mu[\mathbf{F} - \mathbf{f}^t], \quad (4.1)$$

$$\mathbf{S}(\mathbf{C}) := 2\partial_{\mathbf{C}} \Psi(\mathbf{C}) = \lambda \ln J \mathbf{C}^{-1} + \mu[\mathbf{I} - \mathbf{C}^{-1}], \quad (4.2)$$

and are related via

$$\mathbf{S} = \mathbf{f} \cdot \mathbf{P} \quad \text{and} \quad \mathbf{P} = \mathbf{F} \cdot \mathbf{S}.$$

It is of particular interest to linearise these stress measures at the material configuration to obtain their small strain counterparts. In doing so, recall that $\mathbf{F} - \mathbf{I} = \text{Grad } \mathbf{u}$ where $\mathbf{u}$ denotes the displacement vector and the infinitesimal strain is defined by $\epsilon := [\text{Grad } \mathbf{u}]^{\text{sym}}$. The symmetric part of a second-order tensor $\{\bullet\}$ can be obtained via the definition $\{\bullet\}^{\text{sym}} := \mathbb{I}^{\text{sym}} : \{\bullet\} = \{\bullet\} : \mathbb{I}^{\text{sym}}$ where $\mathbb{I}^{\text{sym}} := \frac{1}{2}[\mathbf{I} \otimes \mathbf{I} + \mathbf{I} \otimes \mathbf{I}]$ denotes the fourth-order symmetric identity tensor. The fourth-order volumetric identity tensor is defined by $\mathbb{I}^{\text{vol}} := \frac{1}{3}\mathbf{I} \otimes \mathbf{I}$. Furthermore, $\{\bullet\}^{\text{vol}} := \mathbb{I}^{\text{vol}} : \{\bullet\} = \{\bullet\} : \mathbb{I}^{\text{vol}}$ represents the volumetric part of a second-order tensor $\{\bullet\}$.

The linearisation of the Piola stress $\mathbf{P}$ in Eq. (4.1) at the material configuration is

$$\text{Lin } \mathbf{P}|_{\mathbf{F}=\mathbf{I}} = \mathbf{P}|_{\mathbf{F}=\mathbf{I}} + \mathbb{A}|_{\mathbf{F}=\mathbf{I}} : [\mathbf{F} - \mathbf{I}] = 3\lambda\epsilon^{\text{vol}} + 2\mu\epsilon, \quad (4.3)$$

where

$$\mathbb{A} := \partial_{\mathbf{F}} \mathbf{P} = \lambda[\mathbf{f}^t \otimes \mathbf{f}^t + \ln J \mathbb{D}] + \mu[\mathbb{I} - \mathbb{D}],$$

with

$$\mathbb{D} := \partial_F \mathbf{f}^t = -\mathbf{f}^t \underline{\otimes} \mathbf{f} \quad \text{and} \quad \mathbb{I} := \partial_F \mathbf{F} = \mathbf{i} \underline{\otimes} \mathbf{I}.$$

Next, the Piola–Kirchhoff stress $\mathbf{S}$ given in Eq. (4.2) is linearised at the material configuration:

$$\text{Lin } \mathbf{S}|_{C=I} = \mathbf{S}|_{C=I} + \frac{1}{2} \mathbb{C}|_{C=I} : [\mathbf{C} - \mathbf{I}] = 3\lambda \epsilon^{\text{vol}} + 2\mu \epsilon, \quad (4.4)$$

where

$$\mathbb{C} := 2\partial_C \mathbf{S} = \lambda [\frac{1}{2} \mathbf{C}^{-1} \underline{\otimes} \mathbf{C}^{-1} + \ln J \mathbb{H}] - \mu \mathbb{H},$$

with

$$\mathbb{H} := \partial_C \mathbf{C}^{-1} = -\frac{1}{2} [\mathbf{C}^{-1} \underline{\otimes} \mathbf{C}^{-1} + \mathbf{C}^{-1} \underline{\otimes} \mathbf{C}^{-1}].$$

Comparing the Eq. (4.3) and (4.4), it is obvious that

$$\text{Lin } \mathbf{P}|_{F=I} = \text{Lin } \mathbf{S}|_{C=I} =: \boldsymbol{\sigma}_{\text{Lin}} \quad \text{or} \quad \boldsymbol{\sigma}_{\text{Lin}} = \mathbb{E} : \epsilon, \quad (4.5)$$

with

$$\mathbb{E} := [3\lambda \mathbb{I}^{\text{vol}} + 2\mu \mathbb{I}^{\text{sym}}],$$

where $\boldsymbol{\sigma}_{\text{Lin}}$ denotes the linearised stress tensor and $\mathbb{E}$ is the fourth-order tensor of elastic moduli.

It is common to decompose the linearised stress $\boldsymbol{\sigma}_{\text{Lin}}$ and infinitesimal strain ϵ into their volumetric and deviatoric contributions as

$$\boldsymbol{\sigma}_{\text{Lin}} = \boldsymbol{\sigma}_{\text{Lin}}^{\text{vol}} + \boldsymbol{\sigma}_{\text{Lin}}^{\text{dev}} \quad \text{and} \quad \epsilon = \epsilon^{\text{vol}} + \epsilon^{\text{dev}}.$$

It follows from Eq. (4.5) that

$$\boldsymbol{\sigma}_{\text{Lin}}^{\text{vol}} = 3\kappa \epsilon^{\text{vol}} \quad \text{and} \quad \boldsymbol{\sigma}_{\text{Lin}}^{\text{dev}} = 2\mu \epsilon^{\text{dev}},$$

with $\kappa := \lambda + 2/3\mu$ denoting the bulk compression modulus. For the sake of completeness, the elastic modulus and Poisson ratio are denoted as E and ν , respectively. The relation between different material parameters are summarised in Table 4.1 [see 127, for further details].

	λ	$\mu = G$	E	ν	κ
$\lambda \quad \mu$	λ	μ	$\frac{\mu(3\lambda + 2\mu)}{\lambda + \mu}$	$\frac{\lambda}{2(\lambda + \mu)}$	$\lambda + \frac{2}{3}\mu$
$\lambda \quad E$	λ	$\frac{E - 3\lambda + \sqrt{\Delta}}{4}$	E	$\frac{2\lambda}{E + \lambda + \sqrt{\Delta}}$	$\frac{E + 3\lambda + \sqrt{\Delta}}{6}$
$\lambda \quad \nu$	λ	$\frac{\lambda(1 - 2\nu)}{2\nu}$	$\frac{\lambda(1 + \nu)(1 - 2\nu)}{\nu}$	ν	$\frac{\lambda(1 + \nu)}{3\nu}$
$\lambda \quad \kappa$	λ	$\frac{3}{2}(\kappa - \lambda)$	$\frac{9\kappa(\kappa - \lambda)}{3\kappa - \lambda}$	$\frac{\lambda}{3\kappa - \lambda}$	κ
$\mu \quad E$	$\frac{\mu(E - 2\mu)}{3\mu - E}$	μ	E	$\frac{E - 2\mu}{2\mu}$	$\frac{\mu E}{3(3\mu - E)}$
$\mu \quad \nu$	$\frac{2\mu\nu}{1 - 2\nu}$	μ	$2\mu(1 + \nu)$	ν	$\frac{2\mu(1 + \nu)}{3(1 - 2\nu)}$
$\mu \quad \kappa$	$\kappa - \frac{2}{3}\mu$	μ	$\frac{9\kappa\mu}{3\kappa + \mu}$	$\frac{3\kappa - 2\mu}{6\kappa + 2\mu}$	κ
$E \quad \nu$	$\frac{E\nu}{(1 + \nu)(1 - 2\nu)}$	$\frac{E}{2(1 + \nu)}$	E	ν	$\frac{E}{3(1 - 2\nu)}$
$E \quad \kappa$	$\frac{3\kappa(3\kappa - E)}{9\kappa - E}$	$\frac{3\kappa E}{9\kappa - E}$	E	$\frac{3\kappa - E}{6\kappa}$	κ
$\nu \quad \kappa$	$\frac{3\kappa\nu}{1 + \nu}$	$\frac{3\kappa(1 - 2\nu)}{2(1 + \nu)}$	$3\kappa(1 - 2\nu)$	ν	κ

Table 4.1: Classical relations between material parameters in the bulk where $\Delta := E^2 + 9\lambda^2 + 2E\lambda$.

4.2 HYPERELASTIC MATERIAL ON THE SURFACE

As in the bulk, assume a hyperelastic response on the surface. The surface Helmholtz energy $\hat{\Psi}$ is selected as follows:

$$\hat{\Psi}(\hat{\mathbf{F}}) = \hat{\gamma}\hat{J} + \frac{1}{2}\hat{\lambda}\ln^2\hat{J} + \frac{1}{2}\hat{\mu}[\hat{\mathbf{F}} : \hat{\mathbf{F}} - 2 - 2\ln\hat{J}] \quad \text{with} \quad \hat{J} = \widehat{\text{Det}}\hat{\mathbf{F}} > 0. \quad (4.6)$$

The surface Helmholtz energy consists of a surface tension part characterised through the surface tension $\hat{\gamma}$ and a neo-Hookean part, formally similar to that of the bulk, characterised through the two surface Lamé constants $\hat{\mu}$ and $\hat{\lambda}$. The surface tension part represents a constant Helmholtz energy per unit area of the spatial configuration and corresponds to possible fluid-like behaviour of the surface. The neo-Hookean part represents the elastic, solid-like response of the surface. Alternatively, the surface Helmholtz energy

can be expressed in terms of the surface right Cauchy–Green stretch tensor $\hat{\mathbf{C}} := \hat{\mathbf{F}}^t \cdot \hat{\mathbf{F}}$ as follows:

$$\hat{\Psi}(\hat{\mathbf{C}}) = \gamma \hat{J} + \frac{1}{2} \hat{\lambda} \ln^2 \hat{J} + \frac{1}{2} \hat{\mu} [\widehat{\text{Tr}} \hat{\mathbf{C}} - 2 - 2 \ln \hat{J}] \quad \text{with} \quad \hat{J} = \widehat{\text{Det}} \hat{\mathbf{F}} = [\widehat{\text{Det}} \hat{\mathbf{C}}]^{\frac{1}{2}} > 0,$$

where $\widehat{\text{Tr}} \{\bullet\} = \{\bullet\} : \hat{\mathbf{I}}$ denotes the surface trace operator.

The surface Piola stress $\hat{\mathbf{P}}$ and the surface Piola–Kirchhoff stress $\hat{\mathbf{S}}$ are given by

$$\hat{\mathbf{P}}(\hat{\mathbf{F}}) = \partial_{\hat{\mathbf{F}}} \hat{\Psi}(\hat{\mathbf{F}}) = \gamma \hat{J} \hat{\mathbf{f}}^t + \hat{\lambda} \ln \hat{J} \hat{\mathbf{f}}^t + \hat{\mu} [\hat{\mathbf{F}} - \hat{\mathbf{f}}^t], \quad (4.7)$$

$$\hat{\mathbf{S}}(\hat{\mathbf{C}}) := 2 \partial_{\hat{\mathbf{C}}} \hat{\Psi}(\hat{\mathbf{C}}) = \gamma \hat{J} \hat{\mathbf{C}}^{-1} + \hat{\lambda} \ln \hat{J} \hat{\mathbf{C}}^{-1} + \hat{\mu} [\hat{\mathbf{I}} - \hat{\mathbf{C}}^{-1}]. \quad (4.8)$$

These stress measures are related via

$$\hat{\mathbf{S}} = \hat{\mathbf{f}} \cdot \hat{\mathbf{P}} \quad \text{and} \quad \hat{\mathbf{P}} = \hat{\mathbf{F}} \cdot \hat{\mathbf{S}}.$$

In an identical fashion to the bulk, these stress measures are linearised at the material configuration to obtain their small-strain counterparts. Recall that $\hat{\mathbf{F}} - \hat{\mathbf{I}} = \widehat{\text{Grad}} \hat{\mathbf{u}}$ where $\hat{\mathbf{u}}$ denotes the surface displacement vector and the infinitesimal surface strain is defined by $\hat{\epsilon} := [\widehat{\text{Grad}} \hat{\mathbf{u}}]^{\text{sym}}$. The symmetric part of a surface second-order tensor $\{\bullet\}$ can be obtained as $\{\bullet\}^{\text{sym}} := \hat{\mathbb{I}}^{\text{sym}} : \{\bullet\} = \{\bullet\} : \hat{\mathbb{I}}^{\text{sym}}$ where $\hat{\mathbb{I}}^{\text{sym}} := \frac{1}{2} [\hat{\mathbf{I}} \otimes \hat{\mathbf{I}} + \hat{\mathbf{I}} \otimes \hat{\mathbf{I}}]$ is the surface fourth-order symmetric identity tensor¹. The surface fourth-order volumetric, or rather spherical², identity tensor is defined by $\hat{\mathbb{I}}^{\text{vol}} := \frac{1}{2} \hat{\mathbf{I}} \otimes \hat{\mathbf{I}}$. Furthermore, $\{\bullet\}^{\text{vol}} := \hat{\mathbb{I}}^{\text{vol}} : \{\bullet\} = \{\bullet\} : \hat{\mathbb{I}}^{\text{vol}}$ denotes the volumetric part of a surface second-order tensor $\{\bullet\}$.

The linearisation of the surface Piola stress $\hat{\mathbf{P}}$ given in Eq. (4.7) at the material configuration reads

$$\begin{aligned} \text{Lin } \hat{\mathbf{P}}|_{\hat{\mathbf{F}}=\hat{\mathbf{I}}} &= \hat{\mathbf{P}}|_{\hat{\mathbf{F}}=\hat{\mathbf{I}}} + \hat{\mathbb{A}}|_{\hat{\mathbf{F}}=\hat{\mathbf{I}}} : [\hat{\mathbf{F}} - \hat{\mathbf{I}}] \\ &= \gamma \hat{\mathbf{I}} + [\gamma \hat{\mathbf{I}} \otimes \hat{\mathbf{I}} + 2[\hat{\lambda} + \gamma] \hat{\mathbb{I}}^{\text{vol}} + 2[\hat{\mu} - \gamma] \hat{\mathbb{I}}^{\text{sym}}] : \widehat{\text{Grad}} \hat{\mathbf{u}} \\ &= \gamma \hat{\mathbf{I}} + \gamma \widehat{\text{Grad}} \hat{\mathbf{u}} + 2[\hat{\lambda} + \gamma] \hat{\epsilon}^{\text{vol}} + 2[\hat{\mu} - \gamma] \hat{\epsilon}, \end{aligned} \quad (4.9)$$

where

$$\hat{\mathbb{A}} := \partial_{\hat{\mathbf{F}}} \hat{\mathbf{P}} = \gamma \hat{J} [\hat{\mathbf{f}}^t \otimes \hat{\mathbf{f}}^t + \hat{\mathbb{D}}] + \hat{\lambda} [\hat{\mathbf{f}}^t \otimes \hat{\mathbf{f}}^t + \ln \hat{J} \hat{\mathbb{D}}] + \hat{\mu} [\hat{\mathbb{I}} - \hat{\mathbb{D}}],$$

¹ Note that $\hat{\epsilon} := [\widehat{\text{Grad}} \hat{\mathbf{u}}]^{\text{sym}} \neq \frac{1}{2} [[\widehat{\text{Grad}} \hat{\mathbf{u}}] + [\widehat{\text{Grad}} \hat{\mathbf{u}}]^t]$ in contrast to the bulk. This is due to the fact that $\widehat{\text{Grad}} \hat{\mathbf{u}}$ is only superficial, and not tangential, where $\hat{\epsilon}$ is the tangential surface strain.

² The term *volumetric* is used in analogy to the bulk. Nevertheless, it has a different meaning on the surface. A volumetric deformation in the bulk is a deformation mode which changes the *volume* uniformly. A volumetric surface deformation, however, is a deformation mode which changes the *area* uniformly. In this sense the term *spherical* seems more appropriate. Nonetheless, for the sake of consistency, the term *volumetric* is used henceforth.

with

$$\widehat{\mathbb{D}} := \partial_{\widehat{\mathbf{F}}} \widehat{\mathbf{f}}^t = -\widehat{\mathbf{f}}^t \underline{\otimes} \widehat{\mathbf{f}} + [\mathbf{i} - \widehat{\mathbf{i}}] \underline{\otimes} [\widehat{\mathbf{f}} \cdot \widehat{\mathbf{f}}^t] \quad \text{and} \quad \widehat{\mathbb{I}} := \partial_{\widehat{\mathbf{F}}} \widehat{\mathbf{F}} = \mathbf{i} \underline{\otimes} \widehat{\mathbf{I}}.$$

Next, the surface Piola–Kirchhoff stress $\widehat{\mathbf{S}}$ given in Eq. (4.8) is linearised at the material configuration:

$$\text{Lin } \widehat{\mathbf{S}}|_{\widehat{\mathbf{C}}=\widehat{\mathbf{I}}} = \widehat{\mathbf{S}}|_{\widehat{\mathbf{C}}=\widehat{\mathbf{I}}} + \frac{1}{2}\widehat{\mathbb{C}}|_{\widehat{\mathbf{C}}=\widehat{\mathbf{I}}} : [\widehat{\mathbf{C}} - \widehat{\mathbf{I}}] = \widehat{\gamma} \widehat{\mathbf{I}} + 2[\widehat{\lambda} + \widehat{\gamma}] \widehat{\epsilon}^{\text{vol}} + 2[\widehat{\mu} - \widehat{\gamma}] \widehat{\epsilon} \quad (4.10)$$

where

$$\widehat{\mathbb{C}} := 2\partial_{\widehat{\mathbf{C}}} \widehat{\mathbf{S}} = \widehat{\gamma} \widehat{\mathbf{J}} [\frac{1}{2}\widehat{\mathbf{C}}^{-1} \otimes \widehat{\mathbf{C}}^{-1} + \widehat{\mathbb{H}}] + \widehat{\lambda} [\frac{1}{2}\widehat{\mathbf{C}}^{-1} \otimes \widehat{\mathbf{C}}^{-1} + \ln \widehat{\mathbf{J}} \widehat{\mathbb{H}}] - \widehat{\mu} \widehat{\mathbb{H}},$$

with

$$\widehat{\mathbb{H}} := \partial_{\widehat{\mathbf{C}}} \widehat{\mathbf{C}}^{-1} = -\frac{1}{2}[\widehat{\mathbf{C}}^{-1} \underline{\otimes} \widehat{\mathbf{C}}^{-1} + \widehat{\mathbf{C}}^{-1} \underline{\otimes} \widehat{\mathbf{C}}^{-1}].$$

Comparing the Eq. (4.9) and (4.10), it is obvious that on the surface, and in contrast to the bulk, $\text{Lin } \widehat{\mathbf{P}}|_{\widehat{\mathbf{F}}=\widehat{\mathbf{I}}} \neq \text{Lin } \widehat{\mathbf{S}}|_{\widehat{\mathbf{C}}=\widehat{\mathbf{I}}}$ but rather

$$\text{Lin } \widehat{\mathbf{P}}|_{\widehat{\mathbf{F}}=\widehat{\mathbf{I}}} = \text{Lin } \widehat{\mathbf{S}}|_{\widehat{\mathbf{C}}=\widehat{\mathbf{I}}} + \widehat{\gamma} \widehat{\text{Grad}} \widehat{\mathbf{u}}.$$

Therefore, the two surface stress measures corresponding to the small-strain assumption are

$$\begin{aligned} \widehat{\mathbf{P}} \widehat{\sigma}_{\text{Lin}} &:= \text{Lin } \widehat{\mathbf{P}}|_{\widehat{\mathbf{F}}=\widehat{\mathbf{I}}} = \widehat{\gamma} \widehat{\mathbf{I}} + \widehat{\mathbb{E}} : \widehat{\epsilon} + \widehat{\gamma} \widehat{\text{Grad}} \widehat{\mathbf{u}} && \text{(non-symmetric)}, \\ \widehat{\mathbf{S}} \widehat{\sigma}_{\text{Lin}} &:= \text{Lin } \widehat{\mathbf{S}}|_{\widehat{\mathbf{C}}=\widehat{\mathbf{I}}} = \widehat{\gamma} \widehat{\mathbf{I}} + \widehat{\mathbb{E}} : \widehat{\epsilon} && \text{(symmetric)}, \end{aligned} \quad (4.11)$$

with

$$\widehat{\mathbb{E}} := [2\widehat{\lambda}_{\text{eff}} \widehat{\mathbb{I}}^{\text{vol}} + 2\widehat{\mu}_{\text{eff}} \widehat{\mathbb{I}}^{\text{sym}}] \quad \text{where} \quad \widehat{\lambda}_{\text{eff}} := \widehat{\lambda} + \widehat{\gamma} \quad \text{and} \quad \widehat{\mu}_{\text{eff}} := \widehat{\mu} - \widehat{\gamma}.$$

The mistake made by Gurtin and Murdoch [32] in their widely-cited paper was to omit the surface tension in the definition of the effective quantities $\widehat{\lambda}_{\text{eff}}$ and $\widehat{\mu}_{\text{eff}}$. This error was rectified in an addendum to their original work [122].

Both of the linearised stress measures given in Eq. (4.11) are used in the literature. In the absence of surface tension they are obviously equivalent. In the presence of surface tension care must be taken to ensure that they are used in combination with their corresponding balance equation. In the author's opinion the non-symmetric version should be used in conjunction with Eq. (2.25)₂.

