Universidad Politécnica de Madrid

**Energy-Entropy-Momentum Time
Integration Methods for Coupled
Smooth Dissipative Problems**

T E S I S D O C T O R A L

**Sergio Conde Martín
Ingeniero Industrial**

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DEPARTAMENTO DE MECÁNICA DE MEDIOS CONTINUOS
Y TEORÍA DE ESTRUCTURAS
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INTEGRATION METHODS FOR COUPLED
SMOOTH DISSIPATIVE PROBLEMS

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SERGIO CONDE MARTÍN
INGENIERO INDUSTRIAL

D I R E C T O R

JUAN CARLOS GARCÍA ORDEN
DOCTOR INGENIERO AERONÁUTICO

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Author: Sergio Conde Martín

Email: sergio.conde@upm.es

Tribunal nombrado por el Mgfco. y Excmo. Sr. Rector de la Universidad Politécnica de Madrid, el día 18 de Diciembre de 2015.

Presidente D.

Vocal D.

Vocal D.

Vocal D.

Secretario D.

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To Vicky and Laura

Abstract

This dissertation is concerned with the formulation, analysis and implementation of structure-preserving time integration methods for the solution of the initial(-boundary) value problems describing the dynamics of smooth dissipative systems, either finite- or infinite-dimensional ones. Such systems are understood as those involving thermo-mechanical coupling and/or internal dissipative effects modeled by internal state variables considered to be smooth in the sense that their evolutions follow continuous laws. The dynamics of such systems are ruled by the laws of thermodynamics and symmetries which constitutes the structure meant to be preserved in the numerical setting.

For that, dissipative systems are geometrically described by metriplectic structures which clearly identify the reversible and irreversible parts of their dynamical evolution. In particular, the framework known by the acronym GENERIC is used to reveal the systems' dissipative structure in the same way as the Hamiltonian is for conserving systems. Given that, energy-preserving, entropy-producing and momentum-preserving (EEM) second-order accurate methods are formulated using the discrete derivative operator that enabled the formulation of Energy-Momentum methods ensuring the preservation of the Hamiltonian and symmetries for conservative systems.

Following these guidelines, two kind of EEM methods are formulated in terms of entropy and temperature as a thermodynamical state variable, involving important implications discussed throughout the dissertation. Remarkably, the formulation in temperature becomes central to accommodate Dirichlet boundary conditions.

EEM methods are finally validated and proved to exhibit enhanced numerical stability and robustness properties compared to standard ones.

Resumen

Esta tesis aborda la formulación, análisis e implementación de métodos numéricos de integración temporal para la solución de sistemas disipativos suaves de dimension finita o infinita de manera que su estructura continua sea conservada. Se entiende por dichos sistemas aquellos que involucran acoplamiento termo-mecánico y/o efectos disipativos internos modelados por variables internas que siguen leyes continuas, de modo que su evolución es considerada suave. La dinámica de estos sistemas está gobernada por las leyes de la termodinámica y simetrías, las cuales constituyen la estructura que se pretende conservar de forma discreta.

Para ello, los sistemas disipativos se describen geoméricamente mediante estructuras metripléticas que identifican claramente las partes reversible e irreversible de la evolución del sistema. Así, usando una de estas estructuras conocida por las siglas (en inglés) de GENERIC, la estructura disipativa de los sistemas es identificada del mismo modo que lo es la Hamiltoniana para sistemas conservativos. Con esto, métodos (EEM) con precisión de segundo orden que conservan la energía, producen entropía y conservan los impulsos lineal y angular son formulados mediante el uso del operador derivada discreta introducido para asegurar la conservación de la Hamiltoniana y las simetrías de sistemas conservativos.

Siguiendo estas directrices, se formulan dos tipos de métodos EEM basados en el uso de la temperatura o de la entropía como variable de estado termodinámica, lo que presenta importantes implicaciones que se discuten a lo largo de esta tesis. Entre las cuales cabe destacar que las condiciones de contorno de Dirichlet son naturalmente impuestas con la formulación basada en la temperatura.

Por último, se validan dichos métodos y se comprueban sus mejores prestaciones en términos de la estabilidad y robustez en comparación con métodos estándar.

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Introduction

CHAPTER 1

The main goal of this dissertation is to provide robust and stable numerical integration methods that make use of all the mathematically rich structure that continuous dissipative systems have so as to provide reliably physical solutions.

1.1 Motivation

The current technological paradigm relies inevitably on computational simulations not only because of their positive impact on both production time and costs but also because of their ability to provide solutions for not even testable real phenomena. In parallel, a crucial factor for the consolidation of this technological paradigm lies at the extraordinary and still in progress increment of computer power, which has enabled the addressing of every more demanding problems.

The simulation of the dynamics of nonlinear mechanic systems often lies at the formulation of numerical methods whose solution, obtained through computational means, provides an discrete approximation of the exact model. The aim of discrete solutions is not only to obtain approximated forces and trajectories, but also to extract qualitative information so that a comprehensive understanding of the dynamical behavior of systems can be achieved. For this reason, numerical methods must not only be numerically accurate but also be reliable in the capture of the main features of the dynamical behavior.

The development of numerical methods of such characteristics for the solution of any type of nonlinear problems has significantly progressed in the last decades. Thus, Hamiltonian systems have attracted most of the attention due to its well-known mathematical (geometric) structure and its importance in different areas of the engineering and physics. The success of such numerical methods, known in the specialized literature as *geometric*, is founded on their efficiency to provide reliable solutions as well as their stability and accuracy for long term simulations, that are outstandingly superior to standards numerical methods.

However, there are still a bunch of appealing problems in industry that are not Hamiltonian, such as those involving any type of dissipative mechanisms: viscous or frictional ones; or those involving thermo effects that modify the mechanic behavior of the systems. These problems will be referred to as *dissipative/non-conserving* problems as opposed to *Hamiltonian/conserving* ones. Provided that these scenarios are very often in materials with industrial interest, developing geometric-like methods for the obtention of reliable simulations has become central. Unfortunately, the mathematical structure of these problems is not thus far as understood as the Hamiltonian one, although recent works have made their way to provide a general understanding of them from an unified perspective, which will doubtlessly contribute to reach these lofty objectives. In this sense, this dissertation is a humble contribution towards that target.

Among the most representative applications in different areas of industry would be:

- **Material engineering.** Simulation of vulcanize rubber materials in any of the situations that can be required in everyday industry: from tires to conveyor belts, marine products, windshield wipers, etc. Not only the simulation of the type of aforementioned materials is of interest but also their analyses can contribute to better understand their physical and mechanical features, thus guiding the search for new materials that outperform them.
 - **Mechanical engineering.** Shock absorbers of both automotive and railway vehicles. Dynamical behavior of machinery whose parts can suffer high gradient of temperatures that modifies the mechanical properties.
 - **Civil engineering.** Shock absorber elements such as the Tune-mass-Damper (TMD) typically used in the construction of bridges and high-rise buildings.
-

- **Aerospace engineering.** Solar panels of aircraft exposed to the direct radiation due to The Sun during their maneuvers.

1.2 Geometric Integration

For the last decades, the formulation of geometric (or structure-preserving) methods have played a major role in the development of numerical methods within the domain of computational mechanics. Monographs, such as Hairer et al. (2006), summarize the large number of recent contribution to the field. The emergence of this sort of formulations has completely changed the way of approaching integration methods. Whereas they were traditionally regarded as mere approximations to continuous problems, they are now also considered as dynamic discrete systems with their own characteristics.

Such methods primarily aim to integrate numerically evolution equations arising from deformable or rigid solid dynamics, in such way that they inherit as many qualitative features as possible from the continuous system. This approach arose in order to obtain more physically accurate solutions, which comply with each inherited feature modeled by the continuous problem. The inherited features range from geometric aspects, symmetries of the equations, to first integrals. A well-known example prior to this approach is the Midpoint method. Even though it was not developed within this context, it preserves symmetries and *symplecticity*, and can therefore be considered as a structure-preserving method.

Initially, nonlinear elastodynamics attracted most of the researchers' interest. Monographs such as Leimkuhler & Reich (2005) show evidence of the maturity of the field. The evolution equations involving nonlinear elastodynamics contain Hamiltonian or Lagrangian structures with suitable properties to define preserving methods. Soon, this suitability enabled the formulation of methods whose solutions successfully preserved (part of) the continuous structure of the evolution equations, obtaining the expected physical accuracy. In addition, structure preserving methods exhibit excellent numerical accuracy and robustness when compared with standard methods. Analyses have shown that these methods are remarkably accurate in long term simulations and allow for the use of larger time steps than traditional implicit methods. Moreover, energy preservation significantly improves stability and robustness, as demonstrated, for example, in Stuart & Humphries (1998). These observations inspired a fast development in different fields, among which the most prominent are rigid body dynamics, nonlinear hyperelasticity, nonlinear structural mechanics and contact.

Chronologically, the first binding ideas relating the energy control to the stability are due to Haug et al. (1977), establishing that, in the nonlinear regime, any integration method is unconditionally stable provided that the energy of the system at any time step is less or equal to the energy at its predecessor one for any time step size. Based on this criteria, the authors therein proposed an energy-bounded integration method which collapses to the Trapezoidal method for linear problems. Similar conclusions were made by Hughes et al. (1978), proposing an unconditionally stable energy-conserving method for nonlinear problems based on a modification of the Trapezoidal method. Later, Simó & Wong (1991) developed a second-order accurate integration method for the solution of the solid rigid dynamics without constraints that preserves both energy and angular momentum and is hence unconditionally stable. Following this work, the so-called Energy-Momentum method was formulated for general Hamiltonian systems with symmetries, particularly, for nonlinear elastodynamics of solids, beams and shells in Simó & González (1993); Simó & Tarnow (1992); Simó et al. (1995, 1992). These works laid the foundation for the formulation of Energy-Momentum methods that, by design, preserve first integrals of Hamiltonian systems: the linear and angular momentum maps and the Hamiltonian of the system. Later, González (1996) systematized the formulation by fully developing the concept of the *discrete derivative operator* or *discrete gradient operator*, which was previously discussed, at least, in Gotusso (1985) (see also Itoh & Abe (1988), McLachlan et al. (1999)). This operator is based on properties that ensure both the preservation of the first integrals and the second order accuracy of the discrete system.

Based on this systematic procedure, other authors proposed energy-momentum methods for particular applications such as N-body systems Betsch & Steinmann (2000, 2001a), mechanical systems with holonomic constraints Betsch & Steinmann (2002) and rigid body with restrictions Betsch & Steinmann (2001b).

In the context of flexible multi-body system (FMS), García Orden (1999); García Orden & Goicolea (2000, 2005) developed an Energy-Momentum method for the dynamics of flexible multi-body system formulated with fully geometrically nonlinear displacement-based FEM for deformable bodies and with the penalty method for joints, instead of other extended approaches such as the Floating Frame of Reference (FFR) due to Shabana (2013). Therein, the preserving evaluation of the forces involved in different types of joints are provided. In the same way, an alternative Energy-Momentum method for FMSs based on Augmented Lagrangian was proposed in García Orden & Ortega Aguilera (2006). Also, the stabilization properties for the formulation of

Energy-Momentum methods for problems with constraints were reviewed in García Orden & Dopico (2007). On the other hand, the Energy-Momentum method has also resulted in a powerful tool to study other numerical difficulties whose treatment alters the energy of the system. That is the case of the velocity projection technique to alleviate the *drift* of the constraints when they are approached by the penalty method, discussed in García Orden (2009) and García Orden & Conde Martín (2012).

1.3 The role of dissipation

The previous energy criteria also led to the construction of time integration methods that introduced numerical, viz. artificial, *dissipation* so that the method's stability can be guaranteed by design for both linear and nonlinear problems.

When a solid, structure or body is discretized, low frequency deformation modes are well captured whereas high frequencies modes are very poorly represented. Traditionally, the high frequencies have been considered “spurious”, as they seemed to be related with the spatial discretization performed to find numerical solutions. This consideration suggested their elimination so that the energy of the system can be controlled and hence stable integration can be achieved. In addition, as experimental observations suggested that high frequencies were “naturally” damped out (air, viscosity, friction, ...), it was blindly accepted that the introduced artificial dissipation somehow compensated the physical (real) dissipation, being seldom considered in mathematical models due to the lack of knowledge about it. This modification may alter the dynamics of the system and, consequently may undermine the physical certainty of the solution thus obtained.

Often, spatial discretization techniques applied to nonlinear elastodynamics result in *stiff* ordinary differential equations which are difficult to solve. The main drawbacks come from the coexistence of two highly different ranges of frequencies which usually pose instabilities in the integration. The alleviation of these difficulties were attained by introducing controllable numerical dissipation so that the high frequencies are damped out. First, the HHT method named after their authors in Hilber et al. (1977), then its generalization called α -Generalized method due to Chung & Hulbert (1993) or even the Wilson- θ method Wilson (1968) became very successful in commercial software (Abaqus HHT, ADINA Wilson- θ , etc). Nevertheless, neither non-unconditionally stable classical time integration methods nor the stabilized ones due to high frequencies cut-off are able to control the energy

(rather damped out in long time simulations) or to preserve momenta, thus losing most of the rich features posed by elastodynamics problems.

Energy momentum methods are able to neatly deal with stiff problems, although some cases, very *stiff* ones, presented instabilities in solutions or simply stopped converging. Discrete *FFT* analyses on solutions suggested that these instabilities may appear because the existence of energy transfer from low to high frequency modes of the solution. The size of the discretization seemed not to be crucial. In those situations, high frequencies dissipative methods seem to be the only way to provide solutions. These ideas motivated the development of conserving methods endowed by the capacity of dissipating high frequencies in a controlled manner, in an attempt to combine the benefits of both strategies. In this sense, several methods were proposed as the Constraint Energy Methods due to Hughes et al. (1978), the Energy decaying schemes by Bauchau & Theron (1996), the modified Energy-Momentum methods in the context of contact introduced by Armero & Petöcz (1998, 1999), the methods due to Crisfield et al. (1997) and Ibrahimbegovic & Mamouri (2002) for beams, or the Constraint Energy-Momentum Method for shells Kuhl & Ramm (1999), none of them devoid of drawbacks. Also, using a discontinuous Galerkin approach, Lens & Cardona (2007) proposed an energy preserving/decaying method for nonlinearly constrained multi-body systems.

Finally, based on consistent perturbations of the Energy-momentum stress and velocity formulas, Armero & Romero (2001a,b) proposed the Energy-Dissipative-Momentum-Conserving (EDMC) methods which were proved to successfully handle *stiff* problems by dissipating high frequencies while preserving the linear and angular momentum and relative equilibria. Later, Armero & Romero (2003) extended this approach to the dynamics of nonlinear Cosserat beams. Furthermore, EDMC methods were also proposed for the solution of exactly geometric beams and shells in Romero & Armero (2002a,b).

The spirit of this dissertation can be summarized by the idea of consistently incorporating physical dissipation in numerical methods to stabilize them so that they additionally provide physically certain solutions.

1.4 Structure-preserving integration for dissipative systems

The geometric integration applied to dissipative systems is usually referred to as structure-preserving or thermodynamically consistent time integration methods. Namely, any numerical integration method intended to solve thermodynamical systems in such a way that the laws of thermodynamics are discretely satisfied by construction. The practical engineering interest that thermodynamical systems have together with the success of the Energy-momentum time methods for Hamiltonian (conservative) systems, see González (2000); Simó & Tarnow (1992), motivated many works towards this end, such as Armero & Simó (1992); Gross & Betsch (2010, 2011); Meng (2002); Meng & Laursen (2002); Ortiz et al. (2000). However, these methods -unlike the Hamiltonian case- were not developed within a uniform procedure. In other words, each different problem required a different formulation of the structure-preserving method. Furthermore, there was as yet evidence (within the computational mechanics community) that this was possible, due to the lack of a general formalism that comprises every dissipative system.

In point of fact, a general formalism for dissipative systems did exist in the geometry induced by *metriplectic structures* on smooth manifolds. These structures were first discussed in Morrison (1986) and Kaufman (1984), and are the result of coupling the Poisson structure defining conservative (Hamiltonian) systems with purely dissipative ones described by the so called Gradient structures. In this way, the derived structure is able to reproduce both reversible and irreversible evolutions and provides an unified framework for most of the systems ruled by the laws of thermodynamics.

Thanks to a particular metriplectic structure known as GENERIC, due to Öttinger (2005) and co-workers, Romero (2009, 2010a,b) devised a general procedure for the formulation of Energy-Momentum-Entropy (EEM) methods for any thermodynamical system. The acronym GENERIC stands for “*General Equation for the Non-Equilibrium Reversible Irreversible Coupling*” and, as a metriplectic structure, provides the evolution equations of any thermodynamical system by separating its reversible and irreversible parts. While the reversible part is connected to the derivative of the total energy of the system, the irreversible one depends on the derivative of the total entropy.

The design of the procedure to systematically attain EEM integration methods is applicable to both finite and infinite dimensional systems and relies on the use of the discrete gradient operator which is a second order approximation of the standard gradient operator evaluated at midpoint,

and satisfies two important properties: *directionality* and *consistency*, see González (1996). This key ingredient makes EEM methods share some of the appealing properties derived from conservation of structure, such as the conservation of the symmetries.

Within this approach, GENERIC formalism plays a similar role to the Hamiltonian formalism does in a purely mechanical context. Therefore, with this new approach, every non-conserving continuous evolution system might be considered as a conserving-like, i.e consistent with the laws of thermodynamics. Thermodynamically speaking, the term *consistent* acts as does the term *conservative* in a purely mechanical context. In fact, for the particular case of reversibility the GENERIC formalism simplifies to the Hamiltonian one, as pointed out in Romero (2009), so that it can be interpreted as a natural generalization of the latter.

Based on this framework, García Orden & Romero (2011) proposed an *Energy-Entropy-Momentum* method for the numerical solution of the dynamics of a particular discrete system (finite dimensional), which consists of point masses linked by thermo-viscoelastic springs. In this work, the authors did not use the underlying GENERIC formalism in order to derive the structure-preserving method which satisfies the laws of thermodynamics. On the other hand, Krüger et al. (2011) performed a complete comparison of this framework with several structure-preserving methods for the discrete thermo-elastic case. Also isothermal dissipative problems can be addressed within this novel framework. Thus, the work of Mielke (2011) contains the GENERIC representation for the limit case of isothermal dissipative systems which could be of interest to derive EEM methods for isothermal viscoelasticity or plasticity.

1.4.1 On the selection of the thermodynamic variable

In theory, the thermodynamical state of any dissipative system can be described either by the absolute temperature or by the entropy or by the internal energy or by any other quantity that is a combination of these three. Due to its intuitive physical interpretation, temperature is often used as the variable for the thermodynamical state. However, the use of the entropy as thermodynamical state variable has been reported to be the most suitable choice to yield EEM methods, see for instance García Orden & Romero (2011); Romero (2009, 2010a,b). Although therein the entropy was successfully employed, additional restrictions had to be assumed such as the necessity for material models to enable the analytical provision of its potentials in

terms of the entropy. In addition, many of the thermodynamical problems of practical interest require Dirichlet boundary conditions which can only be defined by means of the temperature, concluding that the entropy choice does not allow or at least substantially hinders the solution of a wide range of problems.

The search for GENERIC form of the evolution equations has so far become cumbersome when the temperature was considered, consequently preventing the formulation of a corresponding EEM method in the sense of Romero (2009). Recently, Mielke (2011) has thoroughly elaborated a fairly systematic procedure to reach the GENERIC form departing from any thermodynamic variable, demonstrating that a GENERIC form in terms of temperature may be achieved for dissipative thermo-mechanical systems. However, its application to any particular system remains non-trivial at all and, therefore, the way to formulate a Temperature-based EEM method has so far been an issue. In this dissertation this issue is successfully resolved, proving that the election of the temperature as state variable does not involve a complex GENERIC form to deal with and hence facilitating the design of a new temperature-based EEM method.

Furthermore, the election of the temperature as thermodynamical state variable offers advantages from the analytical and numerical point of view. In this way, as the temperature can directly be measured, it is normally the preferable variable to work with in the material modeling community, see for instance Dillon Jr. (1962, 1963); Holzapfel (1996); Holzapfel & Simó (1996b); Reese & Govindjee (1998a). The use of any thermodynamical variable other than the temperature would automatically involve the redefinition of the thermo-mechanical potentials such that they are expressed in terms of that other variable. For realistic models this step could become cumbersome or even impossible from an analytical point of view, so that a full implementation would then require a numerical strategy which would complicate in excess the formulation without any doubt. This factor along with the necessity of imposing Dirichlet boundary conditions in continuous approaches (normally based on the FE method) motivated the search for a EEM method in terms of the temperature.

These methods have recently reached a considerable maturity after the works García Orden & Romero (2011), Romero (2013) or Conde Martín et al. (2014), enabling a wide variety of dissipative problems to be formulated within an unified procedure. As a result of the investigations carried out for this dissertation, this procedure has currently adopted two different approaches based on the election of the thermodynamic variable: entropy

or temperature. Thereby, the choice of the thermodynamical variable is not an issue any longer and can be made according to the particular application. Roughly speaking, the use of entropy provides a more straightforward formulation, assuming certain restrictions, and enables the formulation of staggered (first order accurate) methods in which the mechanical and thermal steps are thermodynamically consistent, see Romero (2010b). On the other hand, the use of temperature successfully deals with typically temperature-based (even non-standard) material models and is practically mandatory for considering Dirichlet boundary conditions. Apart from these technical considerations, both strategies present superior numerical stability and robustness and enable the use of larger time steps compared to standard integration methods.

1.4.2 Dissipative effects: internal variables framework

A widespread way for the modeling of material irreversible processes is provided by the internal variables framework introduced by Coleman & Gurtin (1967). Internal or *hidden* variables are supposed to describe aspects of the internal structure of materials related with dissipative effects which cannot externally be measurable nor controllable. These variables are supplemented by (thermodynamically consistent) constitutive laws that macroscopically collect all these effects, influencing on the history of the system thermodynamic evolution. In this dissertation, the focus is put on *smooth* irreversible effects in the sense that they can be described by continuous laws. That is the case of viscoelastic effects in contrast with *non-smooth* changes typically present in plastic or damage transformations.

Internal variables naturally fit in the GENERIC formalism, contributing directly to the irreversible part of the thermodynamic evolution. In the continuous context, this issue has been addressed at least in Mielke (2011), where also the basis for the consideration of non-smooth kinetic processes were established. However, few works have hitherto addressed the formulation of Energy-Entropy-Momentum time-stepping methods involving internal variables. Some remarkable exceptions are García Orden & Romero (2011), Conde Martín et al. (2014) and Conde Martín & García Orden (2015), although they were not rigorously Energy-Entropy-Momentum methods since no use of the unified formalism was involved to reveal their thermodynamic structure in order to formulate their structure-preserving discrete counterparts. However, they fully correspond to those that would have been achieved within the Energy-Entropy-Momentum approach. In particular, García Orden & Romero (2011) demonstrates that the choice of the entropy facilitates

the comprehension of the *geometric* structure of coupled thermo-mechanic dissipative problems whereas Conde Martín et al. (2014) shows that isothermal considerations simplify the formulation of structure-preserving methods, as it closely follows the guidelines provided by the Energy-Momentum method.

Although the unified procedure has never been applied in the literature to evolution equations defined in terms of internal variables, the preserving structure method could nonetheless be achieved.

1.4.3 Variational Integrators

As previously commented, structure-preserving time integration algorithms have become an active topic of research due to their proved reliability and stability, crucially in long term simulations. Apart from the Energy-Entropy-Momentum approach, Variational Integrators has found their place in the solution of dissipative systems preserving some of their (quality) features.

Ultimately, Energy-Entropy-Momentum methods are formulated via the temporal discretization of the evolution equations, previously derived from the GENERIC framework, that define the particular dissipative problem. In contrast, Variational Integrators perform the temporal approximation on an early stage, that is, directly on the variational principle of the problem. This approach dates back to the seventies in the context of Hamiltonian problems Cadzow (1970), although it was fully consolidated in the nineties Moser & Veselov (1991), Marsden & Wendlandt (1997), Kane et al. (1999); Marsden & Ratiu (1999), Marsden & West (2001), Lew et al. (2004) and Romero (2008). More recently, the same idea has been applied to the particular dissipative problem of adiabatic thermo-mechanics Mata & Lew (2011), by introducing the concept of *thermal displacement*. It plays the role of the mechanical displacements but on the thermal evolution of the system so that the temperature can be recovered as the *thermal velocity*. Based on this concept, attempts towards the consideration of thermodynamic systems involving irreversible processes, such as viscoelastic, damage or plastic effects, are being addressed by using a discrete version of Lagrange-D'Alembert principle, see Kern et al. (2014). However, regarding heat conduction, there are still important unresolved issues as the use of Fourier's type heat conduction laws, see also Kern et al. (2014). The problem in this case is that the evolution equations do not derive from an autonomous Lagrangian (or equivalently, an autonomous Hamiltonian).

Above all these considerations, it should be mentioned that Variational Integrators are not *strictly* thermodynamically consistent methods since they are symplectic by design and hence unlikely to be energy-preserving, see Simó et al. (1992). Nevertheless, they manage to maintain the energy bounded provided the time step is small enough, see Hairer et al. (2006); Leimkuhler & Reich (2005), and, therefore, present superior numerical performances compared to standard methods.

1.5 Objectives

The main goal of this work is to formulate, analyze and implement second-order accurate structure-preserving time integration methods for the solution of general coupled smooth dissipative problems, that is, methods that, by design, are thermodynamically consistent and respect the symmetries of the equations. To this end, six principal objectives have been set:

1. To select appropriated finite- and infinite-dimensional smooth dissipative systems so as to study their thermodynamical soundness and symmetries, essential requisites to formulate EEM methods. Among them all, nonlinear thermo-dissipative continuum dynamics will be the final target.
2. To study and elaborate their formulations in terms of both temperature and entropy variables, identifying their main drawbacks in what regards to applicability and conservation properties of both the continuous and discrete settings, the latter being provided by standard time integration methods.
2. To find their descriptions within the GENERIC framework to serve as departing points to formulate abstract time integration methods endowed by conservation properties.
3. To further develop the recently proposed unified methodology to derive EEM methods from the GENERIC evolution equations of the dissipative systems of interest.
4. To elaborate the said methodology to arrive at second-order accurate time integration methods that inherit all the preservation properties previously identified in the continuous descriptions for both temperature and entropy descriptions.

5. To prove the performance of the resulting methods respect both conservation properties, stability and robustness.
6. To provide general guidelines for the formulation of EEM methods for general smooth dissipative systems.

1.6 Overview

This dissertation is organized in seven chapters, in which the first chapter has covered the motivation, state-of-the-art and objectives. Next, an outline of the contents of the rest of the chapters are provided:

Chapter 2 deals with the descriptions of two simple finite-dimensional smooth dissipative systems so as to set the scope of the problems addressed in this dissertation. They are in-depth studied regarding their conservation properties and how they are breached when using standard time integration methods to find numerical solutions of the nonlinear initial value problems.

Chapter 3 contains a detailed description of the concepts involved in the formulation of nonlinear thermo-dissipative continuum dynamics from the most general perspective. Special attention is paid to the entropy and temperature forms of the underlying partial differential equations as well as the isolated dynamics that lead to the laws of thermodynamics and symmetries. Also, the particular case of isothermal changes is addressed. Then, the resulting infinite-dimensional system is spatially approximated by the classical Galerkin FE-based approach and standard time integration methods are formulated to provide approximated solutions.

Chapter 4 stars with a brief introduction on metriplectic structures induced on manifolds so as to then include one of the key point of the present dissertation. That is, the reformulation of the previously studied smooth dissipative systems within the GENERIC formalism (a particular metriplectic structure) that confers an abstract description from which thermodynamically consistent discrete counterparts can be derived. Also, the symmetries of the equations are used to identify the momentum maps that, according to Noether's theorem, are first integrals of the systems evolution.

Chapter 5 provides full details of the unified methodology employed to derived EEM methods from the previously introduced GENERIC form of the systems studied in this dissertation. Therein, the key points for successful implementations of these new methods are provided and reasoned.

Chapter 6 contains simulations that claim to be useful for modeling real

scenarios in industry.

Chapter 7 contains the main conclusions derived from this work and suggests future works that can be addressed to further exploit the investigation carried out in this dissertation.

1.7 Publications

The following scientific publications, conference presentations and seminars contain parts of this thesis:

Journal articles

- **Sergio Conde Martín** and Juan C. García Orden. “Temperature-based thermodynamically consistent integration for finite thermoelastodynamics”, in preparation.
 - Dominik Kern, Ignacio Romero, **Sergio Conde Martín**, Juan C. García Orden. “Performance Assessment of Variational Integrators for Thermomechanical Problems”, submitted in October 2015.
 - **Sergio Conde Martín** and Juan C. García Orden. “On GENERIC-based integration methods for discrete thermo-visco-elastodynamics”, Selected for C&S Special Issue: ACME-UK 2015, submitted in August 2015.
 - **Sergio Conde Martín**, Juan C. García Orden. “Energy-consistent integration scheme for multi-body systems with dissipation”, *Proceedings of the Institution of Mechanical Engineers, Part K: Journal of Multi-body Dynamics. S.I.: New Trends in Mechanism and Machine Science*, **24**, 413-421, 2015. DOI: 10.1177/1464419315615068 .
 - **Sergio Conde Martín**, Peter Betsch, Juan C. García Orden. “A Temperature-based thermodynamically consistent integration scheme for discrete thermo-elastodynamics”, *Commun Nonlinear Sci Numer Simulat*, **32**, 63-80, 2016. DOI: 10.1016/j.cnsns.2015.08.006
 - **Sergio Conde Martín**, Juan C. García Orden, Ignacio Romero. “Energy-consistent time integration for nonlinear viscoelasticity”, *Computational Mechanics*, **54**(2), 473 - 488, 2014. DOI: 10.1007/s00466-014-1000-x.
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- Juan C. García Orden and **Sergio Conde Martín**. “Controllable velocity projection for constraint stabilization in multibody dynamics”, *Nonlinear Dynamic*, **68**(1-2), 245-257, 2012. DOI: 10.1007/s11071-011-0224-y

Conference proceedings

- **Sergio Conde Martín**, Juan C. García Orden, Peter Betsch. “A Temperature-based thermodynamically consistent integration scheme for discrete thermo-elastodynamics”, *ACME-UK 2015*, Swansea (UK), April 2015.
- **Sergio Conde Martín**, Juan C. García Orden, Ignacio Romero. “Energy-consistent integration scheme for multi-body systems with dissipation”, *EUCOMES*, Guimarães (Portugal), IFToMM, September 2014.

Conference abstracts

- **Sergio Conde Martín**, Juan C. García Orden. “Temperature-based thermodynamically consistent time integration for nonlinear thermoelasticity”, *Coupled Problems*, San Servolo, Venice (Italy), IACM-ECCOMAS, May 2015.
- **Sergio Conde Martín**, Juan C. García Orden, Ignacio Romero. “Energy-consistent time integration for nonlinear viscoelasticity”, *WCCM XI*, Barcelona (Spain), IACM-ECCOMAS, July 2014.
- Juan C. García Orden and **Sergio Conde Martín**. “Controllable velocity projection for constraint stabilization in multibody dynamics”, *CNME*, Coimbra (Portugal), SEMNI & APMTAC, June 2011.

Seminars

- **Sergio Conde Martín**, Juan C. García Orden. “GENERIC-based thermodynamically consistent time integration methods for coupled dissipative problems”, *Applied Mathematics Seminar (2014-15)*, Pavia (Italy), I.M.A.T.I-C.N.R., November 25, 2014.
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Nonlinear thermo-dissipative discrete dynamics

CHAPTER 2

In order to set the scope of this dissertation, two nonlinear discrete dissipative systems containing every significant concept involved in the formulation and solution of thermo-dissipative mechanic problems are discussed. In particular, an isolated system composed of two thermo-springs exchanging heat and an isolated system formed by a thermo-viscoelastic element exchanging heat with its environment are considered. The first system addresses the thermo-elastic coupling and the heat conduction phenomenon, which breaks the Hamiltonian structure of the thermo-elastic problem, or, in other words, converts the system into a dissipative one. On the other hand, the second system goes further to include a dissipative mechanism of type *smooth*, specifically of viscoelastic type, which leads the problem to be dissipative by construction. The characterization of the viscoelastic evolution is modeled by an internal variable which introduces a common framework to deal with dissipative behaviors.

Special attention is paid to the conservation properties of these thermodynamic systems as well as the typical breach of them due to standard numerical integrations. Particularly, as a representative standard integration method, the Midpoint method is discussed regarding the discrete conservation properties.

Framed in the same context as this dissertation, the first system was at least studied in Romero (2009) and Krüger et al. (2011) whereas the second one can be found in García Orden & Romero (2011). Therein, the authors addressed the formulation of these systems in terms of entropy to propose Energy-Entropy-Momentum methods. In this chapter, also a formulation

based on temperature is proposed and discussed so that temperature-based Energy-Entropy-Momentum methods can be achieved in subsequent Chapters.

2.1 Two thermo-spring system

The two thermo-spring system is a thermally isolated system consisting of two point masses m_1 and m_2 connected with thermo-springs of natural lengths λ_1^0 and λ_2^0 , as depicted in **Figure 2.1**. The first spring connects m_1 to a fixed point and the second spring connects m_2 to m_1 . The position of the particles are provided by vectors $\mathbf{q}_1$ and $\mathbf{q}_2$ relative to an inertial reference frame $\{\mathbf{e}_a\}_{a=1}^d$ with, for simplicity, the origin located at the fixed point in an euclidean space of dimension d . The two thermo-springs exchange heat according to a unidimensional Fourier's law of the form

$$h := k (\theta_2 - \theta_1), \quad (2.1)$$

$\theta_a \in \mathbb{R}_+$ being the absolute temperature of the spring $a = 1, 2$ and $k \geq 0$ being the coefficient of thermal conductivity.

Figure 2.1. Thermo-spring system

Then, the thermo-springs are assumed to response according to a smooth and convex Helmholtz free-energy function $\Psi_a : (\lambda_a, \theta_a) \in \mathbb{R}_+ \times \mathbb{R}_+ \rightarrow$

$\Psi_a(\lambda_a, \theta_a) \in \mathbb{R}$ defined in terms of the spring temperature θ_a and the spring elongation λ_a , provided by the l^2 -norm, denoted as $\|\cdot\|$, of the relative position vectors as

$$\lambda_1(\mathbf{q}_1) = \|\mathbf{q}_1\|, \quad \lambda_2(\mathbf{q}_1, \mathbf{q}_2) = \|\mathbf{q}_2 - \mathbf{q}_1\| \quad (2.2)$$

The dynamics of the system is governed by the linear momentum balance and the laws of thermodynamics. Thus, the first balance for each mass establishes that

$$m_a \ddot{\mathbf{q}}_a = - \sum_{b=1}^2 \frac{\partial \Psi_b}{\partial \lambda_b} \frac{\partial \lambda_b}{\partial \mathbf{q}_a} + \mathbf{f}_a, \quad (2.3)$$

$\mathbf{f}_a$ being the external forces applied to the particles, see Figure 2.1, whose existence, strictly speaking, makes the system be non-isolated from the mechanical perspective. In view of (2.2), the partial derivatives of the elongations respect to the position vectors result in

$$\frac{\partial \lambda_1}{\partial \mathbf{q}_1} = \frac{\mathbf{q}_1}{\|\mathbf{q}_1\|}, \quad \frac{\partial \lambda_1}{\partial \mathbf{q}_2} = \mathbf{0}, \quad \frac{\partial \lambda_2}{\partial \mathbf{q}_1} = \frac{\mathbf{q}_1 - \mathbf{q}_2}{\|\mathbf{q}_2 - \mathbf{q}_1\|}, \quad \frac{\partial \lambda_2}{\partial \mathbf{q}_2} = \frac{\mathbf{q}_2 - \mathbf{q}_1}{\|\mathbf{q}_2 - \mathbf{q}_1\|}, \quad (2.4)$$

enabling the spring internal force to be identified by

$$\mathbf{f}_a := \frac{\partial \Psi_a}{\partial \lambda_a}, \quad (2.5)$$

On the other hand, the first law of thermodynamics, or energy balance, establishes that the total energy of any isolated thermodynamic system must be preserved. Focusing on each spring it can be stated as

$$\begin{aligned} f_1 \dot{\lambda}_1 &= \dot{e}_1 - h, \\ f_2 \dot{\lambda}_2 &= \dot{e}_2 + h, \end{aligned} \quad (2.6)$$

e_a being the internal energy of the spring a which accounts for both elastic and thermal energy stored in the spring.

Remark 2.1. In classic thermodynamics, the internal energy is intimately related to the free-energy function via the Legendre transform, see Truesdell et al. (2004), according to

$$e := \Psi - \theta \frac{\partial \Psi}{\partial \theta}, \quad (2.7)$$

where the partial derivative is identified with the entropy

$$\eta := - \frac{\partial \Psi}{\partial \theta} \quad (2.8)$$

two important properties of the Legendre transform are unveiled by taking partial differentiation with respect to temperature to give

$$\frac{\partial e}{\partial \theta} = \frac{\partial \Psi}{\partial \theta} - \frac{\partial \Psi}{\partial \theta} - \theta \frac{\partial^2 \Psi}{\partial \theta^2} = \theta \frac{\partial \eta}{\partial \theta}, \quad (2.9)$$

and partial differentiation with respect to entropy, considering that, by definition, the free-energy function depends on temperature and, accordingly, using the chain rule to obtain its derivative respect to entropy

$$\frac{\partial e}{\partial \eta} = \frac{\partial \Psi}{\partial \theta} \frac{\partial \theta}{\partial \eta} - \frac{\partial \theta}{\partial \eta} \frac{\partial \Psi}{\partial \theta} - \theta \frac{\partial^2 \Psi}{\partial \theta^2} \frac{\partial \theta}{\partial \eta} = \theta \frac{\partial \eta}{\partial \theta} \frac{\partial \theta}{\partial \eta} = \theta \quad (2.10)$$

In Chapter 3 these crucial relations will be in-depth analyzed in the context of continuous media.

2.1.1 Two thermo-spring system in temperature variables

Now, the two thermo-spring system is formulated in terms of spring temperatures as thermodynamic variables. As the free-energy function is defined to depend on temperature by construction, the relation (2.7) straightforwardly yields the internal energy in terms of temperature

$$e_a(\lambda_a, \theta_a) = \Psi_a(\lambda_a, \theta_a) + \theta_a \eta_a(\lambda_a, \theta_a), \quad (2.11)$$

with the entropy of each spring being

$$\eta_a(\lambda_a, \theta_a) = -\frac{\partial \Psi_a(\lambda_a, \theta_a)}{\partial \theta_a} \quad (2.12)$$

Furthermore, the energy balance (2.6) is rewritten so that the rate of temperature explicitly appears. It suffices to apply the chain rule to the function $\dot{e}_a(\lambda_a, \theta_a)$, expressed in terms of positions via (2.2), to give

$$\dot{\theta}_a = \left(\frac{\partial e_a}{\partial \theta_a} \right)^{-1} \left[(-1)^{a-1} h - \theta_a \frac{\partial \eta_a}{\partial \lambda_a} \sum_{b=1}^2 \frac{\partial \lambda_a}{\partial \mathbf{q}_b} \cdot \dot{\mathbf{q}}_b \right] \quad (2.13)$$

Interestingly, using relation (2.9) and the chain rule yields the above balance in entropy form

$$\dot{\eta}_a(\lambda_a, \theta_a) = (-1)^{a-1} \frac{h}{\theta_a} \quad (2.14)$$

Remark 2.2. In the traditional calorimetry approach, the partial derivatives appearing in (2.13) are linked to the spring specific heat capacity

$$c_a := \theta_a \frac{\partial \eta_a}{\partial \theta_a} = \frac{\partial e_a}{\partial \theta_a} > 0, \quad (2.15)$$

and the spring latent heat

$$v_a := \theta_a \frac{\partial \eta_a}{\partial \lambda_a} \quad (2.16)$$

The first indicates the amount of energy required to produce unit increase in the temperature while keeping the deformation fixed, and the second accounts for the Gough-Joule heat due to the thermo-mechanical coupling, see for instance Holzapfel (2000).

Then, by introducing the momenta $\mathbf{p}_a \in \mathbb{R}^d$ the evolution equations can be recast in a first order PDE fashion, that is

$$\begin{aligned} \dot{\mathbf{q}}_a &= \frac{\mathbf{p}_a}{m_a} \\ \dot{\mathbf{p}}_a &= - \sum_{b=1}^2 \frac{\partial \Psi_b}{\partial \lambda_b} \frac{\partial \lambda_b}{\partial \mathbf{q}_a} + \mathbf{f}_a \\ \dot{\theta}_a &= \left(\frac{\partial e_a}{\partial \theta_a} \right)^{-1} \left[(-1)^{a-1} h - \theta_a \frac{\partial \eta_a}{\partial \lambda_a} \sum_{b=1}^2 \frac{\partial \lambda_a}{\partial \mathbf{q}_b} \cdot \frac{\mathbf{p}_b}{m_b} \right], \end{aligned} \quad (2.17)$$

Alternatively, using the constitutive relations (2.5), (2.15) and (2.16) they also can be expressed as follows

$$\begin{aligned} \dot{\mathbf{q}}_a &= \frac{\mathbf{p}_a}{m_a} \\ \dot{\mathbf{p}}_a &= - \sum_{b=1}^2 f_b \frac{\partial \lambda_b}{\partial \mathbf{q}_a} + \mathbf{f}_a \\ \dot{\theta}_a &= \frac{1}{c_a} \left[(-1)^{a-1} h - v_a \sum_{b=1}^2 \frac{\partial \lambda_a}{\partial \mathbf{q}_b} \cdot \frac{\mathbf{p}_b}{m_b} \right] \end{aligned} \quad (2.18)$$

It only remains to set initial conditions for the positions $\mathbf{q}_a^0$, the momenta $\mathbf{p}_a^0$ and the temperatures θ_a^0 and the specification of the free-energy function. For example, consider the following Helmholtz free-energy function, used in

Romero (2009),

$$\begin{aligned} \Psi_a(\lambda_a, \theta_a) = & \frac{C_a(\theta_a)}{2} \log^2 \frac{\lambda_a}{\lambda_a^0} - \alpha_a(\theta_a - \theta_{\text{ref}}) \log \frac{\lambda_a}{\lambda_a^0} \\ & + c_a \left(\theta_a - \theta_{\text{ref}} - \theta_a \log \frac{\theta_a}{\theta_{\text{ref}}} \right), \end{aligned} \quad (2.19)$$

where $C_a(\theta_a)$ is the a -th spring stiffness considered to be temperature-dependent, α_a accounts for the thermo-mechanical coupling, c_a is the specific heat capacity and θ_{ref} is the reference temperature at which the unstressed deformation is defined to be zero. Accordingly, the entropy function follows from differentiating once to get

$$\eta_a(\lambda_a, \theta_a) = -\frac{C'_a(\theta_a)}{2} \log^2 \frac{\lambda_a}{\lambda_a^0} + \alpha_a \log \frac{\lambda_a}{\lambda_a^0} + c_a \log \frac{\theta_a}{\theta_{\text{ref}}}, \quad (2.20)$$

$C'_a(\theta_a)$ being the absolute derivative of the function $C_a(\theta_a)$.

Then, according to the Legendre transform (2.7), the internal energy function can directly be obtained as

$$e_a(\lambda_a, \theta_a) = \frac{C_a(\theta_a) - \theta_a C'_a(\theta_a)}{2} \log^2 \frac{\lambda_a}{\lambda_a^0} + \alpha_a \theta_{\text{ref}} \log \frac{\lambda_a}{\lambda_a^0} + c_a (\theta_a - \theta_{\text{ref}}) \quad (2.21)$$

2.1.2 Two thermo-spring system in entropy variables

If the spring entropies are chosen as thermodynamic variables the problem needs to be described with thermodynamic potentials in terms of them. To do that, the Legendre transform is applied to the free-energy function respect to the temperature to arrive at the internal energy in terms of the entropy, which are the transformed potential and the conjugate variable, respectively, that is

$$e_a(\lambda_a, \eta_a) = \Psi_a(\lambda_a, \theta_a(\lambda_a, \eta_a)) + \theta_a(\lambda_a, \eta_a) \eta_a \quad (2.22)$$

In the above expression, it is assumed that the function $\theta_a(\lambda_a, \eta_a)$ can be reached from (2.12). Moreover, the properties of the Legendre transform allow to conclude that

$$f_a = \frac{\partial e_a}{\partial \lambda_a}, \quad \theta_a = \frac{\partial e_a}{\partial \eta_a} \quad (2.23)$$

In view of this, applying the chain rule in (2.7) so that the rates of entropies appear, the entropy formulation of the evolution equation yields

$$\begin{aligned}
\dot{\mathbf{q}}_a &= \frac{\mathbf{p}_a}{m_a} \\
\dot{\mathbf{p}}_a &= - \sum_{b=1}^2 \frac{\partial e_b}{\partial \lambda_b} \frac{\partial \lambda_b}{\partial \mathbf{q}_a} + \mathbf{f}_a \\
\dot{\eta}_1 &= \left(\frac{\partial e_1}{\partial \eta_1} \right)^{-1} k \left(\frac{\partial e_2}{\partial \eta_2} - \frac{\partial e_1}{\partial \eta_1} \right) \\
\dot{\eta}_2 &= \left(\frac{\partial e_2}{\partial \eta_2} \right)^{-1} k \left(\frac{\partial e_1}{\partial \eta_1} - \frac{\partial e_2}{\partial \eta_2} \right)
\end{aligned} \tag{2.24}$$

More compactly, they are expressed in terms of the constitutive relations (2.23) as

$$\begin{aligned}
\dot{\mathbf{q}}_a &= \frac{\mathbf{p}_a}{m_a} \\
\dot{\mathbf{p}}_a &= - \sum_{b=1}^2 f_b \frac{\partial \lambda_b}{\partial \mathbf{q}_a} + \mathbf{f}_a \\
\dot{\eta}_a &= (-1)^{a-1} \frac{h}{\theta_a}
\end{aligned} \tag{2.25}$$

The problem is closed by setting initial conditions for the positions $\mathbf{q}_a^0$, the momenta $\mathbf{p}_a^0$ and the entropies η_a^0 . However, it is usual to know the initial temperature θ_a^0 instead of the initial entropy η_a^0 . In this case, the following relation should be solved in order to properly set the initial conditions

$$\eta_a^0 = - \frac{\partial \Psi_a}{\partial \theta_a}(\lambda_a^0, \theta_a^0) \tag{2.26}$$

Finally, when specifying the free energy function an important issue arises. That is, the temperature function $\theta_a(\lambda_a, \theta_a)$ should be obtained by inverting (2.12) but, it is the case that this only can analytically be done under certain conditions, limiting the range of potential problems that can be addressed with this formulation.

If the free-energy function (2.20) is used, the restriction falling on it is that the dependence of the elastic parameter with temperature must be at most linear, i.e $C'_a(\theta_a) = C$, with C being a real constant. In such a case,

the temperature function results in

$$\theta_a(\lambda_a, \eta_a) = \theta_{\text{ref}} \exp \left(\frac{\eta_a + \frac{C}{2} \log^2 \frac{\lambda_a}{\lambda_a^0} - \alpha_a \log \frac{\lambda_a}{\lambda_a^0}}{c_a} \right) \quad (2.27)$$

Accordingly, the particular form of internal energy in terms of the entropy is provided by

$$\begin{aligned} e_a(\lambda_a, \eta_a) = & \frac{C_a(\theta_a) - \theta_a C}{2} \log^2 \frac{\lambda_a}{\lambda_a^0} + \alpha_a \theta_{\text{ref}} \log \frac{\lambda_a}{\lambda_a^0} \\ & + c_a \theta_{\text{ref}} \left[\exp \left(\frac{\eta_a + \frac{C}{2} \log^2 \frac{\lambda_a}{\lambda_a^0} - \alpha_a \log \frac{\lambda_a}{\lambda_a^0}}{c_a} \right) - 1 \right] \end{aligned} \quad (2.28)$$

2.1.3 Symmetries and laws of thermodynamics

Associated with the dynamics of isolated systems, there exist conserved quantities throughout the motion, imposing in effect a mathematical or natural constraint on it. Particularly, for discrete thermo-dissipative systems, these are the total linear and angular momentum, associated with the symmetries of the equations, and the total energy and entropy of the system.

The proof for the linear and angular momentum is a classical result which departs from the definition of the total linear and angular momentum as

$$\mathbf{L} = \sum_{a=1}^2 \mathbf{p}_a, \quad \mathbf{J} = \sum_{a=1}^2 \mathbf{q}_a \wedge \mathbf{p}_a, \quad (2.29)$$

with $(\cdot) \wedge (\cdot)$ meaning cross product.

Then, it is proved that the rate of these quantities becomes zero, that is

$$\dot{\mathbf{L}} = \sum_{a=1}^2 \dot{\mathbf{p}}_a = \mathbf{0}, \quad \dot{\mathbf{J}} = \sum_{a=1}^2 (\dot{\mathbf{q}}_a \wedge \mathbf{p}_a + \mathbf{q}_a \wedge \dot{\mathbf{p}}_a) = \mathbf{0} \quad (2.30)$$

By using either (2.18)₂ or (2.25)₂ along with (2.4) the proof for the linear momentum follows from

$$\dot{\mathbf{L}} = - \left(f_1 \frac{\mathbf{q}_1}{\lambda_1} + f_2 \frac{\mathbf{q}_1 - \mathbf{q}_2}{\lambda_2} \right) + \mathbf{f}_1 - f_2 \frac{\mathbf{q}_2 - \mathbf{q}_1}{\lambda_2} + \mathbf{f}_2 = -f_1 \frac{\mathbf{q}_1}{\lambda_1} + \mathbf{f}_1 + \mathbf{f}_2, \quad (2.31)$$

which vanishes due to the consideration of the resulting terms to be external. That is, the mechanical isolation of the system involves only the two point masses and the second spring. Given that, the force due to the first spring is considered as external and, hence, it should vanish for the linear momentum to be preserved. In other words, the inclusion of the fixed point into the system leads the total linear momentum (2.29)₁ conservation to be breached, as in this case the system is not mechanically isolated.

The angular momentum, however, is not affected by the previous consideration (although strictly speaking the mechanical isolated system remains equal) as the external force due to the first spring does not contribute to the moment respect to the fixed point, that is

$$\dot{\mathbf{J}} = \sum_{a=1}^2 \mathbf{q}_a \wedge \dot{\mathbf{p}}_a = \mathbf{q}_1 \wedge \left(f_1 \frac{\mathbf{q}_1}{\lambda_1} + f_2 \frac{\mathbf{q}_1 - \mathbf{q}_2}{\lambda_2} \right) + \mathbf{q}_2 \wedge f_2 \frac{\mathbf{q}_2 - \mathbf{q}_1}{\lambda_2} = \mathbf{0}, \quad (2.32)$$

where the external forces have been neglected and use has been made of the cross product property¹.

On the other hand, the total energy $E : \mathcal{S} \rightarrow \mathbb{R}$, $\mathcal{S}$ being the state space, involves the kinetic energy $K : \mathcal{S} \rightarrow \mathbb{R}$ due to the dynamics of the system, provided by

$$K(\|\mathbf{p}_1\|, \|\mathbf{p}_2\|) := \sum_{a=1}^2 \frac{\|\mathbf{p}_a\|^2}{2m_a}, \quad (2.33)$$

and the total internal energy $U : \mathcal{S} \rightarrow \mathbb{R}$ of the springs provided by

$$U(\mathbf{q}_1, \mathbf{q}_2, s_1, s_2) := e_1(\lambda_1(\mathbf{q}_1), s_1) + e_2(\lambda_2(\mathbf{q}_1, \mathbf{q}_2), s_2), \quad (2.34)$$

s_a being either temperatures or entropies, depending on the formulations (2.17) or (2.24).

Then, it is easy to show that the rate of the total energy vanishes in absence of external forces with the help of (2.18)_{1,2} or (2.25)_{1,2} and (2.6)

¹ $\mathbf{a} \wedge \mathbf{b} = -\mathbf{b} \wedge \mathbf{a}$

together with the chain rule on the rate of the elongations to give

$$\begin{aligned}
 \dot{E} = \dot{K} + \dot{U} &= \sum_{a=1}^2 \frac{1}{m_a} \mathbf{p}_a \cdot \dot{\mathbf{p}}_a + \sum_{a=1}^2 \dot{e}_a(\lambda_a, s_a) \\
 &= \sum_{a=1}^2 \frac{1}{m_a} \mathbf{p}_a \cdot \left(- \sum_{b=1}^2 f_b \frac{\partial \lambda_b}{\partial \mathbf{q}_a} \right) + \sum_{a=1}^2 f_a \dot{\lambda}_a \\
 &= - \sum_{a=1}^2 \dot{\mathbf{q}}_a \cdot \sum_{b=1}^2 f_b \frac{\partial \lambda_b}{\partial \mathbf{q}_a} + \sum_{a=1}^2 f_a \sum_{b=1}^2 \frac{\partial \lambda_a}{\partial \mathbf{q}_b} \cdot \dot{\mathbf{q}}_b = 0
 \end{aligned} \tag{2.35}$$

Finally, the entropy formulation of the energy balance (2.24)₃ easily provides the proof for the system to agree with the second law of thermodynamics. Defining the total entropy of the system $S : \mathcal{S} \rightarrow \mathbb{R}_+$ as the sum of the spring entropies, its rate can be demonstrated to be non-negative by additionally using (2.1), that is

$$\dot{S} = \dot{\eta}_1 + \dot{\eta}_2 = h \left(\frac{1}{\theta_1} - \frac{1}{\theta_2} \right) = k \frac{(\theta_2 - \theta_1)^2}{\theta_1 \theta_2} \geq 0 \tag{2.36}$$

This result is also valid for the temperature formulation (2.17) because (2.24)₃ can be recovered by (2.17)₃, as demonstrated in (2.14).

2.2 Thermo-visco-elastic system

The isolated thermo-visco-elastic system is formed by a thermo-visco-elastic element and its environment, which is considered to have a variable temperature and whose thermodynamics is defined by an unique thermal variable. Another option for the thermodynamic isolated system is to consider two thermo-visco-elastic elements exchanging heat between them as the previous example. Similarly, in the previous system, the environment could have been included for the exchange of heat. In any case, the thermodynamic features intended to be studied are present in both alternatives so such decision is not crucial at all.

A thermo-visco-elastic element consists of a generalized Maxwell element connecting two point masses m_1 and m_2 , as depicted in Figure 2.2. The generalized Maxwell element in turn consists of a thermo-spring arranged in parallel with a thermo-Maxwell element, i.e a thermo-spring in series with a dashpot.

Figure 2.2. Thermo-visco-elastic system

Then, the thermo-visco-elastic element is connected to the environment by the exchange of heat which follows an unidimensional Fourier's law of the type

$$h = k(\theta - \vartheta), \quad (2.37)$$

where $\theta \in \mathbb{R}_+$ and $\vartheta \in \mathbb{R}_+$ are the absolute element and the absolute environment temperatures and the scalar $k \geq 0$ is the thermal conductivity parameter.

Analogously to the two thermo-spring system, the position of the point masses are provided by position vectors $\mathbf{q}_1, \mathbf{q}_2 \in \mathbb{R}^d$, d being the problem dimension, relative to an inertia frame of reference $\{\mathbf{e}_i\}_{i=1}^d$ so that the elongation or shortening of the element is

$$\lambda(\mathbf{q}_1, \mathbf{q}_2) = \|\mathbf{q}_2 - \mathbf{q}_1\| = \sqrt{(\mathbf{q}_2 - \mathbf{q}_1) \cdot (\mathbf{q}_2 - \mathbf{q}_1)}, \quad (2.38)$$

whose partial derivatives respect to the positions vectors fully correspond to those of the second spring of the previous system (2.4)_{3,4}.

The new feature that incorporates this system is the flow behavior of the Maxwell element's dashpot, which is characterized by an internal variable $\gamma \in \mathbb{R}$ in the sense of Simó & Hughes (2000), and originally introduced

by Coleman & Gurtin (1967). The viscous effects are thus modeled by a Newtonian viscous fluid specified by a viscosity parameter $\nu > 0$ which may generally depend on temperature. In addition, the viscosity parameter can directly be related to the relaxation/retardation time $\tau > 0$ through the shear moduli of the spring in series with the dashpot $\mu > 0$, that is, $\nu = 2\mu\tau$, see Holzapfel (2000).

As a state variable, the internal variable contributes to the element constitutive behavior, entering the thermo-visco-elastic element free-energy function $\Psi(\lambda, \theta, \gamma): \mathbb{R}_+ \times \mathbb{R}_+ \times \mathbb{R} \rightarrow \mathbb{R}$. Moreover, the Legendre transform (2.7) still applies, leading to the definitions of the element internal energy e and the element entropy η .

The dynamics of this system also relies on the balance laws of linear momentum, energy and entropy. Following Newton's law, the first one can be stated for each mass as

$$m_a \ddot{\mathbf{q}}_a = - \frac{\partial \Psi}{\partial \lambda} \frac{\partial \lambda}{\partial \mathbf{q}_a} + \mathbf{f}_a \quad \text{with } a = 1, 2, \quad (2.39)$$

$\mathbf{f}_a$ being the external forces applied to the point masses. Following the first law of thermodynamics, the energy balance applied to both the element and the environment reads

$$\begin{aligned} \frac{\partial \Psi}{\partial \lambda} \dot{\lambda} &= \dot{e} + h \\ 0 &= \dot{\epsilon} - h, \end{aligned} \quad (2.40)$$

ϵ being the internal energy of the environment.

In addition, the second law of thermodynamics bounds the rate of the internal variable to be proportional to the viscous driving force via the viscosity parameter

$$\dot{\gamma} = - \frac{1}{\nu(\theta)} \frac{\partial \Psi(\lambda, \theta, \gamma)}{\partial \gamma}, \quad (2.41)$$

defining the evolution equation for the internal variable.

2.2.1 Thermo-visco-elastic system in temperature variables

According to (2.7), the element internal energy defined in terms of the element temperature results directly from using the free-energy function $\Psi(\lambda, \theta, \gamma)$, that is

$$e(\lambda, \theta, \gamma) := \Psi(\lambda, \theta, \gamma) - \theta \frac{\partial \Psi(\lambda, \theta, \gamma)}{\partial \theta}, \quad (2.42)$$

where the entropy function of the element is identified to be

$$\eta(\lambda, \theta, \gamma) := -\frac{\partial \Psi(\lambda, \theta, \gamma)}{\partial \theta} \quad (2.43)$$

On the other hand, the environment is thermodynamically determined by either its internal energy $\epsilon(\vartheta)$ or its entropy $\sigma(\vartheta)$ defined in terms of its temperature so that the following identity hold

$$\varsigma = \frac{d\epsilon}{d\vartheta} = \vartheta \frac{d\sigma}{d\vartheta} > 0, \quad (2.44)$$

which is the definition of the specific heat capacity of the environment.

As in the case of the two thermo-spring system, the evolution equations (2.39)-(2.41) can be rewritten as a first order PDE system by introducing the momenta $\mathbf{p}_a \in \mathbb{R}^d$ to give

$$\begin{aligned} \dot{\mathbf{q}}_a &= \frac{\mathbf{p}_a}{m_a} \\ \dot{\mathbf{p}}_a &= -\frac{\partial \Psi}{\partial \lambda} \frac{\partial \lambda}{\partial \mathbf{q}_a} + \mathbf{f}_a \\ \dot{\gamma} &= -\frac{1}{\nu} \frac{\partial \Psi}{\partial \gamma} \\ \dot{\theta} &= \frac{1}{\theta} \left(\frac{\partial \eta}{\partial \theta} \right)^{-1} \left[-\theta \sum_{a=1}^2 \frac{\partial \eta}{\partial \lambda} \frac{\partial \lambda}{\partial \mathbf{q}_a} \cdot \frac{\mathbf{p}_a}{m_a} + \frac{1}{\nu} \frac{\partial \Psi}{\partial \gamma} \left(\frac{\partial \Psi}{\partial \gamma} + \theta \frac{\partial \eta}{\partial \gamma} \right) - h \right] \\ \dot{\vartheta} &= \left(\frac{d\epsilon}{d\vartheta} \right)^{-1} h \end{aligned} \quad (2.45)$$

Alternatively, the appearing partial derivatives are also linked with the element internal force f , the dashpot viscous driving force g and the classical calorimetry coefficients, i.e the specific heat capacities c and ς and latent heats v and w , according to

$$\begin{aligned} f &= \frac{\partial \Psi}{\partial \lambda}, & g &= -\frac{\partial \Psi}{\partial \gamma}, & c &= \frac{\partial e}{\partial \theta} = \theta \frac{\partial \eta}{\partial \theta} > 0, \\ v &= \theta \frac{\partial \eta}{\partial \lambda}, & w &= \theta \frac{\partial \eta}{\partial \gamma}, & \varsigma &= \frac{d\epsilon}{d\vartheta} = \vartheta \frac{d\sigma}{d\vartheta} > 0 \end{aligned} \quad (2.46)$$

Thus, the evolution equations can be expressed in a more compact form

as

$$\begin{aligned}
\dot{\mathbf{q}}_a &= \frac{\mathbf{p}_a}{m_a} \\
\dot{\mathbf{p}}_a &= -f \frac{\partial \lambda}{\partial \mathbf{q}_a} + \mathbf{f}_a \\
\dot{\gamma} &= \frac{g}{\nu} \\
\dot{\theta} &= \frac{1}{c} \left[-v \sum_{a=1}^2 \frac{\partial \lambda}{\partial \mathbf{q}_a} \cdot \frac{\mathbf{p}_a}{m_a} + \frac{g}{\nu} (g - w) - h \right] \\
\dot{\vartheta} &= \frac{h}{\varsigma}
\end{aligned} \tag{2.47}$$

By setting initial conditions for the positions $\mathbf{q}_a^0$, the momentum $\mathbf{p}_a^0$ and temperatures θ^0, ϑ^0 the initial value problem becomes closed, since the internal variable γ^0 is assumed to be zero, at the expense of the specification of the Helmholtz free-energy function. For instance, the one used in García Orden & Romero (2011) and provided by

$$\Psi(\lambda, \theta, \gamma) = (1 + \beta) \Psi^\infty(\lambda, \theta) + \mu(\theta) \gamma^2 - \beta \gamma \frac{\partial \Psi^\infty(\lambda, \theta)}{\partial \lambda}, \tag{2.48}$$

being $\Psi^\infty(\lambda, \theta)$ the free-energy function of the main spring, which is responsible for the whole response of the element when the viscous effects vanish, $\mu(\theta)$ being a parameter associated to the stiffness of the Maxwell element and $\beta = 2\mu(\theta_{\text{ref}})/C(\theta_{\text{ref}})$ relating both parameters at the reference temperature.

General smooth and convex free-energy functions $\Psi^\infty(\lambda, \theta)$ can be considered, as the one used for the two thermo-spring system (2.19). Then, the entropy function follows from differentiating (2.48) once to obtain

$$\eta(\lambda, \theta, \gamma) = -(1 + \beta) \frac{\partial \Psi^\infty}{\partial \theta} - \mu'(\theta) \gamma^2 + \beta \gamma \frac{\partial^2 \Psi^\infty}{\partial \theta \partial \lambda}, \tag{2.49}$$

$\mu'(\theta)$ being the absolute derivative of the function $\mu(\theta)$. Moreover, according to the Legendre transform (2.42), the internal energy function can be directly obtained in terms of temperature

$$\begin{aligned}
e(\lambda, \theta, \gamma) &= (1 + \beta) \left(\Psi^\infty - \theta \frac{\partial \Psi^\infty}{\partial \theta} \right) + (\mu(\theta) - \theta \mu'(\theta)) \gamma^2 \\
&\quad + \beta \gamma \left(\theta \frac{\partial^2 \Psi^\infty}{\partial \theta \partial \lambda} - \frac{\partial \Psi^\infty}{\partial \lambda} \right)
\end{aligned} \tag{2.50}$$

Furthermore, general non-linear expressions for the stiffness $C(\theta)$, the Maxwell element parameter $\mu(\theta)$ and the viscosity parameter $\nu(\theta)$ could be considered. Particularly, the viscosity parameter $\nu(\theta)$ is assumed to follow an exponential law with the inverse of temperature as follows

$$\nu(\theta) = \nu_0 \exp \left[a \left(\frac{1}{\theta} - \frac{1}{\theta_{\text{ref}}} \right) \right] \quad \text{with} \quad \nu_0, a > 0 \quad (2.51)$$

Finally, it is necessary to define a thermodynamical model for the environment. The easiest way is to consider the ideal-gas type model with an internal energy provided by

$$\epsilon(\vartheta) = \varsigma(\vartheta - \theta_{\text{ref}}), \quad (2.52)$$

and the entropy by

$$\sigma(\vartheta) = \varsigma \log(\vartheta/\theta_{\text{ref}}) \quad (2.53)$$

2.2.2 Thermo-visco-elastic system in entropy variables

Alternatively, the thermo-visco-elastic system can be formulated in terms of entropies. Thus, provided $e(\lambda, \eta, \gamma)$ and $\epsilon(\sigma)$, the entropy formulation of the evolution equations reads

$$\begin{aligned} \dot{\mathbf{q}}_a &= \frac{\mathbf{p}_a}{m_a} \\ \dot{\mathbf{p}}_a &= -\frac{\partial e}{\partial \lambda} \frac{\partial \lambda}{\partial \mathbf{q}_a} + \mathbf{f}_a \\ \dot{\gamma} &= -\frac{1}{\nu} \frac{\partial e}{\partial \gamma} \\ \dot{\eta} &= \left(\frac{\partial e}{\partial \eta} \right)^{-1} \left[\frac{1}{\nu} \left(\frac{\partial e}{\partial \gamma} \right)^2 + k \left(\frac{d\epsilon}{d\sigma} - \frac{\partial e}{\partial \eta} \right) \right] \\ \dot{\sigma} &= \left(\frac{d\epsilon}{d\sigma} \right)^{-1} k \left(\frac{\partial e}{\partial \eta} - \frac{d\epsilon}{d\sigma} \right) \end{aligned} \quad (2.54)$$

Identifying now the partial derivatives of the internal energies with the internal force f , the viscous driving force g and the temperatures θ and ϑ , according to

$$f = \frac{\partial e}{\partial \lambda}, \quad g = -\frac{\partial e}{\partial \gamma}, \quad \theta = \frac{\partial e}{\partial \eta} \quad \vartheta = \frac{d\epsilon}{d\sigma}, \quad (2.55)$$

the evolution equations are also expressed as follows

$$\begin{aligned}
\dot{\mathbf{q}}_a &= \frac{\mathbf{p}_a}{m_a} \\
\dot{\mathbf{p}}_a &= -f \frac{\partial \lambda}{\partial \mathbf{q}_a} + \mathbf{f}_a \\
\dot{\gamma} &= \frac{g}{\nu} \\
\dot{\eta} &= \frac{1}{\theta} \left(\frac{g^2}{\nu} - h \right) \\
\dot{\sigma} &= \frac{h}{\vartheta}
\end{aligned} \tag{2.56}$$

To fully bound the problem, initial conditions for the positions $\mathbf{q}_a^0$, the momenta $\mathbf{p}_a^0$ and the entropies η^0 and σ^0 must be set. Again, what it is usual to know is the initial temperatures θ^0 and ϑ_0 for which the following relations must be considered in order to set properly the initial conditions

$$\eta^0 = -\frac{\partial \Psi}{\partial \theta}(\lambda^0, \theta^0, \gamma^0), \quad \sigma^0 = \sigma(\vartheta^0) \tag{2.57}$$

Also, this formulation has the same constraints as those pointed out for the two thermo-spring system. Namely, the relation (2.43) must be analytically invertible to obtain $\theta(\lambda, \eta, \gamma)$. Then, the temperature-dependent stiffness $C(\theta)$, in case of assuming (2.19) for the potential $\Psi^\infty(\lambda, \theta)$, and the parameter $\mu(\theta)$ must be at most linear, that is, $C'(\theta) = C$ and $\mu'(\theta) = \mu$, with C and μ being constants.

With these considerations, the element temperature function in terms of entropy reads

$$\begin{aligned}
\theta(\lambda, \eta, \gamma) = \\
\theta_{\text{ref}} \exp \left[\frac{\frac{C}{2} \log^2 \frac{\lambda}{\lambda_0} - \alpha \log \frac{\lambda}{\lambda_0}}{c} + \frac{\eta + \mu \gamma^2 - \beta \gamma \left(\frac{C}{\lambda} \log \frac{\lambda}{\lambda_0} - \frac{\alpha}{\lambda} \right)}{(1 + \beta)c} \right]
\end{aligned} \tag{2.58}$$

Accordingly, the internal energy function can be directly obtained in terms of entropy by using the above function in (2.50). Also, the viscosity parameter (2.51) must be evaluated via this temperature function

$$\nu(\theta(\lambda, \eta, \gamma)) = \nu_0 \exp \left[a \left(\frac{1}{\theta(\lambda, \eta, \gamma)} - \frac{1}{\theta_{\text{ref}}} \right) \right] \quad \text{with } \nu_0, a > 0 \tag{2.59}$$

In the same way, this formulation requires the inversion of the function (2.53) to obtain the environment temperature in terms of the environment entropy

$$\vartheta(\sigma) = \theta_{\text{ref}} \exp\left(\frac{\sigma}{\varsigma}\right), \quad (2.60)$$

leading the environment internal energy to be

$$\epsilon(\sigma) = \varsigma \theta_{\text{ref}} \left[\exp\left(\frac{\sigma}{\varsigma}\right) - 1 \right] \quad (2.61)$$

2.2.3 Symmetries and law of thermodynamics

This subsection reviews the conservation properties of the thermo-visco-elastic system. For this case, the invariants of a free-motion are also identified with the total linear and angular momentum and the total energy and entropy.

Then, the same definitions (2.29)₁ and (2.29)₂ of the linear and angular momentums apply so, neglecting the external forces, the verification of the linear momentum conservation is achieved by using either (2.47)₂ or (2.56)₂ along with (2.4) to give

$$\dot{\mathbf{L}} = -f \frac{\mathbf{q}_1 - \mathbf{q}_2}{\lambda} - f \frac{\mathbf{q}_2 - \mathbf{q}_1}{\lambda} = \mathbf{0} \quad (2.62)$$

Likewise, the angular momentum conservation is also derived from (2.47)₂ and (2.56)₂, yielding

$$\dot{\mathbf{J}} = \mathbf{q}_1 \wedge f \frac{\mathbf{q}_1 - \mathbf{q}_2}{\lambda} + \mathbf{q}_2 \wedge f \frac{\mathbf{q}_2 - \mathbf{q}_1}{\lambda} = \mathbf{0} \quad (2.63)$$

Regarding the total energy conservation, the kinetic energy answers to the same expression as in the previous system (2.33) whereas the total internal energy now becomes

$$U(\mathbf{q}_1, \mathbf{q}_2, s_1, s_2, \gamma) := e(\lambda(\mathbf{q}_1, \mathbf{q}_2), s_1, \gamma) + \epsilon(s_2), \quad (2.64)$$

s_a being either the element and the environment temperatures or entropies, depending on the formulation.

Then, the proof for the total energy to be preserved in absence of external forces is deduced with the help of (2.47)_{1,2} or (2.56)_{1,2} and (2.40) together

with the chain rule on the rate of the elongations to obtain

$$\begin{aligned}
 \dot{E} &= \dot{K} + \dot{U} = \sum_{a=1}^2 \frac{1}{m_a} \mathbf{p}_a \cdot \dot{\mathbf{p}}_a + \dot{e}(\lambda, s_1, \gamma) + \dot{e}(s_2) \\
 &= \sum_{a=1}^2 \frac{1}{m_a} \mathbf{p}_a \cdot \left(-f \frac{\partial \lambda}{\partial \mathbf{q}_a} \right) + f \dot{\lambda} \\
 &= - \sum_{a=1}^2 \dot{\mathbf{q}}_a \cdot f \frac{\partial \lambda}{\partial \mathbf{q}_a} + f \sum_{a=1}^2 \frac{\partial \lambda}{\partial \mathbf{q}_a} \cdot \dot{\mathbf{q}}_a = 0
 \end{aligned} \tag{2.65}$$

On the other hand, the total entropy is the sum of the element and the environment entropies, whose rate can be proved to be non-negative via the entropy formulation of the energy balance (2.54)₃ and the Fourier law (2.37), that is

$$\dot{S} = \dot{\eta}_1 + \dot{\eta}_2 = \frac{g^2}{\theta \nu} + h \left(\frac{1}{\theta} - \frac{1}{\vartheta} \right) = \frac{g^2}{\theta \nu} + k \frac{(\theta - \vartheta)^2}{\theta \vartheta} \geq 0, \tag{2.66}$$

which also applies to the temperature formulation (2.45) for the same reasons as those argued in the previous Section.

2.3 Standard numerical time integration methods

Each of the initial-value problems discussed so far can be recast in the following simplified form

$$\dot{\mathbf{y}}(t) = \mathbf{f}(\mathbf{y}(t), t) \quad \forall t \in [0, T], \tag{2.67}$$

where the vector $\mathbf{y} \in \mathcal{S}$ collects every state variable and $\mathbf{f}: \mathcal{S} \mapsto \mathbb{R}^{\dim(\mathbf{y})}$ is a nonlinear vector-valued function. Such general nonlinearity is responsible for an analytical integration to be unaffordable, thus requiring a numerical approach in order to provide approximate solutions.

To this end, the continuous time interval of interest $[0, T]$ is decomposed into $N - 1$ subintervals, such that

$$[0, T] = \bigcup_{n=0}^{N-1} [t_n, t_{n+1}], \tag{2.68}$$

whose lengths are provided by $\Delta t_{n+1} = t_{n+1} - t_n$, and are normally assumed to be constant for simplicity although it is not a necessary condition.

The time-evolution of the state variables vector is thus sampled by a sequence of approximated state values at each subinterval extremities, that is

$$\mathbf{y}(t) \approx \{\mathbf{y}_n\}_{n=0}^N, \quad (2.69)$$

where $\mathbf{y}_k$ is the approximation of $\mathbf{y}(t_k)$. The relation between any state and its predecessor depends on the integration method and is obtained via a particular approximation of (2.67) inside every time subinterval, such that

$$\mathbf{y}_{n+1} = \mathbf{y}_n + \int_{t_n}^{t_{n+1}} \mathbf{f}(\mathbf{y}(t), t) dt \quad (2.70)$$

Any method thus constructed is said to be a *one-step* integration method and it will be *consistent* provided that in the limit case of $\Delta t_{n+1} \rightarrow dt$ the continuous evolution is fully recovered. Hence, the approximated solution will be closer to the exact one as the time subintervals are reduced.

Remark 2.3. There exist integration methods that also involve states other than just the previous one, referred to as *multi-step* methods. The most representative methods are the BDF ones, which stands for *Backward Differentiation Methods*, see Dong (2010).

Each one-step time integration method emerges from different approximations of the analytically non-accessible integral of (2.70). Thus, the standard *Forward-Euler*, *Backward-Euler*, *Trapezoidal*, *Midpoint* or *Simpson* methods responds to the following quadratures

$$\begin{aligned} \int_{t_n}^{t_{n+1}} \mathbf{f}(\mathbf{y}(t), t) dt &\approx \Delta t \mathbf{f}(\mathbf{y}_n, t_n) \\ \int_{t_n}^{t_{n+1}} \mathbf{f}(\mathbf{y}(t), t) dt &\approx \Delta t \mathbf{f}(\mathbf{y}_{n+1}, t_{n+1}) \\ \int_{t_n}^{t_{n+1}} \mathbf{f}(\mathbf{y}(t), t) dt &\approx \frac{\Delta t}{2} [\mathbf{f}(\mathbf{y}_{n+1}, t_{n+1}) + \mathbf{f}(\mathbf{y}_n, t_n)] \\ \int_{t_n}^{t_{n+1}} \mathbf{f}(\mathbf{y}(t), t) dt &\approx \Delta t \mathbf{f}(\mathbf{y}_{n+\frac{1}{2}}, t_{n+\frac{1}{2}}) \\ \int_{t_n}^{t_{n+1}} \mathbf{f}(\mathbf{y}(t), t) dt &\approx \frac{\Delta t}{6} [\mathbf{f}(\mathbf{y}_{n+1}, t_{n+1}) + 4\mathbf{f}(\mathbf{y}_{n+\frac{1}{2}}, t_{n+\frac{1}{2}}) + \mathbf{f}(\mathbf{y}_n, t_n)], \end{aligned} \quad (2.71)$$

with $(\cdot)_{n+\frac{1}{2}} = \frac{1}{2} [(\cdot)_{n+1} + (\cdot)_n]$ being the evaluation at the subinterval midpoint.

A valid method needs to be *stable* for moderate time step sizes Δt which, by definition, means that given two perturbations in (2.70), the difference

between the respective solutions are bounded for $0 \leq \Delta t \leq \Delta t_0$, with Δt_0 being the maximum time step size for which the method is stable. The stability issue can only be in-depth developed for partial differential equations with the format $\mathbf{f}(\mathbf{y}(t), t) = \mathbf{A}\mathbf{y}(t)$, $\mathbf{A}$ being a real matrix of constant components whose eigenvalues' real part are negative. In such a case, the concept of *unconditionally stable area* is of importance since it defines all the possible choices for the time step sizes ensuring stable integrations.

For generally non-linear problems, standard methods cannot guarantee stability. However, in the literature different works, e.g. Simó et al. (1992), Stuart & Humphries (1998) or García Orden & Goicolea (2000), have reported that the preservation of qualitative features, particularly the energy, at every time step considerably enhances the stability. This conclusion motivated the search for non-standard integration methods with structure-preserving features, origin of the methods analyzed in this dissertation.

An important conclusion of integration methods' theory asserts that *stability* and *consistency* are necessary and sufficient conditions for a method to be *convergent*, meaning that the maximal error among all time steps is limited and tends to zero as the time step is diminishing, that is

$$\max_{0 \leq n \leq N} \|\mathbf{y}(t_n) - \mathbf{y}_n\| \rightarrow 0 \quad \text{when } \Delta t \rightarrow 0 \quad (2.72)$$

Another important concept is the order of accuracy of the approximation. It measures the rate at which the method converge to the exact solution when diminishing the time step size. That is, second-order accurate methods will converge quadratically to the exact solution as the time step is reduced. In other words, the error can be demonstrated to be bounded by a proportional part of the time step to the power of the order of accuracy z , that is $e(\Delta t) \leq C \Delta t^z$. It is also intimately related to the power of the polynomials that can exactly be integrated. Thus, the *Euler* methods are just first-order accurate and only integrate exactly linear functions, both the *Trapezoidal* and *Midpoint* methods are second-order, exactly integrating parabolic functions, while the *Simpson* method is third-order accurate. The order of accuracy can be enhanced not only by incrementing the degree of the polynomial exactly integrated but by performing the integral approximation in successive stages within the time subinterval, each of them with low order of accuracy. One of the most prominent example of the latter approach is the family of *Runge-Kutta* methods, see Butcher (1996); Kutta (1901).

In addition, if the approximation involves the value of the unknown state at t_{n+1} , the resulting method is said to be *implicit*, as an implicit equation

needs to be solved. If not, the resulting method is *explicit*. Generally speaking, the explicit methods require smaller time step sizes than implicit ones to be stable. Interestingly, there exist implicit methods that, in the linear context, show unconditional stability for any time step size, that is, their unconditional stable area is infinite.

On the other hand, on-purpose methods for the solution of structural dynamics have become widespread. The structural dynamic evolution equations are dominated by second order ODE so the methods are defined in terms of first and second time derivative. The family of β -Newmark (Newmark (1959)) and of α -Generalized (Chung & Hulbert (1993)) methods are the most representative examples of these methods, usually referred to as *structural* methods. An important particular case of the last family is the HHT method named after Hilber et al. (1977) and intended for the elimination of non-desirable high frequencies due to the spatial discretization.

Particularly, given the typical structural dynamic second order ODE evaluated at some instant time $t = t_{n+1}$

$$\mathbf{M}_{n+1}\ddot{\mathbf{q}}_{n+1} + \mathbf{C}_{n+1}\dot{\mathbf{q}}_{n+1} + \mathbf{K}_{n+1}\mathbf{q}_{n+1} = \mathbf{F}_{n+1}, \quad (2.73)$$

the β -Newmark family provides the following formulas

$$\begin{aligned} \mathbf{q}_{n+1} &= \mathbf{q}_n + \Delta t \dot{\mathbf{q}}_n + \left(\frac{1}{2} - \beta\right) \Delta t^2 \ddot{\mathbf{q}}_n + \beta \Delta t^2 \ddot{\mathbf{q}}_{n+1} \\ \dot{\mathbf{q}}_{n+1} &= \dot{\mathbf{q}}_n + (1 - \gamma) \Delta t \ddot{\mathbf{q}}_n + \gamma \Delta t \ddot{\mathbf{q}}_{n+1} \end{aligned} \quad (2.74)$$

with β, γ being two constant limited by the method's stability to be $0 \leq \gamma \leq 1$ and $0 \leq \beta \leq \frac{1}{2}$.

The most important methods of this family are the trapezoidal rule or the constant acceleration method (implicit), the modified trapezoidal rule (implicit), the linear acceleration method (implicit) and the central differences method (explicit). For instance, the trapezoidal rule corresponds to $\beta = \frac{1}{4}$ and $\gamma = \frac{1}{2}$.

Among all these choices, from now on the interest will be in the standard Midpoint and Trapezoidal methods because they are implicit and second-order accurate and entail some conservation properties. For instance, the Midpoint method is *symplectic*, see Simó et al. (1992), and preserves the symmetries of dynamic equations: total linear and angular momentum. In fact, as it will be demonstrated in subsequent Chapters, the Midpoint method can be interpreted as a first approach of the Energy-Entropy-Momentum methods to be presented. Interestingly, both Trapezoidal and Midpoint methods

collapse to the same method for linear problems and preserve first integrals in such a context.