Remark Note that

$$\widehat{\text{Div}} \left(\widehat{\rho} \widehat{\sigma}_{\text{Lin}} \right) = \widehat{\text{Div}} \left(\widehat{s} \widehat{\sigma}_{\text{Lin}} \right) + \widehat{\gamma} \widehat{\text{Div}} \left(\widehat{\text{Grad}} \widehat{u} \right),$$

which shall be compared with equation (13) of [123] where the author explains geometrically the displacement-gradient term. Ru [123] argues that the controversial displacement-gradient term appears due to the fact that the infinitesimal elastic deformation is indeed an incremental deformation superposed on the initial (finite) deformation due to the surface tension. In this manuscript, the reference configuration is assumed to be strain-free as well as stress-free. The surface tension $\widehat{\gamma}$ introduces a residual stress in the body and deforms it into a state from which the infinitesimal deformation is externally applied. In this sense, the final deformed configuration may be understood as a 1st-order deformation of the bulk and 2nd-order deformation of the surface [see 123, for further details of this approach]. $\square$

	$\widehat{\lambda}$	$\widehat{\mu} = \widehat{G}$	$\widehat{E}$	$\widehat{\nu}$	$\widehat{\kappa}$
$\widehat{\lambda} \quad \widehat{\mu}$	$\widehat{\lambda}$	$\widehat{\mu}$	$\frac{4\widehat{\mu}(\widehat{\lambda} + \widehat{\mu})}{\widehat{\lambda} + 2\widehat{\mu}}$	$\frac{\widehat{\lambda}}{\widehat{\lambda} + 2\widehat{\mu}}$	$\widehat{\lambda} + \widehat{\mu}$
$\widehat{\lambda} \quad \widehat{E}$	$\widehat{\lambda}$	$\frac{\widehat{E} - 2\widehat{\lambda} \pm \sqrt{\widehat{\Delta}}}{4}$	$\widehat{E}$	$\frac{2\widehat{\lambda}}{\widehat{E} \pm \sqrt{\widehat{\Delta}}}$	$\frac{\widehat{E} + 2\widehat{\lambda} \pm \sqrt{\widehat{\Delta}}}{4}$
$\widehat{\lambda} \quad \widehat{\nu}$	$\widehat{\lambda}$	$\frac{\widehat{\lambda}(1 - \widehat{\nu})}{2\widehat{\nu}}$	$\frac{\widehat{\lambda}(1 - \widehat{\nu}^2)}{\widehat{\nu}}$	$\widehat{\nu}$	$\frac{\widehat{\lambda}(1 + \widehat{\nu})}{2\widehat{\nu}}$
$\widehat{\lambda} \quad \widehat{\kappa}$	$\widehat{\lambda}$	$\widehat{\kappa} - \widehat{\lambda}$	$\frac{4\widehat{\kappa}(\widehat{\kappa} - \widehat{\lambda})}{2\widehat{\kappa} - \widehat{\lambda}}$	$\frac{\widehat{\lambda}}{2\widehat{\kappa} - \widehat{\lambda}}$	$\widehat{\kappa}$
$\widehat{\mu} \quad \widehat{E}$	$\frac{2\widehat{\mu}(\widehat{E} - 2\widehat{\mu})}{4\widehat{\mu} - \widehat{E}}$	$\widehat{\mu}$	$\widehat{E}$	$\frac{\widehat{E} - 2\widehat{\mu}}{2\widehat{\mu}}$	$\frac{\widehat{\mu}\widehat{E}}{4\widehat{\mu} - \widehat{E}}$
$\widehat{\mu} \quad \widehat{\nu}$	$\frac{2\widehat{\mu}\widehat{\nu}}{1 - \widehat{\nu}}$	$\widehat{\mu}$	$2\widehat{\mu}(1 + \widehat{\nu})$	$\widehat{\nu}$	$\frac{\widehat{\mu}(1 + \widehat{\nu})}{1 - \widehat{\nu}}$
$\widehat{\mu} \quad \widehat{\kappa}$	$\widehat{\kappa} - \widehat{\mu}$	$\widehat{\mu}$	$\frac{4\widehat{\mu}\widehat{\kappa}}{\widehat{\mu} + \widehat{\kappa}}$	$\frac{\widehat{\kappa} - \widehat{\mu}}{\widehat{\kappa} + \widehat{\mu}}$	$\widehat{\kappa}$
$\widehat{E} \quad \widehat{\nu}$	$\frac{\widehat{E}\widehat{\nu}}{1 - \widehat{\nu}^2}$	$\frac{\widehat{E}}{2(1 + \widehat{\nu})}$	$\widehat{E}$	$\widehat{\nu}$	$\frac{\widehat{E}}{2(1 - \widehat{\nu})}$
$\widehat{E} \quad \widehat{\kappa}$	$\frac{2\widehat{\kappa}(2\widehat{\kappa} - \widehat{E})}{4\widehat{\kappa} - \widehat{E}}$	$\frac{\widehat{E}\widehat{\kappa}}{4\widehat{\kappa} - \widehat{E}}$	$\widehat{E}$	$\frac{2\widehat{\kappa} - \widehat{E}}{2\widehat{\kappa}}$	$\widehat{\kappa}$
$\widehat{\nu} \quad \widehat{\kappa}$	$\frac{2\widehat{\kappa}\widehat{\nu}}{1 + \widehat{\nu}}$	$\frac{\widehat{\kappa}(1 - \widehat{\nu})}{1 + \widehat{\nu}}$	$2\widehat{\kappa}(1 - \widehat{\nu})$	$\widehat{\nu}$	$\widehat{\kappa}$

Table 4.2: Relations between material parameters at the boundary where $\widehat{\Delta}$ is defined by $\widehat{\Delta} := \widehat{E}^2 + 4\widehat{\lambda}^2$.

It is shown in the literature [e.g. 128] that for some solids the influence of surface tension is negligible relative to that of surface elasticity. Thus, in order to study the elastic effects of the surface as compared to the bulk, it is assumed, for the majority of the remainder of this work, that $\hat{\gamma} \equiv 0$. The role of surface tension will be explained further in the subsequent Young–Laplace example.

In analogy to the bulk, the symmetric linearised surface stress denoted as $\hat{\sigma}_{\text{Lin}} = \hat{s}\hat{\sigma}_{\text{Lin}}$ and infinitesimal surface strain $\hat{\epsilon}$ can be decomposed into their volumetric and deviatoric contributions via

$$\hat{\sigma}_{\text{Lin}} = \hat{\sigma}_{\text{Lin}}^{\text{vol}} + \hat{\sigma}_{\text{Lin}}^{\text{dev}} \quad \text{and} \quad \hat{\epsilon} = \hat{\epsilon}^{\text{vol}} + \hat{\epsilon}^{\text{dev}}.$$

It follows from Eq. (4.11)₂ that

$$\hat{\sigma}_{\text{Lin}}^{\text{vol}} = 2\hat{\kappa}\hat{\epsilon}^{\text{vol}} \quad \text{and} \quad \hat{\sigma}_{\text{Lin}}^{\text{dev}} = 2\hat{\mu}\hat{\epsilon}^{\text{dev}},$$

with $\hat{\kappa} := \hat{\lambda} + \hat{\mu}$ denoting the surface compression modulus. Note that the definition of the surface modulus $\hat{\kappa}$ follows from in the spirit of that in the bulk. This parameter has been defined differently, i.e. by incorporating a factor of two, in the literature [see e.g. 59, 129], nevertheless, it seems that the current definition is more stringent. For the sake of completeness, the surface elastic modulus and surface Poisson ratio are denoted as $\hat{E}$ and $\hat{\nu}$, respectively. The relation between different surface material parameters are summarised in Table 4.2 (see Javili and Steinmann [90] for further details). In the view of Table 4.1, note that the surface incompressibility limit, i.e. the upper bound for the surface Poisson ratio $\hat{\nu}$, in contrast to the bulk, assumes the value of 1 and not 1/2. This can be justified geometrically.

Finally, the admissible range for the surface material parameters shall be identified. This can be accomplished by analysing the well-posedness of the boundary value problem. The necessary and sufficient conditions for the loss of well-posedness of the boundary value problem governing linear elastic, homogeneous solids are well known [see e.g. 130–139]. They are the loss of ellipticity of the governing equations and the boundary complementing condition, respectively.

Table 4.3: Summary of the conditions for the strong ellipticity and pointwise stability of the elasticity tensors in the bulk and on the surface in terms of the Lamé moduli.

Strong ellipticity requires	$\mu > 0 \quad \text{and} \quad \lambda + 2\mu > 0$	$\hat{\mu} > 0 \quad \text{and} \quad \hat{\lambda} + 2\hat{\mu} > 0$
Pointwise stability requires	$\mu > 0 \quad \text{and} \quad 3\lambda + 2\mu > 0$	$\hat{\mu} > 0 \quad \text{and} \quad \hat{\lambda} + \hat{\mu} > 0$

Javili et al. [96] show that the sufficient conditions for the well-posedness of the boundary value problem at hand are the pointwise stability both in the bulk and on the surface. The results are summarised in Table 4.3 which shows that the strong-ellipticity of the surface is necessary but not sufficient for the well-posedness. Shenoy [140] argues that, within the context of an atomistic model, the calculated surface elasticity tensor need not be pointwise stable as the “surface cannot exist independent of the bulk” and that it is the “total energy (bulk + surface)” that needs to “satisfy the positive definiteness condition”, where positive definiteness refers to pointwise stability. The definition of pointwise stability is, however, a local concept. An argument similar to that of Shenoy [140] is applicable when discussing the stability of the weak approximation to the governing equations, for example as the basis for finite element computations.

Example: Young–Laplace equation

In order to further clarify the theory and to demonstrate its generality, the classical example of the Young–Laplace equation is investigated. This well-known equation states that for static fluids the balance equation on the surface is given by

$$p = -\hat{\gamma} \hat{c}, \quad (4.12)$$

where p is the fluid pressure³, and $\hat{c}$ is twice the mean curvature⁴ in the spatial configuration defined in Eq. (2.11). The spatial balance of the linear momentum on the surface (2.26)₂ in the absence of external tractions reads

$$\widehat{\text{div}} \hat{\sigma} = \sigma \cdot \mathbf{n}. \quad (4.13)$$

Using the relation between the hydrostatic pressure p and Cauchy stress σ for inviscid fluids $\sigma = -p \mathbf{i}$ on the right-hand side, gives

$$\widehat{\text{div}} \hat{\sigma} = -p \mathbf{n}. \quad (4.14)$$

In order to compare Eq. (4.14) and the Young–Laplace equation (4.12), the surface material model proposed in Eq. (4.6) with vanishing elastic parameters is employed, i.e.

$$\hat{\Psi} = \hat{\gamma} \hat{J} \quad \Rightarrow \quad \hat{\mathbf{P}} = \partial_{\hat{\mathbf{F}}} \hat{\Psi} = \hat{\gamma} \hat{J} \hat{\mathbf{f}}^t \quad \Rightarrow \quad \hat{\sigma} = \hat{j} \hat{\mathbf{P}} \cdot \hat{\mathbf{F}}^t = \hat{\gamma} \hat{\mathbf{i}}. \quad (4.15)$$

Inserting $\hat{\sigma} = \hat{\gamma} \hat{\mathbf{i}}$ in Eq. (4.14) yields

$$\widehat{\text{div}}(\hat{\gamma} \hat{\mathbf{i}}) = -p \mathbf{n} \quad \Rightarrow \quad \hat{\gamma} \widehat{\text{div}} \hat{\mathbf{i}} = -p \mathbf{n}, \quad (4.16)$$

and finally using the relation $\widehat{\text{div}} \hat{\mathbf{i}} = \hat{c} \mathbf{n}$ yields $\hat{\gamma} \hat{c} = -p$. Thus, it is clear that the curvature is embedded in the surface divergence operator.

³ For the sake of simplicity, it is assumed that the surface is an interface between the fluid and an outside vacuum.

⁴ Often in the literature $\hat{c}$ is written as sum of the principal curvatures $\hat{c} = -[1/r_1 + 1/r_2]$ where r_1 and r_2 denote the principal radii of curvature. Based on this definition, the curvature is negative if the surface curves away from the normal.

4.3 THERMOHYPERELASTIC MATERIAL

The material models proposed in Section 4.1 and 4.2 can capture the mechanical behaviour of materials. Nevertheless, they do not possess enough structure to capture the thermal behaviour and possible thermomechanically coupled phenomena. The objective of this section is to introduce material models that include not only mechanical and thermal but also thermomechanical contributions.

The focus of this work is on *energetic elasticity* as compared to *entropic elasticity*. For entropic elastic materials, e.g. polymers, the temperature increases due to stretching. On the contrary, energetic elastic materials, e.g. metals, cool down when stretched. The thermomechanical coupling, whether for energetic or entropic elasticity, is termed henceforth the *Gough–Joule* effect. The Gough–Joule effect is often used for entropic elastic materials as it was originally realised for rubbers (see Gough [92] and Joule [93]). It is noteworthy, that the Gough–Joule effect is not solely due to the deformation but, it is rather the rate of a deformation which induces a change in the temperature field.

4.3.1 Bulk

For the simple case of thermohyperelasticity, the Helmholtz energy of the bulk is chosen as⁵

$$\begin{aligned} \Psi(\mathbf{F}, \Theta) := & \frac{1}{2} \lambda \ln^2 J + \frac{1}{2} \mu [\mathbf{F} : \mathbf{F} - 3 - 2 \ln J] \\ & - 3\alpha\kappa [\Theta - \Theta_0] \frac{\ln J}{J} + c_F \left[\Theta - \Theta_0 - \Theta \ln \frac{\Theta}{\Theta_0} \right] - \Xi_0 [\Theta - \Theta_0]. \end{aligned} \quad (4.17)$$

The term $\frac{1}{2} \lambda \ln^2 J + \frac{1}{2} \mu [\mathbf{F} : \mathbf{F} - 3 - 2 \ln J]$ is the classical Helmholtz energy function of neo-Hookean type characterised by the two Lamé constants λ and μ . Thermomechanical coupling is captured by the term $-3\alpha\kappa [\Theta - \Theta_0] \ln J/J$, where the thermal expansion coefficient α weights the product of the bulk compression modulus κ and the difference between the current and the reference temperatures $[\Theta - \Theta_0]$. The term $c_F [\Theta - \Theta_0 - \Theta \ln \Theta/\Theta_0]$ represents the purely thermal behaviour in terms of the specific heat capacity c_F . The final term Ξ_0 accounts for the material specific absolute entropy.

For the bulk Helmholtz energy Eq. (4.17), the Piola stress and the entropy in the bulk follow in the familiar format of thermohyperelasticity from the constitutive laws (2.42)₁ as

$$\mathbf{P} = \partial_{\mathbf{F}} \Psi = [\lambda \ln J - \mu] \mathbf{f}^t + \mu \mathbf{F} - 3\alpha\kappa \frac{1}{J} [\Theta - \Theta_0] [1 - \ln J] \mathbf{f}^t,$$

and

$$\Xi = -\partial_{\Theta} \Psi = 3\alpha\kappa \frac{\ln J}{J} + c_F \ln \frac{\Theta}{\Theta_0} + \Xi_0.$$

⁵ The thermohyperelastic Helmholtz energy is chosen similar to that proposed by Kuhl et al. [141]. For further details see also [115, 116] and references therein.

Next the corresponding tangent contributions in Table 3.1 are derived. The partial derivatives of the Piola stress $\mathbf{P}$ with respect to deformation gradient $\mathbf{F}$ and temperature Θ are given by

$$\begin{aligned}\partial_{\mathbf{F}}\mathbf{P} &= \lambda \mathbf{f}^t \otimes \mathbf{f}^t + \mu \mathbb{I} + [\lambda \ln J - \mu] \mathbb{D} \\ &\quad + 3\alpha\kappa [\Theta - \Theta_0] \left[\frac{2 - \ln J}{J} \mathbf{f}^t \otimes \mathbf{f}^t - \frac{1 - \ln J}{J} \mathbb{D} \right], \\ \partial_{\Theta}\mathbf{P} &= -3\alpha\kappa \frac{1 - \ln J}{J} \mathbf{f}^t.\end{aligned}$$

The partial derivatives of the heat flux vector $\mathbf{Q}$ with respect to deformation gradient $\mathbf{F}$ and temperature Θ are given by

$$\partial_{\text{Grad}\Theta}\mathbf{Q} = -Jk \mathbf{G} \quad \text{and} \quad \partial_{\mathbf{F}}\mathbf{Q} = -Jk \mathbb{G} : \text{Grad}\Theta,$$

where, for the case of isotropic thermal conduction in the spatial configuration,⁶

$$\mathbf{G} \equiv \mathbf{f} \cdot \mathbf{f}^t \quad \text{and} \quad \mathbb{G} \equiv \mathbf{f} \cdot \mathbf{f}^t \otimes \mathbf{f}^t + \mathbb{B},$$

with

$$\mathbb{B} := \partial_{\mathbf{F}}(\mathbf{f} \cdot \mathbf{f}^t) = {}^t[\mathbf{f} \cdot \mathbb{D}] + \mathbf{f} \cdot \mathbb{D} = -[\mathbf{f} \otimes \mathbf{f}] \cdot \mathbf{f}^t - \mathbf{f} \cdot [\mathbf{f}^t \otimes \mathbf{f}].$$

Finally, for the partial derivatives of the Gough–Joule contribution, one makes use of the identity

$$\mathbf{f}^t : \mathbf{D}_t \mathbf{F} = \mathbf{f}^t : \text{Grad}\mathbf{V} = \text{div}\mathbf{V},$$

to obtain

$$\begin{aligned}\partial_{\Theta}(\Theta \partial_{\Theta}\mathbf{P} : \mathbf{D}_t \mathbf{F}) &= -3\alpha\kappa \frac{1 - \ln J}{J} \text{div}\mathbf{V}, \\ \partial_{\mathbf{F}}(\Theta \partial_{\Theta}\mathbf{P} : \mathbf{D}_t \mathbf{F}) &= -3\alpha\kappa \Theta \left[\frac{\ln J - 2}{J} \text{div}\mathbf{V} \mathbf{f}^t + \frac{1 - \ln J}{J} \mathbf{D} \right],\end{aligned}$$

where

$$\begin{aligned}\mathbf{D} &:= \partial_{\mathbf{F}} \text{div}\mathbf{V} = \partial_{\mathbf{F}}(\mathbf{f}^t : \mathbf{D}_t \mathbf{F}) \\ &= \mathbf{D}_t \mathbf{F} : \partial_{\mathbf{F}} \mathbf{f}^t + \mathbf{f}^t : \partial_{\mathbf{F}}(\mathbf{D}_t \mathbf{F}),\end{aligned}$$

and using the Euler-backward approximation,

$$\approx \mathbf{D}_t \mathbf{F} : \mathbb{D} + \frac{1}{\Delta t} \mathbf{f}^t : \mathbb{I}.$$

⁶For isotropic thermal conduction in the material configuration $\mathbf{G} \equiv \mathbf{I}$ and $\mathbb{G} \equiv \mathbf{I} \otimes \mathbf{f}^t$.

4.3.2 Surface

As in the bulk, a simple thermohyperelastic surface Helmholtz energy of the following form is chosen

$$\begin{aligned} \hat{\Psi}(\hat{\mathbf{F}}, \hat{\Theta}) := & \frac{1}{2} \hat{\lambda} \ln^2 \hat{J} + \frac{1}{2} \hat{\mu} [\hat{\mathbf{F}} : \hat{\mathbf{F}} - 2 - 2 \ln \hat{J}] + \hat{\gamma} \hat{J} \\ & - 2 \hat{\alpha} \hat{\kappa} [\hat{\Theta} - \hat{\Theta}_0] \frac{\ln \hat{J}}{\hat{J}} + \hat{c}_{\hat{\mathbf{F}}} \left[\hat{\Theta} - \hat{\Theta}_0 - \hat{\Theta} \ln \frac{\hat{\Theta}}{\hat{\Theta}_0} \right] - \hat{\Xi}_0 [\hat{\Theta} - \hat{\Theta}_0]. \end{aligned} \quad (4.18)$$

The term $\frac{1}{2} \hat{\lambda} \ln^2 \hat{J} + \frac{1}{2} \hat{\mu} [\hat{\mathbf{F}} : \hat{\mathbf{F}} - 2 - 2 \ln \hat{J}]$ mimics the classical Helmholtz-energy function of neo-Hookean type characterised through the two surface Lamé constants $\hat{\lambda}$ and $\hat{\mu}$. The surface tension is denoted as $\hat{\gamma}$. The thermomechanical coupling is captured by the term $-2 \hat{\alpha} \hat{\kappa} [\hat{\Theta} - \hat{\Theta}_0] \ln \hat{J} / \hat{J}$ where $\hat{\alpha}$ is the surface thermal expansion coefficient and $\hat{\kappa} = \hat{\mu} + \hat{\lambda}$ the surface compression modulus. The surface temperatures in the reference and current configurations are denoted as $\hat{\Theta}_0$ and $\hat{\Theta}$, respectively. The surface specific heat capacity $\hat{c}_{\hat{\mathbf{F}}}$ represents the purely thermal behaviour. Finally, the surface specific entropy $\hat{\Xi}_0$ is included. The surface Piola stress and entropy corresponding to the surface Helmholtz energy Eq. (4.18) follow from the constitutive laws (2.42)₂ as

$$\hat{\mathbf{P}} = \partial_{\hat{\mathbf{F}}} \hat{\Psi} = \left[\hat{\lambda} \ln \hat{J} - \hat{\mu} + \hat{\gamma} \hat{J} \right] \hat{\mathbf{f}}^t + \hat{\mu} \hat{\mathbf{F}} - 2 \hat{\alpha} \hat{\kappa} \frac{1}{\hat{J}} [\hat{\Theta} - \hat{\Theta}_0] [1 - \ln \hat{J}] \hat{\mathbf{f}}^t,$$

and

$$\hat{\Xi} = -\partial_{\hat{\Theta}} \hat{\Psi} = 2 \hat{\alpha} \hat{\kappa} \frac{\ln \hat{J}}{\hat{J}} + \hat{c}_{\hat{\mathbf{F}}} \ln \frac{\hat{\Theta}}{\hat{\Theta}_0} + \hat{\Xi}_0.$$

4.3.3 Interface

In an identical fashion to the surface, a simple thermohyperelastic interface Helmholtz energy of the following form is chosen

$$\begin{aligned} \bar{\Psi}(\bar{\mathbf{F}}, \bar{\Theta}) := & \frac{1}{2} \bar{\lambda} \ln^2 \bar{J} + \frac{1}{2} \bar{\mu} [\bar{\mathbf{F}} : \bar{\mathbf{F}} - 2 - 2 \ln \bar{J}] + \bar{\gamma} \bar{J} \\ & - 2 \bar{\alpha} \bar{\kappa} [\bar{\Theta} - \bar{\Theta}_0] \frac{\ln \bar{J}}{\bar{J}} + \bar{c}_{\bar{\mathbf{F}}} \left[\bar{\Theta} - \bar{\Theta}_0 - \bar{\Theta} \ln \frac{\bar{\Theta}}{\bar{\Theta}_0} \right] - \bar{\Xi}_0 [\bar{\Theta} - \bar{\Theta}_0]. \end{aligned} \quad (4.19)$$

The term $\frac{1}{2} \bar{\lambda} \ln^2 \bar{J} + \frac{1}{2} \bar{\mu} [\bar{\mathbf{F}} : \bar{\mathbf{F}} - 2 - 2 \ln \bar{J}]$ mimics the classical Helmholtz-energy function of neo-Hookean type characterised through the two Lamé constants $\bar{\lambda}$ and $\bar{\mu}$. The term $\bar{\gamma}$ represents a surface-tension-like behaviour. The thermomechanical coupling is captured by the term $-2 \bar{\alpha} \bar{\kappa} [\bar{\Theta} - \bar{\Theta}_0] \ln \bar{J} / \bar{J}$ where $\bar{\alpha}$ is the interface thermal expansion coefficient and $\bar{\kappa} := \bar{\mu} + \bar{\lambda}$ the interface compression modulus. The interface temperatures in the reference and current configurations are denoted as $\bar{\Theta}_0$ and $\bar{\Theta}$, respectively. The interface

specific heat capacity $\bar{c}_{\bar{F}}$ represents the purely thermal behaviour. Finally, the interface specific entropy $\bar{\Xi}_0$ is included.

From the constitutive laws (2.42)₃ the interface Piola stress and entropy corresponding to the interface Helmholtz energy Eq. (4.19) are obtained as

$$\bar{\mathbf{P}} = \partial_{\bar{\mathbf{F}}} \bar{\Psi} = \left[\bar{\lambda} \ln \bar{J} - \bar{\mu} + \bar{\gamma} \bar{J} \right] \bar{\mathbf{f}}^t + \bar{\mu} \bar{\mathbf{F}} - 2 \bar{\alpha} \bar{\kappa} \frac{1}{\bar{J}} \left[\bar{\Theta} - \bar{\Theta}_0 \right] \left[1 - \ln \bar{J} \right] \bar{\mathbf{f}}^t,$$

and

$$\bar{\Xi} = -\partial_{\bar{\Theta}} \bar{\Psi} = 2 \bar{\alpha} \bar{\kappa} \frac{\ln \bar{J}}{\bar{J}} + \bar{c}_{\bar{F}} \ln \frac{\bar{\Theta}}{\bar{\Theta}_0} + \bar{\Xi}_0.$$

The interfaces contributions to the tangent as per the equations given in Table 3.1 are formally identical to those in the bulk. However, due to the rank-deficiency, subtle modifications need to be taken into account. Thus

$$\begin{aligned} \partial_{\bar{\mathbf{F}}} \bar{\mathbf{P}} &= \left[\bar{\lambda} + \bar{\gamma} \bar{J} \right] \bar{\mathbf{f}}^t \otimes \bar{\mathbf{f}}^t + \bar{\mu} \bar{\mathbb{I}} + \left[\bar{\lambda} \ln \bar{J} - \bar{\mu} + \bar{\gamma} \bar{J} \right] \bar{\mathbb{D}} \\ &\quad + 2 \bar{\alpha} \bar{\kappa} \left[\bar{\Theta} - \bar{\Theta}_0 \right] \left[\frac{2 - \ln \bar{J}}{\bar{J}} \bar{\mathbf{f}}^t \otimes \bar{\mathbf{f}}^t - \frac{1 - \ln \bar{J}}{\bar{J}} \bar{\mathbb{D}} \right], \\ \partial_{\bar{\Theta}} \bar{\mathbf{P}} &= -2 \bar{\alpha} \bar{\kappa} \frac{1 - \ln \bar{J}}{\bar{J}} \bar{\mathbf{f}}^t, \end{aligned}$$

with

$$\bar{\mathbb{I}} := \partial_{\bar{\mathbf{F}}} \bar{\mathbf{F}} = \bar{\mathbf{i}} \otimes \bar{\mathbf{I}} \quad \text{and} \quad \bar{\mathbb{D}} := \partial_{\bar{\mathbf{F}}} \bar{\mathbf{f}}^t = -\bar{\mathbf{f}}^t \otimes \bar{\mathbf{f}} + [\bar{\mathbf{i}} - \bar{\mathbf{i}}] \otimes \bar{\mathbf{f}} \cdot \bar{\mathbf{f}}^t.$$

The partial derivatives of the interface heat flux vector $\bar{\mathbf{Q}}$ with respect to interface deformation gradient $\bar{\mathbf{F}}$ and temperature $\bar{\Theta}$ are

$$\partial_{\text{Grad} \bar{\Theta}} \bar{\mathbf{Q}} = -\bar{J} \bar{k} \bar{\mathbf{G}} \quad \text{and} \quad \partial_{\bar{\mathbf{F}}} \bar{\mathbf{Q}} = -\bar{J} \bar{k} \bar{\mathbf{G}} \cdot \text{Grad} \bar{\Theta},$$

where for isotropic thermal conduction along the interface in the spatial configuration⁷

$$\bar{\mathbf{G}} \equiv \bar{\mathbf{f}} \cdot \bar{\mathbf{f}}^t \quad \text{and} \quad \bar{\mathbb{G}} \equiv \bar{\mathbf{f}} \cdot \bar{\mathbf{f}}^t \otimes \bar{\mathbf{f}}^t + \bar{\mathbb{B}},$$

with

$$\bar{\mathbb{B}} := \partial_{\bar{\mathbf{F}}} (\bar{\mathbf{f}} \cdot \bar{\mathbf{f}}^t) = {}^t[\bar{\mathbf{f}} \cdot \bar{\mathbb{D}}] + \bar{\mathbf{f}} \cdot \bar{\mathbb{D}}.$$

⁷For isotropic thermal conduction in the material configuration $\bar{\mathbf{G}} \equiv \bar{\mathbf{I}}$ and $\bar{\mathbb{G}} \equiv \bar{\mathbf{I}} \otimes \bar{\mathbf{f}}^t$.

Finally, for the partial derivatives of the Gough–Joule contribution, one makes use of the identity

$$\bar{\mathbf{f}}^t : \mathbf{D}_t \bar{\mathbf{F}} = \bar{\mathbf{f}}^t : \overline{\text{Grad}} \bar{\mathbf{V}} = \overline{\text{div}} \bar{\mathbf{V}},$$

to obtain

$$\begin{aligned} \partial_{\bar{\Theta}}(\bar{\Theta} \partial_{\bar{\Theta}} \bar{\mathbf{P}} : \mathbf{D}_t \bar{\mathbf{F}}) &= -2 \bar{\alpha} \bar{\kappa} \frac{1 - \ln \bar{J}}{\bar{J}} \overline{\text{div}} \bar{\mathbf{V}}, \\ \partial_{\bar{\mathbf{F}}}(\bar{\Theta} \partial_{\bar{\Theta}} \bar{\mathbf{P}} : \mathbf{D}_t \bar{\mathbf{F}}) &= -2 \bar{\alpha} \bar{\kappa} \bar{\Theta} \left[\frac{\ln \bar{J} - 2}{\bar{J}} \overline{\text{div}} \bar{\mathbf{V}} \bar{\mathbf{f}}^t + \frac{1 - \ln \bar{J}}{\bar{J}} \bar{\mathbf{D}} \right], \end{aligned}$$

where

$$\bar{\mathbf{D}} := \partial_{\bar{\mathbf{F}}} \overline{\text{div}} \bar{\mathbf{V}} = \partial_{\bar{\mathbf{F}}}(\bar{\mathbf{f}}^t : \mathbf{D}_t \bar{\mathbf{F}}) \approx \mathbf{D}_t \bar{\mathbf{F}} : \bar{\mathbb{D}} + \frac{1}{\Delta t} \bar{\mathbf{f}}^t : \bar{\mathbb{I}}.$$

Remark The interface Helmholtz energy given in Eq. (4.19) accounts for thermomechanical coupling and the interface heat capacity. For a Kapitza interface these two contributions, as well as the heat conduction along the interface and the interface prescribed heat source, should vanish to satisfy the Kapitza assumption of continuity of the normal heat flux across the interface (see Eq. (2.59)₃). Therefore, the form of the Helmholtz energy for the generalised Kapitza interface simplifies to

$$\bar{\Psi}(\bar{\mathbf{F}}, \bar{\Theta}) = \frac{1}{2} \bar{\lambda} \ln^2 \bar{J} + \frac{1}{2} \bar{\mu} [\bar{\mathbf{F}} : \bar{\mathbf{F}} - 2 - 2 \ln \bar{J}] + \bar{\gamma} \bar{J} - \bar{\Xi}_0 [\bar{\Theta} - \bar{\Theta}_0]. \quad (4.20)$$

□

4.3.4 Curve

Finally, for the sake of completeness, and in a very similar fashion to the surface and interface, a simple thermohyperelastic curve Helmholtz energy of the following form is chosen

$$\begin{aligned} \tilde{\Psi}(\tilde{\mathbf{F}}, \tilde{\Theta}) &:= \frac{1}{2} \tilde{\mu} [\tilde{\mathbf{F}} : \tilde{\mathbf{F}} - 1 - 2 \ln \tilde{J}] + \tilde{\gamma} \tilde{J} \\ &\quad - \tilde{\alpha} \tilde{\mu} [\tilde{\Theta} - \tilde{\Theta}_0] \frac{\ln \tilde{J}}{\tilde{J}} + \tilde{c}_{\tilde{\mathbf{F}}} \left[\tilde{\Theta} - \tilde{\Theta}_0 - \tilde{\Theta} \ln \frac{\tilde{\Theta}}{\tilde{\Theta}_0} \right] - \tilde{\Xi}_0 [\tilde{\Theta} - \tilde{\Theta}_0]. \end{aligned} \quad (4.21)$$

The term $\frac{1}{2} \tilde{\mu} [\tilde{\mathbf{F}} : \tilde{\mathbf{F}} - 1 - 2 \ln \tilde{J}]$ mimics the classical Helmholtz-energy function of neo-Hookean type characterised through a constant $\tilde{\mu}$. Due to the one-dimensional nature of the curve, one mechanical parameter suffices to model the elastic behaviour of the curve. In this sense, the curve parameter $\tilde{\mu}$ can be understood as the elastic-modulus or the compression modulus of the curve and shear modulus is no longer meaningful. A surface-tension-like term is introduced by $\tilde{\gamma}$. The thermomechanical coupling is captured by the

term $-\tilde{\alpha}\tilde{\mu}[\tilde{\Theta} - \tilde{\Theta}_0] \ln \tilde{J}/J$ where $\tilde{\alpha}$ is the curve thermal expansion coefficient. The curve temperatures in the reference and current configurations are denoted as $\tilde{\Theta}_0$ and $\tilde{\Theta}$, respectively. The curve specific heat capacity $\tilde{c}_{\tilde{F}}$ represents the purely thermal behaviour. Finally, the curve specific entropy $\tilde{\Xi}_0$ is included.

From the constitutive laws (2.42)₄ the curve Piola stress and entropy corresponding to the curve Helmholtz energy Eq. (4.21) are obtained as

$$\tilde{\mathbf{P}} = \partial_{\tilde{\mathbf{F}}} \tilde{\Psi} = \left[-\tilde{\mu} + \tilde{\gamma}\tilde{J} \right] \tilde{\mathbf{f}}^t + \tilde{\mu}\tilde{\mathbf{F}} - \tilde{\alpha}\tilde{\mu}\frac{1}{\tilde{J}} \left[\tilde{\Theta} - \tilde{\Theta}_0 \right] \left[1 - \ln \tilde{J} \right] \tilde{\mathbf{f}}^t,$$

and

$$\tilde{\Xi} = -\partial_{\tilde{\Theta}} \tilde{\Psi} = \tilde{\alpha}\tilde{\mu}\frac{\ln \tilde{J}}{\tilde{J}} + \tilde{c}_{\tilde{F}} \ln \frac{\tilde{\Theta}}{\tilde{\Theta}_0} + \tilde{\Xi}_0.$$

Chapter 5

Numerical examples

The objective of this section is to briefly elucidates the theory presented in the previous sections. In particular, the role of a surface or an interface on the overall response of a body using a series of numerical examples is studied. Attention is paid to the influence of the material parameters. These examples are of particular relevance to problems involving materials at the nanoscale. The influence of decreasing specimen size on the overall response can be captured by fixing the bulk material parameters and increasing those of the surface and interface. This is equivalent to fixing the bulk Helmholtz energy and increasing the Helmholtz energy of the surface and interface. In the following examples, heat conduction in the bulk is assumed to be spatially isotropic, i.e. $\mathbf{k} = k \mathbf{i}$. It should be noted that the solution procedure is robust and shows the asymptotically quadratic rate of convergence associated with a Newton–Raphson scheme. The material behaviour in the bulk is characterised by the thermohyperelastic Helmholtz energy function given in Eq. (4.17). The corresponding material parameters for the bulk are given in Table 5.1, unless specified otherwise.

5.1 SURFACE

The following examples illustrate the effects of the surface Helmholtz energy (4.18). In particular, the role of the different terms in the energy are studied by varying their corresponding coefficients. First, in Section 5.1.1 the influence of the surface tension $\hat{\gamma}$ is shown. The contribution of this term, in contrast to all other terms in the energy form, does not vanish at the reference (strain-free) configuration and acts similar to an external force field.

Table 5.1: Bulk properties for the numerical examples.

Lamé constant	μ	80193.8	N/mm ²
Lamé constant	λ	110743.5	N/mm ²
Thermal expansion coefficient	α	1.0×10^{-5}	1/K
Conductivity	k	45.0	N/[s K]
Specific capacity	c_F	3.588	N/[mm ² K]
Reference temperature	Θ_0	298.0	K

In this sense, it should be treated as a prescribed force and therefore is applied incrementally.

The surface energy may or may not be isotropic. The theory here is not confined to the isotropic case and, in principle, an anisotropic behaviour can be captured if the form of the energy includes the anisotropy via a dependence on the surface normal, see Eq. (2.42). For the case of surface tension a simple anisotropic model is introduced and the results are shown which proves the flexibility and generality of the proposed scheme.

Next, in Section 5.1.2 the surface tension is assumed to be zero and the thermomechanical behaviour of the surface and its coupling with the bulk is illustrated via several examples. In these examples, heat conduction on the surface is assumed to be spatially isotropic, i.e. $\hat{k} = \hat{k} \hat{i}$.

5.1.1 Surface tension

Consider a unit-cube model as depicted in Fig. 5.1 (top-left). The cube is discretised using 1728 trilinear hexahedral elements and 2197 nodes. Assume that the cube is covered by an energetic surface with the surface Helmholtz energy given in Eq. (4.18) where all the surface parameters except the surface tension $\hat{\gamma}$ vanish. Rigid body motion is prevented by fixing the cube against translational and rotational degrees of freedom. Symmetry boundary conditions are applied on the mid-planes. A surface tension of $\hat{\gamma} = \mu$ is prescribed on the surface in 20 equal steps.

For a non-vanishing surface tension the reference configuration does not coincide with that of an equilibrium state. Thus the cube deforms in order to reach the equilibrium state, i.e. to minimise the total energy of the bulk plus surface. Clearly, any deformation introduces an increase in the bulk energy as it is zero at the reference configuration, nevertheless, that can be compensated by a decrease in the surface energy. Recall that the surface tension is equivalent to a constant energy per unit deformed area. Therefore, the surface energy can decrease by decreasing the surface area. As a result, the cube tends to transform into a shape where the surface to volume ratio is minimal, i.e. a sphere. The

surface also, tends to shrink. The transformation of the cube into a spherical shape is illustrated in Fig. 5.1.

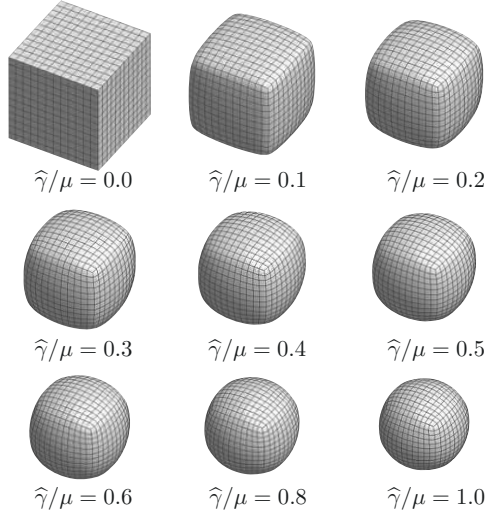


Figure 5.1: Transformation of a unit-cube into a sphere due to an incrementally prescribed surface tension of $\hat{\gamma}/\mu = 1.0\text{mm}$.

Next, the issue of anisotropy is investigated. This example is identical to the previous one except that the surface tension $\hat{\gamma}$ is not constant, but depends on the surface normal and the surface Jacobian via the relation

$$\hat{\gamma} = \mu[1 + \hat{\beta} \hat{J} [\mathbf{n} \cdot \mathbf{e}]^2],$$

where the material parameter $\hat{\beta}$ is chosen to control the anisotropic contribution compared to the isotropic part and the unit vector $\mathbf{e}$ is a given unit vector characterising a preferred direction. The anisotropic effects will be maximum where the normal to the surface is parallel to $\mathbf{e}$ and will vanish where the normal to the surface is orthogonal to $\mathbf{e}$. The vector $\mathbf{e} = (0, 0, 1)$ for the current example is shown in Fig. 5.2. Thus the anisotropic effects will be maximum on the top and the bottom of the model and will vanish on the lateral walls of the model (elsewhere is something between these two extremes). The model is expected therefore to shrink more on the top and the bottom and less at the lateral walls of the cube. Consequently the model cube is expected to transform to an ellipsoidal shape instead of a spherical one. The resulting ellipsoidal shapes for different values of $\hat{\beta}$ are shown in Fig. 5.2.

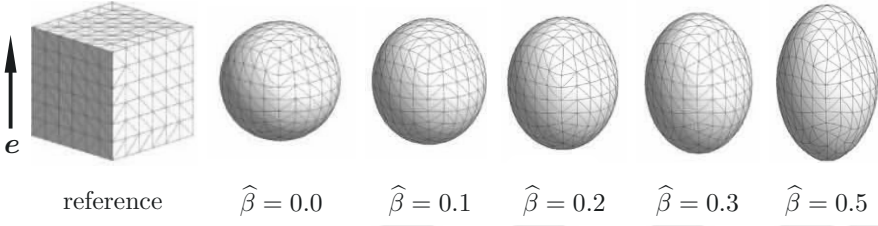


Figure 5.2: Transformation of a model unit-cube to ellipsoid due to a prescribed anisotropic surface tension $\hat{\gamma}/\mu = [1 + \hat{\beta} \hat{J} [\mathbf{n} \cdot \mathbf{e}]^2] \text{mm}$.

5.1.2 Thermomechanical surface

Consider the three-dimensional strip shown in Fig. 5.3. The strip is subjected to plane-strain-like conditions across the thickness. In the middle of the specimen a geometric imperfection is introduced in the form of a hole with a radius of 0.2mm. Lateral deformations are prevented, i.e. the width of the strip can not change. A displacement of 0.5mm is prescribed at the edges resulting in a tensile loading. The resulting amount of deformation is clearly in the finite strain regime. The deformation is assumed to be applied adiabatically at the level of the specimen. Therefore thermally homogeneous Neumann boundary conditions are applied to all boundaries of the bulk. The displacement loading is applied in 20 equal steps and the total time is 10ms. The strip is discretised using 576 trilinear hexahedral elements and 1008 nodes. Assume that the surface of the hole in the specimen is energetic. The surface Helmholtz energy is chosen to be of the form given in Eq. (4.18) with vanishing $\hat{\gamma}$. The response of the material without the energetic surface is studied in Section 5.1.2.1. Thereafter, mechanical and thermomechanical surface effects are detailed in Section 5.1.2.2 and 5.1.2.3, respectively.

5.1.2.1 Bulk effect

Consider first a thermomechanical bulk without energetic surfaces. Under the prescribed boundary conditions the tensile stress increases. This increase of the tensile stress, or more precisely the divergence of the strain rate, cools the specimen due to the Gough–Joule effect. The fact that a geometrical imperfection is introduced leads to the non-uniform stress distribution in the specimen illustrated in Fig. 5.4. Consequently, the non-uniform temperature profile depicted in Fig. 5.5 is obtained.

5.1.2.2 Mechanical surface effect

Consider next a purely mechanical surface. That is $\hat{k} = \hat{c}_{\hat{\mathbf{F}}} = \hat{\alpha} = 0$. The mechanical material parameters for the surface are assumed to be $\hat{\mu}/\mu = \hat{\lambda}/\lambda = 2 \text{mm}$. The mechanical

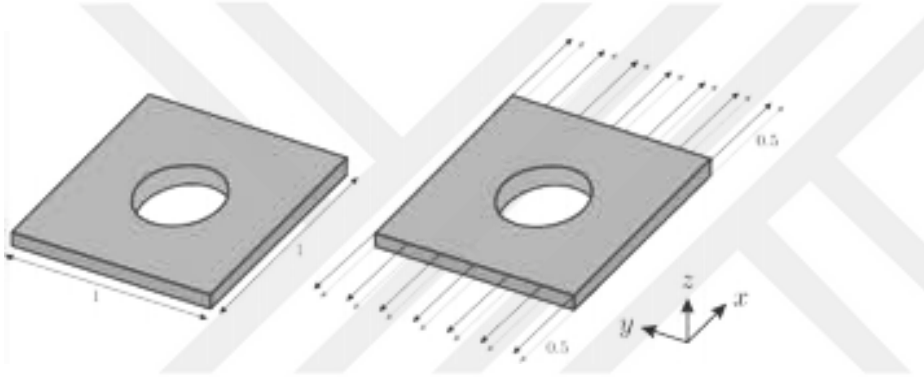


Figure 5.3: Strip with surface: geometry (left) and applied boundary conditions (right). Dimensions are in mm. The thickness is 0.1mm.

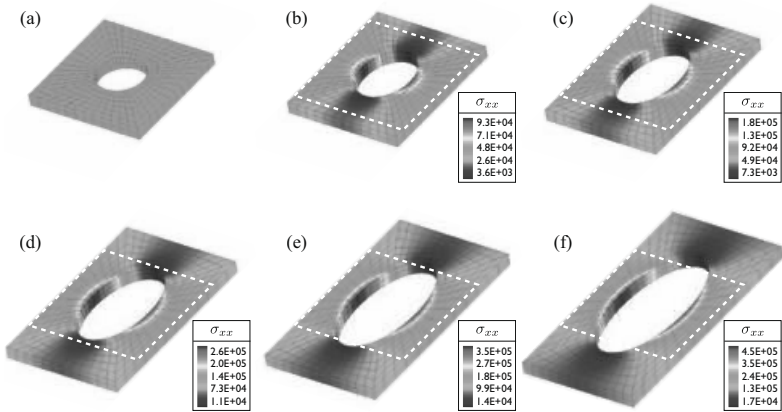


Figure 5.4: The stress distribution for a thermomechanical bulk. The results (a)–(f) correspond to the reference configuration and 20%, 40%, 60%, 80% and 100% of the final deformation, respectively. The stress depicted is the xx -component of the Cauchy stress tensor. The reference configuration is indicated using a dashed (white) line.

resistance of the surface influences the bulk, resulting in a different stress distribution compared to Fig. 5.4. The evolution of the stress field is illustrated in Fig. 5.6. The tensile stress increases with increasing load. Thus, due to the Gough–Joule effect, the temperature is expected to decrease as the applied deformation increases. The non-homogeneous stress distribution produces the non-homogeneous temperature distribution shown in Fig. 5.7.

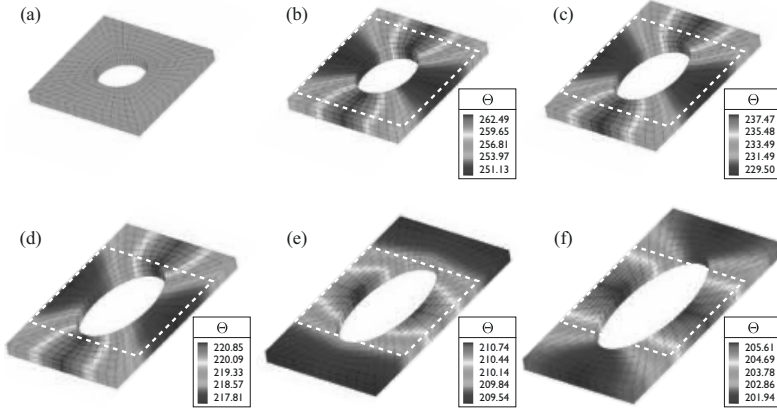


Figure 5.5: The temperature distribution for a thermomechanical bulk. The results (a)–(f) correspond to the reference configuration and 20%, 40%, 60%, 80% and 100% of the final deformation, respectively. The reference configuration is indicated using a dashed (white) line.