2.3.1 Midpoint method for the two thermo-spring system

According to (2.67), (2.70) and (2.71)₄, the following midpoint formulas can be deduced

$$\begin{aligned} \mathbf{y}_{n+\frac{1}{2}} &= \frac{1}{2}(\mathbf{y}_{n+1} + \mathbf{y}_n) \\ \dot{\mathbf{y}}_{n+\frac{1}{2}} &= \frac{1}{2}(\dot{\mathbf{y}}_{n+1} + \dot{\mathbf{y}}_n) = \frac{\mathbf{y}_{n+1} - \mathbf{y}_n}{\Delta t} \end{aligned} \quad (2.75)$$

Furthermore, it is appropriated to introduce the following notation to make clear the midpoint-type formulations to be developed from now on

$$\begin{aligned} (\cdot)_{n+\frac{1}{2}} &= \frac{1}{2}[(\cdot)_{n+1} + (\cdot)_n] \\ (\cdot)|_{n+\frac{1}{2}} &= \text{evaluation at midpoint} \end{aligned} \quad (2.76)$$

Then, identifying the right hand side of (2.17) with the nonlinear vector-valued function $\mathbf{f}(\mathbf{y}(t), t)$ of (2.67), the midpoint temporal discretization of the two thermo-spring system formulated in temperature variables (2.45) results in

$$\begin{aligned} \frac{\mathbf{q}_{1,n+1} - \mathbf{q}_{1,n}}{\Delta t} &= \frac{1}{m_1} \mathbf{p}_{1,n+\frac{1}{2}} \\ \frac{\mathbf{q}_{2,n+1} - \mathbf{q}_{2,n}}{\Delta t} &= \frac{1}{m_2} \mathbf{p}_{2,n+\frac{1}{2}} \\ \frac{\mathbf{p}_{1,n+1} - \mathbf{p}_{1,n}}{\Delta t} &= - \frac{\partial \Psi_1}{\partial \lambda_1} \Big|_{n+\frac{1}{2}} \frac{\mathbf{q}_{1,n+\frac{1}{2}}}{\lambda_1|_{n+\frac{1}{2}}} - \frac{\partial \Psi_2}{\partial \lambda_2} \Big|_{n+\frac{1}{2}} \frac{(\mathbf{q}_1 - \mathbf{q}_2)_{n+\frac{1}{2}}}{\lambda_2|_{n+\frac{1}{2}}} + \bar{\mathbf{f}}_1 \\ \frac{\mathbf{p}_{2,n+1} - \mathbf{p}_{2,n}}{\Delta t} &= - \frac{\partial \Psi_2}{\partial \lambda_2} \Big|_{n+\frac{1}{2}} \frac{(\mathbf{q}_2 - \mathbf{q}_1)_{n+\frac{1}{2}}}{\lambda_2|_{n+\frac{1}{2}}} + \bar{\mathbf{f}}_2 \\ \frac{\theta_{1,n+1} - \theta_{1,n}}{\Delta t} &= \frac{1}{c_1} \left[-\theta_{1,n+\frac{1}{2}} \frac{\partial \eta_1}{\partial \lambda_1} \Big|_{n+\frac{1}{2}} \frac{\mathbf{q}_{1,n+\frac{1}{2}}}{\lambda_1|_{n+\frac{1}{2}}} \cdot \frac{\mathbf{p}_{1,n+\frac{1}{2}}}{m_1} + h|_{n+\frac{1}{2}} \right] \\ \frac{\theta_{2,n+1} - \theta_{2,n}}{\Delta t} &= \frac{1}{c_2} \left[-\theta_{1,n+\frac{1}{2}} \frac{\partial \eta_1}{\partial \lambda_1} \Big|_{n+\frac{1}{2}} \frac{(\mathbf{q}_1 - \mathbf{q}_2)_{n+\frac{1}{2}}}{\lambda_2|_{n+\frac{1}{2}}} \cdot \frac{\mathbf{p}_{1,n+\frac{1}{2}}}{m_1} \right. \\ &\quad \left. - \theta_{2,n+\frac{1}{2}} \frac{\partial \eta_2}{\partial \lambda_2} \Big|_{n+\frac{1}{2}} \frac{(\mathbf{q}_2 - \mathbf{q}_1)_{n+\frac{1}{2}}}{\lambda_2|_{n+\frac{1}{2}}} \cdot \frac{\mathbf{p}_{2,n+\frac{1}{2}}}{m_2} - h|_{n+\frac{1}{2}} \right], \end{aligned} \quad (2.77)$$

where use has been made of (2.4).

In view of the resulting formulation, the key point in a midpoint-type approximation of (nonlinear) evolution equations is that only the state variables and their time derivatives are approximated in any time interval by their midpoint values (2.75). Thus, all functions depending on the state variables are necessarily evaluated at midpoint via them. That is, for instance, the spring elongations (2.2) are provided by

$$\begin{aligned}\lambda_1|_{n+\frac{1}{2}} &= \lambda_1(\mathbf{q}_{1,n+\frac{1}{2}}) = \|\mathbf{q}_{1,n+\frac{1}{2}}\| \\ \lambda_2|_{n+\frac{1}{2}} &= \lambda_2(\mathbf{q}_{1,n+\frac{1}{2}}, \mathbf{q}_{2,n+\frac{1}{2}}) = \|(\mathbf{q}_2 - \mathbf{q}_1)_{n+\frac{1}{2}}\|,\end{aligned}\tag{2.78}$$

whereas the heat flux (2.1) evaluated at midpoint results in

$$h|_{n+\frac{1}{2}} = k(\theta_{2,n+\frac{1}{2}} - \theta_{1,n+\frac{1}{2}})\tag{2.79}$$

Likewise, the constitutive relations (2.5) and (2.16), for $a = 1, 2$, evaluated at midpoint are provided by

$$\begin{aligned}f_a|_{n+\frac{1}{2}} &= \left. \frac{\partial \Psi_a}{\partial \lambda_a} \right|_{n+\frac{1}{2}} = \frac{\partial \Psi_a}{\partial \lambda_a}(\lambda_a|_{n+\frac{1}{2}}, \theta_{a,n+\frac{1}{2}}) \\ v_a|_{n+\frac{1}{2}} &= \theta_{a,n+\frac{1}{2}} \left. \frac{\partial \eta_a}{\partial \lambda_a} \right|_{n+\frac{1}{2}} = \theta_{a,n+\frac{1}{2}} \frac{\partial \eta_a}{\partial \lambda_a}(\lambda_a|_{n+\frac{1}{2}}, \theta_{a,n+\frac{1}{2}})\end{aligned}\tag{2.80}$$

In the same way, the Midpoint method applied to the entropy formulation (2.24) reads

$$\begin{aligned}\frac{\mathbf{q}_{1,n+1} - \mathbf{q}_{1,n}}{\Delta t} &= \frac{1}{m_1} \mathbf{p}_{1,n+\frac{1}{2}} \\ \frac{\mathbf{q}_{2,n+1} - \mathbf{q}_{2,n}}{\Delta t} &= \frac{1}{m_2} \mathbf{p}_{2,n+\frac{1}{2}} \\ \frac{\mathbf{p}_{1,n+1} - \mathbf{p}_{1,n}}{\Delta t} &= - \left. \frac{\partial e_1}{\partial \lambda_1} \right|_{n+\frac{1}{2}} \frac{\mathbf{q}_{1,n+\frac{1}{2}}}{\lambda_1|_{n+\frac{1}{2}}} - \left. \frac{\partial e_2}{\partial \lambda_2} \right|_{n+\frac{1}{2}} \frac{(\mathbf{q}_1 - \mathbf{q}_2)_{n+\frac{1}{2}}}{\lambda_2|_{n+\frac{1}{2}}} + \tilde{\mathbf{f}}_1 \\ \frac{\mathbf{p}_{2,n+1} - \mathbf{p}_{2,n}}{\Delta t} &= - \left. \frac{\partial e_2}{\partial \lambda_2} \right|_{n+\frac{1}{2}} \frac{(\mathbf{q}_2 - \mathbf{q}_1)_{n+\frac{1}{2}}}{\lambda_2|_{n+\frac{1}{2}}} + \tilde{\mathbf{f}}_2 \\ \frac{\eta_{1,n+1} - \eta_{1,n}}{\Delta t} &= \frac{1}{\theta_1|_{n+\frac{1}{2}}} h|_{n+\frac{1}{2}} \\ \frac{\eta_{2,n+1} - \eta_{2,n}}{\Delta t} &= \frac{-1}{\theta_2|_{n+\frac{1}{2}}} h|_{n+\frac{1}{2}},\end{aligned}\tag{2.81}$$

with the temperatures being in this case a function of the state variables (2.27) whose midpoint evaluations are provided by

$$\theta_a|_{n+\frac{1}{2}} = \frac{\partial e_a}{\partial \eta_a}(\lambda_a|_{n+\frac{1}{2}}, \eta_{a,n+\frac{1}{2}}) = \theta_a(\lambda_a|_{n+\frac{1}{2}}, \eta_{a,n+\frac{1}{2}}) \quad (2.82)$$

Accordingly, the heat flux results in

$$h|_{n+\frac{1}{2}} = k(\theta_2|_{n+\frac{1}{2}} - \theta_1|_{n+\frac{1}{2}}), \quad (2.83)$$

and the internal force constitutive relation in

$$f_a|_{n+\frac{1}{2}} = \frac{\partial e_a}{\partial \lambda_a} \Big|_{n+\frac{1}{2}} = \frac{\partial e_a}{\partial \lambda_a}(\lambda_a|_{n+\frac{1}{2}}, \eta_{a,n+\frac{1}{2}}) \quad (2.84)$$

Laws of thermodynamics and symmetries. The performed approximation is not harmless at all regarding the conservation properties (2.31) - (2.36). In fact, the loss of energy conservation for force-free evolution is a well-known result for solutions of nonlinear Hamiltonian problems provided by the midpoint method, see Simó & Tarnow (1992). On the positive side, the midpoint method does possess the conservation of the symplectic structure of the Hamiltonian flow, details can be found in Feng (1986), and of the angular momentum. The latter can be verified by computing the angular momentum balance in any time interval as

$$\begin{aligned} \mathbf{J}_{n+1} - \mathbf{J}_n &= \sum_{a=1}^2 (\mathbf{p}_{a,n+1} \wedge \mathbf{q}_{a,n+1} - \mathbf{p}_{a,n} \wedge \mathbf{q}_{a,n}) \\ &= \sum_{a=1}^2 \left[\mathbf{q}_{a,n+\frac{1}{2}} \wedge (\mathbf{p}_{a,n+1} - \mathbf{p}_{a,n}) - \mathbf{p}_{a,n+\frac{1}{2}} \wedge (\mathbf{q}_{a,n+1} - \mathbf{q}_{a,n}) \right] \\ &= \Delta t \left[\mathbf{q}_{1,n+\frac{1}{2}} \wedge \left(-f_1|_{n+\frac{1}{2}} \frac{\mathbf{q}_{1,n+\frac{1}{2}}}{\lambda_{1,n+\frac{1}{2}}} \right) \right. \\ &\quad \left. + \mathbf{q}_{2,n+\frac{1}{2}} \wedge \left(-f_2|_{n+\frac{1}{2}} \frac{(\mathbf{q}_1 - \mathbf{q}_2)_{n+\frac{1}{2}}}{\lambda_{2,n+\frac{1}{2}}} - f_2|_{n+\frac{1}{2}} \frac{(\mathbf{q}_2 - \mathbf{q}_1)_{n+\frac{1}{2}}}{\lambda_{2,n+\frac{1}{2}}} \right) \right] = \mathbf{0} \end{aligned} \quad (2.85)$$

This result applies for the both formulations (2.77) and (2.81) since it is independent of the definition of the internal force provided by either (2.80)₁ or (2.84).

On the other hand, the loss of the energy conservation can also be proved by computing its balance in any time step as

$$\begin{aligned}
E_{n+1} - E_n &= K_{n+1} + U_{n+1} - K_n - U_n \\
&= \sum_{a=1}^2 \left(\frac{1}{2m_a} \|\mathbf{p}_{a,n+1}\|^2 - \frac{1}{2m_a} \|\mathbf{p}_{a,n}\|^2 + e_{a,n+1} - e_{a,n} \right) \\
&= \sum_{a=1}^2 \left(\frac{1}{2m_a} (\mathbf{p}_{a,n+1} + \mathbf{p}_{a,n}) \cdot (\mathbf{p}_{a,n+1} - \mathbf{p}_{a,n}) + e_{a,n+1} - e_{a,n} \right)
\end{aligned} \tag{2.86}$$

Using either (2.77) or (2.81) and discarding the external forces, the energy balance can be further elaborated to give

$$\begin{aligned}
E_{n+1} - E_n &= -f_1|_{n+\frac{1}{2}} \frac{\lambda_1|_{n+1}^2 - \lambda_1|_n^2}{\lambda_1|_{n+\frac{1}{2}}} - f_2|_{n+\frac{1}{2}} \frac{\lambda_2|_{n+1}^2 - \lambda_2|_n^2}{\lambda_2|_{n+\frac{1}{2}}} \\
&\quad - f_2|_{n+\frac{1}{2}} \frac{\lambda_2|_{n+1}^2 - \lambda_2|_n^2}{\lambda_2|_{n+\frac{1}{2}}} + e_{1,n+1} - e_{1,n} + e_{2,n+1} - e_{2,n} \neq 0,
\end{aligned} \tag{2.87}$$

which generally holds non-zero, concluding that the energy balance is not satisfied by the Midpoint method.

Regarding the entropy balance, the entropy formulation (2.81) readily allows to write

$$\begin{aligned}
S_{n+1} - S_n &= \sum_{a=1}^2 (\eta_{a,n+1} - \eta_{a,n}) = \left(\frac{1}{\theta_1|_{n+\frac{1}{2}}} - \frac{1}{\theta_2|_{n+\frac{1}{2}}} \right) h|_{n+\frac{1}{2}} \\
&= k \frac{\left(\theta_2|_{n+\frac{1}{2}} - \theta_1|_{n+\frac{1}{2}} \right)^2}{\theta_1|_{n+\frac{1}{2}} \theta_2|_{n+\frac{1}{2}}} \geq 0,
\end{aligned} \tag{2.88}$$

demonstrating the fulfillment of the second law by this formulation. In contrast, the temperature formulation (2.77) does not inherit this feature as the entropy balance cannot be reached from the discrete equation written in terms of temperature (2.77).

2.3.2 Midpoint method for the thermo-viscoelastic system

Similarly, the thermo-visco-elastic system evolution equations are approximated by the Midpoint method (2.75). The temperature formulation (2.45) thus results in

$$\begin{aligned}
\frac{\mathbf{q}_{1,n+1} - \mathbf{q}_{1,n}}{\Delta t} &= \frac{1}{m_1} \mathbf{p}_{1,n+\frac{1}{2}} \\
\frac{\mathbf{q}_{2,n+1} - \mathbf{q}_{2,n}}{\Delta t} &= \frac{1}{m_2} \mathbf{p}_{2,n+\frac{1}{2}} \\
\frac{\mathbf{p}_{1,n+1} - \mathbf{p}_{1,n}}{\Delta t} &= - \left. \frac{\partial \Psi}{\partial \lambda} \right|_{n+\frac{1}{2}} \frac{(\mathbf{q}_1 - \mathbf{q}_2)_{n+\frac{1}{2}}}{\lambda|_{n+\frac{1}{2}}} + \tilde{\mathbf{f}}_1 \\
\frac{\mathbf{p}_{2,n+1} - \mathbf{p}_{2,n}}{\Delta t} &= - \left. \frac{\partial \Psi}{\partial \lambda} \right|_{n+\frac{1}{2}} \frac{(\mathbf{q}_2 - \mathbf{q}_1)_{n+\frac{1}{2}}}{\lambda|_{n+\frac{1}{2}}} + \tilde{\mathbf{f}}_2 \\
\frac{\gamma_{n+1} - \gamma_n}{\Delta t} &= - \frac{1}{\nu|_{n+\frac{1}{2}}} \left. \frac{\partial \Psi}{\partial \gamma} \right|_{n+\frac{1}{2}} \\
\frac{\theta_{n+1} - \theta_n}{\Delta t} &= \frac{1}{c} \left[-\theta_{n+\frac{1}{2}} \left. \frac{\partial \eta}{\partial \lambda} \right|_{n+\frac{1}{2}} \frac{(\mathbf{q}_2 - \mathbf{q}_1)_{n+\frac{1}{2}}}{\lambda|_{n+\frac{1}{2}}} \cdot \frac{\mathbf{p}_{1,n+\frac{1}{2}}}{m_1} \right. \\
&\quad \left. + \frac{1}{\nu|_{n+\frac{1}{2}}} \left. \frac{\partial \Psi}{\partial \gamma} \right|_{n+\frac{1}{2}} \left(\left. \frac{\partial \Psi}{\partial \gamma} \right|_{n+\frac{1}{2}} + \theta_{n+\frac{1}{2}} \left. \frac{\partial \eta}{\partial \gamma} \right|_{n+\frac{1}{2}} \right) - h|_{n+\frac{1}{2}} \right] \\
\frac{\vartheta_{n+1} - \vartheta_n}{\Delta t} &= \frac{1}{\varsigma} h|_{n+\frac{1}{2}}
\end{aligned} \tag{2.89}$$

with the midpoint evaluated functions (2.46) and (2.51) being provided by

$$\begin{aligned}
f|_{n+\frac{1}{2}} &= \left. \frac{\partial \Psi}{\partial \lambda} \right|_{n+\frac{1}{2}}, \quad g|_{n+\frac{1}{2}} = - \left. \frac{\partial \Psi}{\partial \gamma} \right|_{n+\frac{1}{2}}, \quad v|_{n+\frac{1}{2}} = \theta_{n+\frac{1}{2}} \left. \frac{\partial \eta}{\partial \lambda} \right|_{n+\frac{1}{2}} \\
w|_{n+\frac{1}{2}} &= \theta_{n+\frac{1}{2}} \left. \frac{\partial \Psi}{\partial \gamma} \right|_{n+\frac{1}{2}}, \quad \nu|_{n+\frac{1}{2}} = \nu(\theta_{n+\frac{1}{2}})
\end{aligned} \tag{2.90}$$

The midpoint approximation of the entropy formulation (2.54) then reads

$$\begin{aligned}
\frac{\mathbf{q}_{1,n+1} - \mathbf{q}_{1,n}}{\Delta t} &= \frac{1}{m_1} \mathbf{p}_{1,n+\frac{1}{2}} \\
\frac{\mathbf{q}_{2,n+1} - \mathbf{q}_{2,n}}{\Delta t} &= \frac{1}{m_2} \mathbf{p}_{2,n+\frac{1}{2}} \\
\frac{\mathbf{p}_{1,n+1} - \mathbf{p}_{1,n}}{\Delta t} &= - \left. \frac{\partial e}{\partial \lambda} \right|_{n+\frac{1}{2}} \frac{(\mathbf{q}_1 - \mathbf{q}_2)_{n+\frac{1}{2}}}{\lambda|_{n+\frac{1}{2}}} + \tilde{\mathbf{f}}_1 \\
\frac{\mathbf{p}_{2,n+1} - \mathbf{p}_{2,n}}{\Delta t} &= - \left. \frac{\partial e}{\partial \lambda} \right|_{n+\frac{1}{2}} \frac{(\mathbf{q}_2 - \mathbf{q}_1)_{n+\frac{1}{2}}}{\lambda|_{n+\frac{1}{2}}} + \tilde{\mathbf{f}}_2 \\
\frac{\gamma_{n+1} - \gamma_n}{\Delta t} &= - \frac{1}{\nu|_{n+\frac{1}{2}}} \left. \frac{\partial e}{\partial \gamma} \right|_{n+\frac{1}{2}} \\
\frac{\eta_{n+1} - \eta_n}{\Delta t} &= \frac{1}{\theta|_{n+\frac{1}{2}}} \left[\frac{1}{\nu|_{n+\frac{1}{2}}} \left(\left. \frac{\partial e}{\partial \gamma} \right|_{n+\frac{1}{2}} \right)^2 - h|_{n+\frac{1}{2}} \right] \\
\frac{\sigma_{n+1} - \sigma_n}{\Delta t} &= \frac{h|_{n+\frac{1}{2}}}{\vartheta|_{n+\frac{1}{2}}}
\end{aligned} \tag{2.91}$$

In this formulation, the temperatures are functions of the state variables so they must be computed through the midpoint evaluation of them

$$\theta|_{n+\frac{1}{2}} = \frac{\partial e}{\partial \eta}(\lambda|_{n+\frac{1}{2}}, \eta_{n+\frac{1}{2}}, \gamma_{n+\frac{1}{2}}), \quad \vartheta|_{n+\frac{1}{2}} = \frac{d\epsilon}{d\sigma}(\sigma_{n+\frac{1}{2}}) \tag{2.92}$$

Accordingly, the viscosity function (2.51) must be evaluated by the element temperature function as

$$\nu|_{n+\frac{1}{2}} = \nu(\theta|_{n+\frac{1}{2}}) = \nu(\theta(\lambda|_{n+\frac{1}{2}}, \eta_{n+\frac{1}{2}}, \gamma_{n+\frac{1}{2}})) \tag{2.93}$$

Laws of thermodynamics and symmetries. As in the two thermo-spring system, the balances of the continuous first integrals (linear and angular momentum, energy) and the entropy in any time interval lead to the preservation of both linear and angular momentums, the breach of the energy preservation and the satisfaction of the entropy inequality by the entropy formulation (2.91) and the breach of such inequality by the temperature formulation (2.89).

2.3.3 Numerical Experiments

All the identified features of the midpoint-based time integration of the two thermo-spring system and the thermo-viscoelastic system are illustrated next based on five numerical experiments.

For the two thermo-spring system, three numerical examples are proposed with the following characteristics:

- Example 1 reproduces one of the examples proposed in Romero (2009). Specifically, the first one based on a constant spring stiffnesses $C_a > 0$ and the following constant data: $m_1 = 1$ kg, $m_2 = 2$ kg, $C_1 = 0.1$ Pa, $C_2 = 1$ Pa, $\lambda_1^0 = 2$ m, $\lambda_2^0 = 1$ m, $k = 300$ Js⁻¹K⁻¹, $\alpha_1 = \alpha_2 = 0.2$ JK⁻¹, $c_1 = c_2 = 5$ JK⁻¹ and $\theta_{\text{ref}} = 300$ K. Then, the system is set in motion by the following initial conditions:

$$\mathbf{q}_1^0 = \mathbf{e}_1, \quad \mathbf{p}_1^0 = 2\mathbf{e}_2, \quad \mathbf{q}_2^0 = 2.2\mathbf{e}_1, \quad \mathbf{p}_2^0 = \mathbf{e}_1, \quad \theta_1^0 = 380, \quad \theta_2^0 = 310$$

- Example 2 is taken from Krüger et al. (2011) and is dominated by high frequencies giving raise to a *stiff* problem. It is based on constant spring stiffness and uses the following constant data: $m_1 = 1$ kg, $m_2 = 2$ kg, $C_1 = 100$ Pa, $C_2 = 100$ Pa, $\lambda_1^0 = 2$ m, $\lambda_2^0 = 1$ m, $k = 10$ Js⁻¹K⁻¹, $\alpha_1 = \alpha_2 = 0.2$ JK⁻¹, $c_{0,1} = c_{0,2} = 1000$ JK⁻¹ and $\theta_{\text{ref}} = 300$ K; and with the following initial conditions

$$\mathbf{q}_{1,0} = 1\mathbf{e}_1, \quad \mathbf{p}_{1,0} = 1\mathbf{e}_2, \quad \mathbf{q}_{2,0} = 2.2\mathbf{e}_1, \quad \mathbf{p}_{2,0} = 4.4\mathbf{e}_2, \quad \theta_{1,0} = 380, \quad \theta_{2,0} = 310$$

- Example 3 further explores the applicability of the temperature formulation in a case impossible to be solved by formulations based on entropy. It is based on a non-linear temperature-dependent function for the spring stiffness expressed by

$$C_a(\theta_\alpha) = C_a^0 - C_a^1 \theta_{\text{ref}} \log \left(\frac{\theta_a}{\theta_{\text{ref}}} \right) \quad (2.94)$$

The data employed in the simulation is:

$m_1 = 10$ kg; $m_2 = 20$ kg; $C_1^0 = 5000$ Pa; $C_2^0 = 10000$ Pa; $C_1^1 = 50$ PaK⁻¹; $C_2^1 = 60$ PaK⁻¹; $\lambda_1^0 = 2$ m; $\lambda_2^0 = 1$ m; $k = 300$ Js⁻¹K⁻¹; $\alpha_1 = \alpha_2 = 20$ JK⁻¹; $c_{0,1} = 5000$ JK⁻¹; $c_{0,2} = 2000$ JK⁻¹; $\theta_{\text{ref}} = 300$ K.

The initial conditions are provided by:

$$\mathbf{q}_{1,0} = 3\mathbf{e}_1 + 0.5\mathbf{e}_3, \quad \mathbf{p}_{1,0} = 10\mathbf{e}_2, \quad \mathbf{q}_{2,0} = 3\mathbf{e}_1 + \mathbf{e}_2 + \mathbf{e}_3, \quad \mathbf{p}_{2,0} = -20\mathbf{e}_3$$

$$\theta_{1,0} = 380, \quad \theta_{2,0} = 298$$

The first numerical example is integrated within the time interval $[0, 25]$ s with constant time step size $\Delta t = 0.3$ s using the Midpoint method applied to the temperature formulation (2.77) and the entropy formulation (2.81). Figure 2.3 and Figure 2.4 show the obtained degrees of freedom and the evolutions of total energy, total entropy and the norm of the total angular momentum.

Figure 2.3. Example 1: solution obtained with the Midpoint method formulated in temperature variables with $\Delta t = 0.3$ s

Figure 2.4. Example 1: solution obtained with the Midpoint method formulated in entropy variables with $\Delta t = 0.3$ s

Both methods are stable for the time step used as they manage to maintain the evolution of energy bounded although, as expected, none of them provides the correct first law of thermodynamics, confirming the theoretical result deduced by (2.87). Significantly, the dissatisfaction of the first law is much more pronounced at the beginning of the simulation when the evolu-

tions of temperatures are dramatically oscillating. Such oscillations are due to the time step size used suggesting that it is not an appropriated one to capture the dynamics of the problem.

Figure 2.5. Example 2: solution obtained with the Midpoint method formulated in temperature variables with $\Delta t = 0.1$ s

On the other hand, the total entropy evolution seems to be less problematic although, once again, at the beginning of the simulation, the temperature

formulation, **Figure 2.3**, breaks the second law. In contrast, the entropy formulation agrees with the second law as was dictated by (2.88). In both cases, the angular momentum preservation is satisfied according to (2.85).

Now, the second example is integrated using the temperature-based and the entropy-based midpoint methods within the time interval $[0, 500]$ s with constant time step size $\Delta t = 0.1$ s.

This moderate time step leads both methods to a non-physical solution for the elongations, as shown in **Figure 2.5** and **Figure 2.6**, highlighting that a solution disagreeing with the essential physical features may be completely spurious despite a successful integration. Thus, the first law of thermodynamics is breached by both methods although, once again, they manage to have the total energy bounded, hence its successful integration. In contrast, the second law is satisfied by the entropy-based Midpoint method while the temperature-based Midpoint method is clearly unable to meet it. The angular momentum, on the other hand, is correctly computed by both methods, as expected.

Finally, the third example is solved just by the temperature-based Midpoint method (2.77) since the entropy-based Midpoint method cannot handle with the non-linear dependency of spring stiffnesses. This examples additionally brings into play a 3D motion of the two masses and a high thermomechanic coupling.

Then, the temperature-based Midpoint is used with a time step of $\Delta t = 0.1$ s to integrate the motion up to 25 s. The results are summarized in **Figure 2.7** and clearly show that the simulation became unstable at the half of whole time interval. The behavior of the total energy reveals that the method fails when it dramatically and uncontrollably decays. Before this event, both law of thermodynamics are breached although the angular momentum adheres to its conservation law.

With these three simple examples, the limitations for the standard Midpoint method to handle a simple nonlinear dissipative problem have been highlighted and reasoned that are intimately related to its inability to fulfill essential physical rules, chiefly with the first law of thermodynamics. Thus, the preservation of the angular momentum does not seem to be crucial for the stability of the method, neither the agreement with the second law seems to provide with extra stability's features as shows the entropy-based Midpoint solutions. Of course, the Midpoint method is consistent meaning that by diminishing the time step these limitation are alleviated although incrementing the computational costs and times. All these problems are to be bypassed

Figure 2.6. Example 2: solution obtained with the Midpoint method formulated in entropy variables with $\Delta t = 0.1$ s

Figure 2.7. Example 3: solution obtained with the Midpoint method formulated in temperature variables with $\Delta t = 0.1$ s

with methods based precisely on the conservation of all the underlying essential physical features.

For the thermo-viscoelastic system, consider a system composed of a particle of mass m connected by a thermo-viscoelastic element to a fixed point of space. In addition, the parameter $\mu(\theta)$ associated with the free energy function of the Maxwell element is assumed to have a linear dependence with the temperature, provided by $\mu(\theta) = \mu_0 - \mu_1(\theta - \theta_{\text{ref}})$, with $\mu_0, \mu_1 > 0$.

The parameters employed in the simulation are $\theta_{\text{ref}} = 300$ K, $m = 1$ kg, $\lambda_0 = 1$ m, $\alpha = 4$ JK⁻¹, $c = 1$ JK⁻¹, $\mu_0 = 5$ Jm⁻², $\mu_1 = 0.1$ Jm⁻²K⁻¹, $\nu_0 = 100$ Nsm⁻¹, $a = 10$ K, $k = 10$ Js⁻¹K⁻¹. The motion is integrated with a constant time step size and initial conditions:

$$\mathbf{q}^0 = [3, 0] \text{ m} \quad , \quad \dot{\mathbf{q}}^0 = [0, 1] \text{ m/s} \quad , \quad \gamma^0 = 0 \text{ m} \quad , \quad \theta^0 = 380 \text{ K} \quad (2.95)$$

Then, two different cases are considered:

- Case I. Constant environment temperature $\vartheta = \theta_{\text{ref}}$ and a linear temperature-dependent stiffness $C(\theta) = C_0 - C_1(\theta - \theta_{\text{ref}})$, with $C_0 = 100$ Pa and $C_1 = 0.5$ PaK⁻¹.

This case corresponds to the model solved in García Orden & Romero (2011) with the entropy formulation and validated with a reference solution.

- Case II. Non-constant environment temperature ϑ and non-linear temperature-dependent stiffness

$$C(\theta) = C_0 - C_1 \theta_{\text{ref}} \log(\theta/\theta_{\text{ref}}), \quad (2.96)$$

with $C_0 = 100$ Pa and $C_1 = 0.5$ PaK⁻¹.

Specific heat capacity $\varsigma = 120$ JK⁻¹. The initial environment temperature is set to $\vartheta_0 = \theta_{\text{ref}} = 300$ K.

Note that Case I is the limit case of Case II for large values of ς and small temperature changes with respect to the environment temperature.

Results for Case I. First, the entropy formulation is analyzed. Since no analytical results are available, the solution obtained with the entropy-based Midpoint method (2.91) and a time step size $\Delta t_{\text{ref}} = 10^{-2}$ s has been adopted as a reference. Figure 2.8 collects the curves of the reference trajectory, temperature, internal variable, total energy, total entropy and total angular momentum up to 20 s. These results suggest that there is a limit configuration

of relative equilibrium, where the trajectory is circular and the element temperature equals the environment one. The initial temperature oscillations are caused by the viscous dissipation of the dashpot, while the smooth long-term behavior is dominated by the heat conduction process. The whole evolution is controlled by the laws of thermodynamics and symmetries as shows the curves for the total energy, total entropy and total angular momentum. The time step size is then small enough to not spoil the preservation features of the system, thus demonstrating the physical consistency of the Midpoint method.

Figure 2.9 contains the results obtained with the Midpoint method formulated in entropy variables and with a time step twenty times larger, that is $\Delta t = 0.2$ s. This time step size makes the method become unstable leading to the failure of integration before the 15 s. Once again, the wrong behavior of the total energy evolution explains the occurring instability since the total entropy and total angular momentum are satisfied, without seemingly contributing to stabilize the integration.

In contrast, the same time step size of $\Delta t = 0.2$ s is not critical for the temperature-based Midpoint method (2.89) to provide a stable solution as shows Figure 2.10. In this solution, the total energy does not neither adhere to the constraint of the first law, however, it does not drift significantly apart from it, definitely stabilizing the method's performance with this time step size. Unexpectedly, the second law is satisfied even though the temperature evolution clearly suggests the time step size to be inappropriate to capture the initial oscillations.

Results for Case II. The reference solution has been obtained with the temperature-based Midpoint method and a time step size of $\Delta t_{\text{ref}} = 10^{-2}$ s. The results are displayed in Figure 2.11 and show the expected long term convergence of the evolution of both element and environment temperatures due to the heat transfer between them while agreeing with the preservation features.

Then, a time step size of $\Delta t = 0.3$ is used to obtain the results contained in Figure 2.12. For this time step size, the temperature-based Midpoint method fails to satisfy the first law of thermodynamics. However, as in Case I, the behavior of the energy is good enough to attain a stable integration. Although the evolution of the total entropy does not strictly agree with the second law, it is quite satisfactory whereas the angular momentum is exactly preserved, as expected.

All these numerical experiments further corroborate the limitations of the

Figure 2.8. Case I: reference solution obtained with the Midpoint method formulated in entropy variables with $\Delta t = 0.01$ s

Figure 2.9. Case I: solution obtained with the Midpoint method formulated in entropy variables with $\Delta t = 0.2$ s

Figure 2.10. Case I: solution obtained with the Midpoint method formulated in temperature variables with $\Delta t = 0.2$ s

Midpoint method to deal with the first law of thermodynamics when using moderate time step sizes, as was also observed in the numerical experiments on the two thermo-spring system.

Figure 2.11. Case II: reference solution obtained with the Midpoint method formulated in temperature variables with $\Delta t = 0.01$ s

Figure 2.12. Case II: solution obtained with the Midpoint method formulated in temperature variables with $\Delta t = 0.3$ s

Nonlinear thermo-dissipative continuum dynamics

CHAPTER 3

The concern of this Chapter is to establish a general framework that encompasses the dynamics of thermo-dissipative continua, understood as continua that may experience geometrically nonlinear displacements and deformation coupled with temperature changes and transformations of the internal structure of the material which macroscopically result in dissipative (irreversible) changes. First, the Chapter starts with the kinematic assumptions for deformable continua, then, a thorough description of the generalized standard materials is provided to enable the formulation of general thermo-dissipative material behaviors. Along with these ingredients, balance laws are established to arrive at the strong form of the governing equations. Furthermore, the conservation properties of the resulting system of equations are deduced from the isolated dynamic equations. These developments have been based on some classical references such as Marsden & Hughes (1983) or Holzapfel (2000). A recent review on this topic can be found in Gurtin et al. (2010).

Once the continuous description is fully elaborated, the Galerkin FE-based spatial approximation is performed to transform the original infinite-dimensional problem into a finite-dimensional one. A brief summary on different spatial discretization techniques is also introduced. Among them all, the Galerkin approach is used due to its simplicity and ability to not damage the conservation properties identified in continuous systems. Finally, a subsequent temporal discretization based on standard time integration methods is proposed and studied regarding the laws of thermodynamics and symmetries.

3.1 Kinematics

Consider a continuum occupying a set of points in the undeformed (reference) configuration $\mathcal{B}_0 \subset \mathbb{R}^d$ with boundary $\partial\mathcal{B}_0$, d being the spatial dimension ($d = 1, 2, 3$), whose positions are collected in $\mathbf{X} \in \mathcal{B}_0$ (respect to an inertial frame of reference) and undergoing a time-dependent motion described by

$$\varphi : \mathcal{B}_0 \times [0, T] \ni (\mathbf{X}, t) \mapsto \varphi(\mathbf{X}, t) \in \mathbb{R}^d, \quad (3.1)$$

which maps any material point $\mathbf{X}$ to the point $\mathbf{x} = \varphi(\mathbf{X}, t) \in \mathbb{R}^d$ in the deformed configuration $\mathcal{B}_t = \varphi(\mathcal{B}_0, t) \subset \mathbb{R}^d$.

Figure 3.1. Continuum kinematics

The motion function (3.1) is assumed to be smooth so the tangent map, denoted as $\mathbf{F}$ and called the *deformation gradient*, can be defined at each point and time as

$$\mathbf{F}(\mathbf{X}, t) := \frac{\partial \varphi(\mathbf{X}, t)}{\partial \mathbf{X}} = \nabla_0 \varphi(\mathbf{X}, t), \quad (3.2)$$

∇_0 being the gradient operator in the reference configuration.

The deformation gradient transforms vectors in the tangent reference space $T_{\mathbf{X}}\mathcal{B}_0$ to vectors in the tangent spatial space $T_{\varphi}\mathcal{B}_t$. Thus, $\mathbf{F} : T_{\mathbf{X}}\mathcal{B}_0 \mapsto T_{\varphi}\mathcal{B}_t$ is a linear transformation for each $\mathbf{X} \in \mathcal{B}_0$. Given the (inertial) frames of reference for each of the reference (Lagrangian) (X_1, X_2, X_3) and spatial

(Eulerian) (x_1, x_2, x_3) spaces, the deformation gradient is a second-order two-point tensor $\mathbf{F} \in \mathbb{T}_d^2$, with $\mathbb{T}_d^q$ being the space of q th-order tensors of dimension d , whose components are provided by

$$F_{aB} = \frac{\partial \varphi_a}{\partial X_B} \quad (3.3)$$

An infinitesimal element volume in the reference (material) configuration is then mapped to the current (spatial) configuration by the non-negative Jacobian determinant or volume ratio J provided by

$$J(\mathbf{X}, t) := \det [\mathbf{F}(\mathbf{X}, t)] > 0, \quad (3.4)$$

in accordance with the principle of the *local impenetrability of the matter*. As a result, the deformation gradient tensor is positive-definite $\mathbf{F} \in (\mathbb{T}_d^2)_+$, i.e it has positive eigenvalues.

On the other hand, the time derivative of the motion is the material velocity $\mathbf{v} : \mathcal{B}_0 \times [0, T] \rightarrow \mathbb{R}^d$ provided in the reference configuration by

$$\mathbf{v}(\mathbf{X}, t) := \frac{\partial \boldsymbol{\varphi}(\mathbf{X}, t)}{\partial t} = \dot{\boldsymbol{\varphi}}(\mathbf{X}, t), \quad (3.5)$$

($\dot{\cdot}$) indicating time differentiation hereafter.

Accordingly, the linear momentum per unit of reference volume $\mathbf{p} : \mathcal{B}_0 \times [0, T] \rightarrow \mathbb{R}^d$ is defined as

$$\mathbf{p}(\mathbf{X}, t) := \rho_0(\mathbf{X}) \mathbf{v}(\mathbf{X}, t), \quad (3.6)$$

where $\rho_0 : \mathcal{B}_0 \rightarrow \mathbb{R}$ is the density in the reference configuration. All the foregoing kinematic relations are depicted in Figure 3.1.

Interestingly, the rate of the deformation gradient is linked with the velocity vector (3.5) or the linear momentum (3.6) as follows

$$\dot{\mathbf{F}}(\mathbf{X}, t) := \frac{\partial}{\partial t} \nabla_0 \boldsymbol{\varphi}(\mathbf{X}, t) = \nabla_0 \mathbf{v}(\mathbf{X}, t) = \nabla_0 \left[\frac{\mathbf{p}(\mathbf{X}, t)}{\rho_0(\mathbf{X})} \right], \quad (3.7)$$

as the material coordinates $\mathbf{X}$ are time-independent, so the velocity gradient tensor measures the rate at which the deformation gradient changes.

Remark 3.1. Materials phenomenologically present distinct behavior according to different modes of deformation. Often, volumetric and isochoric deformation modes are observed to response in clearly distinguishable manners, for which the assumption of the dilatational-deviatoric multiplicative split of the deformation gradient is normally considered. It is based on a modified deformation gradient tensor whose dilatational part vanishes

$$\mathbf{F} = J^{\frac{1}{3}} \bar{\mathbf{F}} \quad \text{with} \quad \det \bar{\mathbf{F}} = 1 \quad (3.8)$$

3.2 Generalized Standard Materials

The types of constitutive behaviors considered in this dissertation are encompassed by the generalized standard materials framework Celigoj (1998); Mielke (2006). Such materials may generally undergo geometrically nonlinear deformations coupled with thermal effects and dissipative mechanisms derived from transformations of the internal structure. Within this general framework, any phenomenological effect can be considered, such as plastic, viscoelastic or damage, piezoelectric effects, microstructure defects, etc. In this sense, the material response will generally be history-dependent since both elastic or inelastic evolutions will be involved.

For the consideration of coupling thermal effects the *Lagrangian* absolute temperature field is introduced as

$$\Theta : \mathcal{B}_0 \times [0, T] \ni (\mathbf{X}, t) \rightarrow \Theta(\mathbf{X}, t) \in \mathbb{R}_+ \quad (3.9)$$

On the other hand, general irreversible effects are described by additional variables that capture the dissipative transformations which take place in the internal structure of materials. Despite existing different approaches to choose these variables, the concept of *internal variables* Coleman & Gurtin (1967) has extensively been used when facing irreversible evolutions of materials. Its use is motivated by numerical considerations, as it easily suits simulations based on the Finite Element method. That is why, this dissertation will hereafter restrict to this framework. They are also referred to as *hidden* variables emphasizing their non-measurable character. For continuous media, they are symmetric strain-like tensors

$$\mathbf{\Lambda}^\alpha : \mathcal{B}_0 \times [0, T] \ni (\mathbf{X}, t) \rightarrow \mathbf{\Lambda}^\alpha(\mathbf{X}, t) \in \text{Sym}(\mathbb{T}_d^2), \quad (3.10)$$

where $\alpha \in [1, m]$ is the number of internal variables and $\text{Sym}(\mathbb{T}_d^2) \subset \mathbb{T}_d^2$ is the space of symmetric second-order tensors. For further developments, also the space of symmetric and positive-definite (positive eigenvalues) second-order tensor is introduced as a subset of the space of symmetric second-order tensors, that is $\text{Sym}(\mathbb{T}_d^2)_+ \subset \text{Sym}(\mathbb{T}_d^2)$

Generalized standard materials are then described by the deformation $\boldsymbol{\varphi}$, the absolute temperature Θ and the internal state variables $\mathbf{\Lambda}^\alpha$. The material thermodynamic evolution is fully determined by knowing these three quantities at any instant time and at any point of the body composed by the general standard material. Specifically, objectivity requirements lead to the

measure of the deformations provided by either the symmetric right Cauchy-Green deformation tensor

$$\mathbf{C} := \mathbf{F}^T \mathbf{F} \in \text{Sym}(\mathbb{T}_d^2)_+, \quad (3.11)$$

in the undeformed configuration $\mathcal{B}_0$, or by the symmetric left Cauchy-Green deformation tensor

$$\mathbf{b} := \mathbf{F} \mathbf{F}^T \in \text{Sym}(\mathbb{T}_d^2)_+, \quad (3.12)$$

in the deformed configuration $\mathcal{B}_t$. Both deformation tensors are bidirectionally related through either the *push-forward* or *pull-back* tensor operations.

3.2.1 Physical constitutive laws

The material behavior can uniquely be defined by the *Helmholtz free-energy* function, measured per unit reference volume, which, in the *Lagrangian description*, is

$$\Psi : \mathcal{B}_0 \times [0, T] \ni (\mathbf{C}, \Theta, \mathbf{\Lambda}^\alpha) \rightarrow \Psi(\mathbf{C}, \Theta, \mathbf{\Lambda}^\alpha) \in \mathbb{R} \quad (3.13)$$

It follows from the constitutive theory, see Truesdell et al. (2004), which is based on the three general principles of *determinism*, *local action* and *frame-indifference*. Particularly, the *frame-indifference* principle is responsible for the free-energy function to depend on the Cauchy-Green tensors, as previously indicated, see Holzapfel (2000).

Furthermore, it is assumed to be a smooth function with the following properties

$$\Psi(\mathbf{1}, \Theta_{\text{ref}}, \mathbf{1}) = 0, \quad \Psi(\mathbf{C}, \Theta, \mathbf{\Lambda}^\alpha) \geq 0, \quad (3.14)$$

which physically means that the material contains no energy in the undeformed configuration and at a given temperature known as a reference temperature Θ_{ref} and that the energy increases with deformation, temperature or dissipative changes in the material.

These properties limit specific types of material behaviors, some of which will be discussed in subsequent chapters.

Remark 3.2. If the material behaves isotropically, the free-energy function depend only on the invariants of Cauchy-Green tensors, normally defined as

$$\begin{aligned} I_{\mathbf{C}} &:= \text{tr}(\mathbf{C}) = \text{tr}(\mathbf{b}) = I_{\mathbf{b}} \\ II_{\mathbf{C}} &:= \frac{1}{2} [I_{\mathbf{C}}^2 - \text{tr}(\mathbf{C}^2)] = \frac{1}{2} [I_{\mathbf{b}}^2 - \text{tr}(\mathbf{b}^2)] = II_{\mathbf{b}} \\ III_{\mathbf{C}} &:= \det \mathbf{C} = \det \mathbf{b} = III_{\mathbf{b}} = J^2 \end{aligned} \quad (3.15)$$

Also, it is usual to define isotropy free-energy functions in terms of the principal stretches, i.e the square root of the eigenvalues of the Cauchy-Green tensors, denoted as $\lambda_i^{\mathbf{C}}, \lambda_i^{\mathbf{b}}$ for $i = 1, 2, 3$, which are related to the above invariants by

$$\begin{aligned} I_{\mathbf{C}} &= (\lambda_1^{\mathbf{C}})^2 + (\lambda_2^{\mathbf{C}})^2 + (\lambda_3^{\mathbf{C}})^2 \\ II_{\mathbf{C}} &= (\lambda_1^{\mathbf{C}})^2 (\lambda_2^{\mathbf{C}})^2 + (\lambda_1^{\mathbf{C}})^2 (\lambda_3^{\mathbf{C}})^2 + (\lambda_2^{\mathbf{C}})^2 (\lambda_3^{\mathbf{C}})^2 \\ III_{\mathbf{C}} &= (\lambda_1^{\mathbf{C}})^2 (\lambda_2^{\mathbf{C}})^2 (\lambda_3^{\mathbf{C}})^2 \end{aligned} \quad (3.16)$$

Remark 3.3. Often, the Helmholtz free-energy function (3.13) is assumed to be additively decoupled into volumetric and isochoric contributions Bonet & Wood (2008). Under this assumption, the thermal effects are commonly considered to contribute to the volumetric part (Holzapfel, 1996; Reese & Govindjee, 1998a) whereas internal dissipative transformations are observed to be related mainly with the isochoric deformations, see for instance (Holzapfel & Simó, 1996b; Reese & Govindjee, 1998b).

Remark 3.4. The described generalized standard material model may generally rely on any hyperelastic model either defined in terms of the invariants $\Psi(I_{\mathbf{C}}, II_{\mathbf{C}}, III_{\mathbf{C}})$ or in terms of the principal stretches $\Psi(\lambda_1^{\mathbf{C}}, \lambda_2^{\mathbf{C}}, \lambda_3^{\mathbf{C}})$ of the right Green-Lagrange tensor.

For thermodynamic consistency, the previously introduced free-energy function (3.13) must satisfy the Clausius-Planck inequality, see Truesdell et al. (2004), which establishes that the rate of internal dissipation must always be non-negative at any particle and any instant time and reads

$$\dot{\mathcal{D}} := \frac{1}{2} \mathbf{S} : \dot{\mathbf{C}} - \dot{\Psi} - \eta \dot{\Theta} \geq 0, \quad (3.17)$$

$(\cdot) : (\cdot)$ meaning the inner product in the space of second-order tensors $\mathbb{T}_d^2$, $\mathbf{S} : \mathcal{B}_0 \times [0, T] \rightarrow \text{Sym}(\mathbb{T}_d^2)$ being the symmetry Piola-Kirchhoff stress tensor and $\eta : \mathcal{B}_0 \times [0, T] \rightarrow \mathbb{R}$ being the entropy function measured per unit reference volume, which are the work conjugated quantities to the right Cauchy-Green deformation tensor (3.12) and the absolute temperature (3.32), respectively.

The chain rule applied to the free-energy function (3.13) along with further thermodynamic arguments, see Coleman & Gurtin (1967), leads to the following constitutive laws for the symmetry Piola-Kirchhoff stress tensor

$$\mathbf{S} := 2 \frac{\partial \Psi(\mathbf{C}, \Theta, \Lambda^\alpha)}{\partial \mathbf{C}}, \quad (3.18)$$

and for the entropy function per unit reference volume

$$\eta := -\frac{\partial \Psi(\mathbf{C}, \Theta, \mathbf{\Lambda}^\alpha)}{\partial \Theta} \quad (3.19)$$

With these definitions the rate of internal dissipation yields

$$\dot{\mathcal{D}} = \sum_{\alpha=0}^m -\frac{\partial \Psi(\mathbf{C}, \Theta, \mathbf{\Lambda}^\alpha)}{\partial \mathbf{\Lambda}^\alpha} : \dot{\mathbf{\Lambda}}^\alpha \geq 0, \quad (3.20)$$

from where the constitutive law for the work conjugated quantities to internal variables, i.e the dissipative driving stress tensors $\mathbf{Q}^\alpha : \mathcal{B}_0 \times [0, T] \rightarrow \text{Sym}(\mathbb{T}_d^2)$, can be deduced to be

$$\mathbf{Q}^\alpha := -\frac{\partial \Psi(\mathbf{C}, \Theta, \mathbf{\Lambda}^\alpha)}{\partial \mathbf{\Lambda}^\alpha} \quad (3.21)$$

More importantly, the condition (3.20) determines the evolution equation for each internal variables. In view of it, the rate of any internal variables must generally pertain to a positive semidefinite functional $\mathcal{K} : \mathbb{T}_d^2 \mapsto \mathbb{T}_d^2 \mid \mathbf{A} : \mathcal{K}(\mathbf{A}) \geq 0, \quad \forall \mathbf{A} \in \mathbb{T}_d^2$ depending on its work conjugate quantity to yield a quadratic form that ensures the fulfillment of the inequality, that is

$$\dot{\mathbf{\Lambda}}^\alpha = \mathcal{K}(\mathbf{Q}^\alpha) \quad \forall \alpha = 1, \dots, m \quad (3.22)$$

A material thus described is said to be *dissipative*.

Remark 3.5. Each different dissipative effect requires a particular form of such functional. For instance, linear smooth dissipative effects are provided by a linear fourth order mapping of the form

$$\mathcal{K}(\mathbf{Q}^\alpha) = \mathbb{V}^\alpha : \mathbf{Q}^\alpha, \quad (3.23)$$

$\mathbb{V}^\alpha$ being a general positive semidefinite fourth order tensor specified by material parameters which may depend on time-dependent variables.

The constitutive laws (3.18) - (3.21) are physical in the sense that they are functions of the *physical* variable temperature.

3.2.2 Heat conduction

The existence of a non-uniform temperature field in the body produces the conduction phenomenon which tends to homogenize the temperature field

in the body by flowing heat from the warmer to the colder region of the body. The sense of the flow, naturally defined in the *Eulerian description* by the Cauchy heat flux vector $\mathbf{h} : \mathcal{B}_t \times [0, T] \rightarrow \mathbb{R}^d$, is prescribed by the *heat conduction inequality* Holzapfel (2000), which reads

$$\mathbf{h} \cdot \nabla \left[\frac{1}{\Theta} \right] \geq 0, \quad (3.24)$$

∇ being the spatial gradient, and determines the way the heat must flow, that is, opposed to the temperature gradient. A suitable constitutive law for the Cauchy heat flux is thus furnished by

$$\mathbf{h}(\boldsymbol{\varphi}, t) := \Theta^2 \boldsymbol{\kappa}(\Theta) \nabla \left[\frac{1}{\Theta} \right], \quad (3.25)$$

which is further supported by experimental observations and known as *Duhamel's law of heat conduction*.

In this law, the symmetric second-order tensor $\boldsymbol{\kappa} : \mathcal{B}_t \times [0, T] \rightarrow \text{Sym}(\mathbb{T}_d^2)_+$ is the spatial thermal conductivity tensor, required to be positive semidefinite and possibly temperature dependent. If the material is thermally isotropic, the conductivity tensor becomes $\boldsymbol{\kappa}(\Theta) = \kappa(\Theta) \mathbf{1}$, $\kappa \geq 0$ being the thermal conductivity parameter.

The Lagrangian form of the Duhamel's law (3.25) can be achieved by using the relation between the spatial and the material gradient $\nabla(\bullet) = \mathbf{F}^{-T} \nabla_0(\bullet)$ and the pull-back operation on the Cauchy heat flux to arrive at the Piola-Kirchhoff heat flux $\mathbf{H} : \mathcal{B}_0 \times [0, T] \rightarrow \mathbb{R}^d$, see Holzapfel (2000),

$$\mathbf{H}(\mathbf{X}, t) := \Theta^2 J \mathbf{F}^{-1} \boldsymbol{\kappa}(\Theta) \mathbf{F}^{-T} \nabla_0 \left[\frac{1}{\Theta} \right] \quad (3.26)$$

Finally, the following simplified notation for the Lagrangian conductivity tensor $\mathbf{K} : \mathcal{B}_0 \times [0, T] \rightarrow \text{Sym}(\mathbb{T}_d^2)_+$ is introduced

$$\mathbf{K}(\mathbf{X}, t) := J \mathbf{F}^{-1} \boldsymbol{\kappa}(\Theta) \mathbf{F}^{-T}, \quad (3.27)$$

which, in the case of thermal isotropy, simplifies to

$$\mathbf{K}(\mathbf{X}, t) := J \kappa(\Theta) \mathbf{C}^{-1} \quad (3.28)$$

3.2.3 The internal energy function

The internal energy is an important thermodynamic potential that macroscopically collects every present microscopic form of energy in materials. The

canonical form of this potential, defined per unit reference volume, is provided as a function of the entropy and other mechanical or internal variables, see Truesdell et al. (2004), that is

$$e : \mathcal{B}_0 \times [0, T] \ni (\mathbf{C}, \eta, \mathbf{\Lambda}^\alpha) \rightarrow e(\mathbf{C}, \eta, \mathbf{\Lambda}^\alpha) \in \mathbb{R}, \quad (3.29)$$

because it is defined through the Legendre transformation of the free-energy function (3.13) when replacing the temperature with its work conjugate entropy as the thermodynamic state variable. The Legendre transformation of the free-energy function with respect to the entropy thus results in

$$e = \Psi + \Theta \eta, \quad (3.30)$$

which defines the *caloric equation of state*.

Remark 3.6. Although the internal energy is canonically a function of the entropy, one can readily obtain internal energy functions in terms of temperature through the Legendre transform applied to free energy functions canonically defined in terms of temperature (3.13), see Dillon Jr. (1962, 1963). Accordingly, the internal energy defined in terms of temperature results in

$$e(\mathbf{C}, \Theta, \mathbf{\Lambda}^\alpha) = \Psi(\mathbf{C}, \Theta, \mathbf{\Lambda}^\alpha) + \Theta \eta(\mathbf{C}, \Theta, \mathbf{\Lambda}^\alpha), \quad (3.31)$$

This form of the internal energy will play a central role in subsequent chapters.

In order for the internal energy function to be defined from canonically temperature-based free-energy functions (3.13), the entropy function (3.19) must be uniquely invertible respect to Θ at fixed $\mathbf{C}$ and $\mathbf{\Lambda}^\alpha$ so that the function

$$\Theta : \mathcal{B}_0 \times [0, T] \ni (\mathbf{C}, \eta, \mathbf{\Lambda}^\alpha) \rightarrow \Theta(\mathbf{C}, \eta, \mathbf{\Lambda}^\alpha) \in \mathbb{R}_+, \quad (3.32)$$

might be achieved. Assuming this, the canonical form of the internal energy can be obtained, following (3.30), as

$$e(\mathbf{C}, \eta, \mathbf{\Lambda}^\alpha) := \Psi(\mathbf{C}, \Theta(\mathbf{C}, \eta, \mathbf{\Lambda}^\alpha), \mathbf{\Lambda}^\alpha) + \Theta(\mathbf{C}, \eta, \mathbf{\Lambda}^\alpha) \eta \quad (3.33)$$

Remark 3.7. The above requirement has to be viewed as an important technical restriction to the description of specific thermoelastic models using the entropy as a thermodynamic state variable.

Provided that, the entropy-based description of generalized standard materials can be achieved from the canonical form of the internal energy potential (3.29) by deriving new constitutive laws for the symmetric Piola-Kirchhoff stress tensor, the temperature function and the dissipative driving

stress tensor. To do that, the rate of internal dissipation is accordingly expressed in terms of this potential using (3.30) to give

$$\dot{\mathcal{D}} = \frac{1}{2} \mathbf{S} : \dot{\mathbf{C}} - \dot{e} + \Theta \dot{\eta} \geq 0 \quad (3.34)$$

Then, applying the chain rule to the function (3.29) yields

$$\dot{\mathcal{D}} = \frac{1}{2} \mathbf{S} : \dot{\mathbf{C}} - \left(\frac{\partial e}{\partial \mathbf{C}} : \dot{\mathbf{C}} + \frac{\partial e}{\partial \eta} \dot{\eta} + \sum_{\alpha=1}^m \frac{\partial e}{\partial \mathbf{\Lambda}^\alpha} : \dot{\mathbf{\Lambda}}^\alpha \right) + \Theta \dot{\eta} \geq 0 \quad (3.35)$$

Thus, following the same arguments as before, the symmetric Piola-kirchhoff stress tensor is now provided by

$$\mathbf{S} := 2 \frac{\partial e(\mathbf{C}, \eta, \mathbf{\Lambda}^\alpha)}{\partial \mathbf{C}} \quad (3.36)$$

Then, the temperature function (3.32) is defined as

$$\Theta := \frac{\partial e(\mathbf{C}, \eta, \mathbf{\Lambda}^\alpha)}{\partial \eta}, \quad (3.37)$$

which is consistent to the relation (3.33) and, finally, the dissipative driving stress tensor now becomes

$$\mathbf{Q}^\alpha := - \frac{\partial e(\mathbf{C}, \eta, \mathbf{\Lambda}^\alpha)}{\partial \mathbf{\Lambda}^\alpha} \quad (3.38)$$

Assuming these new definitions, the resulting rate of internal dissipation will agree with the thermodynamics as long as the evolution equations for the internal variables follow the general law (3.22), now using the new constitutive law for the dissipative driving stress tensor (3.38).

3.2.4 Constitutive behaviors for limit cases

The just discussed generalized standard materials framework is suitable to derive any kind of material behavior ranging from the purely reversible case to general irreversible cases both adiabatic or isothermal. It has been introduced in the most general way to describe general thermo-dissipative material models so that it encompasses every particular case.

Thus, one merely needs to neglect either the thermal or the dissipative effects to arrive at either isothermal models or purely elastic behaviors. To

this end, the thermodynamic potentials dependencies must be reduced accordingly. That is, if the dissipative effects are ignored the general form of the thermodynamic potentials will be

$$s := s(\mathbf{C}, \Theta) \quad \text{or} \quad s := s(\mathbf{C}, \eta), \quad (3.39)$$

s representing any thermodynamic potential. This case corresponds with nonlinear thermoelasticity which can be described either in terms of temperature or entropy via the canonical form of the free-energy or the internal energy potentials, respectively.

On the other hand, in the case of neglecting the thermal effects the resulting material behavior will be isothermal but can still dissipate energy. Therefore, the thermodynamics reduces to *mechanical dynamics* with dissipation, thereby the thermodynamic potentials collapse to the stored energy function that might generally depend on deformation and internal variables

$$\Psi := \Psi(\mathbf{C}, \mathbf{\Lambda}^\alpha) = e(\mathbf{C}, \mathbf{\Lambda}^\alpha) + A, \quad (3.40)$$

with A being some constant of the motion.

Thus, the reversible nonlinear hyperelastic behavior can be recovered ignoring dissipative effects, leading to the well-known deformation-dependent free-energy function

$$\Psi := \Psi(\mathbf{C}) = e(\mathbf{C}) + A \quad (3.41)$$

In subsequent sections and chapters we will be considering every case pointed out before.

3.3 Balance laws: strong form of the initial-boundary value problem

In this section the global balance laws, from which the strong form of the governing equations are derived, are briefly summarized. Also, the Cauchy's stress theorem and its thermodynamic counterpart Stokes' heat flux theorem are introduced.

The evolution of a continuous body composed of a generalized standard material is determined by global balance laws of mass, momenta and energy.

3.3.1 Balance of mass

Any continuum contains a fundamental property called *mass* that accounts for the amount of matter contained inside its boundary. A basic principle of non-relativistic mechanics is that mass cannot be created or destroyed, leading to the balance of mass expressed as

$$m := \int_{\mathcal{B}_0} \rho_0(\mathbf{X}) dV_0 = \int_{\mathcal{B}_t} \rho(\mathbf{X}, t) dv > 0, \quad (3.42)$$

$\rho_0: \mathcal{B}_0 \rightarrow \mathbb{R}_+$ and $\rho: \mathcal{B}_0 \times [0, T] \rightarrow \mathbb{R}_+$ being the density field in material and spatial description respectively. Therefore, the rate of change of the mass throughout time must vanish

$$\dot{m} = \int_{\mathcal{B}_0} \dot{\rho}_0(\mathbf{X}) dV_0 = 0, \quad (3.43)$$

which is automatically fulfilled since the reference mass density is independent of time.

3.3.2 Balance of linear and angular momentum

Classical mechanics is grounded on the axioms of momentum balance principles: linear or translational and angular or rotational. The *total linear momentum* is a vector-valued function $\mathbf{L}: [0, T] \rightarrow \mathbb{R}^d$ defined by the volume integral of the linear momentum per unit (reference) volume (3.6) as follows

$$\mathbf{L}(t) := \int_{\mathcal{B}_0} \mathbf{p}(\mathbf{X}, t) dV_0 \quad (3.44)$$

The balance of linear momentum establishes that the change of this vector magnitude equals to the resultant of external forces, $\mathbf{F}_{\text{ext}}: [0, T] \rightarrow \mathbb{R}^d$ over the body, that is

$$\dot{\mathbf{L}}(t) = \mathbf{F}_{\text{ext}}(t) \quad (3.45)$$

In other words, the action of external forces on a body causes the total linear momentum to change which is the classical statement of the second Newton's law.

The resultant of external forces is the sum of all forces acting in the body or on its boundary, as sketched in Figure 3.2, and can be expressed as

$$\mathbf{F}_{\text{ext}}(t) = \int_{\mathcal{B}_0} \mathbf{B}_0(\mathbf{X}, t) dV_0 + \int_{\partial\mathcal{B}_0} \mathbf{T}_0(\mathbf{X}, t, \mathbf{N}) dA_0, \quad (3.46)$$

Figure 3.2. Volume forces and tractions in the reference configuration.

$\mathbf{B}_0 : \mathcal{B}_0 \times [0, T] \rightarrow \mathbb{R}^d$ being any volumetric force expressed in the reference configuration, such as the gravitational force $\rho_0 \mathbf{g}$, $\mathbf{T}_0 : \partial \mathcal{B}_0 \rightarrow \mathbb{R}^d$ being the traction vector on the boundary measured per unit reference surface area and $\mathbf{N}$ denoting the unit outward normal field on $\partial \mathcal{B}_0$.

As the reference configuration remains invariable along the time the change of the total linear momentum is the volume integral of the rate of the linear momentum per unit reference volume, enabling the balance principle to be expressed as

$$\int_{\mathcal{B}_0} \dot{\mathbf{p}}(\mathbf{X}, t) dV_0 = \int_{\mathcal{B}_0} \mathbf{B}_0(\mathbf{X}, t) dV_0 + \int_{\partial \mathcal{B}_0} \mathbf{T}_0(\mathbf{X}, t, \mathbf{N}) dA_0 \quad (3.47)$$

Furthermore, the *Cauchy's stress theorem*, see Holzapfel (2000), relates the current traction vector $\bar{\mathbf{t}} : \partial \mathcal{B}_t \times [0, T] \rightarrow \mathbb{R}^d$ with the symmetric Cauchy stress tensor $\boldsymbol{\sigma} : \mathcal{B}_t \times [0, T] \rightarrow \text{Sym}(\mathbb{T}_d^2)$, defined in the spatial configuration, which can be translated to the reference configuration as

$$\mathbf{T}_0(\mathbf{X}, t, \mathbf{N}) = (\mathbf{F}\mathbf{S})(\mathbf{X}, t) \cdot \mathbf{N} \quad (3.48)$$

The Gauss' theorem¹ thus allows to transform the resulting surface integral into the volume integral through the material divergence operator $\nabla_0 \cdot (\bullet)$, that is

$$\int_{\mathcal{B}_0} \dot{\mathbf{p}} dV_0 = \int_{\mathcal{B}_0} \mathbf{B}_0 dV_0 + \int_{\mathcal{B}_0} \nabla_0 \cdot (\mathbf{F}\mathbf{S}) dV_0, \quad (3.49)$$

¹ $\int_{A_0} \mathbf{F} \cdot \mathbf{N} dA_0 = \int_{V_0} \nabla_0 \cdot \mathbf{F} dV_0$

where the magnitudes' dependencies have been omitted to simplify the notation.

Finally, reallocating terms and arguing that the above identity must hold for any reference volume, the integrand must identically be nil at any material point and at any time, leading to the strong form or the linear momentum balance in the Lagrangian description

$$\dot{\mathbf{p}} = \nabla_0 \cdot (\mathbf{FS}) + \mathbf{B}_0 \quad (3.50)$$

Similarly, the *total angular momentum* is defined as vector-valued function $\mathbf{J} : [0, T] \rightarrow \mathbb{R}^d$ resulting from the overall volume integral of the moment of the linear momentum vector per unit (reference) volume (3.6) with respect to any fixed point of space, e.g the origin of the inertial frame of reference, that is

$$\mathbf{J}(t) = \int_{\mathcal{B}_0} \boldsymbol{\varphi}(\mathbf{X}, t) \wedge \mathbf{p}(\mathbf{X}, t) dV_0 \quad (3.51)$$

The angular momentum balance states that the just introduced magnitude changes due to the presence of a resultant of external moment (or torques) $\mathbf{M}_{\text{ext}} : [0, T] \rightarrow \mathbb{R}^d$ acting over the body

$$\dot{\mathbf{J}}(t) = \mathbf{M}_{\text{ext}}(t) \quad (3.52)$$

Accordingly, the resultant of external moments is provided by the sum of all volumetric forces and tractions moments

$$\mathbf{M}_{\text{ext}}(t) = \int_{\mathcal{B}_0} \boldsymbol{\varphi}(\mathbf{X}, t) \wedge \mathbf{B}_0(\mathbf{X}, t) dV_0 + \int_{\partial \mathcal{B}_0} \boldsymbol{\varphi}(\mathbf{X}, t) \wedge \mathbf{T}_0(\mathbf{X}, t, \mathbf{N}) dA_0 \quad (3.53)$$

Further elaboration of this principle leads to the already introduced symmetry of the Cauchy stress tensor $\boldsymbol{\sigma} \in \text{Sym}(\mathbb{T}_d^2)$ which is a well-known result whose demonstration can be found in classical references, for instance Malvern (1969), and hence omitted.

3.3.3 Balance of energy

In pure mechanics the balance of energy is a natural consequence of the momentum postulations. Particularly, the total energy of a conservative mechanic system is said to be a *first integral* of the system evolution, see Hand & Finch (1998). However, the consideration of coupled thermo-dissipative

effects leads to the thermodynamic context in which the momentum balances must be supplemented by the balance of energy (first law) and the entropy inequality (second law).

Every internal form of energy in the continuum is collected by the total internal energy $U : [0, T] \rightarrow \mathbb{R}$, provided by

$$U(t) := \int_{\mathcal{B}_0} e(\mathbf{X}, t) dV_0 \quad (3.54)$$

On the other hand, related to the motion, the continuum develops the kinetic energy $K : [0, T] \rightarrow \mathbb{R}$, defined as

$$K(t) := \int_{\mathcal{B}_0} \frac{1}{2\rho_0(\mathbf{X})} \|\mathbf{p}(\mathbf{X}, t)\|^2 dV_0, \quad (3.55)$$

$\|\cdot\|$ being the l^2 -norm in the euclidean space.

Furthermore, the continuum interacts with its surroundings through external sources of energies coming from external forces and heats generally present either in the continuum or on its boundary.

The way these forms of energy interact follows the first law of thermodynamics: the energy balance. It postulates that the external mechanical and thermal power supplied to a thermodynamic continuum is employed to change both its kinetic and its total internal energy

$$\dot{K}(t) + \dot{U}(t) = P_{\text{ext}}(t) + Q(t), \quad (3.56)$$

The power of external mechanical forces or the rate of the work done by the external forces (3.46), $P_{\text{ext}} : [0, T] \rightarrow \mathbb{R}$, may generally be expressed as

$$P_{\text{ext}}(t) := \int_{\mathcal{B}_0} \mathbf{B}_0(\mathbf{X}, t) \cdot \mathbf{v}(\mathbf{X}, t) dV_0 + \int_{\partial\mathcal{B}_0} \mathbf{T}_0(\mathbf{X}, t, \mathbf{N}) \cdot \mathbf{v}(\mathbf{X}, t) dA_0 \quad (3.57)$$

On the other hand, the thermal power is supplied to the continuum through either heat reservoirs, $\mathcal{R} : \mathcal{B}_0 \times [0, T] \rightarrow \mathbb{R}$ measured per unit time and unit reference volume, or heat fluxes, $H_N : \partial\mathcal{B}_0 \times [0, T] \rightarrow \mathbb{R}$ per unit reference surface area, entering or escaping its boundary, see Figure 3.3. Therefore, the rate of thermal work $Q : [0, T] \rightarrow \mathbb{R}$ may be expressed as

$$Q(t) := \int_{\mathcal{B}_0} \mathcal{R}(\mathbf{X}, t) dV_0 + \int_{\partial\mathcal{B}_0} H_N(\mathbf{X}, t, \mathbf{N}) dA_0 \quad (3.58)$$

Figure 3.3. Volumetric source or sink of heat and heat flux escaping through the boundary in the reference configuration

Similarly to the Cauchy's stress theorem (3.48) in continuum mechanics, the *Stokes' heat flux theorem* postulates that the scalar function H_N is a linear function of the outward unit normal

$$H_N(\mathbf{X}, t, \mathbf{N}) := -\mathbf{H}(\mathbf{X}, t) \cdot \mathbf{N}, \quad (3.59)$$

where $\mathbf{H}(\mathbf{X}, t)$ follows the Duhamel's law of heat conduction provided in (3.26).

Considering each of the above contributions the *first law* (3.56) can be rewritten in the Lagrangian description as

$$\begin{aligned} \int_{\mathcal{B}_0} \frac{1}{\rho_0} \dot{\mathbf{p}} \cdot \mathbf{p} dV_0 + \int_{\mathcal{B}_0} \dot{e} dV_0 &= \int_{\mathcal{B}_0} \mathbf{B}_0 \cdot \mathbf{v} dV_0 + \int_{\partial \mathcal{B}_0} (\mathbf{FS}) \mathbf{N} \cdot \mathbf{v} dA_0 \\ &+ \int_{\mathcal{B}_0} \mathcal{R} dV_0 - \int_{\partial \mathcal{B}_0} \mathbf{H} \cdot \mathbf{N} dA_0 \end{aligned} \quad (3.60)$$

The surface integral depending on the stress tensor must be elaborated in order to properly apply the Gauss' theorem, that is

$$\int_{\partial \mathcal{B}_0} (\mathbf{FS}) \mathbf{N} \cdot \mathbf{v} dA_0 = \int_{\partial \mathcal{B}_0} (\mathbf{FS})^T \mathbf{v} \cdot \mathbf{N} dA_0 = \int_{\mathcal{B}_0} \nabla_0 \cdot [(\mathbf{FS})^T \mathbf{v}] dV_0 \quad (3.61)$$

The product rule of the divergence² then allows to obtain

$$\int_{\mathcal{B}_0} \nabla_0 \cdot [(\mathbf{FS})^T \mathbf{v}] dV_0 = \int_{\mathcal{B}_0} (\mathbf{FS}) : \nabla_0 \mathbf{v} dV_0 + \int_{\mathcal{B}_0} \mathbf{v} \cdot \nabla_0 \cdot (\mathbf{FS}) dV_0 \quad (3.62)$$

Using this last result in (3.60), the linear momentum balance (3.49) and applying the Gauss' theorem on the heat flux term, the energy balance results in

$$\int_{\mathcal{B}_0} (\dot{e} - \mathbf{FS} : \nabla_0 \mathbf{v} - \mathcal{R} + \nabla_0 \cdot \mathbf{H}) dV_0 = 0 \quad (3.63)$$

Following the definition of the rate of the deformation gradient (3.7) and some tensor algebra^{3,4}, the second term of (3.63) can be related to the rate of the right Cauchy-Green deformation tensor (3.11) as follows

$$\mathbf{FS} : \nabla_0 \mathbf{v} = \mathbf{FS} : \dot{\mathbf{F}} = \mathbf{S} : \mathbf{F}^T \dot{\mathbf{F}} = \mathbf{S} : \text{Sym}(\mathbf{F}^T \dot{\mathbf{F}}) = \frac{1}{2} \mathbf{S} : \dot{\mathbf{C}}, \quad (3.64)$$

where use has been made of the symmetry of the second Piola-Kirchhoff stress tensor.

As the reference volume is arbitrary, the local form of the energy balance results in

$$\dot{e} = \frac{1}{2} \mathbf{S} : \dot{\mathbf{C}} - \nabla_0 \cdot \mathbf{H} + \mathcal{R} \quad (3.65)$$

The balance (3.65) clearly couples the energy involved in the deformation process with the thermal processes taking place in the continuum.

Finally, the entropy inequality is ensured by the dissipation inequality together with the heat conduction inequality introduced in subsections 3.2.1 and 3.2.2.

3.3.4 Strong form of the governing equations

The above introduced balance laws expressed in local form (3.50), (3.65) and the evolution equations for internal variables (3.22) define the strong form of the governing equations for a thermo-dissipative continuum. That is, given $\mathbf{B}_0 : \mathcal{B}_0 \rightarrow \mathbb{R}^d$, $\mathcal{R} : \mathcal{B}_0 \rightarrow \mathbb{R}$ and constants $\mathbf{T}_0 : \partial \mathcal{B}_0 \rightarrow \mathbb{R}^d$,

² $\nabla_0 \cdot (\mathbf{A}^T \mathbf{b}) = \mathbf{A} : \nabla_0 \mathbf{b} + \mathbf{b} \cdot \nabla_0 \cdot \mathbf{A}$

³ $\mathbf{AB} : \mathbf{C} = \mathbf{A} : \mathbf{B}^T \mathbf{C}$

⁴ $\text{Sym}(\mathbf{A}) = \frac{1}{2}(\mathbf{A} + \mathbf{A}^T)$

$H_N : \partial\mathcal{B}_0 \rightarrow \mathbb{R}$, find $(\boldsymbol{\varphi}, \mathbf{p}, e, \boldsymbol{\Lambda}^\alpha) : \mathcal{B}_0 \rightarrow \mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R} \times \text{Sym}(\mathbb{T}_d^2)^m$, such that

$$\left. \begin{aligned} \dot{\boldsymbol{\varphi}} &= \frac{1}{\rho_0} \mathbf{p} \\ \dot{\mathbf{p}} &= \nabla_0 \cdot (\mathbf{F}\mathbf{S}) + \mathbf{B}_0 \\ \dot{e} &= \frac{1}{2} \mathbf{S} : \dot{\mathbf{C}} - \nabla_0 \cdot \mathbf{H} + \mathcal{R} \\ \dot{\boldsymbol{\Lambda}}^\alpha &= \mathcal{K}(\mathbf{Q}^\alpha) \quad \forall \alpha = 1, \dots, m \end{aligned} \right\} \quad \text{in } \mathcal{B}_0 \times [0, T] \quad (3.66)$$

It is a fully coupled first order partial differential equations (1st order PDE) system whose solution provides the thermodynamics evolution of a continuum from prescribed initial and boundary conditions.

In this way, initial conditions in $\mathcal{B}_0$ and at time $t = 0$ may generally be provided by

$$\left. \begin{aligned} \boldsymbol{\varphi}(\mathbf{X}, 0) &= \mathbf{X} \\ \mathbf{p}(\mathbf{X}, 0) &= \rho_0 \mathbf{v}_0(\mathbf{X}) \\ s(\mathbf{X}, 0) &= s_0(\mathbf{X}) \\ \boldsymbol{\Lambda}^\alpha(\mathbf{X}, 0) &= \mathbf{1} \end{aligned} \right\} \quad \text{in } \mathcal{B}_0, \quad (3.67)$$

where $\mathbf{v}_0(\mathbf{X})$ is a prescribed field, $s_0(\mathbf{X})$ represents a prescribed scalar field for any of the thermodynamic state variable employed to describe the system thermodynamics, in this case $s = e$, and the initial strain-like internal variables are assumed to depart from an undeformed state.

The boundary $\partial\mathcal{B}_0$ is usually decomposed into the subsets $\partial\mathcal{B}_0^\varphi$, $\partial\mathcal{B}_0^\sigma$, $\partial\mathcal{B}_0^\theta$ and $\partial\mathcal{B}_0^H$ in which Dirichlet or Neumann boundary conditions might be imposed. These subsets have the following properties $\partial\mathcal{B}_0^\sigma \cup \partial\mathcal{B}_0^\varphi = \partial\mathcal{B}_0$ and $\partial\mathcal{B}_0^\sigma \cap \partial\mathcal{B}_0^\varphi = \emptyset$, $\partial\mathcal{B}_0^H \cup \partial\mathcal{B}_0^\theta = \partial\mathcal{B}_0$ and $\partial\mathcal{B}_0^H \cap \partial\mathcal{B}_0^\theta = \emptyset$.

Thus, Dirichlet boundary conditions on $\partial\mathcal{B}_0$ at times $t \geq 0$ might be specified by

$$\begin{aligned} \boldsymbol{\varphi} &= \bar{\boldsymbol{\varphi}} \quad \text{on } \partial\mathcal{B}_0^\varphi \times [0, T], \\ s &= \bar{s} \quad \text{on } \partial\mathcal{B}_0^\theta \times [0, T], \end{aligned} \quad (3.68)$$

$\bar{\boldsymbol{\varphi}}$ being the prescribed motions on the boundary $\partial\mathcal{B}_0^\varphi$ and $\bar{s}$ representing one more time a prescribed field of any of the thermal variables.

Likewise, Neumann boundary conditions might be provided by

$$\begin{aligned} (\mathbf{F}\mathbf{S}) \cdot \mathbf{N} &= \mathbf{T}_0 \quad \text{on } \partial\mathcal{B}_0^\sigma \times [0, T], \\ \mathbf{H} \cdot \mathbf{N} &= -H_N \quad \text{on } \partial\mathcal{B}_0^H \times [0, T] \end{aligned} \quad (3.69)$$

Remark 3.8. The initial-boundary value problem (IBVP) (3.66) - (3.68) can further be particularized according to the election of the thermodynamic state variable. The most representative formulations are based on either entropy or temperature, although there are no mathematical restrictions to consider any other variable, for instance, the internal energy per unit reference volume as been already presented. However, from the practical point of view, this election is essential when Dirichlet's boundary conditions are required since, generally, variables other than temperature cannot technically be measured on boundaries. For this reason, the implications of both entropy and temperature formulations will become central in the rest of this dissertation and, therefore, we will pay special attention to their particularities in the subsequent subsections.

3.3.5 Entropy formulation of the IBVP

The use of the canonical form of the internal energy (3.33) along with its corresponding constitutive laws (3.36) - (3.38) enables the rate of internal energy to be expressed as

$$\dot{e}(\mathbf{C}, \eta, \mathbf{\Lambda}^\alpha) = \frac{1}{2} \mathbf{S} : \dot{\mathbf{C}} + \Theta \dot{\eta} - \sum_{\alpha=1}^m \mathbf{Q}^\alpha : \dot{\mathbf{\Lambda}}^\alpha \quad (3.70)$$

Identifying the last term on the right hand side of (3.70) as the rate of internal dissipation according to (3.34) and substituting it into (3.65) the *entropy form* of the local energy balance yields

$$\dot{\eta} = \frac{1}{\Theta} \left(-\nabla_0 \cdot \mathbf{H} + \mathcal{R} + \dot{\mathcal{D}} \right), \quad (3.71)$$

with Θ being a function of the entropy, the deformation and the internal variables according to (3.37).

The above form of the energy balance must be complemented with initial and boundary conditions expressed in terms of the state variable entropy. Without loss of generality, the initial condition for entropy can be assumed to be zero, that is

$$\eta(\mathbf{X}, 0) = 0 \quad \text{in } \mathcal{B}_0 \quad (3.72)$$

However, in some applications an initial prescribed field of temperature $\Theta_0(\mathbf{X})$ in the body is required so an initial non-zero entropy needs to be specified by solving

$$\Theta(\mathbf{X}, 0) = \frac{\partial e}{\partial \eta}(\mathbf{C}(\mathbf{X}, 0), \eta(\mathbf{X}, 0), \mathbf{\Lambda}^\alpha(\mathbf{X}, 0)) = \Theta_0(\mathbf{X}) \quad (3.73)$$

Regarding Dirichlet's boundary conditions, the value of the entropy in the Dirichlet boundary subset $\partial\mathcal{B}_0^\theta$ would then required. However, what is normally available is the value of the temperature on some parts of the boundary, $\bar{\Theta}$ on $\partial\mathcal{B}_0^\theta \times [0, T]$, so the solution of the identity

$$\Theta = \frac{\partial e}{\partial \eta}(\mathbf{C}, \bar{\eta}, \mathbf{\Lambda}^\alpha) = \bar{\Theta} \quad \text{on } \partial\mathcal{B}_0^\theta, \quad (3.74)$$

is required at all instant times in order to translate the temperature values into entropy ones, thereby they could be imposed as follows

$$\eta = \bar{\eta} \quad \text{on } \partial\mathcal{B}_0^\theta \times [0, T] \quad (3.75)$$

This complicates in excess its numerical solution, practically bounding the use of this formulation to applications with no initial conditions of temperatures and no Dirichlet's boundary conditions.

3.3.6 Temperature formulation of the IBVP

The temperature-based formulation of the IBVP (3.66) - (3.68) is derived from the use of the temperature form of the internal energy (3.31) provided by the canonical form of the free-energy function (3.13) and its constitutive laws (3.18) - (3.21). Thus, the rate of change of the internal energy is computed through the chain rule as

$$\dot{e}(\mathbf{C}, \Theta, \mathbf{\Lambda}^\alpha) = \left(\frac{1}{2} \mathbf{S} + \Theta \frac{\partial \eta}{\partial \mathbf{C}} \right) : \dot{\mathbf{C}} + \frac{\partial e}{\partial \Theta} \dot{\Theta} - \sum_{\alpha=1}^m \left(\mathbf{Q}^\alpha - \Theta \frac{\partial \eta}{\partial \mathbf{\Lambda}^\alpha} \right) : \dot{\mathbf{\Lambda}}^\alpha \quad (3.76)$$

The appearing partial derivatives of the entropy function (3.19) are linked with the calorimetric concepts of *latent heat* tensor defined as

$$\mathbf{V}(\mathbf{C}, \Theta, \mathbf{\Lambda}^\alpha) := 2\Theta \frac{\partial \eta(\mathbf{C}, \Theta, \mathbf{\Lambda}^\alpha)}{\partial \mathbf{C}}, \quad (3.77)$$

the *specific heat capacity* assumed to be a real positive number because of the material's stability, see Silhavy (2013), measured per unit reference volume and provided by

$$c := \Theta \frac{\partial \eta(\mathbf{C}, \Theta, \mathbf{\Lambda}^\alpha)}{\partial \Theta} = \frac{\partial e(\mathbf{C}, \Theta, \mathbf{\Lambda}^\alpha)}{\partial \Theta} > 0, \quad (3.78)$$

and the dissipative counterpart to the just introduced latent heat tensor, generally referred to as *dissipative latent heat* tensor, provided by

$$\mathbf{W}^\alpha(\mathbf{C}, \Theta, \mathbf{\Lambda}^\alpha) := \Theta \frac{\partial \eta(\mathbf{C}, \Theta, \mathbf{\Lambda}^\alpha)}{\partial \mathbf{\Lambda}^\alpha} \quad (3.79)$$

Using expressions (3.76) to (3.79) in (3.65), and the definition of the rate of the dissipation (3.20), the *temperature form* of the energy balance is

$$\dot{\Theta} = \frac{1}{c} \left(-\frac{1}{2} \mathbf{V} : \dot{\mathbf{C}} - \sum_{\alpha=1}^m \mathbf{W}^\alpha : \dot{\mathbf{\Lambda}}^\alpha - \nabla_0 \cdot \mathbf{H} + \mathcal{R} + \dot{\mathcal{D}} \right) \quad (3.80)$$

where terms linked with the latent heat tensors (3.77) and (3.79) are referred to as *structural thermoelastic heating* and *structural thermodissipative heating* which accounts for the Gough-Joule effects arising from the coupling thermo-mechanic response and for the same physic phenomenon but related to the dissipative transformations in the continuum, respectively.

The structural thermoelastic heating is thus a scalar-valued function $\mathcal{H}_e : \mathcal{B}_0 \times [0, T] \rightarrow \mathbb{R}$ that provides the heat generated due to mechanical deformations

$$\mathcal{H}_e(\mathbf{X}, t) := -\frac{1}{2} \mathbf{V} : \dot{\mathbf{C}} \quad (3.81)$$

Similarly, the scalar-valued function $\mathcal{H}_d : \mathcal{B}_0 \times [0, T] \rightarrow \mathbb{R}$ is introduced as the structural thermodissipative heating which accounts for the heat dissipated due to dissipative changes in the material

$$\mathcal{H}_d(\mathbf{X}, t) := - \sum_{\alpha=1}^m \mathbf{W}^\alpha : \dot{\mathbf{\Lambda}}^\alpha \quad (3.82)$$

Moreover, by taking into account the symmetry of the latent heat tensor (3.77) along with the relation (3.64), the structural thermoelastic heating may be written as

$$\mathcal{H}_e = -\frac{1}{2} \mathbf{V} : \dot{\mathbf{C}} = -\mathbf{FV} : \nabla_0 \left[\frac{\mathbf{p}}{\rho_0} \right] \quad (3.83)$$

In this way, the *temperature form* of the energy balance (3.80) in terms of the state variables is

$$\dot{\Theta} = \frac{1}{c} \left(-\mathbf{FV} : \nabla_0 \left[\frac{\mathbf{p}}{\rho_0} \right] - \nabla_0 \cdot \mathbf{H} + \mathcal{R} + \dot{\mathcal{D}} + \mathcal{H}_d \right) \quad (3.84)$$

In contrast to the entropy formulation, the resulting local energy balance involves more terms but easily allows to handle with both initial and Dirichlet and Neumann boundary conditions, commonly provided in temperature variables by

$$\begin{aligned} \Theta(\mathbf{X}, 0) &= \Theta_0(\mathbf{X}) && \text{in } \mathcal{B}_0 \\ \Theta &= \bar{\Theta} && \text{on } \partial \mathcal{B}_0^\theta \times [0, T] \\ \mathbf{H} \cdot \mathbf{N} &= -H_N && \text{on } \partial \mathcal{B}_0^H \times [0, T] \end{aligned} \quad (3.85)$$

3.4 Specific thermo-dissipative material models

To close the presented dynamics of thermo-dissipative solids, specific forms of the free-energy function (3.13) must be proposed so that all derived constitutive quantities can be elaborated. Typically, generalized standard material models are built from thermoelastic models which in turn rely on simple hyperelastic models. Taking this into account, a particular isotropic thermoelastic model is introduced to serve also as a base for the formulation of generalized standard materials, particularly, for the purpose of this dissertation, nonlinear (smooth) thermoviscoelastic material models will be considered.

The nonlinear thermoelastic regime accounts for the nonlinear deformations with significant thermal effects and without permanent structural changes or cracks even in the high strain ranges. Elastomeric (high-polymeric) substances such as rubber naturally behave in this regime. A representative model for them responds to the following free-energy function structure

$$\Psi(\mathbf{C}, \Theta) = f(\Theta)\Psi(\mathbf{C}) + T(J, \Theta), \quad (3.86)$$

with $\Psi(\mathbf{C})$ being any hyperelastic free-energy function, $f(\Theta)$ is a temperature-dependent function for the variations of material parameters with temperature and $T(J, \Theta)$ a function accounting for the thermal behavior and for the thermoelastic coupling effects.

As was previously remarked, the thermal effects are observed to be coupled with dilatational deformations. The form of the function T consequently agrees with so by considering two different effect, namely, a pure thermal response and a thermo-volumetric coupling effect via a thermal coefficient expansion α , that is

$$T(J, \Theta) = -3B_0\alpha(\Theta - \Theta_{\text{ref}})G(J) + c \left(\Theta - \Theta_{\text{ref}} - \Theta \log \frac{\Theta}{\Theta_{\text{ref}}} \right), \quad (3.87)$$

where $G(J)$ is a potential that penalizes the change of volume, $B(\Theta)$ is the bulk modulus which may depend on temperature such that at reference temperature Θ_{ref} its value is $B(\Theta_{\text{ref}}) = B_0$.

This structure of the thermoelastic free-energy function can be found in Holzapfel & Simó (1996a) with $f(\Theta) = \Theta/\Theta_{\text{ref}}$. Romero (2010a) also employed it to derive entropy-dependent thermodynamic potentials for which additional assumptions must be made on the above free-energy function. Particularly, the function f must at most be linear, that is $f'(\Theta) = C$, so

that the following identity can analytically be inverted

$$\eta = -\frac{\partial \Psi}{\partial \Theta}(\mathbf{C}, \Theta) = -f'(\Theta)\Psi(\mathbf{C}) + 3B_0\alpha G(J) + c \log \frac{\Theta}{\Theta_{\text{ref}}} \quad (3.88)$$

The result of this inversion thus defines the temperature function in terms of the right Cauchy-Green deformation tensor and the density entropy

$$\Theta(\mathbf{C}, \eta) = \Theta_{\text{ref}} \exp \left[\frac{1}{c} (\eta + C\Psi(\mathbf{C}) - 3B_0\alpha G(J)) \right] \quad (3.89)$$

This model can be extended to account for smooth thermoviscoelastic behavior by attaching to (3.86) a term depending on internal variables which typically vanishes at mechanical equilibrium

$$\Psi(\mathbf{C}, \Theta, \mathbf{\Lambda}^\alpha) = \Psi(\mathbf{C}, \Theta) + \Gamma(\mathbf{C}, \Theta, \mathbf{\Lambda}^\alpha) \quad (3.90)$$

The function Γ defines the particular thermoviscoelastic model. Thus, Holzapfel & Simó (1996b) proposed a quadratically-dependent function on internal variables as follows

$$\Gamma(\mathbf{C}, \Theta, \mathbf{\Lambda}^\alpha) = \sum_{\alpha=1}^m \left[\mu_\alpha(\Theta) |\mathbf{\Lambda}^\alpha|^2 - 2 \frac{\partial \Psi_{\text{iso}}^\alpha(\bar{\mathbf{C}}, \Theta)}{\partial \mathbf{C}} : \mathbf{\Lambda}^\alpha + \Psi_{\text{iso}}^\alpha(\bar{\mathbf{C}}, \Theta) \right], \quad (3.91)$$

where $\mu_\alpha \in \mathbb{R}_+$ is a non-negative parameter associated to the α -thermoviscoelastic process and $\Psi_{\text{iso}}^\alpha : \mathcal{B}_0 \times [0, T] \rightarrow \mathbb{R}$ is a hyperelastic potential related to the viscoelastic processes. This last potential is expressed in terms of isochoric deformations $\bar{\mathbf{F}}$ because, according to real experiments on polymers, see Malvern (1969), the viscoelastic effects occur strongly in shear and weaker in dilatation. For objectivity considerations, this function depends on the modified strain Green-Lagrange tensor $\bar{\mathbf{C}}$ defined as

$$\bar{\mathbf{C}} := J^{-\frac{2}{3}} \mathbf{C} \quad (3.92)$$

Unless stated otherwise the hyperelastic free-energy function is also assumed to be additively split into volumetric and isochoric parts, see Holzapfel (2000), as follows

$$\Psi^\infty(\mathbf{C}, \Theta) := \Psi_{\text{vol}}^\infty(J, \Theta) + \Psi_{\text{iso}}^\infty(\bar{\mathbf{C}}, \Theta) \quad (3.93)$$

Associated with this model, the dissipative functional becomes

$$\mathcal{K}(\mathbf{Q}^\alpha) = \frac{1}{\nu^\alpha(\Theta)} \mathbf{Q}^\alpha, \quad \nu_\alpha(\Theta) = 2\mu_\alpha(\Theta)\tau_\alpha > 0, \quad (3.94)$$

where $\nu_\alpha(\Theta)$ is a viscosity parameter and $\tau_\alpha \in \mathbb{R}_+$ is the relaxation/retardation time, both characterizing the viscous evolution.

Alternatively, based on the multiplicative split of the deformation gradient tensor, Reese & Govindjee (1998a) proposed a function Γ that takes the form of the free-energy function Ψ but evaluated by an objective tensor deriving from the multiplicative structure of the deformation gradient, which is identified with the internal variable.

3.5 Symmetries and laws of thermodynamics

The evolution of isolated thermo-dissipative continua is determined by equation symmetries associated to conserved quantities. These quantities are revealed by the balances laws (3.45) - (3.56) when no external forces and heats are present, that is $\mathbf{F}(t) = \mathbf{M}(t) = \mathbf{0}$ and $Q(t) = 0$. Thus, following the momentum balances, the total linear and angular momentum must be preserved

$$\dot{\mathbf{L}}(t) = \dot{\mathbf{J}}(t) = \mathbf{0} \quad (3.95)$$

According to Noether's theorem, see Goldstein et al. (1965), these conserved quantities are related to the symmetries of the thermo-dissipative continuum evolution equations, which will be in-depth discussed in subsequent Chapters.

On the other hand, the first laws of thermodynamics for isolated systems lead to the conservation of the total energy $E : [0, T] \rightarrow \mathbb{R}$, defined as the kinetic energy (3.55) plus the total internal energy (3.54), that is

$$E(t) := K(t) + U(t) \quad (3.96)$$

The proof for the conservation of the total energy directly follows from the energy balance (3.60) for isolated continua, that is

$$\dot{E}(t) = 0 \quad (3.97)$$

Likewise, the second law of thermodynamics leads to the preservation (reversible processes) or increment (irreversible processes) of the total entropy $S : [0, T] \rightarrow \mathbb{R}_+$ provided by

$$S(t) := \int_{\mathcal{B}_0} \eta(\mathbf{X}, t) dV_0 \quad (3.98)$$

Then, the second law can be verified by using either the entropy formulation (3.71) or the temperature formulation (3.80) to express the rate of entropy per unit reference volume as

$$\dot{S}(t) = \int_{\mathcal{B}_0} \dot{\eta}(\mathbf{X}, t) dV_0 = \int_{\mathcal{B}_0} \frac{1}{\Theta} \left[-\nabla_0 \cdot \mathbf{H} + \dot{\mathcal{D}} \right] dV_0 \quad (3.99)$$

Further elaboration of (3.99) is performed by making use of divergence product rule⁵ and the Gauss' theorem to obtain

$$\dot{S}(t) = - \int_{\partial \mathcal{B}_0} \frac{1}{\Theta} \mathbf{H} \cdot \mathbf{N} dA_0 + \int_{\mathcal{B}_0} \nabla_0 \left[\frac{1}{\Theta} \right] \cdot \mathbf{H} dV_0 + \int_{\mathcal{B}_0} \frac{1}{\Theta} \dot{\mathcal{D}} dV_0 \quad (3.100)$$

As the continuum is isolated the flux on its boundary must be zero so the first term of (3.100) vanishes. Using the Duhamel's law (3.26) along with (3.27), the rate of total entropy can be demonstrated to be always non-negative

$$\dot{S}(t) = \int_{\mathcal{B}_0} \frac{1}{\Theta^2} \nabla_0 \Theta \mathbf{K} \nabla_0 \Theta dV_0 + \int_{\mathcal{B}_0} \frac{1}{\Theta} \sum_{\alpha=1}^m \mathbf{Q}^\alpha : \mathcal{K}(\mathbf{Q}^\alpha) dV_0 \geq 0, \quad (3.101)$$

because both the conductivity tensor (3.27) and the functional $\mathcal{K}$ (3.22) are positive semidefinite.

3.6 Isothermal dynamics as a limit case

In many engineering applications the thermal effects can be disregarded as observations show they do not significantly contribute to the system evolution, although dissipative effects might still condition it. Thus, the limit case of isothermal changes represents a useful framework to study these types of phenomena.

To derive this limit case, the temperature of the continuum is assumed to be constant so that the material behavior might depend only on the deformation and internal variables, as previously introduced in (3.40). The absence of temperature changes obliges to consider the Clausius-Planck inequality for isothermal processes, also called *internal dissipation inequality*, to ensure that the possible dissipated energy flows according to the second principle of thermodynamics. Such inequality reads

$$\dot{\mathcal{D}} = \frac{1}{2} \mathbf{S} : \dot{\mathbf{C}} - \dot{\Psi} \geq 0 \quad (3.102)$$

⁵ $f \nabla_0 \cdot \mathbf{v} = \nabla_0 \cdot (f \mathbf{v}) - \mathbf{v} \cdot \nabla_0 f$

Remark 3.9. When there is no dissipation the above inequality becomes an identity, giving rise to the reversible pure elastic deformation case in which the free-energy function depends only on deformations (3.41).

Following analogous arguments as those which led from (3.18) to (3.21) the ensuing constitutive laws are obtained

$$\mathbf{S} = 2 \frac{\partial \Psi(\mathbf{C}, \mathbf{\Lambda}^\alpha)}{\partial \mathbf{C}}, \quad \mathbf{Q}^\alpha = - \frac{\partial \Psi(\mathbf{C}, \mathbf{\Lambda}^\alpha)}{\partial \mathbf{\Lambda}^\alpha} \quad (3.103)$$

With this assumption, the isothermal formulation can be derived from the previous one (3.66) by neglecting all temperature-dependent terms. Proceeding this way the strong form of isothermal dynamics reduces to

$$\left. \begin{aligned} \dot{\boldsymbol{\varphi}} &= \frac{1}{\rho_0} \mathbf{p} \\ \dot{\mathbf{p}} &= \nabla_0 \cdot (\mathbf{F}\mathbf{S}) + \mathbf{B}_0 \\ \dot{\mathbf{\Lambda}}^\alpha &= \mathcal{K}(\mathbf{Q}^\alpha) \quad \forall \alpha = 1, \dots, m \end{aligned} \right\} \quad \text{in } \mathcal{B}_0 \times [0, T] \quad (3.104)$$

The isothermal consideration brings the system back to the mechanic context in which the energy balance is no longer required to be fulfilled but it is a consequence of the momentum balances (3.45) and (3.52). However, for consistency, the total energy must include the total dissipated energy $D : [0, T] \rightarrow \mathbb{R}$ provided by

$$D(t) := \int_{\mathcal{B}_0} \mathcal{D}(\mathbf{X}, t) dV_0 = \int_{\mathcal{B}_0} \left(\int_0^t \dot{\mathcal{D}} ds \right) dV_0 \quad (3.105)$$

Thus, the energy balance now postulates that the external mechanical power (3.57) supplied to the continuum is employed to change the total energy (3.96) and to produce dissipated energy (3.105) due to the development of dissipative processes, that is

$$\dot{E}(t) + \dot{D}(t) = P_{\text{ext}}(t) \quad (3.106)$$

In this context, the total energy (3.96) is redefined to account for the dissipated energy

$$\bar{E}(t) := E(t) + D(t) \quad (3.107)$$

Then, the energy balance (3.106) applied to isolated systems ($P_{\text{ext}}(t) = 0$) reveals that this *new* energy is preserved. As it is usually expressed using the

phase space variables, that is, coordinates and momenta, it is also referred to as *Augmented Hamiltonian*, see Mohr (2008).

Within the just introduced isothermal framework, classical nonlinear *viscoelasticity*, *plasticity* or *damage* could be formulated by defining appropriate functionals $\mathcal{K}$. We will hereafter focus on smooth changes, that is, viscoelasticity, although we will also give a brief summary of the canonical case of non-smooth problems: plasticity.

3.6.1 Viscoelasticity at finite strain

The most representative isothermal smooth dissipative problem is viscoelasticity. Considering a linear law for the evolution equations of internal variables, it is provided by a dissipative functional $\mathcal{K}$ of the form (3.23), leading to the ensuing general form of the evolution equations

$$\left. \begin{aligned} \dot{\varphi} &= \frac{1}{\rho_0} \mathbf{p} \\ \dot{\mathbf{p}} &= \nabla_0 \cdot (\mathbf{FS}) + \mathbf{B}_0 \\ \dot{\mathbf{A}}^\alpha &= \mathbb{V}^\alpha : \mathbf{Q}^\alpha \quad \forall \alpha = 1, \dots, m \end{aligned} \right\} \quad \text{in } \mathcal{B}_0 \times [0, T] \quad (3.108)$$

This form of the evolution equations fully reproduces the typical viscoelastic behavior characterized by the irreversible processes known as *relaxation* and *creep*. These time-dependent processes connect two consecutive states of mechanic equilibrium under the specific boundary conditions of either fixed strain or fixed stress, sketched in Figure 3.4, and are determined by the relaxation/retardation time $\tau \in \mathbb{R}_+$ which measures the rate of decay/rise of the stress/strain.

In this context, the dissipative driving stress tensor $\mathbf{Q}^\alpha$ is referred to as *non-equilibrium stress tensor* since it tends to disappear as the mechanical equilibrium is reached.

Many different viscoelastic models at finite strain can be found in the literature depending on how the internal variable is defined and how the fourth order tensor viscoelastic tensor is furnished, including linear or non-linear evolution equations for the internal variables. Next, some important examples are summarized.

Holzapfel and Simó. The thermoviscoelastic model due to Holzapfel & Simó (1996b) and provided by (3.91) can be used as isothermal viscoelastic

Figure 3.4. Relaxation and creep processes

model neglecting the temperature field such that

$$\Psi(\mathbf{C}, \mathbf{\Lambda}^\alpha) = \Psi^\infty(\mathbf{C}) + \sum_{\alpha=1}^m \left[\mu_\alpha |\mathbf{\Lambda}^\alpha|^2 - 2 \frac{\partial \Psi_{\text{iso}}^\alpha(\bar{\mathbf{C}})}{\partial \mathbf{C}} : \mathbf{\Lambda}^\alpha + \Psi_{\text{iso}}^\alpha(\bar{\mathbf{C}}) \right], \quad (3.109)$$

where $\Psi^\infty : \mathcal{B}_0 \times [0, T] \rightarrow \mathbb{R}$ represents any hyperelastic potential, $\mu_\alpha \in \mathbb{R}_+$ is a non-negative parameter associated to the α -viscoelastic process and $\Psi_{\text{iso}}^\alpha : \mathcal{B}_0 \times [0, T] \rightarrow \mathbb{R}$ is a hyperelastic potential related to the viscoelastic processes. Accordingly, the free-energy function is additively split into volumetric and isochoric parts, see Holzapfel (2000), as follows

$$\Psi^\infty(\mathbf{C}) := \Psi_{\text{vol}}^\infty(J) + \Psi_{\text{iso}}^\infty(\bar{\mathbf{C}}) \quad (3.110)$$

The above viscoelastic free energy function (3.109) ensures positive dissipation if the rate of internal variables follows a linear law which results from the following fourth order *viscoelastic* tensor

$$\mathbb{V}^\alpha = \frac{1}{\nu^\alpha} \mathbb{I} \quad \forall \alpha = 1, \dots, m, \quad (3.111)$$

with $\mathbb{I}$ being the four rank identity tensor and ν_α being the viscosity coefficient linked to the relaxation/retardation time, inspired by linear viscoelasticity, via

$$\nu_\alpha = 2\mu_\alpha\tau_\alpha \quad (3.112)$$

Furthermore, the viscoelastic free-energy function (3.109) depends quadratically on internal variables and hence the non-equilibrium stress tensor (3.103)₂ will result in a linear function of them

$$\mathbf{Q}^\alpha = -2\mu_\alpha \mathbf{\Lambda}^\alpha + 2 \frac{\partial \Psi_{\text{iso}}^\alpha(\bar{\mathbf{C}})}{\partial \mathbf{C}}, \quad (3.113)$$

so that the evolution equations become linear first order differential equations

$$\dot{\mathbf{\Lambda}}^\alpha + \frac{1}{\tau_\alpha} \mathbf{\Lambda}^\alpha = \frac{2}{\nu_\alpha} \frac{\partial \Psi_{\text{iso}}^\alpha(\bar{\mathbf{C}})}{\partial \mathbf{C}}, \quad (3.114)$$

where use has been made of (3.112). Hence, it can analytically be integrated⁶ to give

$$\mathbf{\Lambda}^\alpha(\mathbf{X}, t) = \int_0^t \exp \left[\frac{-(t-s)}{\tau_\alpha} \right] \frac{2}{\nu_\alpha} \frac{\partial \Psi_{\text{iso}}^\alpha}{\partial \mathbf{C}}(\mathbf{X}, s) ds + \exp \left[\frac{-t}{\tau_\alpha} \right] \mathbf{\Lambda}_0^\alpha \quad (3.115)$$

The history-dependent character of such variables is reflected on the time integration over all previous instant times. Obviously, the above expression needs the partial derivative of the deformation-dependent potential Ψ_{iso}^α to be known at each instant time and material point.

In the literature, such potential Ψ_{iso}^α , associated to the α -dissipative process, is widely assumed to be a proportional part of the hyperelastic potential Ψ_{iso}^∞ by defining non-dimensional constitutive parameters Govindjee & Simó (1992), known as strain-energy factors $\beta_\alpha \geq 0$, such that

$$\Psi_{\text{iso}}^\alpha(\bar{\mathbf{C}}) = \beta_\alpha \Psi_{\text{iso}}^\infty(\bar{\mathbf{C}}) \quad \text{with} \quad \beta_\alpha = \frac{2\mu_\alpha}{E^\infty} \quad \forall \alpha = 1, \dots, m, \quad (3.116)$$

with E^∞ being the Young's modulus defining the hyperelastic potential.

This assumption is further supported by experimental tests on elastomers with viscoelastic behavior characterized by a medium composed of identical polymer chains.

Remark 3.10. Regarding the numerical solution of this model, an important drawback may emerge when applying iterative strategies, i.e Newton-Rapshon method, in which the linearization of the governing equations are required. This step would involve the computation of a rank six tensor arising from the linearization of the stress tensor, known as the linearized material tensor, that is

$$\mathbb{C} = 2 \frac{\partial \mathbf{S}}{\partial \mathbf{C}} = 4 \frac{\partial^2 \Psi}{\partial \mathbf{C}^2} = 4 \left(1 + \sum_{\alpha=1}^m \beta_\alpha \right) \frac{\partial^2 \Psi_{\text{iso}}^\infty}{\partial \mathbf{C}^2} - 8 \sum_{\alpha=1}^m \beta_\alpha \underbrace{\frac{\partial^3 \Psi_{\text{iso}}^\infty}{\partial \mathbf{C}^3}}_{\in \mathbb{T}_d^6} : \mathbf{\Lambda}^\alpha \quad (3.117)$$

Nevertheless, as this sixth order tensor is scaled by the internal variables, in most of the cases this term can be neglected respect to the others such that they could be enough for a successful convergence process.

⁶ $y' + P(x)y = Q(x) \rightarrow y(x) = \exp \left[- \int P(x) dx \right] \int \exp \left[\int P(x) dx \right] Q(x) dx$

Remark 3.11. The described viscoelastic model can be based on anisotropic models as demonstrated in Holzapfel & Gasser (2001).

On the other hand, Holzapfel & Simó (1996b) introduced the following simple form of this potential to provide a rheological interpretation of their model

$$\Psi_{\text{iso}}^{\alpha}(\mathbf{C}) = \frac{1}{8}(\mathbf{C} - \mathbf{1}) : 2\mu_{\alpha}\mathbb{I} : (\mathbf{C} - \mathbf{1}) \quad (3.118)$$

This function is defined through the whole right Cauchy-Green deformation tensor (3.11) instead of its isochoric part (3.92) as was presented. It is the classical Saint-Venant hyperelastic model with the stiffness parameter expressed in terms of the positive parameter μ_{α} . In this particular case, it can be proved that the constitutive (3.103) laws are related in the following way

$$\mathbf{S} = \mathbf{S}^{\infty} + \sum_{\alpha=1}^m \mathbf{Q}^{\alpha} \quad (3.119)$$

Thus, the model follows the rheological behavior provided by the generalized Maxwell element, composed of a spring arranged in parallel with as many as Maxwell-elements as required for the viscoelastic response, sketched in Figure 3.5. That is, at the beginning of the deformation the material response is distributed among the elastic (main) spring and the Maxwell-elements ($\mathbf{Q}^{\alpha} \neq \mathbf{0}$). Instead, as the viscoelastic effects fully develop the whole response is only due to the main spring ($\mathbf{Q}^{\alpha} = \mathbf{0}$).

Now, it is convenient to approach the evolution equations for the internal variables by using the non-equilibrium stress tensor, via time differentiation of (3.108)₃ and (3.114) with (3.111), that is

$$\dot{\mathbf{Q}}^{\alpha} + \frac{1}{\tau_{\alpha}}\mathbf{Q}^{\alpha} = 2\frac{d}{dt} \left[\frac{\partial \Psi_{\text{iso}}^{\alpha}}{\partial \mathbf{C}} \right], \quad (3.120)$$

whose analytical solution is of the form

$$\mathbf{Q}^{\alpha} = \exp \left[-\frac{T}{\tau_{\alpha}} \right] \mathbf{Q}_0^{\alpha} + \int_0^T \exp \left[\frac{-(T-t)}{\tau_{\alpha}} \right] 2\frac{d}{dt} \left[\frac{\partial \Psi_{\text{iso}}^{\alpha}}{\partial \mathbf{C}} \right] dt \quad (3.121)$$

This final expression thus enters (3.119) directly, so the specification of the strain-like internal variables are no longer needed to determine the viscoelastic response.

Mandel stress tensor. A common way to construct isotropic viscoelastic model relies on the concept of the Mandel stress tensor, extensively used in

Figure 3.5. Rheological model

formulations of inelastic material, see Gross & Betsch (2010); Miehe (1995). The departure point is to consider an isotropic material behavior which depends only on invariants of the tensor

$$\mathbf{\Gamma} := \mathbf{C}\mathbf{\Lambda}^{-1}, \quad (3.122)$$

$\mathbf{\Lambda}$ being the symmetric strain-like internal variable, such that

$$\Psi(\mathbf{C}, \mathbf{\Lambda}) := \Psi(\mathbf{\Gamma}) = \Psi(I_{\mathbf{\Gamma}}, II_{\mathbf{\Gamma}}, III_{\mathbf{\Gamma}}) \quad (3.123)$$

This special structure of the viscoelastic free-energy function leads to the definition of the symmetric *Mandel* stress tensor $\mathbf{Y} : \mathcal{B}_0 \times [0, T] \mapsto \text{Sym}(\mathbb{T}_d^2)$ which directly derives from the constitutive relationships (3.103) and reads

$$\mathbf{Y}(\mathbf{X}, t) := \frac{\partial \Psi}{\partial \mathbf{\Gamma}} = 2\mathbf{\Lambda}\mathbf{Q} = \mathbf{C}\mathbf{S} \quad (3.124)$$

Then, the evolution equation for the internal variable is defined through this new stress-like tensor rather than directly through the non-equilibrium

stress tensor, as previously proposed in (3.104)₃, observing that the dissipation inequality (3.102) can be expressed by

$$\dot{\mathcal{D}} = \mathbf{Q} : \dot{\mathbf{\Lambda}} = \mathbf{\Lambda} \mathbf{Q} : \mathbf{\Lambda}^{-1} \dot{\mathbf{\Lambda}} = \mathbf{Y} : \frac{1}{2} \mathbf{\Lambda}^{-1} \dot{\mathbf{\Lambda}} \geq 0 \quad (3.125)$$

In this connection, the second factor in the last term is viewed as a measure of the viscous deformation rate collected in a second order tensor $\mathbf{Z} : \mathcal{B}_0 \times [0, T] \mapsto \text{Sym}(\mathbb{T}_d^2)$ as follows

$$\mathbf{Z} := \frac{1}{2} \mathbf{\Lambda}^{-1} \dot{\mathbf{\Lambda}}, \quad (3.126)$$

such that the evolution equation emanates from making the above inequality a quadratic form, that is

$$\mathbf{Z} = \mathbb{V} : \mathbf{Y}, \quad (3.127)$$

with the viscoelastic fourth order tensor $\mathbb{V}$ being positive semidefinite. Furthermore, it can naturally be expressed in terms of the internal variables and the non-equilibrium stress tensor as follows

$$\dot{\mathbf{\Lambda}} = 2\mathbf{\Lambda} \mathbb{V} : (\mathbf{\Lambda} \mathbf{Q}), \quad (3.128)$$

which is an alternative form of (3.23).

Reese and Govindjee. When facing inelastic effects at finite strains, often the locally multiplicative decomposition of the deformation gradient (3.2) into *elastic* $\mathbf{F}_e$ and *inelastic* (in this case *viscous*) $\mathbf{F}_i$ components, as proposed in Lubliner (1985), is introduced

$$\mathbf{F} := \mathbf{F}_e \mathbf{F}_i \quad (3.129)$$

In this decomposition, it is implicitly assumed the existence of a generally incompatible stress-free configuration $\tilde{\mathbf{x}} \in \tilde{\mathcal{B}}$, called *elastic*, at each neighborhood of every particle point p in the current configuration, as showed in Figure 3.6.

Accordingly, new frame-invariance strain measures are directly derived such as

$$\mathbf{C}_e := \mathbf{F}_e^T \mathbf{F}_e, \quad \mathbf{C}_i := \mathbf{F}_i^T \mathbf{F}_i, \quad \mathbf{b}_e := \mathbf{F}_e \mathbf{F}_e^T, \quad \mathbf{b}_i := \mathbf{F}_i \mathbf{F}_i^T, \quad (3.130)$$

with the following crucial relationships among them

$$\mathbf{C}_e = \mathbf{F}_i^{-T} \mathbf{C} \mathbf{F}_i^{-1}, \quad \mathbf{b}_e = \mathbf{F} \mathbf{C}_i^{-1} \mathbf{F}^T, \quad (3.131)$$

Figure 3.6. Multiplicative decomposition in the small neighborhood of a particle

The inelastic right Cauchy-Green deformation tensor $\mathbf{C}_i$ is defined in the reference configuration, whereas its elastic counterpart $\mathbf{C}_e$ is defined with reference to the elastic configuration.

This decomposition can also be viewed as a rheological model such as the one sketched in Figure 3.5 but with one Maxwell-element. Thus, the elastic deformation gradient can be interpreted as a deformation measure of the main spring whereas the inelastic one is seen as a deformation of the Maxwell-element spring, so that the latter plays the role of an internal variable.

Based on this interpretation, Reese & Govindjee (1998b) proposed a viscoelastic free-energy function expressed as

$$\Psi(\mathbf{C}, \mathbf{F}_i^{-1}) := \Psi^\infty(\mathbf{C}) + \Psi^i(\mathbf{F}_i^{-T} \mathbf{C} \mathbf{F}_i^{-1}) \quad (3.132)$$

The potential Ψ^i accounts for the viscoelastic effects and is chosen in a way that it vanishes when no viscous deformations are present so that the body responds elastically according to the hyperelastic free-energy function Ψ^∞ . In addition, the viscoelastic constitutive response is actually a function of the elastic right Cauchy-Green deformation tensor $(3.130)_1$ via $(3.131)_1$. Accordingly, Ψ^i is widely assumed to be the same potential as Ψ^∞ but evaluated by $\mathbf{C}_e$ since it complies with the requirement of vanishing when no viscoelastic deformations occurs, i.e $\mathbf{C}_e = \mathbf{1}$.

The above viscoelastic free-energy function (3.132) is fully consistent

with the previously introduced Mandel stress tensor approach in the case of isotropy. With this assumption, the above viscoelastic free-energy function can indifferently be expressed in terms of the invariants of the tensors $\mathbf{C}_e$ and $\mathbf{C}\mathbf{C}_i^{-1}$ such that

$$\Psi(\mathbf{C}, \mathbf{F}^{-1}) = \Psi^\infty(\mathbf{C}) + \Psi^i(\mathbf{C}_e) = \Psi^\infty(\mathbf{C}) + \Psi^i(\mathbf{C}\mathbf{C}_i^{-1}) \quad (3.133)$$

In view of that, the Mandel stress tensor approach follows directly from identifying the symmetric strain-like internal variable to be

$$\mathbf{\Lambda} := \mathbf{C}_i \quad (3.134)$$

Hence, the evolution equation for the internal variable is

$$\dot{\mathbf{C}}_i = 2\mathbf{C}_i \mathbb{V} : (\mathbf{Q}\mathbf{C}_i), \quad (3.135)$$

where $\mathbb{V}$ is a positive semidefinite fourth order tensor specified by two positive material parameters $\nu_D \in \mathbb{R}^+$ and $\nu_V \in \mathbb{R}^+$ referred to as deviatoric and volumetric viscosity, respectively, which may generally be deformation-dependent, so that

$$\mathbb{V} = \frac{1}{2\nu_D} \left(\mathbb{I} - \frac{1}{3} \mathbf{1} \otimes \mathbf{1} \right) + \frac{1}{9\nu_V} \mathbf{1} \otimes \mathbf{1} \quad (3.136)$$

Following the classic plasticity theory, Reese & Govindjee (1998a,b) presented the above evolution equations in the current configuration via the relation between the inverse of the inelastic right Cauchy-Green tensor and the elastic left Cauchy-Green deformation tensor (3.131)₂.

Bonet. Also based on the locally multiplicative split of the deformation gradient (3.129), Bonet (2001) proposed the same structure of the viscoelastic free-energy function as (3.132) to arrive at the additive structure of the constitutive law for the symmetric Piola-Kirchhoff stress tensor

$$\mathbf{S} = \mathbf{S}^\infty + \mathbf{S}^i \quad (3.137)$$

Then, relying on kinematic assumptions rather than thermodynamic consistency the following evolution equation was proposed

$$\dot{\mathbf{C}}_i = -\frac{2}{\tau} \left[\frac{\partial^2 \Psi^i(\mathbf{C}, \mathbf{C}_i)}{\partial \mathbf{C} \partial \mathbf{C}_i} \right]^{-1} : \mathbf{S}^i \quad (3.138)$$

The above relation ensures that the viscoelastic effects truly occur due to deviatoric deformations. Nevertheless, unlike the previous models, it does not rely on the dissipation inequality (3.102) so, generally, it does not have to agree with the thermodynamics. This does not mean that one cannot find particular material models which matches this crucial requirement while complying with (3.138), but it does mean that any material model used must be checked to fulfill the required thermodynamic consistency.

All presented models would require only the specification of a hyperelastic Helmholtz free-energy function $\Psi^\infty(\mathbf{C})$ to provide particular viscoelastic models.

In the rest of this dissertation the model due to Holzapfel and Simó will be chosen without losing of generality.

3.6.2 Nonlinear plasticity at finite strain

Although plasticity is a non-smooth dissipative effect and hence out of the scope of this dissertation, it is interesting to include some notes about how it can be described from the framework previously presented.

The non-smooth nature of the plasticity can mathematically be described by using the concept of sub-differentials, denoted as ∂ , see Studer (2009) for the application to non-smooth dynamics. Thus, the positive semidefinite functional $\mathcal{K}$ (3.22) becomes a sub-differential of a positive convex functional $\mathcal{J}$, key details can be found in Mielke (2011), so that the nonlinear plasticity can be cast into the following general form

$$\left. \begin{aligned} \dot{\boldsymbol{\varphi}} &= \frac{1}{\rho_0} \mathbf{p} \\ \dot{\mathbf{p}} &= \nabla_0 \cdot (\mathbf{F}\mathbf{S}) + \mathbf{B}_0 \\ \dot{\mathbf{A}}^\alpha &\in \partial_{\mathbf{Q}} \mathcal{J}(\mathbf{Q}^\alpha) \quad \forall \alpha = 1, \dots, m \end{aligned} \right\} \quad \text{in } \mathcal{B}_0 \times [0, T] \quad (3.139)$$

The convex functional is thus linked with the flow rule, the consistency condition and the loading-unloading conditions that define the plastic behavior. These ingredients have traditionally been proposed to handle the non-smooth plastic evolution. For example, assuming the multiplicative decomposition (3.129), any finite strain plastic model is proved to be thermodynamically sound if

$$-\frac{1}{2} \mathcal{L}_v(\mathbf{b}_e) \mathbf{b}_e^{-1} = \zeta \frac{\partial \phi}{\partial \boldsymbol{\tau}}, \quad (3.140)$$

ϕ being the yield function and $\dot{\zeta}$ being the consistency parameter (Lagrangian multiplier) satisfying the loading-unloading conditions

$$\dot{\zeta} \geq 0, \quad \phi \geq 0, \quad \dot{\zeta}\phi = 0, \quad (3.141)$$

and the consistency condition

$$\dot{\zeta}\dot{\phi} = 0 \quad \text{for } \phi = 0, \quad (3.142)$$

see, for instance, Simó & Miehe (1992) or Bergstrom & Boyce (1998). Defining appropriated convex functionals $\mathcal{J}$ these models can be generated from (3.139).

3.7 Semidiscrete thermo-dissipative dynamics

The modeling of thermo-dissipative continuum dynamics has resulted in an infinite-dimensional evolution system that is nonlinear in space and time and hence it only allows for numerical solutions. Thereby, the infinite-dimensional problem should be transformed into an approximated finite-dimensional one in which the number of variables are bounded. In this process, the partial differential equation system becomes a set of algebraic ones which are recursively solved. This transformation may spoil the original continuous structure of the problem and hence the numerical solution may be quite different (the longer the simulation the worse) from the exact one in terms of physical behavior, not of numerical errors that will inevitably appear. Recall that one of the main objectives of this dissertation is to propose numerical tools that do not ideally introduce *physical* spuriousness in the final numerical method.

Traditionally, the strategies to numerically address continuous problems in space and time are to perform two subsequent discretizations: spatial and temporal. However, space-temporal monolithic discretizations can also be found in the literature, see for instance Gross & Betsch (2011). For the purpose of this dissertations, the first (classical) approach will be adopted as its main contribution is intended for the time integration. In this sense, the spatial discretization performed in this dissertation will be standard, meaning that no further contribution will be made, and no degradation of the time-conservation properties will be involved. Next, a brief summary of the current state-of-the-art for spatial discretization techniques available to face general partial differential equations is carried out.

Since the beginning of numerical methods, different spatial discretization techniques have been proposed. Among them, the most prominent is the Finite Element Method (FEM) Bathe (1982); Hughes (1987); Oñate (2008), mainly because it can accommodate multi-physic problems, not to mention that it was the pioneer in numerical methods as they are understood nowadays. In the last decades, the FEM has widely been developed for the solutions of many physic, mathematical and engineering problems, having highlighted its shortcomings. In order to improve its performance in particular applications many enhancements have been proposed, in some cases even giving rise to new methods such as the Extended Finite Element Method (XFEM) Moës et al. (1999) for the solution of crack propagation, or B-bar FEM or Mixed FEM for incompressible solid deformations Simó et al. (1985). Also, the search for better order of accuracy in the approximation yielded the families of high order FEMs known as hp-FEM or hpk-FEM, see Babuška & Guo (1992).

On the other hand, the fluid dynamics particular demands made its own way on the development of numerical solutions. Thus, the Discontinuous Galerkin (DG) or Petrov-Galerkin (PG) FEM were developed for the solution of diffusion-advection problems, then extended to general first order conservation laws. Also, the Finite Volume Method (FVM) LeVeque (2002) has been successful in this area. Interestingly, these methods have recently been incorporated for the solution of fast solid dynamics Aguirre et al. (2014, 2015); Bonet et al. (2015); Gil et al. (2014); Lee et al. (2013, 2014), thus circumventing the locking phenomenon related to the standard displacement-based FEM applied to incompressible or cuasi-incompressible deformations.

More recently, Mesh-free methods Liu & Gu (2010) and Isogeometric Analysis (IGA) Cottrell et al. (2009); Hughes et al. (2005) have attracted most of the efforts of computational mechanics' community. In the first group, the SPH method Lucy (1977); Monaghan (1988) intended for the solution of strong forms, the Meshfree Galerkin methods with Moving-Least-Square (MLS) approximation functions Belytschko et al. (1994) (named EFG) or the Max-Ent method due to Arroyo & Ortiz (2006) have been advocated for the solution of several types of demanding problems. For instance, a Galerkin Mesh-free method using Radial Basis functions (RBF) has been proposed for the solution of Flexible Multibody Systems with holonomic constraints in Iglesias Ibáñez & García Orden (2011); Iglesias Ibáñez et al. (2013). Also, the Max-Ent approach has been the basis for developing a new framework for the fluid-structure interaction using the Lagrangian description for both solids and fluids in Urrecha (2014).

In theory, any of these spatial discretization techniques could be combined with structure-preserving integration methods provided that they do not spoil the conservation properties of the continuous model. An appealing proof is due to Hesch & Betsch (2012) where an Energy-Momentum method is embedded within a spatial discretization based on IGA.

3.7.1 Variational statement of the IBVP

Most of discretization techniques rely on the variational statement of the (partial) differential equations under consideration, also referred to as the *weak* form of the (partial) differential equations. This choice is based mainly on the fact that the weak form straightforwardly enables the imposition of Neumann boundary conditions, and on the fact that the continuity of the solution may be relaxed compared to the one required by strong forms. Furthermore, the fundamental lemma of the Calculus ensures that the solution of the weak statement fully corresponds with the solution of the strong one, justifying the use of weak forms in discretization techniques.

Weak forms can be derived from strong forms by defining the *trial* and the *weighting* (or *test*) functions. The first ones must comply with the Dirichlet boundary conditions while the second ones must be compatible with them. They are defined in the trial and weighting spaces as

$$\mathcal{V} = \{v | v \in \mathcal{M}, v = \bar{v} \text{ on } \partial\mathcal{B}_0^{\varphi, \theta} \times [0, T]\}, \quad (3.143)$$

$$\mathcal{W} = \{w | w \in \mathcal{N}, w = 0 \text{ on } \partial\mathcal{B}_0^{\varphi, \theta} \times [0, T]\}, \quad (3.144)$$

where $\bar{v}$ represents the prescribed Dirichlet boundary conditions and $\mathcal{M}$ and $\mathcal{N}$ are any two infinite-dimensional spaces.

The procedure consists in first multiplying the strong form by the *weighting* function and then integrating it over the volume occupied by the continuum. The weighting functions and the terms of strong forms thus furnish an inner product space such that $\mathcal{U} = \{v, u | v, u \in \mathcal{V} \times \mathcal{W}, \langle u, v \rangle : \mathcal{V} \times \mathcal{W} \rightarrow \mathbb{R}\}$. A more detailed explanation of this procedure can be found in Hughes (1987).

Let $\mathbf{w}_\varphi, \mathbf{w}_p, w_e, \mathbf{w}_\Lambda^\alpha \in \mathcal{W}$ be a set of weighting functions for each of the trial functions $\varphi, p, e, \Lambda^\alpha \in \mathcal{V}$, then the variational statement of the initial-

boundary value problem (3.66) may be stated by

$$\begin{aligned}
\langle \mathbf{w}_\varphi, \dot{\varphi} \rangle_{\mathcal{B}_0} - \langle \mathbf{w}_\varphi, \frac{1}{\rho_0} \mathbf{p} \rangle_{\mathcal{B}_0} &= 0 \\
\langle \mathbf{w}_\mathbf{p}, \dot{\mathbf{p}} \rangle_{\mathcal{B}_0} + \langle \nabla_0 \mathbf{w}_\mathbf{p}, \mathbf{FS} \rangle_{\mathcal{B}_0} - \langle \mathbf{w}_\mathbf{p}, \mathbf{B}_0 \rangle_{\mathcal{B}_0} - \langle \mathbf{w}_\mathbf{p}, \mathbf{T}_0 \rangle_{\partial \mathcal{B}_0} &= 0 \\
\langle w_e, \dot{e} \rangle_{\mathcal{B}_0} - \langle w_e, \frac{1}{2} \mathbf{S} : \dot{\mathbf{C}} \rangle_{\mathcal{B}_0} - \langle \nabla_0 w_e, \mathbf{H} \rangle_{\mathcal{B}_0} & \\
- \langle w_e, \mathcal{R} \rangle_{\mathcal{B}_0} + \langle w_e, H_N \rangle_{\partial \mathcal{B}_0} &= 0 \\
\langle \mathbf{w}_\Lambda^\alpha, \dot{\Lambda}^\alpha \rangle_{\mathcal{B}_0} - \langle \mathbf{w}_\Lambda^\alpha, \mathcal{K}(\mathbf{Q}^\alpha) \rangle_{\mathcal{B}_0} &= 0 \quad \forall \alpha = 1, \dots, m,
\end{aligned} \tag{3.145}$$

where use has been made of the notation $\langle \cdot, \cdot \rangle_\Delta = \int_\Delta (\cdot) \cdot (\cdot) d\Delta$.

In order to achieve the formulations based on entropy and temperature, weak forms of the energy balances (3.71) and (3.84) must be provided. Thus, let $w_\eta \in \mathcal{W}$ be the test function for the entropy variable $\eta \in \mathcal{V}$ such that the weak form of the energy balance in entropy form (3.71) may be expressed as

$$\begin{aligned}
\langle w_\eta, \dot{\eta} \rangle_{\mathcal{B}_0} - \langle \nabla_0 \left[\frac{w_\eta}{\Theta} \right], \mathbf{H} \rangle_{\mathcal{B}_0} - \langle \frac{w_\eta}{\Theta}, \dot{\mathbf{p}} \rangle_{\mathcal{B}_0} & \\
+ \langle \frac{w_\eta}{\Theta}, H_N \rangle_{\partial \mathcal{B}_0} - \langle \frac{w_\eta}{\Theta}, \mathcal{R} \rangle_{\mathcal{B}_0} &= 0
\end{aligned} \tag{3.146}$$

Likewise, the weak form of the energy balance in temperature form (3.84) is defined via the test function $w_\Theta \in \mathcal{W}$ for the temperature variable $\Theta \in \mathcal{V}$ to give

$$\begin{aligned}
\langle w_\Theta, \dot{\Theta} \rangle_{\mathcal{B}_0} - \langle \nabla_0 \left[\frac{w_\Theta}{c} \right], \mathbf{H} \rangle_{\mathcal{B}_0} + \langle \frac{w_\Theta}{c} \mathbf{FV}, \nabla_0 \left[\frac{\mathbf{p}}{\rho_0} \right] \rangle_{\mathcal{B}_0} & \\
- \langle \frac{w_\Theta}{c}, \dot{\mathbf{D}} + \mathcal{H}_d \rangle_{\mathcal{B}_0} + \langle \frac{w_\Theta}{c}, H_N \rangle_{\partial \mathcal{B}_0} - \langle \frac{w_\Theta}{c}, \mathcal{R} \rangle_{\mathcal{B}_0} &= 0
\end{aligned} \tag{3.147}$$

The full entropy-based or temperature-based weak formulations are then obtained by replacing (3.146) or (3.147) with (3.145)₃ and accordingly considering the correct constitutive laws.

On the other hand, the particular forms of (3.66)₁ and (3.66)₄ lead to the pointless weak forms (3.145)₁ and (3.145)₄, in the sense that it remains necessary for them to be satisfied point-wise so the weak form of the IBVP

(3.66) may equivalently be written as

$$\begin{aligned}
\dot{\boldsymbol{\varphi}} - \frac{1}{\rho_0} \mathbf{p} &= \mathbf{0} \\
\langle \mathbf{w}_p, \dot{\mathbf{p}} \rangle_{\mathcal{B}_0} + \langle \nabla_0 \mathbf{w}_p, \mathbf{FS} \rangle_{\mathcal{B}_0} - \langle \mathbf{w}_p, \mathbf{B}_0 \rangle_{\mathcal{B}_0} - \langle \mathbf{w}_p, \mathbf{T}_0 \rangle_{\partial \mathcal{B}_0} &= 0 \\
\langle w_e, \dot{e} \rangle_{\mathcal{B}_0} - \langle w_e, \frac{1}{2} \mathbf{S} : \dot{\mathbf{C}} \rangle_{\mathcal{B}_0} - \langle \nabla_0 w_e, \mathbf{H} \rangle_{\mathcal{B}_0} & \\
- \langle w_e, \mathcal{R} \rangle_{\mathcal{B}_0} + \langle w_e, H_N \rangle_{\partial \mathcal{B}_0} &= 0 \\
\dot{\mathbf{L}}^\alpha - \mathcal{K}(\mathbf{Q}^\alpha) &= \mathbf{0} \quad \forall \alpha = 1, \dots, m.
\end{aligned} \tag{3.148}$$

Finally, the weak statement for the isothermal dissipative dynamics (3.104) reads

$$\begin{aligned}
\dot{\boldsymbol{\varphi}} - \frac{1}{\rho_0} \mathbf{p} &= \mathbf{0} \\
\langle \mathbf{w}_p, \dot{\mathbf{p}} \rangle_{\mathcal{B}_0} + \langle \nabla_0 \mathbf{w}_p, \mathbf{FS} \rangle_{\mathcal{B}_0} - \langle \mathbf{w}_p, \mathbf{B}_0 \rangle_{\mathcal{B}_0} - \langle \mathbf{w}_p, \mathbf{T}_0 \rangle_{\partial \mathcal{B}_0} &= 0 \\
\dot{\mathbf{L}}^\alpha - \mathcal{K}(\mathbf{Q}^\alpha) &= \mathbf{0} \quad \forall \alpha = 1, \dots, m,
\end{aligned} \tag{3.149}$$

where the symmetry Piola-Kirchhoff stress tensor and the dissipative driving stress tensor accordingly respond to the constitutive laws (3.103).

Remark 3.12. The weak statement of the linear momentum balance (3.148)₂ becomes the classical virtual work principle by choosing the test function $\mathbf{w}_p$ as the virtual displacement $\delta\boldsymbol{\varphi} \in \mathcal{W}$, that is

$$\langle \dot{\mathbf{p}}, \delta\boldsymbol{\varphi} \rangle_{\mathcal{B}_0} + \langle \mathbf{FS}, \nabla_0 \delta\boldsymbol{\varphi} \rangle_{\mathcal{B}_0} - \langle \mathbf{B}_0, \delta\boldsymbol{\varphi} \rangle_{\mathcal{B}_0} - \langle \mathbf{T}_0, \delta\boldsymbol{\varphi} \rangle_{\partial \mathcal{B}_0} = 0 \tag{3.150}$$

Remark 3.13. In the pure mechanical context, unlike the weak form presented for the linear momentum balance, a multi-field variational statement can be constructed to deal with special demands, such as multi-body dynamics governed by Differential-Algebraic Equations (DAEs) or displacement-constrained formulations. The most representative example in solid mechanics is the Hu-Washizu three-field variational principle Hu (1955); Pompe & Washizu (1969) which is used to arrive at aforementioned B-bar FEM methods, see Simó et al. (1985).

3.7.2 Bunov-Galerkin Finite Element spatial discretization

The Finite Element discretization is based on a partition of the continuum $\mathcal{B}_0$, schematically depicted in Figure 3.7, into a conforming regular mesh of

N_e finite elements, each denoted $\mathcal{B}_e^0$, connecting $\mathcal{N}$ nodes, defining a discrete configuration $\mathcal{B}_0^h$ as

$$\mathcal{B}_0^h = \bigcup_{e=1}^{N_e} \mathcal{B}_0^e \quad (3.151)$$

Figure 3.7. Finite elements partition of the continuum

This partition is used to build continuous trial and weighting functions in terms of unknowns on the nodes. The way these functions are specified determines the particular FE method. Thus, the Bunov-Galerkin, or just Galerkin, method is constructed by finite-dimensional approximation of the spaces $\mathcal{V}$ and $\mathcal{W}$, denoted by $\mathcal{V}^h$ and $\mathcal{W}^h$, such that $\mathcal{V}^h \subset \mathcal{V}$ and $\mathcal{W}^h \subset \mathcal{W}$. These approximations consist of all linear combinations of global *shape* functions $N^a : \mathcal{B}_0^h \rightarrow \mathbb{R}$, such that

$$\mathcal{V}^h = \{v^h = \sum_{a=1}^{\mathcal{N}} N^a v^a | v^h \in \mathcal{H}^1, v^h = \bar{v}^h \text{ on } \partial \mathcal{B}_0^{h,\varphi,\theta} \times [0, T]\}, \quad (3.152)$$

$$\mathcal{W}^h = \{w^h = \sum_{a=1}^{\mathcal{N}} N^a w^a | w^h \in \mathcal{H}^1, w^h = 0 \text{ on } \partial \mathcal{B}_0^{h,\varphi,\theta} \times [0, T]\}, \quad (3.153)$$

where v^a , w^a denote (unknown) values on the node a and $\mathcal{H}^l$ is the Hilbert space defined as

$$\mathcal{H}^m = \{v | v \in L_2, D^\alpha v \in L_2, |\alpha| \leq l\}, \quad (3.154)$$

with L_2 being the (Lebesgue) space of square integrable functions.

Remark 3.14. Petrov-Galerkin methods approximate differently the weighting functions to deal with partial differential equations with odd order, such as the advection-dominated diffusion-advection problem, see Fenaux (2013). Also, collocation methods Liu & Gu (2010), those that satisfy the partial differential equations only at certain chosen points, can be understood as a FEM in which the weighting space is approached by Dirac delta functions.

Specifically, the spatial-dependent variables that defines the thermo-dissipative dynamics are spatially discretized by

$$\begin{aligned} \boldsymbol{\varphi}^h(\mathbf{X}, t) &= \sum_{a=1}^{\mathcal{N}} N^a(\mathbf{X}) \boldsymbol{x}^a(t), \\ \boldsymbol{p}^h(\mathbf{X}, t) &= \sum_{a=1}^{\mathcal{N}} N^a(\mathbf{X}) \boldsymbol{p}^a(t), \\ s^h(\mathbf{X}, t) &= \sum_{a=1}^{\mathcal{N}} N^a(\mathbf{X}) s^a(t), \\ \boldsymbol{\Lambda}^{\alpha, h}(\mathbf{X}, t) &= \sum_{a=1}^{\mathcal{N}} N^a(\mathbf{X}) \boldsymbol{\Lambda}^{\alpha, a}(t), \end{aligned} \quad (3.155)$$

where $\boldsymbol{x}^a$, $\boldsymbol{p}^a$, s^a (being either entropy η^a or temperature Θ^a) and $\boldsymbol{\Lambda}^{\alpha, a}$ denote the respective fields' values on the node a . As a result, the problem boils down to finding this set of nodal values, known as degree of freedom of the system. It is precisely in this set of variables where the time-evolution problem remains continuous.

Thus, each spatial-dependent magnitude is spatially approximated by using the above discretization (3.155). For instance, the fundamental deformation gradient tensor and the right Cauchy-Green deformation tensor result in

$$\begin{aligned} \mathbf{F}^h(\mathbf{X}, t) &= \sum_{a=1}^{\mathcal{N}} \boldsymbol{x}^a(t) \otimes \nabla_0 N^a(\mathbf{X}), \\ \mathbf{C}^h(\mathbf{X}, t) &= \sum_{a=1}^{\mathcal{N}} \sum_{b=1}^{\mathcal{N}} \boldsymbol{x}^a(t) \cdot \boldsymbol{x}^b(t) \nabla_0 N^a(\mathbf{X}) \otimes \nabla_0 N^b(\mathbf{X}), \end{aligned} \quad (3.156)$$

where $(\cdot) \otimes (\cdot)$ means external product and the superscript h indicates spatially-discretized counterparts.

Apart from the direct discretization provided by (3.155)₄, the internal variables could also be approximated indirectly by observing that the solution of the spatial discrete form of the dissipative evolution equation throughout time provides a discrete form of $\mathbf{\Lambda}^{\alpha,h}$, that is

$$\dot{\mathbf{\Lambda}}^{\alpha,h} = \mathcal{K}(\mathbf{Q}^{\alpha,h}) \quad \text{in } \mathcal{B}_0^h \times [0, T] \quad \forall \alpha = 1, \dots, m. \quad (3.157)$$

For instance, in the isothermal viscoelastic case due to Simó and Holzapfel (3.114) they would turn out to be

$$\mathbf{\Lambda}^{\alpha,h}(t) = \int_0^t \exp\left[\frac{-(t-s)}{\tau_\alpha}\right] \frac{2}{\nu_\alpha} \frac{\partial \Psi_{\text{iso}}^\alpha}{\partial \mathbf{C}}(\mathbf{C}^h, s) ds + \exp\left[\frac{-t}{\tau_\alpha}\right] \mathbf{\Lambda}_0^\alpha \quad (3.158)$$

Introducing the approximations $\boldsymbol{\varphi}^h, \mathbf{p}^h, \eta^h, \mathbf{\Lambda}^{\alpha,h} \in \mathcal{V}^h$ and $\mathbf{w}_p^h, w_\eta^h \in \mathcal{W}^h$ into the weak form (3.146), the spatially-discrete entropy formulation of evolution equation is obtained

$$\begin{aligned} \dot{\boldsymbol{\varphi}}^h - \frac{1}{\rho_0^h} \mathbf{p}^h &= \mathbf{0}, \\ \langle \mathbf{w}_p^h, \dot{\mathbf{p}}^h \rangle_{\mathcal{B}_0^h} + \langle \nabla_0 \mathbf{w}_p^h, \mathbf{F}^h \mathbf{S}^h \rangle_{\mathcal{B}_0^h} - \langle \mathbf{w}_p^h, \mathbf{B}_0 \rangle_{\mathcal{B}_0^h} - \langle \mathbf{w}_p^h, \mathbf{T}_0 \rangle_{\partial \mathcal{B}_0^h} &= 0, \\ \langle w_\eta^h, \dot{\eta}^h \rangle_{\mathcal{B}_0^h} - \langle \nabla_0 \left[\frac{w_\eta^h}{\Theta^h} \right], \mathbf{H}^h \rangle_{\mathcal{B}_0^h} - \langle \frac{w_\eta^h}{\Theta^h}, \dot{\mathcal{D}}^h \rangle_{\mathcal{B}_0^h} & \\ &+ \langle \frac{w_\eta^h}{\Theta^h}, H_N \rangle_{\partial \mathcal{B}_0^h} - \langle \frac{w_\eta^h}{\Theta^h}, \mathcal{R} \rangle_{\mathcal{B}_0^h} = 0, \\ \dot{\mathbf{\Lambda}}^{\alpha,h} - \mathcal{K}(\mathbf{Q}^{\alpha,h}) &= \mathbf{0} \quad \forall \alpha = 1, \dots, m, \end{aligned} \quad (3.159)$$

where the spatial discretization of the entropy-based constitutive relations (3.36)-(3.38) are computed as follows

$$\left. \begin{aligned} \mathbf{S}^h &= 2 \frac{\partial e}{\partial \mathbf{C}}(\mathbf{C}^h, \eta^h, \mathbf{\Lambda}^{\alpha,h}) \\ \Theta^h &= \frac{\partial e}{\partial \eta}(\mathbf{C}^h, \eta^h, \mathbf{\Lambda}^{\alpha,h}) \\ \mathbf{Q}^{\alpha,h} &= - \frac{\partial e}{\partial \mathbf{\Lambda}^\alpha}(\mathbf{C}^h, \eta^h, \mathbf{\Lambda}^{\alpha,h}) \end{aligned} \right\} \quad \text{in } \mathcal{B}_0^h \times [0, T] \quad (3.160)$$

Similarly, the spatially-discretized temperature formulation derives from

the weak form (3.147) and reads

$$\begin{aligned}
\dot{\boldsymbol{\varphi}}^h - \frac{1}{\rho_0^h} \mathbf{p}^h &= \mathbf{0}, \\
\langle \mathbf{w}_p^h, \dot{\mathbf{p}}^h \rangle_{\mathcal{B}_0^h} + \langle \nabla_0 \mathbf{w}_p^h, \mathbf{F}^h \mathbf{S}^h \rangle_{\mathcal{B}_0^h} - \langle \mathbf{w}_p^h, \mathbf{B}_0 \rangle_{\mathcal{B}_0^h} - \langle \mathbf{w}_p^h, \mathbf{T}_0 \rangle_{\partial \mathcal{B}_0^h} &= 0, \\
\langle w_\Theta^h, \dot{\Theta}^h \rangle_{\mathcal{B}_0^h} - \langle \nabla_0 \left[\frac{w_\Theta^h}{c^h} \right], \mathbf{H}^h \rangle_{\mathcal{B}_0^h} + \langle \frac{w_\Theta^h}{c^h}, \mathbf{F}^h \mathbf{V}^h : \nabla_0 \left[\frac{\mathbf{p}^h}{\rho_0} \right] \rangle_{\mathcal{B}_0^h} & \\
- \langle \frac{w_\Theta^h}{c^h}, \dot{\mathcal{D}}^h + \mathcal{H}_d^h \rangle_{\mathcal{B}_0^h} + \langle \frac{w_\Theta^h}{c^h}, H_N \rangle_{\partial \mathcal{B}_0^h} - \langle \frac{w_\Theta^h}{c^h}, \mathcal{R} \rangle_{\mathcal{B}_0^h} &= 0, \\
\dot{\boldsymbol{\Lambda}}^{\alpha,h} - \mathcal{K}(\mathbf{Q}^{\alpha,h}) &= \mathbf{0} \quad \forall \alpha = 1, \dots, m,
\end{aligned} \tag{3.161}$$

in where the spatial discrete constitutive laws (3.18)-(3.21) and (3.77)-(3.79) now becomes

$$\left. \begin{aligned}
\mathbf{S}^h &= 2 \frac{\partial \Psi}{\partial \mathbf{C}}(\mathbf{C}^h, \Theta^h, \boldsymbol{\Lambda}^{\alpha,h}) \\
\eta^h &= - \frac{\partial \Psi}{\partial \Theta}(\mathbf{C}^h, \Theta^h, \boldsymbol{\Lambda}^{\alpha,h}) \\
\mathbf{Q}^{\alpha,h} &= - \frac{\partial \Psi}{\partial \boldsymbol{\Lambda}^\alpha}(\mathbf{C}^h, \Theta^h, \boldsymbol{\Lambda}^{\alpha,h}) \\
\mathbf{V}^h &= 2 \Theta^h \frac{\partial \eta}{\partial \mathbf{C}}(\mathbf{C}^h, \Theta^h, \boldsymbol{\Lambda}^{\alpha,h}) \\
c^h &= \Theta^h \frac{\partial \eta}{\partial \Theta}(\mathbf{C}^h, \Theta^h, \boldsymbol{\Lambda}^{\alpha,h}) = c > 0 \\
\mathbf{W}^{\alpha,h} &= \Theta^h \frac{\partial \eta}{\partial \boldsymbol{\Lambda}^\alpha}(\mathbf{C}^h, \Theta^h, \boldsymbol{\Lambda}^{\alpha,h})
\end{aligned} \right\} \quad \text{in } \mathcal{B}_0^h \times [0, T] \tag{3.162}$$

As was introduced in section 3.3.6, the thermodynamics obliges the specific heat capacity (3.78) c to be a constant positive real number, simplifying the manipulation of the energy balance weak form (3.161)₃.

Furthermore, in both formulations the heat flux vector (3.26) is spatially discretized according to

$$\mathbf{H}^h = -J^h \mathbf{F}^{h,-1} \boldsymbol{\kappa}(\Theta^h) \mathbf{F}^{h,-T} \nabla_0 \Theta^h = -\mathbf{K}^h \nabla_0 \Theta^h, \tag{3.163}$$

where the temperature field Θ^h is provided either by (3.155)₃ or (3.160)₂. The same applies to the rate of dissipation counterpart which is

$$\dot{\mathcal{D}}^h = \sum_{\alpha=1}^m \mathbf{Q}^{\alpha,h} : \dot{\boldsymbol{\Lambda}}^{\alpha,h} = \sum_{\alpha=1}^m \mathbf{Q}^{\alpha,h} : \mathcal{K}(\mathbf{Q}^{\alpha,h}) \geq 0, \tag{3.164}$$

with the proper constitutive law for the dissipative driving stress tensor: (3.21) or (3.38).

To close the temperature formulation a spatially-discretized counterpart for the thermo-dissipative heating (3.82) needs to be obtained as

$$\dot{\mathcal{H}}_d^h = \sum_{\alpha=1}^m \mathbf{W}^{\alpha,h} : \dot{\mathbf{\Lambda}}^{\alpha,h} = \sum_{\alpha=1}^m \mathbf{W}^{\alpha,h} : \mathcal{K}(\mathbf{Q}^{\alpha,h}) \quad (3.165)$$

On the other hand, the discretized spatial equations of the isothermal dissipative dynamics (3.104) reads

$$\begin{aligned} \dot{\boldsymbol{\varphi}}^h - \frac{1}{\rho_0^h} \mathbf{p}^h &= \mathbf{0}, \\ \langle \mathbf{w}_p^h, \dot{\mathbf{p}}^h \rangle_{\mathcal{B}_0^h} + \langle \nabla_0 \mathbf{w}_p^h, \mathbf{F}^h \mathbf{S}^h \rangle_{\mathcal{B}_0^h} - \langle \mathbf{w}_p^h, \mathbf{B}_0 \rangle_{\mathcal{B}_0^h} - \langle \mathbf{w}_p^h, \mathbf{T}_0 \rangle_{\partial \mathcal{B}_0^h} &= 0, \\ \dot{\mathbf{\Lambda}}^{\alpha,h} - \mathcal{K}(\mathbf{Q}^{\alpha,h}) &= \mathbf{0} \quad \forall \alpha = 1, \dots, m, \end{aligned} \quad (3.166)$$

with the spatial discretized constitutive laws (3.103) being

$$\mathbf{S}^h = 2 \frac{\partial \Psi}{\partial \mathbf{C}}(\mathbf{C}^h, \mathbf{\Lambda}^{\alpha,h}) \quad \text{and} \quad \mathbf{Q}^{\alpha,h} = - \frac{\partial \Psi}{\partial \mathbf{\Lambda}^{\alpha}}(\mathbf{C}^h, \mathbf{\Lambda}^{\alpha,h}) \quad (3.167)$$

Remark 3.15. The introduced spatial discretization does not spoil the time-evolution preserved quantities stated by the continuous formulation (3.95)-(3.101). These quantities have to do with the continuous nature in time and not with spatial aspects. In addition, no use of artificial (numerical) stabilization techniques have been involved and, therefore, some drawbacks might appear such as the widely-known phenomenon of *locking* related to incompressible or nearly incompressible deformations when the standard Galerkin approach is carried out. Some of the methods proposed to fix this phenomenon are based on adding non-physically motivated terms which may compromise the conservation properties. The reader is referred to Hughes (1987) for more details.

3.7.3 Element implementation

In order for Galerkin FEM to be convergent as the mesh is refined the shape functions must be smooth (at least C^1) on each element so the global shape functions are, at worse, continuous but not differentiable in the vicinity of the nodes, that is $N^a \in C^0$. The element functions are commonly defined in the isoparametric space in where a parent domain, e.g. the closed biunit

cube in $\mathbb{R}^3$, is denoted by $\square$, such that any point in the element $\mathbf{X}^e : \square \rightarrow \mathcal{B}_0^e$ is provided, in the Lagrangian description, by

$$\mathbf{X}^e(\boldsymbol{\xi}) = \sum_{i=1}^n N_i(\boldsymbol{\xi}) \mathbf{X}_i^e, \quad (3.168)$$

with n being the number of the nodes per element. The relationship between the isoparametric and the Lagrangian spaces is then provided by the Jacobian transformation

$$\mathbf{J}_0^e := \frac{\partial \mathbf{X}^e}{\partial \boldsymbol{\xi}} = \sum_{i=1}^n \mathbf{X}_i^e \otimes \frac{\partial N_i(\boldsymbol{\xi})}{\partial \boldsymbol{\xi}} \quad (3.169)$$

A FEM based on these functions is said to be *isoparametric*. As examples of 3D-elements, Figure 3.8 shows the shape functions for the linear tetrahedral and the trilinear hexahedral elements which allow for geometrically nonlinear formulations.

Figure 3.8. Shape functions

Finally, the standard Galerkin FEM is complemented by Gaussian quadratures for the evaluation of the integrals appearing in weak forms. By using the isoparametric space, the integral of any function $f : \mathcal{B}_0 \rightarrow \mathbb{R}$ is approximated as follows

$$\begin{aligned} \int_{\mathcal{B}_0} f(\mathbf{X}) dV_0 &\approx \sum_{e=1}^{N_e} \int_{\mathcal{B}_0^e} f(\mathbf{X}^e) dV_0^e \\ &= \sum_{e=1}^{N_e} \int_{\square} f(\boldsymbol{\xi}) \det(\mathbf{J}_0^e) d\square \approx \sum_{e=1}^{N_e} \sum_{i=1}^{n_g} \sum_{j=1}^{n_g} \sum_{k=1}^{n_g} w_i w_j w_k f(\boldsymbol{\xi}_g) \det(\mathbf{J}_{0,g}^e), \end{aligned} \quad (3.170)$$

where n_g is the number of Gauss points, ξ_g are the coordinates of the Gauss point g and w_g is the weight of the g -th Gauss point, see Chandrupatla & Belegundu (1991). Particularly, the trilinear hexahedral element has 8 Gauss points and the weighting factors are given by $w_l = 1$, whereas the tetrahedral element has only a Gauss point and the weighting factor is $w_l = 1/\sqrt[3]{6}$.

With these tools, each term of the above weak forms (3.159)-(3.161) can further be elaborated at the element level to achieve the element implementation. In addition, this implementation must be provided with the linearized counterparts. The linear momentum balance terms can easily be found in the literature, e.g Bonet & Wood (2008); De Borst et al. (2012), in contrast with the energy balance ones, at least within the thermo-dissipative dynamic context. For this reason, Appendix B collects the full details of the derivation of both the linearized and the discretized evolution equations, being the latter developed at element level as usual.

3.8 Standard time integration methods

Once the thermo-dissipative continuum dynamics has spatially been discretized, the full discrete formulation is achieved by performing a temporal discretization. This step becomes crucial regarding the conservation properties of the resulting discrete formulation, requiring on-purpose non-standard integration methods that ensure their preservation.

In this section standard temporal techniques are discussed, emphasizing their implications in the preserved features of the system, stated in Section 3.5. In addition, some benchmark simple problems will be introduced and solved to check the methods' properties and to serve as reference solutions that allow to calibrate the new structure-preserving methods to be presented in Chapter 5.

The resulting semidiscrete thermo-dissipative dynamic equations (3.159), (3.161) or (3.166) also answers to the simplified form (2.67), that is

$$\dot{\mathbf{y}}^h(t) = \mathbf{f}(\mathbf{y}^h(t), t) \quad \forall t \in [0, T], \quad (3.171)$$

with $\mathbf{y}^h = (\varphi^h, \mathbf{p}^h, s^h, \Lambda^{\alpha, h})$.

Performing the division into subintervals $[t_{n+1}, t_n]$ of the entire time interval of interest $[0, T]$, the same standard approximations as those discussed in Section 2.3 can be elaborated for the temporal discretization of semidiscrete thermo-dissipative dynamic equations so full discrete counterparts can be

achieved. Next, the standard midpoint and trapezoidal methods are studied, emphasizing their shortcomings regarding the preservation laws.

3.8.1 Midpoint time integration method

As was introduced in Section 2.3, the midpoint method is a one-step implicit second-order accurate integration method that additionally preserves both the linear and the angular momentum, that is, the symmetries of the thermo-dissipative dynamics continuous evolution equations. However, it violates the laws of thermodynamics for moderate time-step sizes (the larger the worse). This characteristics doubtlessly make it interesting for the purpose of this dissertation. In fact, it is quite close to fulfill all requirements falling on the desired structure-preserving time integration algorithms.

The full midpoint-based discrete entropy formulation of thermo-dissipative continuum dynamics is obtained from (3.159) to be

$$\begin{aligned}
& \frac{\varphi_{n+1}^h - \varphi_n^h}{\Delta t} - \frac{1}{\rho_0^h} \mathbf{p}_{n+\frac{1}{2}}^h = \mathbf{0}, \\
& \langle \mathbf{w}_p^h, \frac{\mathbf{p}_{n+1}^h - \mathbf{p}_n^h}{\Delta t} \rangle_{\mathcal{B}_0^h} + \langle \nabla_0 \mathbf{w}_p^h, \mathbf{F}_{n+\frac{1}{2}}^h \mathbf{S}_{n+\frac{1}{2}}^h \rangle_{\mathcal{B}_0^h} \\
& \quad - \langle \mathbf{w}_p^h, \mathbf{B}_{0,n+\frac{1}{2}} \rangle_{\mathcal{B}_0^h} - \langle \mathbf{w}_p^h, \mathbf{T}_{0,n+\frac{1}{2}} \rangle_{\partial \mathcal{B}_0^h} = 0, \\
& \langle w_\eta^h, \frac{\eta_{n+1}^h - \eta_n^h}{\Delta t} \rangle_{\mathcal{B}_0^h} - \langle \nabla_0 \left[\frac{w_\eta^h}{\Theta_{n+\frac{1}{2}}^h} \right], \mathbf{H}_{n+\frac{1}{2}}^h \rangle_{\mathcal{B}_0^h} - \langle \frac{w_\eta^h}{\Theta_{n+\frac{1}{2}}^h}, \dot{\mathcal{D}}_{n+\frac{1}{2}}^h \rangle_{\mathcal{B}_0^h} \\
& \quad + \langle \frac{w_\eta^h}{\Theta_{n+\frac{1}{2}}^h}, H_{N,n+\frac{1}{2}} \rangle_{\partial \mathcal{B}_0^h} - \langle \frac{w_\eta^h}{\Theta_{n+\frac{1}{2}}^h}, \mathcal{R}_{n+\frac{1}{2}} \rangle_{\mathcal{B}_0^h} = 0, \\
& \frac{\Lambda_{n+1}^{\alpha,h} - \Lambda_n^{\alpha,h}}{\Delta t} - \mathcal{K}(\mathbf{Q}_{n+\frac{1}{2}}^{\alpha,h}) = \mathbf{0} \quad \forall \alpha = 1, \dots, m,
\end{aligned} \tag{3.172}$$

where, contrary to the notation used in Subsection 2.3.1, the notation $(\cdot)_{n+\frac{1}{2}}^h$ has been saturated for the sake of simplicity. The important fact to be considered is that each state variable is evaluated at the subinterval midpoint according to $(\cdot)_{n+\frac{1}{2}}^h = \frac{1}{2}[(\cdot)_{n+1}^h + (\cdot)_n^h]$ whereas all derived quantities and functions are evaluated via them. Thus, the constitutive laws are correspondingly

evaluated as

$$\left. \begin{aligned} \mathbf{S}_{n+\frac{1}{2}}^h &= 2 \frac{\partial e}{\partial \mathbf{C}}(\mathbf{C}_{n+\frac{1}{2}}^h, \eta_{n+\frac{1}{2}}^h, \mathbf{\Lambda}_{n+\frac{1}{2}}^{\alpha,h}) \\ \Theta_{n+\frac{1}{2}}^h &= \frac{\partial e}{\partial \eta}(\mathbf{C}_{n+\frac{1}{2}}^h, \eta_{n+\frac{1}{2}}^h, \mathbf{\Lambda}_{n+\frac{1}{2}}^{\alpha,h}) \\ \mathbf{Q}_{n+\frac{1}{2}}^{\alpha,h} &= -\frac{\partial e}{\partial \mathbf{\Lambda}^\alpha}(\mathbf{C}_{n+\frac{1}{2}}^h, \eta_{n+\frac{1}{2}}^h, \mathbf{\Lambda}_{n+\frac{1}{2}}^{\alpha,h}) \end{aligned} \right\} \quad \text{in } \mathcal{B}_0^h \times [t_n, t_{n+1}], \quad (3.173)$$

with the right Cauchy-Green deformation tensor evaluated at midpoint being

$$\mathbf{C}_{n+\frac{1}{2}}^h = \mathbf{F}_{n+\frac{1}{2}}^{h,T} \mathbf{F}_{n+\frac{1}{2}}^h = \left(\nabla_0 \boldsymbol{\varphi}_{n+\frac{1}{2}}^h \right)^T \nabla_0 \boldsymbol{\varphi}_{n+\frac{1}{2}}^h \quad (3.174)$$

Moreover, the heat flux vector (3.163) evaluated at midpoint results in

$$\mathbf{H}_{n+\frac{1}{2}}^h = -J_{n+\frac{1}{2}}^h \mathbf{F}_{n+\frac{1}{2}}^{h,-1} \boldsymbol{\kappa}(\Theta_{n+\frac{1}{2}}^h) \mathbf{F}_{n+\frac{1}{2}}^{h,-T} \nabla_0 \Theta_{n+\frac{1}{2}}^h = -\mathbf{K}_{n+\frac{1}{2}}^h \nabla_0 \Theta_{n+\frac{1}{2}}^h, \quad (3.175)$$

with $J_{n+\frac{1}{2}}^h = \det \mathbf{F}_{n+\frac{1}{2}}^h$. Note that the evaluation of the material gradient requires the application of the chain rule to give

$$\nabla_0 \Theta_{n+\frac{1}{2}}^h = \frac{\partial \Theta}{\partial \mathbf{C}} : \nabla_0 \mathbf{C}_{n+\frac{1}{2}}^h + \frac{\partial \Theta}{\partial \eta} \nabla_0 \eta_{n+\frac{1}{2}}^h + \frac{\partial \Theta}{\partial \mathbf{\Lambda}^\alpha} : \nabla_0 \mathbf{\Lambda}_{n+\frac{1}{2}}^{\alpha,h} \quad (3.176)$$

The last two terms follow directly from the spatial discretization (3.155) but the first one needs further elaboration by using (3.156)₂, making necessary the implementation of the second partial derivatives of the shape functions, details can be found in Appendix B.

On the other hand, the midpoint evaluation of the rate of dissipation reads

$$\dot{\mathcal{D}}_{n+\frac{1}{2}}^h = \sum_{\alpha=1}^m \mathbf{Q}_{n+\frac{1}{2}}^{\alpha,h} : \dot{\mathbf{\Lambda}}_{n+\frac{1}{2}}^{\alpha,h} = \sum_{\alpha=1}^m \mathbf{Q}_{n+\frac{1}{2}}^{\alpha,h} : \mathcal{K}(\mathbf{Q}_{n+\frac{1}{2}}^{\alpha,h}) \geq 0, \quad (3.177)$$

In a similar way, the full midpoint-based discrete temperature formula-

tion is derived from (3.161) and reads

$$\begin{aligned}
& \frac{\varphi_{n+1}^h - \varphi_n^h}{\Delta t} - \frac{1}{\rho_0^h} \mathbf{p}_{n+\frac{1}{2}}^h = \mathbf{0}, \\
& \langle \mathbf{w}_p^h, \frac{\mathbf{p}_{n+1}^h - \mathbf{p}_n^h}{\Delta t} \rangle_{\mathcal{B}_0^h} + \langle \nabla_0 \mathbf{w}_p^h, \mathbf{F}_{n+\frac{1}{2}}^h \mathbf{S}_{n+\frac{1}{2}}^h \rangle_{\mathcal{B}_0^h} \\
& \quad - \langle \mathbf{w}_p^h, \mathbf{B}_{0,n+\frac{1}{2}} \rangle_{\mathcal{B}_0^h} - \langle \mathbf{w}_p^h, \mathbf{T}_{0,n+\frac{1}{2}} \rangle_{\partial \mathcal{B}_0^h} = 0, \\
& \langle w_\Theta^h, \frac{\Theta_{n+1}^h - \Theta_n^h}{\Delta t} \rangle_{\mathcal{B}_0^h} + \langle \frac{w_\Theta^h}{c}, \mathbf{F}_{n+\frac{1}{2}}^h \mathbf{V}_{n+\frac{1}{2}}^h : \nabla_0 \left[\frac{\mathbf{p}_{n+\frac{1}{2}}^h}{\rho_0^h} \right] \rangle_{\mathcal{B}_0^h} \\
& \quad - \langle \frac{1}{c} \nabla_0 w_\Theta^h, \mathbf{H}_{n+\frac{1}{2}}^h \rangle_{\mathcal{B}_0^h} - \langle \frac{w_\Theta^h}{c}, \dot{\mathbf{D}}_{n+\frac{1}{2}}^h + \mathcal{H}_{d,n+\frac{1}{2}}^h \rangle_{\mathcal{B}_0^h} \\
& \quad + \langle \frac{w_\Theta^h}{c}, H_{N,n+\frac{1}{2}} \rangle_{\partial \mathcal{B}_0^h} - \langle \frac{w_\Theta^h}{c}, \mathcal{R}_{n+\frac{1}{2}} \rangle_{\mathcal{B}_0^h} = 0, \\
& \frac{\Lambda_{n+1}^{\alpha,h} - \Lambda_n^{\alpha,h}}{\Delta t} - \mathcal{K}(\mathbf{Q}_{n+\frac{1}{2}}^{\alpha,h}) = \mathbf{0} \quad \forall \alpha = 1, \dots, m,
\end{aligned} \tag{3.178}$$

where the midpoint constitutive laws are defined in terms of the temperature at midpoint $\Theta_{n+\frac{1}{2}}^h = \frac{1}{2}(\Theta_{n+1}^h + \Theta_n^h)$ according to

$$\left. \begin{aligned}
\mathbf{S}_{n+\frac{1}{2}}^h &= 2 \frac{\partial \Psi}{\partial \mathbf{C}}(\mathbf{C}_{n+\frac{1}{2}}^h, \Theta_{n+\frac{1}{2}}^h, \Lambda_{n+\frac{1}{2}}^{\alpha,h}) \\
\eta_{n+\frac{1}{2}}^h &= - \frac{\partial \Psi}{\partial \Theta}(\mathbf{C}_{n+\frac{1}{2}}^h, \Theta_{n+\frac{1}{2}}^h, \Lambda_{n+\frac{1}{2}}^{\alpha,h}) \\
\mathbf{Q}_{n+\frac{1}{2}}^{\alpha,h} &= - \frac{\partial \Psi}{\partial \Lambda^\alpha}(\mathbf{C}_{n+\frac{1}{2}}^h, \Theta_{n+\frac{1}{2}}^h, \Lambda_{n+\frac{1}{2}}^{\alpha,h}) \\
\mathbf{V}_{n+\frac{1}{2}}^h &= 2 \Theta_{n+\frac{1}{2}}^h \frac{\partial \eta}{\partial \mathbf{C}}(\mathbf{C}_{n+\frac{1}{2}}^h, \Theta_{n+\frac{1}{2}}^h, \Lambda_{n+\frac{1}{2}}^{\alpha,h}) \\
c_{n+\frac{1}{2}}^h &= \Theta_{n+\frac{1}{2}}^h \frac{\partial \eta}{\partial \Theta}(\mathbf{C}_{n+\frac{1}{2}}^h, \Theta_{n+\frac{1}{2}}^h, \Lambda_{n+\frac{1}{2}}^{\alpha,h}) = c > 0 \\
\mathbf{W}_{n+\frac{1}{2}}^{\alpha,h} &= \Theta_{n+\frac{1}{2}}^h \frac{\partial \eta}{\partial \Lambda^\alpha}(\mathbf{C}_{n+\frac{1}{2}}^h, \Theta_{n+\frac{1}{2}}^h, \Lambda_{n+\frac{1}{2}}^{\alpha,h})
\end{aligned} \right\} \quad \text{in } \mathcal{B}_0^h \times [t_n, t_{n+1}] \tag{3.179}$$

Accordingly, the heat vector counterpart (3.175) also becomes a function of the temperature at midpoint, facilitating the evaluation of the involved material gradient as readily follows from (3.155). Moreover, the thermo-dissipative heating (3.82) reads

$$\mathcal{H}_{d,n+\frac{1}{2}}^h = \sum_{\alpha=1}^m \mathbf{W}_{n+\frac{1}{2}}^{\alpha,h} : \dot{\Lambda}_{n+\frac{1}{2}}^{\alpha,h} = \sum_{\alpha=1}^m \mathbf{W}_{n+\frac{1}{2}}^{\alpha,h} : \mathcal{K}(\mathbf{Q}_{n+\frac{1}{2}}^{\alpha,h}) \tag{3.180}$$

Finally, the midpoint-based discrete isothermal-dissipative continuum dynamic equations simplifies to

$$\begin{aligned}
\frac{\varphi_{n+1}^h - \varphi_n^h}{\Delta t} - \frac{1}{\rho_0^h} \mathbf{p}_{n+\frac{1}{2}}^h &= \mathbf{0}, \\
\langle \mathbf{w}_p^h, \frac{\mathbf{p}_{n+1}^h - \mathbf{p}_n^h}{\Delta t} \rangle_{\mathcal{B}_0^h} + \langle \nabla_0 \mathbf{w}_p^h, \mathbf{F}_{n+\frac{1}{2}}^h \mathbf{S}_{n+\frac{1}{2}}^h \rangle_{\mathcal{B}_0^h} \\
&\quad - \langle \mathbf{w}_p^h, \mathbf{B}_{0,n+\frac{1}{2}} \rangle_{\mathcal{B}_0^h} - \langle \mathbf{w}_p^h, \mathbf{T}_{0,n+\frac{1}{2}} \rangle_{\partial \mathcal{B}_0^h} = 0, \\
\frac{\Lambda_{n+1}^{\alpha,h} - \Lambda_n^{\alpha,h}}{\Delta t} - \mathcal{K}(\mathbf{Q}_{n+\frac{1}{2}}^{\alpha,h}) &= \mathbf{0} \quad \forall \alpha = 1, \dots, m,
\end{aligned} \tag{3.181}$$

with the corresponding constitutive laws being evaluated at midpoint as follows

$$\left. \begin{aligned} \mathbf{S}_{n+\frac{1}{2}}^h &= 2 \frac{\partial \Psi}{\partial \mathbf{C}}(\mathbf{C}_{n+\frac{1}{2}}^h, \Lambda_{n+\frac{1}{2}}^{\alpha,h}) \\ \mathbf{Q}_{n+\frac{1}{2}}^{\alpha,h} &= - \frac{\partial \Psi}{\partial \Lambda^\alpha}(\mathbf{C}_{n+\frac{1}{2}}^h, \Lambda_{n+\frac{1}{2}}^{\alpha,h}) \end{aligned} \right\} \quad \text{in } \mathcal{B}_0^h \times [t_n, t_{n+1}] \tag{3.182}$$

Particularly, the internal variables of the Simó and Holzapfel viscoelastic model (3.114) result in

$$\Lambda_{n+1}^{\alpha,h} = \Delta t \exp \left[\frac{-\Delta t}{2\tau_\alpha} \right] \frac{2}{\nu_\alpha} \frac{\partial \Psi_{\text{iso}}^\alpha}{\partial \mathbf{C}}(\mathbf{C}_{n+\frac{1}{2}}^h) + \exp \left[\frac{-\Delta t}{\tau_\alpha} \right] \Lambda_n^\alpha \tag{3.183}$$

Discrete symmetries and thermodynamic laws. The just introduced midpoint approximation preserves the equation's symmetries associated to the free motion of the continuum in space. As was introduced in Section 3.5, these symmetries lead to the conservation of the linear and angular momentum. In a discrete setting, the conservation of any quantity can be checked by balancing it inside any time subinterval. Then, the quantity is discretely conserved if its balance is zero for all time steps. For the global linear (3.44) and angular (3.51) momentum, that is expressed as follows

$$\mathbf{L}_{n+1}^h - \mathbf{L}_n^h = \mathbf{0}, \quad \mathbf{J}_{n+1}^h - \mathbf{J}_n^h = \mathbf{0} \quad \forall [t_n, t_{n+1}] \tag{3.184}$$

To verify the linear momentum balance it suffices to take $\mathbf{w}_p^h = \Delta t \bar{\mathbf{w}}$, $\bar{\mathbf{w}} \in \mathbb{R}^d$ being a constant vector such that $\nabla_0 \mathbf{w}_p^h = \mathbf{0}$, in either (3.172)₂, (3.178)₂ or (3.181)₂ to obtain

$$\begin{aligned}
(\mathbf{L}_{n+1}^h - \mathbf{L}_n^h) \cdot \bar{\mathbf{w}} &= \langle \mathbf{p}_{n+1}^h - \mathbf{p}_n^h, \bar{\mathbf{w}} \rangle_{\mathcal{B}_0^h} \\
&= \Delta t \left[\langle \mathbf{B}_{0,n+\frac{1}{2}}, \bar{\mathbf{w}} \rangle_{\mathcal{B}_0^h} + \langle \mathbf{T}_{0,n+\frac{1}{2}}, \bar{\mathbf{w}} \rangle_{\partial \mathcal{B}_0^h} \right],
\end{aligned} \tag{3.185}$$

which clearly vanishes in absence of external actions.