5.1.2.3 Thermomechanical surface effect

The surface is now endowed with thermal properties. The mechanical properties of the surface are fixed as before by setting $\hat{\mu}/\mu = \hat{\lambda}/\lambda = 2\text{mm}$. In order to better understand the role of the surface thermal properties, the surface conductivity $\hat{k}$, heat capacity $\hat{c}_F$ and heat expansion coefficient $\hat{\alpha}$ are investigated separately.

The effect of surface heat conductivity The surface heat conduction coefficient $\hat{k}$ is increased from zero to $\hat{k}/k = 100\text{mm}$. The remaining surface thermal parameters are set to zero. Figure 5.8 shows the temperature distributions at the end of the applied loading for a range of $\hat{k}/k$. The effect of increasing the surface conductivity is clearly to produce an increasingly uniform temperature distribution along the surface. Note, the result shown in Fig. 5.8 for $\hat{k}/k = 0$ is the same as shown in Fig. 5.7(f).

The effect of surface heat capacity The surface heat capacity $\hat{c}_F$ is now varied from zero to $\hat{c}_F/c_F = 1\text{mm}$. The remaining surface thermal parameters are set as zero. The surface heat capacity causes the surface to conserve its initial temperature and resist temperature change. A higher value of the surface heat capacity results in less temperature decrease at the surface. This can be observed in Fig. 5.9 which shows the final temperature distributions for different surface heat capacities.

The effect of the surface Gough–Joule contribution Finally, the effect of the surface heat

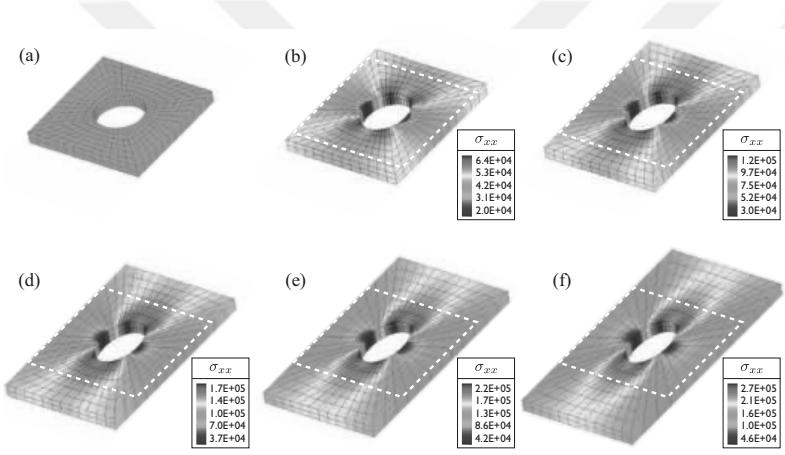


Figure 5.6: The influence a purely mechanical surface on the stress distribution for $\hat{\mu}/\mu = \hat{\lambda}/\lambda = 2\text{mm}$. The results (a)–(f) correspond to the reference configuration and 20%, 40%, 60%, 80% and 100% of the final deformation, respectively. The stress depicted is the xx -component of the Cauchy stress tensor. The reference configuration is indicated using a dashed (white) line.

expansion coefficient $\hat{\alpha}$ on the temperature distribution is studied. The surface heat expansion coefficient $\hat{\alpha}$ is varied from zero to $\hat{\alpha}/\alpha = 0.75$ while the remaining surface thermal parameters are specified as zero. According to Eq. (4.18), increasing the surface heat expansion coefficient increases the surface thermomechanical coupling. As a result of the Gough–Joule effect, the surface cools due to the positive strain rate applied to the surface from the surrounding bulk material. The surface cooling is proportional to $\hat{\alpha}/\alpha$. This explains the temperature distributions shown in Fig. 5.10.

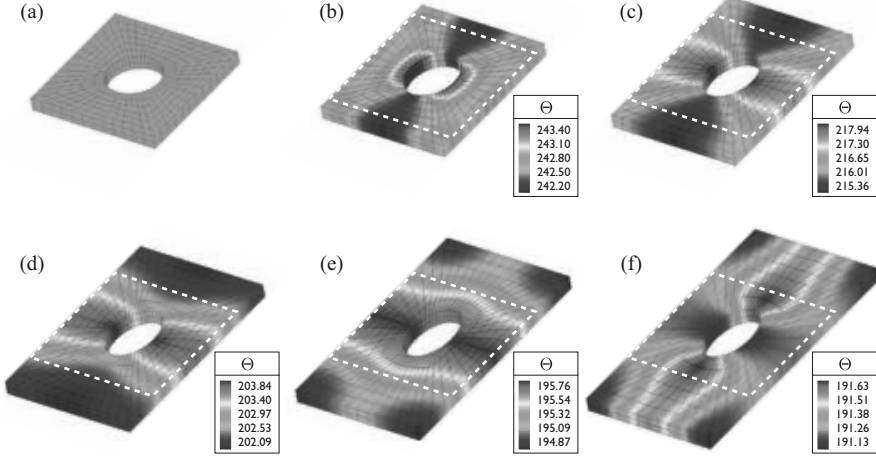


Figure 5.7: The influence of a purely mechanical surface on the temperature distribution for $\hat{\mu}/\mu = \hat{\lambda}/\lambda = 2\text{mm}$. The results (a)–(f) correspond to the reference configuration and 20%, 40%, 60%, 80% and 100% of the final deformation, respectively. The reference configuration is indicated using a dashed (white) line.

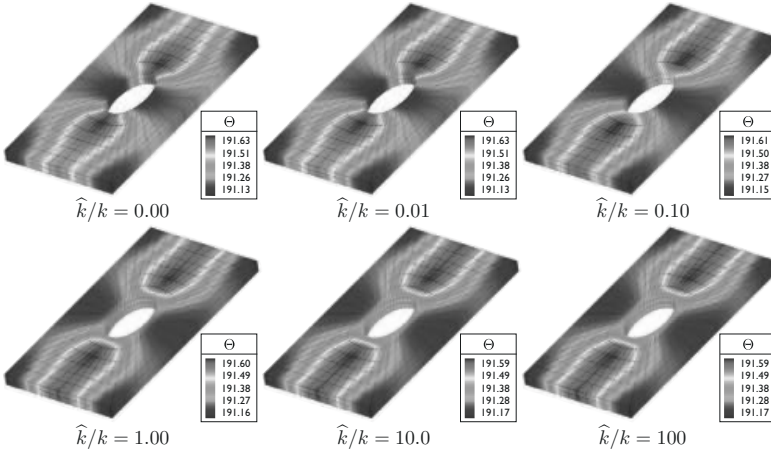


Figure 5.8: The influence of interface conduction on the temperature distribution for $\hat{\mu}/\mu = \hat{\lambda}/\lambda = 2\text{mm}$ and $\hat{k}/k = 0 - 100\text{mm}$.

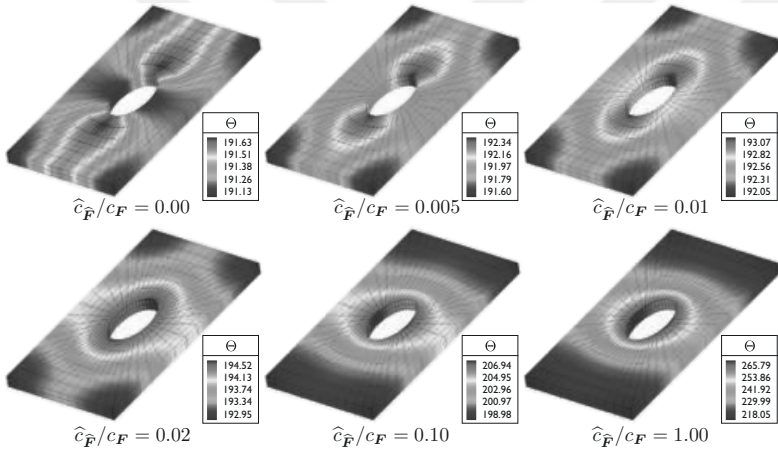


Figure 5.9: The influence of the interface heat capacity on the temperature distribution for $\hat{\mu}/\mu = \hat{\lambda}/\lambda = 2\text{mm}$ and $\hat{c}_F/c_F = 0 - 1\text{mm}$.

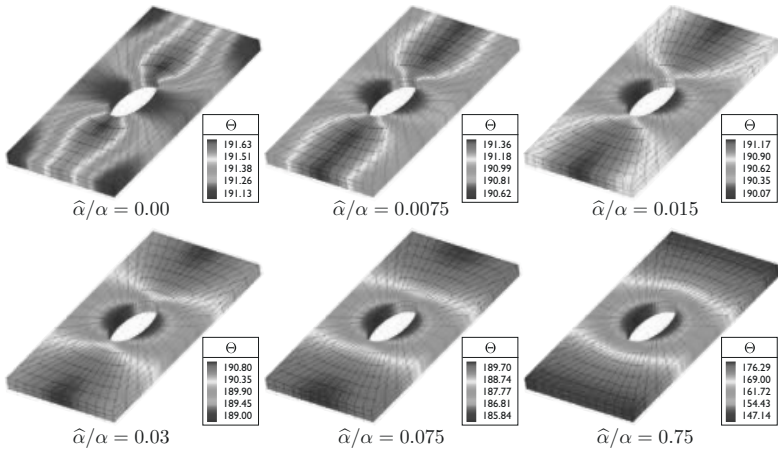


Figure 5.10: The influence of the interface heat expansion coefficient on temperature distribution for $\hat{\mu}/\mu = \hat{\lambda}/\lambda = 2\text{mm}$ and $\hat{\alpha}/\alpha = 0 - 0.75$.

5.2 INTERFACE

Consider the three-dimensional strip shown in Fig. 5.11. The strip is subjected to plane-strain-like conditions across the thickness. The strip is partitioned into two homogeneous domains by an interface. Lateral deformations are prevented, i.e. the width of the strip can not change. A displacement of 0.5mm is prescribed at the edges resulting in a tensile loading. The resulting deformation is clearly in the finite strain regime. The deformation is assumed to be applied adiabatically. Therefore thermally homogeneous Neumann boundary conditions are applied to all boundaries of the bulk. The displacement loading is applied in 20 equal steps and the total time is 10ms. The strip is discretised using 1600 trilinear hexahedral elements.

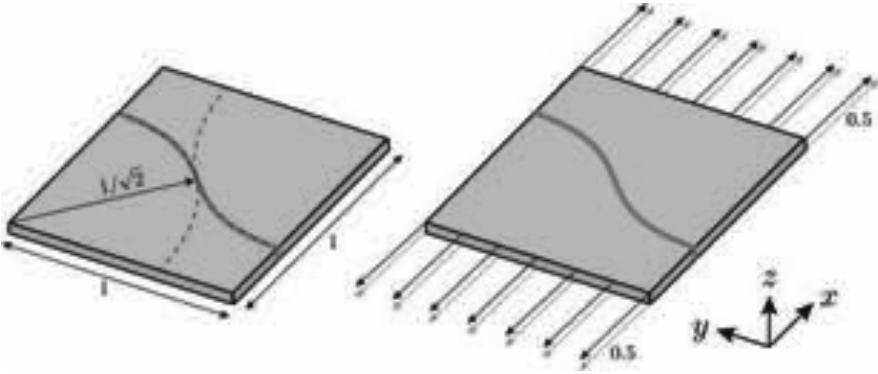


Figure 5.11: Strip with interface: geometry (left) and applied boundary conditions (right). Dimensions are in mm. The thickness is 0.05mm.

5.2.1 Thermomechanical highly-conductive interface

This section details on thermomechanical behaviour of highly-conductive interfaces. The interface Helmholtz energy is chosen to be of the form given in Eq. (4.19) with vanishing $\bar{\gamma}$. In the following examples, heat conduction on the interface is assumed to be spatially isotropic, i.e. $\bar{\mathbf{k}} = \bar{k} \bar{\mathbf{i}}$.

5.2.1.1 Mechanical interface effect

Consider first a purely mechanical interface. That is $\bar{k} = \bar{c}_{\bar{F}} = \bar{\alpha} = 0$. The mechanical material parameters for the interface are assumed to be $\bar{\mu}/\mu = \bar{\lambda}/\lambda = 2\text{mm}$. The mechanical resistance of the interface influences the bulk, resulting in a non-homogeneous stress distribution. The evolution of the stress field is illustrated in Fig. 5.12. The tensile stress increases with increasing load. This increase of the tensile stress, or more precisely

the divergence of the strain rate, cools the specimen due to the Gough–Joule effect. Thus the temperature is expected to decrease as the applied deformation increases. The non-homogeneous stress distribution produces the non-homogeneous temperature distribution shown in Fig. 5.13. Note that the temperature field is continuous across the interface while the stress is not. The jump of the stress field across the interface is equal to the interface divergence of the interface stress according to Eq. (2.25)₃.

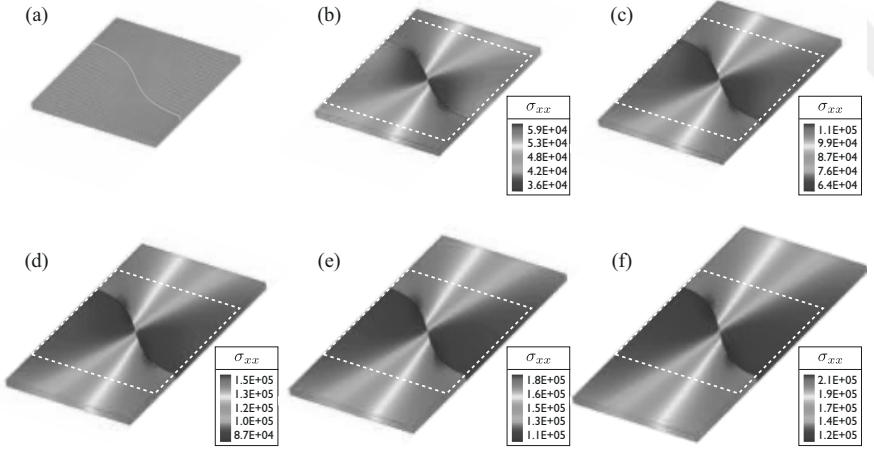


Figure 5.12: The influence a purely mechanical interface on the stress distribution for $\bar{\mu}/\mu = \bar{\lambda}/\lambda = 2\text{mm}$. The results (a)–(f) correspond to the reference configuration and 20%, 40%, 60%, 80% and 100% of the final deformation, respectively. The stress depicted is the xx -component of the Cauchy stress tensor. The reference configuration is indicated using a dashed (white) line.

5.2.1.2 Thermomechanical interface effect

The interface is now endowed with thermal properties. The mechanical properties of the interface are fixed as before by setting $\bar{\mu}/\mu = \bar{\lambda}/\lambda = 2\text{mm}$. In order to better understand the role of the interface thermal properties, the interface conductivity $\bar{k}$, heat capacity $\bar{c}_F$ and heat expansion coefficient $\bar{\alpha}$ are investigated separately.

The effect of interface conductivity The interface heat conduction coefficient $\bar{k}$ is increased from zero to $\bar{k}/k = 100\text{mm}$. The remaining interface thermal parameters are set to zero. Figure 5.14 shows the temperature distributions at the end of the applied loading for a range of $\bar{k}/k$. The effect of increasing the interface conductivity is clearly to produce an increasingly uniform temperature distribution along the interface. Note, the result shown

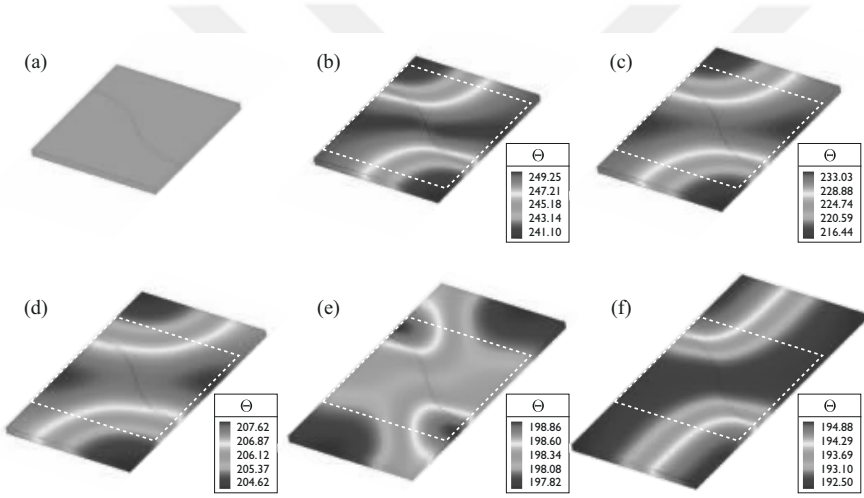


Figure 5.13: The influence of a purely mechanical interface on the temperature distribution for $\bar{\mu}/\mu = \bar{\lambda}/\lambda = 2\text{mm}$. The results (a)–(f) correspond to the reference configuration and 20%, 40%, 60%, 80% and 100% of the final deformation, respectively. The reference configuration is indicated using a dashed (white) line.

in Fig. 5.14 for $\bar{k}/k = 0$ is the same as shown in Fig. 5.13(f). The x -component of the Cauchy heat flux vector is shown in Fig. 5.15. The Cauchy heat flux clearly exhibits a discontinuity across the interface. This is due to the existence of heat flux along the interface. More precisely, the jump of the heat flux across the interface is equal to the negative of the interface divergence of the heat flux along the interface. This can be explained by the temperature evolution equation Eq. (2.59)₃ which, for the current assumptions, simplifies to

$$[[Q]] \cdot \bar{N} = -\overline{\text{Div}} Q.$$

The effect of interface heat capacity The interface heat capacity $\bar{c}_F$ is now varied from zero to $\bar{c}_F/c_F = 1\text{mm}$. The remaining interface thermal parameters are set as zero.

The interface heat capacity causes the interface to conserve its initial temperature and resist temperature change. A higher value for the interface heat capacity results in less temperature decrease at the interface. This can be observed in Fig. 5.16 which shows the final temperature distributions for different interface heat capacities. The x -component of the Cauchy heat flux vector is shown in Fig. 5.17. Increasing the interface heat capacity results in an increasing jump in the Cauchy heat flux vector across the interface. This can

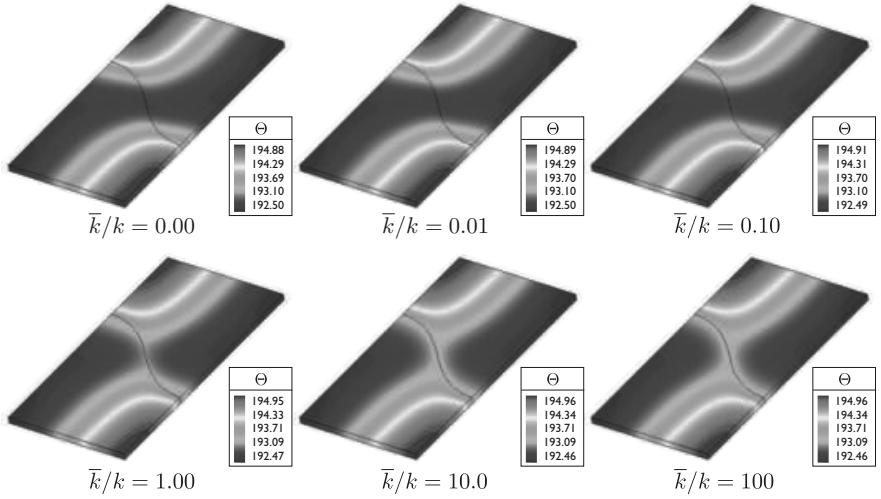


Figure 5.14: The influence of interface conduction on the temperature distribution for $\bar{\mu}/\mu = \bar{\lambda}/\lambda = 2\text{mm}$ and $\bar{k}/k = 0 - 100\text{mm}$.

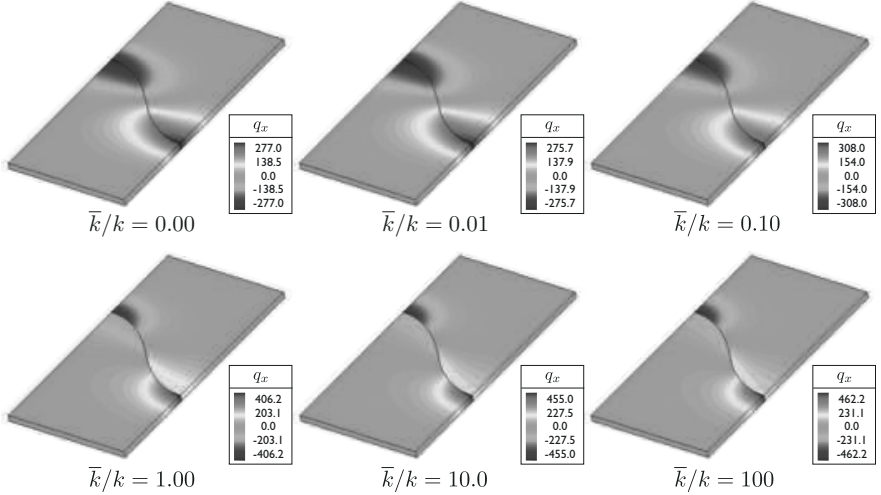


Figure 5.15: The influence of interface conduction on the x -component of the Cauchy heat flux vector for $\bar{\mu}/\mu = \bar{\lambda}/\lambda = 2\text{mm}$ and $\bar{k}/k = 0 - 100\text{mm}$.

be understood from the temperature evolution equation Eq. (2.59)₃ which simplifies to

$$[[Q]] \cdot \bar{N} = -\bar{c}_{\bar{F}} D_t \bar{\Theta}.$$

It states that the jump of the heat flux across the interface is equal to the negative of the interface heat capacity multiplied by the time derivative of the interface temperature.

The effect of interface Gough–Joule effect Finally, the effect of the interface heat expansion coefficient $\bar{\alpha}$ on the temperature distribution is studied. The interface heat expansion coefficient $\bar{\alpha}$ is varied from zero to $\bar{\alpha}/\alpha = 1.5$ while the remaining interface thermal parameters are specified as zero. According to Eq. (4.19), increasing the interface heat expansion coefficient increases the interface thermomechanical coupling. As a result of the Gough–Joule effect, the interface cools due to the positive strain rate applied to the interface from the surrounding bulk material. The interface cooling is proportional to $\bar{\alpha}/\alpha$. This explains the temperature distributions shown in Fig. 5.18. Figure 5.19 shows the Cauchy heat flux distributions for different ratios of $\bar{\alpha}/\alpha$. The temperature evolution equation Eq. (2.59)₃ in this case simplifies into

$$[[Q]] \cdot \bar{N} = \bar{\Theta} \bar{P}_{,\bar{\Theta}} : D_t \bar{F} = -2 \bar{\alpha} \bar{\kappa} \bar{\Theta} \frac{1 - \ln \bar{J}}{\bar{J}} \text{div } \bar{V},$$

and clearly shows that the jump of the heat flux across the interface is proportional to the interface heat expansion coefficient $\bar{\alpha}$.