On the other hand, the verification for the angular momentum conservation follows from noting that

$$\mathbf{J}_{n+1}^h - \mathbf{J}_n^h = \int_{\mathcal{B}_0^h} \left[\boldsymbol{\varphi}_{n+\frac{1}{2}}^h \wedge (\mathbf{p}_{n+1}^h - \mathbf{p}_n^h) - \mathbf{p}_{n+\frac{1}{2}}^h \wedge (\boldsymbol{\varphi}_{n+1}^h - \boldsymbol{\varphi}_n^h) \right] dV_0, \quad (3.186)$$

Then, the second term of the right hand side of (3.186) vanishes according to either (3.172)₁, (3.178)₁ or (3.181)₁.

Now, considering $\mathbf{w}_p^h = \Delta t \bar{\mathbf{w}} \wedge \boldsymbol{\varphi}_{n+\frac{1}{2}}^h$, $\bar{\mathbf{w}} \in \mathbb{R}^d$ being an arbitrary constant vector, and furnishing the associated skew-symmetric tensor $\bar{\mathbf{w}} \in \text{Skw}(\mathbb{T}_d^2)$ such that $\bar{\mathbf{w}} \times \boldsymbol{\varphi}_{n+\frac{1}{2}}^h = \bar{\mathbf{w}} \boldsymbol{\varphi}_{n+\frac{1}{2}}^h$ and hence $\nabla_0 \mathbf{w}_p^h = \Delta t \bar{\mathbf{w}} \mathbf{F}_{n+\frac{1}{2}}^h$, the angular momentum balance yields

$$\begin{aligned} (\mathbf{J}_{n+1}^h - \mathbf{J}_n^h) \cdot \bar{\mathbf{w}} &= \langle \boldsymbol{\varphi}_{n+\frac{1}{2}}^h \wedge (\mathbf{p}_{n+1}^h - \mathbf{p}_n^h), \bar{\mathbf{w}} \rangle_{\mathcal{B}_0^h} \\ &= \langle \mathbf{p}_{n+1}^h - \mathbf{p}_n^h, \bar{\mathbf{w}} \wedge \boldsymbol{\varphi}_{n+\frac{1}{2}}^h \rangle_{\mathcal{B}_0^h} \\ &= \Delta t \left[-\langle \mathbf{F}_{n+\frac{1}{2}}^h \mathbf{S}_{n+\frac{1}{2}}^h \mathbf{F}_{n+\frac{1}{2}}^{h,T}, \bar{\mathbf{w}} \rangle_{\mathcal{B}_0^h} \right. \\ &\quad \left. + \langle \mathbf{B}_{0,n+\frac{1}{2}}, \bar{\mathbf{w}} \wedge \boldsymbol{\varphi}_{n+\frac{1}{2}}^h \rangle_{\mathcal{B}_0^h} + \langle \mathbf{T}_{0,n+\frac{1}{2}}, \bar{\mathbf{w}} \wedge \boldsymbol{\varphi}_{n+\frac{1}{2}}^h \rangle_{\partial \mathcal{B}_0^h} \right] \end{aligned} \quad (3.187)$$

The first term on the right hand side of (3.187) vanishes due to the symmetry of the tensor $\mathbf{F}_{n+\frac{1}{2}}^h \mathbf{S}_{n+\frac{1}{2}}^h \mathbf{F}_{n+\frac{1}{2}}^{h,T}$ and the skew-symmetry of $\bar{\mathbf{w}}$. Therefore, the absence of external actions makes the angular momentum balance be zero since (3.187) must hold for all $\bar{\mathbf{w}}$, proving that the midpoint scheme keeps the symmetries of the continuous counterpart.

Unlike the momentum balances, the total energy balance does not result in energy conservation since it reads

$$\begin{aligned} E_{n+1}^h - E_n^h &= K_{n+1}^h - K_n^h + U_{n+1}^h - U_n^h \\ &= \int_{\mathcal{B}_0^h} \frac{1}{2\rho_0^h} (\|\mathbf{p}_{n+1}^h\|^2 - \|\mathbf{p}_n^h\|^2) dV_0 + \int_{\mathcal{B}_0^h} (e_{n+1}^h - e_n^h) dV_0 \\ &= \int_{\mathcal{B}_0^h} \frac{1}{\rho_0^h} \mathbf{p}_{n+\frac{1}{2}}^h \cdot (\mathbf{p}_{n+1}^h - \mathbf{p}_n^h) dV_0 + \int_{\mathcal{B}_0^h} (e_{n+1}^h - e_n^h) dV_0 \end{aligned} \quad (3.188)$$

The first term in the above expression can be further elaborated by considering $\mathbf{w}_p^h = \mathbf{p}_{n+\frac{1}{2}}^h / \rho_0^h$ in either (3.172)₂, (3.178)₂ or (3.181)₂ along with a

particular tensorial property⁷ to give

$$\begin{aligned} E_{n+1}^h - E_n^h = & -\langle \mathbf{S}_{n+\frac{1}{2}}^h, \frac{1}{2}(\mathbf{C}_{n+1}^h - \mathbf{C}_n^h) \rangle_{\mathcal{B}_0^h} + \langle \mathbf{B}_{0,n+\frac{1}{2}}, \Delta \boldsymbol{\varphi}^h \rangle_{\mathcal{B}_0^h} \\ & + \langle \mathbf{T}_{0,n+\frac{1}{2}}, \Delta \boldsymbol{\varphi}^h \rangle_{\partial \mathcal{B}_0^h} + \int_{\mathcal{B}_0^h} (e_{n+1}^h - e_n^h) dV_0, \end{aligned} \quad (3.189)$$

which in absence of external forces yields

$$E_{n+1}^h - E_n^h = - \int_{\mathcal{B}_0^h} \mathbf{S}_{n+\frac{1}{2}}^h : \frac{1}{2}(\mathbf{C}_{n+1}^h - \mathbf{C}_n^h) dV_0 + \int_{\mathcal{B}_0^h} (e_{n+1}^h - e_n^h) dV_0 \quad (3.190)$$

Unfortunately, this last expression cannot be further detailed unless assuming some loss of generality, thus concluding that the midpoint-based energy conservation cannot be generally ensured.

Remark 3.16. The energy balance (3.190) also applies in the reversible elastic case in which the internal energy is identified with the Helmholtz free-energy hyperelastic potential $\Psi := \Psi(\mathbf{C})$ according to (3.41). In such a case, the energy conservation is clearly not fulfilled as the following inequality generally holds

$$\Psi(\mathbf{C}_{n+1}^h) - \Psi(\mathbf{C}_n^h) \neq \mathbf{S}_{n+\frac{1}{2}}^h : \frac{1}{2}(\mathbf{C}_{n+1}^h - \mathbf{C}_n^h) \quad (3.191)$$

This observation reveals the key for a method to be energy-conserving in the Hamiltonian context, which was devised in Simó & Tarnow (1992).

Interestingly, the entropy formulation complies with the second law of thermodynamics, which directly derives from choosing $w_\eta^h = \Delta t$ in (3.172)₃ to give

$$\begin{aligned} S_{n+1}^h - S_n^h = & \int_{\mathcal{B}_0^h} (\eta_{n+1}^h - \eta_n^h) dV_0 \\ = & -\left\langle \frac{\Delta t}{(\Theta_{n+\frac{1}{2}}^h)^2} \nabla_0 \Theta_{n+\frac{1}{2}}^h, \mathbf{H}_{n+\frac{1}{2}}^h \right\rangle_{\mathcal{B}_0^h} + \left\langle \frac{\Delta t}{\Theta_{n+\frac{1}{2}}^h}, \dot{\mathcal{D}}_{n+\frac{1}{2}}^h \right\rangle_{\mathcal{B}_0^h} \\ & - \left\langle \frac{\Delta t}{\Theta_{n+\frac{1}{2}}^h}, H_{N,n+\frac{1}{2}} \right\rangle_{\partial \mathcal{B}_0^h} + \left\langle \frac{\Delta t}{\Theta_{n+\frac{1}{2}}^h}, \mathcal{R}_{n+\frac{1}{2}} \right\rangle_{\mathcal{B}_0^h} \end{aligned} \quad (3.192)$$

Assuming the isolation of the continuum, that is $H_N = \mathcal{R} = 0$, together

⁷ $\mathbf{AB} : \mathbf{C} = \mathbf{B} : \mathbf{A}^T \mathbf{C}$

with the expressions (3.175) and (3.177) the entropy balance gives

$$\begin{aligned} S_{n+1}^h - S_n^h = & \left\langle \frac{\Delta t}{(\Theta_{n+\frac{1}{2}}^h)^2} \nabla_0 \Theta_{n+\frac{1}{2}}^h, \mathbf{K}_{n+\frac{1}{2}}^h \nabla_0 \Theta_{n+\frac{1}{2}}^h \right\rangle_{\mathcal{B}_0^h} \\ & + \left\langle \frac{\Delta t}{\Theta_{n+\frac{1}{2}}^h}, \dot{\mathcal{D}}_{n+\frac{1}{2}}^h \right\rangle_{\mathcal{B}_0^h} \geq 0, \end{aligned} \quad (3.193)$$

which proves the fulfillment of the second law in a midpoint-based discrete fashion.

The temperature formulation (3.178), on the other hand, does not inherit this important feature as it is impossible to relate the entropy balance to the temperature balance appearing in (3.178)₃.

3.8.2 Trapezoidal time integration method

The standard second-order trapezoidal method also provides a straightforward formulation although it does not possess any preservation features other than the linear momentum one for general nonlinear problems as the dynamics of thermo-dissipative continua. As a representative full discrete formulation of trapezoidal-type, consider the temperature formulation which reads

$$\begin{aligned} \frac{\varphi_{n+1}^h - \varphi_n^h}{\Delta t} - \frac{1}{\rho_0} \bar{\mathbf{p}}_{n+\frac{1}{2}}^h &= \mathbf{0}, \\ \langle \mathbf{w}_{\mathbf{p}}^h, \frac{\mathbf{p}_{n+1}^h - \mathbf{p}_n^h}{\Delta t} \rangle_{\mathcal{B}_0^h} + \langle \nabla_0 \mathbf{w}_{\mathbf{p}}^h, \overline{\mathbf{F}^h \mathbf{S}^h}_{n+\frac{1}{2}} \rangle_{\mathcal{B}_0^h} \\ &\quad - \langle \mathbf{w}_{\mathbf{p}}^h, \overline{\mathbf{B}}_{0,n+\frac{1}{2}} \rangle_{\mathcal{B}_0^h} - \langle \mathbf{w}_{\mathbf{p}}^h, \overline{\mathbf{T}}_{0,n+\frac{1}{2}} \rangle_{\partial \mathcal{B}_0^h} = 0, \\ \langle w_{\Theta}^h, \frac{\Theta_{n+1}^h - \Theta_n^h}{\Delta t} \rangle_{\mathcal{B}_0^h} + \langle \frac{w_{\Theta}^h}{c}, \overline{\mathbf{F}^h \mathbf{V}^h} : \nabla_0 [\mathbf{p}^h / \rho_0]_{n+\frac{1}{2}} \rangle_{\mathcal{B}_0^h} \\ &\quad - \langle \nabla_0 \left[\frac{w_{\Theta}^h}{c} \right], \overline{\mathbf{H}}_{n+\frac{1}{2}}^h \rangle_{\mathcal{B}_0^h} - \langle \frac{w_{\Theta}^h}{c}, \overline{\mathcal{D}}_{n+\frac{1}{2}}^h + \overline{\mathcal{H}}_{d,n+\frac{1}{2}}^h \rangle_{\mathcal{B}_0^h} \\ &\quad + \langle \frac{w_{\Theta}^h}{c}, \overline{\mathbf{H}}_{N,n+\frac{1}{2}}^h \rangle_{\partial \mathcal{B}_0^h} - \langle \frac{w_{\Theta}^h}{c}, \overline{\mathcal{R}}_{n+\frac{1}{2}}^h \rangle_{\mathcal{B}_0^h} = 0 \\ \frac{\Lambda_{n+1}^{\alpha,h} - \Lambda_n^{\alpha,h}}{\Delta t} - \overline{\mathcal{K}}(\mathbf{Q}^{\alpha,h})_{n+\frac{1}{2}} &= \mathbf{0} \quad \forall \alpha = 1, \dots, m, \end{aligned} \quad (3.194)$$

with $\overline{(\cdot)}_{n+\frac{1}{2}} = \frac{1}{2} [(\cdot)_{n+1} + (\cdot)_n]$ indicating the mean value, which coincides with the midpoint evaluation for linear functions.

As an example of its inability to preserve the invariants of a free-motion, the angular momentum is elaborated using (3.194)₂ in (3.187) to give

$$\begin{aligned}
(\mathbf{J}_{n+1}^h - \mathbf{J}_n^h) \cdot \bar{\mathbf{w}} &= \Delta t \left[-\langle \overline{\mathbf{F}^h \mathbf{S}^h}_{n+\frac{1}{2}} \mathbf{F}_{n+\frac{1}{2}}^{h,T}, \bar{\mathbf{w}} \rangle_{\mathcal{B}_0^h} \right. \\
&\quad \left. + \langle \overline{\mathbf{B}}_{0,n+\frac{1}{2}}, \bar{\mathbf{w}} \wedge \boldsymbol{\varphi}_{n+\frac{1}{2}}^h \rangle_{\mathcal{B}_0^h} + \langle \overline{\mathbf{T}}_{0,n+\frac{1}{2}}, \bar{\mathbf{w}} \wedge \boldsymbol{\varphi}_{n+\frac{1}{2}}^h \rangle_{\partial \mathcal{B}_0^h} \right] \\
&= \Delta t \left[-\langle \frac{1}{2} (\mathbf{F}_{n+1}^h \mathbf{S}_{n+1}^h + \mathbf{F}_n^h \mathbf{S}_n^h) \mathbf{F}_{n+\frac{1}{2}}^{h,T}, \bar{\mathbf{w}} \rangle_{\mathcal{B}_0^h} \right. \\
&\quad \left. + \langle \overline{\mathbf{B}}_{0,n+\frac{1}{2}}, \bar{\mathbf{w}} \wedge \boldsymbol{\varphi}_{n+\frac{1}{2}}^h \rangle_{\mathcal{B}_0^h} + \langle \overline{\mathbf{T}}_{0,n+\frac{1}{2}}, \bar{\mathbf{w}} \wedge \boldsymbol{\varphi}_{n+\frac{1}{2}}^h \rangle_{\partial \mathcal{B}_0^h} \right],
\end{aligned} \tag{3.195}$$

where the term depending on the stress tensor is generally non-zero and hence the angular momentum is not preserved in a force-free motion. The laws of thermodynamics are also breached by this approximation.

Metriplectic structures: GENERIC formalism

CHAPTER 4

Somehow hidden for the computational mechanics' community but quite apparent for mathematicians it was the concept of metriplectic structure developed in the context of differential geometry' theory, see the monograph due to Frankel (2011). The metriplectic structure on a smooth manifold possesses all the mathematical features involved in the dynamic equations associated with general dissipative systems. This geometrical description of dissipative systems dates back to the work of Morrison (1984), Kaufman (1985), Grmela (1986), Brockett (1993) and Nguyen & Turski (2001). With this structure, most of the dissipative problems of interest can be generated from a general abstract (unifying) form that guarantees certain properties of their solutions. Not only that but also, such abstract form further contributes to the understanding of the equations that pose thermodynamic soundness, to discard non thermodynamically consistent terms, or even to suggest admissible candidates for the time evolution equations in new physical theories.

A particular metriplectic structure is the framework introduced by Öttinger (2005) and co-workers Grmela & Öttinger (1997); Öttinger & Grmela (1997) for “*General Equilibrium Non-Equilibrium Reversible-Irreversible Coupling*”, known by the acronym GENERIC. It exploits the geometric description provided by metriplectic structures to formulate isolated thermodynamic systems of interest in the fields of physics or engineering. Thus, the evolution equations describing any isolated thermodynamical system are derived via an additive decomposition into the system reversible evolution, which is associated with a differential operator on the total energy, and its irreversible one, which is connected with a differential operator on the total entropy.

For the purposes of this dissertation, the key issue in the GENERIC framework is that, for dissipative systems, it naturally plays the role of the Hamiltonian framework for conserving ones, which revealed the general formulation of conserving time integration counterparts: Energy-Momentum methods. Furthermore, from the formal point of view, the metriplectic GENERIC framework shares the key features of Hamiltonian framework so that the same reasoning which led from Hamiltonian systems to Energy-momentum methods can be applied to reveal thermodynamically consistent time integration counterparts for general dissipative systems that, following the parallelism, will be referred to as Energy-Entropy-Momentum methods. These ideas were first devised in the works of Romero (2009, 2010a,b).

In this Chapter, the fundamental concepts on metriplectic structures are introduced. Then, the GENERIC framework is used to define *smooth* dissipative systems in unified fashion for both finite and infinite dimensional problems. Finally, the different dissipative problems dealt with so far are formulated within this general framework so that full equivalence can easily be checked and, accordingly, discrete thermodynamically consistent counterparts can be derived in the following Chapter.

4.1 Metriplectic structures

In the context of differential geometry, a metriplectic structure is a structure arising from the combination of a Poisson structure and a Gradient (or metric) structure, see Fish (2005). The resulting structure is suitable to model the geometry of the dissipative systems which generally pose reversible (conserving) and irreversible (dissipative) qualities along trajectories. Thus, the Poisson structure assumes the generation of the reversible part of the system evolution while the Gradient structure controls the irreversible evolution.

Conservative systems on a phase space $\mathcal{P}$ can be described by a Poisson (or symplectic) structure of the form

$$\dot{f} = \{f, H\} \quad \forall f : \mathcal{P} \rightarrow \mathbb{R}, \quad (4.1)$$

where $H : \mathcal{P} \rightarrow \mathbb{R}$ is the Hamiltonian function and the bracket $\{\cdot, \cdot\}$ is the Poisson bracket. This bracket is a bilinear and skew-symmetric operator on the phase space that additionally satisfies the Jacobi identity and the Leibniz rule, see Goldstein et al. (1965). These properties of the bracket ensure the conservation of the Hamiltonian, defining a conserving system, which directly

follows from taking $f = H$ to give

$$\dot{H} = \{H, H\} = 0, \quad (4.2)$$

due to the skew-symmetry of the Poisson bracket.

Gradient or metric systems, however, were devised for the modeling of purely dissipative systems, that is, systems which evolve by increasing its entropy. Geometrically, a metric tensor (in a Riemannian geometry) is responsible for inducing such evolution on a phase space $\mathcal{T}$, hence its name. Thus, the system evolution is provided by the following structure

$$\dot{f} = [f, S] \quad \forall f : \mathcal{T} \rightarrow \mathbb{R}, \quad (4.3)$$

$S : \mathcal{T} \rightarrow \mathbb{R}$ being a function on a phase space identified with a type of entropy, and the bracket $[\cdot, \cdot]$ being the metric bracket which is a bilinear, symmetric and positive semi-definite operator. Then, the production of entropy is guaranteed as can be demonstrated by choosing $f = S$ to give

$$\dot{S} = [S, S] \geq 0, \quad (4.4)$$

due to the metric bracket being positive semi-definite.

These two mutually exclusive structures can be combined, thus defining a metriplectic structure, with the idea of attaching dissipation terms to Hamiltonian systems so that general dissipative system can be modeled by

$$\dot{f} = \{f, E\} + [f, S] \quad \forall f : \mathcal{S} \rightarrow \mathbb{R}, \quad (4.5)$$

where $E : \mathcal{S} \rightarrow \mathbb{R}$ is the total energy of the system and $S : \mathcal{S} \rightarrow \mathbb{R}$ the total entropy defined on a state space $\mathcal{S}$.

For the metriplectic system (4.5) to exhibit trajectories in agreement with the laws of thermodynamics, additional requirements must be imposed on the introduced brackets, specifically

$$\{S, E\} = [E, S] = 0 \quad (4.6)$$

Thus, in view of (4.5) and (4.6) it follows that the law of thermodynamics are satisfied, that is

$$\begin{aligned} \dot{E} &= \{E, E\} + [E, S] = 0 \\ \dot{S} &= \{S, E\} + [S, S] \geq 0 \end{aligned} \quad (4.7)$$

More details about metriplectic structures for the modeling of dissipative problems can be found in Guha (2007) and the pioneering work of Morrison (1984), Kaufman (1985) and Grmela (1986).

4.2 Finite-dimensional smooth dissipative systems

As commented at the beginning of the Chapter, a metriplectic structure that has gained popularity in the last years among the physic and computational mechanic communities is the GENERIC formalism introduced by Grmela & Öttinger (1997); Öttinger & Grmela (1997), and fully revised in the monograph Öttinger (2005). This framework intends for a physical approach rather than geometric (mathematical) of metriplectic structures, that is why, for instance, the introduced metric bracket, responsible for generating the dissipative part, is accordingly named *dissipative* or *friction* bracket, making clear the effect of its contribution.

Due to any metriplectic structure (4.5) contains a Poisson structure (reversible), the GENERIC formalism can be considered as a natural extension of the Hamiltonian formalism. Based on this idea, the GENERIC framework allows for an unified definition of isolated (thermo)dissipative systems.

Definition 4.1. Let $\mathcal{S}$ be a finite-dimensional state space that contains the $2k$ -dimensional phase space $\mathcal{P}$ defining a Hamiltonian system by the pair $(\mathbf{q}, \mathbf{p}) \in \mathbb{R}^k$ and all the internal variables $(\gamma_1, \dots, \gamma_m) \in \mathbb{R}^m$ and the thermal variables $(s_1, \dots, s_t) \in \mathbb{R}^t$ required to fully represent the isolated system' thermodynamics, furnishing each two finite-dimensional spaces $\mathcal{D}, \mathcal{T}$ of dimension t and m , respectively, that is

$$\mathcal{S} = \{\mathbf{z} = (\mathbf{q}, \mathbf{p}, \gamma_1, \dots, \gamma_m, s_1, \dots, s_t) \in (\mathcal{P} \times \mathcal{D} \times \mathcal{T}) \subset \mathbb{R}^{2k+m+t}\} \quad (4.8)$$

Then, the tangent space at some given state $\mathbf{z}$ and its dual are denoted as $T_{\mathbf{z}}\mathcal{S}$ and $T_{\mathbf{z}}^*\mathcal{S}$, respectively.

Definition 4.2. An finite-dimensional smooth dissipative system is an isolated system whose evolution equations are provided by the GENERIC equations

$$\dot{\mathbf{z}} = \mathbf{L}(\mathbf{z})DE(\mathbf{z}) + \mathbf{M}(\mathbf{z})DS(\mathbf{z}), \quad (4.9)$$

$E: \mathbf{z} \in \mathcal{S} \rightarrow \mathbb{R}$ being the total energy function and $S: \mathbf{z} \in \mathcal{S} \rightarrow \mathbb{R}$ being the total entropy function, $D(\cdot)^1$ being the gradient operator with respect to the state space vector $\mathbf{z}$ and $\mathbf{L}^2, \mathbf{M}: T_{\mathbf{z}}^*\mathcal{S} \mapsto T_{\mathbf{z}}\mathcal{S}$ being the Poisson and Dissipative matrices.

Remark 4.1. Following Mielke (2011), any *non-smooth* dissipative system is an isolated system whose evolution equations are provided by

$$\dot{\mathbf{z}} = \mathbf{L}(\mathbf{z})DE(\mathbf{z}) + \partial\mathcal{M}(\mathbf{z}, DS), \quad (4.10)$$

¹not to be confused with the total dissipated energy D defined by (3.105).

²not to be confused with the total linear momentum vector $\mathbf{L}$.

where $\partial\mathcal{M}(\mathbf{z}, \cdot)$ is the subdifferential of a non-negative and convex functional $\mathcal{M} : \mathcal{S} \times T_{\mathbf{z}}^*\mathcal{S} \mapsto \mathbb{R}$ with $\mathcal{M}(\mathbf{z}, \mathbf{0}) = 0$.

Proposition 4.1. *The system $(\mathcal{S}, \mathbf{L}, \mathbf{M}, E, S)$ is thermodynamically sound iff $\mathbf{L}$ is skew-symmetric, $\mathbf{M}$ is symmetric and positive semi-definite, and both satisfy the following degeneracy or non-interaction conditions*

$$\mathbf{L}(\mathbf{z})DS(\mathbf{z}) = \mathbf{M}(\mathbf{z})DE(\mathbf{z}) = \mathbf{0} \quad (4.11)$$

Proof. The proof follows from the elaboration of the rate of the total energy and the total entropy of the system via the chain rule

$$\dot{E} = DE \cdot \dot{\mathbf{z}} = DE \cdot \mathbf{L}DE + DE \cdot \mathbf{M}DS = DS \cdot \mathbf{M}DE = 0, \quad (4.12)$$

$$\begin{aligned} \dot{S} &= DS \cdot \dot{\mathbf{z}} = DS \cdot \mathbf{L}DE + DS \cdot \mathbf{M}DS \\ &= -DE \cdot \mathbf{L}DS + DS \cdot \mathbf{M}DS \geq 0, \end{aligned} \quad (4.13)$$

where use has been made of (4.9) and (4.11) along with the properties previously stated for the matrices. $\square$

Remark 4.2. Equations (4.9) - (4.13) constitute the GENERIC formalism for finite-dimensional systems which are a finite-dimensional version of the general metriplectic structure defined by (4.5) - (4.7).

In contrast to the Hamiltonian framework, there no exist canonical forms of the Poisson and Dissipative matrices. Their obtention in terms of the chosen state variables determines their components which, of course, depend on the particular thermo-dissipative problem. The search of their components could be cumbersome depending mainly on the thermodynamical state variable. However, the introduced structure of the state space $\mathcal{S}$ leads the matrices to have a block structure, from which some general conclusions can be made based on physical assumptions. Thus, due to the dissipative nature of internal variables, they do not contribute to the reversible evolution of the system, provided by the Poisson matrix $\mathbf{L}$, so its blocks $\mathbf{L}_{q\gamma}$, $\mathbf{L}_{p\gamma}$ must vanish. In the same way, the phase variables $(\mathbf{q}, \mathbf{p})$ are responsible for the reversible changes, suggesting that the blocks of the Dissipative matrix $\mathbf{M}_{qq}$, $\mathbf{M}_{qp}$, $\mathbf{M}_{pp}$ are identically zero.

Moreover, Mielke (2011) provides a fairly systematic procedure to obtain them for dissipative systems defined in a state space as (4.8). The systematization is achieved by noticing that there are a set of thermodynamical state variables, i.e $s_i \in \mathcal{T}$, for which the matrices $\mathbf{L}$ and $\mathbf{M}$ become simpler, thus defining the nearest thing of *canonical* forms of them. These simple forms

are the basis to unveil them for any choice of the thermodynamical variables by resorting to change of variables techniques. Such canonical-like forms are revealed by the orthogonality imposed by the degeneracy conditions (4.11).

Specifically, if the total entropy function S is identified in the state space $\mathcal{S}$, the Poisson matrix becomes the classical symplectic matrix, see Alan J. & Meyer (1972), denoted as $\mathbf{\Omega}_0$, plus zero components out of the phase variables, that is

$$\mathbf{L}_0 = \left(\begin{array}{c|c|c} \mathbf{\Omega}_0 & \mathbf{0}_{2k \times m} & \mathbf{0}_{2k \times t} \\ \hline \mathbf{0}_{2k \times m}^T & \mathbf{0}_m & \mathbf{0}_{m \times t} \\ \hline \mathbf{0}_{2k \times t}^T & \mathbf{0}_{m \times t}^T & \mathbf{0}_t \end{array} \right) \text{ if } S \in \mathcal{S}, \text{ with } \mathbf{\Omega}_0 = \left(\begin{array}{c|c} \mathbf{0}_k & \mathbf{1}_k \\ \hline -\mathbf{1}_k & \mathbf{0}_k \end{array} \right), \quad (4.14)$$

where $\mathbf{0}_{i \times j}$ and $\mathbf{1}_{i \times j}$ are the null and the identity matrices of dimension ij , with a single index i meaning square matrices of dimension i .

Similarly, if the total energy function E is used to describe the system thermodynamics, the Dissipative matrix adopts the following simple form

$$\mathbf{M}_0 = M \left(\begin{array}{c|c|c} \mathbf{0}_{2k} & \mathbf{0}_{2k \times m} & \mathbf{0}_{2k \times t} \\ \hline \mathbf{0}_{2k \times m}^T & \mathbf{g}_m & \mathbf{0}_{m \times t} \\ \hline \mathbf{0}_{2k \times t}^T & \mathbf{0}_{m \times t}^T & \mathbf{0}_t \end{array} \right) \text{ if } E \in \mathcal{S}, \quad (4.15)$$

$\mathbf{g}_m$ being the metric tensor in the space $\mathcal{D}$ and $M \geq 0$ some scalar factor depending on the particular system.

With this reasoning, the matrices for any choice of the state variable can be generated from two changes of variables, namely

$$\hat{\mathbf{z}} = \mathcal{S}(\mathbf{z}), \quad \hat{\mathbf{z}} = \mathcal{E}(\mathbf{z}), \quad (4.16)$$

so that the new Poisson matrix is provided by

$$\mathbf{L} = \left(\frac{\partial \mathcal{S}}{\partial \mathbf{z}} \right)^{-1} (\mathbf{L}_0 \circ \mathcal{S}) \left(\frac{\partial \mathcal{S}}{\partial \mathbf{z}} \right)^{-T}, \quad (4.17)$$

whereas the novel Dissipative matrix responds to

$$\mathbf{M} = \left(\frac{\partial \mathcal{E}}{\partial \mathbf{z}} \right)^{-1} (\mathbf{M}_0 \circ \mathcal{E}) \left(\frac{\partial \mathcal{E}}{\partial \mathbf{z}} \right)^{-T}, \quad (4.18)$$

$(\cdot) \circ (\cdot)$ meaning composition. From (4.17), it is clear that the resulting Poisson matrix always contains the canonical symplectic matrix for all vector state $\mathbf{z} \in \mathcal{S}$.

4.2.1 Finite-dimensional dissipative systems with symmetries

For dissipative systems, a symmetry is the action of a Lie group on the state space that preserves both reversible and irreversible operators. Noether's theorem indicates that associated with these actions are momentum maps that are constant along the solution. A detailed description of the purely Hamiltonian case can be found in Marsden & Ratiu (1999), while its natural extension to the GENERIC framework was developed in Romero (2013). Next, these results are used to define dissipative systems with symmetries.

Thus, let G be a Lie group with an associated algebra $\mathfrak{g}$ and its dual $\mathfrak{g}^*$, endowed by an exponential map $\exp[\cdot]: \mathfrak{g} \mapsto G$ which takes elements of the Lie algebra onto the group G . The group G acts on the state space $\mathcal{S}$ via an action $\Phi: G \times \mathcal{S} \mapsto \mathcal{S}$ denoted by $\Phi_g(\mathbf{z}) = \Phi(g, \mathbf{z})$. Furthermore, the one-parameter family of actions $\Phi^\xi: \mathbb{R} \times \mathcal{S} \mapsto \mathcal{S}$ is defined by the format $\Phi^\xi(\epsilon, \mathbf{z}) = \Phi(\exp[\epsilon\xi], \mathbf{z})$ for any $\xi \in \mathfrak{g}$. The tangent of this curve at the origin is provided by

$$\xi_{\mathcal{S}}(\mathbf{z}) = \left. \frac{d}{d\epsilon} \right|_{\epsilon=0} \Phi^\xi(\epsilon, \mathbf{z}), \quad (4.19)$$

which is the infinitesimal generator of the action corresponding to ξ .

Then, an action Φ is said to preserve the metriplectic structure of GENERIC if, for any $g \in G$, the following holds

$$D\Phi_g(\mathbf{z}) \cdot \mathbf{L} \cdot D\Phi_g(\mathbf{z})^T = \mathbf{L} \circ \Phi_g \text{ and } D\Phi_g(\mathbf{z}) \cdot \mathbf{M} \cdot D\Phi_g(\mathbf{z})^T = \mathbf{M} \circ \Phi_g \quad (4.20)$$

Definition 4.3. A smooth dissipative system $(\mathcal{S}, \mathbf{L}, \mathbf{M}, E, S)$ has a momentum map if an action Φ of a Lie group G in the state space $\mathcal{S}$ is an invariant of the total energy of the system, that is, it is verified that

$$E \circ \Phi_g = E(\Phi(g, \mathbf{z})) = E(\mathbf{z}) \quad \forall g \in G, \quad \forall \mathbf{z} \in \mathcal{S}, \quad (4.21)$$

then, the system $(\mathcal{S}, G, \mathbf{L}, \mathbf{M}, E, S)$ is a dissipative system with symmetries and the total energy E is said to be a G -invariant function, see Appendix A.

Definition 4.4. A mapping $\mathbf{J}: \mathbf{z} \in \mathcal{S} \mapsto \mathfrak{g}^*$ is a momentum map associated with the action Φ iff the action preserves the GENERIC structure, i.e satisfies (4.20), and for any $\xi \in \mathfrak{g}$, the scalar function $J_\xi: \mathcal{S} \mapsto \mathbb{R}$, defined as

$$J_\xi(\mathbf{z}) = \mathbf{J}(\mathbf{z}) \cdot \xi, \quad (4.22)$$

satisfies

$$\xi_{\mathcal{S}} = \mathbf{L} D J_\xi, \quad \mathbf{0} = \mathbf{M} D J_\xi \quad (4.23)$$

Theorem 4.2. *The momentum maps of a dissipative system with symmetries $(\mathcal{S}, \mathbf{L}, \mathbf{M}, E, S)$ are conserved quantities (first integrals) of the system.*

Proof. The chain rule together with the evolution equations (4.9) lead the rate of the scalar function (4.22) to be

$$\dot{J}_{\xi} = DJ_{\xi} \cdot \dot{z} = DJ_{\xi} \cdot \mathbf{L}DE + DJ_{\xi} \cdot \mathbf{M}DS \quad (4.24)$$

that, by using (4.23), simplifies to

$$\dot{J}_{\xi} = -DE \cdot \xi_{\mathcal{S}} \quad (4.25)$$

As the scalar function (4.22) depends on an arbitrary ξ , the momentum map $\mathbf{J}$ is preserved if the right hand side of (4.25) identically vanishes. This is proved by choosing $g = \exp[\epsilon \xi]$ in (4.21) so the derivative with respect ϵ gives

$$DE \cdot \xi_{\mathcal{S}} = 0, \quad (4.26)$$

demonstrating that the mapping $\mathbf{J}$ defined according to Def. 4.4 is conserved along the system evolution. $\square$

4.3 GENERIC forms of the two thermo-spring system

The two thermo-spring system presented in Section 2.1 is a finite-dimensional dissipative system in the sense of the Def. 4.2, where the space $\mathcal{D}$ vanishes. This particularity invalidates the application of the systematic procedure due to Mielke (2011) previously reviewed. However, its evolution equations (2.24) or (2.17) can still be written in the GENERIC format. For that, two GENERIC forms need to be elaborated according to two choices of the thermodynamical variables in the state vector based on either entropy or temperature variables. The entropy-based GENERIC form of this system was first proposed in Romero (2009) while the temperature-based (so far thought to be difficult to attain) was recently revealed in Conde Martín et al. (2016). Both forms are briefly reviewed in the following subsections.

4.3.1 Entropy-based GENERIC formulation

The entropy-based GENERIC description of the two thermo-spring system departs from the definition of the finite-dimensional phase space to be

$\mathcal{P} = \mathbb{R}^{2d} \times \mathbb{R}^{2d}$ and the thermodynamical space to be $\mathcal{T} = \mathbb{R}^2$ which together define the state space as follows

$$\mathcal{S} = \{ \mathbf{z} = (\mathbf{q}_1, \mathbf{q}_2, \mathbf{p}_1, \mathbf{p}_2, \eta_1, \eta_2) \in \mathbb{R}^{2d} \times \mathbb{R}^{2d} \times \mathbb{R}^2, \mathbf{q}_1 \neq \mathbf{0}, \mathbf{q}_2 \neq \mathbf{q}_1 \} \quad (4.27)$$

With this state space, the total energy of the system is provided by the sum of the kinetic energy of the point masses (2.33) and the the internal energies of the springs in terms of entropies (2.22) to give

$$E(\mathbf{z}) = K(\|\mathbf{p}_1\|, \|\mathbf{p}_2\|) + \sum_{b=1}^2 e_b(\lambda_b, \eta_b), \quad (4.28)$$

Recall that the entropy formulation is restricted to those cases in which the analytical function $e_i(\lambda_i, \eta_i)$ can be achieved.

For the state space (4.27), the total entropy of the system is provided by the sum of the two of the state variables, namely the spring entropies, as

$$S(\mathbf{z}) = \sum_{a=1}^2 \eta_a \quad (4.29)$$

Thus, the first step to find the GENERIC equations is to derive the total energy and total entropy with respect to the state vector (4.27), yielding

$$DE = \begin{pmatrix} \frac{\partial e_1}{\partial \lambda_1} \frac{\partial \lambda_1}{\partial \mathbf{q}_1} + \frac{\partial e_2}{\partial \lambda_2} \frac{\partial \lambda_2}{\partial \mathbf{q}_1} \\ \frac{\partial e_2}{\partial \lambda_2} \frac{\partial \lambda_2}{\partial \mathbf{q}_2} \\ \frac{\mathbf{p}_1}{m_1} \\ \frac{\mathbf{p}_2}{m_2} \\ \frac{\partial e_1}{\partial \eta_1} \\ \frac{\partial e_2}{\partial \eta_2} \end{pmatrix}, \quad DS = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 1 \end{pmatrix} \quad (4.30)$$

Due to the simplicity of the system, the Poisson and Dissipative matrices required to recast the evolution equations (2.24) in the GENERIC form (4.9)

can be constructed by inspection. The Poisson thus results in the *canonical* one provided by (4.14), that is

$$\mathbf{L}(\mathbf{z}) = \left(\begin{array}{cccc|cc} \mathbf{0} & \mathbf{0} & \mathbf{1} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{1} & \mathbf{0} & \mathbf{0} \\ -\mathbf{1} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & -\mathbf{1} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \hline \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & 0 & 0 \\ \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & 0 & 0 \end{array} \right) \quad (4.31)$$

The Dissipative matrix, however, is a bit more involved, that is

$$\mathbf{M}(\mathbf{z}) = k \left(\begin{array}{cccc|cc} \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & \frac{\partial e_2}{\partial \eta_2} \left(\frac{\partial e_1}{\partial \eta_1} \right)^{-1} & -1 \\ \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & -1 & \frac{\partial e_1}{\partial \eta_1} \left(\frac{\partial e_2}{\partial \eta_2} \right)^{-1} \end{array} \right), \quad (4.32)$$

where the partial derivatives are identified with the spring temperatures via (2.23)₂, that is

$$\frac{\partial e_1}{\partial \eta_1} = \theta_1, \quad \frac{\partial e_2}{\partial \eta_2} = \theta_2 \quad (4.33)$$

Finally, the use of these matrices and gradients in (4.9) leads to the evolution equations (2.24) except for the external forces applied to the point masses which are out of the GENERIC expressions due to being external. In any case, they can be inserted a posteriori taking into account that their presence will breach the conservation properties stated by the GENERIC formulation.

4.3.2 Temperature-based GENERIC formulation

Consider a state vector which includes the temperatures of the springs as the thermodynamical variables so the state space is defined by

$$\mathcal{S} = \{ \mathbf{z} = (\mathbf{q}_1, \mathbf{q}_2, \mathbf{p}_1, \mathbf{p}_2, \theta_1, \theta_2) \in \mathbb{R}^{2d} \times \mathbb{R}^{2d} \times \mathbb{R}_+^2, \mathbf{q}_1 \neq \mathbf{0}, \mathbf{q}_2 \neq \mathbf{q}_1 \} \quad (4.34)$$

The total energy of the two thermo-spring system was introduced in 2.1 as the sum of the kinetic energy of the point masses (2.33) and the internal energy of the springs (2.7), that is

$$E(\mathbf{z}) = K(\|\mathbf{p}_1\|, \|\mathbf{p}_2\|) + \sum_{b=1}^2 e_b(\lambda_b, \theta_b), \quad (4.35)$$

The total entropy of the system is provided by the sum of the spring entropy (2.12) to be

$$S(\mathbf{z}) = \sum_{a=1}^2 \eta_a(\lambda_a, \theta_a) = \sum_{a=1}^2 -\frac{\partial \Psi_a(\lambda_a, \theta_a)}{\partial \theta_a} \quad (4.36)$$

Again, the gradient of the total energy and total entropy with respect to the state vector need to be elaborated, that is

$$DE = \begin{pmatrix} \frac{\partial e_1}{\partial \lambda_1} \frac{\partial \lambda_1}{\partial \mathbf{q}_1} + \frac{\partial e_2}{\partial \lambda_2} \frac{\partial \lambda_2}{\partial \mathbf{q}_1} \\ \frac{\partial e_2}{\partial \lambda_2} \frac{\partial \lambda_2}{\partial \mathbf{q}_2} \\ \frac{\mathbf{p}_1}{m_1} \\ \frac{\mathbf{p}_2}{m_2} \\ \frac{\partial e_1}{\partial \theta_1} \\ \frac{\partial e_2}{\partial \theta_2} \end{pmatrix}, \quad DS = \begin{pmatrix} \frac{\partial \eta_1}{\partial \lambda_1} \frac{\partial \lambda_1}{\partial \mathbf{q}_1} + \frac{\partial \eta_2}{\partial \lambda_2} \frac{\partial \lambda_2}{\partial \mathbf{q}_1} \\ \frac{\partial \eta_2}{\partial \lambda_2} \frac{\partial \lambda_2}{\partial \mathbf{q}_2} \\ 0 \\ 0 \\ \frac{\partial \eta_1}{\partial \theta_1} \\ \frac{\partial \eta_2}{\partial \theta_2} \end{pmatrix} \quad (4.37)$$

The associated Poisson and Dissipative matrices required to recast the evolution equations (2.17) in the GENERIC form (4.9) are provided by

$$\mathbf{L}(\mathbf{z}) = \left(\begin{array}{cccc|cc} \mathbf{0} & \mathbf{0} & \mathbf{1} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{1} & \mathbf{0} & \mathbf{0} \\ -\mathbf{1} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{L}_{11} & \mathbf{L}_{12} \\ \mathbf{0} & -\mathbf{1} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{L}_{22} \\ \hline \mathbf{0}^T & \mathbf{0}^T & \bar{\mathbf{L}}_{11} & \mathbf{0}^T & 0 & 0 \\ \mathbf{0}^T & \mathbf{0}^T & \bar{\mathbf{L}}_{21} & \bar{\mathbf{L}}_{22} & 0 & 0 \end{array} \right) \quad (4.38)$$

Interestingly, new terms taking into account the thermo-mechanical coupling appears with this choice of the state vector, which are provided by

$$\mathbf{L}_{ab} = -\bar{\mathbf{L}}_{ba}^T = \left(\frac{\partial \eta_b}{\partial \theta_b} \right)^{-1} \frac{\partial \eta_b}{\partial \lambda_b} \frac{\partial \lambda_b}{\partial \mathbf{q}_a}, \quad (4.39)$$

Similar ones appear when the internal energies are considered in the state vector, see Romero (2009), demonstrating that the temperature election is not much more involved than the other common choices.

The Dissipative matrix can be expressed in the following way

$$\mathbf{M}(\mathbf{z}) = k\theta_1\theta_2 \begin{pmatrix} \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & M_{11} & M_{12} \\ \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & M_{21} & M_{22} \end{pmatrix}, \quad (4.40)$$

with the scalar values M_{ab} being provided by

$$M_{ab} = (-1)^{a+b} \left(\frac{\partial e_a}{\partial \theta_a} \right)^{-1} \left(\frac{\partial e_b}{\partial \theta_b} \right)^{-1} \quad (4.41)$$

Remark 4.3. The fact that the temperatures appear as factors of the matrix will have an impact in the formulation of Energy-Entropy-Momentum methods as will be explained in Chapter 5.

Due to the state vector including the temperatures, the GENERIC equations (4.9) provides the evolution equations of the system in the following particular form

$$\begin{aligned} \dot{\mathbf{q}}_a &= \frac{\mathbf{p}_a}{m_a} \\ \dot{\mathbf{p}}_a &= - \sum_{b=1}^2 \left(\frac{\partial e_b}{\partial \lambda_b} - \theta_b \frac{\partial \eta_b}{\partial \lambda_b} \right) \frac{\partial \lambda_b}{\partial \mathbf{q}_a} \\ \dot{\theta}_a &= \left(\frac{\partial e_a}{\partial \theta_a} \right)^{-1} \left[(-1)^{a-1} h - \theta_a \frac{\partial \eta_a}{\partial \lambda_a} \sum_{b=1}^2 \frac{\partial \lambda_a}{\partial \mathbf{q}_b} \cdot \frac{\mathbf{p}_b}{m_b} \right], \end{aligned} \quad (4.42)$$

for $a = 1, 2$.

The form (2.17), besides the external forces, is then recast by using relation provided by the Legendre transform (2.7) in the linear momentum balance (4.42)₂.

4.3.3 Laws of thermodynamics and symmetries

The laws of thermodynamics are ensured by the GENERIC equations (4.9) and by the properties of the Poisson and Dissipative matrices. Thus, the energy conservation results trivial from (4.12). The second law, however, can be further elaborated by using the Dissipative matrix provided by either (4.32) or (4.40) along with the gradient (4.30)₂ or (4.37)₂, leading to the rate of entropy

$$\dot{S}(\mathbf{z}) = DS \cdot \dot{\mathbf{z}} = DS \cdot \mathbf{M}DS = k \frac{(\theta_2 - \theta_1)^2}{\theta_1 \theta_2} \geq 0, \quad (4.43)$$

that demonstrates the two thermo-spring system is thermodynamically sound. Note that for the entropy-based formulation the appearing temperatures are functions of the entropy via (4.33).

As was demonstrated in Section 2.1.3, the two thermo-spring system only has a symmetry respect to rotational orbits. Recall that the isolation of the system includes the fixed point so the linear momentum (a symmetry respect to translational orbits) is breached.

Then, the preserved momentum map is identified with the classical angular momentum. To reveal it within the GENERIC formalism, consider the action of the rotation group $G = \text{SO}(3) = \{\mathbf{G}: \mathbb{R}^3 \mapsto \mathbb{R}^3 | \mathbf{G}^T \mathbf{G} = \mathbf{1}, \det(\mathbf{G}) = 1\}$ on $\mathcal{S}$, $\Phi: G \times \mathcal{S} \mapsto \mathcal{S}$ defined by

$$\Phi_{\mathbf{G}} = \Phi(\mathbf{G}, \mathbf{z}) = (\mathbf{G}\mathbf{q}_1, \mathbf{G}\mathbf{q}_2, \mathbf{G}\mathbf{p}_1, \mathbf{G}\mathbf{p}_2, s_1, s_2) \quad \text{with } \mathbf{G} \in \text{SO}(3), \quad (4.44)$$

where s_i is either entropies η_i or temperatures θ_i .

First, it is easily proved that this action preserves the total energy of the system by noting that

$$\begin{aligned} \|\mathbf{G}\mathbf{q}_1\| &= \sqrt{\mathbf{q}_1^T \mathbf{G}^T \mathbf{G} \mathbf{q}_1} = \sqrt{\mathbf{q}_1^T \mathbf{q}_1} = \|\mathbf{q}_1\| \\ \|\mathbf{G}(\mathbf{q}_2 - \mathbf{q}_1)\| &= \sqrt{(\mathbf{q}_2 - \mathbf{q}_1)^T \mathbf{G}^T \mathbf{G} (\mathbf{q}_2 - \mathbf{q}_1)} = \|\mathbf{q}_2 - \mathbf{q}_1\| \\ \|\mathbf{G}\mathbf{p}_a\| &= \sqrt{\mathbf{p}_a^T \mathbf{G}^T \mathbf{G} \mathbf{p}_a} = \sqrt{\mathbf{p}_a^T \mathbf{p}_a} = \|\mathbf{p}_a\| \quad \text{with } a = 1, 2, \end{aligned} \quad (4.45)$$

so that the action Φ on it gives

$$\begin{aligned} E \circ \Phi_{\mathbf{G}} &= K(\|\mathbf{G}\mathbf{p}_1\|, \|\mathbf{G}\mathbf{p}_2\|) + e_1(\lambda_1(\mathbf{G}\mathbf{q}_1), s_1) + e_2(\lambda_2(\mathbf{G}\mathbf{q}_2, \mathbf{G}\mathbf{q}_1), s_2) \\ &= K(\|\mathbf{G}\mathbf{p}_1\|, \|\mathbf{G}\mathbf{p}_2\|) + e_1(\|\mathbf{G}\mathbf{q}_1\|, s_1) + e_2(\|\mathbf{G}(\mathbf{q}_2 - \mathbf{q}_1)\|, s_2) \\ &= E(\mathbf{z}), \end{aligned} \quad (4.46)$$

where use has been made of the relations (2.2).

Similarly, the preservation of the reversible and irreversible operators (4.20) when applied this action can be demonstrated using the same arguments as above, the full details can be found in Romero (2013).

On the other hand, the infinitesimal generator of actions (4.19) results, for any $\xi \in G$, in

$$\xi_{\mathcal{S}}(z) = \left. \frac{d}{d\epsilon} \right|_{\epsilon=0} \Phi^{\xi}(\epsilon, z) = (\xi \wedge q_1, \xi \wedge q_2, \xi \wedge p_1, \xi \wedge p_2, 0, 0)^T \quad (4.47)$$

Given that, the angular momentum defined by $(2.29)_2$ is a momentum map associated with the action Φ_G if the scalar function $J_{\xi} : \mathcal{S} \mapsto \mathbb{R}$, provided by

$$J_{\xi}(z) = \xi \cdot J = \xi \cdot \sum_{a=1}^2 q_a \wedge p_a, \quad (4.48)$$

satisfies the relations (4.23). Hence, the proof must be done separately for each of the formulations employed. The first step, however, is to compute the gradient of the scalar function which gives

$$DJ_{\xi} = (p_1 \wedge \xi, p_2 \wedge \xi, \xi \wedge q_1, \xi \wedge q_2, 0, 0)^T \quad (4.49)$$

Thus, the entropy-based GENERIC form is readily proved by

$$\mathbf{L}DJ_{\xi} = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ 0^T & 0^T & 0^T & 0^T & 0 & 0 \\ 0^T & 0^T & 0^T & 0^T & 0 & 0 \end{pmatrix} \begin{pmatrix} p_1 \wedge \xi \\ p_2 \wedge \xi \\ \xi \wedge q_1 \\ \xi \wedge q_2 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} \xi \wedge q_1 \\ \xi \wedge q_2 \\ -p_1 \wedge \xi \\ -p_2 \wedge \xi \\ 0 \\ 0 \end{pmatrix}, \quad (4.50)$$

which coincides with $\xi_{\mathcal{S}}$ provided by (4.47). Furthermore, the second requisite is also fulfilled as proves the following

$$\mathbf{M}DJ_{\xi} = k \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0^T & 0^T & 0^T & 0^T & \frac{\theta_2}{\theta_1} & -1 \\ 0^T & 0^T & 0^T & 0^T & -1 & \frac{\theta_1}{\theta_2} \end{pmatrix} \begin{pmatrix} p_1 \wedge \xi \\ p_2 \wedge \xi \\ \xi \wedge q_1 \\ \xi \wedge q_2 \\ 0 \\ 0 \end{pmatrix} = 0 \quad (4.51)$$

All this is the proof for the angular momentum (2.29) to be a first integral of the two thermo-spring system formulated in terms of entropy.

On the other hand, for the temperature-based GENERIC matrices, the following is obtained

$$\begin{aligned}
 \mathbf{L}D J_\xi &= \begin{pmatrix} 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 & \mathbf{L}_{11} & \mathbf{L}_{12} \\ 0 & -1 & 0 & 0 & 0 & \mathbf{L}_{22} \\ \mathbf{0}^T & \mathbf{0}^T & \bar{\mathbf{L}}_{11} & \mathbf{0}^T & 0 & 0 \\ \mathbf{0}^T & \mathbf{0}^T & \bar{\mathbf{L}}_{21} & \bar{\mathbf{L}}_{22} & 0 & 0 \end{pmatrix} \begin{pmatrix} \mathbf{p}_1 \wedge \xi \\ \mathbf{p}_2 \wedge \xi \\ \xi \wedge \mathbf{q}_1 \\ \xi \wedge \mathbf{q}_2 \\ 0 \\ 0 \end{pmatrix} \\
 &= \begin{pmatrix} \xi \wedge \mathbf{q}_1 \\ \xi \wedge \mathbf{q}_2 \\ -\mathbf{p}_1 \wedge \xi \\ -\mathbf{p}_2 \wedge \xi \\ \bar{\mathbf{L}}_{11} \cdot (\xi \wedge \mathbf{q}_1) \\ \bar{\mathbf{L}}_{21} \cdot (\xi \wedge \mathbf{q}_1) + \bar{\mathbf{L}}_{22} \cdot (\xi \wedge \mathbf{q}_2) \end{pmatrix} = \begin{pmatrix} \xi \wedge \mathbf{q}_1 \\ \xi \wedge \mathbf{q}_2 \\ -\mathbf{p}_1 \wedge \xi \\ -\mathbf{p}_2 \wedge \xi \\ 0 \\ 0 \end{pmatrix} \quad (4.52)
 \end{aligned}$$

The two last components of the resulting vector can be demonstrated to be zero by elaborating the terms $\bar{\mathbf{L}}_{ab}$ according to (4.38) together with properties of the cross product³. Lastly, the second requirement is trivially satisfied as follows

$$\mathbf{M}D J_\xi = k\theta_1\theta_2 \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & M_{11} & M_{12} \\ \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & M_{21} & M_{22} \end{pmatrix} \begin{pmatrix} \mathbf{p}_1 \wedge \xi \\ \mathbf{p}_2 \wedge \xi \\ \xi \wedge \mathbf{q}_1 \\ \xi \wedge \mathbf{q}_2 \\ 0 \\ 0 \end{pmatrix} = \mathbf{0}, \quad (4.53)$$

concluding that the angular momentum (2.29) is a preserved quantity of the two thermospring system formulated in terms of temperatures.

4.4 GENERIC form of the thermo-visco-elastic system

The thermo-visco-elastic system introduced in Section 2.2 is also a dissipative system in the sense of (4.9). Then, it can be described within

³ $\mathbf{a} \cdot (\mathbf{b} \wedge \mathbf{a}) = 0, \mathbf{a} \cdot (\mathbf{b} \wedge \mathbf{c}) = \mathbf{b} \cdot (\mathbf{c} \wedge \mathbf{a}) = \mathbf{c} \cdot (\mathbf{a} \wedge \mathbf{b})$

the GENERIC formalism for both choices of the thermodynamical variable: entropy or temperature. Although García Orden & Romero (2011) dealt with the formulation of the thermo-visco-elastic system using entropies, its GENERIC form has never been advocated. In the following subsections both entropy-based and temperature-based GENERIC forms are elaborated, thus fulfilling this gap.

4.4.1 Entropy-based GENERIC formulation

The entropy-based GENERIC form relies on a state space composed by a phase space $\mathcal{P} = \mathbb{R}^{2d} \times \mathbb{R}^{2d}$, a space $\mathcal{D} = \mathbb{R}$ and a space $\mathcal{T} = \mathbb{R}^2$ to altogether be

$$\mathcal{S} = \{ \mathbf{z} = (\mathbf{q}_1, \mathbf{q}_2, \mathbf{p}_1, \mathbf{p}_2, \gamma, \eta, \sigma) \in \mathbb{R}^{2d} \times \mathbb{R}^{2d} \times \mathbb{R} \times \mathbb{R}^2, \mathbf{q}_2 \neq \mathbf{q}_1 \} \quad (4.54)$$

This choice needs the internal energy of the element and of the environment to be redefined in terms of their entropies. As has already been pointed out, this step may not be feasible for particular thermodynamic models, being an important technical constraint for the formulation. Then, assuming that the constitutive models employed for both the element and the environment enable their internal energies to be functions of their respective entropies, the total energy of the system is provided by

$$E(\mathbf{z}) = K(\|\mathbf{p}_1\|, \|\mathbf{p}_2\|) + e(\lambda, \eta, \gamma) + \epsilon(\sigma), \quad (4.55)$$

where K is the kinetic energy provided by (2.33).

For its part, the total entropy of the system is just the sum of two state variables

$$S(\mathbf{z}) = \eta + \sigma \quad (4.56)$$

This simplicity is responsible for the simple form that acquires the Poisson matrix, which in essence becomes the classical symplectic matrix, i.e its *canonical* form (4.14), that is

$$\mathbf{L}(\mathbf{z}) = \left(\begin{array}{cccc|ccc} \mathbf{0} & \mathbf{0} & \mathbf{1} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{1} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ -\mathbf{1} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & -\mathbf{1} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \hline \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & 0 & 0 & 0 \\ \hline \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & 0 & 0 & 0 \\ \hline \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & 0 & 0 & 0 \end{array} \right) \quad (4.57)$$

Nevertheless, the Dissipative matrix requires to be carefully obtained to account for the both dissipative phenomena present in the system: heat conduction and internal viscous dissipation. Either by using the ideas of Mielke (2011), summarized at the beginning of this Section, or by bearing in mind the evolution equations (2.54) the Dissipative matrix can be demonstrated to be

$$\mathbf{M}(\mathbf{z}) = \begin{pmatrix} \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & \frac{1}{\nu} \frac{\partial e}{\partial \eta} & -\frac{1}{\nu} \frac{\partial e}{\partial \gamma} & 0 \\ \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & -\frac{1}{\nu} \frac{\partial e}{\partial \gamma} & \left(\frac{\partial e}{\partial \eta} \right)^{-1} \left[\frac{1}{\nu} \left(\frac{\partial e}{\partial \gamma} \right)^2 + k \frac{\partial \epsilon}{\partial \sigma} \right] & -k \\ \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & 0 & -k & k \left(\frac{\partial \epsilon}{\partial \sigma} \right)^{-1} \frac{\partial e}{\partial \eta} \end{pmatrix} \quad (4.58)$$

In agreement with these matrices, the resulting evolutions equations derived from the use of (4.9) are those provided by (2.54) with the exception of the external forces and taking into account that in this case the temperatures are provided by

$$\theta(\lambda, \eta, \gamma) = \frac{\partial e(\lambda, \eta, \gamma)}{\partial \eta}, \quad \vartheta(\sigma) = \frac{d\epsilon(\sigma)}{d\sigma} \quad (4.59)$$

4.4.2 Temperature-based GENERIC formulation

For the temperature choice, the state vector is defined in a state space of the form

$$\mathcal{S} = \{ \mathbf{z} = (\mathbf{q}_1, \mathbf{q}_2, \mathbf{p}_1, \mathbf{p}_2, \gamma, \theta, \vartheta) \in \mathbb{R}^{2d} \times \mathbb{R}^{2d} \times \mathbb{R} \times \mathbb{R}_+^2, \mathbf{q}_2 \neq \mathbf{q}_1 \} \quad (4.60)$$

Given this state space, the total energy of the system is provided by

$$E(\mathbf{z}) = K(\|\mathbf{p}_1\|, \|\mathbf{p}_2\|) + e(\lambda, \theta, \gamma) + \epsilon(\vartheta), \quad (4.61)$$

The total entropy is the sum of both the element and the environment entropies which can be expressed in terms of the above state vector as

$$S(\mathbf{z}) = \eta(\lambda, \gamma, \theta) + \sigma(\vartheta) = -\frac{\partial \Psi(\lambda, \gamma, \theta)}{\partial \theta} + \sigma(\vartheta) \quad (4.62)$$

Recalling that the elongation λ depends on the state vector via relation (2.38), the energy and entropy gradients results in

$$DE = \begin{pmatrix} \frac{\partial e}{\partial \lambda} \frac{\partial \lambda}{\partial \mathbf{q}_1} \\ \frac{\partial e}{\partial \lambda} \frac{\partial \lambda}{\partial \mathbf{q}_2} \\ \frac{\mathbf{p}_1}{m_1} \\ \frac{\mathbf{p}_2}{m_2} \\ \frac{\partial e}{\partial \gamma} \\ \frac{\partial e}{\partial \theta} \\ \frac{d\epsilon}{d\vartheta} \end{pmatrix}, \quad DS = \begin{pmatrix} \frac{\partial \eta}{\partial \lambda} \frac{\partial \lambda}{\partial \mathbf{q}_1} \\ \frac{\partial \eta}{\partial \lambda} \frac{\partial \lambda}{\partial \mathbf{q}_2} \\ \mathbf{0} \\ \mathbf{0} \\ \frac{\partial \eta}{\partial \gamma} \\ \frac{\partial \eta}{\partial \theta} \\ \frac{d\sigma}{d\vartheta} \end{pmatrix} \quad (4.63)$$

A brief inspection of them reveals that they contain every term involved in the evolution equations written in the form (2.45). Therefore, the Poisson and Dissipative matrices must be built such that they comply with their respective requirements and yield the correct set of the system evolution equations. Accordingly, the Poisson matrix is found to be

$$\mathbf{L}(\mathbf{z}) = \left(\begin{array}{cccc|c|cc} \mathbf{0} & \mathbf{0} & \mathbf{1} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{1} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ -\mathbf{1} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{L}_1 & \mathbf{0} \\ \mathbf{0} & -\mathbf{1} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{L}_2 & \mathbf{0} \\ \hline \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & 0 & 0 & 0 \\ \hline \mathbf{0}^T & \mathbf{0}^T & \bar{\mathbf{L}}_1 & \bar{\mathbf{L}}_2 & 0 & 0 & 0 \\ \hline \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & 0 & 0 & 0 \end{array} \right), \quad (4.64)$$

with

$$\mathbf{L}_a = -\bar{\mathbf{L}}_a^T = \left(\frac{\partial \eta}{\partial \theta} \right)^{-1} \frac{\partial \eta}{\partial \lambda} \frac{\partial \lambda}{\partial \mathbf{q}_a} \quad (4.65)$$

As expected, it comprises the symplectic Hamiltonian matrix plus terms derived from the thermo-mechanical coupling, i.e the heat generated when changing the elongation of the device.

Likewise, the Dissipative matrix has the following structure

$$\mathbf{M}(\mathbf{z}) = \theta \begin{pmatrix} \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & M_{11} & M_{12} & 0 \\ \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & M_{12} & M_{22} + M'_{11} & M'_{12} \\ \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & 0 & M'_{12} & M'_{22} \end{pmatrix}, \quad (4.66)$$

in which the appearing scalars are provided by

$$M_{ab} = (-1)^{a+b} \frac{1}{\nu} \left(\frac{\partial e}{\partial \gamma} \right)^{a(b-1)} \left(\frac{\partial e}{\partial \theta} \right)^{-a(b-1)}, \quad (4.67)$$

and

$$M'_{ab} = (-1)^{a+b} k \vartheta \left(\frac{\partial e}{\partial \theta} \right)^{a(b-1)-2} \left(\frac{d\epsilon}{d\vartheta} \right)^{-a(b-1)} \quad (4.68)$$

Each of them accounts for the two dissipative mechanisms involved in the system evolution, i.e the viscous flow taking place in the dashpot and the heat transfer, respectively.

Remark 4.4. The element temperature can be factorized out of the matrix which means that the structural properties stated over the Dissipative matrix hold for any value it may take. This issue will have consequences in the formulation of Energy-Entropy-Momentum methods.

Then, using (4.63) - (4.68) in (4.9) the system evolution equations are

obtained with the following format

$$\begin{aligned}
\dot{\mathbf{q}}_a &= \frac{\mathbf{p}_a}{m_a} \\
\dot{\mathbf{p}}_a &= - \left(\frac{\partial e}{\partial \lambda} - \theta \frac{\partial \eta}{\partial \lambda} \right) \frac{\partial \lambda}{\partial \mathbf{q}_a} \\
\dot{\gamma} &= - \frac{1}{\nu} \left(\frac{\partial e}{\partial \gamma} - \theta \frac{\partial \eta}{\partial \gamma} \right) \\
\dot{\theta} &= \left(\frac{\partial e}{\partial \theta} \right)^{-1} \left[-\theta \sum_{a=1}^2 \frac{\partial \eta}{\partial \lambda} \frac{\partial \lambda}{\partial \mathbf{q}_a} \cdot \frac{\mathbf{p}_a}{m_a} + \frac{1}{\nu} \left(\frac{\partial e}{\partial \gamma} - \theta \frac{\partial \eta}{\partial \gamma} \right) \frac{\partial e}{\partial \gamma} - h \right] \\
\dot{\vartheta} &= \left(\frac{d\epsilon}{d\vartheta} \right)^{-1} h,
\end{aligned} \tag{4.69}$$

which are the same as those obtained in Chapter 2 provided by (2.45) after using the relation between the free energy and the internal energy provided by the Legendre transform (2.7) along with its direct consequence (2.9), except for the external forces applied in the point masses.

4.4.3 Laws of thermodynamics and symmetries

For both choices, the change of total energy is trivially demonstrated to be zero

$$\dot{E}(\mathbf{z}) = DE \cdot \dot{\mathbf{z}} = DE \cdot \mathbf{L}DE + DS \cdot \mathbf{M}DE = 0 \tag{4.70}$$

The change of the total entropy, on the other hand, needs separate elaboration. Thus, the entropy formulation yields

$$\begin{aligned}
\dot{S}(\mathbf{z}) &= DS \cdot \dot{\mathbf{z}} = -DE \cdot \mathbf{L}DS + DS \cdot \mathbf{M}DS \\
&= \frac{1}{\nu\theta} \left(\frac{\partial e}{\partial \gamma} \right)^2 + k \frac{(\theta - \vartheta)^2}{\theta\vartheta} \geq 0,
\end{aligned} \tag{4.71}$$

whereas the temperature-based one gives

$$\begin{aligned}
\dot{S}(\mathbf{z}) &= DS \cdot \dot{\mathbf{z}} = -DE \cdot \mathbf{L}DS + DS \cdot \mathbf{M}DS \\
&= \frac{1}{\theta\nu} \left(\theta \frac{\partial \eta}{\partial \gamma} - \frac{\partial e}{\partial \gamma} \right)^2 + k \frac{(\theta - \vartheta)^2}{\theta\vartheta} \\
&= \frac{1}{\theta\nu} \left(-\frac{\partial \Psi}{\partial \gamma} \right)^2 + k \frac{(\theta - \vartheta)^2}{\theta\vartheta} \geq 0
\end{aligned} \tag{4.72}$$

The difference between both results comes from the different definitions that adopt the viscous force g in each formulation $(2.55)_2$ or $(2.46)_2$

Regarding the symmetries of the system, in Section 2.2.3 two preserved quantities other than energy were identified to be the linear and the angular momentum. The same can be concluded within the GENERIC formalism. For instance, the linear momentum is associated with the action of the additive group $G = \mathbb{R}^d$ on $\mathcal{S}$, $\Phi: G \times \mathcal{S} \mapsto \mathcal{S}$ defined by

$$\Phi_{\mathbf{a}} = \Phi(\mathbf{a}, \mathbf{z}) = (\mathbf{q}_1 + \mathbf{a}, \mathbf{q}_2 + \mathbf{a}, \mathbf{p}_1, \mathbf{p}_2, \gamma, s_1, s_2) \quad \text{with } \mathbf{a} \in \mathbb{R}^d, \quad (4.73)$$

where s_i is either entropies η_i or temperatures θ_i .

This action preserves the total energy of the system as proved the following

$$\begin{aligned} E \circ \Phi_{\mathbf{a}} &= K(\|\mathbf{p}_1\|, \|\mathbf{p}_2\|) + e(\lambda(\mathbf{q}_2 + \mathbf{a}, \mathbf{q}_1 + \mathbf{a}), \gamma, s_1) + \epsilon(s_2) \\ &= K(\|\mathbf{p}_1\|, \|\mathbf{p}_2\|) + e(\|\mathbf{q}_2 + \mathbf{a} - \mathbf{q}_1 - \mathbf{a}\|, \gamma, s_1) + \epsilon(s_2) \\ &= E(\mathbf{z}), \end{aligned} \quad (4.74)$$

Also, this action preserves the reversible and irreversible operators (4.20). To prove it, first the gradient of the action is computed to give

$$D\Phi_{\mathbf{a}} = (\mathbf{1}, \mathbf{1}, \mathbf{1}, \mathbf{1}, 1, 1, 1)^T \quad (4.75)$$

For this gradient, it is trivial to show that the products $D\Phi_{\mathbf{a}}(\mathbf{z}) \cdot \mathbf{L} \cdot D\Phi_{\mathbf{a}}(\mathbf{z})^T$ or $D\Phi_{\mathbf{a}}(\mathbf{z}) \cdot \mathbf{M} \cdot D\Phi_{\mathbf{a}}(\mathbf{z})^T$ results in the matrices $\mathbf{L}, \mathbf{M}$ themselves. On the other hand, the action composition operation on them yields the same results as their components depend on the action-perturbed state variables, i.e the positions coordinates, via the norm of the relative vector so the same as shown in (4.74) applies.

Moreover, the infinitesimal generator of actions (4.19) for any $\boldsymbol{\xi} \in \mathfrak{g}$ yields

$$\boldsymbol{\xi}_{\mathcal{S}}(\mathbf{z}) = \left. \frac{d}{d\epsilon} \right|_{\epsilon=0} \Phi_{\mathbf{a}}^{\boldsymbol{\xi}}(\epsilon, \mathbf{z}) = (\boldsymbol{\xi}, \boldsymbol{\xi}, \mathbf{0}, \mathbf{0}, 0, 0, 0)^T \quad (4.76)$$

To prove that the linear momentum $(2.29)_1$ is a momentum map associated with the action $\Phi_{\mathbf{a}}$, consider the scalar function $J_{\boldsymbol{\xi}}: \mathcal{S} \mapsto \mathbb{R}$, provided by

$$J_{\boldsymbol{\xi}}(\mathbf{z}) = \boldsymbol{\xi} \cdot \mathbf{L} = \boldsymbol{\xi} \cdot \sum_{a=1}^2 \mathbf{p}_a, \quad (4.77)$$

Then, it must comply with (4.23) for which the elaboration of the gradient of the scalar function is required, that is

$$DJ_\xi = (\mathbf{0}, \mathbf{0}, \boldsymbol{\xi}, \boldsymbol{\xi}, 0, 0, 0)^T \quad (4.78)$$

Thus, for the entropy-based GENERIC form it follows that

$$\mathbf{L}DJ_\xi = \begin{pmatrix} \mathbf{0} & \mathbf{0} & \mathbf{1} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{1} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ -\mathbf{1} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & -\mathbf{1} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & 0 & 0 & 0 \\ \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & 0 & 0 & 0 \\ \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \mathbf{0} \\ \mathbf{0} \\ \boldsymbol{\xi} \\ \boldsymbol{\xi} \\ 0 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} \boldsymbol{\xi} \\ \boldsymbol{\xi} \\ \mathbf{0} \\ \mathbf{0} \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad (4.79)$$

which coincides with $\boldsymbol{\xi}_{\mathcal{J}}$ provided by (4.76). Now, looking at the requisite for the Dissipative matrix the following is obtained

$$\mathbf{M}DJ_\xi = \begin{pmatrix} \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & \frac{1}{\nu} \frac{\partial e}{\partial \eta} & -\frac{1}{\nu} \frac{\partial e}{\partial \gamma} & 0 \\ \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & -\frac{1}{\nu} \frac{\partial e}{\partial \gamma} & \frac{1}{\theta \nu} \left(\frac{\partial e}{\partial \gamma} \right)^2 + k \frac{\vartheta}{\theta} & -k \\ \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & 0 & -k & k \frac{\theta}{\vartheta} \end{pmatrix} \begin{pmatrix} \mathbf{0} \\ \mathbf{0} \\ \boldsymbol{\xi} \\ \boldsymbol{\xi} \\ 0 \\ 0 \\ 0 \end{pmatrix} = \mathbf{0} \quad (4.80)$$

Finally, for the temperature-based GENERIC matrices, the following is obtained

$$\mathbf{L}DJ_\xi = \begin{pmatrix} \mathbf{0} & \mathbf{0} & \mathbf{1} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{1} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ -\mathbf{1} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{L}_1 & \mathbf{0} \\ \mathbf{0} & -\mathbf{1} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{L}_2 & \mathbf{0} \\ \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & 0 & 0 & 0 \\ \mathbf{0}^T & \mathbf{0}^T & \bar{\mathbf{L}}_1 & \bar{\mathbf{L}}_2 & 0 & 0 & 0 \\ \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \mathbf{0} \\ \mathbf{0} \\ \boldsymbol{\xi} \\ \boldsymbol{\xi} \\ 0 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} \boldsymbol{\xi} \\ \boldsymbol{\xi} \\ \mathbf{0} \\ \mathbf{0} \\ 0 \\ \bar{\mathbf{L}}_1 \cdot \boldsymbol{\xi} + \bar{\mathbf{L}}_2 \cdot \boldsymbol{\xi} \\ 0 \end{pmatrix} \quad (4.81)$$

The remaining term in the above vector vanishes due to the definition of terms $\bar{\mathbf{L}}_a$ which leads them to satisfy $\bar{\mathbf{L}}_1 = -\bar{\mathbf{L}}_2$. Lastly, in this case, the Dissipative term $\mathbf{M}D\mathbf{J}_\xi$ also yields zero due to the form of the scalar function gradient (4.78).

These results are the proof for the linear momentum (2.29)₁ to be a first integral of the thermo-visco-elastic system for the both formulations considered.

The thermo-visco-elastic system also has a symmetry associated with a rotation group. As with the two thermo-spring system, the corresponding momentum map is the angular momentum provided by (2.29). The proof closely follows the one done for the two thermo-spring system (4.44) - (4.53).

4.5 Infinite-dimensional dissipative systems

In this Section the GENERIC formalism is discussed for infinite-dimensional spaces so as to provide a unified definition for infinite-dimensional smooth dissipative systems. From a practical perspective, such systems are basically those defined in continua. Therefore, the resulting unified theory will enable the formulation of the nonlinear thermo-dissipative continuum dynamics discussed in Chapter 3. In order to make statements clear, the pure coupled finite strain thermoelastic case will be first studied and, then, the more general thermo-dissipative case will be addressed. Finally, the isothermal limit case, described in Section 3.6, will be also formulated within this unified framework under certain assumptions.

For the definition of infinite-dimensional dissipative systems, consider an infinite-dimensional domain identified with a reference configuration occupying an open subset $\mathcal{B}_0 \subset \mathbb{R}^d$. Then, the thermodynamic state of all the particles contained in $\mathcal{B}_0$ at a given instant is defined by smooth mappings $\mathbf{z}: \mathcal{B}_0 \times [0, T] \mapsto \mathbb{R}^k \times \text{Sym}(\mathbb{T}_d^2)^m$, furnishing the infinite-dimensional state space $\mathcal{S}$ assumed to be a subset of an infinite-dimensional vector space $\mathcal{X}$ with inner product $\langle \cdot, \cdot \rangle: \mathcal{X} \times \mathcal{X} \mapsto \mathbb{R}$ identified with its dual $\mathcal{X}^*$.

If $\mathbf{z}$ is a state in $\mathcal{S}$, then the set of tangent vectors at $\mathbf{z}$ furnishes the infinite-dimensional vector space called tangent space and denoted by $T_{\mathbf{z}}\mathcal{S}$. For subsequent developments, only linear manifolds are considered so each of the tangent spaces are identified with the same vector space, denoted as $\mathcal{X}_{\mathbf{z}}$, that is, $T_{\mathbf{z}}\mathcal{S} \cong \mathcal{X}_{\mathbf{z}}$, where $\mathcal{X}_{\mathbf{z}}$ is a subset of $\mathcal{X}$.

Then, given a tangent element $\mathbf{U} \in \mathcal{X}_{\mathbf{z}}$ and any functional $\mathcal{F}: \mathcal{S} \mapsto \mathbb{R}$,

the functional derivative at $\mathbf{z}$ is introduced as a mapping $\delta\mathcal{F}/\delta\mathbf{z}: \mathcal{S} \mapsto \mathcal{X}$ defined by

$$\left\langle \frac{\delta\mathcal{F}}{\delta\mathbf{z}}, \mathbf{U} \right\rangle = D\mathcal{F}(\mathbf{z}) \cdot \mathbf{u} + \sum_{\alpha=1}^m D\mathcal{F}(\mathbf{z}): \mathbf{U}^\alpha, \quad (4.82)$$

for all $\mathbf{U} = (\mathbf{u}, \mathbf{U}^\alpha) \in \mathbb{R}^k \times \text{Sym}(\mathbb{T}_d^2)^m$.

The gradient operator in the Euclidian space $\mathbb{R}^k$ and the gradient operator in the symmetric second-order tensor space $\text{Sym}(\mathbb{T}_d^2)^m$ are canonically defined⁴ via the directional derivative as follows

$$D\mathcal{F}(\mathbf{z}) \cdot \mathbf{u} = \left. \frac{d}{d\epsilon} \right|_{\epsilon=0} \mathcal{F}(\mathbf{v} + \epsilon\mathbf{u}, \mathbf{Z}^\alpha), \quad D\mathcal{F}(\mathbf{z}): \mathbf{U}^\alpha = \left. \frac{d}{d\epsilon} \right|_{\epsilon=0} \mathcal{F}(\mathbf{v}, \mathbf{Z}^\alpha + \epsilon\mathbf{U}^\alpha), \quad (4.83)$$

for all $\mathbf{z} = (\mathbf{v}, \mathbf{Z}^\alpha) \in \mathbb{R}^k \times \text{Sym}(\mathbb{T}_d^2)^m$.

All the functionals involved in the derivation of infinite-dimensional dissipative systems are based on scalar-valued density functions $f: \mathcal{S} \rightarrow \mathbb{R}$ integrated over the volume occupied by the continuum as follows

$$\mathcal{F}(\mathbf{z}) = \int_{\mathcal{B}_0} f(\mathbf{z}) dV_0 \quad (4.84)$$

The previous definition of the functional derivative applied to this type of functionals leads to the following identity

$$\begin{aligned} \left\langle \frac{\delta\mathcal{F}}{\delta\mathbf{z}}, \mathbf{U} \right\rangle &= \int_{\mathcal{B}_0} Df(\mathbf{z}) \cdot \mathbf{u} dV_0 + \sum_{\alpha=1}^m \int_{\mathcal{B}_0} Df(\mathbf{z}): \mathbf{U}^\alpha dV_0 \\ &= \langle Df(\mathbf{z}), \mathbf{U} \rangle_{\mathcal{B}_0}, \end{aligned} \quad (4.85)$$

which will often appear for the derivation of the evolution equations of infinite-dimensional dissipative systems.

Definition 4.5. The infinite-dimensional state space $\mathcal{S}$ defining dissipative systems consists of an infinite-dimensional phase space $\mathcal{P}$, defined by the set of smooth mappings $\boldsymbol{\varphi}, \mathbf{p}: \mathcal{B}_0 \mapsto \mathbb{R}^d \times \mathbb{R}^d$, an infinite-dimensional thermal space $\mathcal{T}$, defined by a smooth mapping $s: \mathcal{B}_0 \mapsto \mathbb{R}$ and an infinite-dimensional *dissipative* space $\mathcal{D}$, provided by the set of m internal variable smooth mappings $\boldsymbol{\Lambda}^\alpha: \mathcal{B}_0 \mapsto \text{Sym}(\mathbb{T}_d^2)$ with $\alpha = 1, \dots, m$, altogether collected in

$$\mathcal{S} = \{ \mathbf{z} = (\boldsymbol{\varphi}, \mathbf{p}, s, \boldsymbol{\Lambda}^1, \dots, \boldsymbol{\Lambda}^m) : \mathcal{B}_0 \times [0, T] \mapsto \mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R} \times \text{Sym}(\mathbb{T}_d^2)^m \} \quad (4.86)$$

⁴note that both gradients use the same notation in order to keep it simple.