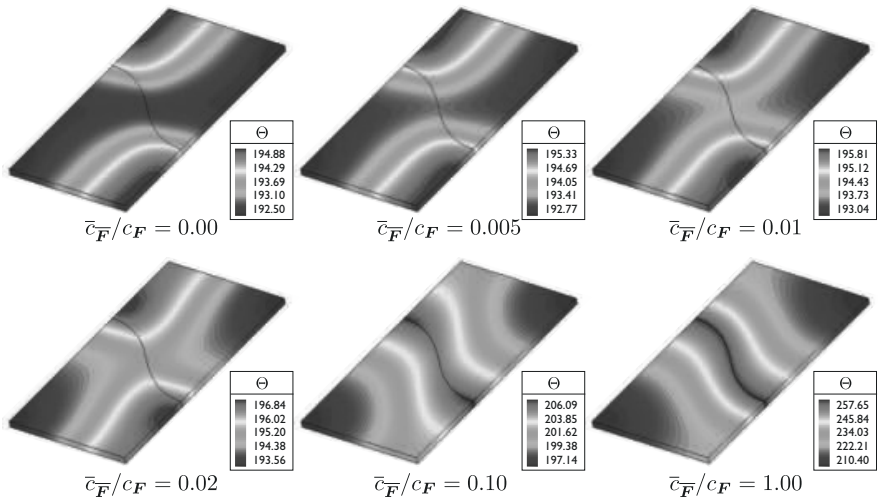


Figure 5.16: The influence of the interface heat capacity on the temperature distribution for $\bar{\mu}/\mu = \bar{\lambda}/\lambda = 2\text{mm}$ and $\bar{c}_F/c_F = 0 - 1\text{mm}$.

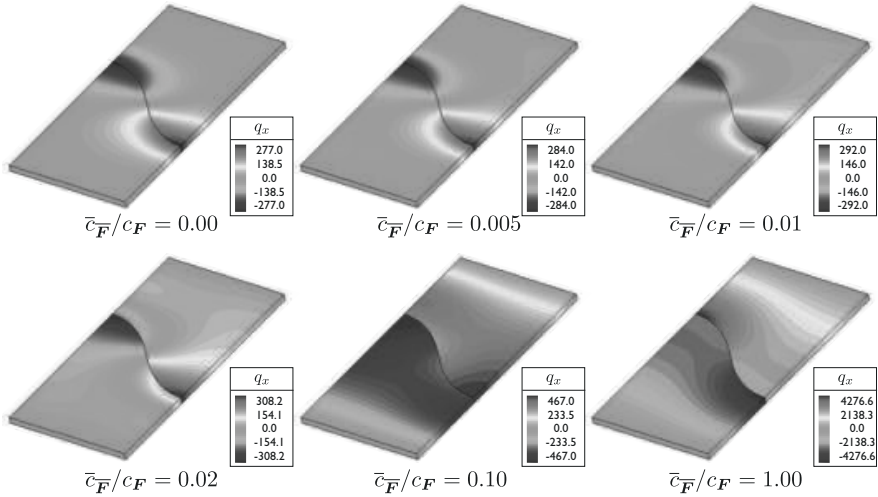


Figure 5.17: The influence of the interface heat capacity on Cauchy heat flux vector for $\bar{\mu}/\mu = \bar{\lambda}/\lambda = 2\text{mm}$ and $\bar{c}_F/c_F = 0 - 1\text{mm}$.

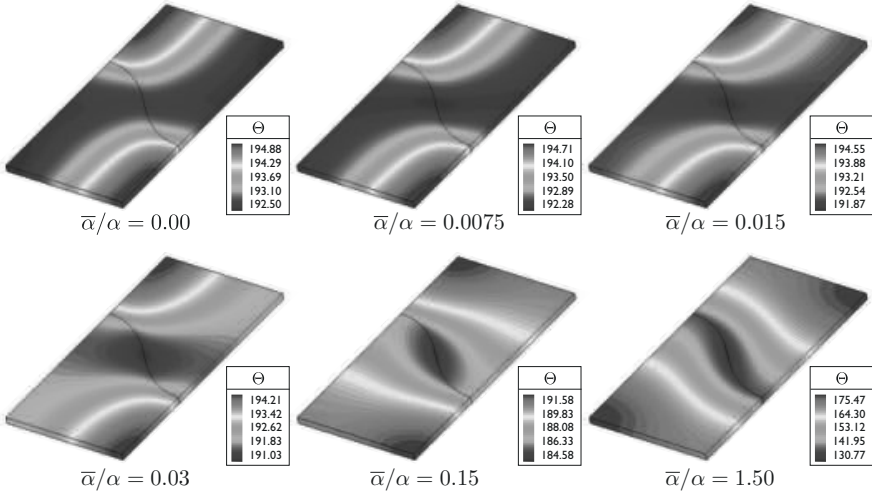


Figure 5.18: The influence of the interface heat expansion coefficient on temperature distribution for $\bar{\mu}/\mu = \bar{\lambda}/\lambda = 2\text{mm}$ and $\bar{\alpha}/\alpha = 0 - 1.5$.

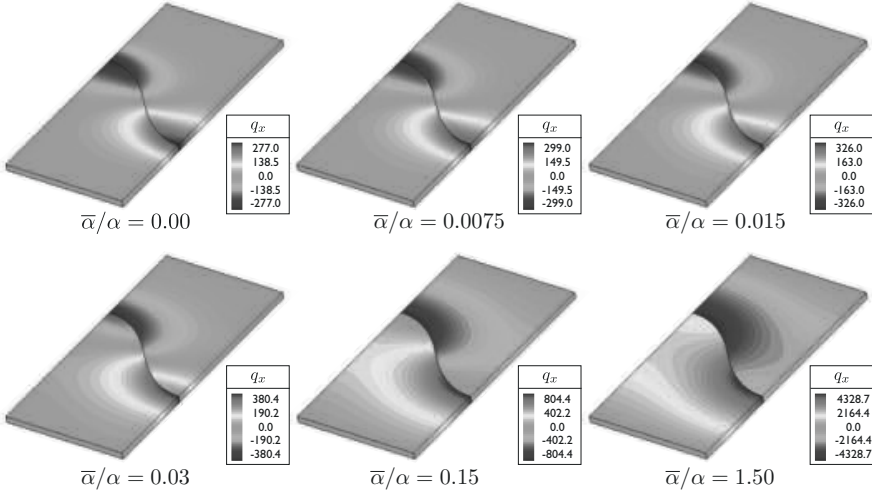


Figure 5.19: The influence of the interface heat expansion coefficient on the temperature distribution for $\bar{\mu}/\mu = \bar{\lambda}/\lambda = 2\text{mm}$ and $\bar{\alpha}/\alpha = 0 - 1.5$.

5.2.2 Generalised Kapitza interface

The objective of this section is to elucidate the role of a Kapitza interface on the the overall response of a body using a series of numerical examples. The interface Helmholtz energy is chosen to be of the form given in Eq. (4.20) with vanishing $\bar{\gamma}$.

The mechanical material parameters for the Kapitza interface shown in Fig. 5.11 are assumed to be $\bar{\mu}/\mu = \bar{\lambda}/\lambda = 2\text{mm}$. The mechanical resistance of the interface influences the bulk, resulting in a non-homogeneous stress distribution. The evolution of the stress field is illustrated in Fig. 5.20. Note that the stress field is discontinuous across the interface. The jump of the stress field across the interface is equal to the interface divergence of the interface stress according to the relationships given in Eq. (2.25)₃. The tensile stress increases with increasing load. The increase in the tensile stress or, more precisely, the divergence of the strain rate cools the specimen due to the Gough–Joule effect. Thus the temperature is expected to decrease as the applied deformation increases. The non-homogeneous stress distribution produces the temperature distribution shown in Fig. 5.21 for a Kapitza thermal resistance $\bar{r}_Q = 1.0 \times 10^{-5}$. Note that in Fig. 5.21–5.23 the temperature field is discontinuous across the interface, however, this discontinuity is not visible in Fig. 5.21 due to the very small Kapitza thermal resistance.

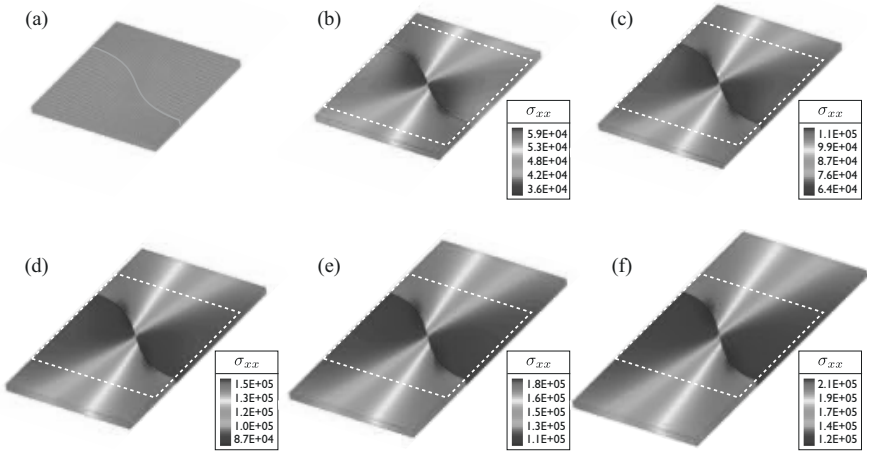


Figure 5.20: The influence the interface on the stress distribution for $\bar{\mu}/\mu = \bar{\lambda}/\lambda = 2\text{mm}$. The results (a)–(f) correspond to the reference configuration and 20%, 40%, 60%, 80% and 100% of the final deformation, respectively. The stress depicted is the xx -component of the Cauchy stress tensor. The reference configuration is indicated using a dashed (white) line.

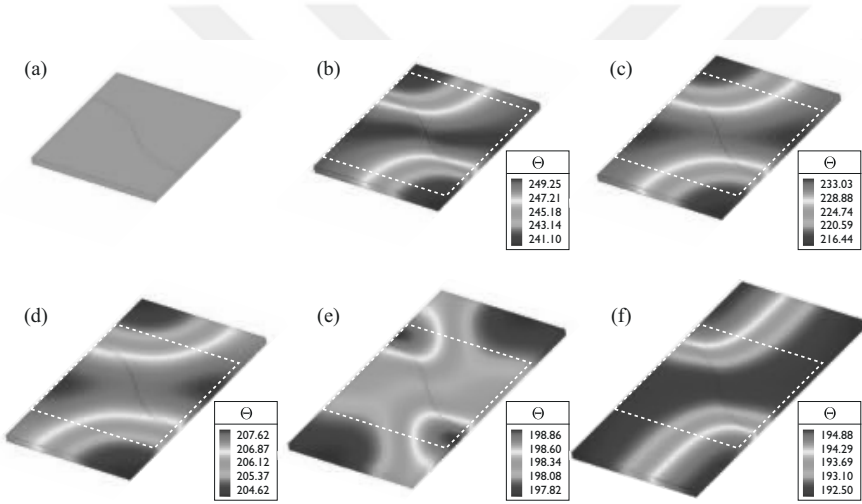


Figure 5.21: The influence of the interface on the temperature distribution for $\bar{\mu}/\mu = \bar{\lambda}/\lambda = 2\text{mm}$ and $\bar{\tau}_Q = 0.00001$. The results (a)–(f) correspond to the reference configuration and 20%, 40%, 60%, 80% and 100% of the final deformation, respectively. The reference configuration is indicated using a dashed (white) line.

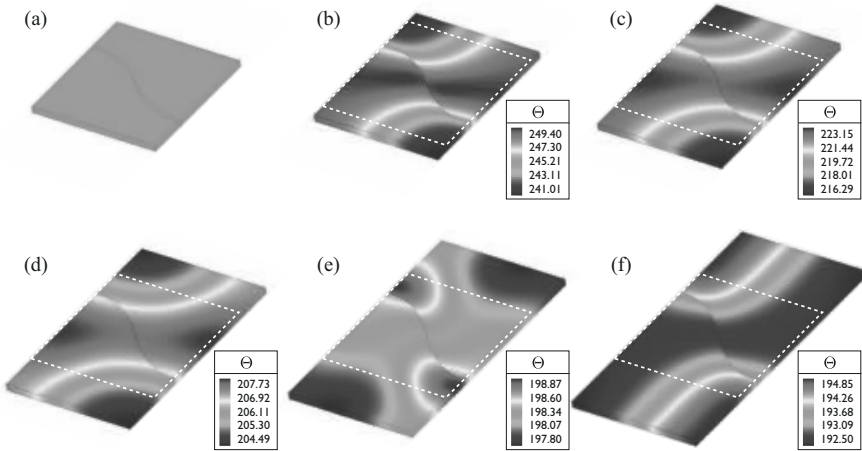


Figure 5.22: The influence of a purely mechanical interface on the temperature distribution for $\bar{\mu}/\mu = \bar{\lambda}/\lambda = 2\text{mm}$ and $\bar{\tau}_Q = 0.001$. The results (a)–(f) correspond to the reference configuration and 20%, 40%, 60%, 80% and 100% of the final deformation, respectively. The reference configuration is indicated using a dashed (white) line.

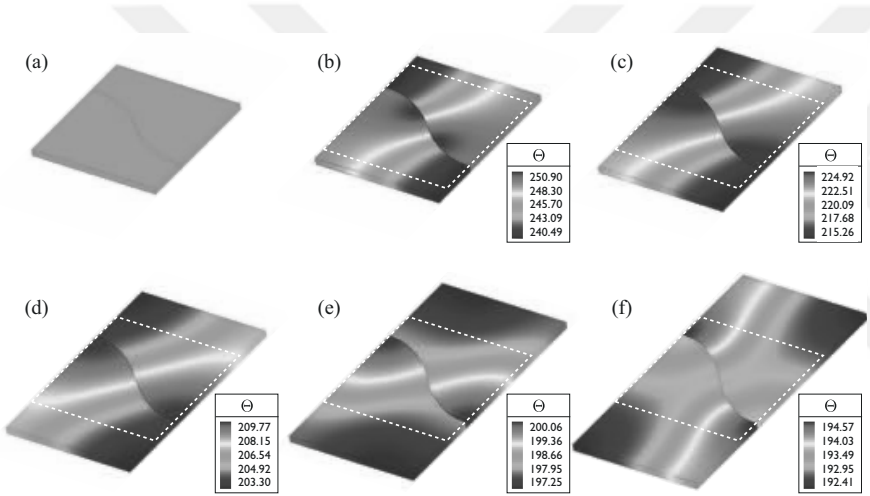


Figure 5.23: The influence of a purely mechanical interface on the temperature distribution for $\bar{\mu}/\mu = \bar{\lambda}/\lambda = 2\text{mm}$ and $\bar{r}_Q = 0.1$. The results (a)–(f) correspond to the reference configuration and 20%, 40%, 60%, 80% and 100% of the final deformation, respectively. The reference configuration is indicated using a dashed (white) line.

In order to better understand the effects of the Kapitza thermal resistance $\bar{r}_Q$, a strip with straight interface is studied next.

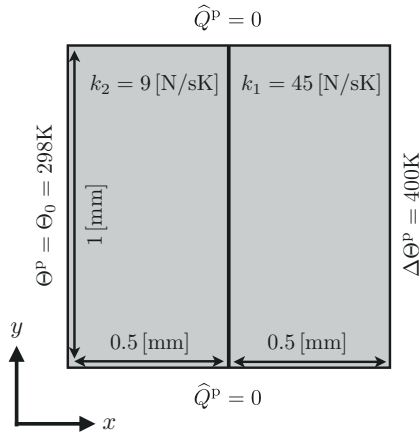


Figure 5.24: Strip with a straight interface: problem definition.

Consider the strip shown in Fig. 5.24 which is subjected to plane-strain conditions across the thickness. The strip is partitioned into two homogeneous domains by a straight interface in the middle. The thermal and mechanical properties of both domains are identical except for the heat conduction coefficient which is five times smaller on the left-hand side of the interface. A temperature increase of 400K is prescribed at the right edge. The temperature at the left edge is maintained at the reference temperature of 298K resulting in heat flux (conduction) from right to left. The left and the right edges are subject to mechanically homogeneous Dirichlet boundary conditions. On the lateral edges thermally and mechanically homogeneous Neumann boundary conditions are applied. The strip is discretised using bilinear quadrilateral elements.

The temperature and heat flux profiles for different Kapitza thermal resistances $\bar{r}_Q$ at the final time $t_{\text{end}} = 0.2\text{s}$ are depicted in Fig. 5.25. The temperature jump across the interface increases with increasing Kapitza thermal resistance. By contrast, the heat flux remains continuous across the interface. The results shown in Fig. 5.25 correspond to the time $t = t_{\text{end}}$ where the solution is nearly stationary. The evolution from the non-linear transient solution to the linear stationary one is illustrated in Fig. 5.26. These results clearly show the discontinuity of the temperature and continuity of the heat flux across the interface. Furthermore, the results serve as a benchmark for future investigations. The stationary temperature profiles correspond to the analytical solution [see e.g. 81].

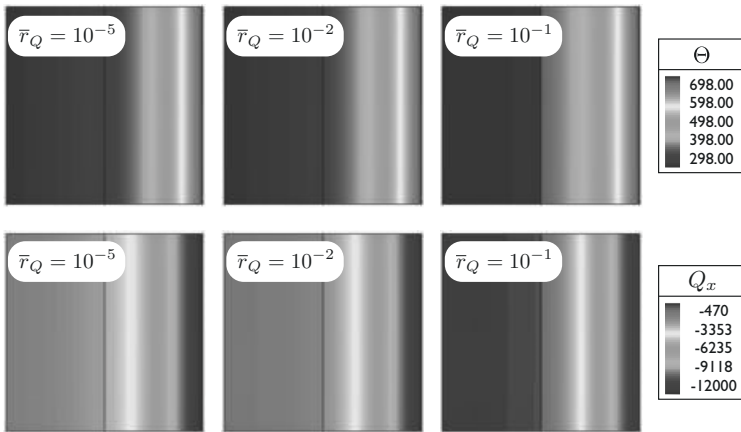
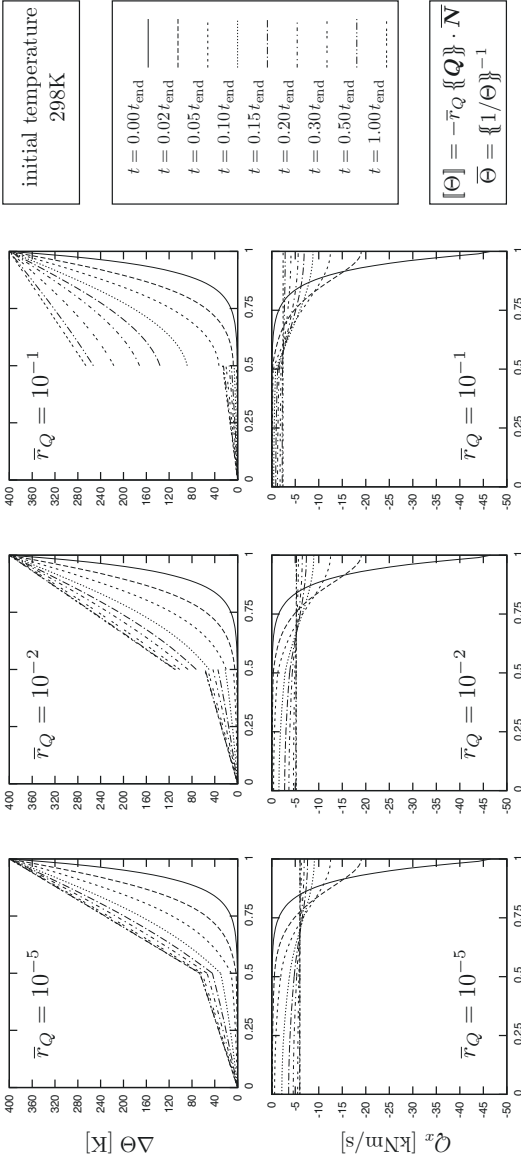


Figure 5.25: Strip with a straight interface: the computed temperature and normal heat flux distribution for various Kapitza resistances $\bar{r}_Q$.



t/t_{end}	$\bar{r}_Q = 10^{-5}$				$\bar{r}_Q = 10^{-2}$				$\bar{r}_Q = 10^{-1}$			
	$[\Theta]$	$\{[\Theta]\}$	$\bar{\Theta}$	$\{[Q]\} \cdot \bar{N}$	$[\Theta]$	$\{[\Theta]\}$	$\bar{\Theta}$	$\{[Q]\} \cdot \bar{N}$	$[\Theta]$	$\{[\Theta]\}$	$\bar{\Theta}$	$\{[Q]\} \cdot \bar{N}$
0.00	0.0006	298.37	298.37	-6.4E+01	0.34	298.44	298.44	-3.60E+01	0.65	298.50	298.50	-9.40E+00
0.02	0.0056	300.67	300.67	-5.6E+02	3.31	301.31	301.30	-3.40E+02	7.01	302.02	301.98	-8.90E+01
0.05	0.0190	309.23	309.23	-1.9E+03	12.69	311.74	311.61	-1.30E+03	30.79	315.31	314.56	-3.50E+02
0.10	0.0376	327.80	327.80	-3.8E+03	28.23	333.89	333.29	-2.80E+03	82.12	345.25	340.36	-8.70E+02
0.15	0.0476	342.32	342.32	-4.8E+03	37.95	351.42	350.39	-3.80E+03	125.11	371.47	360.94	-1.30E+03
0.20	0.0530	351.55	351.55	-5.3E+03	43.62	363.04	361.73	-4.40E+03	156.82	391.36	375.65	-1.60E+03
0.30	0.0577	360.22	360.22	-5.8E+03	49.00	374.83	373.23	-4.90E+03	196.36	416.57	393.43	-2.00E+03
0.50	0.0597	364.04	364.04	-6.0E+03	51.68	380.89	379.13	-5.20E+03	227.87	436.80	407.09	-2.30E+03
1.00	0.0599	364.50	364.50	-6.0E+03	52.10	381.84	380.06	-5.20E+03	239.34	444.18	411.94	-2.40E+03

Figure 5.26: The influence of the Kapitza thermal resistance $\bar{r}_Q$ on the temperature and heat flux distributions.