Definition 4.6. A infinite-dimensional dissipative system is an isolated system ruled by the infinite-dimensional GENERIC evolution equations defined, for any functional $\mathcal{F}: \mathcal{S} \mapsto \mathbb{R}$, as

$$\dot{\mathcal{F}}(\mathbf{z}) = \{\mathcal{F}(\mathbf{z}), E(\mathbf{z})\} + [\mathcal{F}(\mathbf{z}), S(\mathbf{z})], \quad (4.87)$$

where $E: \mathcal{S} \mapsto \mathbb{R}$ is the total energy of the system, $S: \mathcal{S} \mapsto \mathbb{R}$ is the total entropy of the system, $\{\cdot, \cdot\}: \mathcal{S} \times \mathcal{S} \mapsto \mathbb{R}$ is the bilinear Poisson operator satisfying the skew-symmetry, Jacobi and Leibniz properties, as introduced in Section 4.1, and $[\cdot, \cdot]: \mathcal{S} \times \mathcal{S} \mapsto \mathbb{R}$ is the bilinear Dissipative (metric) operator being symmetric and positive-definite as also introduced in Section 4.1.

Proposition 4.3. *Any infinite-dimensional dissipative system provided by (4.87) agrees with the law of thermodynamics if the bilinear operators additionally satisfy the degeneracy or non-interaction conditions*

$$\{S(\mathbf{z}), \mathcal{F}(\mathbf{z})\} = [E(\mathbf{z}), \mathcal{F}(\mathbf{z})] = 0, \quad (4.88)$$

for every functional $\mathcal{F}: \mathcal{S} \rightarrow \mathbb{R}$.

Proof. The proof relies on the brackets properties along with the just introduced degeneracy conditions as was reasoned in Section 4.1 for general metriplectic structures to arrive at (4.7). $\square$

Furthermore, the Poisson and Dissipative brackets are associated to reversible and irreversible differential operators $\mathbf{L}, \mathbf{M}: \mathcal{S} \times \mathcal{X} \rightarrow \mathcal{X}$ as follows

$$\{\mathcal{F}, \mathcal{G}\} = \left\langle \frac{\delta \mathcal{F}}{\delta \mathbf{z}}, \mathbf{L} \left[\frac{\delta \mathcal{G}}{\delta \mathbf{z}} \right] \right\rangle, \quad [\mathcal{F}, \mathcal{G}] = \left\langle \frac{\delta \mathcal{F}}{\delta \mathbf{z}}, \mathbf{M} \left[\frac{\delta \mathcal{G}}{\delta \mathbf{z}} \right] \right\rangle \quad (4.89)$$

Analogously to the finite-dimensional case, essential physical considerations allow to conclude that the reversible (Poisson) operator cannot be generated by the dissipative space $\mathcal{D}$ while the irreversible (Dissipative) one can only depend on the thermal and dissipative spaces $\mathcal{T}$ and $\mathcal{D}$.

4.5.1 Infinite-dimensional smooth dissipative systems with symmetries

The notion of symmetries and momentum maps can be generalized for infinite-dimensional systems. Assuming the algebra of Lie Groups introduced in the previous Section, an action Φ on the state space $\mathcal{S}$ of a Lie group G

preserves the infinite-dimensional GENERIC structure if, for any two functionals $\mathcal{F}, \mathcal{G}: \mathcal{S} \mapsto \mathbb{R}$, it is satisfied that

$$\{\mathcal{F} \circ \Phi_g, \mathcal{G} \circ \Phi_g\} = \{\mathcal{F}, \mathcal{G}\} \circ \Phi_g \quad \text{and} \quad [\mathcal{F} \circ \Phi_g, \mathcal{G} \circ \Phi_g] = [\mathcal{F}, \mathcal{G}] \circ \Phi_g, \quad (4.90)$$

for any $g \in G$.

Definition 4.7. Let G be a Lie group on a state space with an associated action Φ that preserve the infinite-dimensional GENERIC structure. Then, if the total energy of an infinite-dimensional dissipative system is a G -invariant function, that is

$$E \circ \Phi_g = E \quad \forall g \in G, \quad (4.91)$$

the system is a infinite-dimensional dissipative with symmetries and has a momentum map associated with the action.

Definition 4.8. Given a Lie group G with associated algebra $\mathfrak{g}$ and dual $\mathfrak{g}^*$, a mapping $\mathbf{J}: \mathcal{S} \rightarrow \mathfrak{g}^*$ is a momentum map associated with the action Φ if, for any $\boldsymbol{\xi} \in \mathfrak{g}$, the scalar functional $J_{\boldsymbol{\xi}}: \mathcal{S} \rightarrow \mathbb{R}$ defined as

$$J_{\boldsymbol{\xi}}(\mathbf{z}) = \langle \mathbf{J}(\mathbf{z}), \boldsymbol{\xi} \rangle, \quad (4.92)$$

satisfies

$$\boldsymbol{\xi}_{\mathcal{S}} = \mathbf{L} \left[\frac{\delta J_{\boldsymbol{\xi}}}{\delta \mathbf{z}} \right], \quad \mathbf{0} = \mathbf{M} \left[\frac{\delta J_{\boldsymbol{\xi}}}{\delta \mathbf{z}} \right], \quad (4.93)$$

where $\boldsymbol{\xi}_{\mathcal{S}}$ is the infinitesimal generator of the action defined in (4.19).

Theorem 4.4. *The momentum map of a infinite-dimensional dissipative system with symmetries is a conserved quantity of the system evolution.*

Proof. The proof directly follows from the calculation of the rate of the scalar functional $J_{\boldsymbol{\xi}}$ using (4.87) along with the properties of the brackets and (4.93), altogether yielding

$$\dot{J}_{\boldsymbol{\xi}} = -\{E, J_{\boldsymbol{\xi}}\} = -\left\langle \frac{\delta E}{\delta \mathbf{z}}, \mathbf{L} \left[\frac{\delta J_{\boldsymbol{\xi}}}{\delta \mathbf{z}} \right] \right\rangle = -\left\langle \frac{\delta E}{\delta \mathbf{z}}, \boldsymbol{\xi}_{\mathcal{S}} \right\rangle \quad (4.94)$$

Finally, the term on the right hand side results from differentiating (4.91), considering (4.19), to give the identity

$$\left\langle \frac{\delta E}{\delta \mathbf{z}}, \boldsymbol{\xi}_{\mathcal{S}} \right\rangle = 0, \quad (4.95)$$

□

The above theorem corresponds with the Noether's theorem for infinite-dimensional dissipative system with symmetries in the sense of Def. 4.7.

4.6 GENERIC form of nonlinear thermoelasticity

The previous definition of infinite-dimensional dissipative system encompasses, for instance, the dynamics of isolated thermoelastic continua experiencing finite strains and thermal coupled with heat conduction. The complete description of such a system results from defining appropriated Poisson and Dissipative operators in terms of a given state variables with the format (5.18), among which different pure thermodynamical variables can be adopted, fundamentally either density entropy or temperature, although many others could be used. The choice of the entropy can be found in either Romero (2010a,b, 2013). In contrast, the choice of temperature has so far presented drawbacks and, therefore, it has not apparently been addressed until this work.

4.6.1 Entropy formulation

The description based on the density entropy relies on the following infinite-dimensional vector state space

$$\mathcal{S} = \{z = (\varphi, \mathbf{p}, \eta) : \mathcal{B}_0 \times [0, T] \mapsto \mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}, \det(\nabla_0 \varphi) > 0\}, \quad (4.96)$$

whose tangent space is

$$T\mathcal{S} = \{w = (w_\varphi, w_p, w_\eta) : \mathcal{B}_0 \mapsto \mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}\} \quad (4.97)$$

Accordingly, the total energy function and total entropy function are defined by (3.96) (with (3.55) and (3.54)) and (3.98). Taking into account that the material dissipative effects are neglected, that is the thermodynamic potentials are of the form (3.39)₂, and the above state vector (4.96), their particular expressions are

$$E(z) = \int_{\mathcal{B}_0} \left(\frac{1}{2\rho_0} \|\mathbf{p}\|^2 + e(\mathbf{C}, \eta) \right) dV_0, \quad S(z) = \int_{\mathcal{B}_0} \eta dV_0, \quad (4.98)$$

Then, the directional derivatives of these functionals can be calculated by (4.82) for any element on the tangent space (4.97) to give

$$\begin{aligned} \left\langle \frac{\delta E}{\delta \varphi}, w_\varphi \right\rangle &= \left\langle 2 \frac{\partial e}{\partial \mathbf{C}}, \nabla_0 \varphi^T \nabla_0 w_\varphi \right\rangle_{\mathcal{B}_0} & \left\langle \frac{\delta S}{\delta \varphi}, w_\varphi \right\rangle &= 0 \\ \left\langle \frac{\delta E}{\delta \mathbf{p}}, w_p \right\rangle &= \left\langle \frac{\mathbf{p}}{\rho_0}, w_p \right\rangle_{\mathcal{B}_0} & \left\langle \frac{\delta S}{\delta \mathbf{p}}, w_p \right\rangle &= 0 \\ \left\langle \frac{\delta E}{\delta \eta}, w_\eta \right\rangle &= \left\langle \frac{\partial e}{\partial \eta}, w_\eta \right\rangle_{\mathcal{B}_0} = \langle \Theta, w_\eta \rangle_{\mathcal{B}_0} & \left\langle \frac{\delta S}{\delta \eta}, w_\eta \right\rangle &= \langle 1, w_\eta \rangle_{\mathcal{B}_0}, \end{aligned} \quad (4.99)$$

where the first result can be explained by considering the following result on real-valued functions $f : \mathcal{S} \rightarrow \mathbb{R}$ that depend on the motion function φ via the right Cauchy-Green deformation tensor $\mathbf{C}(\varphi) := \nabla_0 \varphi^T \nabla_0 \varphi$, which results from nothing more than applying the chain rule of the directional derivative and using the symmetry of the said tensor to give

$$Df(\mathbf{C}(\varphi), \dots) \cdot \mathbf{u} = Df : (D\mathbf{C} \cdot \mathbf{u}) = 2 \frac{\partial f}{\partial \mathbf{C}} : \nabla_0 \varphi^T \nabla_0 \mathbf{u} \quad (4.100)$$

The resulting partial derivatives of the internal energy in (4.99) are identified to be the symmetric Piola-Kirchhoff stress tensor $\mathbf{S} : \mathcal{S} \mapsto \text{Sym}(\mathbb{T}_d^2)$ and the temperature field $\Theta : \mathcal{S} \mapsto \mathbb{R}_+$ provided by (3.36) and (3.37) (ignoring the dependency on internal variables), that is

$$\mathbf{S}(\mathbf{C}(\varphi), \eta) = 2 \frac{\partial e}{\partial \mathbf{C}}(\mathbf{C}(\varphi), \eta), \quad \Theta(\mathbf{C}(\varphi), \eta) = \frac{\partial e}{\partial \eta}(\mathbf{C}(\varphi), \eta) \quad (4.101)$$

Given that, it only remains to specify proper reversible and irreversible operators that generate the balance laws governing the thermoelastic continuum dynamics which are, following Chapter 3, the linear momentum and energy balances.

As with the finite-dimensional case (4.14), the use of the entropy as thermodynamical state variable leads the reversible operator to be provided by the canonical one of Hamiltonian mechanics, see Marsden & Ratiu (1999), which, for any two functionals $\mathcal{F}, \mathcal{G} : \mathcal{S} \rightarrow \mathbb{R}$, reads

$$\{\mathcal{F}, \mathcal{G}\} = \left\langle \frac{\delta \mathcal{F}}{\delta \varphi}, \frac{\delta \mathcal{G}}{\delta \mathbf{p}} \right\rangle - \left\langle \frac{\delta \mathcal{F}}{\delta \mathbf{p}}, \frac{\delta \mathcal{G}}{\delta \varphi} \right\rangle \quad (4.102)$$

For its part, the bilinear Dissipative operator is built to account for the conduction phenomenon (of dissipative nature), see Romero (2010a), for any two functionals $\mathcal{F}, \mathcal{G} : \mathcal{S} \rightarrow \mathbb{R}$, as follows

$$[\mathcal{F}, \mathcal{G}] = \left\langle \nabla_0 \left[\frac{1}{\Theta} \frac{\delta \mathcal{F}}{\delta \eta} \right], \Theta^2 \mathbf{K} \nabla_0 \left[\frac{1}{\Theta} \frac{\delta \mathcal{G}}{\delta \eta} \right] \right\rangle \quad (4.103)$$

In the above expression, $\mathbf{K}$ is the material conductivity tensor (3.27) which is symmetric and positive semidefinite, thus granting the bracket with these properties.

The above Poisson and Dissipative brackets comply with the required degeneracy conditions (4.88). The proofs easily follow from (4.99) to give

$$\begin{aligned}\{S, \mathcal{F}\} &= \left\langle \frac{\delta S}{\delta \boldsymbol{\varphi}}, \frac{\delta \mathcal{F}}{\delta \mathbf{p}} \right\rangle - \left\langle \frac{\delta S}{\delta \mathbf{p}}, \frac{\delta \mathcal{F}}{\delta \boldsymbol{\varphi}} \right\rangle = 0 \\ [E, \mathcal{F}] &= \left\langle \nabla_0 \left[\frac{1}{\Theta} \right], \Theta^2 \mathbf{K} \nabla_0 \left[\frac{1}{\Theta} \frac{\delta \mathcal{F}}{\delta \eta} \right] \right\rangle = 0\end{aligned}\tag{4.104}$$

In order to derive the evolution equations of the thermoelastic continuum dynamics, the time derivative of a functional $\mathcal{F}: \mathcal{S} \mapsto \mathbb{R}$ is calculated as follows

$$\dot{\mathcal{F}} = \left\langle \frac{\delta \mathcal{F}}{\delta \mathbf{z}}, \dot{\mathbf{z}} \right\rangle = \left\langle \frac{\delta \mathcal{F}}{\delta \boldsymbol{\varphi}}, \dot{\boldsymbol{\varphi}} \right\rangle + \left\langle \frac{\delta \mathcal{F}}{\delta \mathbf{p}}, \dot{\mathbf{p}} \right\rangle + \left\langle \frac{\delta \mathcal{F}}{\delta \eta}, \dot{\eta} \right\rangle\tag{4.105}$$

On the other hand, the reversible part generated by the Poisson bracket has the following expression

$$\{\mathcal{F}, E\} = -\{E, \mathcal{F}\} = -\left\langle \frac{\delta E}{\delta \boldsymbol{\varphi}}, \frac{\delta \mathcal{F}}{\delta \mathbf{p}} \right\rangle + \left\langle \frac{\delta E}{\delta \mathbf{p}}, \frac{\delta \mathcal{F}}{\delta \boldsymbol{\varphi}} \right\rangle\tag{4.106}$$

In the same way, the irreversible part is provided by

$$[\mathcal{F}, S] = \left\langle \nabla_0 \left[\frac{1}{\Theta} \frac{\delta \mathcal{F}}{\delta \eta} \right], \Theta^2 \mathbf{K} \nabla_0 \left[\frac{1}{\Theta} \frac{\delta S}{\delta \eta} \right] \right\rangle\tag{4.107}$$

Choosing the functional derivative to be a tangent vector $\langle \delta \mathcal{F} / \delta \mathbf{z}, \dot{\mathbf{z}} \rangle = \langle \mathbf{w}, \dot{\mathbf{z}} \rangle_{\mathcal{B}_0}$ and using the functional derivatives (4.99) along with (4.101), the weak statement of the balance laws read

$$\begin{aligned}\langle \mathbf{w}_{\boldsymbol{\varphi}}, \dot{\boldsymbol{\varphi}} \rangle_{\mathcal{B}_0} &= \langle \mathbf{w}_{\boldsymbol{\varphi}}, \frac{1}{\rho_0} \mathbf{p} \rangle_{\mathcal{B}_0} \\ \langle \mathbf{w}_{\mathbf{p}}, \dot{\mathbf{p}} \rangle_{\mathcal{B}_0} &= -\langle \nabla_0 \mathbf{w}_{\mathbf{p}}, \mathbf{F} \mathbf{S} \rangle_{\mathcal{B}_0} \\ \langle w_{\eta}, \dot{\eta} \rangle_{\mathcal{B}_0} &= -\langle \nabla_0 \left[\frac{w_{\eta}}{\Theta} \right], \mathbf{K} \nabla_0 \Theta \rangle_{\mathcal{B}_0} = \langle \nabla_0 \left[\frac{w_{\eta}}{\Theta} \right], \mathbf{H} \rangle_{\mathcal{B}_0}\end{aligned}\tag{4.108}$$

As expected, these equations only describe the isolated dynamics of a thermoelastic continuum as external contributions are intrinsically excluded in the GENERIC formalism. However, a posteriori consideration of them could be done to arrive at the weak statement provided by (3.146), considering $\dot{\mathcal{D}} = 0$, by attaching them to the above equations.

Accordingly, the total energy of the system is preserved which can be proved by choosing $\mathcal{F} = E$ in the GENERIC equations (4.105), (4.106) and (4.107) to give

$$\dot{E}(\mathbf{z}) = \{E, E\} + [E, S] = \langle \nabla_0 \left[\frac{1}{\Theta} \right], \Theta^2 \mathbf{K} \nabla_0 \left[\frac{1}{\Theta} \right] \rangle_{\mathcal{B}_0} = 0 \quad (4.109)$$

Similarly, the rate of the total entropy follows from taking $\mathcal{F} = S(\mathbf{z})$ to give

$$\begin{aligned} \dot{S}(\mathbf{z}) &= \{S, E\} + [S, S] = \langle \nabla_0 \left[\frac{1}{\Theta} \right], \Theta^2 \mathbf{K} \nabla_0 \left[\frac{1}{\Theta} \right] \rangle_{\mathcal{B}_0} \\ &= \langle \frac{1}{\Theta^2} \nabla_0 \Theta, \mathbf{K} \nabla_0 \Theta \rangle_{\mathcal{B}_0} \geq 0, \end{aligned} \quad (4.110)$$

which coincides with the first term of (3.101) due to the heat conduction phenomenon since is the only dissipative process involved in coupled thermoelastic solids.

4.6.2 Temperature formulation

Now, the temperature formulation of thermoelasticity is addressed within the GENERIC formalism. To this end, the state space of the thermoelastic continuum is defined to be the infinite dimensional set

$$\mathcal{S} = \{\mathbf{z} = (\boldsymbol{\varphi}, \mathbf{p}, \Theta) : \mathcal{B}_0 \times [0, T] \mapsto \mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}_+, \det(\nabla_0 \boldsymbol{\varphi}) > 0\}, \quad (4.111)$$

whose tangent space is

$$T\mathcal{S} = \{\mathbf{w} = (\mathbf{w}_\varphi, \mathbf{w}_p, w_\Theta) : \mathcal{B}_0 \times [0, T] \mapsto \mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}\} \quad (4.112)$$

To express the total energy and total entropy of the system in terms of this state space, the thermodynamic potentials in terms of temperature (3.39)₁ need to be used to obtain

$$E(\mathbf{z}) = \int_{\mathcal{B}_0} \left(\frac{1}{2\rho_0} \|\mathbf{p}\|^2 + e(\mathbf{C}, \Theta) \right) dV_0, \quad S(\mathbf{z}) = \int_{\mathcal{B}_0} \eta(\mathbf{C}, \Theta) dV_0 \quad (4.113)$$

Accordingly, the functional derivatives now are

$$\begin{aligned}
 \left\langle \frac{\delta E}{\delta \boldsymbol{\varphi}}, \mathbf{w}_{\boldsymbol{\varphi}} \right\rangle &= \left\langle 2 \frac{\partial e}{\partial \mathbf{C}}, \nabla_0 \boldsymbol{\varphi}^T \nabla_0 \mathbf{w}_{\boldsymbol{\varphi}} \right\rangle_{\mathcal{B}_0} & \left\langle \frac{\delta S}{\delta \boldsymbol{\varphi}}, \mathbf{w}_{\boldsymbol{\varphi}} \right\rangle &= \left\langle 2 \frac{\partial \eta}{\partial \mathbf{C}}, \nabla_0 \boldsymbol{\varphi}^T \nabla_0 \mathbf{w}_{\boldsymbol{\varphi}} \right\rangle_{\mathcal{B}_0} \\
 \left\langle \frac{\delta E}{\delta \mathbf{p}}, \mathbf{w}_{\mathbf{p}} \right\rangle &= \left\langle \frac{\mathbf{p}}{\rho_0}, \mathbf{w}_{\mathbf{p}} \right\rangle_{\mathcal{B}_0} & \left\langle \frac{\delta S}{\delta \mathbf{p}}, \mathbf{w}_{\mathbf{p}} \right\rangle &= 0 \\
 \left\langle \frac{\delta E}{\delta \Theta}, w_{\Theta} \right\rangle &= \left\langle \frac{\partial e}{\partial \Theta}, w_{\Theta} \right\rangle_{\mathcal{B}_0} & \left\langle \frac{\delta S}{\delta \Theta}, w_{\Theta} \right\rangle &= \left\langle \frac{\partial \eta}{\partial \Theta}, w_{\Theta} \right\rangle_{\mathcal{B}_0}
 \end{aligned} \tag{4.114}$$

Then, the appearing partial derivatives are linked with the symmetric Piola-Kirchhoff stress tensor $\mathbf{S}$, the latent heat tensor $\mathbf{V}$ and the specific heat capacity c by the constitutive laws (neglecting the internal variables) (3.18), (3.77) and (3.78) in the following manner

$$2 \frac{\partial e}{\partial \mathbf{C}} = \mathbf{S} + 2\Theta \frac{\partial \eta}{\partial \mathbf{C}}, \quad 2 \frac{\partial \eta}{\partial \mathbf{C}} = \frac{1}{\Theta} \mathbf{V}, \quad \frac{\partial e}{\partial \Theta} = \Theta \frac{\partial \eta}{\partial \Theta} = c \tag{4.115}$$

For this choice, the Poisson bracket needs to be extended to account for reversible mechanism of the thermo-deformation coupling, which for any two functionals $\mathcal{F}, \mathcal{G} : \mathcal{S} \rightarrow \mathbb{R}$ are

$$\begin{aligned}
 \{\mathcal{F}, \mathcal{G}\} &= \left\langle \frac{\delta \mathcal{F}}{\delta \boldsymbol{\varphi}}, \frac{\delta \mathcal{G}}{\delta \boldsymbol{\varphi}} \right\rangle - \left\langle \frac{\delta \mathcal{F}}{\delta \mathbf{p}}, \frac{\delta \mathcal{G}}{\delta \mathbf{p}} \right\rangle + \left\langle \nabla_0 \left[\frac{\delta \mathcal{F}}{\delta \mathbf{p}} \right], \mathbf{FV} \frac{1}{c} \frac{\delta \mathcal{G}}{\delta \Theta} \right\rangle \\
 &\quad - \left\langle \mathbf{FV} \frac{1}{c} \frac{\delta \mathcal{F}}{\delta \Theta}, \nabla_0 \left[\frac{\delta \mathcal{G}}{\delta \mathbf{p}} \right] \right\rangle
 \end{aligned} \tag{4.116}$$

The Dissipative bracket, however, is slightly modified due to the change of the thermal variable. Thus, for any two functionals $\mathcal{F}, \mathcal{G} : \mathcal{S} \rightarrow \mathbb{R}$, it is

$$[\mathcal{F}, \mathcal{G}] = \left\langle \nabla_0 \left[\frac{1}{c} \frac{\delta \mathcal{F}}{\delta \Theta} \right], \Theta^2 \mathbf{K} \nabla_0 \left[\frac{1}{c} \frac{\delta \mathcal{G}}{\delta \Theta} \right] \right\rangle \tag{4.117}$$

Again, the material conductivity tensor $\mathbf{K}$ is responsible for the Dissipative operator to be positive semidefinite.

The degeneracy conditions (4.88) are readily verified as follows

$$\begin{aligned}
 \{S, \mathcal{F}\} &= \left\langle \frac{1}{\Theta} \mathbf{FV}, \nabla_0 \left[\frac{\delta \mathcal{F}}{\delta \mathbf{p}} \right] \right\rangle - \left\langle \frac{1}{\Theta} \mathbf{FV}, \nabla_0 \left[\frac{\delta \mathcal{F}}{\delta \mathbf{p}} \right] \right\rangle = 0 \\
 [E, \mathcal{F}] &= \left\langle \nabla_0 \left[\frac{1}{c} \right], \Theta^2 \mathbf{K} \nabla_0 \left[\frac{1}{c} \frac{\delta \mathcal{F}}{\delta \Theta} \right] \right\rangle = 0
 \end{aligned} \tag{4.118}$$

Following the same arguments as before, the evolution equations provided by the GENERIC formalism for the isolated dynamics of a thermoelastic continuum described in terms of the temperature are

$$\begin{aligned}
\langle \mathbf{w}_\varphi, \dot{\varphi} \rangle_{\mathcal{B}_0} &= \langle \mathbf{w}_\varphi, \frac{1}{\rho_0} \mathbf{p} \rangle_{\mathcal{B}_0} \\
\langle \mathbf{w}_\mathbf{p}, \dot{\mathbf{p}} \rangle_{\mathcal{B}_0} &= -\langle \nabla_0 \mathbf{w}_\mathbf{p}, \mathbf{F} \left(2 \frac{\partial e}{\partial \mathbf{C}} - \mathbf{V} \right) \rangle_{\mathcal{B}_0} = -\langle \nabla_0 \mathbf{w}_\mathbf{p}, \mathbf{F} \mathbf{S} \rangle_{\mathcal{B}_0} \\
\langle w_\Theta, \dot{\Theta} \rangle_{\mathcal{B}_0} &= -\langle \frac{w_\Theta}{c} \mathbf{F} \mathbf{V}, \nabla_0 \left[\frac{\mathbf{p}}{\rho_0} \right] \rangle_{\mathcal{B}_0} - \langle \nabla_0 \left[\frac{w_\Theta}{c} \right], \mathbf{K} \nabla_0 \Theta \rangle_{\mathcal{B}_0},
\end{aligned} \tag{4.119}$$

which are the isolated version of the weak statement provided in (3.147).

Also, the laws of thermodynamics can easily be derived to prove the energy preservation and the entropy production. Thus, the rate of the total energy is elaborated by choosing $\mathcal{F} = E(\mathbf{z})$, provided by (4.113)₁, in the GENERIC equations (4.87) with the definition of the brackets provided by (4.116) and (4.117) to yield

$$\begin{aligned}
\dot{E}(\mathbf{z}) &= \{E(\mathbf{z}), E(\mathbf{z})\} + [E(\mathbf{z}), S(\mathbf{z})] \\
&= \langle 2\mathbf{F} \frac{\partial e}{\partial \mathbf{C}}, \nabla_0 \left[\frac{\mathbf{p}}{\rho_0} \right] \rangle_{\mathcal{B}_0} - \langle \nabla_0 \left[\frac{\mathbf{p}}{\rho_0} \right], 2\mathbf{F} \frac{\partial e}{\partial \mathbf{C}} \rangle_{\mathcal{B}_0} \\
&\quad - \langle \frac{1}{c} \mathbf{F} \mathbf{V}, \nabla_0 \left[\frac{\mathbf{p}}{\rho_0} \right] \rangle_{\mathcal{B}_0} + \langle \nabla_0 \left[\frac{\mathbf{p}}{\rho_0} \right], \mathbf{F} \mathbf{V} \frac{1}{c} \rangle_{\mathcal{B}_0} \\
&\quad + \langle \nabla_0 \left[\frac{1}{c} \right], \Theta^2 \mathbf{K} \nabla_0 \left[\frac{1}{c} \frac{c}{\Theta} \right] \rangle_{\mathcal{B}_0} = 0
\end{aligned} \tag{4.120}$$

Finally, the rate of the total entropy follows from choosing $\mathcal{F} = S(\mathbf{z})$, provided by (4.113)₂, to give

$$\begin{aligned}
\dot{S}(\mathbf{z}) &= \{S(\mathbf{z}), E(\mathbf{z})\} + [S(\mathbf{z}), S(\mathbf{z})] \\
&= \langle \frac{1}{\Theta} \mathbf{F} \mathbf{V}, \nabla_0 \left[\frac{\mathbf{p}}{\rho_0} \right] \rangle_{\mathcal{B}_0} - \langle \frac{1}{c} \frac{c}{\Theta} \mathbf{F} \mathbf{V}, \nabla_0 \left[\frac{\mathbf{p}}{\rho_0} \right] \rangle_{\mathcal{B}_0} \\
&\quad + \langle \nabla_0 \left[\frac{1}{c} \frac{c}{\Theta} \right], \Theta^2 \mathbf{K} \nabla_0 \left[\frac{1}{c} \frac{c}{\Theta} \right] \rangle_{\mathcal{B}_0} = \langle \frac{1}{\Theta^2} \nabla_0 \Theta, \mathbf{K} \nabla_0 \Theta \rangle_{\mathcal{B}_0} \geq 0,
\end{aligned} \tag{4.121}$$

with the temperature field, in this case, being a state variable rather than a function of the state variables as in (4.110).

4.7 GENERIC form of thermo-dissipative dynamics

Consider now the general case of the thermo-dissipative continuum dynamics introduced in Chapter 3. This general case complements the previously discussed thermoelastic case by including internal variables to describe any dissipative transformation taking place in the material interior. In the same way, the entropy and the temperature formulations are elaborated which, to the best of the author's knowledge, have so far not been addressed.

4.7.1 Entropy formulation

Focusing on the entropy-based description of the problem, the infinite-dimensional state space now incorporates m strain-like internal variables tensors to be

$$\mathcal{S} = \{\mathbf{z} = (\boldsymbol{\varphi}, \mathbf{p}, \eta, \boldsymbol{\Lambda}^\alpha) : \mathcal{B}_0 \mapsto \mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R} \times \text{Sym}(\mathbb{T}_d^2)^m, \det(\nabla_0 \boldsymbol{\varphi}) > 0\} \quad (4.122)$$

Accordingly, the tangent space becomes

$$T\mathcal{S} = \{\mathbf{w} = (\mathbf{w}_\varphi, \mathbf{w}_p, w_\eta, \mathbf{w}_{\Lambda^\alpha}) : \mathcal{B}_0 \mapsto \mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R} \times \text{Sym}(\mathbb{T}_d^2)^m\} \quad (4.123)$$

Given that, the total energy of the system in terms of state vector variables $\mathbf{z}$ is attained by using the thermodynamic potential (3.33) while the total entropy is provided by one of the state variables, that is

$$E(\mathbf{z}) = \int_{\mathcal{B}_0} \left(\frac{1}{2\rho_0} \|\mathbf{p}\|^2 + e(\mathbf{C}, \eta, \boldsymbol{\Lambda}^\alpha) \right) dV_0, \quad S(\mathbf{z}) = \int_{\mathcal{B}_0} \eta dV_0 \quad (4.124)$$

As a result of the above definitions, the functional derivatives now read

$$\begin{aligned} \left\langle \frac{\delta E}{\delta \boldsymbol{\varphi}}, \mathbf{w}_\varphi \right\rangle &= \left\langle 2 \frac{\partial e}{\partial \mathbf{C}}, \nabla_0 \boldsymbol{\varphi}^T \nabla_0 \mathbf{w}_\varphi \right\rangle_{\mathcal{B}_0} & \left\langle \frac{\delta S}{\delta \boldsymbol{\varphi}}, \mathbf{w}_\varphi \right\rangle &= 0 \\ \left\langle \frac{\delta E}{\delta \mathbf{p}}, \mathbf{w}_p \right\rangle &= \left\langle \frac{\mathbf{p}}{\rho_0}, \mathbf{w}_p \right\rangle_{\mathcal{B}_0} & \left\langle \frac{\delta S}{\delta \mathbf{p}}, \mathbf{w}_p \right\rangle &= 0 \\ \left\langle \frac{\delta E}{\delta \eta}, w_\eta \right\rangle &= \left\langle \frac{\partial e}{\partial \eta}, w_\eta \right\rangle_{\mathcal{B}_0} & \left\langle \frac{\delta S}{\delta \eta}, w_\eta \right\rangle &= \langle 1, w_\eta \rangle_{\mathcal{B}_0} \\ \left\langle \frac{\delta E}{\delta \boldsymbol{\Lambda}^\alpha}, \mathbf{w}_{\Lambda^\alpha} \right\rangle &= \left\langle \frac{\partial e}{\partial \boldsymbol{\Lambda}^\alpha}, \mathbf{w}_{\Lambda^\alpha} \right\rangle_{\mathcal{B}_0} & \left\langle \frac{\delta S}{\delta \boldsymbol{\Lambda}^\alpha}, \mathbf{w}_{\Lambda^\alpha} \right\rangle &= 0 \end{aligned} \quad (4.125)$$

From this result, the constitutive laws (3.36), (3.37) and (3.38) are identified with

$$\mathbf{S} = 2 \frac{\partial e}{\partial \mathbf{C}}, \quad \mathbf{Q}^\alpha = - \frac{\partial e}{\partial \mathbf{\Lambda}^\alpha}, \quad \Theta = \frac{\partial e}{\partial \eta} \quad (4.126)$$

The GENERIC form of general thermo-dissipative continuum dynamics based on the entropy as a state variable is provided by the canonical Poisson bracket (4.102), related to the election of the entropy, and by the Dissipative bracket which, in addition to the conduction phenomenon, also involves the dissipation due to the presence of irreversible transformations in the continuum. For any two functionals $\mathcal{F}, \mathcal{G}: \mathcal{S} \rightarrow \mathbb{R}$, they are

$$\begin{aligned} \{\mathcal{F}, \mathcal{G}\} &= \left\langle \frac{\delta \mathcal{F}}{\delta \boldsymbol{\varphi}}, \frac{\delta \mathcal{G}}{\delta \mathbf{p}} \right\rangle - \left\langle \frac{\delta \mathcal{F}}{\delta \mathbf{p}}, \frac{\delta \mathcal{G}}{\delta \boldsymbol{\varphi}} \right\rangle \\ [\mathcal{F}, \mathcal{G}] &= \left\langle \nabla_0 \left[\frac{1}{\Theta} \frac{\delta \mathcal{F}}{\delta \eta} \right], \Theta^2 \mathbf{K} \nabla_0 \left[\frac{1}{\Theta} \frac{\delta \mathcal{G}}{\delta \eta} \right] \right\rangle + \left\langle \frac{1}{\Theta} \frac{\delta \mathcal{F}}{\delta \eta}, \dot{\mathcal{D}} \frac{\delta \mathcal{G}}{\delta \eta} \right\rangle \\ &\quad + \sum_{\alpha=1}^m \left\langle \frac{\delta \mathcal{F}}{\delta \mathbf{\Lambda}^\alpha}, \mathcal{K}(\mathbf{Q}^\alpha) \frac{\delta \mathcal{G}}{\delta \eta} \right\rangle, \end{aligned} \quad (4.127)$$

where $\mathbf{K}$ is the material conductivity tensor (3.27), $\mathcal{K}$ is the positive semidefinite dissipation functional and $\dot{\mathcal{D}}$ is the dissipation provided by (3.34), also defined to be positive for thermodynamical soundness. As all of these quantities are positive semidefinite, the Dissipative bracket itself will also be positive semidefinite.

Remark 4.5. The last term in the Dissipative bracket breaks the symmetry of the operator. However, this fact does not seem to be crucial for it to provide the thermodynamically consistent evolution equations.

Regarding the degeneracy conditions, the one falling on the Poisson bracket was proved in (4.104)₁ whereas, using (4.125), the degeneracy condition for the Dissipative bracket (4.11)₂ yields

$$\begin{aligned} [E, \mathcal{F}] &= \left\langle \nabla_0 \left[\frac{1}{\Theta} \Theta \right], \Theta^2 \mathbf{K} \nabla_0 \left[\frac{1}{\Theta} \frac{\delta \mathcal{F}}{\delta \eta} \right] \right\rangle \\ &\quad + \left\langle \frac{1}{\Theta} \Theta, \dot{\mathcal{D}} \frac{\delta \mathcal{F}}{\delta \eta} \right\rangle + \sum_{\alpha=1}^m \left\langle -\mathbf{Q}^\alpha, \mathcal{K}(\mathbf{Q}^\alpha) \frac{\delta \mathcal{F}}{\delta \eta} \right\rangle, \end{aligned} \quad (4.128)$$

which identically vanishes since the rate of dissipation is just provided by the form

$$\dot{\mathcal{D}} = \sum_{\alpha=1}^m \mathbf{Q}^\alpha : \mathcal{K}(\mathbf{Q}^\alpha) \geq 0 \quad (4.129)$$

The time derivative of any function defined on the state space (4.122) now becomes

$$\dot{\mathcal{F}} = \left\langle \frac{\delta \mathcal{F}}{\delta \boldsymbol{\varphi}}, \dot{\boldsymbol{\varphi}} \right\rangle + \left\langle \frac{\delta \mathcal{F}}{\delta \mathbf{p}}, \dot{\mathbf{p}} \right\rangle + \left\langle \frac{\delta \mathcal{F}}{\delta \eta}, \dot{\eta} \right\rangle + \sum_{\alpha=1}^m \left\langle \frac{\delta \mathcal{F}}{\delta \boldsymbol{\Lambda}^\alpha}, \dot{\boldsymbol{\Lambda}}^\alpha \right\rangle \quad (4.130)$$

Then, the evolution equations derived from the GENERIC formalism for the thermo-dissipative dynamics of continua described in terms of the density entropy are

$$\begin{aligned} \langle \mathbf{w}_\varphi, \dot{\boldsymbol{\varphi}} \rangle_{\mathcal{B}_0} &= \langle \mathbf{w}_\varphi, \frac{1}{\rho_0} \mathbf{p} \rangle_{\mathcal{B}_0} \\ \langle \mathbf{w}_\mathbf{p}, \dot{\mathbf{p}} \rangle_{\mathcal{B}_0} &= -\langle \nabla_0 \mathbf{w}_\mathbf{p}, \mathbf{FS} \rangle_{\mathcal{B}_0} \\ \langle w_\eta, \dot{\eta} \rangle_{\mathcal{B}_0} &= -\langle \nabla_0 \left[\frac{w_\eta}{\Theta} \right], \mathbf{K} \nabla_0 \Theta \rangle_{\mathcal{B}_0} + \langle \frac{w_\eta}{\Theta}, \dot{\mathcal{D}} \rangle_{\mathcal{B}_0} \\ \langle \mathbf{w}_{\boldsymbol{\Lambda}^\alpha}, \dot{\boldsymbol{\Lambda}}^\alpha \rangle_{\mathcal{B}_0} &= \langle \mathbf{w}_{\boldsymbol{\Lambda}^\alpha}, \mathcal{K}(\mathbf{Q}^\alpha) \rangle_{\mathcal{B}_0}, \quad \alpha = 1, \dots, m \end{aligned} \quad (4.131)$$

The above set of weak equations corresponds with the one provided by (3.146) with the exception of the external actions on the continuum.

The laws of thermodynamics can easily be verified by computing the rate of the total energy system using $\mathcal{F} = E(\mathbf{z})$ in (4.87) to give

$$\dot{E}(\mathbf{z}) = \{E(\mathbf{z}), E(\mathbf{z})\} + [E(\mathbf{z}), S(\mathbf{z})] = 0 \quad (4.132)$$

and the rate of the total entropy choosing $\mathcal{F} = S(\mathbf{z})$ to give

$$\begin{aligned} \dot{S}(\mathbf{z}) &= \{S(\mathbf{z}), E(\mathbf{z})\} + [S(\mathbf{z}), S(\mathbf{z})] \\ &= -\langle \nabla_0 \left[\frac{1}{\Theta} \right], \mathbf{K} \nabla_0 \Theta \rangle_{\mathcal{B}_0} + \langle \frac{1}{\Theta}, \dot{\mathcal{D}} \rangle_{\mathcal{B}_0} \\ &= \langle \frac{1}{\Theta^2} \nabla_0 \Theta, \mathbf{K} \nabla_0 \Theta \rangle_{\mathcal{B}_0} + \langle \frac{1}{\Theta}, \dot{\mathcal{D}} \rangle_{\mathcal{B}_0} \geq 0 \end{aligned} \quad (4.133)$$

This last result fully coincides with (3.101) obtained by the classic approach carried out in Chapter 3.

4.7.2 Temperature formulation

Finally, the GENERIC formalism for the thermo-dissipative continuum dynamics described by the temperature is presented. To this end, the state

space is defined as follows

$$\mathcal{S} = \{\mathbf{z} = (\boldsymbol{\varphi}, \mathbf{p}, \Theta, \boldsymbol{\Lambda}^\alpha): \mathcal{B}_0 \mapsto \mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}_+ \times \text{Sym}(\mathbb{T}_d^2)^m, \det(\nabla_0 \boldsymbol{\varphi}) > 0\}, \quad (4.134)$$

and the tangent space is

$$T\mathcal{S} = \{\mathbf{w} = (\mathbf{w}_\varphi, \mathbf{w}_p, w_\Theta, \mathbf{w}_{\Lambda^\alpha}): \mathcal{B}_0 \mapsto \mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R} \times \text{Sym}(\mathbb{T}_d^2)^m\} \quad (4.135)$$

Hence, the total energy and entropy of the system are provided by

$$\begin{aligned} E(\mathbf{z}) &= \int_{\mathcal{B}_0} \left(\frac{1}{2\rho_0} \|\mathbf{p}\|^2 + e(\mathbf{C}, \Theta, \boldsymbol{\Lambda}^\alpha) \right) dV_0, \\ S(\mathbf{z}) &= \int_{\mathcal{B}_0} \eta(\mathbf{C}, \Theta, \boldsymbol{\Lambda}^\alpha) dV_0 \end{aligned} \quad (4.136)$$

Their functional derivatives then result in

$$\begin{aligned} \left\langle \frac{\delta E}{\delta \boldsymbol{\varphi}}, \mathbf{w}_\varphi \right\rangle &= \left\langle 2 \frac{\partial e}{\partial \mathbf{C}}, \mathbf{F}^T \nabla_0 \mathbf{w}_\varphi \right\rangle_{\mathcal{B}_0} & \left\langle \frac{\delta S}{\delta \boldsymbol{\varphi}}, \mathbf{w}_\varphi \right\rangle &= \left\langle 2 \frac{\partial \eta}{\partial \mathbf{C}}, \mathbf{F}^T \nabla_0 \mathbf{w}_\varphi \right\rangle_{\mathcal{B}_0} \\ \left\langle \frac{\delta E}{\delta \mathbf{p}}, \mathbf{w}_p \right\rangle &= \left\langle \frac{\mathbf{p}}{\rho_0}, \mathbf{w}_p \right\rangle_{\mathcal{B}_0} & \left\langle \frac{\delta S}{\delta \mathbf{p}}, \mathbf{w}_p \right\rangle &= 0 \\ \left\langle \frac{\delta E}{\delta \Theta}, w_\Theta \right\rangle &= \left\langle \frac{\partial e}{\partial \Theta}, w_\Theta \right\rangle_{\mathcal{B}_0} & \left\langle \frac{\delta S}{\delta \Theta}, w_\Theta \right\rangle &= \left\langle \frac{\partial \eta}{\partial \Theta}, w_\Theta \right\rangle_{\mathcal{B}_0} \\ \left\langle \frac{\delta E}{\delta \boldsymbol{\Lambda}^\alpha}, \mathbf{w}_{\Lambda^\alpha} \right\rangle &= \left\langle \frac{\partial e}{\partial \boldsymbol{\Lambda}^\alpha}, \mathbf{w}_{\Lambda^\alpha} \right\rangle_{\mathcal{B}_0} & \left\langle \frac{\delta S}{\delta \boldsymbol{\Lambda}^\alpha}, \mathbf{w}_{\Lambda^\alpha} \right\rangle &= \left\langle \frac{\partial \eta}{\partial \boldsymbol{\Lambda}^\alpha}, \mathbf{w}_{\Lambda^\alpha} \right\rangle_{\mathcal{B}_0} \end{aligned} \quad (4.137)$$

As usual, the above partial derivatives are linked with the symmetric Piola-Kirchhoff stress tensor $\mathbf{S}$, the driving stress tensor $\mathbf{Q}^\alpha$, the latent heat tensor $\mathbf{V}$, the visco-latent heat tensor $\mathbf{W}^\alpha$ and the specific heat capacity c . These relations were revealed in Chapter 3, subsection 3.3.6, and are summarized next

$$\begin{aligned} 2 \frac{\partial e}{\partial \mathbf{C}} &= \mathbf{S} + 2\Theta \frac{\partial \eta}{\partial \mathbf{C}}, & 2 \frac{\partial \eta}{\partial \mathbf{C}} &= \frac{1}{\Theta} \mathbf{V}, \\ \frac{\partial e}{\partial \Theta} &= \Theta \frac{\partial \eta}{\partial \Theta} = c & & \\ \frac{\partial e}{\partial \boldsymbol{\Lambda}^\alpha} &= -\mathbf{Q}^\alpha + \Theta \frac{\partial \eta}{\partial \boldsymbol{\Lambda}^\alpha}, & \frac{\partial \eta}{\partial \boldsymbol{\Lambda}^\alpha} &= \frac{1}{\Theta} \mathbf{W}^\alpha \end{aligned} \quad (4.138)$$

The Poisson bracket is not modified respect to the pure thermoelastic case (4.116), now the symmetric latent heat $\mathbf{V}$ tensor also depending on internal

variables. In contrast, the Dissipative bracket must add new terms to deal with the new source of dissipation due to the internal variables. Thereby, for any two functionals $\mathcal{F}, \mathcal{G}: \mathcal{S} \rightarrow \mathbb{R}$, they are

$$\begin{aligned} \{\mathcal{F}, \mathcal{G}\} &= \left\langle \frac{\delta \mathcal{F}}{\delta \boldsymbol{\varphi}}, \frac{\delta \mathcal{G}}{\delta \boldsymbol{p}} \right\rangle - \left\langle \frac{\delta \mathcal{F}}{\delta \boldsymbol{p}}, \frac{\delta \mathcal{G}}{\delta \boldsymbol{\varphi}} \right\rangle - \left\langle \mathbf{FV} \frac{1}{c} \frac{\delta \mathcal{F}}{\delta \Theta}, \nabla_0 \left[\frac{\delta \mathcal{G}}{\delta \boldsymbol{p}} \right] \right\rangle \\ &\quad + \left\langle \nabla_0 \left[\frac{\delta \mathcal{F}}{\delta \boldsymbol{p}} \right], \mathbf{FV} \frac{1}{c} \frac{\delta \mathcal{G}}{\delta \Theta} \right\rangle \\ [\mathcal{F}, \mathcal{G}] &= \left\langle \nabla_0 \left[\frac{1}{c} \frac{\delta \mathcal{F}}{\delta \Theta} \right], \Theta^2 \mathbf{K} \nabla_0 \left[\frac{1}{c} \frac{\delta \mathcal{G}}{\delta \Theta} \right] \right\rangle + \left\langle \frac{1}{c} \frac{\delta \mathcal{F}}{\delta \Theta}, (\dot{\mathcal{D}} + \mathcal{H}_d) \frac{\Theta}{c} \frac{\delta \mathcal{G}}{\delta \Theta} \right\rangle \\ &\quad + \sum_{\alpha=1}^m \left\langle \frac{\delta \mathcal{F}}{\delta \boldsymbol{\Lambda}^\alpha}, \mathcal{K}(\mathbf{Q}^\alpha) \frac{\Theta}{c} \frac{\delta \mathcal{G}}{\delta \Theta} \right\rangle, \end{aligned} \quad (4.139)$$

where the term $\mathcal{H}_d$ is the thermodissipative heating provided by (3.82). The same arguments as before applies to conclude the positive semi-definiteness and the lack of symmetry of the Dissipative bracket.

Using (4.129) and (3.82), the degeneracy conditions are verified as follows

$$\begin{aligned} \{S, \mathcal{F}\} &= \left\langle \frac{1}{\Theta} \mathbf{FV}, \nabla_0 \left[\frac{\delta \mathcal{F}}{\delta \boldsymbol{p}} \right] \right\rangle - \left\langle \frac{1}{c} \frac{c}{\Theta} \mathbf{FV}, \nabla_0 \left[\frac{\delta \mathcal{F}}{\delta \boldsymbol{p}} \right] \right\rangle = 0 \\ [E, \mathcal{F}] &= \left\langle \nabla_0 \left[\frac{1}{c} \right], \Theta^2 \mathbf{K} \nabla_0 \left[\frac{1}{c} \frac{\delta \mathcal{F}}{\delta \Theta} \right] \right\rangle + \left\langle \frac{1}{c} c, (\dot{\mathcal{D}} + \mathcal{H}_d) \frac{\Theta}{c} \frac{\delta \mathcal{F}}{\delta \Theta} \right\rangle \\ &\quad + \sum_{\alpha=1}^m \left\langle (-\mathbf{Q}^\alpha + \mathbf{W}^\alpha), \mathcal{K}(\mathbf{Q}^\alpha) \frac{\Theta}{c} \frac{\delta \mathcal{F}}{\delta \Theta} \right\rangle = 0, \end{aligned} \quad (4.140)$$

where use has been made of the definition of the thermodissipative heating (3.82).

Applying the GENERIC formulas, the weak form of the isolated evolution equations for the thermo-dissipative continuum dynamics equations reads

$$\begin{aligned} \langle \mathbf{w}_\varphi, \dot{\boldsymbol{\varphi}} \rangle_{\mathcal{B}_0} &= \langle \mathbf{w}_\varphi, \frac{1}{\rho_0} \boldsymbol{p} \rangle_{\mathcal{B}_0} \\ \langle \mathbf{w}_p, \dot{\boldsymbol{p}} \rangle_{\mathcal{B}_0} &= -\langle \nabla_0 \mathbf{w}_p, \mathbf{F} \left(2 \frac{\partial e}{\partial \mathbf{C}} - \mathbf{V} \right) \rangle_{\mathcal{B}_0} = -\langle \nabla_0 \mathbf{w}_p, \mathbf{FS} \rangle_{\mathcal{B}_0} \\ \langle w_\Theta, \dot{\Theta} \rangle_{\mathcal{B}_0} &= -\left\langle \frac{w_\Theta}{c} \mathbf{FV}, \nabla_0 \left[\frac{\boldsymbol{p}}{\rho_0} \right] \right\rangle_{\mathcal{B}_0} - \left\langle \nabla_0 \left[\frac{w_\Theta}{c} \right], \mathbf{K} \nabla_0 \Theta \right\rangle_{\mathcal{B}_0} \\ &\quad + \left\langle \frac{w_\Theta}{c}, \dot{\mathcal{D}} + \mathcal{H}_d \right\rangle_{\mathcal{B}_0} \\ \langle \mathbf{w}_{\boldsymbol{\Lambda}^\alpha}, \dot{\boldsymbol{\Lambda}^\alpha} \rangle_{\mathcal{B}_0} &= \langle \mathbf{w}_{\boldsymbol{\Lambda}^\alpha}, \mathcal{K}(\mathbf{Q}^\alpha) \rangle_{\mathcal{B}_0}, \quad \alpha = 1, \dots, m, \end{aligned} \quad (4.141)$$

which are the same as those obtained in (3.147) but without considering external actions.

To finish, the laws of thermodynamics are verified by taking $\mathcal{F} = E(\mathbf{z})$ in (4.87) to calculate the rate of total energy as follows

$$\dot{E}(\mathbf{z}) = \{E(\mathbf{z}), E(\mathbf{z})\} + [E(\mathbf{z}), S(\mathbf{z})] = 0, \quad (4.142)$$

and by choosing $\mathcal{F} = S(\mathbf{z})$ to arrive at the following rate of total entropy

$$\begin{aligned} \dot{S}(\mathbf{z}) &= \{S(\mathbf{z}), E(\mathbf{z})\} + [S(\mathbf{z}), S(\mathbf{z})] \\ &= -\langle \nabla_0 \left[\frac{1}{c} \frac{c}{\Theta} \right], \mathbf{K} \nabla_0 \Theta \rangle_{\mathcal{B}_0} \\ &\quad + \sum_{\alpha=1}^m \left\langle \frac{1}{\Theta} \mathbf{W}^\alpha, \mathcal{K}(\mathbf{Q}^\alpha) \frac{\Theta}{c} \frac{c}{\Theta} \right\rangle_{\mathcal{B}_0} + \left\langle \frac{1}{c} \frac{c}{\Theta}, (\dot{\mathcal{D}} + \mathcal{H}_d) \frac{\Theta}{c} \frac{c}{\Theta} \right\rangle_{\mathcal{B}_0} \\ &= \left\langle \frac{1}{\Theta^2} \nabla_0 \Theta, \mathbf{K} \nabla_0 \Theta \right\rangle_{\mathcal{B}_0} + \sum_{\alpha=1}^m \left\langle \frac{1}{\Theta}, \mathbf{Q}^\alpha : \mathcal{K}(\mathbf{Q}^\alpha) \right\rangle_{\mathcal{B}_0} \geq 0 \end{aligned} \quad (4.143)$$

4.8 Metriplectic structure for isothermal dissipative dynamics

Isothermal dissipative systems can be approached from the metriplectic structure perspective following Bloch et al. (1996). Therein, the authors introduced a metriplectic structure based on an energy function on a state space $E : \mathcal{S} \rightarrow \mathbb{R}$ that decreases over time, which is what happens in the context of isothermal dissipative systems with the total energy resulting from the sum of the kinetic energy plus the total free energy function. With this premise, the flow of a metriplectic structure is provided by

$$\dot{f} = \{[f, E]\} = \{f, E\} + (f, E) \quad \forall f : \mathcal{S} \rightarrow \mathbb{R}, \quad (4.144)$$

defining the Poisson-Dissipative bracket, denoted as $\{[\cdot, \cdot]\}$, so that

$$\dot{E} = \{[E, E]\} = \{E, E\} + (E, E) = (E, E) \leq 0, \quad (4.145)$$

where the bracket $(\cdot, \cdot) : \mathcal{S} \times \mathcal{S} \mapsto \mathbb{R}$ is a bilinear and negative semidefinite operator. The above definition is the proof for the system to develop dissipation along its evolution.

In this particular metriplectic structure, the energy function E is responsible for generating both the reversible and irreversible flows. In fact, the

limit case of its rate $\dot{E}$ being zero corresponds with the purely Hamiltonian case. For general positive functions E , its rate is always negative so it serves as a strong Lyapunov function. As a result, the system will surely relax to a state of equilibrium, i.e. to a surface of minimal energy.

On the other hand, by making certain physic assumptions, see Mielke (2011), isothermal dissipative dynamics can be described consistently from the GENERIC approach, which, observe, is not a metriplectic structure of the format just introduced.

For the infinite-dimensional case, the above introduced metriplectic structure is defined over functionals on the infinite-dimensional state space $\mathcal{F} : \mathcal{S} \rightarrow \mathbb{R}$.

Definition 4.9. An infinite-dimensional isothermal dissipative system is a system governed by the following differential equations

$$\dot{\mathcal{F}} = \{[\mathcal{F}, E]\}, \quad (4.146)$$

where $E : \mathcal{S} \rightarrow \mathbb{R}$ is the total energy of the system understood as the sum of the kinetic energy plus the total free-energy function, as was introduced in (3.96) taking into account the relation (3.40), which is to be decreasing along the system evolution.

Thus, to derive the evolution equations of isothermal dissipative continuum dynamics, consider the infinite-dimensional state space

$$\mathcal{S} = \{\mathbf{z} = (\boldsymbol{\varphi}, \mathbf{p}, \boldsymbol{\Lambda}^\alpha) : \mathcal{B}_0 \mapsto \mathbb{R}^d \times \mathbb{R}^d \times \text{Sym}(\mathbb{T}_d^2)^m, \det(\nabla_0 \boldsymbol{\varphi}) > 0\}, \quad (4.147)$$

along with its tangent space

$$T\mathcal{S} = \{\mathbf{w} = (\mathbf{w}_\varphi, \mathbf{w}_p, \mathbf{w}_{\Lambda^\alpha}) : \mathcal{B}_0 \mapsto \mathbb{R}^d \times \mathbb{R}^d \times \text{Sym}(\mathbb{T}_d^2)^m\} \quad (4.148)$$

Then, the total energy of the system in terms of this state variables is provided by

$$E(\mathbf{z}) = \int_{\mathcal{B}_0} \left(\frac{1}{2\rho_0} \|\mathbf{p}\|^2 + \Psi(\mathbf{C}, \boldsymbol{\Lambda}^\alpha) \right) dV_0, \quad (4.149)$$

whose functional derivative results in

$$\begin{aligned} \left\langle \frac{\delta E}{\delta \boldsymbol{\varphi}}, \mathbf{w}_\varphi \right\rangle &= \left\langle 2 \frac{\partial \Psi}{\partial \mathbf{C}}, \mathbf{F}^T \nabla_0 \mathbf{w}_\varphi \right\rangle_{\mathcal{B}_0} \\ \left\langle \frac{\delta E}{\delta \mathbf{p}}, \mathbf{w}_p \right\rangle &= \left\langle \frac{\mathbf{p}}{\rho_0}, \mathbf{w}_p \right\rangle_{\mathcal{B}_0} \\ \left\langle \frac{\delta E}{\delta \boldsymbol{\Lambda}^\alpha}, \mathbf{w}_{\Lambda^\alpha} \right\rangle &= \left\langle \frac{\partial \Psi}{\partial \boldsymbol{\Lambda}^\alpha}, \mathbf{w}_{\Lambda^\alpha} \right\rangle_{\mathcal{B}_0} \end{aligned} \quad (4.150)$$

The Poisson-Dissipative bracket is then provided by

$$\{[\mathcal{F}, \mathcal{G}]\} = \left\langle \frac{\delta \mathcal{F}}{\delta \boldsymbol{\varphi}}, \frac{\delta \mathcal{G}}{\delta \mathbf{p}} \right\rangle - \left\langle \frac{\delta \mathcal{F}}{\delta \mathbf{p}}, \frac{\delta \mathcal{G}}{\delta \boldsymbol{\varphi}} \right\rangle + \sum_{\alpha=1}^m \left\langle \frac{\delta \mathcal{F}}{\delta \boldsymbol{\Lambda}^\alpha}, \mathcal{K} \left(-\frac{\delta \mathcal{G}}{\delta \boldsymbol{\Lambda}^\alpha} \right) \right\rangle \quad (4.151)$$

The time derivative of any function defined on the state space (4.147) now becomes Poisson-Dissipative

$$\dot{\mathcal{F}} = \left\langle \frac{\delta \mathcal{F}}{\delta \mathbf{z}}, \dot{\mathbf{z}} \right\rangle = \left\langle \frac{\delta \mathcal{F}}{\delta \boldsymbol{\varphi}}, \dot{\boldsymbol{\varphi}} \right\rangle + \left\langle \frac{\delta \mathcal{F}}{\delta \mathbf{p}}, \dot{\mathbf{p}} \right\rangle + \sum_{\alpha=1}^m \left\langle \frac{\delta \mathcal{F}}{\delta \boldsymbol{\Lambda}^\alpha}, \dot{\boldsymbol{\Lambda}^\alpha} \right\rangle \quad (4.152)$$

Identifying the partial derivatives of (4.150) with the isothermal constitutive laws (3.103) and choosing $\delta \mathcal{F} / \delta \mathbf{z} = \mathbf{w}$, the weak statement of isolated evolution equations for the isothermal dissipative dynamics reads

$$\begin{aligned} \langle \mathbf{w}_\varphi, \dot{\boldsymbol{\varphi}} \rangle_{\mathcal{B}_0} &= \langle \mathbf{w}_\varphi, \frac{1}{\rho_0} \mathbf{p} \rangle_{\mathcal{B}_0} \\ \langle \mathbf{w}_p, \dot{\mathbf{p}} \rangle_{\mathcal{B}_0} &= -\langle \nabla_0 \mathbf{w}_p, \mathbf{F} \mathbf{S} \rangle_{\mathcal{B}_0} \\ \langle \mathbf{w}_{\Lambda^\alpha}, \dot{\boldsymbol{\Lambda}^\alpha} \rangle_{\mathcal{B}_0} &= \langle \mathbf{w}_{\Lambda^\alpha}, \mathcal{K}(\mathbf{Q}^\alpha) \rangle_{\mathcal{B}_0}, \quad \alpha = 1, \dots, m \end{aligned} \quad (4.153)$$

Finally, choosing $\mathcal{F} = E$ in (4.146) the rate of the total energy yields

$$\dot{E} = \{[E, E]\} = - \sum_{\alpha=1}^m \langle \mathbf{Q}^\alpha, \mathcal{K}(\mathbf{Q}^\alpha) \rangle_{\mathcal{B}_0} = -\dot{D} \leq 0 \rightarrow \dot{E} + \dot{D} = 0, \quad (4.154)$$

which reveals that the so called Augmented Hamiltonian (3.107) is preserved along the isolated system evolution, as was demonstrated in Chapter 3.

Remark 4.6. The viscoelastic model due to Holzapfel & Simó (1996b) introduced in subsection 3.6.1 is thus attained by specifying the dissipative functional $\mathcal{K}$ according to (3.23).

4.9 Symmetries of infinite-dimensional dissipative systems

As was identified in Chapter 3, the evolution equations of thermo-dissipative/isothermal isolated dynamics of continua pose symmetries associated with conserved quantities (first integrals) of the motion. That is, general thermo-dissipative continua are dissipative system with symmetries according to Def. 4.7.

In Section 3.5 of Chapter 3, the first integrals of the motion were identified with the total linear momentum (3.44) and the total angular momentum (3.51). Within the GENERIC approach, they are derived from the action of certain Lie Groups that preserve the GENERIC operators according to (4.90).

Thus, the total linear momentum (3.44) is a momentum map associated with an additive group $G = \mathbb{R}^d$ whose action $\Phi: \mathbb{R}^d \times \mathcal{S} \rightarrow \mathcal{S}$ is defined by

$$\Phi_{\mathbf{a}}(\mathbf{z}) = \Phi(\mathbf{a}, \mathbf{z}) = (\boldsymbol{\varphi} + \mathbf{a}, \mathbf{p}, s, \boldsymbol{\Lambda}^1, \dots, \boldsymbol{\Lambda}^m) \quad \forall \mathbf{a} \in \mathbb{R}^d, \quad (4.155)$$

where the state space $\mathcal{S}$ has been chosen in the more general way. Then, the infinitesimal generator of the action is provided by

$$\boldsymbol{\xi}_{\mathcal{S}} = \left. \frac{d}{d\epsilon} \right|_{\epsilon=0} \Phi_{\boldsymbol{\xi}}(\epsilon, \mathbf{z}) = (\boldsymbol{\xi}, \mathbf{0}, 0, \mathbf{0}, \dots, \mathbf{0}), \quad (4.156)$$

This action preserves all the GENERIC operators presented in previous sections. The proof for the pure thermoelastic case in terms of entropy, i.e for the operators (4.102) and (4.103), can be found in Romero (2013). For the rest, similar arguments can be used to verify their preservation.

Now, to demonstrate that the linear momentum is a momentum map that is preserved along the system evolution, a scalar functional is built as follows

$$J_{\boldsymbol{\xi}} = \langle \mathbf{p}, \boldsymbol{\xi} \rangle_{\mathcal{B}_0} = \mathbf{L} \cdot \boldsymbol{\xi} \quad \forall \boldsymbol{\xi} \in \mathbb{R}^d \quad (4.157)$$

whose rate can be elaborated by using the GENERIC equations (4.87) to give

$$\dot{J}_{\boldsymbol{\xi}} = \{J_{\boldsymbol{\xi}}, E(\mathbf{z})\} + [J_{\boldsymbol{\xi}}, S(\mathbf{z})] \quad (4.158)$$

For each of the forms of the Dissipative brackets presented for each of the cases considered in previous subsections and for the last term of the Poisson-Dissipative bracket of the isothermal case (4.151), it can be concluded that

$$[J_{\boldsymbol{\xi}}, S(\mathbf{z})] = 0, \quad (4.159)$$

as the scalar functional does not depend on internal variables nor on thermodynamical ones that are responsible for furnishing the Dissipative operators. Then, to proceed further, the Poisson brackets must be particularized for each of the cases considered. Essentially, there are two different definitions of them, each for the entropy formulation (the isothermal case can be included here) and for the temperature formulation. In the first case, either

(4.102) or (4.127)₁ or the first two terms in (4.151), the rate of the scalar functional (4.157) yields

$$\dot{J}_\xi = \{J_\xi, E(\mathbf{z})\} = -\{E(\mathbf{z}), J_\xi\} = -\left\langle \frac{\delta E}{\delta \boldsymbol{\varphi}}, \frac{\delta J_\xi}{\delta \mathbf{p}} \right\rangle = -\left\langle \frac{\delta E}{\delta \boldsymbol{\varphi}}, \boldsymbol{\xi} \right\rangle \quad (4.160)$$

For the temperature formulations, that is, the Poisson brackets provided by (4.116) or (4.139), the same result is obtained, that is

$$\dot{J}_\xi = -\{E(\mathbf{z}), J_\xi\} = -\left\langle \frac{\delta E}{\delta \boldsymbol{\varphi}}, \boldsymbol{\xi} \right\rangle - \left\langle \mathbf{FV} \frac{1}{c} \frac{\delta E}{\delta \Theta}, \nabla_0 \boldsymbol{\xi} \right\rangle = -\left\langle \frac{\delta E}{\delta \boldsymbol{\varphi}}, \boldsymbol{\xi} \right\rangle \quad (4.161)$$

The verification is completed by noticing that the resulting term vanishes because the total energy of the system is invariant respect to the action $\Phi_{\mathbf{u}}$ of the additive Group, as it depends on the motion $\boldsymbol{\varphi}$ only through the right Cauchy deformation tensor, thus concluding that the global linear momentum (3.44) is preserved for each of the systems perviously presented.

On the other hand, the total angular momentum (3.51) is a momentum map associated with the rotation group $G = \text{SO}(3) = \{\mathbf{G}: \mathbb{R}^3 \mapsto \mathbb{R}^3 | \mathbf{G}\mathbf{G}^T = \mathbf{1}, \det(\mathbf{G}) = 1\}$ whose action $\Phi: \text{SO}(3) \times \mathcal{S} \rightarrow \mathcal{S}$ is provided by

$$\Phi_{\mathbf{G}}(\mathbf{z}) = \Phi(\mathbf{G}, \mathbf{z}) = (\mathbf{G}\boldsymbol{\varphi}, \mathbf{G}\mathbf{p}, s, \boldsymbol{\Lambda}^1, \dots, \boldsymbol{\Lambda}^m) \quad \forall \mathbf{G} \in \text{SO}(3), \quad (4.162)$$

and its infinitesimal generator of actions provided by

$$\boldsymbol{\xi}_{\mathcal{S}} = \left. \frac{d}{d\epsilon} \right|_{\epsilon=0} \Phi^{\boldsymbol{\xi}}(\epsilon, \mathbf{z}) = (\boldsymbol{\xi} \wedge \boldsymbol{\varphi}, \boldsymbol{\xi} \wedge \mathbf{p}, 0, \mathbf{0}) \quad (4.163)$$

This action also preserves all the GENERIC operators introduced above as can be seen in Romero (2013) for the pure thermoelastic case formulated in terms of entropy (4.102) and (4.103). The proofs for the rest would closely follow the same guidelines.

Then, the verification for the angular momentum (3.51) to be a conserved momentum map follows from building the following scalar functional

$$J_\xi = \langle \boldsymbol{\varphi} \wedge \mathbf{p}, \boldsymbol{\xi} \rangle_{\mathcal{B}_0} = \mathbf{J} \cdot \boldsymbol{\xi} \quad (4.164)$$

According to the GENERIC equations (4.87), its rate read

$$\dot{J}_\xi = \{J_\xi, E(\mathbf{z})\} + [J_\xi, S(\mathbf{z})], \quad (4.165)$$

where the second term on the right hand side vanishes for all of the cases considered due to the same reasons as for the linear momentum. Then, the Poisson brackets of the entropy formulations and the isothermal one, (4.102), (4.127)₁ or (4.151), are used to arrive at

$$\dot{J}_{\boldsymbol{\xi}} = \{J_{\boldsymbol{\xi}}, E(\mathbf{z})\} = -\{E(\mathbf{z}), J_{\boldsymbol{\xi}}\} = \left\langle \frac{\delta E}{\delta \boldsymbol{\varphi}}, \boldsymbol{\xi} \wedge \boldsymbol{\varphi} \right\rangle - \left\langle \frac{\delta E}{\delta \mathbf{p}}, \mathbf{p} \wedge \boldsymbol{\xi} \right\rangle \quad (4.166)$$

Now, using the Poisson brackets for the temperature formulations (4.116) and (4.139), it follows that

$$\begin{aligned} \dot{J}_{\boldsymbol{\xi}} = \{J_{\boldsymbol{\xi}}, E(\mathbf{z})\} = -\{E(\mathbf{z}), J_{\boldsymbol{\xi}}\} &= \left\langle \frac{\delta E}{\delta \boldsymbol{\varphi}}, \boldsymbol{\xi} \wedge \boldsymbol{\varphi} \right\rangle - \left\langle \frac{\delta E}{\delta \mathbf{p}}, \mathbf{p} \wedge \boldsymbol{\xi} \right\rangle \\ &+ \left\langle \mathbf{FV} \frac{1}{c} \frac{\delta E}{\delta \Theta}, \nabla_0[\boldsymbol{\xi} \wedge \boldsymbol{\varphi}] \right\rangle \end{aligned} \quad (4.167)$$

The last term of the right hand side identically vanishes because it results in the product of a symmetric tensor and a skew-symmetric tensor which arises from the matrix format of the cross product $\boldsymbol{\xi} \wedge \boldsymbol{\varphi} = \hat{\boldsymbol{\xi}}\boldsymbol{\varphi}$, that is

$$\left\langle \mathbf{FV} \frac{1}{c} \frac{\delta E}{\delta \Theta}, \nabla_0[\hat{\boldsymbol{\xi}}\boldsymbol{\varphi}] \right\rangle = \left\langle \mathbf{FV} \frac{1}{c} \frac{\delta E}{\delta \Theta}, \hat{\boldsymbol{\xi}}\mathbf{F} \right\rangle = \left\langle \frac{1}{c} \frac{\delta E}{\delta \Theta} \mathbf{FV}\mathbf{F}^T, \hat{\boldsymbol{\xi}} \right\rangle = 0 \quad (4.168)$$

Finally, due to the objectivity of the total energy functions of the systems previously described, the action $\Phi_{\mathbf{G}}$ does not modify them so the rate of the scalar function (4.164) is an invariant of any of the above systems evolution and hence, the angular momentum (3.51) is a first integral of the motion of them.

Thermodynamically Consistent Algorithms

CHAPTER 5

The aim of this Chapter is to present a general methodology to derive thermodynamically consistent second-order accurate time integration methods for general dissipative systems defined as in the previous Chapter. The resulting methods not only agree with the laws of thermodynamics but also preserve the first integrals associated with the symmetries of the system while being second-order accurate. The key ingredient of this methodology is a *discrete derivative operator* satisfying two essential properties, namely, the directionality and the consistency properties. The first property is responsible for the preservation of the geometric structure of the systems, revealed in the previous Chapter, whereas the second properties ensures the second-order accuracy.

In the same way as in the continuous modeling the metriplectic structure extended the Poisson structure to include dissipative terms, this new methodology extends the formulation to derive Energy-Momentum methods for conserving systems to the formulation of Energy-Entropy-Momentum methods for dissipative systems. In fact, such extension rests on the same key concepts that led to the formulation of Energy-Momentum methods, thus sharing most of their appealing features.

5.1 Energy-Entropy-Momentum time integration methods

For concreteness, Energy-Entropy-Momentum (EEM) integration methods are those derived from the fairly general methodology devised in the work of Romero (2009, 2010a,b), which provides discrete counterparts of the GENERIC equations in such a way that their intrinsic metriplectic structure is preserved. Hence, counterparts thus constructed are automatically thermodynamically consistent and momentum maps-preserving, that is, Energy-preserving, Entropy-producing and Momentum-preserving by design, hence their names: Energy-Entropy-Momentum methods.

The methodology basically follows the guidelines that led to the general formulation of Energy-Momentum methods. In short, it consists in a temporal approximation of the GENERIC equations defining general dissipative systems of mid-point type (2.75) combined with a discrete derivative operator satisfying two essential properties: directionality and consistency. As a result of these two key elements in the formulation, the resulting time integration methods are canonically structure-preserving and second order accurate. Among all possible candidates for the discrete derivative operator studied in Romero (2012), the one proposed in González (1996) for the formulation of Energy-Momentum methods presents advantages from the implementation point of view, thus being the optimal candidate to develop Energy-Entropy-Momentum methods.

This general methodology can adopt several approaches mainly regarding the strategy to deal with thermo-coupled problems, which might affect the order of accuracy of resulting methods, and regarding the thermodynamical state variable used to describe the system's thermodynamics. This last alternative has been recently open after the investigations carried out for the composition of this dissertation that have enabled the formulation of temperature-based EEM methods as an alternative of the so far favored entropy-based ones due to its apparent simplicity.

Thus, motivated by the natural partition of coupling problems into a mechanical and a thermal problems, their solutions are commonly obtained with staggered strategies, so that advantages of the different time scales involved in each problem can be exploited, see for instance Holzapfel & Simó (1996a). This strategy is further backed by the metriplectic structure of dissipative systems which clearly separates the reversible (isentropic) and the irreversible (entropic) contributions to the system evolution. In fact, Romero (2009, 2010b) proved that using the entropy as state variable, stag-

gered methods in which each step remains thermodynamically consistent can be formulated within the proposed methodology. However, the second order accuracy cannot be retained.

Alternatively, the methodology can be performed by adopting a monolithic strategy, that this, solving the coupled equations at once. With this approach, in contrast to the staggered strategy, second order accurate methods are automatically achieved and the choice of the thermodynamical variable is theoretically not restricted. In this dissertation, the scope is restricted to this monolithic second-order accurate approach considering the most significant thermodynamical state variables: entropy or temperature; so that the stability, the accuracy and the conservation properties of the both approaches can be thoroughly discussed.

For methods with higher order of accuracy, sub-stepping procedures were proposed by Tarnow & Simó (1994) to raise the order of accuracy while preserving the stability and conserving properties. However, the presence of a ‘Dissipative bracket’ in the problems of interest seems to lead methods formulated backward in time to be ill-posed, thus preventing an effective increment of the order of accuracy.

5.2 General formulation of EEM methods

For any finite-dimensional system, either of the form of Def. 4.2 or resulting from the spatial discretization of infinite-dimensional systems in the sense of Def. 4.6, for instance, using the Galerkin approach summarized in subsection 3.7.2, consider the classical partition of the time integration interval $[0, T]$ into constant subintervals of length $\Delta t = t_{n+1} - t_n$. Then, the state vector $\mathbf{z} \in \mathcal{S}, \mathcal{S}^h$ at certain instants of time t_i is approximated as $\mathbf{z}_i \simeq \mathbf{z}(t_i)$ so that the construction of EEM counterparts rests on the following definitions.

Definition 5.1. For any subinterval $[t_n, t_{n+1}]$, the time derivative of the vector state $\dot{\mathbf{z}}$ is approximated by the following second-order accurate formula

$$\dot{\mathbf{z}}_{n+\frac{1}{2}} = \frac{\mathbf{z}_{n+1} - \mathbf{z}_n}{\Delta t}, \quad \forall [t_n, t_{n+1}] \quad (5.1)$$

Definition 5.2. Discrete derivative operator. This operator is a second order approximation of the standard derivative operator evaluated at midpoint of the time interval. According to González (1996), for any smooth function defined in an inner product space $(\mathcal{S}, \langle \cdot, \cdot \rangle_{\mathcal{S}})$, $f : \mathcal{S} \rightarrow \mathbb{R}$, this second-order

operator $D: \mathcal{S} \times \mathcal{S} \mapsto T\mathcal{S}$ is provided by

$$Df(\mathbf{z}_{n+1}, \mathbf{z}_n) = Df(\mathbf{z}_{n+\frac{1}{2}}) + \frac{f(\mathbf{z}_{n+1}) - f(\mathbf{z}_n) - \langle Df(\mathbf{z}_{n+\frac{1}{2}}), \Delta \mathbf{z} \rangle_{\mathcal{S}}}{\langle \Delta \mathbf{z}, \Delta \mathbf{z} \rangle_{\mathcal{S}}} \Delta \mathbf{z}, \quad (5.2)$$

where $\mathbf{z}_{n+1}, \mathbf{z}_n \in \mathcal{S}$, $\mathbf{z}_{n+\frac{1}{2}} = (\mathbf{z}_{n+1} + \mathbf{z}_n)/2$, $\Delta \mathbf{z} = \mathbf{z}_{n+1} - \mathbf{z}_n$ and D^1 being standard derivative.

For state spaces with structure of products $\mathcal{S} = L_1 \times \dots \times L_k$ for some $k \geq 1$, with every $L_i, i = 1, \dots, k$ endowed with an inner product $\langle \cdot, \cdot \rangle_{L_i}$, as in the systems considered, the discrete derivative operator with respect to the product structure of $\mathcal{S}$, for any smooth function $f: \mathcal{S} \rightarrow \mathbb{R}$, is provided by

$$\langle Df(\mathbf{z}_{n+1}, \mathbf{z}_n), \Delta \mathbf{z} \rangle_{\mathcal{S}} = \sum_{i=1}^k \langle D_{z_i} f(\mathbf{z}_{n+1}, \mathbf{z}_n), \Delta z_i \rangle_{L_i}, \quad (5.3)$$

where the term $D_{z_i} f(\mathbf{z}_{n+1}, \mathbf{z}_n)$ is the i -th second order accurate discrete counterpart to the i -th partial derivative of the function f at midpoint; for more details about its computation consult Appendix A.

These definitions of the discrete derivative operator satisfy the required properties of *directionality* and *consistency*, that is

$$\langle Df(\mathbf{z}_{n+1}, \mathbf{z}_n), \mathbf{z}_{n+1} - \mathbf{z}_n \rangle_{\mathcal{S}} = f(\mathbf{z}_{n+1}) - f(\mathbf{z}_n), \quad (5.4)$$

$$Df(\mathbf{z}_{n+1}, \mathbf{z}_n) = Df(\mathbf{z}_{n+\frac{1}{2}}) + \mathcal{O}(\|\mathbf{z}_{n+1} - \mathbf{z}_n\|^2) \quad (5.5)$$

The first one holds the key to preserve discretely the evolution structure identified in continuous systems. The second one ensures the second order accuracy. The proofs for the operator to satisfy these properties can be also found in Appendix A.

Associated with functions being invariant to the action Φ of a Lie Group G with algebra $\mathfrak{g}$ and dual $\mathfrak{g}^*$, whose infinitesimal generator of actions is denoted as $\xi_{\mathcal{S}}(\mathbf{z})$, i.e G -invariant functions, the G -equivariant discrete derivative operator is introduced.

Definition 5.3. The G -equivariant discrete derivative operator is a discrete derivative operator operator $D^G: \mathcal{S} \times \mathcal{S} \mapsto T\mathcal{S}$ in the sense of (5.2) that satisfies two additional properties:

¹notice the different notations used for the standard derivative D and for the discrete derivative D .

1. Equivariance

$$D^G f(\Phi_g(\mathbf{z}_{n+1}), \Phi_g(\mathbf{z}_n)) = \left[D\Phi_g(\mathbf{z}_{n+\frac{1}{2}}) \right]^{-T} D^G f(\mathbf{z}_{n+1}, \mathbf{z}_n), \quad (5.6)$$

for all $g \in G$ and $\mathbf{z}_{n+1}, \mathbf{z}_n \in \mathcal{S}$.

2. Orthogonality

$$\left\langle D^G f(\mathbf{z}_{n+1}, \mathbf{z}_n), \boldsymbol{\xi}_{\mathcal{S}}(\mathbf{z}_{n+\frac{1}{2}}) \right\rangle_{\mathcal{S}} = 0 \quad \forall \boldsymbol{\xi} \in \mathfrak{g}^*, \quad (5.7)$$

for all $\mathbf{z}_{n+1}, \mathbf{z}_n \in \mathcal{S}$.

Proposition 5.1. *Let $f : \mathcal{S} \rightarrow \mathbb{R}$ be a smooth G -invariant function, $\pi : \mathcal{S} \rightarrow \mathbb{R}^r$ be a set of r functions $\pi_i : \mathcal{S} \rightarrow \mathbb{R}$ which are invariant respect to an action Φ of a Lie group G . Let $\tilde{f} : \pi(\mathcal{S}) \rightarrow \mathbb{R}$ be the associated reduced function defined by $\tilde{f}(\pi(\mathbf{z})) = f(\mathbf{z})$, for all $\mathbf{z}$. If the invariant $\pi_i : \mathcal{S} \rightarrow \mathbb{R}$ is at most of degree two, then a G -equivariant discrete derivative for f is provided by*

$$D^G f(\mathbf{z}_{n+1}, \mathbf{z}_n) = \left[D\pi(\mathbf{z}_{n+\frac{1}{2}}) \right]^T D\tilde{f}(\pi(\mathbf{z}_{n+1}), \pi(\mathbf{z}_n)), \quad (5.8)$$

where for any $\mathbf{z} \in \mathcal{S}$, $D\pi(\mathbf{z}) \in \mathbb{R}^{r \times \dim(\mathcal{S})}$ and $r = \dim(\mathcal{S}) - o$, o being the number of orbits associated with the Lie group G .

These properties become important to define discrete counterparts of dissipative systems with symmetries and are verified in Appendix A.

5.2.1 Discrete finite-dimensional smooth dissipative systems

In this subsection, the previous definitions are employed to define discrete finite-dimensional smooth dissipative systems with symmetries, thus providing the general form of EEM methods for finite-dimensional dissipative systems provided by Def. 4.2.

Definition 5.4. A discrete finite-dimensional smooth dissipative system with symmetries is a discrete system governed by the following discrete GENERIC equations

$$\frac{\mathbf{z}_{n+1} - \mathbf{z}_n}{\Delta t} = \mathbf{L}(\mathbf{z}_{n+1}, \mathbf{z}_n) D^G E(\mathbf{z}_{n+1}, \mathbf{z}_n) + \mathbf{M}(\mathbf{z}_{n+1}, \mathbf{z}_n) D^G S(\mathbf{z}_{n+1}, \mathbf{z}_n), \quad (5.9)$$

where $\mathbf{L}(\mathbf{z}_{n+1}, \mathbf{z}_n)$ and $\mathbf{M}(\mathbf{z}_{n+1}, \mathbf{z}_n)$ are second order approximations of the continuous Poisson and Dissipative matrices evaluated at midpoint

$$\begin{aligned} \mathbf{L}(\mathbf{z}_{n+1}, \mathbf{z}_n) &= \mathbf{L}(\mathbf{z}_{n+\frac{1}{2}}) + \mathcal{O}(\mathbf{z}_{n+1} - \mathbf{z}_n)^2, \\ \mathbf{M}(\mathbf{z}_{n+1}, \mathbf{z}_n) &= \mathbf{M}(\mathbf{z}_{n+\frac{1}{2}}) + \mathcal{O}(\mathbf{z}_{n+1} - \mathbf{z}_n)^2 \end{aligned} \quad (5.10)$$

In analogy to the continuous case, the discrete versions of the Poisson and Dissipative matrices must satisfy the degeneracy or non-interaction conditions in the following form

$$\mathbf{L}(\mathbf{z}_{n+1}, \mathbf{z}_n) \mathbf{D}^G S(\mathbf{z}_{n+1}, \mathbf{z}_n) = \mathbf{0}, \quad \mathbf{M}(\mathbf{z}_{n+1}, \mathbf{z}_n) \mathbf{D}^G E(\mathbf{z}_{n+1}, \mathbf{z}_n) = \mathbf{0} \quad (5.11)$$

Discrete laws of thermodynamics. The satisfaction of the laws of thermodynamics by the discrete setting (5.9) directly follows from directionality property (5.4) to give

$$\begin{aligned} E_{n+1} - E_n &= \mathbf{D}^G E(\mathbf{z}_{n+1}, \mathbf{z}_n) \cdot (\mathbf{z}_{n+1} - \mathbf{z}_n) \\ &= \Delta t \mathbf{D}^G E(\mathbf{z}_{n+1}, \mathbf{z}_n) \cdot \mathbf{L}(\mathbf{z}_{n+1}, \mathbf{z}_n) \mathbf{D}^G E(\mathbf{z}_{n+1}, \mathbf{z}_n) \\ &\quad + \Delta t \mathbf{D}^G E(\mathbf{z}_{n+1}, \mathbf{z}_n) \cdot \mathbf{M}(\mathbf{z}_{n+1}, \mathbf{z}_n) \mathbf{D}^G S(\mathbf{z}_{n+1}, \mathbf{z}_n) \\ &= \Delta t \mathbf{D}^G S(\mathbf{z}_{n+1}, \mathbf{z}_n) \cdot \mathbf{M}(\mathbf{z}_{n+1}, \mathbf{z}_n) \mathbf{D}^G E(\mathbf{z}_{n+1}, \mathbf{z}_n) = 0 \end{aligned} \quad (5.12)$$

This result can be directly deduced from the skew-symmetry of the discrete Poisson matrix together with the non-interaction conditions (5.11). Similarly, the total entropy balance results in

$$\begin{aligned} S_{n+1} - S_n &= \mathbf{D}^G S(\mathbf{z}_{n+1}, \mathbf{z}_n) \cdot (\mathbf{z}_{n+1} - \mathbf{z}_n) \\ &= \Delta t \mathbf{D}^G S(\mathbf{z}_{n+1}, \mathbf{z}_n) \cdot \mathbf{L}(\mathbf{z}_{n+1}, \mathbf{z}_n) \mathbf{D}^G E(\mathbf{z}_{n+1}, \mathbf{z}_n) \\ &\quad + \Delta t \mathbf{D}^G S(\mathbf{z}_{n+1}, \mathbf{z}_n) \cdot \mathbf{M}(\mathbf{z}_{n+1}, \mathbf{z}_n) \mathbf{D}^G S(\mathbf{z}_{n+1}, \mathbf{z}_n) \\ &= -\Delta t \mathbf{D}^G E(\mathbf{z}_{n+1}, \mathbf{z}_n) \cdot \mathbf{L}(\mathbf{z}_{n+1}, \mathbf{z}_n) \mathbf{D}^G S(\mathbf{z}_{n+1}, \mathbf{z}_n) \\ &\quad + \Delta t \mathbf{D}^G S(\mathbf{z}_{n+1}, \mathbf{z}_n) \cdot \mathbf{M}(\mathbf{z}_{n+1}, \mathbf{z}_n) \mathbf{D}^G S(\mathbf{z}_{n+1}, \mathbf{z}_n) \geq 0 \end{aligned} \quad (5.13)$$

Accordingly, the total entropy is always non-decreasing because of the symmetry and positive semi-definiteness of the discrete Dissipative matrix together with the non-interaction conditions.

Discrete symmetries. As discrete dissipative systems have been defined via the G -equivariant discrete derivative operator of the G -invariant total energy function $E: \mathcal{S} \mapsto \mathbb{R}$ and total entropy function $S: \mathcal{S} \mapsto \mathbb{R}$, their equations (5.9) pose symmetries with which discrete counterparts $\tilde{\mathbf{J}}$ of the continuous momentum maps $\mathbf{J}$ are associated. Thus, a mapping $\tilde{\mathbf{J}}: \mathcal{S} \mapsto \mathfrak{g}^*$ is a discrete momentum maps if the scalar function $\tilde{J}_\xi: \mathcal{S} \mapsto \mathbb{R}$ defined as

$$\tilde{J}_\xi(\mathbf{z}) = \tilde{\mathbf{J}}(\mathbf{z}) \cdot \xi, \quad (5.14)$$

for any $\xi \in \mathfrak{g}$, satisfies

$$\begin{aligned} \xi_{\mathcal{S}(\mathbf{z}_{n+\frac{1}{2}})} &= \mathbf{L}(\mathbf{z}_{n+1}, \mathbf{z}_n) \mathbf{D}^G \tilde{J}_\xi(\mathbf{z}_{n+1}, \mathbf{z}_n), \\ \mathbf{0} &= \mathbf{M}(\mathbf{z}_{n+1}, \mathbf{z}_n) \mathbf{D}^G \tilde{J}_\xi(\mathbf{z}_{n+1}, \mathbf{z}_n) \end{aligned} \quad (5.15)$$

Theorem 5.2. *The momentum maps of a discrete dissipative system with symmetries $(\mathcal{S}, \mathbf{L}, \mathbf{M}, \mathbf{D}^G, E, S)$ are conserved quantities of the solution of the discrete system (5.9).*

Proof. The directionality property along with the discrete equations (5.9) lead the balance of the scalar function (5.14) in any time subintervals to be

$$\tilde{J}_{\xi, n+1} - \tilde{J}_{\xi, n} = \mathbf{D}^G \tilde{J}_{\xi} \cdot (\mathbf{z}_{n+1} - \mathbf{z}_n) = \Delta t (\mathbf{D}^G \tilde{J}_{\xi} \cdot \mathbf{L} \mathbf{D}^G E + \mathbf{D}^G \tilde{J}_{\xi} \cdot \mathbf{M} \mathbf{D}^G S), \quad (5.16)$$

that, by using (5.15), simplifies to

$$\tilde{J}_{\xi, n+1} - \tilde{J}_{\xi, n} = -\Delta t \mathbf{D}^G E \cdot \boldsymbol{\xi}_{\mathcal{S}}(\mathbf{z}_{n+\frac{1}{2}}) = 0, \quad (5.17)$$

which vanishes due to the orthogonality property of the G -equivariant discrete derivative operator (5.7), demonstrating that the mapping $\tilde{\mathbf{J}}$ is conserved along the discrete system evolution. $\square$

5.2.2 Discrete infinite-dimensional dissipative systems

The formulation of EEM methods for the infinite-dimensional dissipative systems, defined in Chapter 4, encompasses two semi-discretizations: a first one standard in space and, then, a non-standard in time based on the discrete derivative concept.

Thus, any discretization technique commented in Section 3.7 that does not spoil its continuous evolution properties is considered standard and hence might perfectly be used to derive EEM methods. So far, the EEM formalism has been fully developed by performing a standard Galerkin FE-based spatial discretization and hence this approach will be assumed to propose EEM methods for the infinite-dimensional systems discussed in previous Chapters.

Then, as in Section 3.7, the infinite-dimensional state spaces defining dissipative systems are approximated by finite-dimensional subsets $\mathcal{S}^h \subset \mathcal{S}$ provided by the linear combination of shape functions typically defined in a regular partition of the infinite-dimensional domain $\mathcal{B}_0^h \subset \mathcal{B}_0$ such that

$$\mathcal{S}^h = \{\mathbf{z}^h = \sum_{a=1}^{\mathcal{N}} N^a \mathbf{z}^a \mid \mathbf{z}^h \in \mathcal{H}^1, \mathbf{z}^h = \bar{\mathbf{z}}^h \text{ on } \partial \mathcal{B}_0^{h, \varphi, \theta} \times [0, T]\}, \quad (5.18)$$

Similarly, the tangent space is also assumed to be approximated by the same subset such that

$$T\mathcal{S}^h = \{\mathbf{w}^h = \sum_{a=1}^{\mathcal{N}} N^a \mathbf{w}^a \mid \mathbf{w}^h \in \mathcal{H}^1, \mathbf{w}^h = \mathbf{0} \text{ on } \partial \mathcal{B}_0^{h, \varphi, \theta} \times [0, T]\}, \quad (5.19)$$

Once the standard spatial discretization has been performed, the following definition leads to the formulation of EEM methods.

Definition 5.5. A discrete infinite-dimensional smooth dissipative system with symmetries is a discrete system governed by the consistent discrete GENERIC equations

$$\frac{\mathcal{F}(\mathbf{z}_{n+1}^h) - \mathcal{F}(\mathbf{z}_n^h)}{\Delta t} = \{\{\mathcal{F}, E\}\}(\mathbf{z}_{n+1}^h, \mathbf{z}_n^h) + [[\mathcal{F}, S]](\mathbf{z}_{n+1}^h, \mathbf{z}_n^h), \quad (5.20)$$

for all $\mathcal{F} : \mathcal{S}^h \mapsto \mathbb{R}$ and $E : \mathcal{S}^h \mapsto \mathbb{R}$ being the total energy function and $S : \mathcal{S}^h \mapsto \mathbb{R}$ being the total entropy function.

The operator $\{\{\cdot, \cdot\}\} : \mathcal{S}^h \times \mathcal{S}^h \mapsto \mathbb{R}$ is a consistent second-order discrete counterpart of the bilinear Poisson operator satisfying the skew-symmetry, Jacobi and Leibniz properties, whereas the operator $[[\cdot, \cdot]] : \mathcal{S}^h \times \mathcal{S}^h \mapsto \mathbb{R}$ is similarly a consistent second-order discrete counterpart to the bilinear Dissipative operator being symmetric and positive-definite.

Proposition 5.3. *The solution of discrete infinite-dimensional dissipative systems (5.20) agrees with the discrete form of the laws of thermodynamics provided by*

$$E(\mathbf{z}_{n+1}^h) = E(\mathbf{z}_n^h), \quad S(\mathbf{z}_{n+1}^h) \geq S(\mathbf{z}_n^h), \quad (5.21)$$

if the discrete bilinear operators additionally satisfy the following discrete degeneracy or non-interaction conditions

$$\{\{S, \mathcal{F}\}\} = [[E, \mathcal{F}]] = 0, \quad (5.22)$$

for every functional $\mathcal{F} : \mathcal{S}^h \rightarrow \mathbb{R}$.

Proof. The proof relies on the discrete brackets properties along with the just introduced discrete degeneracy conditions. Then, choosing $\mathcal{F}(\mathbf{z}^h) = E(\mathbf{z}^h)$ in (5.20) leads to

$$E(\mathbf{z}_{n+1}^h) - E(\mathbf{z}_n^h) = \Delta t [\{\{E, E\}\}(\mathbf{z}_{n+1}^h, \mathbf{z}_n^h) + [[E, S]](\mathbf{z}_{n+1}^h, \mathbf{z}_n^h)] = 0 \quad (5.23)$$

Similarly, choosing $\mathcal{F}(\mathbf{z}^h) = S(\mathbf{z}^h)$ leads to

$$S(\mathbf{z}_{n+1}^h) - S(\mathbf{z}_n^h) = \Delta t [\{\{S, E\}\}(\mathbf{z}_{n+1}^h, \mathbf{z}_n^h) + [[S, S]](\mathbf{z}_{n+1}^h, \mathbf{z}_n^h)] \geq 0 \quad (5.24)$$

□

The introduced discrete brackets derive from the continuous ones (4.89) through the G -equivariant discrete functional derivative operator $\frac{\Delta^G \mathcal{F}}{\Delta \mathbf{z}}: \mathcal{S}^h \times \mathcal{S}^h \mapsto T\mathcal{S}^h$, also introduced by González (1996) for the formulation of Energy-momentum methods for infinite-dimensional Hamiltonian problems, and discrete differential operators $\mathbf{L}, \mathbf{M}: \mathcal{S}^h \times \mathcal{S}^h \times T\mathcal{S}^h \mapsto T\mathcal{S}^h$ satisfying the same properties as their continuous counterparts, so that, given two functional $\mathcal{F}, \mathcal{G}: \mathcal{S}^h \mapsto \mathbb{R}$, they can generally be expressed by

$$\{\{\mathcal{F}, \mathcal{G}\}\}(z_{n+1}^h, z_n^h) = \left\langle \frac{\Delta^G \mathcal{F}}{\Delta \mathbf{z}}(z_{n+1}^h, z_n^h), \mathbf{L} \left[\frac{\Delta^G \mathcal{G}}{\Delta \mathbf{z}}(z_{n+1}^h, z_n^h) \right] \right\rangle \quad (5.25)$$

$$[[\mathcal{F}, \mathcal{G}]](z_{n+1}^h, z_n^h) = \left\langle \frac{\Delta^G \mathcal{F}}{\Delta \mathbf{z}}(z_{n+1}^h, z_n^h), \mathbf{M} \left[\frac{\Delta^G \mathcal{G}}{\Delta \mathbf{z}}(z_{n+1}^h, z_n^h) \right] \right\rangle \quad (5.26)$$

The G -equivariant discrete functional derivative is then a second-order approximation of the functional derivative $\frac{\delta \mathcal{F}}{\delta \mathbf{z}}$ at the midpoint that possesses the crucial directionality property

$$\left\langle \frac{\Delta^G \mathcal{F}}{\Delta \mathbf{z}}(z_{n+1}^h, z_n^h), z_{n+1}^h - z_n^h \right\rangle = \mathcal{F}(z_{n+1}^h) - \mathcal{F}(z_n^h) \quad (5.27)$$

Accordingly, the left hand side of (5.20) can be expressed in terms of the Def. 5.1, that is

$$\frac{\mathcal{F}(z_{n+1}^h) - \mathcal{F}(z_n^h)}{\Delta t} = \left\langle \frac{\Delta^G \mathcal{F}}{\Delta \mathbf{z}}(z_{n+1}^h, z_n^h), \frac{z_{n+1}^h - z_n^h}{\Delta t} \right\rangle \quad (5.28)$$

On the other hand, for the types of functionals involved in the definition of infinite-dimensional dissipative systems in the sense of Def. 4.6, that is

$$\mathcal{F}(z^h) = \int_{\mathcal{B}_0^h} f(z^h) dV_0, \quad (5.29)$$

the G -equivariant discrete functional derivative is linked with the G -equivariant discrete derivative (5.8) by

$$\left\langle \frac{\Delta^G \mathcal{F}}{\Delta \mathbf{z}}(z_{n+1}^h, z_n^h), \mathbf{V} \right\rangle = \langle \mathbf{D}^G f(z_{n+1}^h, z_n^h), \mathbf{V} \rangle_{\mathcal{B}_0^h}, \quad \forall \mathbf{V} \in T\mathcal{S}^h \quad (5.30)$$

In short, for any element of the tangent space $\mathbf{w}^h \in T\mathcal{S}^h$, the general form of Galerkin-based EEM methods for infinite-dimensional dissipative sys-

tems is provided by the following weak statement

$$\begin{aligned} \left\langle \mathbf{w}^h, \frac{\mathbf{z}_{n+1}^h - \mathbf{z}_n^h}{\Delta t} \right\rangle &= \left\langle \mathbf{w}^h, \mathbf{L} \left[\frac{\Delta^G E}{\Delta \mathbf{z}} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h) \right] \right\rangle \\ &+ \left\langle \mathbf{w}^h, \mathbf{M} \left[\frac{\Delta^G S}{\Delta \mathbf{z}} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h) \right] \right\rangle \end{aligned} \quad (5.31)$$

Discrete laws of thermodynamics. In Galerkin-type formulations the preservation of the continuous structure ultimately relies on the fact that the discrete derivatives in the sense of (5.2) belong to the Galerkin-based space $T\mathcal{S}^h$ since the proof for the total energy and entropy to be discretely preserved follows from replacing the weighting functions by them. Thus, choosing $\mathbf{w}^h = \frac{\Delta^G E}{\Delta \mathbf{z}}$ in (5.31) and using its directionality property, the energy balance gives

$$\begin{aligned} \frac{E(\mathbf{z}_{n+1}^h) - E(\mathbf{z}_n^h)}{\Delta t} &= \left\langle \frac{\Delta^G E}{\Delta \mathbf{z}} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h), \mathbf{L} \left[\frac{\Delta^G E}{\Delta \mathbf{z}} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h) \right] \right\rangle \\ &+ \left\langle \frac{\Delta^G E}{\Delta \mathbf{z}} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h), \mathbf{M} \left[\frac{\Delta^G S}{\Delta \mathbf{z}} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h) \right] \right\rangle = 0, \end{aligned} \quad (5.32)$$

which vanishes due to the skew-symmetry of the discrete Poisson operator and the degeneracy conditions.

Similarly, choosing $\mathbf{w}^h = \frac{\Delta^G S}{\Delta \mathbf{z}}$ in (5.31) and using its directionality property, the entropy balance yields

$$\begin{aligned} \frac{S(\mathbf{z}_{n+1}^h) - S(\mathbf{z}_n^h)}{\Delta t} &= \left\langle \frac{\Delta^G S}{\Delta \mathbf{z}} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h), \mathbf{L} \left[\frac{\Delta^G E}{\Delta \mathbf{z}} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h) \right] \right\rangle \\ &+ \left\langle \frac{\Delta^G S}{\Delta \mathbf{z}} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h), \mathbf{M} \left[\frac{\Delta^G S}{\Delta \mathbf{z}} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h) \right] \right\rangle \geq 0 \end{aligned} \quad (5.33)$$

Further details on this issue can be found in Romero (2010a).

Discrete symmetries. Similarly to the finite-dimensional case, the definition of the discrete dissipative systems via the G -equivariant discrete derivative operator of the G -invariant total energy function $E: \mathcal{S}^h \mapsto \mathbb{R}$ and total entropy function $S: \mathcal{S}^h \mapsto \mathbb{R}$ leads its discrete equations (5.20) to pose symmetries. Hence, discrete momentum maps $\tilde{\mathbf{J}}: \mathcal{S}^h \mapsto \mathfrak{g}^*$, corresponding with

those continuous momentum maps $\mathbf{J}$, are associated satisfying

$$\begin{aligned}\xi_{\mathcal{S}}(z_{n+\frac{1}{2}}^h) &= \mathbf{L}(z_{n+1}^h, z_n^h) \left[\frac{\Delta^G \tilde{J}_{\xi}}{\Delta z}(z_{n+1}^h, z_n^h) \right], \\ \mathbf{0} &= \mathbf{M}(z_{n+1}^h, z_n^h) \left[\frac{\Delta^G \tilde{J}_{\xi}}{\Delta z}(z_{n+1}^h, z_n^h) \right]\end{aligned}\tag{5.34}$$

for any the scalar function $\tilde{J}_{\xi}: \mathcal{S}^h \mapsto \mathbb{R}$ defined as

$$\tilde{J}_{\xi}(z^h) = \tilde{\mathbf{J}}(z^h) \cdot \xi, \quad \forall \xi \in \mathfrak{g}\tag{5.35}$$

Theorem 5.4. *The momentum maps of a discrete infinite-dimensional dissipative system with symmetries are conserved quantities of the solution of the discrete system (5.20).*

Proof. The directionality property along with the discrete equations (5.9) lead the balance of the scalar function (5.14) in any time subintervals to be

$$\begin{aligned}\tilde{J}_{\xi, n+1} - \tilde{J}_{\xi, n} &= \left\langle \frac{\Delta^G \tilde{J}_{\xi}}{\Delta z}, z_{n+1}^h - z_n^h \right\rangle \\ &= \Delta t \left\langle \frac{\Delta^G \tilde{J}_{\xi}}{\Delta z}, \mathbf{L} \left[\frac{\Delta^G E}{\Delta z} \right] \right\rangle + \Delta t \left\langle \frac{\Delta^G \tilde{J}_{\xi}}{\Delta z}, \mathbf{M} \left[\frac{\Delta^G S}{\Delta z} \right] \right\rangle,\end{aligned}\tag{5.36}$$

that, by using (5.34) along with (5.30), simplifies to

$$\tilde{J}_{\xi, n+1} - \tilde{J}_{\xi, n} = -\Delta t \left\langle \frac{\Delta^G E}{\Delta z}(z_{n+1}^h, z_n^h), \xi_{\mathcal{S}}(z_{n+\frac{1}{2}}^h) \right\rangle = 0,\tag{5.37}$$

which vanishes due to the orthogonality property of the G -equivariant discrete derivative operator (5.7), demonstrating that the mapping $\tilde{\mathbf{J}}$ is conserved along the discrete system evolution. $\square$

5.3 EEM methods for the two thermo-spring system

Based on the general format provided by (5.9), EEM methods are attained for the two thermo-spring system based on both the entropy and the temperature descriptions.

5.3.1 Entropy-based EEM method

Departing from the finite-dimensional state space (4.27) and the total energy (4.28) and entropy (4.29) defined on it, the G -equivariant discrete derivative operator applied to them can be elaborated by using (5.8) to give

$$\begin{aligned} D^G E(\mathbf{z}_{n+1}, \mathbf{z}_n) &= \left[D\pi(\mathbf{z}_{n+\frac{1}{2}}) \right]^T D\tilde{E}(\pi(\mathbf{z}_{n+1}), \pi(\mathbf{z}_n)) \\ D^G S(\mathbf{z}_{n+1}, \mathbf{z}_n) &= \left[D\pi(\mathbf{z}_{n+\frac{1}{2}}) \right]^T D\tilde{S}(\pi(\mathbf{z}_{n+1}), \pi(\mathbf{z}_n)), \end{aligned} \quad (5.38)$$

where π is an invariant function respect to the action of Lie groups that is at most quadratic on its argument according to Prop. 5.1.

In subsection 4.3.3, the two thermo-spring system was proved to be symmetric respect to the rotation group $SO(3)$ and associated with this symmetry, a momentum map, identified with the total angular momentum (3.51), was proved to be a conserved quantity of the system evolution according to Noether's theorem. As the state space (4.27) results in the $\mathbb{R}^{10}$ space, nine invariants respect to the said group are identified to be

$$\begin{aligned} \pi_1 &= \lambda_1^2, \quad \pi_2 = \lambda_2^2, \quad \pi_3 = \|\mathbf{p}_1\|^2 \\ \pi_4 &= \|\mathbf{p}_2\|^2, \quad \pi_5 = \eta_1, \quad \pi_6 = \eta_2 \\ \pi_7 &= \mathbf{q}_1 \cdot \mathbf{p}_1, \quad \pi_8 = \mathbf{q}_2 \cdot \mathbf{p}_2, \quad \pi_9 = \mathbf{q}_1 \cdot \mathbf{q}_2 \end{aligned} \quad (5.39)$$

The proof for their invariability respect to the $SO(3)$ group closely follows the arguments used in (4.45). On the other hand, they are crucially linear, bilinear or quadratic functions of the state vector and hence invariants in the sense of Prop. 5.1.

Remark 5.1. The spring elongations λ_i are also invariants respect to the action of the $SO(3)$ as proved (4.45), however, their definitions are not linear, bilinear or quadratic functions of the state variables and hence cannot be used as invariant functions according to Prop. 5.1.

Then, collecting all these invariant functions in a vector-valued function $\pi(\mathbf{z}) = (\pi_1, \pi_2, \pi_3, \pi_4, \pi_5, \pi_6, \pi_7, \pi_8, \pi_9)^T$, its gradient respect to the state

space reads

$$D\pi(\mathbf{z}) = \begin{pmatrix} \frac{\partial \lambda_1^2}{\partial \mathbf{q}_1} & \mathbf{0} & \mathbf{0} & \mathbf{0} & 0 & 0 \\ \frac{\partial \lambda_2^2}{\partial \mathbf{q}_1} & \frac{\partial \lambda_2^2}{\partial \mathbf{q}_2} & \mathbf{0} & \mathbf{0} & 0 & 0 \\ \mathbf{0} & \mathbf{0} & 2\mathbf{p}_1 & \mathbf{0} & 0 & 0 \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & 2\mathbf{p}_2 & 0 & 0 \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & 1 & 0 \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & 0 & 1 \\ \mathbf{p}_1 & \mathbf{0} & \mathbf{q}_1 & \mathbf{0} & 0 & 0 \\ \mathbf{0} & \mathbf{p}_2 & \mathbf{0} & \mathbf{q}_2 & 0 & 0 \\ \mathbf{q}_2 & \mathbf{q}_1 & \mathbf{0} & \mathbf{0} & 0 & 0 \end{pmatrix}, \quad (5.40)$$

where the partial derivatives of the elongations are provided by

$$\frac{\partial \lambda_1^2}{\partial \mathbf{q}_1} = 2\mathbf{q}_1, \quad \frac{\partial \lambda_2^2}{\partial \mathbf{q}_1} = 2(\mathbf{q}_1 - \mathbf{q}_2), \quad \frac{\partial \lambda_2^2}{\partial \mathbf{q}_2} = 2(\mathbf{q}_2 - \mathbf{q}_1), \quad (5.41)$$

Furthermore, the total energy (4.28) can be expressed through these invariants, thus obtaining the reduced total energy function to be

$$\tilde{E}(\pi(\mathbf{z})) = \tilde{K}(\pi_3, \pi_4) + \sum_{a=1}^2 \tilde{e}_a(\pi_a, \pi_{a+4}) = \sum_{a=1}^2 \left(\frac{\pi_{a+2}}{2m_a} + \tilde{e}_a(\pi_a, \pi_{a+4}) \right) \quad (5.42)$$

For its part, the reduced total entropy does not change as just depend on two of the invariants, that is

$$\tilde{S}(\pi(\mathbf{z})) = \pi_5 + \pi_6, \quad (5.43)$$

Accordingly, the partitioned definition of the discrete derivative operator (5.3) is applied to obtain the discrete derivative of them

$$D\tilde{E}(\pi_{n+1}, \pi_n) = \begin{pmatrix} D_{\lambda_1^2} \tilde{e}_1 \\ D_{\lambda_2^2} \tilde{e}_2 \\ (2m_1)^{-1} \\ (2m_2)^{-1} \\ D_{\eta_1} \tilde{e}_1 \\ D_{\eta_2} \tilde{e}_2 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad D\tilde{S}(\pi_{n+1}, \pi_n) = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad (5.44)$$

Each of the previous partitioned discrete derivatives operators applies to scalar-valued functions defined on a Cartesian product space. As an example, the partial discrete derivative of the internal energy function in terms of the first or the second invariants $\pi_a = \lambda_a^2$ is provided by

$$D_{\lambda_a^2} \tilde{e}_a = \frac{\tilde{e}_a(\lambda_{a,n+1}^2, \eta_{a,n+1}) - \tilde{e}_a(\lambda_{a,n}^2, \eta_{a,n+1}) + \tilde{e}_a(\lambda_{a,n+1}^2, \eta_{a,n}) - \tilde{e}_a(\lambda_{a,n}^2, \eta_{a,n})}{2(\lambda_{a,n+1}^2 - \lambda_{a,n}^2)} \quad (5.45)$$

Due to the consistency property of the discrete derivative operator (5.5), the above expression is well-defined when $\lambda_{a,n+1}^2 \rightarrow \lambda_{a,n}^2$, particularly, it becomes

$$\lim_{\lambda_{a,n+1}^2 \rightarrow \lambda_{a,n}^2} D_{\lambda_a^2} \tilde{e}_a = \frac{1}{2} \left(\frac{\partial \tilde{e}_a}{\partial \lambda_a^2}(\lambda_{a,n}^2, \eta_{a,n+1}) + \frac{\partial \tilde{e}_a}{\partial \lambda_a^2}(\lambda_{a,n}^2, \eta_{a,n}) \right) \quad (5.46)$$

Accordingly, the partial discrete derivative respect to the fifth or the sixth invariants, that is, the spring entropies, is provided by

$$D_{\eta_a} \tilde{e}_a = \frac{\tilde{e}_a(\lambda_{a,n+1}^2, \eta_{a,n+1}) - \tilde{e}_a(\lambda_{a,n+1}^2, \eta_{a,n}) + \tilde{e}_a(\lambda_{a,n}^2, \eta_{a,n+1}) - \tilde{e}_a(\lambda_{a,n}^2, \eta_{a,n})}{2(\eta_{a,n+1} - \eta_{a,n})} \quad (5.47)$$

Similarly, in the limit case of $\eta_{a,n+1} \rightarrow \eta_{a,n}$, the above partial derivative becomes

$$\lim_{\eta_{a,n+1} \rightarrow \eta_{a,n}} D_{\eta_a} \tilde{e}_a = \frac{1}{2} \left(\frac{\partial \tilde{e}_a}{\partial \eta_a}(\lambda_{a,n+1}^2, \eta_{a,n}) + \frac{\partial \tilde{e}_a}{\partial \eta_a}(\lambda_{a,n}^2, \eta_{a,n}) \right) \quad (5.48)$$

The proofs of the limit cases and the general format of the partial discrete derivatives for these types of functions can be found in Appendix A.

Furthermore, the definition of the discrete derivative operator (5.2) applied to linear or quadratic functions simply coincides with the standard derivative evaluated at midpoint. This result has been used to obtain the third and fourth components of the discrete derivative vector of the reduced total energy (5.42) as well as the fifth and sixth components of the discrete derivative vector of the reduced total entropy (5.43).

Now, the G -equivariant discrete derivative of the total energy and entropy

are elaborated by using (5.38) with (5.40) and (5.44) to give

$$\mathbf{D}^G E = \begin{pmatrix} \sum_{a=1}^2 \mathbf{D}_{\lambda_a^2} \tilde{e}_a \left(\frac{\partial \lambda_a^2}{\partial \mathbf{q}_1} \right)_{n+\frac{1}{2}} \\ \mathbf{D}_{\lambda_2^2} \tilde{e}_2 \left(\frac{\partial \lambda_2^2}{\partial \mathbf{q}_2} \right)_{n+\frac{1}{2}} \\ \mathbf{p}_{1,n+\frac{1}{2}}/m_1 \\ \mathbf{p}_{2,n+\frac{1}{2}}/m_2 \\ \mathbf{D}_{\eta_1} \tilde{e}_1 \\ \mathbf{D}_{\eta_2} \tilde{e}_2 \end{pmatrix}, \quad \mathbf{D}^G S = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 1 \end{pmatrix}, \quad (5.49)$$

According to the just obtained discrete derivatives, the discrete counterpart of the continuous Poisson matrix is just the continuous matrix itself (4.31), because it is constant, provided by

$$\mathbf{L}(\mathbf{z}_{n+1}, \mathbf{z}_n) = \mathbf{L}(\mathbf{z}) = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & 0 & 0 \\ \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & 0 & 0 \end{pmatrix} \quad (5.50)$$

In addition, the discrete counterpart of the continuous Dissipative matrix (4.32) are defined from the previous discrete derivatives to be

$$\mathbf{M}(\mathbf{z}_{n+1}, \mathbf{z}_n) = k \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & \frac{\mathbf{D}_{\eta_2} \tilde{e}_2}{\mathbf{D}_{\eta_1} \tilde{e}_1} & -1 \\ \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & -1 & \frac{\mathbf{D}_{\eta_1} \tilde{e}_1}{\mathbf{D}_{\eta_2} \tilde{e}_2} \end{pmatrix} \quad (5.51)$$

In view of the continuous Dissipative matrix (4.32), the resulting partitioned discrete derivatives in its discrete version are identified with the algorithmic temperatures θ_1^* and θ_2^* according to

$$\theta_a^* = \mathbf{D}_{\eta_a} \tilde{e}_a, \quad (5.52)$$

which are a second-order approximation of the continuous one (4.33).

Finally, inserting relationships (5.67) through (5.52) into the discrete GENERIC form (5.9), the following representation of the entropy-based EEM method for the two thermo-spring system is achieved

$$\begin{aligned}
\frac{\mathbf{q}_{a,n+1} - \mathbf{q}_{a,n}}{\Delta t} &= \frac{\mathbf{p}_{a,n+\frac{1}{2}}}{m_a} \\
\frac{\mathbf{p}_{a,n+1} - \mathbf{p}_{a,n}}{\Delta t} &= - \sum_{b=1}^2 \mathbf{D}_{\lambda_b^2} \tilde{\mathbf{e}}_b \left(\frac{\partial \lambda_b^2}{\partial \mathbf{q}_a} \right)_{n+\frac{1}{2}} \\
\frac{\eta_{1,n+1} - \eta_{1,n}}{\Delta t} &= k \left(\frac{\theta_2^*}{\theta_1^*} - 1 \right) \\
\frac{\eta_{2,n+1} - \eta_{2,n}}{\Delta t} &= k \left(\frac{\theta_1^*}{\theta_2^*} - 1 \right)
\end{aligned} \tag{5.53}$$

The set of discrete equations (5.53) is clearly recognized as a discrete counterpart of the continuous ones provided by (2.24) or (2.25).

Discrete laws of thermodynamics. The solution of the above discrete equations agrees with the laws of thermodynamics due to the properties of the discrete Poisson (5.50) and Dissipative (5.51) matrices along with the definition of discrete dissipative systems. Then, the energy conservation directly follows from (5.12) whereas the entropy production can be elaborated by using (5.13) to give

$$S_{n+1} - S_n = \Delta t k \frac{(\theta_2^* - \theta_1^*)^2}{\theta_1^* \theta_2^*} \geq 0, \tag{5.54}$$

Discrete symmetries. Due to the use of the G -equivariant discrete derivative operator definition based on the observation for the system to be symmetric respect to the $\text{SO}(3)$ group, the total angular momentum (3.51) is also discretely preserved. The proof closely follows the one performed in the continuous case (4.44) - (4.53), now using the discrete counterparts of the Poisson and Dissipative matrices and of the standard derivatives given by (5.50), (5.51) and (5.67) following (5.14) - (5.15).

Linearization of discrete evolution equations. The resulting entropy-based EEM method is an implicit scheme and, as every implicit scheme, it requires a linearization of the equations in order to employ a Newton-Raphson's strategy to obtain the roots of the residue at machine precision.

Then, the classical tangent matrix of the method has the format

$$\mathbf{K} = \left(\begin{array}{c|c|c} \mathbf{K}_{\mathbf{q}_a \mathbf{q}_b} & \mathbf{K}_{\mathbf{q}_a \mathbf{p}_b} & \mathbf{K}_{\mathbf{q}_a \eta_b} \\ \hline \mathbf{K}_{\mathbf{p}_a \mathbf{q}_b} & \mathbf{K}_{\mathbf{p}_a \mathbf{p}_b} & \mathbf{K}_{\mathbf{p}_a \eta_b} \\ \hline \mathbf{K}_{\eta_a \mathbf{q}_b} & \mathbf{K}_{\eta_a \mathbf{p}_b} & \mathbf{K}_{\eta_a \eta_b} \end{array} \right) \quad a, b = 1, 2 \quad (5.55)$$

Then, each of the blocks is elaborated next. Thus, the linearization of the first two equation respect to the positions and momenta yields

$$\mathbf{K}_{\mathbf{q}_a \mathbf{q}_b} = \frac{1}{\Delta t} \mathbf{1}_d, \quad \mathbf{K}_{\mathbf{q}_a \mathbf{p}_b} = \frac{1}{2m_a} \mathbf{1}_d, \quad \text{if } a = b \text{ otherwise } \mathbf{K}_{\mathbf{q}_a \mathbf{q}_b} = \mathbf{K}_{\mathbf{q}_a \mathbf{p}_b} = \mathbf{0} \quad (5.56)$$

The remaining linearization of these equations vanishes because they do not depend on the spring entropies

$$\mathbf{K}_{\mathbf{q}_a \eta_b} = \mathbf{0} \quad a, b = 1, 2 \quad (5.57)$$

Then, the linearization of the linear momentum balance respect to positions gives

$$\mathbf{K}_{\mathbf{p}_a \mathbf{q}_b} = \sum_{c=1}^2 \left[\frac{\partial \mathbf{D}_{\lambda_c^2} \tilde{e}_c}{\partial \lambda_{c,n+1}^2} \left(\frac{\partial \lambda_c^2}{\partial \mathbf{q}_a} \right)_{n+\frac{1}{2}} \otimes \left(\frac{\partial \lambda_c^2}{\partial \mathbf{q}_b} \right)_{n+1} + \frac{1}{2} \mathbf{D}_{\lambda_c^2} \tilde{e}_c \left(\frac{\partial^2 \lambda_c^2}{\partial \mathbf{q}_a \partial \mathbf{q}_b} \right)_{n+1} \right], \quad (5.58)$$

Now linearizing them respect to the momenta leads to

$$\mathbf{K}_{\mathbf{p}_a \mathbf{p}_b} = \frac{1}{\Delta t} \mathbf{1}_d \quad \text{if } a = b \text{ otherwise } \mathbf{K}_{\mathbf{p}_a \mathbf{p}_b} = \mathbf{0}, \quad (5.59)$$

whereas the linearization in terms of springs entropies yields

$$\mathbf{K}_{\mathbf{p}_a \eta_b} = \sum_{c=1}^2 \frac{\partial \mathbf{D}_{\lambda_c^2} \tilde{e}_c}{\partial \eta_{b,n+1}} \left(\frac{\partial \lambda_c^2}{\partial \mathbf{q}_a} \right)_{n+\frac{1}{2}}, \quad a, b = 1, 2 \quad (5.60)$$

Finally, the last blocks due to the linearization of the discrete energy balance equations result in

$$\begin{aligned} \mathbf{K}_{\eta_a \mathbf{q}_b} &= \frac{\partial \kappa_a}{\partial \lambda_{b,n+1}} \left(\frac{\partial \lambda_b}{\partial \mathbf{q}_b} \right)_{n+1}, \quad a, b = 1, 2 \\ \mathbf{K}_{\eta_a \eta_b} &= \frac{1}{\Delta t} + \frac{\partial \kappa_a}{\partial \eta_{a,n+1}}, \quad \mathbf{K}_{\eta_a \eta_b} = \frac{\partial \kappa_a}{\partial \eta_{b,n+1}}, \quad \text{if } a \neq b, a, b = 1, 2 \end{aligned} \quad (5.61)$$

where the scalars κ_a have been introduced as

$$\kappa_1 = k \left(\frac{\theta_2^*}{\theta_1^*} - 1 \right), \quad \kappa_2 = k \left(\frac{\theta_1^*}{\theta_2^*} - 1 \right) \quad (5.62)$$

Since they do not depend on momenta, the corresponding blocks vanish, that is $\mathbf{K}_{\eta_a \mathbf{p}_b} = \mathbf{0}$.

In the above expressions, the linearizations of the partial discrete derivative follows from the format provided by (5.45) or can be derived from the general linearized discrete derivative provided in Appendix A. Similarly, the second partial derivative of the elongations respect to positions vectors follows from (5.41).

5.3.2 Temperature-based EEM method

Similarly, focusing on the finite-dimensional state space (4.34) and its corresponding total energy (4.35) and entropy (4.36), their G -equivariant discrete derivatives are elaborated by identifying the nine invariants to be

$$\begin{aligned} \pi_1 &= \lambda_1^2, & \pi_2 &= \lambda_2^2, & \pi_3 &= \|\mathbf{p}_1\|^2 \\ \pi_4 &= \|\mathbf{p}_2\|^2, & \pi_5 &= \theta_1, & \pi_6 &= \theta_2 \\ \pi_7 &= \mathbf{q}_1 \cdot \mathbf{p}_1, & \pi_8 &= \mathbf{q}_2 \cdot \mathbf{p}_2, & \pi_9 &= \mathbf{q}_1 \cdot \mathbf{q}_2, \end{aligned} \quad (5.63)$$

whose standard derivative coincides with (5.40). Then, the reduced total energy is provided by

$$\tilde{E}(\pi(\mathbf{z})) = \tilde{K}(\pi_3, \pi_4) + \sum_{a=1}^2 \tilde{e}_a(\pi_a, \pi_{a+4}) = \sum_{a=1}^2 \left(\frac{\pi_{a+2}}{2m_a} + \tilde{e}_a(\pi_a, \pi_{a+4}) \right), \quad (5.64)$$

and the reduced total entropy by

$$\tilde{S}(\pi(\mathbf{z})) = \sum_{a=1}^2 \tilde{\eta}_a(\pi_a, \pi_{a+4}), \quad (5.65)$$

Accordingly, their discrete derivatives directly follow from the partitioned

definition of the discrete derivative operator (5.3) to give

$$\mathbf{D}\tilde{E}(\pi_{n+1}, \pi_n) = \begin{pmatrix} \mathbf{D}_{\lambda_1^2} \tilde{e}_1 \\ \mathbf{D}_{\lambda_2^2} \tilde{e}_2 \\ (2m_1)^{-1} \\ (2m_2)^{-1} \\ \mathbf{D}_{\theta_1} \tilde{e}_1 \\ \mathbf{D}_{\theta_2} \tilde{e}_2 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad \mathbf{D}\tilde{S}(\pi_{n+1}, \pi_n) = \begin{pmatrix} \mathbf{D}_{\lambda_1^2} \tilde{\eta}_1 \\ \mathbf{D}_{\lambda_2^2} \tilde{\eta}_2 \\ 0 \\ 0 \\ \mathbf{D}_{\theta_1} \tilde{\eta}_1 \\ \mathbf{D}_{\theta_2} \tilde{\eta}_2 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad (5.66)$$

Now performing the matrix multiplication of (5.40) by (5.66) according to (5.38), the G -equivariant discrete derivatives of the total energy and the total entropy reads

$$\mathbf{D}^G E = \begin{pmatrix} \sum_{a=1}^2 \mathbf{D}_{\lambda_a^2} \tilde{e}_a \left(\frac{\partial \lambda_a^2}{\partial \mathbf{q}_1} \right)_{n+\frac{1}{2}} \\ \mathbf{D}_{\lambda_2^2} \tilde{e}_2 \left(\frac{\partial \lambda_2^2}{\partial \mathbf{q}_2} \right)_{n+\frac{1}{2}} \\ \mathbf{p}_{1,n+\frac{1}{2}}/m_1 \\ \mathbf{p}_{2,n+\frac{1}{2}}/m_2 \\ \mathbf{D}_{\theta_1} \tilde{e}_1 \\ \mathbf{D}_{\theta_2} \tilde{e}_2 \end{pmatrix}, \quad \mathbf{D}^G S = \begin{pmatrix} \sum_{a=1}^2 \mathbf{D}_{\lambda_a^2} \tilde{\eta}_a \left(\frac{\partial \lambda_a^2}{\partial \mathbf{q}_1} \right)_{n+\frac{1}{2}} \\ \mathbf{D}_{\lambda_2^2} \tilde{\eta}_2 \left(\frac{\partial \lambda_2^2}{\partial \mathbf{q}_2} \right)_{n+\frac{1}{2}} \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{D}_{\theta_1} \tilde{\eta}_1 \\ \mathbf{D}_{\theta_2} \tilde{\eta}_2 \end{pmatrix}, \quad (5.67)$$

In agreement with these discrete gradients, the discrete counterpart of the Poisson matrix is provided by

$$\mathbf{L}(\mathbf{z}_{n+1}, \mathbf{z}_n) = \begin{pmatrix} \mathbf{0} & \mathbf{0} & \mathbf{1} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{1} & \mathbf{0} & \mathbf{0} \\ -\mathbf{1} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{L}_{11} & \mathbf{L}_{12} \\ \mathbf{0} & -\mathbf{1} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{L}_{22} \\ \mathbf{0}^T & \mathbf{0}^T & \bar{\mathbf{L}}_{11} & \mathbf{0}^T & \mathbf{0} & \mathbf{0} \\ \mathbf{0}^T & \mathbf{0}^T & \bar{\mathbf{L}}_{21} & \bar{\mathbf{L}}_{22} & \mathbf{0} & \mathbf{0} \end{pmatrix}, \quad (5.68)$$

with

$$\mathbf{L}_{ab} = -\bar{\mathbf{L}}_{ba}^T = (\mathbf{D}_{\theta_b} \tilde{\eta}_b)^{-1} \mathbf{D}_{\lambda_a^2} \tilde{\eta}_b \left(\frac{\partial \lambda_b^2}{\partial \mathbf{q}_a} \right)_{n+\frac{1}{2}} \quad (5.69)$$

Similarly, the discrete counterpart of the Dissipative matrix reads

$$\mathbf{M}(\mathbf{z}_{n+1}, \mathbf{z}_n) = k\theta_1^*\theta_2^* \begin{pmatrix} \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & M_{11} & M_{12} \\ \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & M_{12} & M_{22} \end{pmatrix}, \quad (5.70)$$

with

$$M_{ab} = (-1)^{a+b} (D_{\theta_a} \tilde{e}_a)^{-1} (D_{\theta_b} \tilde{e}_b)^{-1} \quad (5.71)$$

It can be easily verified that definitions (5.68) and (5.70) do satisfy the crucial structural properties stated by (5.11). In particular, the conditions for the discrete Dissipation matrix (5.70) hold independent of the specific choice for the algorithmic temperatures θ_1^* and θ_2^* . As a result, according to (5.9)-(5.13), any evaluation of them within the time interval would automatically define a discrete dissipative system counterpart and, hence, a second-order accurate monolithic EEM method.

However, among all possible candidates, one choice appears to be more *physical*. Unexpectedly, it is revealed by the discrete Poisson matrix (5.68) when is used to generate the right hand side of the discrete counterpart of the linear momentum balance. That is, multiplying its third and fourth rows by the G -equivariant discrete derivative of the total energy (5.66) to give

$$\sum_{j=1}^6 \mathbf{L}_{(a+2)j} D^G E_j = - \sum_{b=1}^2 \left(D_{\lambda_b^2} \tilde{e}_b - \frac{D_{\theta_b} \tilde{e}_b}{D_{\theta_b} \tilde{\eta}_b} D_{\lambda_b^2} \tilde{\eta}_b \right) \left(\frac{\partial \lambda_b^2}{\partial \mathbf{q}_a} \right)_{n+\frac{1}{2}}, \quad a = 1, 2 \quad (5.72)$$

Then, identifying each of the terms of this discrete counterpart with the ones in the right hand side of the continuous equations (4.42)₂, the appearing ratios in the above expression must be counterparts of the spring temperatures.

With this reasoning, the algorithmic temperatures are chosen to be

$$\theta_a^* = \frac{D_{\theta_a} \tilde{e}_a}{D_{\theta_a} \tilde{\eta}_a} \quad (5.73)$$

Remark 5.2. The above algorithmic temperature can be viewed as a canonical choice that provides an unique discrete counterpart of the specific heat capacity (3.78), that is

$$c_a = D_{\theta_a} \tilde{e}_a = \theta_a^* D_{\theta_a} \tilde{\eta}_a > 0, \quad (5.74)$$

which could not otherwise be achieved by any other definition, provided that use is made of the discrete derivative in the sense of González (1996).

Then, the partial discrete derivative operator respect to temperature applied to both the reduced internal energy and reduced entropy functions follows the format provided in (5.47) replacing entropies with temperatures, so the algorithmic temperature is provided by

$$\theta_a^* = \frac{\tilde{e}_a(\lambda_{a,n+1}^2, \theta_{a,n+1}) - \tilde{e}_a(\lambda_{a,n+1}^2, \theta_{a,n}) + \tilde{e}_a(\lambda_{a,n}^2, \theta_{a,n+1}) - \tilde{e}_a(\lambda_{a,n}^2, \theta_{a,n})}{\tilde{\eta}_a(\lambda_{a,n+1}^2, \theta_{a,n+1}) - \tilde{\eta}_a(\lambda_{a,n+1}^2, \theta_{a,n}) + \tilde{\eta}_a(\lambda_{a,n}^2, \theta_{a,n+1}) - \tilde{\eta}_a(\lambda_{a,n}^2, \theta_{a,n})}, \quad (5.75)$$

which, in the limit case of $\theta_{a,n+1} \rightarrow \theta_{a,n}$, collapses to

$$\lim_{\theta_{a,n+1} \rightarrow \theta_{a,n}} \theta_a^* = \frac{\frac{\partial \tilde{e}_a}{\partial \theta_a}(\lambda_{a,n}^2, \theta_{a,n}) + \frac{\partial \tilde{e}_a}{\partial \theta_a}(\lambda_{a,n}^2, \theta_{a,n})}{\frac{\partial \tilde{\eta}_a}{\partial \theta_a}(\lambda_{a,n+1}^2, \theta_{a,n}) + \frac{\partial \tilde{\eta}_a}{\partial \theta_a}(\lambda_{a,n}^2, \theta_{a,n})} \quad (5.76)$$

Finally, inserting relationships (5.66) through (5.73) into the discrete GENERIC form (5.9), the following representation of the temperature-based EEM method is achieved

$$\begin{aligned} \frac{\mathbf{q}_{a,n+1} - \mathbf{q}_{a,n}}{\Delta t} &= \frac{\mathbf{p}_{a,n+\frac{1}{2}}}{m_a} \\ \frac{\mathbf{p}_{a,n+1} - \mathbf{p}_{a,n}}{\Delta t} &= - \sum_{b=1}^2 \left(\mathbf{D}_{\lambda_b^2} \tilde{e}_b - \theta_b^* \mathbf{D}_{\lambda_b^2} \tilde{\eta}_b \right) \left(\frac{\partial \lambda_b^2}{\partial \mathbf{q}_a} \right)_{n+\frac{1}{2}} \\ \frac{\theta_{1,n+1} - \theta_{1,n}}{\Delta t} &= (\mathbf{D}_{\theta_1} \tilde{e}_1)^{-1} \left[-\theta_1^* \mathbf{D}_{\lambda_1^2} \tilde{\eta}_1 \left(\frac{\partial \lambda_1^2}{\partial \mathbf{q}_1} \right)_{n+\frac{1}{2}} \cdot \frac{\mathbf{p}_{1,n+\frac{1}{2}}}{m_1} + h^* \right] \\ \frac{\theta_{2,n+1} - \theta_{2,n}}{\Delta t} &= (\mathbf{D}_{\theta_2} \tilde{e}_2)^{-1} \left[-\theta_2^* \sum_{b=1}^2 \mathbf{D}_{\lambda_b^2} \tilde{\eta}_b \left(\frac{\partial \lambda_b^2}{\partial \mathbf{q}_b} \right)_{n+\frac{1}{2}} \cdot \frac{\mathbf{p}_{b,n+\frac{1}{2}}}{m_b} - h^* \right], \end{aligned} \quad (5.77)$$

where the consistent evaluation of the heat flux (2.1) is provided by

$$h^* = k(\theta_2^* - \theta_1^*) \quad (5.78)$$

The temperature-based EEM method (5.77) clearly resembles its continuous counterpart (4.42) and, hence (2.17), where the continuous partial derivatives have been replaced by its discrete counterparts and the temperatures have been consistently evaluated in the sense of (5.73).

What is more, the directionality property of the operator (5.4) enables the last two equations in (5.77) to be recast in the form

$$\begin{aligned} \frac{\eta_1(\lambda_{1,n+1}, \theta_{1,n+1}) - \eta_1(\lambda_{1,n}, \theta_{1,n})}{\Delta t} &= k \left(\frac{\theta_2^*}{\theta_1^*} - 1 \right) \\ \frac{\eta_2(\lambda_{2,n+1}, \theta_{2,n+1}) - \eta_2(\lambda_{2,n}, \theta_{2,n})}{\Delta t} &= k \left(\frac{\theta_1^*}{\theta_2^*} - 1 \right) \end{aligned} \quad (5.79)$$

This form resembles the one obtained in the entropy-based EEM method (5.53)_{3,4} with the particularity of the entropies being function of the state vector rather than part of the state vector.

Remark 5.3.

1. Although the use of an algorithmic temperature other than (5.73) is possible, as pointed out before, the method does not assume the easy-interpretable form (5.77), neither the discrete form (5.79) could be achieved. It should be noted, however, that this choice does not in any case alter (5.77)₂ since those algorithmic temperatures are imposed by the discrete Poisson matrix (5.68) and the G -equivariant discrete derivative of the total energy (5.67)₁ to be always provided by (5.73). Further insight on this issued will be provided in subsection 5.3.3 based on a particular example.
2. The thermodynamical consistency of (5.77) algorithmically relies on the application of the discrete derivative to both the internal energy and the entropy functions. In contrast to that, the entropy-based EEM method (5.53) requires only to apply the discrete derivative operator to the internal energy function expressed in terms of the entropy. Therefore, the temperature-based EEM method involves more computational cost which is the price to be paid in order to overcome the problems pointed out along this dissertation regarding provision of the potentials in terms of the entropy and the Dirichlet's boundary conditions for continuous problems.

Discrete laws of thermodynamics and symmetries. Due to the construction of the discrete version of the Poisson and Dissipative matrices according to (5.68) and (5.70), the conservation of energy as well as the production of entropy are guaranteed. It only remains to compute the increment of the entropy in each time step which follows from (5.13) to give

$$S_{n+1} - S_n = \Delta t k \frac{(\theta_2^* - \theta_1^*)^2}{\theta_1^* \theta_2^*} \geq 0, \quad (5.80)$$

and can be viewed as the discrete counterpart of (4.43).

The same reasons as those argued for the entropy-based EEM method applies in this case to assert that the resulting temperature-based EEM method (5.77) preserves the total angular momentum (3.51).

Linearization of discrete evolution equations. In this case the tangent matrix has the following format

$$\mathbf{K} = \left(\begin{array}{c|c|c} \mathbf{K}_{q_a q_b} & \mathbf{K}_{q_a p_b} & \mathbf{K}_{q_a \theta_b} \\ \hline \mathbf{K}_{p_a q_b} & \mathbf{K}_{p_a p_b} & \mathbf{K}_{p_a \theta_b} \\ \hline \mathbf{K}_{\theta_a q_b} & \mathbf{K}_{\theta_a p_b} & \mathbf{K}_{\theta_a \theta_b} \end{array} \right) \quad a, b = 1, 2 \quad (5.81)$$

Then, first row blocks coincide with the one for the entropy-based method (5.56) and (5.57). This time the linearization of the linear momentum balance respect to the positions vectors takes the same expression as (5.58) but in terms of the algorithmic internal forces defined by

$$f_a^* = D_{\lambda_a^2} \tilde{e}_a - \theta_a^* D_{\lambda_a^2} \tilde{\eta}_a, \quad (5.82)$$

so that the said matrix block now reads

$$\mathbf{K}_{p_a q_b} = \sum_{c=1}^2 \left[\frac{\partial f_c^*}{\partial \lambda_{c,n+1}^2} \left(\frac{\partial \lambda_c^2}{\partial \mathbf{q}_a} \right)_{n+\frac{1}{2}} \otimes \left(\frac{\partial \lambda_c^2}{\partial \mathbf{q}_b} \right)_{n+1} + \frac{1}{2} f_c^* \left(\frac{\partial^2 \lambda_c^2}{\partial \mathbf{q}_a \partial \mathbf{q}_b} \right)_{n+1} \right] \quad (5.83)$$

and, accordingly, the partial derivative of the algorithmic internal force respect to the current elongation gives

$$\frac{\partial f_a^*}{\partial \lambda_{a,n+1}} = \frac{\partial D_{\lambda_a^2} \tilde{e}_a}{\partial \lambda_{a,n+1}} - \frac{\partial \theta_a^*}{\partial \lambda_{a,n+1}} D_{\lambda_a^2} \tilde{\eta}_a - \theta_a^* \frac{\partial D_{\lambda_a^2} \tilde{\eta}_a}{\partial \lambda_{a,n+1}} \quad (5.84)$$

Similarly, the block due to the momenta $\mathbf{K}_{p_a p_b}$ coincides with (5.59), whereas the block due to the variation of temperatures is provided by

$$\mathbf{K}_{p_a \theta_b} = \frac{\partial f_b^*}{\partial \theta_{b,n+1}} \left(\frac{\partial \lambda_b^2}{\partial \mathbf{q}_a} \right)_{n+\frac{1}{2}}, \quad a, b = 1, 2. \quad (5.85)$$

In contrast, the blocks for the energy balance equations are much more involved than their counterparts of the entropy-based EEM method. To elaborate them, the scalars ρ_a, κ_a are introduced as

$$\rho_a = \frac{D_{\lambda_a^2} \tilde{\eta}_a}{D_{\theta_a} \tilde{\eta}_a}, \quad \kappa_a = k \frac{\theta_2^* - \theta_1^*}{D_{\theta_a} \tilde{e}_a}, \quad (5.86)$$

whose derivatives respect both elongations and temperatures are

$$\frac{\partial \rho_a}{\partial s_{a,n+1}} = \frac{1}{D_{\theta_a} \tilde{\eta}_a} \left(\frac{\partial D_{\lambda_a^2} \tilde{\eta}_a}{\partial s_{a,n+1}} - \rho_a \frac{\partial D_{\theta_a} \tilde{\eta}_a}{\partial s_{a,n+1}} \right), \quad s_a = \lambda_a, \theta_a \quad (5.87)$$

and

$$\frac{\partial \kappa_a}{\partial s_{c,n+1}} = \frac{1}{D_{\theta_a} \tilde{e}_a} \left[k \left(\frac{\partial \theta_2^*}{\partial s_{c,n+1}} - \frac{\partial \theta_1^*}{\partial s_{c,n+1}} \right) - \kappa_a \frac{\partial D_{\theta_a} \tilde{e}_a}{\partial s_{c,n+1}} \right], \quad s_c = \lambda_c, \theta_c \quad (5.88)$$

Thus, the linearization respect to the position vectors is of the form

$$\begin{aligned} \mathbf{K}_{\theta_a \mathbf{q}_b} = & \sum_{c=1}^2 \left[\frac{\partial \rho_a}{\partial \lambda_{a,n+1}} \left(\frac{\partial \lambda_a^2}{\partial \mathbf{q}_c} \right)_{n+\frac{1}{2}} \otimes \left(\frac{\partial \lambda_a}{\partial \mathbf{q}_b} \right)_{n+1} \right. \\ & \left. + \frac{1}{2} \rho_a \left(\frac{\partial^2 \lambda_a^2}{\partial \mathbf{q}_c \partial \mathbf{q}_b} \right)_{n+1} \right] \frac{\mathbf{p}_{c,n+\frac{1}{2}}}{m_c} + (-1)^a \frac{\partial \kappa_a}{\partial \lambda_{b,n+1}} \left(\frac{\partial \lambda_b}{\partial \mathbf{q}_b} \right)_{n+1} \end{aligned} \quad (5.89)$$

In this case, the linearized energy balances equations contributes to variations of the momenta

$$\mathbf{K}_{\theta_a \mathbf{p}_b} = \frac{\rho_a}{2m_b} \left(\frac{\partial \lambda_a^2}{\partial \mathbf{q}_b} \right)_{n+\frac{1}{2}} \quad (5.90)$$

Finally, the last block of the tangent matrix is provided by

$$\mathbf{K}_{\theta_a \theta_b} = \sum_{c=1}^2 \left[\frac{\partial \rho_a}{\partial \theta_{b,n+1}} \left(\frac{\partial \lambda_a^2}{\partial \mathbf{q}_c} \right)_{n+\frac{1}{2}} \cdot \frac{\mathbf{p}_{c,n+\frac{1}{2}}}{m_c} \right] + (-1)^a \frac{\partial \kappa_a}{\partial \theta_{b,n+1}} \quad (5.91)$$

5.3.3 Validation and comparison with standard methods

In section 2.3.3 three methods were proposed to discuss the performance of the Midpoint methods regarding the conservation properties. Now these examples are solved by the newly proposed EEM methods so that they can be validated and the conservation properties can be verified.

In addition, for the temperature formulation, four different choices for the algorithmic temperatures appearing in the discrete Dissipative matrix (5.70) have been implemented, giving raise to different temperature-based EEM methods, so as to gain insight into how this selection can affect the method's performance. Particularly, they are chosen to be either the current,

the converged, the midpoint or the reference (constant) temperatures. In making these choices, expressions (5.77) are not valid any more, specifically equations (5.77)_{3,4} become slightly different, as pointed out in Remark 5.3. Remarkably, in these implementations the algorithmic temperature of the discrete lineal momentum balance (5.77)₂ is still provided by (5.73) since it is constrained by the Poisson matrix (5.68) and the G -equivariant discrete derivative operator of the total energy (5.67).

First, to validate the EEM methods their order of accuracy based on the Example 1 of subsection 2.3.3 is studied by computing the relative error at different time step sizes with respect to a reference solution as

$$e_z = \frac{\|z - z_{\text{ref}}\|}{\|z_{\text{ref}}\|}, \quad (5.92)$$

z being the solution at $t_f = 25$ and z_{ref} being the reference solution at the same instant t_f obtained with the Midpoint method (5.183) and time step size of $\Delta t = 0.001$ s. The results obtained with the entropy-based and temperature-based EEM methods along with the temperature-based Midpoint and Trapezoidal methods are plotted in Figure 5.1. It shows the second order of accuracy of the EEM methods and the error constants which are very similar to the ones of Midpoint and Trapezoidal methods.

The same analysis is performed with the different temperature-based EEM methods resulting from the aforementioned choices for the algorithmic temperatures. The results are collected in Figure 5.2 and reveal that the choices inside the time interval yield the expected second order accuracy with the practically same exact constant error. Also expected, the constant choice leads to a poor order of accuracy as it is unable to provide a proper approximation of temperatures in each time step. However, Figure 5.3 shows the laws of thermodynamics provided by each of these EEM methods with a time step of $\Delta t = 0.3$ s. All of them, even the constant-temperature one, provide the correct evolution of the total energy and entropy, confirming that the preservation properties of the discrete setting (5.9) relies on the crucial structure of the Dissipative matrix (5.70) and supports the election based on (5.73) due to the reasons discussed in the previous subsection 5.3.2.

Figure 5.4 contains the solution of Example 1 of subsection 2.3.3 obtained with the entropy-based EEM method and a time step size of $\Delta t = 0.3$, which coincides with that reported by Romero (2009). The strains and temperatures evolution are apparently identical to the midpoint solution's shown in Figure 2.4, however, although unappreciable, they are as different as they must be to satisfy the first law of thermodynamics, which is confirmed by the

Figure 5.1. State vector error vs. time step

Figure 5.2. Example 1: State vector error vs. time step

Figure 5.3. Example 1: Total energy and total entropy obtained with each of the temperature-based EEM methods and $\Delta t = 0.3$. (Same legend as Figure 5.2).

curve of the energy evolution. Similarly, the total entropy evolution agrees with the second law of the thermodynamics and the angular momentum evolution is constant, confirming the theoretical results obtained in previous subsections.

The solution of Example 1 obtained with the temperature-based EEM method for $\Delta t = 0.3$ s is collected in Figure 5.5. Expectedly, the total energy, entropy and angular momentum curves agrees with their preservation laws. Interestingly, the final amount of entropy provided by this method is slightly different compared to the one provided by the entropy-based method. The reason is on the large time step size used. In fact, it can be verified that they both produce the same amount as the time step size is reduced. Remarkably, the reference solution provides the same final amount as the one provided by the entropy-based EEM method for the time step size used of $\Delta t = 0.3$ s.

Figure 5.6 and Figure 5.7 show the solution of Example 2 of subsection 2.3.3 obtained with the entropy-based and the temperature-based EEM methods, respectively. First, it is remarkable that the non-physical drift of the elongations observed in the midpoint solutions Figure 2.4 or Figure 2.3 has disappeared in both solutions. That is because the solution complies with the laws of thermodynamics as demonstrates the curves of the total energy and total entropy for both methods. Therefore, it is apparent that both the entropy-based and temperature-based methods allow for larger time steps to provide sound solutions.

Figure 5.4. Example 1: solution obtained with entropy-based EEM method with $\Delta t = 0.3$ s

Figure 5.5. Example 1: solution obtained with the temperature-based EEM method with $\Delta t = 0.3$ s

The evolution of the elongations shows the high frequencies involved by the stiff parameters of the springs. They are even appreciable in the evolution of temperatures by a small ripple around the mean evaluation. These high frequencies might not be correctly captured by the time step chosen, somehow explaining the different results for the elongations provided by the two EEM methods.

Figure 5.6. Example 2: solution obtained with entropy-based EEM method with $\Delta t = 0.1$ s

Figure 5.7. Example 2: solution obtained with temperature-based EEM method with $\Delta t = 0.1$ s

Now, the temperature-based EEM method is used to solve Example 3, which, recall, cannot be approached by an entropy formulation because the thermodynamic potentials in terms of entropy are unreachable. In contrast to the Midpoint method, the time step size of $\Delta t = 0.1$ s allows for the stable solution displayed in Figure 5.5. The stability is mainly attained by the satisfaction of the first law of thermodynamics depicted in the curve of the

total energy. Besides, the temperature-based EEM method provides solutions satisfying the entropy inequality and the preservation of angular momentum, as has theoretically been proved in previous subsections. Looking at the solution, the coupling is clearly visible in the evolution of temperatures.

Figure 5.8. Example 3: solution obtained with temperature-based EEM method with $\Delta t = 0.1$ s

In summary, the EEM methods outperforms their midpoint counterparts

due to their capacity to adhere to the essential conservation laws identified in the continuous equations. Among them all, the fulfillment of the first law of thermodynamics is crucial for the stability of the method for moderately large time step sizes.

5.4 EEM methods for the thermo-visco-elastic system

As in the case of the two thermo-spring system, the general discrete dissipative system equations (5.9) are used to propose EEM methods for the thermo-visco-elastic system presented in Section 2.2 based on the use of the entropies and of the temperatures.

5.4.1 Entropy-based EEM method

The entropy-based EEM method is directly derived from the finite-dimensional state space (4.54). The first step is then to apply the G -equivariant discrete derivative operator (5.8) to the total energy (4.55) and total entropy (4.56). For that, recall that this system poses two symmetries respect to the actions of the additive group $G = \mathbb{R}^d$ and the rotation group $G = \text{SO}(3)$, leading the total linear and angular momentum to be first integrals of the system evolution, as demonstrated in Section 4.4. Then, nine invariants functions respect to these actions are found to be

$$\begin{aligned} \pi_1 &= \lambda^2, & \pi_2 &= \|\mathbf{p}_1\|^2, & \pi_3 &= \|\mathbf{p}_2\|^2 \\ \pi_4 &= \gamma, & \pi_5 &= \eta, & \pi_6 &= \sigma \\ \pi_7 &= (\mathbf{q}_1 - \mathbf{q}_2) \cdot \mathbf{p}_1, & \pi_8 &= (\mathbf{q}_2 - \mathbf{q}_1) \cdot \mathbf{p}_2, & \pi_9 &= (\mathbf{q}_1 - \mathbf{q}_2) \cdot (\mathbf{q}_2 - \mathbf{q}_1) \end{aligned} \quad (5.93)$$

It can be easily verified that these functions are indeed invariants of both actions by following the same arguments as in (4.45) and (4.74). In addition, they all are linear, bilinear or quadratic functions of the state vector so they are appropriated invariants to construct G -equivariant discrete derivatives according to (5.8).

The standard derivative of the vector-valued function that collects all of

the above invariants $\pi(\mathbf{z}) = (\pi_1, \dots, \pi_9)$ results in the following matrix

$$D\pi(\mathbf{z}) = \begin{pmatrix} 2(\mathbf{q}_1 - \mathbf{q}_2) & 2(\mathbf{q}_2 - \mathbf{q}_1) & \mathbf{0} & \mathbf{0} & 0 & 0 & 0 \\ \mathbf{0} & \mathbf{0} & 2\mathbf{p}_1 & \mathbf{0} & 0 & 0 & 0 \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & 2\mathbf{p}_2 & 0 & 0 & 0 \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & 1 & 0 & 0 \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & 0 & 1 & 0 \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & 0 & 0 & 1 \\ \mathbf{p}_1 & -\mathbf{p}_1 & \mathbf{q}_1 - \mathbf{q}_2 & \mathbf{0} & 0 & 0 & 0 \\ -\mathbf{p}_2 & \mathbf{p}_2 & \mathbf{0} & \mathbf{q}_2 - \mathbf{q}_1 & 0 & 0 & 0 \\ \mathbf{q}_2 - \mathbf{q}_1 & \mathbf{q}_1 - \mathbf{q}_2 & \mathbf{0} & \mathbf{0} & 0 & 0 & 0 \end{pmatrix} \quad (5.94)$$

Based on these invariants, the reduced forms of the total energy and total entropy functions (4.55) are

$$\tilde{E}(\pi(\mathbf{z})) = \sum_{a=1}^2 \frac{\pi_{a+1}}{2m_a} + \tilde{e}(\pi_1, \pi_5, \pi_4) + \tilde{\epsilon}(\pi_6), \quad \tilde{S}(\pi(\mathbf{z})) = \pi_5 + \pi_6, \quad (5.95)$$

whose discrete derivatives are obtained via the partitioned definition (5.3) to be

$$D\tilde{E}(\pi_{n+1}, \pi_n) = \begin{pmatrix} D_{\lambda^2} \tilde{e} \\ (2m_1)^{-1} \\ (2m_2)^{-1} \\ D_{\gamma} \tilde{e} \\ D_{\eta} \tilde{e} \\ D_{\sigma} \tilde{\epsilon} \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad D\tilde{S}(\pi_{n+1}, \pi_n) = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad (5.96)$$

In this case, the partial discrete derivative respect to the first invariant is, following the formula for three-variable functions in Appendix A, provided by

$$\begin{aligned} D_{\lambda^2} \tilde{e} &= \frac{\tilde{e}(\lambda_{n+1}^2, \eta_{n+1}, \gamma_{n+1}) - \tilde{e}(\lambda_n^2, \eta_{n+1}, \gamma_n)}{2(\lambda_{n+1}^2 - \lambda_n^2)} \\ &+ \frac{\tilde{e}(\lambda_{n+1}^2, \eta_n, \gamma_{n+1}) - \tilde{e}(\lambda_n^2, \eta_n, \gamma_n)}{2(\lambda_{n+1}^2 - \lambda_n^2)} \end{aligned} \quad (5.97)$$

Due to the consistency property of the discrete derivative operator (5.5), the above expression is well-defined when $\lambda_{n+1}^2 \rightarrow \lambda_n^2$, particularly, it becomes

$$\lim_{\Delta\lambda^2 \rightarrow 0} D_{\lambda^2} \tilde{e} = \frac{1}{2} \left(\frac{\partial \tilde{e}}{\partial \lambda^2}(\lambda_n^2, \eta_{n+1}, \gamma_{n+1}) + \frac{\partial \tilde{e}}{\partial \lambda^2}(\lambda_n^2, \eta_n, \gamma_n) \right) \quad (5.98)$$

On the other hand, the environment internal energy function depends on just one variable so its discrete derivative is simply

$$D_{\sigma} \epsilon = \frac{\epsilon(\sigma_{n+1}) - \epsilon(\sigma_n)}{\sigma_{n+1} - \sigma_n} \quad (5.99)$$

For the rest of the partial discrete derivatives consult Appendix A.

Then, the G -equivariant discrete derivatives derives from these discrete derivatives together with (5.94) evaluated a midpoint $\mathbf{z}_{n+\frac{1}{2}}$ to yield

$$D^G E = \begin{pmatrix} 2(\mathbf{q}_1 - \mathbf{q}_2)_{n+\frac{1}{2}} D_{\lambda^2} \tilde{e} \\ 2(\mathbf{q}_2 - \mathbf{q}_1)_{n+\frac{1}{2}} D_{\lambda^2} \tilde{e} \\ \mathbf{p}_{1,n+\frac{1}{2}}/m_1 \\ \mathbf{p}_{2,n+\frac{1}{2}}/m_2 \\ D_{\gamma} \tilde{e} \\ D_{\eta} \tilde{e} \\ D_{\sigma} \tilde{e} \end{pmatrix}, \quad D^G S = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 1 \end{pmatrix} \quad (5.100)$$

As a result, the discrete counterpart of the Poisson matrix (4.57) are simply provided by

$$\mathbf{L}(\mathbf{z}_{n+1}, \mathbf{z}_n) = \mathbf{L}(\mathbf{z}), \quad (5.101)$$

whereas the discrete Dissipative matrix (4.58) yields

$$\mathbf{M}(\mathbf{z}_{n+1}, \mathbf{z}_n) = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0^T & 0^T & 0^T & 0^T & \frac{D_{\eta} \tilde{e}}{\nu^*} & -\frac{D_{\gamma} \tilde{e}}{\nu^*} & 0 \\ 0^T & 0^T & 0^T & 0^T & -\frac{D_{\gamma} \tilde{e}}{\nu^*} & \frac{(D_{\gamma} \tilde{e})^2 + \nu^* k D_{\sigma} \tilde{e}}{\nu^* D_{\eta} \tilde{e}} & -k \\ 0^T & 0^T & 0^T & 0^T & 0 & -k & k \frac{D_{\eta} \tilde{e}}{D_{\sigma} \epsilon} \end{pmatrix} \quad (5.102)$$

In this case, the discrete derivatives are clearly identified with the algorithmic internal and viscous forces and the temperatures

$$f^* = 2D_{\lambda^2}\tilde{e}, \quad g^* = -D_\gamma\tilde{e}, \quad \theta^* = D_\eta\tilde{e}, \quad \vartheta^* = D_\sigma\tilde{e} \quad (5.103)$$

In principle, the algorithmic counterpart of the viscosity parameter (2.51) is not restricted by the current formulation so any evaluation of the element temperature inside the time interval could be used, particularly, the algorithmic temperature to give

$$\nu^* = \nu_0 \exp \left[a \left(\frac{1}{\theta^*} - \frac{1}{\theta_{\text{ref}}} \right) \right], \quad \nu_0, a > 0 \quad (5.104)$$

Assuming these definitions, expressions (5.100) to (5.104) are used in (5.9) to arrive at the entropy-based EEM discrete evolution equations

$$\begin{aligned} \frac{\mathbf{q}_{a,n+1} - \mathbf{q}_{a,n}}{\Delta t} &= \frac{\mathbf{p}_{a,n+\frac{1}{2}}}{m_a} \\ \frac{\mathbf{p}_{a,n+1} - \mathbf{p}_{a,n}}{\Delta t} &= (-1)^a (\mathbf{q}_1 - \mathbf{q}_2)_{n+\frac{1}{2}} f^* \\ \frac{\gamma_{n+1} - \gamma_n}{\Delta t} &= \frac{g^*}{\nu^*} \\ \frac{\eta_{n+1} - \eta_n}{\Delta t} &= \frac{1}{\theta^*} \left[\frac{(-g^*)^2}{\nu^*} + k(\vartheta^* - \theta^*) \right] \\ \frac{\sigma_{n+1} - \sigma_n}{\Delta t} &= \frac{k}{\vartheta^*} (\theta^* - \vartheta^*) \end{aligned} \quad (5.105)$$

The resulting entropy-based EEM method (5.105) is very similar to its continuous counterpart (2.56).

Discrete laws of thermodynamics. The discrete laws of thermodynamics are guaranteed by the matrices properties according to (5.12) and (5.13). Thus, the increment of the entropy in each time step can be calculated to give

$$S_{n+1} - S_n = \Delta t k \frac{(\theta^* - \vartheta^*)^2}{\theta^* \vartheta^*} + \frac{(-g^*)^2}{\theta^* \nu^*} \geq 0, \quad (5.106)$$

which can be viewed as the discrete analogue of (4.71).

Discrete symmetries. The discrete symmetries are also inherited by the entropy-based EEM method (5.105) because the use of the G -equivariant discrete derivatives based on the invariability of the total energy and total entropy functions respect to the action of the additive and rotation groups.

Thus, the discrete version of the Noether's theorem 5.2 allows to assert that the total linear momentum (3.44) and the total angular momentum (3.51) are preserved quantities on the discrete solution. The proofs is equivalent to those performed in the continuous case in Sections 4.3 and 4.4.

Linearization of discrete evolution equations. The resulting implicit method requires the linearization of its discrete equations (5.105) that are collected in a tangent matrix of the form

$$\mathbf{K} = \left(\begin{array}{c|c|c|c|c} \mathbf{K}_{q_a q_b} & \mathbf{K}_{q_a p_b} & \mathbf{K}_{q_a \gamma} & \mathbf{K}_{q_a \eta} & \mathbf{K}_{q_a \sigma} \\ \hline \mathbf{K}_{p_a q_b} & \mathbf{K}_{p_a p_b} & \mathbf{K}_{p_a \gamma} & \mathbf{K}_{p_a \eta} & \mathbf{K}_{p_a \sigma} \\ \hline \mathbf{K}_{\gamma q_a} & \mathbf{K}_{\gamma p_a} & \mathbf{K}_{\gamma \gamma} & \mathbf{K}_{\gamma \eta} & \mathbf{K}_{\gamma \sigma} \\ \hline \mathbf{K}_{\eta q_b} & \mathbf{K}_{\eta p_b} & \mathbf{K}_{\eta \gamma} & \mathbf{K}_{\eta \eta} & \mathbf{K}_{\eta \sigma} \\ \hline \mathbf{K}_{\sigma q_b} & \mathbf{K}_{\sigma p_b} & \mathbf{K}_{\sigma \gamma} & \mathbf{K}_{\sigma \eta} & \mathbf{K}_{\sigma \sigma} \end{array} \right) \quad a, b = 1, 2 \quad (5.107)$$

Then, the first two blocks in the first row are identical to the blocks for the EEM methods of the two thermo-spring variable (5.56), whereas the last threes blocks are just provided by the null matrix.

Looking now at the second row blocks, the first one corresponding with the linearization of the discrete linear momentum balance respect to the position vectors reads

$$\mathbf{K}_{p_a q_b} = \frac{1}{2} \frac{\partial f^*}{\partial \lambda_{n+1}^2} \left(\frac{\partial \lambda^2}{\partial \mathbf{q}_a} \right)_{n+\frac{1}{2}} \otimes \left(\frac{\partial \lambda^2}{\partial \mathbf{q}_b} \right)_{n+1} + \frac{1}{4} f^* \left(\frac{\partial^2 \lambda^2}{\partial \mathbf{q}_a \partial \mathbf{q}_b} \right)_{n+1} \quad (5.108)$$

The second block fully coincides with (5.59), while the third and the fourth ones yield

$$\mathbf{K}_{p_a \gamma} = \frac{1}{2} \frac{\partial f^*}{\partial \gamma_{n+1}}, \quad \mathbf{K}_{p_a \eta} = \frac{1}{2} \frac{\partial f^*}{\partial \eta_{n+1}} \quad (5.109)$$

To end up with this row, the last block vanishes due to the linear momentum balance being non-dependent on the environment entropy.

The third row provides the linearization of the evolution equation for the internal variables. Thus, the linearization of this term respect to the positions, the element entropy and the internal variable can be elaborated to

give

$$\begin{aligned}
\mathbf{K}_{\gamma q_a} &= - \left(\frac{1}{\nu^*} \frac{\partial g^*}{\partial \lambda_{n+1}} - \frac{g^*}{(\nu^*)^2} \frac{\partial \nu^*}{\partial \lambda_{n+1}} \right) \left(\frac{\partial \lambda}{\partial q_a} \right)_{n+1} \\
\mathbf{K}_{\gamma \eta} &= - \frac{1}{\nu^*} \frac{\partial g^*}{\partial \eta_{n+1}} + \frac{g^*}{(\nu^*)^2} \frac{\partial \nu^*}{\partial \eta_{n+1}} \\
\mathbf{K}_{\gamma \gamma} &= \frac{1}{\Delta t} - \frac{1}{\nu^*} \frac{\partial g^*}{\partial \gamma_{n+1}} + \frac{g^*}{(\nu^*)^2} \frac{\partial \nu^*}{\partial \gamma_{n+1}},
\end{aligned} \tag{5.110}$$

with the rest of the blocks being zero.

On the other hand, all the blocks of the fourth row but one are non-zero. In particular, the linearization respect to the position vectors

$$\begin{aligned}
\mathbf{K}_{\eta q_a} &= \frac{1}{(\theta^*)^2} \frac{\partial \theta^*}{\partial \lambda_{n+1}^2} \left(\frac{(-g^*)^2}{\nu^*} + k(\vartheta^* - \theta^*) \right) \left(\frac{\partial \lambda^2}{\partial q_a} \right)_{n+1} \\
&\quad - \frac{1}{\theta^*} \left(\frac{2g^*}{\nu^*} \frac{\partial g^*}{\partial \lambda_{n+1}^2} - \left(\frac{g^*}{\nu^*} \right)^2 \frac{\partial \nu^*}{\partial \lambda_{n+1}^2} - k \frac{\partial \theta^*}{\partial \lambda_{n+1}^2} \right) \left(\frac{\partial \lambda^2}{\partial q_a} \right)_{n+1}
\end{aligned} \tag{5.111}$$

Similarly, the linearization respect to the internal variable reads

$$\begin{aligned}
\mathbf{K}_{\eta \gamma} &= \frac{1}{(\theta^*)^2} \frac{\partial \theta^*}{\partial \gamma_{n+1}} \left(\frac{(-g^*)^2}{\nu^*} + k(\vartheta^* - \theta^*) \right) \\
&\quad - \frac{1}{\theta^*} \left(\frac{2g^*}{\nu^*} \frac{\partial g^*}{\partial \gamma_{n+1}} - \left(\frac{g^*}{\nu^*} \right)^2 \frac{\partial \nu^*}{\partial \gamma_{n+1}} - k \frac{\partial \theta^*}{\partial \gamma_{n+1}} \right),
\end{aligned} \tag{5.112}$$

and the linearization respect to the element entropy yields

$$\begin{aligned}
\mathbf{K}_{\eta \eta} &= \frac{1}{\Delta t} + \frac{1}{(\theta^*)^2} \frac{\partial \theta^*}{\partial \eta_{n+1}} \left(\frac{(-g^*)^2}{\nu^*} + k(\vartheta^* - \theta^*) \right) \\
&\quad - \frac{1}{\theta^*} \left(\frac{2g^*}{\nu^*} \frac{\partial g^*}{\partial \eta_{n+1}} + \left(\frac{g^*}{\nu^*} \right)^2 \frac{\partial \nu^*}{\partial \eta_{n+1}} + k \frac{\partial \theta^*}{\partial \eta_{n+1}} \right)
\end{aligned} \tag{5.113}$$

The last block of the fourth row is then provided by

$$\mathbf{K}_{\eta \sigma} = -k \frac{1}{\theta^*} \frac{d\vartheta^*}{d\sigma_{n+1}} \tag{5.114}$$

Finally, the blocks in the last row are provided by

$$\begin{aligned}
\mathbf{K}_{\sigma \mathbf{q}_a} &= -\frac{k}{\vartheta^*} \frac{\partial \theta^*}{\partial \lambda_{n+1}} \left(\frac{\partial \lambda}{\partial \mathbf{q}_a} \right)_{n+1}, \quad a = 1, 2 \\
\mathbf{K}_{\sigma \gamma} &= -\frac{k}{\vartheta^*} \frac{\partial \theta^*}{\partial \gamma_{n+1}} \\
\mathbf{K}_{\sigma \eta} &= -\frac{k}{\vartheta^*} \frac{\partial \theta^*}{\partial \eta_{n+1}} \\
\mathbf{K}_{\sigma \sigma} &= \frac{1}{\Delta t} + k \frac{\theta^*}{(\vartheta^*)^2} \frac{d\vartheta^*}{d\sigma_{n+1}}
\end{aligned} \tag{5.115}$$

5.4.2 Temperature-based EEM method

Analogously, the temperature-based EEM method follows from the application of the G -equivariant discrete derivative operator to the total energy (4.61) and total entropy (4.62) expressed in terms of the state vector (4.60) and based on the following invariants

$$\begin{aligned}
\pi_1 &= \lambda^2, \quad \pi_2 = \|\mathbf{p}_1\|^2, \quad \pi_3 = \|\mathbf{p}_2\|^2 \\
\pi_4 &= \gamma, \quad \pi_5 = \theta, \quad \pi_6 = \vartheta \\
\pi_7 &= (\mathbf{q}_1 - \mathbf{q}_2) \cdot \mathbf{p}_1, \quad \pi_8 = (\mathbf{q}_2 - \mathbf{q}_1) \cdot \mathbf{p}_2, \quad \pi_9 = (\mathbf{q}_1 - \mathbf{q}_2) \cdot (\mathbf{q}_2 - \mathbf{q}_1)
\end{aligned} \tag{5.116}$$

These new invariant functions lead the reduced total energy and total entropy functions to be provided by

$$\begin{aligned}
\tilde{E}(\pi(\mathbf{z})) &= \sum_{a=1}^2 \frac{\pi_{a+1}}{2m_a} + \tilde{e}(\pi_1, \pi_5, \pi_4) + \tilde{\epsilon}(\pi_6) \\
\tilde{S}(\pi(\mathbf{z})) &= \tilde{\eta}(\pi_1, \pi_5, \pi_4) + \tilde{\sigma}(\pi_6),
\end{aligned} \tag{5.117}$$

Their respective discrete derivatives respect to the invariants are then derived from the partitioned definition (5.3) to give

$$\mathbf{D}\tilde{E}(\pi_{n+1}, \pi_n) = \begin{pmatrix} \mathbf{D}_{\lambda^2} \tilde{e} \\ (2m_1)^{-1} \\ (2m_2)^{-1} \\ \mathbf{D}_{\gamma} \tilde{e} \\ \mathbf{D}_{\theta} \tilde{e} \\ \mathbf{D}_{\vartheta} \tilde{\epsilon} \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad \mathbf{D}\tilde{S}(\pi_{n+1}, \pi_n) = \begin{pmatrix} \mathbf{D}_{\lambda^2} \tilde{\eta} \\ 0 \\ 0 \\ \mathbf{D}_{\gamma} \tilde{\eta} \\ \mathbf{D}_{\theta} \tilde{\eta} \\ \mathbf{D}_{\vartheta} \tilde{\sigma} \\ 0 \\ 0 \\ 0 \end{pmatrix}, \tag{5.118}$$

The G -equivariant discrete derivative can be elaborated following (5.38) with (5.94) to give

$$D^G E = \begin{pmatrix} 2(\mathbf{q}_1 - \mathbf{q}_2)_{n+\frac{1}{2}} D_{\lambda^2} \tilde{e} \\ 2(\mathbf{q}_2 - \mathbf{q}_1)_{n+\frac{1}{2}} D_{\lambda^2} \tilde{e} \\ \mathbf{p}_{1,n+\frac{1}{2}}/m_1 \\ \mathbf{p}_{2,n+\frac{1}{2}}/m_2 \\ D_\gamma \tilde{e} \\ D_\theta \tilde{e} \\ D_\vartheta \tilde{e} \end{pmatrix}, \quad D^G S = \begin{pmatrix} 2(\mathbf{q}_1 - \mathbf{q}_2)_{n+\frac{1}{2}} D_{\lambda^2} \tilde{\eta} \\ 2(\mathbf{q}_2 - \mathbf{q}_1)_{n+\frac{1}{2}} D_{\lambda^2} \tilde{\eta} \\ \mathbf{0} \\ \mathbf{0} \\ D_\gamma \tilde{\eta} \\ D_\theta \tilde{\eta} \\ D_\vartheta \tilde{\sigma} \end{pmatrix} \quad (5.119)$$

Accordingly, the discrete counterpart of the Poisson (4.64) is constructed in the following way

$$\mathbf{L}(\mathbf{z}_{n+1}, \mathbf{z}_n) = \begin{pmatrix} \mathbf{0} & \mathbf{0} & \mathbf{1} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{1} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ -\mathbf{1} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{L}_1 & \mathbf{0} \\ \mathbf{0} & -\mathbf{1} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{L}_2 & \mathbf{0} \\ \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & 0 & 0 & 0 \\ \mathbf{0}^T & \mathbf{0}^T & \bar{\mathbf{L}}_1 & \bar{\mathbf{L}}_2 & 0 & 0 & 0 \\ \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & 0 & 0 & 0 \end{pmatrix} \quad (5.120)$$

with

$$\mathbf{L}_a = -\bar{\mathbf{L}}_a^T = (-1)^a (D_\theta \tilde{\eta})^{-1} 2D_{\lambda^2} \tilde{\eta} (\mathbf{q}_2 - \mathbf{q}_1)_{n+\frac{1}{2}} \quad (5.121)$$

Similarly, the discrete counterpart of the Dissipative matrix (4.66) becomes

$$\mathbf{M}(\mathbf{z}_{n+1}, \mathbf{z}_n) = \theta^* \begin{pmatrix} \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & \frac{1}{\nu^*} & -\frac{D_\gamma \tilde{e}}{\nu^* D_\theta \tilde{e}} & 0 \\ \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & -\frac{D_\gamma \tilde{e}}{\nu^* D_\theta \tilde{e}} & \frac{(D_\gamma \tilde{e})^2 + \nu^* k \vartheta^*}{\nu^* D_\theta \tilde{e}^2} & -\frac{k \vartheta^*}{D_\theta \tilde{e} D_\vartheta \tilde{e}} \\ \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & \mathbf{0}^T & 0 & -\frac{k \vartheta^*}{D_\theta \tilde{e} D_\vartheta \tilde{e}} & \frac{k \vartheta^*}{D_\vartheta \tilde{e}^2} \end{pmatrix} \quad (5.122)$$

As in the case of the temperature-based EEM method for the two thermo-spring system, provided that the algorithmic temperatures θ^* and ϑ^* are evaluated at any point within the time step, the resulting temperature-based EEM method will be second-order accurate according to (5.9).