Chapter 6

Conclusion

A procedure for deriving the equations governing the response of a solid bulk, surrounded by a surface, and intersected by an interface, all of which are energetic, has been presented. The interaction between the surface and the interface has also been accounted for. The structure of the constitutive relations in the various parts of the body was made clear by assigning these regions distinct Helmholtz energies and following a Coleman–Noll-like procedure. The remaining (reduced) dissipation inequalities suggest the structure of the heat and entropy flux vectors, and permissible restrictions on the temperature field in the various parts of the body; particular attention was paid to the interface. It was shown that the interface temperature is not, in general, equal to the average of the temperature across the interface. In order to sufficiently satisfy the dissipation inequalities it seems rather natural to choose the interface coldness equal to the average of the coldness across the interface.

The weak formulation of the governing equations was then given and compared to six commonly-used restrictions thereof. The finite element and the finite difference methods were used to discretise the problem in space and time, respectively. A three-dimensional finite element framework for thermomechanical continua containing energetic interfaces and surfaces was presented in detail.

Furthermore, aspects of material modelling for the elasticity theory in the various parts of the body were elaborated on. This aspect of the work has particular relevance to applications in nano-mechanics in which (mechanical) surfaces are widely studied. Thus a particular emphasis was placed on the material modelling of the surface. The relationship

between the surface material parameters and their admissible ranges were discussed.

Finally, the theory was elucidated using a series of numerical examples. In particular, the role of a surface or an interface and the choice of constitutive parameters on the overall response of a body was studied. These examples contain the key features associated with materials at the nanoscale. The influence of decreasing specimen size on the overall response can be captured by fixing the bulk material parameters and increasing those of the surface or interface. The solution procedure is robust and shows the asymptotically quadratic rate of convergence associated with a Newton–Raphson scheme.

The work presented here could be extended in various possible ways. This contribution was restricted to thermoelastic materials. An obvious extension would be to account for inelasticity at the nano-scale as recently observed in [142].

The diffusion of mass or chemical species was not accounted for. Such an extension to a formulation which accounts for surface structures and includes the effects of diffusion and viscoelasticity has been considered by McBride et al. [74].

The widely-used assumption relating heat and entropy via the absolute temperature has been here. The validity and necessity of this assumption should be explored using the procedure outlined in Müller [143].

The theory proposed here is often motivated by applications where size effects play a critical role. The ratio of the bulk Helmholtz energy to those in the remaining parts of the body implicitly accounts for the size-effects. However, the theory lacks a physical length scale related to the thickness of the interface or surface. Steigmann and Ogden [40] incorporate local elastic resistance to flexure into the Gurtin and Murdoch surface elasticity theory, thereby introducing an inherent length scale and regularising the associated variational problem. Recent work by Forest et al. [144], comparing first and second strain-gradient theories for capillary effects in elastic fluids at small length scales, emphasises the importance of nonlocality and the associated issue of length scale. An extension to account for the flexural resistance of the surface or interface is therefore suggested. Related works include Gurtin and Jabbour [41], Fried and Todres [42] and Chhapadia et al. [43].

The current presentation has been based on classical deformational mechanics and has not exploited the powerful framework of configurational mechanics, see e.g. Maugin [30], Steinmann et al. [31]. A transferral of the work presented here to the configurational setting would certainly help further understanding of the role of surface and interface energies in coupled problems.

An extension of this work to allow for non-smooth surfaces and thereby account for energetic curves on the surface that arise as geometric entities would allow for an improved description of various problems in nano-mechanics, see e.g. Yvonnet et al. [73] who model ionic nanowires using surface elasticity theory and ab-initio calculations.

A framework for micro-to-macro transitions whereby the surfaces of the microscopic

features are endowed with their own (energetic) structures can be established, see [97]. The surface elasticity theory introduces additional microscopic length scales.

Surface elasticity theory can be applied to allow non-coherent interfaces to capture in-plane stretch in addition to the normal opening mode, see McBride et al. [98] for micro-to-macro transitions for heterogeneous material layers accounting for in-plane stretch. The normal opening mode can be captured by a traction-separation law.

Finally, two main restrictions of this work were the kinematic coherence and material nature of the interface. The extension to non-coherent and evolving interfaces brings various challenges particularly from the computational prospective.



Appendices

Appendix A

Geometry of surfaces and curves

It is enlightening to briefly review some basic terminologies and results on surfaces and curves. For further details the reader is referred to [87, 105–110] among others. Here, some technicalities are borrowed from Steinmann [87].

A.1 SURFACES

A two-dimensional (smooth) surface $\mathcal{S}$ in the three dimensional, embedding Euclidean space with coordinates $\mathbb{x}$ is parameterised by two surface coordinates η^α with $\alpha = 1, 2$ as

$$\mathbb{x} = \mathbb{x}(\eta^\alpha).$$

The corresponding tangent vectors $\mathfrak{a}_\alpha \in T\mathcal{S}$ to the surface coordinate lines η^α , i.e. the covariant (natural) surface basis vectors are given by

$$\mathfrak{a}_\alpha = \partial_{\eta^\alpha} \mathbb{x}.$$

The associated contravariant (dual) surface basis vectors $\mathfrak{a}^\alpha$ are defined by the Kronecker property $\delta^\alpha_\beta = \mathfrak{a}^\alpha \cdot \mathfrak{a}_\beta$ and are explicitly related to the covariant surface basis vectors $\mathfrak{a}_\alpha$ by the co- and contra-variant surface metric coefficients $\mathfrak{a}_{\alpha\beta}$ (first fundamental form of the surface) and $\mathfrak{a}^{\alpha\beta}$, respectively, as

$$\begin{aligned} \mathfrak{a}_\alpha &= \mathfrak{a}_{\alpha\beta} \mathfrak{a}^\beta & \text{with } \mathfrak{a}_{\alpha\beta} &= \mathfrak{a}_\alpha \cdot \mathfrak{a}_\beta = [\mathfrak{a}^{\alpha\beta}]^{-1}, \\ \mathfrak{a}^\alpha &= \mathfrak{a}^{\alpha\beta} \mathfrak{a}_\beta & \text{with } \mathfrak{a}^{\alpha\beta} &= \mathfrak{a}^\alpha \cdot \mathfrak{a}^\beta = [\mathfrak{a}_{\alpha\beta}]^{-1}. \end{aligned}$$

The contra- and covariant base vectors $\mathfrak{a}^3$ and $\mathfrak{a}_3$, normal to $T\mathcal{S}$, are defined by

$$\mathfrak{a}^3 := \mathfrak{a}_1 \times \mathfrak{a}_2 \quad \text{and} \quad \mathfrak{a}_3 := [\mathfrak{a}^{33}]^{-1} \mathfrak{a}^3 \quad \text{so that} \quad \mathfrak{a}^3 \cdot \mathfrak{a}_3 = 1.$$

Thereby, the corresponding contra- and covariant metric coefficients, respectively, $[\mathfrak{a}^{33}]$ and $[\mathfrak{a}_{33}]$ follow as

$$[\mathfrak{a}^{33}] = |\mathfrak{a}_1 \times \mathfrak{a}_2|^2 = \det[\mathfrak{a}_{\alpha\beta}] = [\det[\mathfrak{a}^{\alpha\beta}]]^{-1} = [\mathfrak{a}_{33}]^{-1}.$$

Accordingly, the surface area element ds and the surface normal $\mathfrak{n}$ are computed as

$$ds = |\mathfrak{a}_1 \times \mathfrak{a}_2| d\eta^1 d\eta^2 = [\mathfrak{a}^{33}]^{1/2} d\eta^1 d\eta^2 \quad \text{and} \quad \mathfrak{n} = [\mathfrak{a}_{33}]^{1/2} \mathfrak{a}^3 = [\mathfrak{a}^{33}]^{1/2} \mathfrak{a}_3.$$

Moreover, with $\hat{\mathfrak{i}}$ denoting the ordinary mixed-variant unit tensor of the three-dimensional, embedding Euclidian space, the mixed-variant surface unit tensor $\hat{\mathfrak{i}}$ is defined as

$$\hat{\mathfrak{i}} := \delta^{\alpha\beta} \mathfrak{a}_{\alpha} \otimes \mathfrak{a}^{\beta} = \mathfrak{a}_{\alpha} \otimes \mathfrak{a}^{\alpha} = \hat{\mathfrak{i}} - \mathfrak{a}_3 \otimes \mathfrak{a}^3 = \hat{\mathfrak{i}} - \mathfrak{n} \otimes \mathfrak{n}.$$

Clearly the mixed-variant surface unit tensor acts as a surface (idempotent) projection tensor.

The surface gradient and surface divergence operators for vector fields are defined by

$$\text{grad}_s \{\bullet\} := \partial_{\eta^{\alpha}} \{\bullet\} \otimes \mathfrak{a}^{\alpha} \quad \text{and} \quad \text{div}_s := \partial_{\eta^{\alpha}} \{\bullet\} \cdot \mathfrak{a}^{\alpha}.$$

As a consequence, observe that $\text{grad}_s \{\bullet\} \cdot \mathfrak{n} = 0$ holds by definition. For fields that are smooth in a neighbourhood of the surface, the surface gradient and surface divergence operators are alternatively defined as

$$\text{grad}_s \{\bullet\} := \text{grad} \{\bullet\} \cdot \hat{\mathfrak{i}} \quad \text{and} \quad \text{div}_s := \text{grad}_s \{\bullet\} : \hat{\mathfrak{i}} = \text{grad} \{\bullet\} : \hat{\mathfrak{i}}.$$

Finally, the Gauss formulae for the derivatives of the co- and contra-variant surface basis vectors read

$$\partial_{\eta^{\beta}} \mathfrak{a}_{\alpha} = \Gamma_{\alpha\beta}^{\gamma} \mathfrak{a}_{\gamma} + \hat{k}_{\alpha\beta} \mathfrak{n} \quad \text{and} \quad \partial_{\eta^{\beta}} \mathfrak{a}^{\alpha} = -\Gamma_{\beta\gamma}^{\alpha} \mathfrak{a}^{\gamma} + \hat{k}_{\beta}^{\alpha} \mathfrak{n},$$

where $\Gamma_{\alpha\beta}^{\gamma} = \partial_{\eta^{\beta}} \mathfrak{a}_{\alpha} \cdot \mathfrak{a}^{\gamma}$ denote the surface Christoffel symbols and $\hat{k}_{\alpha\beta}$ are the coefficients of the curvature tensor. The curvature tensor $\hat{\mathbb{k}} = \hat{k}_{\alpha\beta} \mathfrak{a}^{\alpha} \otimes \mathfrak{a}^{\beta}$ and twice the mean curvature $\hat{k} = \hat{k}_{\alpha}^{\alpha}$ of the surface $\mathcal{S}$ are defined as the negative surface gradient and surface divergence of the surface normal $\mathfrak{n}$, respectively,

$$\hat{\mathbb{k}} := -\text{grad}_s \mathfrak{n} = -\partial_{\eta^{\beta}} \mathfrak{n} \otimes \mathfrak{a}^{\beta} \quad \text{and} \quad \hat{k} := -\text{div}_s \mathfrak{n} = -\partial_{\eta^{\beta}} \mathfrak{n} \cdot \mathfrak{a}^{\beta}. \quad (\text{A.1})$$

The covariant coefficients of the curvature tensor (second fundamental form of the surface) are computed by $\hat{k}_{\alpha\beta} = \mathfrak{a}_{\alpha} \cdot \hat{\mathbb{k}} \cdot \mathfrak{a}_{\beta} = -\mathfrak{a}_{\alpha} \cdot \partial_{\eta^{\beta}} \mathfrak{n}$.

A.2 CURVES

A one-dimensional (smooth) curve $\mathcal{C}$ in the three-dimensional, embedding euclidian space with coordinates $\mathbf{x}$ is parameterised by the arc-length η as

$$\mathbf{x} = \mathbf{x}(\eta).$$

The corresponding tangent vector $\mathbf{t} \in T\mathcal{C}$ to the curve, together with the (principal) normal and binormal vectors $\mathbf{m}$ and $\mathbf{b}$, orthogonal to $T\mathcal{C}$, are defined by

$$\mathbf{t} := \partial_\eta \mathbf{x} \quad \text{and} \quad \mathbf{m} := \partial_\eta \mathbf{t} / |\partial_\eta \mathbf{t}| \quad \text{and} \quad \mathbf{b} := \mathbf{t} \times \mathbf{m}.$$

Due to the parametrisation of the curve in its arc-length η , the tangent vector $\mathbf{t}$ has unit length and the curve line element dc is computed as

$$dc = |\partial_\eta \mathbf{x}| d\eta = |\mathbf{t}| d\eta = d\eta.$$

Moreover, we define the mixed-variant curve unit tensor $\tilde{\mathbf{i}}$ as

$$\tilde{\mathbf{i}} := \mathbf{t} \otimes \mathbf{t} = \mathbf{i} - \mathbf{m} \otimes \mathbf{m} - \mathbf{b} \otimes \mathbf{b}.$$

Clearly the mixed-variant curve unit tensor acts as a curve (idempotent) projection tensor.

The curve gradient and curve divergence operators for vector fields are defined by

$$\text{grad}_c \{\bullet\} := \partial_\eta \{\bullet\} \otimes \mathbf{t} \quad \text{and} \quad \text{div}_c := \partial_\eta \{\bullet\} \cdot \mathbf{t}.$$

As a consequence, observe that $\text{grad}_c \{\bullet\} \cdot \mathbf{m} = \mathbf{0}$ and $\text{grad}_c \{\bullet\} \cdot \mathbf{b} = \mathbf{0}$ hold by definition. For fields that are smooth in a of the curve, the curve gradient and curve divergence operators are alternatively defined as

$$\text{grad}_c \{\bullet\} := \text{grad} \{\bullet\} \cdot \tilde{\mathbf{i}} \quad \text{and} \quad \text{div}_c := \text{grad}_c \{\bullet\} : \tilde{\mathbf{i}} = \text{grad} \{\bullet\} : \tilde{\mathbf{i}}.$$

Finally, the Frénet–Serret formulae for the derivatives of the curve basis vectors read

$$\partial_\eta \mathbf{t} = \tilde{k} \mathbf{m} \quad \text{and} \quad \partial_\eta \mathbf{m} = -\tilde{k} \mathbf{t} + \tilde{k}' \mathbf{b} \quad \text{and} \quad \partial_\eta \mathbf{b} = -\tilde{k}' \mathbf{m},$$

where $\tilde{k}$ and $\tilde{k}'$ denote the scalar valued curvature and torsion of the curve. Based on the Frénet–Serret formulae, the curve divergence of the curve unit tensor $\tilde{\mathbf{i}}$ renders

$$\text{div}_c \tilde{\mathbf{i}} = \tilde{k} \mathbf{m}.$$

Likewise, the curvature tensors $\tilde{\mathbf{k}}_{\parallel}$, $\tilde{\mathbf{k}}_{\perp}$ and the scalar valued curvature $\tilde{k}$ are defined as the curve gradient of the curve tangent $\mathbf{t}$ and the negative curve gradient and curve divergence of the curve normal $\mathbf{m}$, respectively,

$$\begin{aligned} \tilde{\mathbf{k}}_{\parallel} &:= \text{grad}_c \mathbf{t} = \partial_\eta \mathbf{t} \otimes \mathbf{t} \quad \text{and} \quad \tilde{\mathbf{k}}_{\perp} := -\text{grad}_c \mathbf{m} = -\partial_\eta \mathbf{m} \otimes \mathbf{t}, \\ \tilde{k} &:= -\text{div}_c \mathbf{m} = -\partial_\eta \mathbf{m} \cdot \mathbf{t}. \end{aligned}$$

The curvature tensors are computed as $\tilde{\mathbf{k}}_{\parallel} = \tilde{k} \mathbf{m} \otimes \mathbf{t}$ and $\tilde{\mathbf{k}}_{\perp} = \tilde{k} \mathbf{t} \otimes \mathbf{t} - \tilde{k}' \mathbf{b} \otimes \mathbf{t}$.

Appendix B

Some mathematical relations and derivations

In this section some useful identities which are employed throughout this work are given. Furthermore, the intermediate steps and technicalities of some proofs are detailed.

B.1 USEFUL IDENTITIES

In order to derive the balance equations in Section 2.2, a number of mathematical identities are needed. They are listed here without proof. For scalars R , $\hat{R}$, $\bar{R}$ and $\tilde{R}$, vectors $\mathbf{Q}$, $\hat{\mathbf{Q}}$, $\bar{\mathbf{Q}}$ and $\tilde{\mathbf{Q}}$, and second-order tensors $\mathbf{P}$, $\hat{\mathbf{P}}$, $\bar{\mathbf{P}}$ and $\tilde{\mathbf{P}}$ the following relations hold:

$$\begin{aligned}\text{Div}(\mathbf{Q} \times \mathbf{P}) &= \mathbf{Q} \times \text{Div} \mathbf{P} + \varepsilon : [\text{Grad} \mathbf{Q} \cdot \mathbf{P}^t] && \text{in } \mathcal{B}_0, \\ \widehat{\text{Div}}(\hat{\mathbf{Q}} \times \hat{\mathbf{P}}) &= \hat{\mathbf{Q}} \times \widehat{\text{Div}} \hat{\mathbf{P}} + \varepsilon : [\widehat{\text{Grad}} \hat{\mathbf{Q}} \cdot \hat{\mathbf{P}}^t] && \text{in } \mathcal{S}_0, \\ \overline{\text{Div}}(\bar{\mathbf{Q}} \times \bar{\mathbf{P}}) &= \bar{\mathbf{Q}} \times \overline{\text{Div}} \bar{\mathbf{P}} + \varepsilon : [\overline{\text{Grad}} \bar{\mathbf{Q}} \cdot \bar{\mathbf{P}}^t] && \text{in } \mathcal{S}_0, \\ \widetilde{\text{Div}}(\tilde{\mathbf{Q}} \times \tilde{\mathbf{P}}) &= \tilde{\mathbf{Q}} \times \widetilde{\text{Div}} \tilde{\mathbf{P}} + \varepsilon : [\widetilde{\text{Grad}} \tilde{\mathbf{Q}} \cdot \tilde{\mathbf{P}}^t] && \text{in } \mathcal{C}_0.\end{aligned}\tag{B.1}$$

$$\begin{aligned}\text{Div}(R \mathbf{Q}) &= R \text{Div} \mathbf{Q} + \mathbf{Q} \cdot \text{Grad} R && \text{in } \mathcal{B}_0, \\ \widehat{\text{Div}}(\hat{R} \hat{\mathbf{Q}}) &= \hat{R} \widehat{\text{Div}} \hat{\mathbf{Q}} + \hat{\mathbf{Q}} \cdot \widehat{\text{Grad}} \hat{R} && \text{in } \mathcal{S}_0, \\ \overline{\text{Div}}(\bar{R} \bar{\mathbf{Q}}) &= \bar{R} \overline{\text{Div}} \bar{\mathbf{Q}} + \bar{\mathbf{Q}} \cdot \overline{\text{Grad}} \bar{R} && \text{in } \mathcal{S}_0, \\ \widetilde{\text{Div}}(\tilde{R} \tilde{\mathbf{Q}}) &= \tilde{R} \widetilde{\text{Div}} \tilde{\mathbf{Q}} + \tilde{\mathbf{Q}} \cdot \widetilde{\text{Grad}} \tilde{R} && \text{in } \mathcal{C}_0.\end{aligned}\tag{B.2}$$

$$\begin{aligned}
\text{Div}(\mathbf{Q} \cdot \mathbf{P}) &= \mathbf{Q} \cdot \text{Div} \mathbf{P} + \mathbf{P} : \text{Grad} \mathbf{Q} && \text{in } \mathcal{B}_0, \\
\widehat{\text{Div}}(\widehat{\mathbf{Q}} \cdot \widehat{\mathbf{P}}) &= \widehat{\mathbf{Q}} \cdot \widehat{\text{Div}} \widehat{\mathbf{P}} + \widehat{\mathbf{P}} : \widehat{\text{Grad}} \widehat{\mathbf{Q}} && \text{in } \mathcal{S}_0, \\
\overline{\text{Div}}(\overline{\mathbf{Q}} \cdot \overline{\mathbf{P}}) &= \overline{\mathbf{Q}} \cdot \overline{\text{Div}} \overline{\mathbf{P}} + \overline{\mathbf{P}} : \overline{\text{Grad}} \overline{\mathbf{Q}} && \text{in } \mathcal{I}_0, \\
\widetilde{\text{Div}}(\widetilde{\mathbf{Q}} \cdot \widetilde{\mathbf{P}}) &= \widetilde{\mathbf{Q}} \cdot \widetilde{\text{Div}} \widetilde{\mathbf{P}} + \widetilde{\mathbf{P}} : \widetilde{\text{Grad}} \widetilde{\mathbf{Q}} && \text{in } \mathcal{C}_0.
\end{aligned} \tag{B.3}$$

B.2 REFORMULATION OF MECHANICAL POWER IN TERMS OF STRESSES

Invoking the balances of momentum in the various parts of the body (2.25), the expression (2.14) for the mechanical power can be reformulated in terms of the stresses. Using the balances of linear momentum (2.25) to express the various stress measures in terms of their associated bulk, surface, interface and curve forces, denoted $\mathbf{B}^p$, $\widehat{\mathbf{B}}^p$, $\overline{\mathbf{B}}^p$ and $\widetilde{\mathbf{B}}^p$, respectively, the global working (2.14) becomes:

$$\begin{aligned}
\mathcal{W}_0 &= \int_{\mathcal{B}_0} \mathbf{V} \cdot [-\text{Div} \mathbf{P}] \, dV + \int_{\mathcal{S}_0^{\text{ext}}} \widehat{\mathbf{V}} \cdot [-\widehat{\text{Div}} \widehat{\mathbf{P}} + \mathbf{P} \cdot \mathbf{N}] \, dA \\
&+ \int_{\mathcal{I}_0} \overline{\mathbf{V}} \cdot [-\overline{\text{Div}} \overline{\mathbf{P}} - \llbracket \mathbf{P} \rrbracket \cdot \overline{\mathbf{N}}] \, dA + \int_{\mathcal{C}_0^{\text{ext}}} \widetilde{\mathbf{V}} \cdot [-\widetilde{\text{Div}} \widetilde{\mathbf{P}} + \overline{\mathbf{P}} \cdot \widetilde{\mathbf{N}}_i - \llbracket \widehat{\mathbf{P}} \rrbracket \cdot \widetilde{\mathbf{N}}_s] \, dL \\
&+ \int_{\mathcal{S}_0^{\text{int}}} \mathbf{V} \cdot [\mathbf{P} \cdot \mathbf{M}] \, dA + \int_{\mathcal{L}_0} \widehat{\mathbf{V}} \cdot [\widehat{\mathbf{P}} \cdot \widehat{\mathbf{N}}] \, dL \\
&+ \int_{\mathcal{C}_0^{\text{int}}} \overline{\mathbf{V}} \cdot [\overline{\mathbf{P}} \cdot \overline{\mathbf{M}}] \, dL + \sum_{\partial \mathcal{C}_0^{\text{ext}}} \widetilde{\mathbf{V}} \cdot [\widetilde{\mathbf{P}} \cdot \widetilde{\mathbf{N}}] \, dL.
\end{aligned}$$

It follows from the definition of the control regions, given in Section 2.1.3, that

$$\begin{aligned}
\int_{\mathcal{S}_0^{\text{int}}} \{\bullet\} \, dA &= \int_{\partial \mathcal{B}_0} \{\bullet\} \, dA - \int_{\mathcal{S}_0^{\text{ext}}} \{\bullet\} \, dA, \\
\int_{\mathcal{C}_0^{\text{int}}} \{\bullet\} \, dL &= \int_{\partial \mathcal{I}_0} \{\bullet\} \, dL - \int_{\mathcal{C}_0^{\text{ext}}} \{\bullet\} \, dL.
\end{aligned}$$

Furthermore, the outward normal to $\partial \mathcal{B}_0$ on the surface is the same as the outward normal to the surface, i.e. $\mathbf{M}|_{\mathcal{S}_0^{\text{ext}}} = \mathbf{N}$. In an identical fashion to the surface $\overline{\mathbf{M}}|_{\mathcal{C}_0^{\text{ext}}} = \widetilde{\mathbf{N}}_i$. Due to kinematic slavery on the surface $\mathbf{V}|_{\mathcal{S}_0^{\text{ext}}} = \widehat{\mathbf{V}}$ and $\overline{\mathbf{V}}|_{\mathcal{C}_0^{\text{ext}}} = \widetilde{\mathbf{V}}$. From these observations, the following two terms in the global working can be restated as follows:

$$\begin{aligned}
\int_{\mathcal{S}_0^{\text{int}}} \mathbf{V} \cdot [\mathbf{P} \cdot \mathbf{M}] \, dA &= \int_{\partial \mathcal{B}_0} \mathbf{V} \cdot [\mathbf{P} \cdot \mathbf{M}] \, dA - \int_{\mathcal{S}_0^{\text{ext}}} \widehat{\mathbf{V}} \cdot [\mathbf{P} \cdot \mathbf{N}] \, dA, \\
\int_{\mathcal{L}_0} \widehat{\mathbf{V}} \cdot [\widehat{\mathbf{P}} \cdot \widehat{\mathbf{N}}] \, dL &= \int_{\partial \mathcal{I}_0} \overline{\mathbf{V}} \cdot [\overline{\mathbf{P}} \cdot \overline{\mathbf{M}}] \, dL - \int_{\mathcal{C}_0^{\text{ext}}} \widetilde{\mathbf{V}} \cdot [\overline{\mathbf{P}} \cdot \widetilde{\mathbf{N}}_i] \, dL.
\end{aligned}$$

Thus, the global working becomes

$$\begin{aligned} \mathcal{W}_0 = & \int_{B_0} \mathbf{V} \cdot [-\text{Div} \mathbf{P}] \, dV + \int_{S_0^{\text{ext}}} \widehat{\mathbf{V}} \cdot [-\widehat{\text{Div}} \widehat{\mathbf{P}}] \, dA \\ & + \int_{I_0} \overline{\mathbf{V}} \cdot [-\overline{\text{Div}} \overline{\mathbf{P}} - \llbracket \mathbf{P} \rrbracket \cdot \overline{\mathbf{N}}] \, dA + \int_{C_0^{\text{ext}}} \widetilde{\mathbf{V}} \cdot [-\widetilde{\text{Div}} \widetilde{\mathbf{P}} - \llbracket \widehat{\mathbf{P}} \rrbracket \cdot \widetilde{\mathbf{N}}_s] \, dL \\ & + \int_{\partial B_0} \mathbf{V} \cdot [\mathbf{P} \cdot \mathbf{M}] \, dA + \int_{\partial I_0} \overline{\mathbf{V}} \cdot [\overline{\mathbf{P}} \cdot \overline{\mathbf{M}}] \, dL \\ & + \int_{\mathcal{L}_0} \widehat{\mathbf{V}} \cdot [\widehat{\mathbf{P}} \cdot \widehat{\mathbf{N}}] \, dL + \sum_{\partial C_0^{\text{ext}}} \widetilde{\mathbf{V}} \cdot [\widetilde{\mathbf{P}} \cdot \widetilde{\mathbf{N}}] \, , \end{aligned}$$

and using the identities (B.3) yields

$$\begin{aligned} = & \int_{B_0} \mathbf{P} : \text{Grad} \mathbf{V} \, dV - \int_{B_0} \text{Div} (\mathbf{V} \cdot \mathbf{P}) \, dV + \int_{S_0^{\text{ext}}} \widehat{\mathbf{P}} : \widehat{\text{Grad}} \widehat{\mathbf{V}} \, dA \\ & - \int_{S_0^{\text{ext}}} \widehat{\text{Div}} (\widehat{\mathbf{V}} \cdot \widehat{\mathbf{P}}) \, dA + \int_{I_0} \overline{\mathbf{P}} : \overline{\text{Grad}} \overline{\mathbf{V}} \, dA - \int_{I_0} \overline{\text{Div}} (\overline{\mathbf{V}} \cdot \overline{\mathbf{P}}) \, dA \\ & - \int_{I_0} \overline{\mathbf{V}} \cdot \llbracket \mathbf{P} \rrbracket \cdot \overline{\mathbf{N}} \, dA + \int_{C_0^{\text{ext}}} \widetilde{\mathbf{P}} : \widetilde{\text{Grad}} \widetilde{\mathbf{V}} \, dL - \int_{C_0^{\text{ext}}} \widetilde{\text{Div}} (\widetilde{\mathbf{V}} \cdot \widetilde{\mathbf{P}}) \, dL \\ & - \int_{C_0^{\text{ext}}} \widetilde{\mathbf{V}} \cdot \llbracket \widehat{\mathbf{P}} \rrbracket \cdot \widetilde{\mathbf{N}}_s \, dL + \int_{\partial B_0} \mathbf{V} \cdot \mathbf{P} \cdot \mathbf{M} \, dA + \int_{\partial I_0} \overline{\mathbf{V}} \cdot \overline{\mathbf{P}} \cdot \overline{\mathbf{M}} \, dL \\ & + \int_{\mathcal{L}_0} \widehat{\mathbf{V}} \cdot \widehat{\mathbf{P}} \cdot \widehat{\mathbf{N}} \, dL + \sum_{\partial C_0^{\text{ext}}} \widetilde{\mathbf{V}} \cdot \widetilde{\mathbf{P}} \cdot \widetilde{\mathbf{N}} \, , \end{aligned}$$

and finally, using the extended divergence theorems for the various parts of the body (2.4)–(2.7) gives

$$\begin{aligned} = & \int_{B_0} \mathbf{P} : \text{Grad} \mathbf{V} \, dV + \int_{S_0^{\text{ext}}} \widehat{\mathbf{P}} : \widehat{\text{Grad}} \widehat{\mathbf{V}} \, dA + \int_{I_0} \overline{\mathbf{P}} : \overline{\text{Grad}} \overline{\mathbf{V}} \, dA + \int_{C_0^{\text{ext}}} \widetilde{\mathbf{P}} : \widetilde{\text{Grad}} \widetilde{\mathbf{V}} \, dL \\ & - \int_{\partial B_0} \mathbf{V} \cdot \mathbf{P} \cdot \mathbf{M} \, dA + \int_{I_0} \llbracket \mathbf{V} \cdot \mathbf{P} \rrbracket \cdot \overline{\mathbf{N}} \, dA - \int_{\mathcal{L}_0} \widehat{\mathbf{V}} \cdot \widehat{\mathbf{P}} \cdot \widehat{\mathbf{N}} \, dL + \int_{S_0^{\text{ext}}} \widehat{\mathbf{C}} \widehat{\mathbf{V}} \cdot \widehat{\mathbf{P}} \cdot \mathbf{N} \, dA \\ & + \int_{C_0^{\text{ext}}} \llbracket \widehat{\mathbf{V}} \cdot \widehat{\mathbf{P}} \rrbracket \cdot \widetilde{\mathbf{N}}_s \, dL - \int_{\partial I_0} \overline{\mathbf{V}} \cdot \overline{\mathbf{P}} \cdot \overline{\mathbf{M}} \, dL + \int_{I_0} \overline{\mathbf{C}} \overline{\mathbf{V}} \cdot \overline{\mathbf{P}} \cdot \overline{\mathbf{N}} \, dA - \sum_{\partial C_0^{\text{ext}}} \widetilde{\mathbf{V}} \cdot \widetilde{\mathbf{P}} \cdot \widetilde{\mathbf{N}} \\ & + \int_{C_0^{\text{ext}}} \widetilde{\mathbf{C}} \widetilde{\mathbf{V}} \cdot \widetilde{\mathbf{P}} \cdot \widetilde{\mathbf{N}}_c \, dL - \int_{I_0} \overline{\mathbf{V}} \cdot \llbracket \mathbf{P} \rrbracket \cdot \overline{\mathbf{N}} \, dA - \int_{C_0^{\text{ext}}} \widetilde{\mathbf{V}} \cdot \llbracket \widehat{\mathbf{P}} \rrbracket \cdot \widetilde{\mathbf{N}}_s \, dL \\ & + \int_{\partial B_0} \mathbf{V} \cdot \mathbf{P} \cdot \mathbf{M} \, dA + \int_{\partial I_0} \overline{\mathbf{V}} \cdot \overline{\mathbf{P}} \cdot \overline{\mathbf{M}} \, dL + \int_{\mathcal{L}_0} \widehat{\mathbf{V}} \cdot \widehat{\mathbf{P}} \cdot \widehat{\mathbf{N}} \, dL + \sum_{\partial C_0^{\text{ext}}} \widetilde{\mathbf{V}} \cdot \widetilde{\mathbf{P}} \cdot \widetilde{\mathbf{N}} \, , \end{aligned}$$

which simplifies to

$$\begin{aligned} \mathcal{W}_0 = & \int_{B_0} \mathbf{P} : \text{Grad} \mathbf{V} \, dV + \int_{S_0^{\text{ext}}} \widehat{\mathbf{P}} : \widehat{\text{Grad}} \widehat{\mathbf{V}} \, dA + \int_{I_0} \overline{\mathbf{P}} : \overline{\text{Grad}} \overline{\mathbf{V}} \, dA \\ & + \int_{C_0^{\text{ext}}} \widetilde{\mathbf{P}} : \widetilde{\text{Grad}} \widetilde{\mathbf{V}} \, dL + \int_{I_0} [\mathbf{V} \cdot \mathbf{P}] \cdot \overline{\mathbf{N}} \, dA + \int_{C_0^{\text{ext}}} [\widehat{\mathbf{V}} \cdot \widehat{\mathbf{P}}] \cdot \widetilde{\mathbf{N}}_s \, dL \\ & - \int_{I_0} \overline{\mathbf{V}} \cdot [\mathbf{P}] \cdot \overline{\mathbf{N}} \, dA - \int_{C_0^{\text{ext}}} \widetilde{\mathbf{V}} \cdot [\widehat{\mathbf{P}}] \cdot \widetilde{\mathbf{N}}_s \, dL. \end{aligned}$$

The interface is assumed to be coherent, thus $[\mathbf{V}] = \mathbf{0}$ and $[\widehat{\mathbf{V}}] = \mathbf{0}$. Therefore, $\overline{\mathbf{V}} \cdot [\mathbf{P}] = [\mathbf{V} \cdot \mathbf{P}]$ and $\widetilde{\mathbf{V}} \cdot [\widehat{\mathbf{P}}] = [\widehat{\mathbf{V}} \cdot \widehat{\mathbf{P}}]$ and the last four terms vanish. What remains is the global working in terms of the stresses

$$\begin{aligned} \mathcal{W}_0 = & \int_{B_0} \mathbf{P} : \text{Grad} \mathbf{V} \, dV + \int_{I_0} \overline{\mathbf{P}} : \overline{\text{Grad}} \overline{\mathbf{V}} \, dA \\ & + \int_{S_0^{\text{ext}}} \widehat{\mathbf{P}} : \widehat{\text{Grad}} \widehat{\mathbf{V}} \, dA + \int_{C_0^{\text{ext}}} \widetilde{\mathbf{P}} : \widetilde{\text{Grad}} \widetilde{\mathbf{V}} \, dL. \end{aligned}$$

B.3 DERIVATION OF THE INTERFACE TEMPERATURE EVOLUTION EQUATION

It is enlightening to review the procedure to obtain the non-standard interface temperature evolution equation (2.59)₃.

The balance of internal energy on the interface (2.30)₃ reads

$$\overline{\mathbf{P}} : \overline{\text{Grad}} \overline{\mathbf{V}} - \overline{\text{Div}} \overline{\mathbf{Q}} + \overline{\mathbf{Q}} = D_t \overline{E} \quad \text{with} \quad \overline{\mathbf{Q}} = \overline{\mathbf{Q}}^p - [\mathbf{Q}] \cdot \overline{\mathbf{N}} \quad \text{on } \mathcal{I}_0.$$

The rate of change of the internal energy on the interface $D_t \overline{E}$ is expanded using the definition of the *Helmholtz* energy (2.39)₃ as follows:

$$D_t \overline{E} = D_t (\overline{\Psi} + \overline{\Theta} \overline{\Xi}),$$

and from the parametrisation of the *Helmholtz* energy given in Eq. (2.41)₃,

$$= \left[\frac{\partial \overline{\Psi}}{\partial \overline{\mathbf{F}}} + \frac{\partial \overline{\Psi}}{\partial \overline{\mathbf{n}}} \cdot \frac{\partial \overline{\mathbf{n}}}{\partial \overline{\mathbf{F}}} \right] : D_t \overline{\mathbf{F}} + \frac{\partial \overline{\Psi}}{\partial \overline{\Theta}} D_t \overline{\Theta} + \overline{\Xi} D_t \overline{\Theta} + \overline{\Theta} D_t \overline{\Xi},$$

and from the constitutive relations (2.42)₃,

$$= \overline{\mathbf{P}} : D_t \overline{\mathbf{F}} + \overline{\Theta} D_t \overline{\Xi}.$$

Inserting this result into balance of energy on the interface (2.30)₃ yields

$$\overline{\mathbf{P}} : \overline{\text{Grad}} \overline{\mathbf{V}} - \overline{\text{Div}} \overline{\mathbf{Q}} + \overline{\mathbf{Q}} = \overline{\mathbf{P}} : D_t \overline{\mathbf{F}} + \overline{\Theta} D_t \overline{\Xi},$$

and recalling that

$$\overline{\text{Grad}} \, \overline{V} = \frac{\partial}{\partial \overline{X}} \left(\overline{V} \right) = \frac{\partial}{\partial \overline{X}} \left(D_t \overline{x} \right) = D_t \left(\frac{\partial \overline{x}}{\partial \overline{X}} \right) = D_t \overline{F},$$

allowing the balance of energy to be expressed as

$$-\overline{\text{Div}} \, \overline{Q} + \overline{Q} = \overline{\Theta} D_t \overline{\Xi}. \quad (\text{B.4})$$

The right-hand side of Eq. (B.4) can be simplified as follows

$$\overline{\Theta} D_t \overline{\Xi} = \overline{\Theta} \frac{\partial \overline{\Xi}}{\partial \overline{\Theta}} D_t \overline{\Theta} + \overline{\Theta} \frac{\partial \overline{\Xi}}{\partial \overline{F}} : D_t \overline{F} + \overline{\Theta} \frac{\partial \overline{\Xi}}{\partial \overline{n}} \cdot D_t \overline{n},$$

and using the constitutive relation $\overline{\Xi} = -\frac{\partial \overline{\Psi}}{\partial \overline{\Theta}}$,

$$\begin{aligned} &= -\overline{\Theta} \frac{\partial^2 \overline{\Psi}}{\partial \overline{\Theta} \partial \overline{\Theta}} D_t \overline{\Theta} - \overline{\Theta} \frac{\partial^2 \overline{\Psi}}{\partial \overline{F} \partial \overline{\Theta}} : D_t \overline{F} + \overline{\Theta} \frac{\partial \overline{\Xi}}{\partial \overline{n}} \cdot \frac{\partial \overline{n}}{\partial \overline{F}} : D_t \overline{n} \\ &= \underbrace{-\overline{\Theta} \frac{\partial^2 \overline{\Psi}}{\partial \overline{\Theta} \partial \overline{\Theta}} D_t \overline{\Theta}}_{\overline{c}_{\overline{F}}} - \underbrace{\overline{\Theta} \frac{\partial}{\partial \overline{\Theta}} \left[\frac{\partial \overline{\Psi}}{\partial \overline{F}} + \frac{\partial \overline{\Psi}}{\partial \overline{n}} \cdot \frac{\partial \overline{n}}{\partial \overline{F}} \right]}_{\overline{P}} : D_t \overline{F}, \end{aligned}$$

where $\overline{c}_{\overline{F}}$ is the interface heat capacity. Finally, inserting this result into Eq. (B.4) gives the equation for the evolution of the interface temperature as in Eq. (2.59)₃.

Bibliography

- [1] P. Pawlow. Über die Abhängigkeit des Schmelzpunktes von der Oberflächenenergie eines festen Körpers. *Z. physik Chemie*, 65:1–35, 1908. [cited at p. 1]
- [2] J. W. Gibbs. *The Scientific Papers of J.W. Gibbs*. Dover Publications, 1961. [cited at p. 1]
- [3] E. A. Guggenheim. The thermodynamics of interfaces in systems of several components. *Trans. Faraday Soc.*, 35:397–412, 1940. [cited at p. 1]
- [4] N. K. Adam. *The Physics and Chemistry of Surfaces*. Oxford University Press, London, 1941. [cited at p. 1, 2]
- [5] R. Shuttleworth. The surface tension of solids. *Proceedings of the Physical Society. Section A*, 63(5):444–457, 1950. [cited at p. 1, 2]
- [6] C. Herring. Some theorems on the free energies of crystal surfaces. *Physical Review*, 82(1):87–93, 1951. [cited at p. 1]
- [7] J. J. Bikerman. Surface energy of solids. *physica status solidi (b)*, 10(1):3–26, 1965. [cited at p. 1]
- [8] E. Orowan. Surface energy and surface tension in solids and liquids. *Proceedings of the Royal Society A*, 316(1527):473–491, 1970. [cited at p. 1]
- [9] J. W. Cahn. Thermodynamics of solid and fluid surfaces, segregation to interfaces. *Segregation to Interfaces, ASM Seminar Series*, pages 3–23, 1978. [cited at p. 1]
- [10] J. W. Cahn. Interfacial free energy and interfacial stress: The case of an internal interface in a solid. *Acta Metallurgica*, 37(3):773–776, 1989. [cited at p. 1]

- [11] L. E. Murr. *Interfacial Phenomena in Metals and Alloys*. Addison Wesley, 1975. [cited at p. 2]
- [12] C. Rottman. Landau theory of coherent interphase interfaces. *Phys. Rev. B*, 38:12031–34, 1988. [cited at p. 2]
- [13] A. W. Adamson. *Physical Chemistry of Surfaces*. John Wiley & Sons, 1990. [cited at p. 2]
- [14] J. M. Howe. *Interfaces in Materials*. John Wiley & Sons, 1997. [cited at p. 2]
- [15] V. A. Marichev. General thermodynamic equations for the surface tension of liquids and solids. *Surface Science*, 604(3–4):458–463, 2010. [cited at p. 2]
- [16] A. I. Rusanov. Surface thermodynamics revisited. *Surface Science Reports*, 58:11–239, 2005. [cited at p. 2]
- [17] A. I. Rusanov. Thermodynamics of solid surfaces. *Surface Science Reports*, 23:173–247, 1996. [cited at p. 2]
- [18] P. Müller and A. Saul. Elastic effects on surface physics. *Surface Science Reports*, 54(5–8):157–258, 2004. [cited at p. 2]
- [19] H. Ibach. The role of surface stress in reconstruction, epitaxial growth and stabilization of mesoscopic structures. *Surface Science Reports*, 29(5–6):195–263, 1997. [cited at p. 2]
- [20] P. H. Leo and R. F. Sekerka. Overview no. 86: The effect of surface stress on crystal-melt and crystal-crystal equilibrium. *Acta Metallurgica*, 37(12):3119–3138, 1989. [cited at p. 2]
- [21] R. C. Cammarata. Surface and interface stress effects on interfacial and nanostructured materials. *Materials Science and Engineering: A*, 237(2):180–184, 1997. [cited at p. 2]
- [22] R. C. Cammarata. Surface and interface stress effects in thin films. *Progress in Surface Science*, 46(1):1–38, 1994. [cited at p. 2]
- [23] R. C. Cammarata, K. Sieradzki, and F. Spaepen. Simple model for interface stresses with application to misfit dislocation generation in epitaxial thin films. *Journal of Applied Physics*, 87(3):1227–1234, 2000. [cited at p. 2]
- [24] R. C. Cammarata. Generalized thermodynamics of surfaces with applications to small solid systems. *Solid State Physics*, 61:1–75, 2009. [cited at p. 2]

- [25] F. D. Fischer, T. Waitz, D. Vollath, and N. K. Simha. On the role of surface energy and surface stress in phase-transforming nanoparticles. *Progress in Materials Science*, 53(3):481–527, 2008. [cited at p. 2, 52]
- [26] E. M. Gutman. On the thermodynamic definition of surface stress. *Journal of Physics: Condensed Matter*, 7(48):L663–L667, 1995. [cited at p. 2, 52]
- [27] D. J. Bottomley and T. Ogino. Alternative to the Shuttleworth formulation of solid surface stress. *Phys. Rev. B*, 63:165412, 2001. [cited at p. 2]
- [28] V. A. Marichev. Structure-mechanical approach to surface tension of solids. *Surface Science*, 600(19):4527–4536, 2006. [cited at p. 2]
- [29] D. Kramer and J. Weissmüller. A note on surface stress and surface tension and their interrelation via Shuttleworth’s equation and the Lippmann equation. *Surface Science*, 601(14):3042–3051, 2007. [cited at p. 2, 52]
- [30] G. A. Maugin. *Configurational Forces: Thermomechanics, Physics, Mathematics, and Numerics*. CRC Press, 2010. [cited at p. 2, 29, 90]
- [31] P. Steinmann, A. McBride, S. Bargmann, and A. Javili. A deformational and configurational framework for geometrically non-linear continuum thermomechanics coupled to diffusion. *International Journal of Non-Linear Mechanics*, 47(2):215–227, 2012. [cited at p. 2, 6, 90]
- [32] M. E. Gurtin and A. Ian Murdoch. A continuum theory of elastic material surfaces. *Archive for Rational Mechanics and Analysis*, 57(4):291–323, 1975. [cited at p. 2, 52, 57, 90]
- [33] M. E. Gurtin and A. Ian Murdoch. Surface stress in solids. *International Journal of Solids and Structures*, 14(6):43–440, 1978. [cited at p. 2]
- [34] R. Dingreville and J. Qu. Surface free energy and its effect on the elastic behavior of nano-sized particles, wires and films. *Journal of the Mechanics and Physics of Solids*, 53(8):1827–1854, 2005. [cited at p. 2]
- [35] J. He and C. M. Lilley. Surface effect on the elastic behavior of static bending nanowires. *Nano Letters*, 8(7):1798–1802, 2008. [cited at p. 2]
- [36] H. L. Duan, J. Wang, and B. L. Karihaloo. Theory of elasticity at the nanoscale. *Advances in Applied Mechanics*, 42:1–68, 2009. [cited at p. 2]