Similar reasons as those used in the mentioned case lead the algorithmic temperatures to be chosen as

$$\theta^* = \frac{D_\theta \tilde{\epsilon}}{D_\theta \tilde{\eta}}, \quad \vartheta^* = \frac{D_\vartheta \tilde{\epsilon}}{D_\vartheta \tilde{\sigma}} \quad (5.123)$$

Also, the algorithmic viscosity parameter can be provided by (5.104) but with the algorithmic element temperature just introduced.

The temperature-based EEM method then results from using the relations (5.118) - (5.123) in (5.9) to give

$$\begin{aligned} \frac{\mathbf{q}_{a,n+1} - \mathbf{q}_{a,n}}{\Delta t} &= \frac{\mathbf{p}_{a,n+\frac{1}{2}}}{m_a} \\ \frac{\mathbf{p}_{a,n+1} - \mathbf{p}_{a,n}}{\Delta t} &= (-1)^a (2D_{\lambda^2} \tilde{\epsilon} - \theta^* 2D_{\lambda^2} \tilde{\eta}) (\mathbf{q}_1 - \mathbf{q}_2)_{n+\frac{1}{2}} \\ \frac{\gamma_{n+1} - \gamma_n}{\Delta t} &= \frac{-1}{\nu^*} (D_\gamma \tilde{\epsilon} - \theta^* D_\gamma \tilde{\eta}) \\ \frac{\theta_{n+1} - \theta_n}{\Delta t} &= \frac{1}{D_\theta \tilde{\epsilon}} \left[-\theta^* 2D_{\lambda^2} \tilde{\eta} \sum_{a=1}^2 (-1)^a (\mathbf{q}_2 - \mathbf{q}_1)_{n+\frac{1}{2}} \cdot \frac{\mathbf{p}_{a,n+\frac{1}{2}}}{m_a} \right. \\ &\quad \left. + \frac{D_\gamma \tilde{\epsilon}}{\nu^*} (D_\gamma \tilde{\epsilon} - \theta^* D_\gamma \tilde{\eta}) + k(\vartheta^* - \theta^*) \right] \\ \frac{\vartheta_{n+1} - \vartheta_n}{\Delta t} &= k \frac{\theta^* - \vartheta^*}{D_\vartheta \tilde{\epsilon}} \end{aligned} \quad (5.124)$$

The resulting temperature-based EEM method (5.124) resembles its continuous counterpart (4.69). The discrete equation of the energy balance of the element (5.124)₄ can be simplified by elaborating the first term on the right hand side as follows

$$\begin{aligned} \sum_{a=1}^2 (-1)^a (\mathbf{q}_2 - \mathbf{q}_1)_{n+\frac{1}{2}} \cdot \frac{\mathbf{p}_{a,n+\frac{1}{2}}}{m_a} &= \sum_{a=1}^2 (-1)^a (\mathbf{q}_2 - \mathbf{q}_1)_{n+\frac{1}{2}} \cdot \frac{\mathbf{q}_{a,n+1} - \mathbf{q}_{a,n}}{\Delta t} \\ &= \frac{\lambda_{n+1}^2 - \lambda_n^2}{2 \Delta t} \end{aligned} \quad (5.125)$$

Then, the discrete equation reads

$$\begin{aligned} \frac{\theta_{n+1} - \theta_n}{\Delta t} = \frac{1}{D_{\theta}\tilde{e}} \left[-\theta^* 2D_{\lambda^2}\tilde{\eta} \frac{\lambda_{n+1}^2 - \lambda_n^2}{2\Delta t} \right. \\ \left. + \frac{D_{\gamma}\tilde{e}}{\nu^*} (D_{\gamma}\tilde{e} - \theta^* D_{\gamma}\tilde{\eta}) + k(\vartheta^* - \theta^*) \right] \end{aligned} \quad (5.126)$$

Furthermore, by introducing the algorithmic viscous force as

$$g^* = -(D_{\gamma}\tilde{e} - \theta^* D_{\gamma}\tilde{\eta}), \quad (5.127)$$

and using (5.124)₃, the second term of the right hand side of (5.126) becomes

$$\begin{aligned} \frac{\theta_{n+1} - \theta_n}{\Delta t} = \frac{1}{D_{\theta}\tilde{e}} \left[-\theta^* D_{\lambda^2}\tilde{\eta} \frac{\lambda_{n+1}^2 - \lambda_n^2}{\Delta t} \right. \\ \left. - (-g^* + \theta^* D_{\gamma}\tilde{\eta}) \frac{\gamma_{n+1} - \gamma_n}{\Delta t} + k(\vartheta^* - \theta^*) \right] \end{aligned} \quad (5.128)$$

Now, the definition of the algorithmic temperature (5.123) is introduced to give

$$\begin{aligned} \frac{\theta_{n+1} - \theta_n}{\Delta t} = -\frac{1}{D_{\theta}\tilde{\eta}} D_{\lambda^2}\tilde{\eta} \frac{\lambda_{n+1}^2 - \lambda_n^2}{\Delta t} - \frac{D_{\gamma}\tilde{\eta}}{D_{\theta}\tilde{\eta}} \frac{\gamma_{n+1} - \gamma_n}{\Delta t} \\ - \frac{-g^*}{D_{\theta}\tilde{e}} \frac{\gamma_{n+1} - \gamma_n}{\Delta t} + \frac{k(\vartheta^* - \theta^*)}{D_{\theta}\tilde{e}} \end{aligned} \quad (5.129)$$

Rearranging terms it can be written as follows

$$\begin{aligned} D_{\theta}\tilde{\eta} \frac{\theta_{n+1} - \theta_n}{\Delta t} + D_{\lambda^2}\tilde{\eta} \frac{\lambda_{n+1}^2 - \lambda_n^2}{\Delta t} + D_{\gamma}\tilde{\eta} \frac{\gamma_{n+1} - \gamma_n}{\Delta t} \\ = \frac{-g^*}{\theta^*} \frac{\gamma_{n+1} - \gamma_n}{\Delta t} + \frac{k(\vartheta^* - \theta^*)}{\theta^*} \end{aligned} \quad (5.130)$$

Finally, the three terms on the left hand side are identified with the directionality property of the discrete derivative operator so the equation takes the following entropy form

$$\frac{\eta(\lambda_{n+1}, \theta_{n+1}, \gamma_{n+1}) - \eta(\lambda_n, \theta_n, \gamma_n)}{\Delta t} = k \left(\frac{\vartheta^*}{\theta^*} - 1 \right) + \frac{(-g^*)^2}{\theta^* \nu^*}, \quad (5.131)$$

where use has also been made of the introduced identity and (5.124)₃.

In a similar but much more direct way, by using the directionality property the last equation in (5.124) can be simplified to

$$\frac{\sigma(\vartheta_{n+1}) - \sigma(\vartheta_n)}{\Delta t} = k \left(\frac{\theta^*}{\vartheta^*} - 1 \right) \quad (5.132)$$

These forms of the last two discrete equations of the temperature-based EEM method can alternatively be used in its implementation.

Discrete laws of thermodynamics. The conservation of the total energy and the production of entropy due to the conduction phenomenon and the internal viscous changes are readily verified by (5.12) and (5.13) using the discrete matrices and gradients used to derive the temperature-based EEM method. Particularly, the increment of the entropy can also be checked by noting that the total entropy balance is the balance of the element entropy plus the balance of environment entropy, provided by (5.131), to give

$$S_{n+1} - S_n = \Delta t k \frac{(\theta^* - \vartheta^*)^2}{\theta^* \vartheta^*} + \frac{(\mathbf{D}_\gamma \tilde{\epsilon} - \theta^* \mathbf{D}_\gamma \tilde{\eta})^2}{\theta^* \nu^*} \geq 0, \quad (5.133)$$

which can be viewed as the discrete analogue of (4.72).

Discrete symmetries the total linear and angular momenta are first integrals of the solution provided by the temperature-based EEM method, since use has been made of the G -equivariant discrete derivatives of the total energy and entropy. These functions are G -invariant functions respect to the additive and rotation groups so, according to the discrete Noether's theorem 5.2, the associated momentum maps are the total linear and angular momentums. Again, the proofs follow the guidelines provided for the continuous case.

Linearization of discrete evolution equations. The linearized discrete equations are assembled in this case in a tangent matrix with the following blocks

$$\mathbf{K} = \left(\begin{array}{c|c|c|c|c} \mathbf{K}_{q_a q_b} & \mathbf{K}_{q_a p_b} & \mathbf{K}_{q_a \gamma} & \mathbf{K}_{q_a \theta} & \mathbf{K}_{q_a \vartheta} \\ \hline \mathbf{K}_{p_a q_b} & \mathbf{K}_{p_a p_b} & \mathbf{K}_{p_a \gamma} & \mathbf{K}_{p_a \theta} & \mathbf{K}_{p_a \vartheta} \\ \hline \mathbf{K}_{\gamma q_a} & \mathbf{K}_{\gamma p_a} & \mathbf{K}_{\gamma \gamma} & \mathbf{K}_{\gamma \theta} & \mathbf{K}_{\gamma \vartheta} \\ \hline \mathbf{K}_{\theta q_a} & \mathbf{K}_{\theta p_a} & \mathbf{K}_{\theta \gamma} & \mathbf{K}_{\theta \theta} & \mathbf{K}_{\theta \vartheta} \\ \hline \mathbf{K}_{\vartheta q_a} & \mathbf{K}_{\vartheta p_a} & \mathbf{K}_{\vartheta \gamma} & \mathbf{K}_{\vartheta \theta} & \mathbf{K}_{\vartheta \vartheta} \end{array} \right) \quad a, b = 1, 2 \quad (5.134)$$

The first two blocks in the first row coincides with (5.56), while the last three blocks result in null matrices. In the second row, the first block is identical to (5.108) but with the algorithmic internal force being provided by

$$f^* = \mathbf{D}_{\lambda^2} \tilde{\epsilon} - \theta^* \mathbf{D}_{\lambda^2} \tilde{\eta} \quad (5.135)$$

Also, the above definition applies for the second block provided by (5.59) and the third and fourth blocks by (5.109).

Similarly, the blocks in the third row are provided by (5.110) in where the definition of the algorithmic viscous force is provided by (5.127) and the entropy variable is replaced by the temperature variable.

For the blocks in the fourth row, the ensuing definitions are introduced

$$\rho = \frac{D_{\lambda^2} \tilde{\eta}}{D_{\theta} \tilde{\eta}}, \quad \xi = \frac{D_{\gamma} \tilde{e}}{D_{\theta} \tilde{e}}, \quad \kappa = k \frac{\theta^* - \vartheta^*}{D_{\theta} \tilde{e}}, \quad (5.136)$$

so that the evolution equation due to the energy balance can be rewritten as follows

$$\frac{\theta_{n+1} - \theta_n}{\Delta t} = -2\rho D_{\lambda^2} \tilde{\eta} \sum_{a=1}^2 (-1)^a (\mathbf{q}_2 - \mathbf{q}_1)_{n+\frac{1}{2}} \cdot \frac{\mathbf{p}_{a,n+\frac{1}{2}}}{m_a} \quad (5.137)$$

$$+ \frac{\xi}{\nu^*} (D_{\gamma} \tilde{e} - \theta^* D_{\gamma} \tilde{\eta}) + \kappa \quad (5.138)$$

To linearize it, the derivatives of the previous scalars respect to the elongation, the internal variable or the temperatures are provided by

$$\frac{\partial \rho}{\partial s_{n+1}} = \frac{1}{D_{\theta} \tilde{\eta}} \left(\frac{\partial D_{\lambda^2} \tilde{\eta}}{\partial s_{n+1}} - \rho \frac{\partial D_{\theta} \tilde{\eta}}{\partial s_{n+1}} \right), \quad s = \lambda, \theta, \gamma, \quad (5.139)$$

$$\frac{\partial \xi}{\partial s_{n+1}} = \frac{1}{D_{\theta} \tilde{e}} \left(\frac{\partial D_{\gamma} \tilde{e}}{\partial s_{n+1}} - \xi \frac{\partial D_{\theta} \tilde{e}}{\partial s_{n+1}} \right), \quad s = \lambda, \theta, \gamma, \quad (5.140)$$

and

$$\frac{\partial \kappa}{\partial s_{n+1}} = \frac{1}{D_{\theta} \tilde{e}} \left[k \left(\frac{\partial \theta^*}{\partial s_{n+1}} - \frac{\partial \vartheta^*}{\partial s_{n+1}} \right) + \kappa \frac{\partial D_{\theta} \tilde{e}}{\partial s_{n+1}} \right], \quad s = \lambda, \theta, \gamma \quad (5.141)$$

Then, the first block can be expressed as follows

$$\begin{aligned} \mathbf{K}_{\theta \mathbf{q}_a} = & \sum_{b=1}^2 \left[\frac{\partial \rho}{\partial \lambda_{n+1}^2} \left(\frac{\partial \lambda^2}{\partial \mathbf{q}_b} \right)_{n+\frac{1}{2}} \otimes \left(\frac{\partial \lambda^2}{\partial \mathbf{q}_a} \right)_{n+1} + \frac{1}{2} \rho \left(\frac{\partial^2 \lambda^2}{\partial \mathbf{q}_b \partial \mathbf{q}_a} \right)_{n+1} \right] \frac{\mathbf{p}_{b,n+\frac{1}{2}}}{m_b} \\ & + \left(\frac{g^*}{\nu^*} \frac{\partial \xi}{\partial \lambda_{n+1}^2} + \frac{\xi}{\nu^*} \frac{\partial g^*}{\partial \lambda_{n+1}^2} - \frac{\xi g^*}{(\nu^*)^2} \frac{\partial \nu^*}{\partial \lambda_{n+1}^2} + \frac{\partial \kappa}{\partial \lambda_{n+1}^2} \right) \left(\frac{\partial \lambda^2}{\partial \mathbf{q}_a} \right)_{n+1} \end{aligned} \quad (5.142)$$

The contribution due to the momenta is then

$$\mathbf{K}_{\theta \mathbf{p}_a} = \frac{\rho}{2m_b} \left(\frac{\partial \lambda^2}{\partial \mathbf{q}_a} \right)_{n+\frac{1}{2}}, \quad a = 1, 2 \quad (5.143)$$

The linearization respect to the element temperature yields

$$\begin{aligned} \mathbf{K}_{\theta\theta} = & \frac{1}{\Delta t} + \sum_{a=1}^2 \left[\frac{\partial \rho}{\partial \theta_{n+1}} \left(\frac{\partial \lambda^2}{\partial \mathbf{q}_a} \right)_{n+\frac{1}{2}} \cdot \frac{\mathbf{p}_{a,n+\frac{1}{2}}}{m_a} \right] \\ & + \frac{g^*}{\nu^*} \frac{\partial \xi}{\partial \theta_{n+1}} + \frac{\xi}{\nu^*} \frac{\partial g^*}{\partial \theta_{n+1}} - \frac{\xi g^*}{(\nu^*)^2} \frac{\partial \nu^*}{\partial \theta_{n+1}} - \frac{\partial \kappa}{\partial \theta_{n+1}} \end{aligned} \quad (5.144)$$

The last block of the fourth row is then provided by

$$\mathbf{K}_{\theta\vartheta} = \frac{\partial \kappa}{\partial \vartheta_{n+1}} = -k \frac{1}{D_{\theta e}} \frac{d\vartheta^*}{d\vartheta_{n+1}} \quad (5.145)$$

Finally, the blocks in the last row are provided by

$$\begin{aligned} \mathbf{K}_{\vartheta \mathbf{q}_a} &= -\frac{k}{D_{\vartheta \tilde{\epsilon}}} \frac{\partial \theta^*}{\partial \lambda_{n+1}^2} \left(\frac{\partial \lambda^2}{\partial \mathbf{q}_a} \right)_{n+1}, \quad a = 1, 2 \\ \mathbf{K}_{\vartheta \gamma} &= -\frac{k}{D_{\vartheta \tilde{\epsilon}}} \frac{\partial \theta^*}{\partial \gamma_{n+1}} \\ \mathbf{K}_{\vartheta \theta} &= -\frac{k}{D_{\vartheta \tilde{\epsilon}}} \frac{\partial \theta^*}{\partial \theta_{n+1}} \\ \mathbf{K}_{\vartheta \vartheta} &= \frac{1}{\Delta t} - \frac{k}{D_{\vartheta \tilde{\epsilon}}^2} \left(\frac{d\vartheta^*}{d\vartheta_{n+1}} D_{\vartheta \tilde{\epsilon}} - \vartheta^* \frac{dD_{\vartheta \tilde{\epsilon}}}{d\vartheta_{n+1}} \right) \end{aligned} \quad (5.146)$$

5.4.3 Validation and comparison with standard methods

Next, the just devised EEM methods are validated and compared with the results for the two cases considered in subsection 2.3.3. In addition, results obtained with the standard Trapezoidal method have been considered. The validation to be performed is based on convergence plots of relative errors computed by (5.92) using the reference solutions provided in subsection 2.3.3.

Results for Case I. Figure 5.9 plots the relative position error. The results corroborate the second order convergence of the temperature-based EEM method and also reveal a superior accuracy compared with both implicit Midpoint method (2.89) and Trapezoidal method applied to the temperature-based system (2.45). On the other hand, the entropy-based EEM method results in this case a little bit more accurate in position than the temperature-based EEM one.

The convergence of temperature is displayed in Figure 5.10. Comparing with the range of relative errors in Figure 5.9, it becomes apparent that, for

this case, temperatures are more accurately computed than positions. Remarkably, the temperature-based EEM method is significantly more accurate than other methods, including the entropy-based EEM one.

The second order accuracy and the smaller constant error of the temperature-based EEM method, compared with the other methods, can also be seen in the convergence plot of the internal variable γ in Figure 5.11. Interestingly, the entropy-based EEM method provides poor accuracy, even compared with the standard Midpoint and Trapezoidal methods.

The solution including the long-term behavior of the laws of thermodynamics and the angular momentum are displayed in Figure 5.12 and Figure 5.13 for $\Delta t = 0.2$ s and for the temperature-based EEM and entropy-based EEM methods, respectively.

Figure 5.9. Case I: Position ($\mathbf{q}$) relative error

Results for Case II. This case can only be faced by the temperature-based EEM method due to the technical difficulties associated with the non-linear dependency of the spring stiffness with temperature that prevent the formulation of an entropy-based EEM method.

Figures 5.14, 5.15 and 5.16 display the relative errors in position ($\mathbf{q}$), element temperature (θ) and internal variable (γ). Again, the quadratic convergence is observed and the accuracy significantly improves compared

Figure 5.10. Case I: Temperature (θ) relative error

Figure 5.11. Case I: Internal variable (γ) relative error

Figure 5.12. Case I: solution obtained with temperature-based EEM method with $\Delta t = 0.2$ s

Figure 5.13. Case I: solution obtained with the entropy-based EEM method with $\Delta t = 0.2$ s

with both Trapezoidal and Midpoint methods. Convergence results for the environment temperature are omitted, since all methods exhibit similar accuracies for this particular case.

Figure 5.17 shows that, for the time step size $\Delta t = 0.3s$ that led the Midpoint method to not satisfy the law of thermodynamics, the temperature-based EEM method provides the right long-term behavior of the laws of thermodynamics and the angular momentum.

All these results confirm the superior stability and robustness features bestowed by the preservation of essential physical rules.

Figure 5.14. Case II: Position (q) relative error

Figure 5.15. Case II: Element temperature (θ) relative error

Figure 5.16. Case II: Internal variable (γ) relative error

Figure 5.17. Case II: solution obtained with temperature-based EEM method with $\Delta t = 0.3$ s

5.5 EEM methods for nonlinear thermoelasticity

In this section, the methodology introduced in subsection 5.2.2 is used to construct EEM time integration methods for the nonlinear dynamics of thermoelastic solids presented in Section 4.6. Once again, two different approaches based on the selection for the thermodynamical variable will be elaborated giving raise to the so called entropy-based EEM method and the temperature-based EEM method. While the first one was fully elaborated in Romero (2010a,b), the second one, to the best of the author's knowledge, has never been advocated.

5.5.1 Entropy-based EEM method

To construct an entropy-based EEM counterpart of nonlinear thermoe-lastodynamics, the infinite-dimensional state space (4.96) containing the density entropy is projected onto an finite-dimensional one defined in a partition of the continuum into regular elements by the linear combination of shape functions as was introduced in Section 3.7, that is

$$\mathcal{S}^h = \{\mathbf{z}^h = \sum_{a=1}^{\mathcal{N}} N^a \mathbf{z}^a = (\boldsymbol{\varphi}^h, \mathbf{p}^h, \eta^h) : \mathcal{B}_0^h \mapsto \mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}, \det(\nabla_0 \boldsymbol{\varphi}^h) > 0\}, \quad (5.147)$$

The tangent space is also projected onto the finite-dimensional space of linear combinations of shape functions to give

$$T\mathcal{S}^h = \{\mathbf{w}^h = \sum_{a=1}^{\mathcal{N}} N^a \mathbf{w}^a = (\mathbf{w}_{\boldsymbol{\varphi}}^h, \mathbf{w}_{\mathbf{p}}^h, w_{\eta}^h) : \mathcal{B}_0^h \mapsto \mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}\} \quad (5.148)$$

Then, in view of the continuous forms for the Poisson and the Dissipative brackets (4.102) and (4.103), their respective discrete counterparts, for two any functionals $\mathcal{F}, \mathcal{G} : \mathcal{S}^h \mapsto \mathbb{R}$, are provided by

$$\begin{aligned} \{\{\mathcal{F}, \mathcal{G}\}\}(\mathbf{z}_{n+1}^h, \mathbf{z}_n^h) &= \left\langle \frac{\Delta^G \mathcal{F}}{\Delta \boldsymbol{\varphi}}(\mathbf{z}_{n+1}^h, \mathbf{z}_n^h), \frac{\Delta^G \mathcal{G}}{\Delta \mathbf{p}}(\mathbf{z}_{n+1}^h, \mathbf{z}_n^h) \right\rangle \\ &\quad - \left\langle \frac{\Delta^G \mathcal{F}}{\Delta \mathbf{p}}(\mathbf{z}_{n+1}^h, \mathbf{z}_n^h), \frac{\Delta^G \mathcal{G}}{\Delta \boldsymbol{\varphi}}(\mathbf{z}_{n+1}^h, \mathbf{z}_n^h) \right\rangle \end{aligned} \quad (5.149)$$

$$\begin{aligned} [[\mathcal{F}, \mathcal{G}]](\mathbf{z}_{n+1}^h, \mathbf{z}_n^h) &= \left\langle \nabla_0 \left[\frac{1}{\Theta^*} \frac{\Delta^G \mathcal{F}}{\Delta \eta}(\mathbf{z}_{n+1}^h, \mathbf{z}_n^h) \right], (\Theta^*)^2 \mathbf{K}_{n+\frac{1}{2}}^h \nabla_0 \left[\frac{1}{\Theta^*} \frac{\Delta^G \mathcal{G}}{\Delta \eta}(\mathbf{z}_{n+1}^h, \mathbf{z}_n^h) \right] \right\rangle, \end{aligned} \quad (5.150)$$

where Θ^* is the algorithmic temperature to be defined within the time interval $[t_n, t_{n+1}]$ and $\mathbf{K}_{n+\frac{1}{2}}^h$ is the second order approximation of the material conductivity tensor provided by

$$\mathbf{K}_{n+\frac{1}{2}}^h = J_{n+\frac{1}{2}}^h \mathbf{F}_{n+\frac{1}{2}}^{h,-1} \boldsymbol{\kappa}(\Theta^*) \mathbf{F}_{n+\frac{1}{2}}^{h,-T}, \quad \text{with } J_{n+\frac{1}{2}}^h = \det \mathbf{F}_{n+\frac{1}{2}}^h \quad (5.151)$$

In order to elaborate the appearing G -equivariant discrete functional derivatives in the discrete brackets, recall that the total energy and the total entropy (4.98) are invariant functions respect to the additive and the rotation groups as was observed in Section 4.9. Then, the following invariant function respect to the actions of these group is identified

$$\pi(\mathbf{z}^h) = (\nabla_0 \boldsymbol{\varphi}^{hT} \nabla_0 \boldsymbol{\varphi}^h, \|\mathbf{p}^h\|^2, \eta^h) = (\mathbf{F}^{h,T} \mathbf{F}^h, \|\mathbf{p}^h\|^2, \eta^h), \quad (5.152)$$

whose components are additionally linear or quadratic functions of the state variables so they can be used as invariant functions in the sense of Prop. 5.1.

Based on this invariant function, the reduced total energy and total entropy read

$$\tilde{E}(\pi(\mathbf{z}^h)) = \int_{\mathcal{B}_0^h} \left(\frac{\pi_2}{2\rho_0} + \tilde{e}(\pi_1, \pi_3) \right) dV_0, \quad \tilde{S}(\pi(\mathbf{z}^h)) = \int_{\mathcal{B}_0^h} \pi_3 dV_0, \quad (5.153)$$

Now, with the help of (5.30) the G -equivariant discrete functional derivative of the total energy can be elaborated by using G -equivariant discrete derivative operator (5.8). To this end, the discrete derivative operator (5.2) of the above reduced functionals along with the standard derivative of the invariant function are used to give

$$\begin{aligned} \left\langle \frac{\Delta^G E}{\Delta \mathbf{z}} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h), \mathbf{w}^h \right\rangle &= \langle \mathbf{D}^G \left[\frac{\|\mathbf{p}^h\|^2}{2\rho_0} + e(\mathbf{C}^h, \eta^h) \right] (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h), \mathbf{w}^h \rangle_{\mathcal{B}_0^h} \\ &= \langle D\pi(\mathbf{z}_{n+\frac{1}{2}}^h)^T \mathbf{D} \left[\frac{\pi_2}{2\rho_0} + \tilde{e}(\pi_1, \pi_3) \right] (\pi_{n+1}, \pi_n), \mathbf{w}^h \rangle_{\mathcal{B}_0^h} \\ &= \langle \mathbf{D} \left[\frac{\pi_2}{2\rho_0} + \tilde{e}(\pi_1, \pi_3) \right] (\pi_{n+1}, \pi_n), D\pi(\mathbf{z}_{n+\frac{1}{2}}^h) \cdot \mathbf{w}^h \rangle_{\mathcal{B}_0^h} \\ &= \langle \mathbf{D}_{\pi_1} \tilde{e}(\pi_{n+1}, \pi_n), D\pi_1 \cdot \mathbf{w}_{\boldsymbol{\varphi}}^h \rangle_{\mathcal{B}_0^h} \\ &\quad + \langle \mathbf{D}_{\pi_2} \left[\frac{\pi_2}{2\rho_0} \right] (\pi_{n+1}, \pi_n), D\pi_2 \cdot \mathbf{w}_{\mathbf{p}}^h \rangle_{\mathcal{B}_0^h} \\ &\quad + \langle \mathbf{D}_{\pi_3} \tilde{e}(\pi_{n+1}, \pi_n), D\pi_3 w_{\eta}^h \rangle_{\mathcal{B}_0^h}, \end{aligned} \quad (5.154)$$

for any vector $\mathbf{w}^h \in T\mathcal{S}^h$.

Similarly, the G -equivariant discrete functional applied to the total entropy results in

$$\begin{aligned} \left\langle \frac{\Delta^G S}{\Delta \mathbf{z}} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h), \mathbf{w}^h \right\rangle &= \langle D^G \eta(\mathbf{z}_{n+1}^h, \mathbf{z}_n^h), \mathbf{w}^h \rangle_{\mathcal{B}_0} \\ &= \langle D\pi(\mathbf{z}_{n+\frac{1}{2}})^T D\pi_3, \mathbf{w}^h \rangle_{\mathcal{B}_0^h} \\ &= \langle D_{\pi_3} \pi_3, D\pi_3 w_\eta^h \rangle_{\mathcal{B}_0^h} \end{aligned} \quad (5.155)$$

Then, their final expressions are revealed by performing the standard derivatives of each component of the invariant function, which are

$$\begin{aligned} D\pi_1 \cdot \mathbf{a} &= D(\mathbf{F}^{h,T} \mathbf{F}^h) \cdot \mathbf{a} = \mathbf{F}^{h,T} \nabla_0 \mathbf{a} + \nabla_0 \mathbf{a}^T \mathbf{F}^h, \quad \forall \mathbf{a} \in \mathbb{R}^d \\ D\pi_2 \cdot \mathbf{a} &= D(\|\mathbf{p}^h\|^2) \cdot \mathbf{a} = 2\mathbf{p}^h \cdot \mathbf{a}, \quad \forall \mathbf{a} \in \mathbb{R}^d \\ D\pi_3 w &= D(\eta^h) w = w, \quad \forall w \in \mathbb{R} \end{aligned} \quad (5.156)$$

Using these results, the G -equivariant partial discrete functionals of the total energy are provided by

$$\begin{aligned} \left\langle \frac{\Delta^G E}{\Delta \boldsymbol{\varphi}} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h), \mathbf{w}_\varphi^h \right\rangle &= \langle 2\mathbf{F}_{n+\frac{1}{2}}^h D_{\pi_1} \tilde{e}(\pi_{n+1}, \pi_n), \nabla_0 \mathbf{w}_\varphi^h \rangle_{\mathcal{B}_0^h} \\ \left\langle \frac{\Delta^G E}{\Delta \mathbf{p}} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h), \mathbf{w}_p^h \right\rangle &= \left\langle \frac{\mathbf{p}_{n+\frac{1}{2}}^h}{\rho_0}, \mathbf{w}_p^h \right\rangle_{\mathcal{B}_0^h} \\ \left\langle \frac{\Delta^G E}{\Delta \eta} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h), w_\eta^h \right\rangle &= \langle D_{\pi_3} \tilde{e}(\pi_{n+1}, \pi_n), w_\eta^h \rangle_{\mathcal{B}_0^h}, \end{aligned} \quad (5.157)$$

where use has been made of the symmetry of the partial discrete derivative of the reduced internal energy density respect to the first invariant, identified with the symmetric right Cauchy-Green deformation tensor $\pi_1 = \mathbf{F}^{h,T} \mathbf{F}^h = \mathbf{C}^h$, and a second-order tensor product property².

For its part, the G -equivariant discrete functional of the total entropy is finally provided by

$$\left\langle \frac{\Delta^G S}{\Delta \eta} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h), w_\eta^h \right\rangle = \langle 1, w_\eta^h \rangle_{\mathcal{B}_0^h} \quad (5.158)$$

The resulting discrete derivatives of the reduced internal energy density function are clearly identified as discrete counterparts of the symmetric Piola-kirchhoff stress tensor and the temperature field, that is

$$\mathbf{S}^* = 2D_{\pi_1} \tilde{e}(\pi_{n+1}, \pi_n) = 2D_{\mathbf{C}} e, \quad \Theta^* = D_{\pi_3} \tilde{e}(\pi_{n+1}, \pi_n) = D_\eta e \quad (5.159)$$

² $\mathbf{A} : \mathbf{B} \mathbf{C} = \mathbf{B}^T \mathbf{A} : \mathbf{C}$

Following the partitioned definition of the discrete derivative operator, they are derived from the first and second discrete derivatives of functions depending on the right Cauchy-Green deformation tensor as a first argument and on a scalar thermodynamical variable, in this case the entropy density, as a second argument. Their elaborated formulas can be found in Appendix A and are summarized next

$$\mathbf{S}^* = 2\mathbf{D}_{\mathbf{C}}e = \bar{\mathbf{S}}_{n+\frac{1}{2}}^h + \frac{\Delta e_{n+1} + \Delta e_n - \bar{\mathbf{S}}_{n+\frac{1}{2}}^h : \Delta \mathbf{C}^h}{\Delta \mathbf{C}^h : \Delta \mathbf{C}^h} \Delta \mathbf{C}^h, \quad (5.160)$$

where

$$\Delta e_i = e(\mathbf{C}_{n+1}^h, \eta_i^h) - e(\mathbf{C}_n^h, \eta_i^h), \quad (5.161)$$

and the following simplified notation has been introduced

$$\bar{\mathbf{S}}_{n+\frac{1}{2}}^h = \frac{1}{2}(\mathbf{S}_{n+1} + \mathbf{S}_n) \text{ with } \mathbf{S}_i = 2 \frac{\partial e}{\partial \mathbf{C}}(\mathbf{C}_{n+\frac{1}{2}}^h, \eta_i^h) \quad (5.162)$$

The key point in the above evaluation relies on the fact that the right Cauchy-Green deformation tensor is provided by its mean value in the time interval $\mathbf{C}_{n+\frac{1}{2}}^h = \frac{1}{2}(\mathbf{C}_{n+1}^h + \mathbf{C}_n^h)$. Recall that in a midpoint-type discretization only the state variables are evaluated in such a way.

In addition, the above formula is well-defined in the limit case of $\Delta \mathbf{C}^h \rightarrow \mathbf{0}$ due to the consistency property of the discrete derivative operator, demonstrated in Appendix A, leading to

$$\lim_{\Delta \mathbf{C}^h \rightarrow \mathbf{0}} \mathbf{S}^* = \frac{\partial e}{\partial \mathbf{C}}(\mathbf{C}_n^h, \eta_{n+1}^h) + \frac{\partial e}{\partial \mathbf{C}}(\mathbf{C}_n^h, \eta_n^h) \quad (5.163)$$

The algorithmic temperature assumes a simplified form due to being a scalar field, that is

$$\Theta^* = \mathbf{D}_{\eta}e = \frac{e(\mathbf{C}_{n+1}^h, \eta_{n+1}^h) - e(\mathbf{C}_{n+1}^h, \eta_n^h) + (\mathbf{C}_n^h, \eta_{n+1}^h) - e(\mathbf{C}_n^h, \eta_n^h)}{2(\eta_{n+1}^h - \eta_n^h)}, \quad (5.164)$$

which in the limit case of $\eta_{n+1}^h = \eta_n^h$ collapses to

$$\lim_{\Delta \eta^h \rightarrow 0} \Theta^* = \frac{1}{2} \left(\frac{\partial e}{\partial \eta}(\mathbf{C}_{n+1}^h, \eta_n^h) + \frac{\partial e}{\partial \eta}(\mathbf{C}_n^h, \eta_n^h) \right) \quad (5.165)$$

Then, all the previous results are used in (5.20) to arrive at the following

representation of the entropy-based EEM method

$$\begin{aligned}
\langle \mathbf{w}_\varphi^h, \frac{\varphi_{n+1}^h - \varphi_n^h}{\Delta t} \rangle_{\mathcal{B}_0^h} &= \langle \mathbf{w}_\varphi^h, \frac{1}{\rho_0} \mathbf{p}_{n+\frac{1}{2}}^h \rangle_{\mathcal{B}_0^h} \\
\langle \mathbf{w}_\mathbf{p}^h, \frac{\mathbf{p}_{n+1}^h - \mathbf{p}_n^h}{\Delta t} \rangle_{\mathcal{B}_0^h} &= -\langle \nabla_0 \mathbf{w}_\mathbf{p}^h, \mathbf{F}_{n+\frac{1}{2}}^h \mathbf{S}^* \rangle_{\mathcal{B}_0^h} \\
\langle w_\eta^h, \frac{\eta_{n+1}^h - \eta_n^h}{\Delta t} \rangle_{\mathcal{B}_0^h} &= -\langle \nabla_0 \left[\frac{w_\eta^h}{\Theta^*} \right], \mathbf{K}_{n+\frac{1}{2}}^h \nabla_0 \Theta^* \rangle_{\mathcal{B}_0^h}
\end{aligned} \tag{5.166}$$

Laws of thermodynamics. According to the formalism that has led to the entropy-based EEM method (5.166), its solution agrees with the laws of thermodynamics and symmetries. In fact, using the discrete brackets (5.149) and (5.150) along with the discrete functional derivatives of the total energy and entropy (5.157) and (5.158) in (5.32) leads the energy balance to be

$$\begin{aligned}
E_{n+1}^h - E_n^h &= \Delta t \langle \mathbf{F}_{n+\frac{1}{2}}^h \mathbf{S}^*, \nabla_0 \left[\frac{\mathbf{p}_{n+\frac{1}{2}}^h}{\rho_0} \right] \rangle_{\mathcal{B}_0^h} \\
&\quad - \Delta t \langle \nabla_0 \left[\frac{\mathbf{p}_{n+\frac{1}{2}}^h}{\rho_0} \right], \mathbf{F}_{n+\frac{1}{2}}^h \mathbf{S}^* \rangle_{\mathcal{B}_0^h} \\
&\quad + \Delta t \langle \nabla_0 \left[\frac{1}{\Theta^*} \Theta^* \right], (\Theta^*)^2 \mathbf{K}_{n+\frac{1}{2}}^h \nabla_0 \left[\frac{1}{\Theta^*} \right] \rangle_{\mathcal{B}_0^h} = 0
\end{aligned} \tag{5.167}$$

For its part, the entropy balance yields

$$\begin{aligned}
S_{n+1}^h - S_n^h &= \Delta t \langle \nabla_0 \left[\frac{1}{\Theta^*} \right], (\Theta^*)^2 \mathbf{K}_{n+\frac{1}{2}}^h \nabla_0 \left[\frac{1}{\Theta^*} \right] \rangle_{\mathcal{B}_0^h} \\
&= \Delta t \langle \frac{1}{(\Theta^*)^2} \nabla_0 \Theta^*, \mathbf{K}_{n+\frac{1}{2}}^h \nabla_0 \Theta^* \rangle_{\mathcal{B}_0^h} \geq 0,
\end{aligned} \tag{5.168}$$

which is the discrete analogous of (3.101) for the dissipation due to the conduction phenomenon.

Remark 5.4. Despite these results, neither the conservation of energy nor the production of entropy can be ensured by the resulting discrete Galerkin-based EEM method, since, the resulting G -equivariant discrete functional derivatives do not belong to the Galerkin space $\mathcal{V}^h$ identified with the tangent space state $T\mathcal{S}^h$. Particularly, the resulting algorithmic temperature (5.159)₂ does not belong to the finite-dimensional Galerkin space $\Theta^* \notin \mathcal{V}^h$, where the temperature field is naturally defined in this context. This issue leads the entropy-based EEM method (5.159) to the dissatisfaction of the

energy conservation. More details about this issue are provided in Romero (2010a) as well as a correction of the entropy-based EEM method consisting in a L_2 projection technique that brings the consistent evaluation of the temperature $(5.159)_2$ back to the Galerkin space.

The positive side of this required projection is that the material gradient of the temperature field needed for heat conduction term is straightforward as the resulting projected temperature will surely be provided by the linear combination of shape functions, as the state variable (3.155). Thus, its gradient can directly be computed through the gradient of the shape functions.

Interestingly, this issue did not arise in the formulation of the Energy-Momentum methods of conserving problems due to the simple forms of the canonical Poisson bracket and the kinetic energy that lead the G -equivariant discrete functional derivative to be defined within the Galerkin-based tangent space.

Discrete symmetries. The devised EEM method does preserve the linear and angular momentum along its discrete solution since, by definition, they both are at most quadratic functions of the state variables, and hence their G -equivariant discrete functional derivatives surely belong to $\mathcal{V}^h$ as happened with the kinetic energy in Hamiltonian problems. The proof is similar to the one performed for the continuous case in Section 4.9, now using the discrete counterparts of the brackets. Also, similar arguments as those provided in (3.185) - (3.187) to demonstrate the preservation of the momentum maps in a midpoint-type discretization can be followed up to arrive at the same conclusion.

5.5.2 Temperature-based EEM method

In order to derive the temperature-based EEM method the state space (4.111) is transformed into a finite-dimensional space using the Galerkin approach presented in Section 3.7 such that

$$\mathcal{S}^h = \{z^h = \sum_{a=1}^{\mathcal{N}} N^a z^a = (\varphi^h, p^h, \Theta^h) : \mathcal{B}_0^h \mapsto \mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}_+, \det(\nabla_0 \varphi^h) > 0\}, \quad (5.169)$$

whose tangent space is

$$T\mathcal{S}^h = \{w^h = \sum_{a=1}^{\mathcal{N}} N^a w^a = (w_\varphi^h, w_p^h, w_\Theta^h) : \mathcal{B}_0^h \mapsto \mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}\} \quad (5.170)$$

In view of the continuous Poisson bracket (4.116), its consistent discrete counterpart based on (5.25) is found, for any two functional $\mathcal{F}, \mathcal{G}: \mathcal{S} \mapsto \mathbb{R}$, to be

$$\begin{aligned} \{[\mathcal{F}, \mathcal{G}]\}(\mathbf{z}_{n+1}^h, \mathbf{z}_n^h) &= \left\langle \frac{\Delta^G \mathcal{F}}{\Delta \boldsymbol{\varphi}}(\mathbf{z}_{n+1}^h, \mathbf{z}_n^h), \frac{\Delta^G \mathcal{G}}{\Delta \mathbf{p}}(\mathbf{z}_{n+1}^h, \mathbf{z}_n^h) \right\rangle \\ &\quad - \left\langle \frac{\Delta^G \mathcal{F}}{\Delta \mathbf{p}}(\mathbf{z}_{n+1}^h, \mathbf{z}_n^h), \frac{\Delta^G \mathcal{G}}{\Delta \boldsymbol{\varphi}}(\mathbf{z}_{n+1}^h, \mathbf{z}_n^h) \right\rangle \\ &\quad + \left\langle \nabla_0 \left[\frac{\Delta^G \mathcal{F}}{\Delta \mathbf{p}}(\mathbf{z}_{n+1}^h, \mathbf{z}_n^h) \right], \mathbf{F}_{n+\frac{1}{2}}^h \mathbf{V}^* \frac{1}{c} \frac{\Delta^G \mathcal{G}}{\Delta \Theta}(\mathbf{z}_{n+1}^h, \mathbf{z}_n^h) \right\rangle \\ &\quad - \left\langle \mathbf{F}_{n+\frac{1}{2}}^h \mathbf{V}^* \frac{1}{c} \frac{\Delta^G \mathcal{F}}{\Delta \Theta}(\mathbf{z}_{n+1}^h, \mathbf{z}_n^h), \nabla_0 \left[\frac{\Delta^G \mathcal{G}}{\Delta \mathbf{p}}(\mathbf{z}_{n+1}^h, \mathbf{z}_n^h) \right] \right\rangle, \end{aligned} \quad (5.171)$$

where $\mathbf{V}^*$ is a discrete second order counterpart of the symmetric latent heat tensor (3.77) (neglecting the internal variables) and c is the constant specific heat capacity defined in (3.78).

Now looking at the continuous Dissipative brackets (4.117), its discrete counterpart is constructed as follows

$$\begin{aligned} [[\mathcal{F}, \mathcal{G}]](\mathbf{z}_{n+1}^h, \mathbf{z}_n^h) &= \left\langle \nabla_0 \left[\frac{1}{c} \frac{\Delta^G \mathcal{F}}{\Delta \Theta}(\mathbf{z}_{n+1}^h, \mathbf{z}_n^h) \right], (\Theta^*)^2 \mathbf{K}_{n+\frac{1}{2}}^h \nabla_0 \left[\frac{1}{c} \frac{\Delta^G \mathcal{G}}{\Delta \Theta}(\mathbf{z}_{n+1}^h, \mathbf{z}_n^h) \right] \right\rangle, \end{aligned} \quad (5.172)$$

with $\mathbf{K}_{n+\frac{1}{2}}^h$ being provided by (5.151) except for the algorithmic temperature yet to be defined in this approach.

Similarly to the entropy-based case, the following invariant function respect to the action of the additive and rotation group is found

$$\pi(\mathbf{z}^h) = (\mathbf{F}^{h,T} \mathbf{F}^h, \|\mathbf{p}^h\|^2, \Theta^h) \quad (5.173)$$

Accordingly, the reduced forms of the total energy and the total entropy (4.113) are provided in terms of the invariant function by

$$\tilde{E}(\pi(\mathbf{z}^h)) = \int_{\mathcal{B}_0} \left(\frac{\pi_2}{2\rho_0} + \tilde{e}(\pi_1, \pi_3) \right) dV_0, \quad \tilde{S}(\pi(\mathbf{z}^h)) = \int_{\mathcal{B}_0} \tilde{\eta}(\pi_1, \pi_3) dV_0, \quad (5.174)$$

Observing that the derivatives of the invariant function coincide with those previously obtained (5.156), the G -equivariant partial discrete deriva-

tives of the total energy results in

$$\begin{aligned}
\left\langle \frac{\Delta^G E}{\Delta \boldsymbol{\varphi}} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h), \mathbf{w}_{\boldsymbol{\varphi}}^h \right\rangle &= \langle 2\mathbf{F}_{n+\frac{1}{2}}^h \mathbf{D}_{\pi_1} \tilde{e}(\pi_{n+1}, \pi_n), \nabla_0 \mathbf{w}_{\boldsymbol{\varphi}}^h \rangle_{\mathcal{B}_0^h} \\
\left\langle \frac{\Delta^G E}{\Delta \mathbf{p}} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h), \mathbf{w}_{\mathbf{p}}^h \right\rangle &= \left\langle \frac{\mathbf{p}_{n+\frac{1}{2}}^h}{\rho_0}, \mathbf{w}_{\mathbf{p}}^h \right\rangle_{\mathcal{B}_0^h} \\
\left\langle \frac{\Delta^G E}{\Delta \Theta} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h), w_{\Theta}^h \right\rangle &= \langle \mathbf{D}_{\pi_3} \tilde{e}(\pi_{n+1}, \pi_n), w_{\Theta}^h \rangle_{\mathcal{B}_0^h},
\end{aligned} \tag{5.175}$$

Similarly, the G -equivariant partial discrete derivatives of the total entropy read

$$\begin{aligned}
\left\langle \frac{\Delta^G S}{\Delta \boldsymbol{\varphi}} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h), \mathbf{w}_{\boldsymbol{\varphi}}^h \right\rangle &= \langle 2\mathbf{F}_{n+\frac{1}{2}}^h \mathbf{D}_{\pi_1} \tilde{\eta}(\pi_{n+1}, \pi_n), \nabla_0 \mathbf{w}_{\boldsymbol{\varphi}}^h \rangle_{\mathcal{B}_0^h} \\
\left\langle \frac{\Delta^G S}{\Delta \mathbf{p}} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h), \mathbf{w}_{\mathbf{p}}^h \right\rangle &= 0 \\
\left\langle \frac{\Delta^G S}{\Delta \Theta} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h), w_{\Theta}^h \right\rangle &= \langle \mathbf{D}_{\pi_3} \tilde{\eta}(\pi_{n+1}, \pi_n), w_{\Theta}^h \rangle_{\mathcal{B}_0^h}
\end{aligned} \tag{5.176}$$

Given that, the requirements imposed by the discrete degeneracy conditions (5.22) on the discrete brackets (5.171) and (5.172) leads to

$$\begin{aligned}
&\{\{S, \mathcal{F}\}\} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h) \\
&= \left\langle 2\mathbf{F}_{n+\frac{1}{2}}^h \mathbf{D}_{\pi_1} \tilde{\eta}(\pi_{n+1}, \pi_n), \nabla_0 \left[\frac{\Delta^G \mathcal{F}}{\Delta \mathbf{p}} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h) \right] \right\rangle \\
&\quad - \left\langle \mathbf{F}_{n+\frac{1}{2}}^h \mathbf{V}^* \frac{\mathbf{D}_{\pi_3} \tilde{\eta}(\pi_{n+1}, \pi_n)}{c}, \nabla_0 \left[\frac{\Delta^G \mathcal{F}}{\Delta \mathbf{p}} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h) \right] \right\rangle = 0,
\end{aligned} \tag{5.177}$$

and

$$\begin{aligned}
&[[E, \mathcal{F}]] (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h) \\
&= \left\langle \nabla_0 \left[\frac{\mathbf{D}_{\pi_3} \tilde{e}(\pi_{n+1}, \pi_n)}{c} \right], (\Theta^*)^2 \mathbf{K}_{n+\frac{1}{2}}^h \nabla_0 \left[\frac{1}{c} \frac{\Delta^G \mathcal{F}}{\Delta \Theta} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h) \right] \right\rangle = 0,
\end{aligned} \tag{5.178}$$

Thus, in order for these degeneracy conditions to be fulfilled, the following relations must hold

$$\frac{\mathbf{D}_{\pi_3} \tilde{\eta}(\pi_{n+1}, \pi_n)}{c} \mathbf{V}^* = 2\mathbf{D}_{\pi_1} \tilde{\eta}(\pi_{n+1}, \pi_n), \quad \mathbf{D}_{\pi_3} \tilde{e}(\pi_{n+1}, \pi_n) = c \tag{5.179}$$

Remarkably, the second relation is always satisfied due to the definition of the specific heat capacity as a positive constant number.

Furthermore, the first relation is elaborated using the second one to give

$$\mathbf{V}^* = 2 \frac{D_{\pi_3} \tilde{e}(\pi_{n+1}, \pi_n)}{D_{\pi_3} \tilde{\eta}(\pi_{n+1}, \pi_n)} D_{\pi_1} \tilde{\eta}(\pi_{n+1}, \pi_n), \quad (5.180)$$

in which, following the continuous definition of the latent heat tensor (3.77), the appearing rate is identified with an algorithmic temperature. What is more, the resulting algorithmic temperature is the one that makes the specific heat capacity (3.78) be univocally defined within any time interval, that is

$$\Theta^* = \frac{D_{\pi_3} \tilde{e}(\pi_{n+1}, \pi_n)}{D_{\pi_3} \tilde{\eta}(\pi_{n+1}, \pi_n)} \rightarrow c = D_{\pi_3} \tilde{e}(\pi_{n+1}, \pi_n) = \Theta^* D_{\pi_3} \tilde{\eta}(\pi_{n+1}, \pi_n), \quad (5.181)$$

The fully elaborated formulas for the above discrete derivative are formally identical to (5.164) changing the density entropy by the temperature and the internal energy function accordingly.

Simplifying the notation, the algorithmic latent heat tensor is expressed as follows

$$\mathbf{V}^* = 2\Theta^* D_C \eta, \quad (5.182)$$

with the appearing discrete derivative being formally provided by (5.160), replacing the internal energy function by the density function and the density entropy state variable by the temperature state variable.

Assuming these definitions and performing the operations in (5.20) using all the above needed expressions, the temperature-based EEM method for the nonlinear thermoelastic continuum dynamics reads

$$\begin{aligned} \langle \mathbf{w}_\varphi^h, \frac{\varphi_{n+1}^h - \varphi_n^h}{\Delta t} \rangle_{\mathcal{B}_0^h} &= \langle \mathbf{w}_\varphi^h, \frac{1}{\rho_0} \mathbf{p}_{n+\frac{1}{2}}^h \rangle_{\mathcal{B}_0^h} \\ \langle \mathbf{w}_p^h, \frac{\mathbf{p}_{n+1}^h - \mathbf{p}_n^h}{\Delta t} \rangle_{\mathcal{B}_0^h} &= - \langle \nabla_0 \mathbf{w}_p^h, \mathbf{F}_{n+\frac{1}{2}}^h (2D_C e - \mathbf{V}^*) \rangle_{\mathcal{B}_0^h} \\ \langle \mathbf{w}_\Theta^h, \frac{\Theta_{n+1}^h - \Theta_n^h}{\Delta t} \rangle_{\mathcal{B}_0^h} &= - \langle \frac{w_\Theta^h}{c} \mathbf{F}_{n+\frac{1}{2}}^h \mathbf{V}^*, \nabla_0 \left[\frac{\mathbf{p}_{n+\frac{1}{2}}^h}{\rho_0} \right] \rangle_{\mathcal{B}_0^h} \\ &\quad - \langle \nabla_0 \left[\frac{w_\Theta^h}{c} \right], \mathbf{K}_{n+\frac{1}{2}}^h \nabla_0 \Theta^* \rangle_{\mathcal{B}_0^h} \end{aligned} \quad (5.183)$$

Finally, from the right hand side of the linear momentum balance, the consistent evaluation of the symmetric Piola-Kirchhoff stress tensor is identified as

$$\mathbf{S}^* = 2D_C e - \mathbf{V}^* = 2(D_C e - \Theta^* D_C \eta) = 2D_C \Psi^*, \quad (5.184)$$

which has been expressed through an artificial function Ψ^* to emphasize its connection with its continuous counterpart (3.18), neglecting the internal variables. Its elaborated formula responds to the format provided by (5.160).

Interestingly, as in the previously developed temperature-based EEM methods for discrete finite-dimensional systems, the directionality property of the discrete derivative operator allows to recast the last equation, i.e the energy balance, into a discrete entropy form

$$\langle w_\Theta^h, \Theta^* \frac{\eta(\mathbf{C}_{n+1}^h, \Theta_{n+1}^h) - \eta(\mathbf{C}_n^h, \Theta_n^h)}{\Delta t} \rangle_{\mathcal{B}_0^h} = -\langle \nabla_0 w_\Theta^h, \mathbf{K}_{n+\frac{1}{2}}^h \nabla_0 \Theta^* \rangle_{\mathcal{B}_0^h} \quad (5.185)$$

Discrete laws of thermodynamics. In contrast to the entropy-based method, the temperature-based method does ensure the preservation of energy and the production of entropy within the Galerkin approximation. The proof for the energy balance follows from choosing the weighting functions in (5.183) according to

$$\mathbf{w}_\varphi^h = \mathbf{p}_{n+1}^h - \mathbf{p}_n^h, \quad \mathbf{w}_p^h = \varphi_{n+1}^h - \varphi_n^h, \quad w_\Theta^h = c = D_\Theta e, \quad (5.186)$$

which, in this case, do belong to the Galerkin space $\mathcal{V}^h$ since the specific heat capacity c has been introduced to be a constant positive number due to the material's stability issues. In other words, the internal energy function in terms of temperature of the materials considered depends linearly on temperature so that its partial discrete derivative operator results in a constant number. Then, they are used in (5.183) to give

$$\begin{aligned} \langle \mathbf{p}_{n+1}^h - \mathbf{p}_n^h, \frac{\varphi_{n+1}^h - \varphi_n^h}{\Delta t} \rangle_{\mathcal{B}_0^h} &= \langle \mathbf{p}_{n+1}^h - \mathbf{p}_n^h, \frac{1}{\rho_0} \mathbf{p}_{n+\frac{1}{2}}^h \rangle_{\mathcal{B}_0^h} \\ \langle \varphi_{n+1}^h - \varphi_n^h, \frac{\mathbf{p}_{n+1}^h - \mathbf{p}_n^h}{\Delta t} \rangle_{\mathcal{B}_0^h} &= -\langle \mathbf{F}_{n+1}^h - \mathbf{F}_n^h, \mathbf{F}_{n+\frac{1}{2}}^h (2D_{\mathbf{C}}e - \mathbf{V}^*) \rangle_{\mathcal{B}_0^h} \\ \langle c, \frac{\Theta_{n+1}^h - \Theta_n^h}{\Delta t} \rangle_{\mathcal{B}_0^h} &= -\langle \frac{c}{c} \mathbf{F}_{n+\frac{1}{2}}^h \mathbf{V}^*, \nabla_0 \left[\frac{\mathbf{p}_{n+\frac{1}{2}}^h}{\rho_0} \right] \rangle_{\mathcal{B}_0^h} \\ &\quad - \langle \nabla_0 \left[\frac{c}{c} \right], \mathbf{K}_{n+\frac{1}{2}}^h \nabla_0 \Theta^* \rangle_{\mathcal{B}_0^h} \end{aligned} \quad (5.187)$$

In view of the two first equations, their right hand sides have to be identical. On the other hand, using the first equation in the right hand side of the second equation the following is obtained

$$\begin{aligned} \langle \mathbf{p}_{n+1}^h - \mathbf{p}_n^h, \frac{1}{\rho_0} \mathbf{p}_{n+\frac{1}{2}}^h \rangle_{\mathcal{B}_0^h} &= -\langle \mathbf{F}_{n+1}^h - \mathbf{F}_n^h, \mathbf{F}_{n+\frac{1}{2}}^h (2D_{\mathbf{C}}e - \mathbf{V}^*) \rangle_{\mathcal{B}_0^h} \\ \langle c, \Theta_{n+1}^h - \Theta_n^h \rangle_{\mathcal{B}_0^h} &= -\Delta t \langle \mathbf{F}_{n+\frac{1}{2}}^h \mathbf{V}^*, \nabla_0 \left[\frac{\varphi_{n+1}^h - \varphi_n^h}{\Delta t} \right] \rangle_{\mathcal{B}_0^h} \end{aligned} \quad (5.188)$$

Finally, adding up these equations and using the directionality property of the discrete gradient operator leads to

$$\langle \mathbf{p}_{n+1}^h - \mathbf{p}_n^h, \frac{1}{\rho_0} \mathbf{p}_{n+\frac{1}{2}}^h \rangle_{\mathcal{B}_0^h} + \langle 1, e(\mathbf{C}_{n+1}^h, \Theta_{n+1}^h) - e(\mathbf{C}_n^h, \Theta_n^h) \rangle_{\mathcal{B}_0^h} = 0, \quad (5.189)$$

in where the first term is identified with the total kinetic energy balance and the second term is the total internal energy balance

$$K_{n+1}^h - K_n^h + U_{n+1}^h - U_n^h = 0, \quad (5.190)$$

demonstrating that the temperature-based EEM method is energy-preserving by design.

The entropy balance can then be derived directly from (5.24) to give

$$\begin{aligned} S_{n+1}^h - S_n^h &= \Delta t \langle \nabla_0 \left[\frac{\mathbf{p}_{n+\frac{1}{2}}^h}{\rho_0} \right], \mathbf{F}_{n+\frac{1}{2}}^h \mathbf{V}^* \frac{1}{c} \frac{c}{\Theta^*} \rangle_{\mathcal{B}_0^h} \\ &\quad - \Delta t \langle \mathbf{F}_{n+\frac{1}{2}}^h \mathbf{V}^* \frac{1}{c} \frac{c}{\Theta^*}, \nabla_0 \left[\frac{\mathbf{p}_{n+\frac{1}{2}}^h}{\rho_0} \right] \rangle_{\mathcal{B}_0^h} \\ &\quad + \Delta t \langle \nabla_0 \left[\frac{1}{c} \frac{c}{\Theta^*} \right], \Theta^{*,2} \mathbf{K}_{n+\frac{1}{2}}^h \nabla_0 \left[\frac{1}{c} \frac{c}{\Theta^*} \right] \rangle_{\mathcal{B}_0^h} \\ &= \Delta t \langle \frac{1}{(\Theta^*)^2} \nabla_0 \Theta^*, \mathbf{K}_{n+\frac{1}{2}}^h \nabla_0 \Theta^* \rangle_{\mathcal{B}_0^h} \geq 0 \end{aligned} \quad (5.191)$$

Discrete symmetries. As in the case of the entropy-based method, it can be demonstrated that the temperature-based poses symmetries respect to the additive and rotation group and hence preserves the total linear and angular momentum. The proof is omitted as firmly follows the steps provided in Section 4.9 for the continuous case or the one that led to the demonstration for the midpoint standard method to preserve the linear and angular momentums (3.185) - (3.187), this time using the symmetry of the algorithmic Piola-Kirchhoff stress tensor instead of the symmetry of midpoint one.

Implementation issues. The discrete thermodynamical consistency of the temperature-based method relies on the special evaluation of the temperature field inside the time interval provided by

$$\Theta^* = \frac{D_{\Theta} e}{D_{\Theta} \eta} = \frac{c}{D_{\Theta} \eta} \quad (5.192)$$

This evaluation generally involves both the motion and the temperature fields values at the interval extremities so the material gradient defining the

heat conduction must be carefully obtained. Doubtlessly, this issue complicates the implementation of the temperature-based EEM method compared to standard integrations methods based on temperature in where the implementation of this gradient is attained by the gradient of the shape functions, see, for instance, Hesch & Betsch (2011).

Then, the material gradient applied to the algorithmic temperatures results in

$$\nabla_0 \Theta^* = \nabla_0 \left[\frac{D_{\Theta} e}{D_{\Theta} \eta} \right] = \frac{-\Theta^*}{D_{\Theta} \eta} \nabla_0 [D_{\Theta} \eta] \quad (5.193)$$

The expression of the partial discrete derivative of the density entropy function respect to the temperature has the same format of (5.164) so its gradient can be elaborated as follows

$$\begin{aligned} \nabla_0 [D_{\Theta} \eta] &= \nabla_0 \left[\frac{\eta(\mathbf{C}_{n+1}^h, \Theta_{n+1}^h) - \eta(\mathbf{C}_{n+1}^h, \Theta_n^h) + \eta(\mathbf{C}_n^h, \Theta_{n+1}^h) - \eta(\mathbf{C}_n^h, \Theta_n^h)}{2(\Theta_{n+1}^h - \Theta_n^h)} \right] \\ &= \frac{\nabla_0 [\eta(\mathbf{C}_{n+1}^h, \Theta_{n+1}^h) - \eta(\mathbf{C}_{n+1}^h, \Theta_n^h) + \eta(\mathbf{C}_n^h, \Theta_{n+1}^h) - \eta(\mathbf{C}_n^h, \Theta_n^h)]}{2(\Theta_{n+1}^h - \Theta_n^h)} \\ &\quad - \frac{D_{\Theta} \eta}{(\Theta_{n+1}^h - \Theta_n^h)} \nabla_0 [\Theta_{n+1}^h - \Theta_n^h] \end{aligned} \quad (5.194)$$

The full elaboration of the first term relies on the following type of identities

$$\begin{aligned} \nabla_0 [\eta(\mathbf{C}_i^h, \Theta_{n+1}^h) - \eta(\mathbf{C}_i^h, \Theta_n^h)] &= \left(\frac{\partial \eta}{\partial \mathbf{C}}(\mathbf{C}_i^h, \Theta_{n+1}^h) - \frac{\partial \eta}{\partial \mathbf{C}}(\mathbf{C}_i^h, \Theta_n^h) \right) : \nabla_0 \mathbf{C}_i^h \\ &\quad + \frac{\partial \eta}{\partial \Theta}(\mathbf{C}_i^h, \Theta_{n+1}^h) \nabla_0 \Theta_{n+1}^h - \frac{\partial \eta}{\partial \Theta}(\mathbf{C}_i^h, \Theta_n^h) \nabla_0 \Theta_n^h, \end{aligned} \quad (5.195)$$

for $i = n, n + 1$.

In view of this result, for general thermoelastic material models, a successful implementation of the temperature-based method requires the elaboration of the material gradient of the temperatures at each of the time interval extremities, which follow from the FE-based discretization (3.155), and the material gradient of the right Cauchy-Green deformation tensor. This last operation is much more involved and requires the implementation of the second derivatives of shape functions. Recall that they also arise in the midpoint standard formulation of entropy-based continuous equations (3.176).

Fortunately, the modeling of most of the thermoelastic materials is based on free-energy functions provided by (3.88) with at most linear dependency on the elastic constants, that is $f'(\Theta) = C$, so that the term multiplying the above involved gradient identically vanishes and the gradient of the algorithmic temperatures simplifies to depend only on the gradients of the temperature evaluated at the extremities of the time interval, thus avoiding the implementation and computation of the second derivatives of shape functions.

In fact, in such a case, the algorithmic temperature can be expressed just in terms of the temperature evaluated at the time interval extremities such that

$$\Theta^* = \frac{D_{\Theta} e}{D_{\Theta} \eta} = \frac{\Theta_{n+1}^h - \Theta_n^h}{\log(\Theta_{n+1}^h / \Theta_n^h)}, \quad (5.196)$$

which in the limit case of $\Theta_{n+1}^h = \Theta_n^h$ is well-defined as

$$\lim_{\Theta_{n+1}^h \rightarrow \Theta_n^h} \Theta^* = \Theta_n^h \quad (5.197)$$

The gradient of the algorithmic temperature results then in

$$\nabla_0 \Theta^* = \frac{\left(1 - \frac{\Theta^*}{\Theta_{n+1}^h}\right) \nabla_0 \Theta_{n+1}^h - \left(1 - \frac{\Theta^*}{\Theta_n^h}\right) \nabla_0 \Theta_n^h}{\log(\Theta_{n+1}^h / \Theta_n^h)}, \quad (5.198)$$

while, in the limit case of $\Theta_{n+1}^h = \Theta_n^h$, it reduces to

$$\lim_{\Theta_{n+1}^h \rightarrow \Theta_n^h} \nabla_0 \Theta^* = \frac{1}{2} \nabla_0 [\Theta_{n+1}^h + \Theta_n^h] = \nabla_0 \Theta_n^h \quad (5.199)$$

Then, as the EEM methods are by construction implicit, the linearization of the equations are required for a full implementation. In the linearization respect to the temperature field, the linearized gradient of the algorithmic temperature will be involved so it is provided next

$$\frac{\partial(\nabla_0 \Theta^*)}{\partial \Theta_{n+1}} = \frac{-\left(\frac{\partial \Theta^*}{\partial \Theta_{n+1}} - \frac{\Theta^*}{\Theta_{n+1}}\right) \nabla_0 \Theta_{n+1} + \frac{\Theta_{n+1}}{\Theta_n} \frac{\partial \Theta^*}{\partial \Theta_{n+1}} \nabla_0 \Theta_n - \nabla_0 \Theta^*}{\Theta_{n+1} \log\left(\frac{\Theta_{n+1}}{\Theta_n}\right)} \quad (5.200)$$

with

$$\frac{\partial \Theta^*}{\partial \Theta_{n+1}} = \frac{\Theta^* \left(1 - \frac{\Theta^*}{\Theta_{n+1}^h}\right)}{\Theta_{n+1}^h - \Theta_n^h} \quad (5.201)$$

Finally, in the limit case $\Theta_{n+1}^h = \Theta_n^h$ the linearized contribution vanishes

$$\lim_{\Theta_{n+1}^h \rightarrow \Theta_n^h} \frac{\partial(\nabla_0 \Theta^*)}{\partial \Theta_{n+1}} = \mathbf{0} \quad (5.202)$$

5.6 EEM methods for nonlinear thermo-dissipative dynamics

EEM methods are derived from the methodology described in subsection 5.2.2 for the dynamics of thermo-dissipative continuum presented in Chapter 3 in a classical fashion and in Chapter 4, Section 4.7, within a geometric approach. As for the dissipative systems discussed so far, two EEM methods are to be proposed in terms of the thermodynamical variable used: entropy or temperature.

5.6.1 Entropy-based EEM method

For the derivation of the entropy-based EEM method, the infinite-dimensional state space (4.122) is transformed into an finite-dimensional by using the shape functions space defined in a regular partition of the continuum of FE-type, that is

$$\begin{aligned} \mathcal{S}^h = \{ \mathbf{z}^h = \sum_{a=1}^{\mathcal{N}} N^a \mathbf{z}^a = (\boldsymbol{\varphi}^h, \mathbf{p}^h, \eta^h, \boldsymbol{\Lambda}^{\alpha, h}) : \mathcal{B}_0^h \mapsto \\ \mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R} \times \text{Sym}(\mathbb{T}_d^2)^m, \det(\nabla_0 \boldsymbol{\varphi}^h) > 0 \}, \end{aligned} \quad (5.203)$$

The tangent space is also identified with the finite-dimensional space of linear combinations of shape functions to give

$$\begin{aligned} T\mathcal{S}^h = \{ \mathbf{w}^h = \sum_{a=1}^{\mathcal{N}} N^a \mathbf{w}^a = (\mathbf{w}_{\boldsymbol{\varphi}}^h, \mathbf{w}_{\mathbf{p}}^h, w_{\eta}^h, \mathbf{w}_{\boldsymbol{\Lambda}^{\alpha}}^h) : \mathcal{B}_0^h \mapsto \\ \mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R} \times \text{Sym}(\mathbb{T}_d^2)^m \} \end{aligned} \quad (5.204)$$

Then, the discrete Poisson bracket is the canonical one provided by

$$\begin{aligned} \{ \{ \mathcal{F}, \mathcal{G} \} \} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h) = \left\langle \frac{\Delta^G \mathcal{F}}{\Delta \boldsymbol{\varphi}} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h), \frac{\Delta^G \mathcal{G}}{\Delta \mathbf{p}} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h) \right\rangle \\ - \left\langle \frac{\Delta^G \mathcal{F}}{\Delta \mathbf{p}} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h), \frac{\Delta^G \mathcal{G}}{\Delta \boldsymbol{\varphi}} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h) \right\rangle \end{aligned} \quad (5.205)$$

The novelty of the thermo-dissipative continuum system rests on the Dissipative bracket which includes terms accounting for the internal dissipation due to the development of internal variables. Then, according to (5.26), its discrete counterparts is provided by

$$\begin{aligned}
& [[\mathcal{F}, \mathcal{G}]](z_{n+1}^h, z_n^h) \\
&= \left\langle \nabla_0 \left[\frac{1}{\Theta^*} \frac{\Delta^G \mathcal{F}}{\Delta \eta}(z_{n+1}^h, z_n^h) \right], \mathbf{K}_{n+\frac{1}{2}}^h (\Theta^*)^2 \nabla_0 \left[\frac{1}{\Theta^*} \frac{\Delta^G \mathcal{G}}{\Delta \eta}(z_{n+1}^h, z_n^h) \right] \right\rangle \\
&- \left\langle \frac{1}{\Theta^*} \frac{\Delta^G \mathcal{F}}{\Delta \eta}(z_{n+1}^h, z_n^h), \dot{\mathcal{D}}^* \frac{\Delta^G \mathcal{G}}{\Delta \eta}(z_{n+1}^h, z_n^h) \right\rangle \\
&+ \sum_{\alpha=1}^m \left\langle \frac{\Delta^G \mathcal{F}}{\Delta \Lambda^\alpha}(z_{n+1}^h, z_n^h), \mathcal{K}(\mathbf{Q}^{\alpha,*}) \frac{\Delta^G \mathcal{G}}{\Delta \eta}(z_{n+1}^h, z_n^h) \right\rangle
\end{aligned} \tag{5.206}$$

where Θ^* is the algorithmic temperature, $\mathbf{K}_{n+\frac{1}{2}}^h$ is the algorithmic conductivity tensor provided by (5.151), $\dot{\mathcal{D}}^*$ is the algorithmic dissipation rate, $\mathbf{Q}^{\alpha,*}$ is the algorithmic thermo-dissipative driving stress tensor and $\mathcal{K}$ is the positive-definite functional defining dissipative materials.

In order to construct a entropy-based EEM method that respects the symmetries of the continuous system, the following invariant function is considered

$$\pi(z^h) = (\nabla_0 \boldsymbol{\varphi}^{h^T} \nabla_0 \boldsymbol{\varphi}^h, \|\mathbf{p}^h\|^2, \eta^h, \Lambda^{h,\alpha}) = (\mathbf{F}^{h,T} \mathbf{F}^h, \|\mathbf{p}^h\|^2, \eta^h, \Lambda^{h,\alpha}), \tag{5.207}$$

with $\alpha = 1, \dots, m$. Then, the reduced internal energy and entropy functions read

$$\begin{aligned}
\tilde{E}(\pi(z^h)) &= \int_{\mathcal{B}_0^h} \left(\frac{\pi_2}{2\rho_0} + \tilde{e}(\pi_1, \pi_3, \pi_{3+\alpha}) \right) dV_0, \quad \alpha = 1, \dots, m \\
\tilde{S}(\pi(z^h)) &= \int_{\mathcal{B}_0^h} \pi_3 dV_0,
\end{aligned} \tag{5.208}$$

Given that, the G -equivariant discrete functional derivative of the total

energy (4.136)₁ is elaborated to yield

$$\begin{aligned}
\left\langle \frac{\Delta^G E}{\Delta \mathbf{z}} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h), \mathbf{w}^h \right\rangle &= \langle D^G \left[\frac{\|\mathbf{p}^h\|^2}{2\rho_0} + e(\mathbf{C}^h, \eta^h, \mathbf{\Lambda}^{h,\alpha}) \right] (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h), \mathbf{w}^h \rangle_{\mathcal{B}_0^h} \\
&= \langle D\pi(\mathbf{z}_{n+\frac{1}{2}}^h)^T D \left[\frac{\pi_2}{2\rho_0} + \tilde{e}(\pi_1, \pi_3, \pi_{3+\alpha}) \right] (\pi_{n+1}, \pi_n), \mathbf{w}^h \rangle_{\mathcal{B}_0^h} \\
&= \langle D \left[\frac{\pi_2}{2\rho_0} + \tilde{e}(\pi_1, \pi_3, \pi_{3+\alpha}) \right] (\pi_{n+1}, \pi_n), D\pi(\mathbf{z}_{n+\frac{1}{2}}^h) \cdot \mathbf{w}^h \rangle_{\mathcal{B}_0^h} \\
&= \langle D_{\pi_1} \tilde{e}(\pi_1, \pi_3, \pi_{3+\alpha}), D\pi_1 \cdot \mathbf{w}_{\boldsymbol{\varphi}}^h \rangle_{\mathcal{B}_0^h} \\
&\quad + \langle D_{\pi_2} \left[\frac{\pi_2}{2\rho_0} \right], D\pi_2 \cdot \mathbf{w}_{\mathbf{p}}^h \rangle_{\mathcal{B}_0^h} \\
&\quad + \langle D_{\pi_3} \tilde{e}(\pi_{n+1}, \pi_n), D\pi_3 w_{\eta}^h \rangle_{\mathcal{B}_0^h} \\
&\quad + \sum_{\alpha=1}^m \langle D_{\pi_{3+\alpha}} \tilde{e}(\pi_{n+1}, \pi_n), D\pi_{3+\alpha} : \mathbf{w}_{\mathbf{\Lambda}^\alpha}^h \rangle_{\mathcal{B}_0^h},
\end{aligned} \tag{5.209}$$

for any vector $\mathbf{w}^h \in T\mathcal{S}^h$. In the same way, the G -equivariant discrete functional derivative of the total entropy (4.124)₂ reads

$$\begin{aligned}
\left\langle \frac{\Delta^G S}{\Delta \mathbf{z}} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h), \mathbf{w}^h \right\rangle &= \langle D^G \eta(\mathbf{z}_{n+1}^h, \mathbf{z}_n^h), \mathbf{w}^h \rangle_{\mathcal{B}_0} \\
&= \langle D\pi(\mathbf{z}_{n+\frac{1}{2}}^h)^T D\tilde{\eta}(\pi_{n+1}, \pi_n), \mathbf{w}^h \rangle_{\mathcal{B}_0^h} \\
&= \langle D_{\pi_3} \pi_3, D\pi_3 \cdot \mathbf{w}^h \rangle_{\mathcal{B}_0^h}
\end{aligned} \tag{5.210}$$

In addition to the standard derivatives of the invariant function provided in (5.156), the derivative of the $(3+\alpha)$ -th invariant must be considered, that is

$$D\pi_{3+\alpha} : \mathbf{w} = \mathbf{w}, \quad \forall \mathbf{w} \in \text{Sym}(\mathbb{T}_d^2) \tag{5.211}$$

Thereby, the G -equivariant partial discrete functional derivatives gives

$$\begin{aligned}
\left\langle \frac{\Delta^G E}{\Delta \boldsymbol{\varphi}} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h), \mathbf{w}_{\boldsymbol{\varphi}}^h \right\rangle &= \langle 2\mathbf{F}_{n+\frac{1}{2}}^h D_{\pi_1} \tilde{e}(\pi_{n+1}, \pi_n), \nabla_0 \mathbf{w}_{\boldsymbol{\varphi}}^h \rangle_{\mathcal{B}_0^h} \\
\left\langle \frac{\Delta^G E}{\Delta \mathbf{p}} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h), \mathbf{w}_{\mathbf{p}}^h \right\rangle &= \left\langle \frac{\mathbf{p}_{n+\frac{1}{2}}^h}{\rho_0}, \mathbf{w}_{\mathbf{p}}^h \right\rangle_{\mathcal{B}_0^h} \\
\left\langle \frac{\Delta^G E}{\Delta \eta} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h), w_{\eta}^h \right\rangle &= \langle D_{\pi_3} \tilde{e}(\pi_{n+1}, \pi_n), w_{\eta}^h \rangle_{\mathcal{B}_0^h} \\
\left\langle \frac{\Delta^G E}{\Delta \mathbf{\Lambda}^\alpha} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h), \mathbf{w}_{\mathbf{\Lambda}^\alpha}^h \right\rangle &= \langle D_{\pi_{3+\alpha}} \tilde{e}(\pi_{n+1}, \pi_n), \mathbf{w}_{\mathbf{\Lambda}^\alpha}^h \rangle_{\mathcal{B}_0^h},
\end{aligned} \tag{5.212}$$

whereas the only G -equivariant partial discrete functional derivative of the total entropy different from zero is

$$\left\langle \frac{\Delta^G S}{\Delta \eta} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h), w_\eta^h \right\rangle = \langle 1, \mathbf{w}_\eta^h \rangle_{\mathcal{B}_0^h} \quad (5.213)$$

As in the pure thermoelastic case, the following definitions for the algorithmic symmetry Piola-Kirchhoff stress tensor and temperature are assumed

$$\mathbf{S}^* = 2\mathbf{D}_{\pi_1} \tilde{e}(\pi_{n+1}, \pi_n) = 2\mathbf{D}_{\mathbf{C}} e, \quad \Theta^* = \mathbf{D}_{\pi_3} \tilde{e}(\pi_{n+1}, \pi_n) = \mathbf{D}_\eta e \quad (5.214)$$

Furthermore, the $(3 + \alpha)$ -th partial discrete derivative of the internal energy is identified with the α -th algorithmic thermo-dissipative driving stress tensor

$$\mathbf{Q}^{\alpha,*} = -\mathbf{D}_{\pi_{3+\alpha}} \tilde{e}(\pi_{n+1}, \pi_n) = -\mathbf{D}_{\mathbf{A}^\alpha} e \quad (5.215)$$

Assuming the above definition, for the Dissipative bracket (5.206) to satisfy the degeneracy condition (5.22), the algorithmic dissipation rate must be

$$\dot{\mathcal{D}}^* = \sum_{\alpha=1}^m \mathbf{Q}^{\alpha,*} : \mathcal{K}(\mathbf{Q}^{\alpha,*}) \geq 0 \quad (5.216)$$

For example, in the common case of one internal variable, the energy function becomes a three-variable function so the partitioned case of the discrete derivative operator respect to the first variable, see Appendix A, leads to

$$\mathbf{S}^* = 2\mathbf{D}_{\mathbf{C}} e = \bar{\mathbf{S}}_{n+\frac{1}{2}}^h + \frac{\Delta e_{n+1} + \Delta e_n - \bar{\mathbf{S}}_{n+\frac{1}{2}}^h : \Delta \mathbf{C}^h}{\Delta \mathbf{C}^h : \Delta \mathbf{C}^h} \Delta \mathbf{C}^h, \quad (5.217)$$

with

$$\Delta e_i = e(\mathbf{C}_{n+1}^h, \eta_i^h, \mathbf{A}_i^{1,h}) - e(\mathbf{C}_n^h, \eta_i^h, \mathbf{A}_i^{1,h}), \quad (5.218)$$

and

$$\bar{\mathbf{S}}_{n+\frac{1}{2}}^h = \frac{1}{2} (\mathbf{S}_{n+1} + \mathbf{S}_n) \quad \text{with} \quad \mathbf{S}_i = 2 \frac{\partial e}{\partial \mathbf{C}} (\mathbf{C}_{n+\frac{1}{2}}^h, \eta_i^h, \mathbf{A}_i^{1,h}) \quad (5.219)$$

Then, respect to the second variable, the partitioned case of the discrete derivative operator gives

$$\begin{aligned} \Theta^* = \mathbf{D}_\eta e = & \frac{e(\mathbf{C}_{n+1}^h, \eta_{n+1}^h, \mathbf{A}_n^{1,h}) - e(\mathbf{C}_{n+1}^h, \eta_n^h, \mathbf{A}_n^{1,h})}{2(\eta_{n+1}^h - \eta_n^h)} \\ & + \frac{e(\mathbf{C}_n^h, \eta_{n+1}^h, \mathbf{A}_{n+1}^{1,h}) - e(\mathbf{C}_n^h, \eta_n^h, \mathbf{A}_{n+1}^{1,h})}{2(\eta_{n+1}^h - \eta_n^h)}, \end{aligned} \quad (5.220)$$

And, finally, the third partitioned discrete derivative is provided by

$$\mathbf{Q}^{1,*} = -\mathbf{D}_{\Lambda^1} e = \overline{\mathbf{Q}}_{n+\frac{1}{2}}^{1,h} - \frac{\Delta e_{n+1} + \Delta e_n + \overline{\mathbf{Q}}_{n+\frac{1}{2}}^{1,h} : \Delta \Lambda^{1,h}}{\Delta \Lambda^{1,h} : \Delta \Lambda^{1,h}} \Delta \Lambda^{1,h}, \quad (5.221)$$

with, in this case, the increment of the internal energy being

$$\Delta e_i = e(\mathbf{C}_{n+1}^h, \eta_i^h, \Lambda_{n+1}^{1,h}) - e(\mathbf{C}_n^h, \eta_i^h, \Lambda_n^{1,h}), \quad (5.222)$$

and

$$\overline{\mathbf{Q}}_{n+\frac{1}{2}}^{1,h} = \frac{1}{2} (\mathbf{Q}_{n+1}^1 + \mathbf{Q}_n^1) \quad \text{with} \quad \mathbf{Q}_i^1 = -\frac{\partial e}{\partial \Lambda}(\mathbf{C}_i^h, \eta_i^h, \Lambda_{n+\frac{1}{2}}^{1,h}) \quad (5.223)$$

Definitely, the entropy-based EEM method for the nonlinear thermo-dissipative dynamics of continua follows from (5.31) using (5.212) and (5.213) to give

$$\begin{aligned} \langle \mathbf{w}_\varphi^h, \frac{\varphi_{n+1}^h - \varphi_n^h}{\Delta t} \rangle_{\mathcal{B}_0^h} &= \langle \mathbf{w}_\varphi^h, \frac{1}{\rho_0} \mathbf{p}_{n+\frac{1}{2}}^h \rangle_{\mathcal{B}_0^h} \\ \langle \mathbf{w}_\mathbf{p}^h, \frac{\mathbf{p}_{n+1}^h - \mathbf{p}_n^h}{\Delta t} \rangle_{\mathcal{B}_0^h} &= -\langle \nabla_0 \mathbf{w}_\mathbf{p}^h, \mathbf{F}_{n+\frac{1}{2}}^h \mathbf{S}^* \rangle_{\mathcal{B}_0^h} \\ \langle \mathbf{w}_\eta^h, \frac{\eta_{n+1}^h - \eta_n^h}{\Delta t} \rangle_{\mathcal{B}_0^h} &= -\langle \nabla_0 \left[\frac{w_\eta^h}{\Theta^*} \right], \mathbf{K}_{n+\frac{1}{2}}^h \nabla_0 \Theta^* \rangle_{\mathcal{B}_0^h} - \langle \frac{w_\eta^h}{\Theta^*}, \dot{\mathbf{D}}^* \rangle_{\mathcal{B}_0^h} \\ \langle \mathbf{w}_\Lambda^h, \frac{\Lambda_{n+1}^{\alpha,h} - \Lambda_n^{\alpha,h}}{\Delta t} \rangle_{\mathcal{B}_0^h} &= \langle \mathbf{w}_\Lambda^h, \mathcal{K}(\mathbf{Q}^{*,\alpha}) \rangle_{\mathcal{B}_0^h} \end{aligned} \quad (5.224)$$

Discrete laws of thermodynamics. The resulting method presents the same problem as the one for the pure thermoelastic case (5.166) regarding the conservation of energy as the algorithmic temperature defined by the discrete derivative operator is out of the Galerkin space $\mathcal{V}^h$. A L_2 -projection strategy would then be required to guarantee the energy conservation of the solution provided by the entropy-based method.