- [37] A. Ian Murdoch. A thermodynamical theory of elastic material interfaces. *The Quarterly Journal of Mechanics and Applied Mathematics*, 29(3):245–275, 1976. [cited at p. 2]
- [38] M. E. Gurtin and A. Struthers. Multiphase thermomechanics with interfacial structure 3. Evolving phase boundaries in the presence of bulk deformation. *Archive for Rational Mechanics and Analysis*, 112(2):97–160, 1990. [cited at p. 2, 10]
- [39] M. E. Gurtin, J. Weissmüller, and F. Larché. A general theory of curved deformable interfaces in solids at equilibrium. *Philosophical Magazine A*, 78(5):1093–1109, 1998. [cited at p. 2]
- [40] D. J. Steigmann and R. W. Ogden. Elastic surface-substrate interactions. *Proceedings of the Royal Society A*, 455(1982):437–474, 1999. [cited at p. 2, 90]
- [41] M. E. E. Gurtin and M. E. Jabbour. Interface evolution in three dimensions with curvature-dependent energy and surface diffusion: Interface-controlled evolution, phase transitions, epitaxial growth of elastic films. *Archive for Rational Mechanics and Analysis*, 163:171–208, 2002. [cited at p. 2, 90]
- [42] E. Fried and R. Todres. Mind the gap: The shape of the free surface of a rubber-like material in proximity to a rigid contactor. *Journal of Elasticity*, 80:97–151, 2005. [cited at p. 2, 90]
- [43] P. Chhapadia, P. Mohammadi, and P. Sharma. Curvature-dependent surface energy and implications for nanostructures. *Journal of the Mechanics and Physics of Solids*, 59(10):2103–2115, October 2011. [cited at p. 2, 90]
- [44] G. P. Moeckel. Thermodynamics of an interface. *Archive for Rational Mechanics and Analysis*, 57:255–280, 1975. [cited at p. 2, 10]
- [45] F. dell’Isola and A. Romano. On the derivation of thermomechanical balance equations for continuous systems with a nonmaterial interface. *International Journal of Engineering Science*, 25(11–12):1459–1468, 1987. [cited at p. 2]
- [46] I. Müller. Entropy, absolute temperature, and coldness in thermodynamics. In *Courses and lectures - International Centre for Mechanical Sciences*. Springer, Vienna, New York, 1971. [cited at p. 2]
- [47] V. V. Gogosov, V. A. Naletova, C. Z. Bin, and G. A. Shaposhnikova. Conservation laws for the mass, momentum, and energy on a phase interface for true and excess surface parameters. *Fluid Dynamics*, 18:923–930, 1983. [cited at p. 2]

- [48] N. Daher and G. A. Maugin. The method of virtual power in continuum mechanics application to media presenting singular surfaces and interfaces. *Acta Mechanica*, 60 (3-4):217–240, 1986. [cited at p. 2, 3, 10, 34, 35]
- [49] P. Germain. The method of virtual power in continuum mechanics. part 2: Microstructure. *SIAM J. Appl. Math.*, 25:556–575, 1973. [cited at p. 2]
- [50] G. A. Maugin. The method of virtual power in continuum mechanics: Application to coupled fields. *Acta Mechanica*, 35:1–70, 1980. [cited at p. 2]
- [51] N. Daher and G. A. Maugin. Deformable semiconductors with interfaces: Basic continuum equations. *International Journal of Engineering Science*, 25(9):1093–1129, 1987. [cited at p. 2]
- [52] N. Daher and G. A. Maugin. Virtual power and thermodynamics for electromagnetic continua with interfaces. *J. Math. Phys.*, 27:3022, 1986. [cited at p. 2]
- [53] A. Ian Murdoch. Some fundamental aspects of surface modelling. *Journal of Elasticity*, 80(1):33–52, 2005. [cited at p. 2]
- [54] M. Šilhavý. Equilibrium of phases with interfacial energy: A variational approach. *Journal of Elasticity*, 105:271–303, 2011. [cited at p. 2]
- [55] H. S. Park, P. A. Klein, and G. J. Wagner. A surface Cauchy-Born model for nanoscale materials. *International Journal for Numerical Methods in Engineering*, 68(10):1072–1095, 2006. [cited at p. 3]
- [56] H. S. Park and P. A. Klein. A Surface Cauchy-Born model for silicon nanostructures. *Computer Methods in Applied Mechanics and Engineering*, 197(41-42):3249–3260, 2008. [cited at p. 3]
- [57] H. S. Park and P. A. Klein. Surface Cauchy-Born analysis of surface stress effects on metallic nanowires. *Physical Review B*, 75(8):1–9, 2007. [cited at p. 3, 52]
- [58] H. S. Park, W. Cai, and H. D. Espinosa. Mechanics of crystalline nanowires. *MRS bulletin*, 34(3):178–183, 2009. [cited at p. 3]
- [59] P. Sharma, S. Ganti, and N. Bhate. Effect of surfaces on the size-dependent elastic state of nano-inhomogeneities. *Applied Physics Letters*, 82(4):535–537, 2003. [cited at p. 3, 59]
- [60] P. Sharma and S. Ganti. Size-dependent Eshelby’s tensor for embedded nano-inclusions incorporating surface/interface energies. *Journal of Applied Mechanics*, 71: 663–671, 2004. [cited at p. 3]

- [61] P. Sharma and L. T. Wheeler. Size-dependent elastic state of ellipsoidal nano-inclusions incorporating surface/interface tension. *Journal of Applied Mechanics*, 74(3):447–454, 2007. [cited at p. 3]
- [62] J. D. Eshelby. The force on an elastic singularity. *Philosophical Transactions of the Royal Society of London. Series A*, 244(877):87, 1951. [cited at p. 3]
- [63] J. D. Eshelby. The determination of the elastic field of an ellipsoidal inclusion, and related problems. *Proceedings of the Royal Society A*, 241(1226):376–396, 1957. [cited at p. 3]
- [64] H. L. Duan, J. Wang, Z. P. Huang, and B. L. Karihalo. Eshelby formalism for nano-inhomogeneities. *Proceedings of the Royal Society A*, 461(2062):3335–3353, 2005. [cited at p. 3]
- [65] H. L. Duan, J. Wang, Z. P. Huang, and B. L. Karihaloo. Size-dependent effective elastic constants of solids containing nano-inhomogeneities with interface stress. *Journal of the Mechanics and Physics of Solids*, 53(7):1574–1596, 2005. [cited at p. 3]
- [66] H. L. Duan and B. L. Karihaloo. Effective thermal conductivities of heterogeneous media containing multiple imperfectly bonded inclusions. *Physical Review B*, 75:064206, 2007. [cited at p. 3]
- [67] Y. Benveniste and T. Miloh. Imperfect soft and stiff interfaces in two-dimensional elasticity. *Mechanics of Materials*, 33(6):309–323, 2001. [cited at p. 3]
- [68] Z. Huang and L. Sun. Size-dependent effective properties of a heterogeneous material with interface energy effect: from finite deformation theory to infinitesimal strain analysis. *Acta Mechanica*, 190:151–163, 2007. [cited at p. 3]
- [69] F. D. Fischer and J. Svoboda. Stresses in hollow nanoparticles. *International Journal of Solids and Structures*, 47(20):2799–2805, 2010. [cited at p. 3]
- [70] A. M. Zöllner, A. Buganza Tepole, and E. Kuhl. On the biomechanics and mechanobiology of growing skin. *Journal of Theoretical Biology*, 297:166–175, 2012. [cited at p. 3]
- [71] C. Q. Sun. Thermo-mechanical behavior of low-dimensional systems: The local bond average approach. *Progress in Materials Science*, 54(2):179–307, 2009. [cited at p. 3]
- [72] W. C. Johnson. Superficial stress and strain at coherent interfaces. *Acta Materialia*, 48(2):433–444, 2000. [cited at p. 3]

- [73] J. Yvonnet, A. Mitrushchenkov, G. Chambaudand, and Q.-C. He. Finite element model of ionic nanowires with size-dependent mechanical properties determined by ab initio calculations. *Computer Methods in Applied Mechanics and Engineering*, 200:614–625, 2011. [cited at p. 3, 90]
- [74] A. McBride, A. Javili, P. Steinmann, and S. Bargmann. Geometrically nonlinear continuum thermomechanics with surface energies coupled to diffusion. *Journal of the Mechanics and Physics of Solids*, 59(10):2116–2133, 2011. [cited at p. 3, 6, 34, 90]
- [75] P. Cermelli, E. Fried, and M. E. Gurtin. Transport relations for surface integrals arising in the formulation of balance laws for evolving fluid interfaces. *Journal of Fluid Mechanics*, 544:339, 2005. [cited at p. 3]
- [76] I. Özdemir, W. A. M. Brekelmans, and M. G. D. Geers. A Thermo-mechanical cohesive zone model. *Computational Mechanics*, 46(5):735–745, 2010. [cited at p. 4]
- [77] Y. Benveniste. A general interface model for a three-dimensional curved thin anisotropic interphase between two anisotropic media. *Journal of the Mechanics and Physics of Solids*, 54(4):708–734, 2006. [cited at p. 4]
- [78] H. Le-Quang, G. Bonnet, and Q.-C. He. Size-dependent Eshelby tensor fields and effective conductivity of composites made of anisotropic phases with highly conducting imperfect interfaces. *Physical Review B*, 81(6):1–15, 2010. [cited at p. 4]
- [79] S. T. Gu and Q.-C. He. Interfacial discontinuity relations for coupled multifield phenomena and their application to the modeling of thin interphases as imperfect interfaces. *Journal of the Mechanics and Physics of Solids*, 59(7):1413–1426, 2011. [cited at p. 4]
- [80] P. L. Kapitza. The study of heat transfer in helium ii. *J. Phys. (USSR)*, 4:181–210, 1941. [cited at p. 4]
- [81] J. Yvonnet, Q.-C. He, Q.-Z. Zhu, and J.-F. Shao. A general and efficient computational procedure for modelling the Kapitza thermal resistance based on XFEM. *Computational Materials Science*, 50(4):1220–1224, 2011. [cited at p. 4, 5, 41, 42, 49, 86]
- [82] J. Yvonnet, Q.-C. He, and C. Toulemonde. Numerical modelling of the effective conductivities of composites with arbitrarily shaped inclusions and highly conducting interface. *Composites Science and Technology*, 68(13):2818–2825, 2008. [cited at p. 4, 5, 41, 42]

- [83] T. Miloh and Y. Benveniste. On the effective conductivity of composites with ellipsoidal inhomogeneities and highly conducting interfaces. *Proceedings of the Royal Society A*, 455(1987):2687–2706, 1999. [cited at p. 4]
- [84] A. Javili, A. McBride, and P. Steinmann. Numerical modelling of thermomechanical solids with highly-conductive energetic interfaces. *International Journal For Numerical Methods In Engineering*, 2012. doi: 10.1002/nme.4402. [cited at p. 4, 6, 41, 43]
- [85] J. Mosler and I. Scheider. A thermodynamically and variationally consistent class of damage-type cohesive models. *Journal of the Mechanics and Physics of Solids*, 59(8): 1647–1668, 2011. [cited at p. 4]
- [86] P. Steinmann and O. Häsner. On material interfaces in thermomechanical solids. *Archive of Applied Mechanics*, 75(1):31–41, 2005. [cited at p. 4, 14]
- [87] P. Steinmann. On boundary potential energies in deformational and configurational mechanics. *Journal of the Mechanics and Physics of Solids*, 56(3):772–800, 2008. [cited at p. 4, 10, 93]
- [88] A. Javili and P. Steinmann. A finite element framework for continua with boundary energies. Part I: The two-dimensional case. *Computer Methods in Applied Mechanics and Engineering*, 198(27-29):2198–2208, 2009. [cited at p. 4, 6]
- [89] A. Javili and P. Steinmann. A finite element framework for continua with boundary energies. Part II: The three-dimensional case. *Computer Methods in Applied Mechanics and Engineering*, 199(9-12):755–765, 2010. [cited at p. 4, 6]
- [90] A. Javili and P. Steinmann. On thermomechanical solids with boundary structures. *International Journal of Solids and Structures*, 47(24):3245–3253, 2010. [cited at p. 4, 6, 21, 59]
- [91] A. Javili and P. Steinmann. A finite element framework for continua with boundary energies. Part III: The thermomechanical case. *Computer Methods in Applied Mechanics and Engineering*, 200(21-22):1963–1977, 2011. [cited at p. 4, 6, 41, 42]
- [92] J. Gough. A description of a property of caoutchouc on indian rubber; with some reflections on the case of the elasticity of this substance. *Memoirs of the Literary and Philosophical Society of Manchester*, 1:288–295, 1805. [cited at p. 5, 61]
- [93] J. P. Joule. On some thermo-dynamic properties of solids. *Philosophical Transactions of the Royal Society A*, 149:91–131, 1859. [cited at p. 5, 61]

- [94] A. Javili, A. McBride, and P. Steinmann. Thermomechanics of solids with lower-dimensional energetics: On the importance of surface, interface and curve structures at the nanoscale. a unifying review. (*in print*), 2012. [cited at p. 6]
- [95] A. Javili, A. McBride, and P. Steinmann. Numerical modelling of thermomechanical solids with mechanically energetic (generalised) kapitza interfaces. *Computational Materials Science*, 65:542–551, 2012. [cited at p. 6, 41, 43]
- [96] A. Javili, A. McBride, P. Steinmann, and B. D. Reddy. Relationships between the admissible range of surface material parameters and stability of linearly elastic bodies. *Philosophical Magazine*, 92:3540–3563, 2012. [cited at p. 6, 59]
- [97] A. Javili, A. McBride, P. Steinmann, J. Mergheim, and U. Schmidt. Micro-to-macro transitions for continua with surface structure at the microscale. (*in review*), 2012. [cited at p. 6, 91]
- [98] A. McBride, J. Mergheim, A. Javili, P. Steinmann, and S. Bargmann. Micro-to-macro transitions for heterogeneous material layers accounting for in-plane stretch. *Journal of the Mechanics and Physics of Solids*, 60(6):1221–1239, 2012. [cited at p. 6, 91]
- [99] J. E. Marsden and T. J. R. Hughes. *Mathematical Foundations of Elasticity*. Dover Publications, 1994. [cited at p. 9, 18]
- [100] M. Šilhavý. *The Mechanics and Thermodynamics of Continuous Media*. Springer, 1997. [cited at p. 9]
- [101] C. Truesdell and W. Noll. *The Non-Linear Field Theories of Mechanics*. Springer, 2004. [cited at p. -]
- [102] M. E. Gurtin, E. Fried, and L. Anand. *The Mechanics and Thermodynamics of Continua*. Cambridge University Press, 2009. [cited at p. 9]
- [103] G. A. Holzapfel. *Nonlinear Solid Mechanics: A Continuum Approach for Engineering*. John Wiley & Sons, 2000. [cited at p. 9]
- [104] J. Besson, G. Cailletaud, J. L. Chaboche, and S. Forest. *Non-Linear Mechanics of Materials*. Springer, 2010. [cited at p. 9]
- [105] R. M. Bowen and C. C. Wang. *Introduction to Vectors and Tensors: Linear and Multilinear Algebra*. Plenum Press, 1976. [cited at p. 10, 93]
- [106] E. Kreyszig. *Differential Geometry*. Dover Publications, 1991. [cited at p. 10, 93]

- [107] P. G. Ciarlet. *An Introduction to Differential Geometry with Applications to Elasticity*. Springer, 2005. [cited at p. 10, 93]
- [108] L. P. Eisenhart. *An Introduction to Differential Geometry: with Use of the Tensor Calculus*. Oxford University Press, 1940. [cited at p. 10, 93]
- [109] S. Lang. *Fundamentals of Differential Geometry*. Springer, 1927. [cited at p. 10, 93]
- [110] M. P. Do Carmo. *Differential Geometry of Curves and Surfaces*. Prentice-Hall, Inc., 1976. [cited at p. 10, 93]
- [111] M. E. Gurtin. *Configurational Forces as Basic Concepts of Continuum Physics*. Springer, 2000. [cited at p. 15, 32]
- [112] A. C. Eringen. *Mechanics of Continua*. Wiley, 1967. [cited at p. 29]
- [113] K. Hutter. The foundations of thermodynamics, its basic postulates and implications. a review of modern thermodynamics. *Acta Mechanica*, 27:1–54, 1977. [cited at p. 29]
- [114] N. K. Simha and K. Bhattacharya. Kinetics of phase boundaries with edges and junctions in a three-dimensional multi-phase body. *Journal of the Mechanics and Physics of Solids*, 48(12):2619 – 2641, 2000. [cited at p. 32]
- [115] C. Miehe. Entropic thermoelasticity at finite strains. Aspects of the formulation and numerical implementation. *Computer Methods in Applied Mechanics and Engineering*, 120(3-4):243–269, 1995. [cited at p. 41, 42, 43, 61]
- [116] J. T. Oden. *Finite Elements of Nonlinear Continua*. McGraw-Hill Advanced Engineering Series, 1972. [cited at p. 43, 61]
- [117] F. Armero and J. C. Simo. A new unconditionally stable fractional step method for non-linear coupled thermomechanical problems. *International Journal for Numerical Methods in Engineering*, 35(4):737–766, 1992. [cited at p. 43]
- [118] G. A. Holzapfel and J. C. Simo. A new viscoelastic constitutive model for continuous media at finite thermomechanical changes. *International Journal of Solids and Structures*, 33(20-22):3019–3034, 1996. [cited at p. 43]
- [119] E. Kuhl. *Theory and Numerics of Open System Thermodynamics - Spatial and Material Settings*. Universität Kaiserslautern, 2004. [cited at p. 43]
- [120] P. G. Ciarlet. *Mathematical elasticity, Vol. 1*. North-Holland, 1988. [cited at p. 51]

- [121] R. W. Ogden. *Non-Linear Elastic Deformations*. Dover Publications, 1997. [cited at p. 51]
- [122] M. E. Gurtin and A. Ian Murdoch. Addenda to our paper A continuum theory of elastic material surfaces. *Archive for Rational Mechanics and Analysis*, 59(4):1–2, 1975. [cited at p. 52, 57]
- [123] C. Q. Ru. Simple geometrical explanation of Gurtin-Murdoch model of surface elasticity with clarification of its related versions. *Science China*, 2010. [cited at p. 52, 58]
- [124] W. Haiss. Surface stress of clean and adsorbate-covered solids. *Reports on Progress in Physics*, 64(5):591–648, 2001. [cited at p. 52]
- [125] R. Dingreville and J. Qu. A semi-analytical method to compute surface elastic properties. *Acta Materialia*, 55(1):141–147, 2007. [cited at p. 52]
- [126] J. Yvonnet, A. Mitrushchenkov, G. Chambaud, and Q.-C. He. Finite element model of ionic nanowires with size-dependent mechanical properties determined by ab initio calculations. *Computer Methods in Applied Mechanics and Engineering*, 200(5-8): 614–625, 2011. [cited at p. 52]
- [127] L. E. Malvern. *Introduction to the Mechanics of a Continuous Medium*. Prentice Hall, 1969. [cited at p. 54]
- [128] R. E. Miller and V. B. Shenoy. Size-dependent elastic properties of nanosized structural elements. *Nanotechnology*, 11(3):139, 2000. [cited at p. 59]
- [129] G. W. Wei, Y. u. Shouwen, and H. Ganyun. Finite element characterization of the size-dependent mechanical behaviour in nanosystems. *Nanotechnology*, 17(4):1118–1122, 2006. [cited at p. 59]
- [130] R. Hill. A general theory of uniqueness and stability in elastic-plastic solids. *Journal of the Mechanics and Physics of Solids*, 6(3):236–249, 1958. [cited at p. 59]
- [131] H. C. Simpson and S. J. Spector. On failure of the complementing condition and nonuniqueness in linear elastostatics. *Journal of Elasticity*, 15:229–231, 1985. [cited at p. 59]
- [132] A. Benallal, R. Billardon, and G. Geymonat. *Bifurcation and localization in rate-independent materials. Some General Considerations*. In: *Bifurcation and Stability of Dissipative Systems CISM Courses and Lectures*, vol. 327, pages 1–44. Springer, 1993. [cited at p. 59]

- [133] B. D. Reddy. Surface instabilities on an equibiaxially stretched elastic half-space. *Mathematical Proceedings of the Cambridge Philosophical Society*, 91:491–501, 1982. [cited at p. 59]
- [134] B. D. Reddy. The occurrence of surface instabilities and shear bands in plane strain deformation of an elastic half-space. *Quarterly Journal of Mechanics and Applied Mathematics*, 36:337–350, 1983. [cited at p. 59]
- [135] D. Bigoni, M. Ortiz, and A. Needleman. Effect of interfacial compliance on bifurcation of a layer bonded to a substrate. *International Journal of Solids and Structures*, 34(97):4305–4326, 1997. [cited at p. 59]
- [136] W. Han and B. D. Reddy. *Plasticity: Mathematical theory and numerical analysis*. Springer, 1999. [cited at p. 59]
- [137] D. Bigoni and M. Gei. Bifurcations of a coated, elastic cylinder. *International Journal of Solids and Structures*, 38(30-31):5117–5148, 2001. [cited at p. 59]
- [138] D. J. Steigmann. Elastic waves interacting with a thin, prestressed, fiber-reinforced surface film. *International Journal of Engineering Science*, 48(11):1604–1609, 2010. [cited at p. 59]
- [139] D. J. Steigmann. Refined theory for linearly elastic plates: Laminae and laminates. *Mathematics and Mechanics of Solids*, 17(4):351–363, 2011. [cited at p. 59]
- [140] V. B. Shenoy. Atomistic calculations of elastic properties of metallic fcc crystal surfaces. *Physical Review B*, 71(9):1–11, 2005. [cited at p. 60]
- [141] E. Kuhl, R. Denzer, F. J. Barth, and P. Steinmann. Application of the material force method to thermo-hyperelasticity. *Computer Methods in Applied Mechanics and Engineering*, 193(30–32):3303–3325, 2004. [cited at p. 61]
- [142] J. C. Ye, J. Lu, C. T. Liu, Q. Wang, and Y. Yang. Atomistic free-volume zones and inelastic deformation of metallic glasses. *Nature Materials*, 9(8):619–623, 2010. [cited at p. 90]
- [143] I. Müller. On the entropy inequality. *Archive for Rational Mechanics and Analysis*, 26:118–141, 1967. [cited at p. 90]
- [144] S. Forest, N. M. Cordero, and E. P. Busso. First vs. second gradient of strain theory for capillarity effects in an elastic fluid at small length scales. *Computational Materials Science*, 50(4):1299–1304, 2011. [cited at p. 90]

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