Discrete symmetries. In contrast to the discrete laws of thermodynamics, the discrete symmetries are respected by the resulting entropy-based method due to the same arguments as those used for the EEM method (5.166).

5.6.2 Temperature-based EEM method

The formulation of the temperature-based EEM method departs from the consideration of the Galerkin-based finite-dimensional state and tangent

spaces

$$\begin{aligned} \mathcal{S}^h = \{ \mathbf{z}^h = \sum_{a=1}^{\mathcal{N}} N^a \mathbf{z}^a = (\boldsymbol{\varphi}^h, \mathbf{p}^h, \Theta^h, \boldsymbol{\Lambda}^{\alpha,h}) : \mathcal{B}_0^h \mapsto \\ \mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R} \times \text{Sym}(\mathbb{T}_d^2)^m, \det(\nabla_0 \boldsymbol{\varphi}^h) > 0 \}, \end{aligned} \quad (5.225)$$

$$\begin{aligned} T\mathcal{S}^h = \{ \mathbf{w}^h = \sum_{a=1}^{\mathcal{N}} N^a \mathbf{w}^a = (\mathbf{w}_{\boldsymbol{\varphi}}^h, \mathbf{w}_{\mathbf{p}}^h, w_{\Theta}^h, \mathbf{w}_{\boldsymbol{\Lambda}^{\alpha}}^h) : \mathcal{B}_0^h \mapsto \\ \mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R} \times \text{Sym}(\mathbb{T}_d^2)^m \} \end{aligned} \quad (5.226)$$

Then, the continuous Poisson brackets (4.139)₁ is approximated using (5.25) to give

$$\begin{aligned} \{ \{ \mathcal{F}, \mathcal{G} \} \} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h) = \left\langle \frac{\Delta^G \mathcal{F}}{\Delta \boldsymbol{\varphi}} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h), \frac{\Delta^G \mathcal{G}}{\Delta \mathbf{p}} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h) \right\rangle \\ - \left\langle \frac{\Delta^G \mathcal{F}}{\Delta \mathbf{p}} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h), \frac{\Delta^G \mathcal{G}}{\Delta \boldsymbol{\varphi}} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h) \right\rangle \\ + \left\langle \nabla_0 \left[\frac{\Delta^G \mathcal{F}}{\Delta \mathbf{p}} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h) \right], \mathbf{F}_{n+\frac{1}{2}}^h \mathbf{V}^* \frac{1}{c} \frac{\Delta^G \mathcal{G}}{\Delta \Theta} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h) \right\rangle \\ - \left\langle \mathbf{F}_{n+\frac{1}{2}}^h \mathbf{V}^* \frac{1}{c} \frac{\Delta^G \mathcal{F}}{\Delta \Theta} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h), \nabla_0 \left[\frac{\Delta^G \mathcal{G}}{\Delta \mathbf{p}} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h) \right] \right\rangle, \end{aligned} \quad (5.227)$$

where $\mathbf{V}^*$ is the algorithmic symmetric latent heat tensor (3.77) and c is the constant specific heat capacity defined in (3.78).

Likewise, the continuous Dissipative brackets (4.139)₂ is approximated using (5.26) to give

$$\begin{aligned} [[\mathcal{F}, \mathcal{G}]] (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h) = \left\langle \frac{1}{c} \frac{\Delta^G \mathcal{F}}{\Delta \Theta} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h), (\dot{\mathcal{D}}^* + \mathcal{H}_d^*) \frac{\Theta^*}{c} \frac{\Delta^G \mathcal{G}}{\Delta \Theta} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h) \right\rangle \\ + \sum_{\alpha=1}^m \left\langle \frac{\Delta^G \mathcal{F}}{\Delta \boldsymbol{\Lambda}^{\alpha}} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h), \mathcal{K}(\mathbf{Q}^{*,\alpha}) \frac{\Theta^*}{c} \frac{\Delta^G \mathcal{G}}{\Delta \Theta} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h) \right\rangle \\ + \left\langle \nabla_0 \left[\frac{1}{c} \frac{\Delta^G \mathcal{F}}{\Delta \Theta} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h) \right], \mathbf{K}_{n+\frac{1}{2}}^h (\Theta^*)^2 \nabla_0 \left[\frac{1}{c} \frac{\Delta^G \mathcal{G}}{\Delta \Theta} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h) \right] \right\rangle, \end{aligned} \quad (5.228)$$

where $\dot{\mathcal{D}}^*$ is the algorithmic dissipation rate, $\mathcal{H}_d^*$ is the algorithmic thermo-dissipative heating, Θ^* is the algorithmic temperature, $\mathbf{Q}^{\alpha,*}$ is the algorithmic thermo-dissipative driving stress tensor and $\mathcal{K}$ is the positive-definite functional defining dissipative materials and $\mathbf{K}_{n+\frac{1}{2}}^h$ is provided by (5.151),

Next, the following invariants are identified

$$\pi(\mathbf{z}^h) = (\nabla_0 \boldsymbol{\varphi}^{h\top} \nabla_0 \boldsymbol{\varphi}^h, \|\mathbf{p}^h\|^2, \Theta^h, \boldsymbol{\Lambda}^{h,\alpha}) = (\mathbf{F}^{h\top} \mathbf{F}^h, \|\mathbf{p}^h\|^2, \Theta^h, \boldsymbol{\Lambda}^{h,\alpha}), \quad (5.229)$$

so that the G -equivariant partial discrete functional derivatives of the total energy and entropy functions (4.136) are provided by

$$\begin{aligned} \left\langle \frac{\Delta^G E}{\Delta \boldsymbol{\varphi}}(\mathbf{z}_{n+1}^h, \mathbf{z}_n^h), \mathbf{w}_{\boldsymbol{\varphi}}^h \right\rangle &= \langle 2\mathbf{F}_{n+\frac{1}{2}}^h \mathbf{D}_{\pi_1} \tilde{e}(\pi_{n+1}, \pi_n), \nabla_0 \mathbf{w}_{\boldsymbol{\varphi}}^h \rangle_{\mathcal{B}_0^h} \\ \left\langle \frac{\Delta^G E}{\Delta \mathbf{p}}(\mathbf{z}_{n+1}^h, \mathbf{z}_n^h), \mathbf{w}_{\mathbf{p}}^h \right\rangle &= \left\langle \frac{\mathbf{p}_{n+\frac{1}{2}}^h}{\rho_0}, \mathbf{w}_{\mathbf{p}}^h \right\rangle_{\mathcal{B}_0^h} \\ \left\langle \frac{\Delta^G E}{\Delta \Theta}(\mathbf{z}_{n+1}^h, \mathbf{z}_n^h), w_{\Theta}^h \right\rangle &= \langle \mathbf{D}_{\pi_3} \tilde{e}(\pi_{n+1}, \pi_n), w_{\Theta}^h \rangle_{\mathcal{B}_0^h} \\ \left\langle \frac{\Delta^G E}{\Delta \boldsymbol{\Lambda}^\alpha}(\mathbf{z}_{n+1}^h, \mathbf{z}_n^h), \mathbf{w}_{\boldsymbol{\Lambda}^\alpha}^h \right\rangle &= \langle \mathbf{D}_{\pi_3+\alpha} \tilde{e}(\pi_{n+1}, \pi_n), \mathbf{w}_{\boldsymbol{\Lambda}^\alpha}^h \rangle_{\mathcal{B}_0^h}, \end{aligned} \quad (5.230)$$

$$\begin{aligned} \left\langle \frac{\Delta^G S}{\Delta \boldsymbol{\varphi}}(\mathbf{z}_{n+1}^h, \mathbf{z}_n^h), \mathbf{w}_{\boldsymbol{\varphi}}^h \right\rangle &= \langle 2\mathbf{F}_{n+\frac{1}{2}}^h \mathbf{D}_{\pi_1} \tilde{\eta}(\pi_{n+1}, \pi_n), \nabla_0 \mathbf{w}_{\boldsymbol{\varphi}}^h \rangle_{\mathcal{B}_0^h} \\ \left\langle \frac{\Delta^G S}{\Delta \mathbf{p}}(\mathbf{z}_{n+1}^h, \mathbf{z}_n^h), \mathbf{w}_{\mathbf{p}}^h \right\rangle &= 0 \\ \left\langle \frac{\Delta^G S}{\Delta \Theta}(\mathbf{z}_{n+1}^h, \mathbf{z}_n^h), w_{\Theta}^h \right\rangle &= \langle \mathbf{D}_{\pi_3} \tilde{\eta}(\pi_{n+1}, \pi_n), w_{\Theta}^h \rangle_{\mathcal{B}_0^h} \\ \left\langle \frac{\Delta^G S}{\Delta \boldsymbol{\Lambda}^\alpha}(\mathbf{z}_{n+1}^h, \mathbf{z}_n^h), \mathbf{w}_{\boldsymbol{\Lambda}^\alpha}^h \right\rangle &= \langle \mathbf{D}_{\pi_3+\alpha} \tilde{\eta}(\pi_{n+1}, \pi_n), \mathbf{w}_{\boldsymbol{\Lambda}^\alpha}^h \rangle_{\mathcal{B}_0^h}, \end{aligned} \quad (5.231)$$

In view of the above and analogously to the thermoelastic case, the discrete degeneracy conditions of the discrete Poisson and Dissipative brackets, (5.228) and (5.227), are satisfied if the following holds

$$\frac{\mathbf{D}_{\pi_3} \tilde{\eta}(\pi_{n+1}, \pi_n)}{c} \mathbf{V}^* = 2\mathbf{D}_{\pi_1} \tilde{\eta}(\pi_{n+1}, \pi_n), \quad \mathbf{D}_{\pi_3} \tilde{e}(\pi_{n+1}, \pi_n) = c, \quad (5.232)$$

leading to the definitions for the algorithmic temperature and latent heat tensor

$$\begin{aligned} c &= \mathbf{D}_{\pi_3} \tilde{e}(\pi_{n+1}, \pi_n) = \Theta^* \mathbf{D}_{\pi_3} \tilde{\eta}(\pi_{n+1}, \pi_n) \rightarrow \Theta^* = \frac{\mathbf{D}_{\Theta} e}{\mathbf{D}_{\Theta} \eta}, \\ \mathbf{V}^* &= 2\Theta^* \mathbf{D}_{\pi_1} \tilde{\eta}(\pi_{n+1}, \pi_n) = 2\Theta^* \mathbf{D}_{\mathbf{C}} \eta, \end{aligned} \quad (5.233)$$

In addition, the same arguments for the degeneracy condition of the discrete Dissipative bracket lead to the following definitions

$$\begin{aligned}\mathbf{Q}^{\alpha,*} &= -\mathbf{D}_{\pi_{3+\alpha}} \tilde{e}(\pi_{n+1}, \pi_n) = -\mathbf{D}_{\mathbf{A}^\alpha} e \\ \mathbf{W}^{\alpha,*} &= \Theta^* \mathbf{D}_{\pi_{3+\alpha}} \tilde{\eta}(\pi_{n+1}, \pi_n) = \Theta^* \mathbf{D}_{\mathbf{A}^\alpha} \eta,\end{aligned}\quad (5.234)$$

and, in agreement with them, the following ones

$$\dot{\mathcal{D}}^* = \sum_{\alpha=1}^m \mathbf{Q}^{\alpha,*} : \mathcal{K}(\mathbf{Q}^{\alpha,*}) \geq 0, \quad \mathcal{H}_d^* = \sum_{\alpha=1}^m \mathbf{W}^{\alpha,*} : \mathcal{K}(\mathbf{Q}^{\alpha,*}) \quad (5.235)$$

Then, the temperature-based EEM method directly derives from (5.31) along with (5.230) and (5.231) to give

$$\begin{aligned}\langle \mathbf{w}_\varphi^h, \frac{\varphi_{n+1}^h - \varphi_n^h}{\Delta t} \rangle_{\mathcal{B}_0^h} &= \langle \mathbf{w}_\varphi^h, \frac{1}{\rho_0} \mathbf{p}_{n+\frac{1}{2}}^h \rangle_{\mathcal{B}_0^h} \\ \langle \mathbf{w}_\mathbf{p}^h, \frac{\mathbf{p}_{n+1}^h - \mathbf{p}_n^h}{\Delta t} \rangle_{\mathcal{B}_0^h} &= -\langle \mathbf{F}_{n+\frac{1}{2}}^h \mathbf{S}^*, \nabla_0 \mathbf{w}_\mathbf{p}^h \rangle_{\mathcal{B}_0^h} \\ \langle \mathbf{w}_\Theta^h, \frac{\Theta_{n+1}^h - \Theta_n^h}{\Delta t} \rangle_{\mathcal{B}_0^h} &= -\langle \nabla_0 \left[\frac{w_\Theta^h}{c} \right], \mathbf{K}_{n+\frac{1}{2}}^h \nabla_0 \Theta^* \rangle_{\mathcal{B}_0^h} \\ &\quad - \langle \frac{w_\Theta^h}{c}, \dot{\mathcal{D}}^* + \mathcal{H}_d^* \rangle_{\mathcal{B}_0^h} \\ &\quad - \langle \frac{w_\Theta^h}{c} \mathbf{F}_{n+\frac{1}{2}}^h \mathbf{V}^*, \nabla_0 \left[\frac{\mathbf{p}_{n+\frac{1}{2}}^h}{\rho_0} \right] \rangle_{\mathcal{B}_0^h} \\ \langle \mathbf{w}_\mathbf{A}^h, \frac{\mathbf{A}_{n+1}^{\alpha,h} - \mathbf{A}_n^{\alpha,h}}{\Delta t} \rangle_{\mathcal{B}_0^h} &= \langle \mathbf{w}_\mathbf{A}^h, \mathcal{K}(\mathbf{Q}^{\alpha,*}) \rangle_{\mathcal{B}_0^h},\end{aligned}\quad (5.236)$$

where the algorithmic symmetric Piola-Kirchhoff stress tensor is provided by (5.184).

In the same way as in the temperature-based EEM method for nonlinear thermoelastic continuum dynamics, the directionality property of the discrete derivative operator allows to rewrite the discrete equation due to the energy balance in an entropy form

$$\begin{aligned}\langle \mathbf{w}_\Theta^h, \Theta^* \frac{\eta(\mathbf{C}_{n+1}^h, \Theta_{n+1}^h, \mathbf{A}_{n+1}^h) - \eta(\mathbf{C}_n^h, \Theta_n^h, \mathbf{A}_n^h)}{\Delta t} \rangle_{\mathcal{B}_0^h} &= -\langle \nabla_0 w_\Theta^h, \mathbf{K}_{n+\frac{1}{2}}^h \nabla_0 \Theta^* \rangle_{\mathcal{B}_0^h} \\ &\quad - \langle \mathbf{w}_\Theta^h, \dot{\mathcal{D}}^* \rangle_{\mathcal{B}_0^h}\end{aligned}\quad (5.237)$$

Discrete laws of thermodynamics. The laws of thermodynamics in their discrete form (5.21) are ensured by the temperature-based EEM method

(5.236) due to the same arguments argued in the pure thermoelastic case. Particularly, the total entropy balance in any time step can be detailed by using (5.231) in (5.33) to give

$$S_{n+1}^h - S_n^h = \Delta t \left\langle \frac{1}{(\Theta^*)^2} \nabla_0 \Theta^*, \mathbf{K}_{n+\frac{1}{2}}^h \nabla_0 \Theta^* \right\rangle_{\mathcal{B}_0^h} + \left\langle \frac{1}{(\Theta^*)^2}, \dot{\mathcal{D}}^* \right\rangle_{\mathcal{B}_0^h} \geq 0, \quad (5.238)$$

which is the discrete counterpart of (3.101).

Discrete symmetries. Based on the same arguments as those used for each of the EEM methods proposed so far, it can be asserted that the temperature-based EEM method for nonlinear thermo-dissipative dynamics is momentum maps-preserving, particularly the total linear and angular momentums are discretely preserved along the system solution.

5.7 EEM method for nonlinear isothermal dissipative dynamics

In order to derive EEM methods for the isothermal limit case studied in Section 3.6, a proper discrete counterpart that preserve the metriplectic structure of such problems (4.146) must be proposed. To this end, the Galerkin formulation is assumed for the spatial discretization of both the infinite-dimensional state space and its tangent space $\mathcal{S}^h \equiv \mathcal{V}^h$ and $T\mathcal{S}^h \equiv \mathcal{W}^h$.

Definition 5.6. A discrete infinite-dimensional smooth isothermal dissipative system with symmetries is a discrete system governed by the consistent discrete equations

$$\frac{\mathcal{F}(\mathbf{z}_{n+1}^h) - \mathcal{F}(\mathbf{z}_n^h)}{\Delta t} = \{ \{ [[\mathcal{F}, E]] \} \} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h), \quad (5.239)$$

for all $\mathcal{F} : \mathcal{S}^h \mapsto \mathbb{R}$ and $E : \mathcal{S}^h \mapsto \mathbb{R}$ the total energy understood as kinetic plus internal with the latter being provided by the free-energy function in terms of deformation and internal variable (4.149).

The operator $\{ \{ [\cdot, \cdot] \} \} : \mathcal{S}^h \times \mathcal{S}^h \mapsto \mathbb{R}$ is a consistent second-order discrete counterpart of the bilinear Poisson-Dissipative operator introduced in (4.144).

Proposition 5.5. *The solution of discrete infinite-dimensional dissipative systems (5.239) agrees with the discrete form of the laws of thermodynamics provided by*

$$E(\mathbf{z}_{n+1}^h) \leq E(\mathbf{z}_n^h), \quad (5.240)$$

if the discrete bilinear operator satisfy

$$\{\{[[E, E]]\}\} \leq 0, \quad (5.241)$$

for every functional $\mathcal{F}: \mathcal{S}^h \rightarrow \mathbb{R}$.

Using this definition, an EEM method for the isothermal dissipative continuum dynamics can be developed by first considering the Galerkin-based finite-dimensional state space

$$\begin{aligned} \mathcal{S}^h = \{ \mathbf{z} = \sum_{a=1}^{\mathcal{N}} N^a \mathbf{z}^a = (\boldsymbol{\varphi}^h, \mathbf{p}^h, \boldsymbol{\Lambda}^{\alpha, h}) : \mathcal{B}_0^h \mapsto \\ \mathbb{R}^d \times \mathbb{R}^d \times \text{Sym}(\mathbb{T}_d^2)^m, \det(\nabla_0 \boldsymbol{\varphi}) > 0 \}, \end{aligned} \quad (5.242)$$

along with its tangent space

$$\begin{aligned} T\mathcal{S}^h = \{ \mathbf{w}^h = \sum_{a=1}^{\mathcal{N}} N^a \mathbf{w}^a = (\mathbf{w}_{\boldsymbol{\varphi}}^h, \mathbf{w}_{\mathbf{p}}^h, \mathbf{w}_{\boldsymbol{\Lambda}^{\alpha}}^h) : \mathcal{B}_0 \mapsto \\ \mathbb{R}^d \times \mathbb{R}^d \times \text{Sym}(\mathbb{T}_d^2)^m \} \end{aligned} \quad (5.243)$$

Then, the Poisson-Dissipative bracket (4.151) is approximated by using the G -equivariant discrete derivative operator to give

$$\begin{aligned} \{\{[[\mathcal{F}, \mathcal{G}]]\}\} = & \left\langle \frac{\Delta^G \mathcal{F}}{\Delta \boldsymbol{\varphi}}(\mathbf{z}_{n+1}^h, \mathbf{z}_n^h), \frac{\Delta^G \mathcal{G}}{\Delta \mathbf{p}}(\mathbf{z}_{n+1}^h, \mathbf{z}_n^h) \right\rangle \\ & - \left\langle \frac{\Delta^G \mathcal{F}}{\Delta \mathbf{p}}(\mathbf{z}_{n+1}^h, \mathbf{z}_n^h), \frac{\Delta^G \mathcal{G}}{\Delta \boldsymbol{\varphi}}(\mathbf{z}_{n+1}^h, \mathbf{z}_n^h) \right\rangle \\ & + \sum_{\alpha=1}^m \left\langle \frac{\Delta^G \mathcal{F}}{\Delta \boldsymbol{\Lambda}^{\alpha}}(\mathbf{z}_{n+1}^h, \mathbf{z}_n^h), \mathcal{K} \left(-\frac{\Delta^G \mathcal{G}}{\Delta \boldsymbol{\Lambda}^{\alpha}}(\mathbf{z}_{n+1}^h, \mathbf{z}_n^h) \right) \right\rangle, \end{aligned} \quad (5.244)$$

with $\mathcal{K}$ being the positive semidefinite functional that defines dissipative materials.

Now, the following invariants respect to the additive group $G = \mathbb{R}^d$ and the rotation $G = \text{SO}(3)$ are identified as

$$\pi(\mathbf{z}^h) = ((\nabla_0 \boldsymbol{\varphi}^h)^T \nabla_0 \boldsymbol{\varphi}^h, \|\mathbf{p}^h\|^2, \boldsymbol{\Lambda}^{h, \alpha}) = (\mathbf{F}^{h, T} \mathbf{F}^h, \|\mathbf{p}^h\|^2, \boldsymbol{\Lambda}^{h, \alpha}), \quad (5.245)$$

so that the total energy (4.149) is expressed through them to obtain its reduced form

$$\tilde{E}(\pi(\mathbf{z}^h)) = \int_{\mathcal{B}_0^h} \left(\frac{\pi_2}{2\rho_0} + \tilde{\Psi}(\pi_1, \pi_{2+\alpha}) \right) dV_0, \quad \alpha = 1, \dots, m \quad (5.246)$$

The definition of the G -equivariant discrete functional (5.30) is elaborated with the help of the reduced energy function and the invariant function to arrive at

$$\begin{aligned} \left\langle \frac{\Delta^G E}{\Delta \boldsymbol{\varphi}} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h), \mathbf{w}_{\boldsymbol{\varphi}}^h \right\rangle &= \langle 2\mathbf{F}_{n+\frac{1}{2}}^h \mathbf{D}_{\pi_1} \tilde{\Psi}(\pi_{n+1}, \pi_n), \nabla_0 \mathbf{w}_{\boldsymbol{\varphi}}^h \rangle_{\mathcal{B}_0^h} \\ \left\langle \frac{\Delta^G E}{\Delta \mathbf{p}} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h), \mathbf{w}_{\mathbf{p}}^h \right\rangle &= \left\langle \frac{\mathbf{p}_{n+\frac{1}{2}}^h}{\rho_0}, \mathbf{w}_{\mathbf{p}}^h \right\rangle_{\mathcal{B}_0^h} \\ \left\langle \frac{\Delta^G E}{\Delta \boldsymbol{\Lambda}^\alpha} (\mathbf{z}_{n+1}^h, \mathbf{z}_n^h), \mathbf{w}_{\boldsymbol{\Lambda}^\alpha}^h \right\rangle &= \langle \mathbf{D}_{\pi_2+\alpha} \tilde{\Psi}(\pi_{n+1}, \pi_n), \mathbf{w}_{\boldsymbol{\Lambda}^\alpha}^h \rangle_{\mathcal{B}_0^h}, \end{aligned} \quad (5.247)$$

from which the following discrete counterparts of the constitutive laws (3.103) are identified

$$\begin{aligned} \mathbf{S}^* &= 2\mathbf{D}_{\pi_3} \tilde{\Psi}(\pi_{n+1}, \pi_n) = 2\mathbf{D}_{\mathbf{C}} \Psi, \\ \mathbf{Q}^{\alpha,*} &= -\mathbf{D}_{\pi_3+\alpha} \tilde{\Psi}(\pi_{n+1}, \pi_n) = -\mathbf{D}_{\boldsymbol{\Lambda}^\alpha} \Psi \end{aligned} \quad (5.248)$$

Now, using (5.244), (5.247) and (5.248) in (5.239), the EEM method for isothermal dissipative continuum dynamics reads

$$\begin{aligned} \left\langle \mathbf{w}_{\boldsymbol{\varphi}}^h, \frac{\boldsymbol{\varphi}_{n+1}^h - \boldsymbol{\varphi}_n^h}{\Delta t} \right\rangle_{\mathcal{B}_0^h} &= \left\langle \mathbf{w}_{\boldsymbol{\varphi}}^h, \frac{1}{\rho_0} \mathbf{p}_{n+\frac{1}{2}}^h \right\rangle_{\mathcal{B}_0^h} \\ \left\langle \mathbf{w}_{\mathbf{p}}^h, \frac{\mathbf{p}_{n+1}^h - \mathbf{p}_n^h}{\Delta t} \right\rangle_{\mathcal{B}_0^h} &= -\langle \nabla_0 \mathbf{w}_{\mathbf{p}}^h, \mathbf{F}_{n+\frac{1}{2}}^h \mathbf{S}^* \rangle_{\mathcal{B}_0^h} \\ \left\langle \mathbf{w}_{\boldsymbol{\Lambda}^\alpha}^h, \frac{\boldsymbol{\Lambda}_{n+1}^{\alpha,h} - \boldsymbol{\Lambda}_n^{\alpha,h}}{\Delta t} \right\rangle_{\mathcal{B}_0^h} &= \langle \mathbf{w}_{\boldsymbol{\Lambda}^\alpha}^h, \mathcal{K}(\mathbf{Q}^{\alpha,*}) \rangle_{\mathcal{B}_0^h} \end{aligned} \quad (5.249)$$

The resulting method is essentially the Energy-Momentum method combined with a consistent integration of the evolution equations for the internal variables that ensure the dissipation.

Discrete laws of thermodynamics. As was discussed in Section 3.6, isothermal dissipative systems can only evolve by dissipating energy. Therefore, the energy balance in each of the time steps of a discrete setting must be non-positive if the discrete setting agrees with the thermodynamics.

$$E_{n+1}^h - E_n^h = \langle -\mathbf{Q}^{\alpha,*}, \mathcal{K}(\mathbf{Q}^{\alpha,*}) \rangle_{\mathcal{B}_0^h} = -\langle 1, \dot{\mathcal{D}}^* \rangle_{\mathcal{B}_0^h} \leq 0 \quad (5.250)$$

In other words, the augmented Hamiltonian in the sense of (3.107) is discretely preserved

$$\bar{E}_{n+1}^h = \bar{E}_n^h \quad (5.251)$$

Discrete symmetries. Likewise the continuous equations (3.166), the linear and angular momentum are preserved quantities (first integrals) of the discrete solution provided by (5.249). This can be verified by both using the discrete counterpart of the Poisson-discrete bracket (5.244) along with the discrete version of the Noether's theorem 5.4 or by resorting to the procedure applied for the midpoint standard method carried out in (3.185) - (3.187).

Viscoelastic continuum dynamics. The viscoelastic continuum dynamics presented in subsection (3.6.1) is based on the free-energy function (3.109) which leads to the following form of the dissipative functional

$$\mathcal{K}(\mathbf{Q}^\alpha) = \frac{1}{\nu^\alpha} \mathbf{Q}^\alpha \quad (5.252)$$

Then, the EEM method simplifies to

$$\begin{aligned} \langle \mathbf{w}_\varphi^h, \frac{\varphi_{n+1}^h - \varphi_n^h}{\Delta t} \rangle_{\mathcal{B}_0^h} &= \langle \mathbf{w}_\varphi^h, \frac{1}{\rho_0} \mathbf{p}_{n+\frac{1}{2}}^h \rangle_{\mathcal{B}_0^h} \\ \langle \mathbf{w}_p^h, \frac{\mathbf{p}_{n+1}^h - \mathbf{p}_n^h}{\Delta t} \rangle_{\mathcal{B}_0^h} &= -\langle \nabla_0 \mathbf{w}_p^h, \mathbf{F}_{n+\frac{1}{2}}^h \mathbf{S}^* \rangle_{\mathcal{B}_0^h} \\ \langle \mathbf{w}_\Lambda^h, \frac{\Lambda_{n+1}^{\alpha,h} - \Lambda_n^{\alpha,h}}{\Delta t} \rangle_{\mathcal{B}_0^h} &= \langle \mathbf{w}_\Lambda^h, \frac{1}{\nu^\alpha} \mathbf{Q}^{\alpha,*} \rangle_{\mathcal{B}_0^h}, \end{aligned} \quad (5.253)$$

which can be seen as a natural generalization of the Energy-momentum method for hyperelastic solids to account for viscoelastic effects.

On the other hand, the energy balance is specified by

$$E_{n+1}^h - E_n^h = -\Delta t \int_{\mathcal{B}_0^h} \frac{1}{\nu^\alpha} \|\mathbf{Q}^{\alpha,*}\|^2 dV_0 \leq 0 \quad (5.254)$$

Remark 5.5. The implementation of the EEM method for viscoelastic continuum dynamics depends on the number of internal variables chosen to model the viscous effects. Not only as many dissipative evolution equations as the total number of internal variables should be solved, but a re-calculation of the expression for the time-discrete constitutive laws (5.248)₂, defined by the discrete derivative operator, according to (A.7). In Appendix A, detailed expressions are considered for models with one, two or three internal variables. In the simulations of Chapter 6, just one internal variable will be employed.

Remark 5.6. An elaboration of expression (5.253)₃, taking into account the discrete derivative operator detailed in the Appendix A and the free energy

function (3.109), reveals that it coincides with the standard trapezoidal approximation of the evolution equations for the internal variables. Note that this coincidence is due to the specific dependency of the free energy function on the internal variables.

Simulations

CHAPTER 6

This Chapter contains a series of simulations to illustrate the potential scope of applications that can be addressed by EEM methods. The selected simulations have been divided into three different areas: isothermal viscoelastic solids, thermoelastic solids and multi-body systems composed of isothermal viscoelastic solids or thermo-viscoelastic stiffeners.

All the simulations make use of trilinear hexahedral eight-nodes meshes with fully nonlinear geometrical formulation, as introduced in Chapter 3 and detailed in Appendix B. EEM methods' solutions will be compared with both Trapezoidal and Midpoint methods in order to highlight their superior performance for the selected time step sizes.

Most of the work of this dissertation has consisted in the implementation of the proposed EEM methods into an C++ open (upon request) code developed within a small division of the Computational Mechanics Group at Technical University of Madrid and led by Dr. Juan Carlos García Orden. The code, called EPPI, was primarily intended for the statics and dynamics of multi-body systems composed by rigid and deformable bodies. After the work done for this dissertation, the code has been extended to deal with thermo-dissipative coupled deformable bodies.

EPPI is an object-oriented and MPI-based parallel computing software with the following main features:

- General purpose: statics and dynamics of multi-body systems, composed by rigid and thermal-dissipative coupled deformable bodies.

- Object-oriented software:
- Parallel computing: MPI.
- Solvers and linear algebra: SuperLU, UMFPACK, Eigen.
- Graphics output:
- Version control system:
- Repositories [access upon request]:

1. <https://bitbucket.org/scondemartin/eppi>
2. <https://code.google.com/p/eppi/>

6.1 Dynamics of isothermal viscoelastic solids

In this section, two representative simulations are carried out in order to illustrate the properties and the performance of the isothermal EEM method provided by (5.253). For the first example, the vibration of a cantilever beam is simulated, demonstrating the strength of accurately dissipating the energy according to the laws of thermodynamics. Finally, the simulation of a tumbling L-shaped block is performed to verify the preservation laws and the corresponding effect on the stability and robustness in a problem with notorious geometrical non-linearities (large motions and deformations).

For the viscoelastic behavior in isothermal conditions, the model due to Holzapfel and Simó described in subsection 3.6.1 is considered with only one internal variable. For the hyperelastic part, the Neo-Hookean material model provided in Bonet & Wood (2008) is used, but it would also be possible to consider other common rubber-like materials, such as Ogden-type models, etc.

6.1.1 Vibrating cantilever beam

The vibration of a cantilever beam, depicted in Figure 6.1, under its own weight is analyzed. The beam is 4 m long, has a 0.5×0.5 m cross section, and the finite element mesh has 160 elements. The material behavior is based on a decoupled Neo-Hookean model, see for instance Bonet & Wood (2008),

Figure 6.1. Cantilever beam and external actions

with constants summarized in Table 6.1. The beam is set in motion by the action of a point load applied at the extreme cross section centroid, described in (6.1), which vanishes at 2 s and g is set to 9.81 ms^{-2} .

$$\mathbf{f}(t) = f(t) \begin{bmatrix} 0 \\ 1000 \\ 1000 \end{bmatrix} N, \quad f(t) = \begin{cases} t & \text{for } t \leq 2 \text{ s} \\ 0 & \text{for } t > 2 \text{ s} \end{cases} \quad (6.1)$$

The evolution of the energy of the system (including the dissipated energy) must remain constant in the free-force phase. In other words, the energy introduced by the force will be partially consumed by the development of the viscoelastic deformations such that the beam vibrations will be damped out.

Table 6.1. Viscoelastic decoupled Neo-hookean model properties

Shear moduli	μ	422.5	kPa
Bulk modulus	B	10^4	kPa
Retardation/Relaxation time	τ_1	1.0	s
Dissipative process parameter	μ_1	542.5	kPa
Density	ρ_0	600	kg/m^3

The motion of the beam is integrated for the time interval $[0, 50] \text{ s}$ with time step size of $\Delta t = 0.1 \text{ s}$ using the Trapezoidal, Midpoint and the isothermal EEM method. Some snapshots of the simulation are plotted in Figure

6.2, where the large deflection of the beam can be observed. Figure 6.3 shows the vertical displacement of the extreme cross section centroid in time, and Figure 6.4 shows the horizontal projection of the three-dimensional trajectory of the same point.

Figure 6.2. Snapshot of the motion of the beam (from left to right, top to bottom)

Finally, Figure 6.5 depicts the evolution of the energy obtained with the classic methods and illustrates that they are unable to comply with the first

Figure 6.3. Vertical displacement of the extreme cross section centroid

Figure 6.4. XY Trajectory of the extreme cross section centroid

law of thermodynamics (they lead to non-decreasing evolution of energy at certain time-steps in the free-force phase of the motion), and ultimately fails before the end of the simulation.

On the other hand, the isothermal EEM method, Figure 6.6, succeeds by assuring the fulfillment of the laws of thermodynamics, providing with stability to the simulation.

Figure 6.5. Beam - Energy: $E = K + U$

Figure 6.6. Beam - Energy: $E = K + U$

6.1.2 A tumbling L-shaped block

In this example the dynamics of an L-shaped block with viscoelastic response in isothermal conditions is considered. The L-shaped geometry is provided by the mesh used, among many other works, in Armero & Zambrana-Rojas (2007); Meng & Laursen (2002); Simó & Tarnow (1992) which is depicted in Figure 6.7. The viscoelastic material behavior is based on a decoupled Neo-Hookean model, whose main characteristics are collected in Table 6.2.

Table 6.2. Viscoelastic decoupled Neo-Hooke model properties

Bulk modulus	B_0	5243	Pa
Shear modulus	μ	1004	Pa
Retardation/Relaxation time	τ	20	s
Dissipative process parameter	μ_1	50.2	Pa
Density	ρ_0	100	kgm^{-3}

Figure 6.7. L-shaped block mesh and external forces

During an initial phase the block is subjected to two resultant loads at the top and left end surfaces, faces A and B, respectively, according to Figure 6.7, where the resultant values are also defined. These resultants arise from a nodal forces distribution, which is symmetric, consisting in the application of the sixteenth part of the resultant in each node in the face. At the end of this phase, these forces vanish and, as a result, the block tumbles free of external forces in the space undergoing finite deformation accompanied by large overall rotations and translations.

This example is integrated for a time interval $[0, 200]$ s with a time step size $\Delta t = 0.5$ s using Trapezoidal, Midpoint and the isothermal EEM method. In accordance with the simulation, the energy evolution of the system must increase during the loaded phase and then must be unconditionally decreasing in the free-force phase.

First of all, a sequence of deformed snapshots calculated with the isothermal EEM method is provided in Figure 6.8. Interestingly, as the simulation progresses, the L-block resembles more to the undeformed shape. That happens because the dilational-derivatoric material model concentrates the viscoelastic effects on the derivatoric deformations.

Finally, Figure 6.9 depicts the evolution of the energy of the system obtained with each of the compared methods and clearly shows that the classical ones provide a non-physical evolution of the energy in the free-force phase of the motion, which eventually cause these methods to collapse. Obviously, the final growth of the energy results in polluted solutions, distorted shapes of the block and non-physical viscoelastic stresses. Instead, the isothermal EEM method reproduces the accurate physical behavior, enhancing the stability

Figure 6.8. Snapshots of the motion of the L-shaped block (from left to right, top to bottom)

Figure 6.9. L-Shaped block - Energy $E = K + U$

and robustness of the method and allowing to calculate long term simulations with the same time step as the one which makes classical methods explode. In order to illustrate this assertion, the evolution of the total energy of the body (kinetic plus internal) is computed in a long term simulation of 2000 s, with the same time step as before, in Figure 6.10. Therein, the loss of energy produced in the unloaded phase of the motion due to the viscoelastic dissipation is clearly visible. Both plots demonstrate that the classical methods fail to satisfy the laws of thermodynamics for moderately large time steps, resulting either in physically inaccurate solutions or in the methods' failure.

In addition to this characteristics, the isothermal EEM method also preserves the angular momentum as demonstrates Figure 6.11. It is also provided a zoom to verify that Midpoint method preserves the angular momentum too, as expected, whereas Trapezoidal method does not.

Figure 6.10. L-Shaped block - Long Term Simulation

Figure 6.11. L-Shaped block - Angular Momentum Norm

6.2 Dynamics of thermoelastic solids

In this section, the performance of the EEM methods for the dynamics of thermoelastic solids devised in Section 5.5 is analyzed. The temperature-based EEM method will attract most of the attention due to its novelty. Two simulations are studied based on a fairly complex mesh resulting from twisting a block and on the L-shaped block mesh previously introduced for the analysis of the isothermal viscoelastic dynamics. The first mesh is used in a simulation with no Dirichlet boundary conditions and, therefore, it can be approached by both the entropy- and temperature-based EEM methods. In contrast, the L-shaped block mesh is employed in a example including natural Dirichlet boundary conditions so only the temperature-based EEM can handle with it.

In both simulations, the thermoelastic behavior is modeled by a free energy function of the form provided in (3.86)-(3.87), introduced in Section 3.4, and based on the decoupled Neo-Hookean hyperelastic model previously introduced.

6.2.1 Twisted Block

The simulation consists in the free flight of a twisted block caused by an initial velocity applied on its top. The twisted block was introduced in Romero (2010b) and is constructed from a block of dimensions $4 \times 4 \times 10\pi$ whose top face is twisted 360° with respect to the opposite one. A finite element mesh of non-regular hexahedra is constructed by partitioning the short edges and long edges, respectively, in 3 and 19 identical divisions. Figure 6.12 depicts the twisted block mesh along with the selected frame of reference in which the initial velocity of all the points of the top surface can be expressed as $\mathbf{v}_0 = 10\mathbf{e}_x + 10\mathbf{e}_z$. The constitutive law of the thermoelastic is based on the material constants collected in Table 6.3.

Then, the long term motion of the free-flying twisted block is integrated up to 500 s with a relatively large time step size of $\Delta t = 2.0$ s using the standard Midpoint method formulated in entropy and temperature variables and the temperature-based EEM method (5.183). The performance of the entropy-based EEM method is thoroughly analyzed in Romero (2010b).

Some snapshots of the motion obtained with the EEM method are shown in Figure 6.20. Also, contour plots of temperatures in the deformed meshes are displayed. The initial velocity induces two main effects; on the one hand,

Figure 6.12. Twisted block and initial conditions

a global rotation of the block which leads it from its initial vertical position to an horizontal one, and, on the other hand, a slight torsion of the block, causing deformations that heat up the block due to the coupling effects. The global variation of temperature is moderate although the temperature dramatically increases at the beginning of the motion, where the deformation are more pronounced. After that, the temperature of the block is slowing homogenizing due to the heat conduction process dominated by a low conductivity parameter.

Table 6.3. Thermoelastic decoupled Neo-Hooke model properties

Lamé parameters	λ, μ	1000	Pa
Specific heat capacity	c	1	JK^{-1}
Dilatation coefficient	α	10^{-4}	JK^{-1}
Conductivity	k	0.1	$\text{JK}^{-1}\text{s}^{-1}$
Ref. Temperature	Θ_{ref}	273	K
Density	ρ_0	4	kgm^{-3}

Apparently, the just described dynamics does not pose special challenges, however, none of the standard methods is able to provide an stable solution for the selected time step size. The total energy evolution, depicted in **Figure 6.14**, reveals that the temperature-based Midpoint method outperforms the entropy-based one, although none of them agrees with the first law of thermodynamics. In **Figure 6.15**, the curves of the total entropy evolution provided by the two standard methods are depicted, confirming that the entropy-based Midpoint method provides the correct non-decreasing behavior dictated by the second law of thermodynamics (3.193), while the temperature-based Midpoint method fails to adhere to such principle. This observation corroborates the general conclusion drawn along this dissertation asserting that the capacity for integration methods to agree with the first law is much more critical regarding the methods' stability than the capacity to meet the second principle of thermodynamics.

In contrast, the temperature-based EEM method manages to meet the two laws of thermodynamics for such a moderately large time step size, as shown in **Figure 6.16** and **Figure 6.17**, allowing for stable solutions in long term simulations. Additionally, the total angular momentum is preserved as can be seen in **Figure 6.18**.

Figure 6.13. Snapshots and contour plots of temperature of the Twisted block (from top to bottom, left to right). Temperature-based EEM integration, $\Delta t = 2$ s

Figure 6.14. Standard methods: Total energy evolution

Figure 6.15. Standard methods: Total Entropy evolution

Figure 6.16. Total energy evolution **Figure 6.17.** Total Entropy evolution

Figure 6.18. Total Angular momentum evolution

6.2.2 L-shaped block with Dirichlet initial-boundary conditions

In order to further exploit the performance of the temperature-based EEM method, consider the L-shaped block of subsection 6.1.2, now made of thermoelastic material and, again, subject to two external forces that vanish at certain time. In addition, in faces A and B , Dirichlet initial-boundary conditions are imposed by setting temperatures other than the reference temperature, as indicated in Figure 6.19. After the initial instant, the temperature of the faces are not imposed any longer so that they will evolve according to the balance laws. This consideration prevents the entropy-based EEM method (5.166) to be directly applied, that is, its application would require an involved preprocess to infer the values of entropy at every node.

Figure 6.19. L-shaped block with Dirichlet initial-boundary conditions

The example is integrated using the standard Midpoint and Trapezoidal methods and the temperature-based EEM up to 100 s and time step size of $\Delta t = 0.2$ s. The rest of the data required to perform the simulation is provided by the thermoelastic material parameters are in Table 6.4

Then, the result provided by the temperature-based EEM method is plotted in Figure 6.20, which contains the contour plots of temperatures for different snapshots of the motion described by the block. The initial external actions induce both large deformations and rotations in the block while the thermal evolution is controlled by the heat conduction process which slowly

Table 6.4. Thermoelastic decoupled Neo-Hooke model properties

Shear modulus	μ	997.5	Pa
Bulk modulus	B_0	5209	Pa
Specific heat capacity	c	100	JK ⁻¹
Dilatation coefficient	α	$2.233 \cdot 10^{-4}$	JK ⁻¹
Conductivity	k	10	JK ⁻¹
Ref. Temperature	Θ_{ref}	293.15	K
Density	ρ_0	100	kgm ⁻³

compensates the gradient of temperature caused by the initial-boundary conditions.

For the selected time step size, only the temperature-based EEM method is able to integrate the whole time interval. The standard methods, formulated in temperature variable to handle with the initial-boundary conditions, become unstable before the end of the integration. The instabilities are directly related to the incapacity to fulfill the first law of thermodynamics in the force-free phase of the evolution as shows **Figure 6.21**. Neither is the second law satisfied by the standard methods as can be observed in **Figure 6.22**. In contrast, both figures clearly show that the temperature-based EEM method provides evolutions of the total energy and total entropy in agreement with the laws of thermodynamics, this way successfully managing to complete the long term simulation. In addition, **Figure 6.23** demonstrates that the solution provided by the EEM method respects the symmetries of the isolated evolution equations by plotting the total angular momentum which is preserved during the force-free phase of the motion of the block.

Figure 6.20. Snapshots and contour plots of temperature of the L-shaped block (from top to bottom, left to right). Temperature-based EEM integration, $\Delta t = 0.2$ s

Figure 6.21. Total energy $E = K + U$

Figure 6.22. Total Entropy

Figure 6.23. Total Angular Momentum

6.3 Isothermal viscoelastic applications to multibody system dynamics

Before presenting particular applications, the multibody framework is briefly introduced, focusing on how to treat the deformable isothermal dissipative solids so that the laws of thermodynamics are satisfied by design.

6.3.1 Multibody framework

All nodal coordinates $\mathbf{x}^a$ and nodal variations $\delta\mathbf{x}^a$ are collected in vectors $\mathbf{q}_D$ and $\delta\mathbf{q}_D$ respectively. As a result, the discrete weak formulation (3.166) can be written in matrix format as

$$(\delta\mathbf{q}_D)^T \left(\underbrace{\int_{\mathcal{B}^h} \rho \mathbf{N}^T \mathbf{N} dV}_{\mathbf{M}_D} \ddot{\mathbf{q}}_D^h - \underbrace{\int_{\mathcal{B}_0^h} \mathbf{B} \mathbf{S}^h dV_0}_{\mathbf{f}_D^{int}} - \mathbf{f}_D^{ext} \right) = 0 \quad (6.2)$$

with $(\delta\mathbf{q}_D) \in \mathcal{V}^n$ defined in a finite-dimensional space. Accordingly, the isothermal EEM method (5.249) can be written in matrix form in terms of the nodal positions $\mathbf{q}_D(t)$ and velocities $\dot{\mathbf{q}}_D(t)$ as follows

$$\begin{aligned} \mathbf{M}_D(\dot{\mathbf{q}}_{D_{n+1}} - \dot{\mathbf{q}}_{D_n}) - \Delta t (\mathbf{f}_D^{int*} + \mathbf{f}_D^{ext*}) &= \mathbf{0} \\ \dot{\mathbf{q}}_{D_{n+1}} &= \frac{2(\mathbf{q}_{D_{n+1}} - \mathbf{q}_{D_n})}{\Delta t} - \dot{\mathbf{q}}_{D_n}, \end{aligned} \quad (6.3)$$

where $\mathbf{f}_D^{int*}$ and $\mathbf{f}_D^{ext*}$ are second-order algorithmic approximations of the internal and external forces respectively in the time interval $[t_{n+1}, t_n]$, that ensure exact discrete energy consistency based on the discrete derivative operator. Note that internal variables $\Lambda^{\alpha,h}$ do not explicitly appear in (6.3) since they are condensed at element level.

A MBS formed by several deformable bodies $(\mathcal{B}_i, i = 1, \dots, N)$ is achieved by simply collecting in $\mathbf{q}_D$ all the variables of the different bodies, assembling the matrices and forces and adding the constraint terms associated with the kinematic pairs. These constraint terms will be explained with some more detail in the following section.

6.3.2 Rigid bodies and constraints

A set of dependent coordinates will be used to define the position of a rigid body $\mathcal{B}_R$, collected in vector $\mathbf{q}_R : [0, T] \rightarrow \mathbb{R}^{3m}$. Deliberately, these

coordinates will always be the spatial (inertial) coordinates of m selected material points in $\mathcal{B}_R$. In terms of them, the kinetic energy (K_R) can always be expressed as

$$K_R = \frac{1}{2} \dot{\mathbf{q}}_R^T \cdot (\mathbf{M}_R \dot{\mathbf{q}}_R) \quad (6.4)$$

$\mathbf{M}_R$ being the mass matrix, which will be constant provided that $m \geq 4$ and the selected points are non-coplanar and non-aligned in groups of three García Orden & Goicolea (2000).

As long as $\mathbf{q}_R$ collects coordinates of material points within the rigid body, constant-distance constraints are necessary. These constraints are holonomic and scleronomic $\Phi : \mathbb{R}^{3m} \ni \mathbf{q}_R \mapsto \Phi(\mathbf{q}_R) \in \mathbb{R}^q$; thus, they do not dissipate energy. The weak form of the constrained problem, based on the introduction of Lagrange multipliers $\lambda \in \mathbb{R}^q$ is

$$\begin{aligned} \delta \mathbf{q}_R^T \cdot \mathbf{M}_R \ddot{\mathbf{q}}_R + \delta \mathbf{q}_R^T \cdot [(\mathbf{D}\Phi)^T \lambda] + \delta \lambda^T \cdot \Phi - \\ - \delta \mathbf{q}_R^T \cdot \mathbf{f}_R^{ext} = 0 \\ \forall \delta \mathbf{q}_R \in \mathcal{V}^{3m}, \forall \delta \lambda \in \mathcal{X}^q, \end{aligned} \quad (6.5)$$

where $\mathbf{f}_R^{ext}$ is the vector of external forces and $\mathbf{f}_{\Phi_R} = -(\mathbf{D}\Phi)^T \lambda$ is the constraint force vector with $\mathbf{D}\Phi = \partial \Phi / \partial \mathbf{q}_R$. The enforcement of the constraints with the penalty method is equivalent to consider $\lambda = \alpha \Phi$ in the former expression, where α is a $(q \times q)$ constant penalty matrix. Generalising the above approach, a MBS formed by several rigid bodies ($\mathcal{B}_{R_i}, i = 1, \dots, N$) is achieved by simply collecting in $\mathbf{q}_R$ all the variables of the different bodies and adding the constraint terms associated with the kinematic pairs.

6.3.3 Flexible multibody system

Consider now a multibody system composed of sets of both rigid ($\mathcal{B}_R$) and deformable ($\mathcal{B}_D$) bodies. Rigid bodies are defined by coordinates $\mathbf{q}_R : [0, T] \rightarrow \mathbb{R}^m$ and the deformable ones by $\mathbf{q}_D : [0, T] \rightarrow \mathbb{R}^n$. Constraints are classified into three categories: a) constraints Φ_R involving rigid body points only; b) constraints Φ_D involving deformable body points only and, finally, c) constraints Φ_{RD} involving rigid and deformable body points.

The weak form of the dynamic equation with Lagrange multipliers may

be written as

$$\begin{aligned}
& \delta \mathbf{q}_R^T \cdot \mathbf{M}_R \ddot{\mathbf{q}}_R + \delta \mathbf{q}_D^T \cdot \mathbf{M}_D \ddot{\mathbf{q}}_D + \delta \mathbf{q}_D^T \cdot \mathbf{f}_D^{int} + \\
& + \delta \mathbf{q}_R^T \cdot [(\mathbf{D}\Phi_R)^T \boldsymbol{\lambda}_R + (\mathbf{D}_R \Phi_{RD})^T \boldsymbol{\lambda}_{RD}] + \\
& + \delta \mathbf{q}_D^T \cdot [(\mathbf{D}\Phi_D)^T \boldsymbol{\lambda}_D + (\mathbf{D}_D \Phi_{RD})^T \boldsymbol{\lambda}_{RD}] - \\
& - \delta \boldsymbol{\lambda}_R^T \cdot \Phi_R - \delta \boldsymbol{\lambda}_D^T \cdot \Phi_D - \delta \boldsymbol{\lambda}_{RD}^T \cdot \Phi_{RD} \\
& - \delta \mathbf{q}_R^T \cdot \mathbf{f}_R^{ext} - \delta \mathbf{q}_D^T \cdot \mathbf{f}_D^{ext} = 0 \\
& \quad \forall \delta \mathbf{q}_R \in \mathcal{V}^m, \quad \forall \delta \mathbf{q}_D \in \mathcal{V}^n, \\
& \quad \forall \delta \boldsymbol{\lambda}_R \in \mathcal{X}^{q_R}, \quad \forall \delta \boldsymbol{\lambda}_D \in \mathcal{X}^{q_D}, \quad \forall \delta \boldsymbol{\lambda}_{RD} \in \mathcal{X}^{q_{RD}}, \quad (6.6)
\end{aligned}$$

where $\mathbf{D}_R$ and $\mathbf{D}_D$ are respectively the derivative operators for Φ_{RD} with respect to $\mathbf{q}_R$ and $\mathbf{q}_D$.

Finally, defining a new global vector of unknowns $\mathbf{q} : [0, T] \rightarrow \mathbb{R}^{m+n}$ merging $\mathbf{q}_R$ and $\mathbf{q}_D$, being $\delta \mathbf{q}, \delta \boldsymbol{\lambda}_R, \delta \boldsymbol{\lambda}_D$ and $\delta \boldsymbol{\lambda}_{RD}$ arbitrary, global dynamics will be expressed by the set of index-3 algebraic-differential equations in matrix form:

$$\begin{aligned}
& \underbrace{\left(\begin{array}{c|c} \mathbf{M}_R & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{M}_D \end{array} \right)}_{\mathbf{M}} \underbrace{\left\{ \begin{array}{c} \ddot{\mathbf{q}}_R \\ \ddot{\mathbf{q}}_D \end{array} \right\}}_{\ddot{\mathbf{q}}} = \\
& \underbrace{\left\{ \begin{array}{c} \mathbf{f}_{\Phi_R} \\ \mathbf{f}_{\Phi_D} \end{array} \right\}}_{\mathbf{f}_{\Phi}} + \mathbf{f}_{\Phi_{RD}} + \underbrace{\left\{ \begin{array}{c} \mathbf{0} \\ \mathbf{f}_D^{int} \end{array} \right\}}_{\mathbf{f}} + \underbrace{\left\{ \begin{array}{c} \mathbf{f}_R^{ext} \\ \mathbf{f}_D^{ext} \end{array} \right\}}_{\mathbf{f}^{ext}} \quad (6.7a)
\end{aligned}$$

$$\Phi_R = \mathbf{0}, \quad \Phi_D = \mathbf{0}, \quad \Phi_{RD} = \mathbf{0}, \quad (6.7b)$$

where $\mathbf{f}_{\Phi_{RD}}$ is the coupling term between the rigid and the deformable sub-systems. If a penalty method is employed, equations (6.7b) disappear and (6.7a) transforms into a purely differential system.

6.3.4 Consistent rigid bodies and constraints

Based on the parametrization for rigid bodies presented in the previous section, with inertial Cartesian coordinates $\mathbf{q}_R$ of selected material points, it becomes apparent that the consistent formulation relies just on the adequate treatment of the constant-distance constraints. This is due to the fact that the mass matrix $\mathbf{M}_R$ is constant, and therefore the conserving formulation of the inertial terms, following (6.3), is given simply by $\mathbf{M}_R(\dot{\mathbf{q}}_{R_{n+1}} - \dot{\mathbf{q}}_{R_n})$.

Note that the constant-distance constraints are holonomic and scleronomous; thus they do not dissipate energy and the consistent formulation is in this case an energy-conserving one.

A conserving formulation of a constant-distance constraint can be obtained with a Lagrange multiplier method González (1999), a penalty method García Orden (1999); García Orden & Goicolea (2000) or an augmented Lagrangian method García Orden & Ortega Aguilera (2006). With the Lagrange multipliers and augmented Lagrange methods, constraints are exactly satisfied with exact discrete energy conservation. With the penalty method, constraints are violated but the stored energy is exactly released if they are exactly fulfilled. This means that, with conserving penalty, the summation of the kinetic energy, the potential energy of the conserving applied forces and the constraint energy is constant.

Constraint forces, specifically formulated to satisfy exact energy conservation, are introduced into the scheme (6.3). Among all available options, the conserving penalty formulation is specially appealing due to its simplicity, as it can be obtained from a constraint potential. For example, consider two points with positions defined by vectors $\mathbf{x}_1$ and $\mathbf{x}_2$. The relative position vector is denoted by $\mathbf{r} = \mathbf{x}_2 - \mathbf{x}_1$ and the absolute distance by $r = |\mathbf{r}|$. The constant-distance constraint is expressed as $\Phi(r) = r - r_0$, being r_0 the initial distance. With this notation, the conserving constraint force is given by:

$$\mathbf{f}_{\Phi_R}^* = -\alpha \left(1 - \frac{r_0}{\tilde{r}_{n+\frac{1}{2}}} \right) \begin{pmatrix} \mathbf{r}_{n+\frac{1}{2}} \\ -\mathbf{r}_{n+\frac{1}{2}} \end{pmatrix}, \quad (6.8)$$

where $\tilde{r}_{n+\frac{1}{2}} = (r_{n+1} + r_n)/2$ and $\alpha \in \mathbb{R}_+$ is the penalty parameter. Full details about the linearization of (6.8) and other important practical issues, as the behaviour in the limit $\Delta \mathbf{r} \rightarrow \mathbf{0}$, can be found in García Orden & Goicolea (2000); Goicolea & García Orden (2002).

Joints connecting different bodies are taken into account with additional constraints, not necessarily of the constant-distance type. These constraints will depend, in general, on the position vectors of many points of the bodies, and will be fully non-linear. If a conserving penalty approach is employed, different strategies can be employed; one option is to directly apply the discrete derivative operator (5.2) to the constraint potential in order to obtain the constraint force $\mathbf{f}_{\Phi}^*$, as in Leyendecker et al. (2004). Other option is to enforce the directionality condition (5.4) with a standard derivative evaluated at an intermediate value in $[t_{n+1}, t_n]$, as proposed in the original energy-momentum method by Simó & Tarnow (1992). Details of this latter approach can be found in García Orden & Goicolea (2000).

6.3.5 Consistent flexible multibody system

In the previous sections a energy-consistent formulation of deformable viscoelastic bodies, rigid bodies and constraints has been obtained. Thus, the energy-consistent global formulation of a flexible multibody system is obtained in a straightforward way, just putting together both the rigid and the deformable subsystems and adding the terms related with the constraints, representing the kinematical joints between them. Following the format given in (6.3) and using the conserving penalty method for the constraints, the following scheme is obtained to be solved for the global positions and velocities $\mathbf{q}_{n+1}$ and $\dot{\mathbf{q}}_{n+1}$:

$$\underbrace{\left(\begin{array}{c|c} \mathbf{M}_R & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{M}_D \end{array} \right)}_{\mathbf{M}} \left[\underbrace{\left\{ \begin{array}{c} \dot{\mathbf{q}}_{R_{n+1}} \\ \dot{\mathbf{q}}_{D_{n+1}} \end{array} \right\}}_{\dot{\mathbf{q}}_{n+1}} - \underbrace{\left\{ \begin{array}{c} \dot{\mathbf{q}}_{R_n} \\ \dot{\mathbf{q}}_{D_n} \end{array} \right\}}_{\dot{\mathbf{q}}_n} \right] - \underbrace{\left\{ \begin{array}{c} \mathbf{f}_{\Phi_R}^* \\ \mathbf{f}_{\Phi_D}^* \end{array} \right\}}_{\mathbf{f}_{\Phi}^*} - \mathbf{f}_{\Phi_{RD}}^* - \underbrace{\left\{ \begin{array}{c} \mathbf{0} \\ \mathbf{f}_D^{int*} \end{array} \right\}}_{\mathbf{f}^*} - \underbrace{\left\{ \begin{array}{c} \mathbf{f}_R^{ext*} \\ \mathbf{f}_D^{ext*} \end{array} \right\}}_{\mathbf{f}^*} = \mathbf{0} \quad (6.9a)$$

$$\dot{\mathbf{q}}_{n+1} = \frac{2(\mathbf{q}_{n+1} - \mathbf{q}_n)}{\Delta t} - \dot{\mathbf{q}}_n, \quad (6.9b)$$

where the symbol (*) represents the EEM algorithmic approximation of the affected magnitude.

6.3.6 Applications

In this section three examples inspired by real mechanisms have been considered to be representative of complex multibody systems with deformable isothermal dissipative bodies, where stable and accurate long-term computational solutions are usually hard to obtain.

It is necessary to remark that these two examples are used just to illustrate the performance and the applicability of the proposed energy-consistent global method for flexible multibody systems; a detailed state-of-the-art survey on computational models for the dynamics of these types of specific systems are out of the scope of this dissertation and, accordingly, no detailed critical comparisons with other methods traditionally applied in these fields are included. Nevertheless, a very brief outline of the key issues affecting their numerical solution are presented for each one of them.

Satellite with viscoelastic solar panels' maneuver. Many references in the literature study the dynamics of spacecrafts with flexible appendages, like solar panels or antennas; e.g. Gao et al. (2008); Lomas (2001); Modi (1974); Sakamoto et al. (2011); Wallrapp & Wiedemann (2002); Zakrzhevskii (2008). Banerjee (2003) presents an interesting overview of the computational difficulties associated to very flexible space structures; namely the stiff character of the equations of motion, the coupling between axial and bending effects and the problems associated with large deformations. Stiffness is tackled using implicit integration schemes, that usually improve stability introducing numerical damping in the high-frequency range. The axial-bending coupling is considered by introducing additional terms to the standard floating frame of reference approach, or by a fully nonlinear formulation for the flexible parts, that has also the advantage of being capable of representing large deformations. The presented approach, based on a full nonlinear finite element formulation combined with the energy-consistent (implicit) integration scheme, is thus a valid framework for dealing with these problems. The advantage of using the energy-consistent time-integration scheme is that it allows to obtain stable long-term solutions with time step sizes larger than those associated to standard methods, while being more physically accurate, as it will be illustrated next.

Consider the maneuver of a satellite with flexible solar panels made of viscoelastic material and depicted in Figure 6.24. The body is a $1 \times 1 \times 1$ m cube with a mass of 500 kg, and each panel is 4 m long, 1 m wide and 0.1 m thick. Each panel is hinged to the satellite body by three smooth spherical joints (see Figure 6.25) and connected by four rigid and massless bars, acting as stiffeners of the panels. The satellite body is equipped with two rockets R_1 and R_2 that provide the necessary thrust, given by (6.10) expressed in kN, to perform the maneuver aimed to change of attitude of the satellite in 90° . The motion is illustrated in Figure 6.26.

Figure 6.24. Satellite: mesh and boundary condition definition.

Figure 6.25. Satellite: spherical joints' position.

$$R_1(t) = -R_2(t) = \begin{cases} -t & \text{for } t \leq 0.5 \text{ s} \\ t - 1 & \text{for } 0.5 < t \leq 1 \text{ s} \\ 0 & \text{for } 1 < t \leq 12.8 \text{ s} \\ 1.15(12.8 - t) & \text{for } 12.8 < t \leq 13.3 \text{ s} \\ 1.15(t - 13.3) & \text{for } 13.3 < t \leq 13.8 \text{ s} \\ 0 & \text{for } t > 13.8 \text{ s} \end{cases} \quad (6.10)$$

The satellite body is modeled with a homogeneous Saint Venant-Kirchhoff material with density $\rho_{0,b} = 500 \text{ kg/m}^3$, a Young modulus $E_b = 1 \text{ GPa}$ and Poisson coefficient $\nu_b = 0.3$. The panels are modeled by the viscoelastic material due to Holzapfel & Simó (1996b) with free-energy provided by (3.109) based on Neo-hookean hyperelasticity and one internal variable, with $\nu_p = 0.4$, $E_p = 100 \text{ kPa}$, $\tau_p = 2 \text{ s}$, $\mu_p = 5 \text{ kPa}$ and $\rho_{0,p} = 100 \text{ kg/m}^3$.

The example is integrated for a time interval $[0, 50] \text{ s}$ with a time step size $\Delta t = 0.2 \text{ s}$ using trapezoidal and energy-consistent methods. In addition, an integration using the Midpoint method is performed with a smaller time step size, i.e $\Delta t = 0.02 \text{ s}$, in order to stress that conserving the angular-momentum does not help to stabilize solutions as conserving the laws of thermodynamics does.

Figure 6.27 depicts the evolution of the energy of the system obtained with each scheme. It clearly shows that the Trapezoidal method provides a non-physical evolution of the energy in the free-force phases of the motion, which eventually cause this method to collapse. The same can be concluded for the midpoint method which is unable to provide a full integration even for a time step size ten times smaller.

On the other hand, the isothermal EEM method successes in simulating

Figure 6.26. Snapshots of the maneuver (from top to bottom, left to right).
Energy-consistent integration, $\Delta t = 0.2$ s

the whole time interval, showing a decreasing total energy during the free-force periods of the motion. It can be concluded that the isothermal EEM method enhances the stability and robustness of the numerical integration of this problem, allowing to calculate long term simulations with the same time step as the one which makes standard methods fail.

Figure 6.28 shows that the energy-consistent method exactly conserves the angular momentum in the free-force periods of the movement, while the trapezoidal rule fails to accomplish it even when it remains stable, during the first seconds of integration.

Finally, Figure 6.29 shows that the dissipation increases as the relaxation times decreases. Note that the energy-consistent integration provides positive dissipation in all cases.

Figure 6.27. Satellite. Evolution of the total energy of the system, kinetic plus potential, obtained with the Trapezoidal, Midpoint and isothermal EEM method. Only the isothermal EEM method provides a full solution which, in addition, is in accordance with the laws of thermodynamics

Figure 6.28. Satellite. Evolution of the angular momentum of the system obtained with the trapezoidal and isothermal EEM methods.

Figure 6.29. Satellite, Total energy (kinetic plus potential), isothermal EEM integration with $\Delta t = 0.2$ s

Satellite with thermoviscoelastic stiffeners' maneuver. This example simulates a maneuver of a satellite with flexible solar panels, as depicted in Figure 6.30. The model is very similar to the one presented in García Orden & Romero (2011) , which was solved with an entropy-based EEM method as well as standard Midpoint and Trapezoidal rules.

The body is a $1 \times 1 \times 1$ m cube with a mass of 500 kg, and each panel is 4 m long, 1 m wide and 0.1 m thick. Each panel is hinged at the lower side to the satellite body by three smooth spherical joints and connected by four discrete thermo-visco-elastic elements, acting as stiffeners.

Figure 6.30. Satellite model, showing the solar panels' hinges and the rockets

The satellite body is equipped with two rockets R_1 and R_2 that provide the necessary thrust to perform the maneuver, aimed to change of attitude of the satellite in 90° . The maneuver starts firing both rockets during 1 s, initiating a rotation of the whole satellite. After one and a quarter turn, the movement of the panels stabilizes and the rockets are fired again; this second firing takes place in the precise moment of time required to stop the rotation leaving the satellite with the new orientation. The time-dependent forces of the rockets are shown in Figure 6.31, and the motion is illustrated in Figure 6.26.

Both the satellite body and the panels are modeled with an homogeneous Saint Venant-Kirchhoff material. The material of the body has a density $\rho_b = 500 \text{ kg/m}^3$, a Young modulus $E_b = 1 \text{ GPa}$ and Poisson coefficient $\nu_b = 0.3$. The panels have a density $\rho_p = 10 \text{ kg/m}^3$, a Young modulus $E_p = 5000 \text{ Pa}$ and a Poisson coefficient $\nu_p = 0.3$. Eight-noded hexahedral finite elements with a fully nonlinear geometrical formulation are employed for both the body and the panels.

Figure 6.31. Rocket forces vs. time

The parameters of the thermo-visco-elastic stiffeners are $\lambda_0 = 1$ m, $\theta_r = 300$ K, $c_{10} = 100$ Nm, $c_{11} = 0.5$ NmK⁻¹, $\beta_c = 4$ NmK⁻¹, $c_0 = 1$ NmK⁻¹, $\mu_0 = 5$ Nm⁻¹, $\mu_1 = 0.1$ Nm⁻¹K⁻¹, $\eta_0 = 100$ Nsm⁻¹, $a = 10$ K. The environment temperature is constant $\theta_{\text{ref}} = 10$ K and the thermal conductivity is $k = 2$ Nms⁻¹K⁻¹.

The motion obtained with the thermodynamically consistent integration of the dynamical equations is shown in Figure 6.26, being the consistent formulation of the elastic parts of the system provided by the energy-momentum scheme (González, 2000; Simó & Tarnow, 1992; Simó et al., 1992), and the dissipative thermo-visco-elastic stiffeners implement the temperature-based TC formulation presented in this paper.

The differences between this model and the one presented in García Orden & Romero (2011) are:

- The number of panels. The increment of the number of panels from two to four has several effects that add some numerical difficulties. Basically, it produces a kinematically richer movement, with two of the panels deforming with a dominant bending mode and the other two with a torsional mode. As a consequence higher frequencies are introduced, because panel torsional frequencies are a little bit higher

than the bending ones.

- The conductivity (k) between the stiffeners and the environment. The decrement of the conductivity will produce higher temperatures in the elements, because the generated heat dissipates at a lower rate.
- The dependency of the main spring stiffness with temperature. Since higher temperatures are expected, the logarithmic expression (2.96) have been adopted, while in García Orden & Romero (2011) is linear. This choice poses additional technical difficulties, as it has already been mentioned in different sections of the paper, when entropy is used to formulate the EEM method. Nevertheless, no special difficulties appear when temperature is used.

Figures 6.33, 6.34 and 6.35 display the angular momentum, the energy and the entropy respectively, obtained with the temperature-based EEM method with $\Delta t = 0.2$ s, which are qualitatively similar to the ones reported in García Orden & Romero (2011). Exact discrete satisfaction of the two laws of thermodynamics and the symmetries (rotational in this case, associated with the angular momentum during the free-force motion) is observed as expected.

Figures 6.36 and 6.37 show the evolution of the representative temperature of the different groups of stiffeners. Specifically, Figure 6.36 displays the temperature of the stiffeners constraining the two panels that have a distinct bending motion (parallel to the plane perpendicular to the angular velocity), while Figure 6.37 shows the temperature of the rest of the stiffeners, associated to the panels that have a distinct torsional motion.

Finally, Figures 6.38, 6.39 and 6.40 have been included to emphasize the robustness of the proposed temperature-based EEM method compared with standard methods, such as Midpoint and Trapezoidal methods. These methods are convergent and can successfully obtain a solution provided the time-step size is reduced. However, the numerical experiment shows that the temperature-based EEM method may obtain a stable solution with time-step sizes larger than those limited by stability in standard methods, with exact satisfaction of the two laws of thermodynamics and the present symmetries.

Figure 6.32. *Snapshots of the maneuver (from top to bottom, left to right).
Consistent integration, $\Delta t = 0.2$ s*

Figure 6.33. Total angular momentum, consistent integration, $\Delta t = 0.2$ s

Figure 6.34. Energy, consistent integration, $\Delta t = 0.2$ s

Figure 6.35. Entropy, consistent integration, $\Delta t = 0.2$ s

Figure 6.36. Stiffeners' temperature, EEM method, $\Delta t = 0.2$ s

Figure 6.37. Stiffeners' temperature, consistent integration, $\Delta t = 0.2$ s

Figure 6.38. Total angular momentum, $\Delta t = 0.2$ s

Figure 6.39. Total energy $\Delta t = 0.2$ s **Figure 6.40.** Total entropy, $\Delta t = 0.2$ s

Rotor blade with elastomeric bearing. For the last example, consider a multibody model of a helicopter rotor blade incorporating an elastomeric bearing.

There are many references in the specialized literature on multibody dynamics devoted to the dynamics of rotorcraft systems; see for instance Bauchau (2009); Chun et al. (2013); Kang et al. (2014); Maqueda et al. (2008) and references therein. Likewise the satellite example of the previous section, the coupling between axial and bending effects along with the stiff character of the related initial value problems are among the main numerical challenges posed by these types of models. The model proposed in this paper is simple but, nevertheless, incorporates these difficulties and, therefore, we have considered it to be representative of this type of engineering systems. Descriptions of suitable numerical approaches described in the literature as well as the advantages of the proposed approach have already been mentioned regarding the satellite example and are omitted here.

The bearing is a $0.3 \times 0.3 \times 0.2$ m block made of viscoelastic material connecting the solid rigid blade and the rotor. The blade is a rigid prism 2.7 m long with a density of 2500 kg/m^3 . Figure 6.41 shows the whole model. The material parameters used for the viscoelastic bearing are: $\nu = 0.49$, $E = 2.1 \text{ MPa}$, $\tau = 10 \text{ s}$, $\mu = 1.05 \text{ MPa}$ and $\rho_0 = 100 \text{ kg/m}^3$.

The internal face of the prismatic bearing is rigid and is rigidly attached to the hub (not shown, located at the center of the reference system XYZ in Figure 6.41). The two lower vertices of the bearing internal face are constrained to frictionless move along the fixed circular path depicted also in Figure 6.41.

Figure 6.41. Rotor blade with elastomeric bearing: mesh and boundary condition definition.

Figure 6.42. Snapshots of the motion of the rotor blade with elastomeric bearing

The system is initially in an horizontal position and at rest, and it is set to motion by the hub with an angular velocity $\omega_0(t)$ around the fixed vertical axis which acts during the first 2 s and is defined by the law:

$$\omega_0(t) = \frac{\omega_s}{2} \left[t - \frac{1}{\pi} \sin(\pi t) \right] \text{ if } 0 \leq t \leq 2 \text{ s} \quad (6.11)$$

with $\omega_s = 0.6124$ rad/s. The time step size is chosen as $\Delta t = 0.1$ s and the motion is integrated up to 30 s with trapezoidal and energy-consistent methods. An extra simulation is carried out by midpoint method and time step size of $\Delta t = 0.01$ s.

Figure 6.42 shows some snapshots of the motion, which is a composition of the main rotation around the vertical axis imposed by the rotor and rotations around other spatial axis due to the deformation of the bearing under the action of gravity and the inertia effects. Figure 6.43 shows the vertical position of the center of mass of the blade, oscillating due to the aforementioned deformation of the bearing under to the weight of the blade.

Figure 6.44 shows that the total energy obtained with the isothermal EEM method is monotonically decreasing during the free-force motion, while the trapezoidal rule shows a non-physical behavior and eventually becomes unstable. As in the previous example, the midpoint method with a smaller time step size is able to integrate further time steps but ends up failing due to an unreasonable growth of the energy.

Figure 6.45 displays the dependency of the energy with the relaxation-time parameter, computed with the isothermal EEM method. As expected, we obtain a positive dissipation that increases as the relaxation time of the viscoelastic model decreases.

Figure 6.43. Vertical position of the blade center of mass

Figure 6.44. Evolution of the total energy of the blade system.

Figure 6.45. Total energy (kinetic plus potential), isothermal EEM with $\Delta t = 0.1$ s

Summary, conclusions and future work

CHAPTER 7

This dissertation has addressed the formulation, analysis and implementation of structure-preserving time integration methods for nonlinear smooth coupled dissipative systems. These time integration methods are able to provide solutions which agree with the fundamental conservation properties identified in continuous models derived from the laws of thermodynamics and symmetries. They are constructed within an uniform methodology consisting of a temporal discretization of mid-point type combined with a special second order accurate discrete operator responsible for preservation of the thermodynamical and symmetrical structure of the continuous equations. Thus, the resulting methods are Energy-preserving Entropy-producing and Momentum-preserving (EEM) by design while rendering second-order accuracy.

The uniform methodology conceptually relies on the underlying metriplectic structure of the initial-boundary value problems defining the evolution of coupled smooth dissipative systems. Such structure provides an unified framework to deal with any dissipative system governed by the laws of thermodynamics. Formally, a metriplectic structure is a generalization of the (reversible) Poisson structure that possesses Hamiltonian (conservative) systems by attaching a (irreversible) Gradient structure that defines pure dissipative systems. Then, the evolution of dissipative systems is generated from the addition of two reversible and irreversible operators. Using a particular metriplectic framework, known by the acronym GENERIC, the methodology has basically consisted in extending the concepts involved in the formulation of Energy-Momentum integration methods to the integration of dissipative

problems defined by its metriplectic structure. Thus, the concept of the discrete derivative operator has enabled the derivation of discrete counterparts that agree with the laws of thermodynamics and respect the symmetries.

Alternative strategies have been adopted deriving from the use of either entropies or temperatures for the thermodynamic state variable. Special attention has been paid to the temperature-based formulation since it has not thus far been developed. With these strategies, most of the real problems of interest can successfully be faced.

The formulation of EEM methods for finite-dimensional dissipative systems directly follows from the introduced methodology with the only requirement of devising its reversible and irreversible operators in the sense of the metriplectic structures in terms of the thermodynamical variable chosen. Thus, the discrete preservation features are completely guaranteed.

For infinite-dimensional dissipative systems, however, the methodology must be supplemented by a spatial discretization that converts the system into a finite-dimensional one in such a way that the preservation features are not altered. The classical Galerkin FE-based technique has been proved to be appropriated for the successful formulations of EEM methods. The final discrete conservation features, however, might not be guaranteed for any formulation based on this methodology. Specifically, Galerkin formulations requires that the resulting discrete derivative operators belong to the finite-dimensional Galerkin space. Unfortunately, this cannot be ensured for any formulation of the system. Particularly, that is the case of the entropy-based approach whose resulting EEM method needs to be corrected with an L_2 -projection technique.

Several representative smooth dissipative systems have been considered from finite- to infinite-dimensional ones addressing the most common sources of dissipation: heat conduction and internal dissipative effects. In all of them, dissipative effects have been considered *smooth*, in the sense that they may be described by continuous laws, and have been approached by internal variables which naturally contributes to the irreversible operator of the metriplectic structure.

Each of the smooth dissipative systems has been thoroughly introduced discussing its conservation features and reasoning the loss of some of such features when standard integration methods are used to obtain approximate solutions. The continuous formulation of these systems has been approached following classical thermodynamical assumptions from different perspectives according to the thermodynamical variable chosen for the description of the

system thermodynamics. Also, the continuous formulation has been addressed by the unified GENERIC framework, carefully developing the reversible and irreversible operators in terms of both entropy and temperatures, guaranteeing the thermodynamical soundness of the formulated systems.

Then, the methodology to construct EEM methods has been fully exploited so that entropy-based and temperature-based EEM methods have been proposed and checked their discrete conservation features. Also, both approaches has been compared regarding conservation features, relative errors, applicability and implementation issues.

Thus, from the formulation point of view, it can be asserted that the temperature-based EEM methods pose three main advantages respect to their entropy-based counterparts:

- Common constitutive formulations in terms of the temperature can directly be applied.
- Dirichlet boundary conditions are naturally imposed.
- In Galerkin formulations, no need for a L_2 -projection technique to ensure the preservation properties.

However, from the computational cost perspective, the thermodynamical consistency of the temperature-based EEM methods relies on the notion of discrete derivative operator applied to the internal energy and entropy functions so they requires about twice as much implementation effort and computational cost compared to the entropy-based EEM ones that only needs the elaboration of the discrete derivative operator for the internal energy expressed in terms of entropy.

Furthermore, the temperature-based EEM methods for infinite-dimensional dissipative systems rest on a special evaluation of the temperature filed within the time interval to ensure the preservation of the structure that complicates the implementation of the heat conduction contribution. Fortunately, the particular form of classic thermo(visco)elastic models helps to simplify the said implementation.

For the finite-dimensional dissipative systems approached with the temperature-based formulation, the issue of the evaluation of the temperatures involved in the discrete evolution equations corresponding to the energy balance ones remains open. That is because any evaluation of them within the time interval ensures both discrete preservation features and second-order

accuracy. However, there exist a candidate that stands out among all because it leads to an unique discrete definition of the specific heat capacity which contributes to the desired discrete thermodynamical consistency. Significantly, such evaluation coincides with the evaluation that univocally arose in the infinite-dimensional case.

All numerical examples proposed throughout this dissertation suggest that EEM methods not only conserves angular and linear momentum, and the laws of thermodynamics, but considerably improves the numerical stability and enables the use of larger time steps compared to standard integration schemes.

In particular, the numerical examples of Chapter 5 have revealed that the temperature-based EEM method for finite-dimensional dissipative systems with internal variables are significantly more accurate for the positions, the internal variable and the temperatures at a fixed time step than the standard implicit methods and the EEM entropy-based method.

Another important aspect to consider when facing dissipative problems is that the inclusion of dissipative effects naturally contributes to the stability of standard methods in the same way as the inclusion of artificial dissipation helps to the stability of standard integration methods for elastodynamics problems. Thereby, solutions can be obtained for moderately large time step sizes; sizes that would produce unstable solutions when no dissipation is present. In fact, as the dissipative effects become important, it is more likely for standard methods to provide stable solutions. However, these solutions might have accumulated an important error (the longer the simulation the worse) since neither the laws of thermodynamics nor the symmetries comply with their essential physical rules. Instead, the EEM method complies with every evolution property inherited from the continuum, providing physical certainty over the solution obtained.

Finally, the main conclusions of the research carried out in this dissertation are summarized in the following six points:

1. Just as in the conserving case, **preserving the structure of dissipative problems** provides solutions with **physical certainty** and poses **numerical advantages**.
 2. The **basic structure** of coupled smooth dissipative systems is provided by the **laws of thermodynamics** and the **symmetries**, and can be formulated within an **unified framework** provided by **metriplectic structures** induced on manifolds.
-

3. General **energy-preserving, entropy-producing, momentum-preserving methods** (EEM) for dissipative problems can be formulated by using the same ideas as those that led to the formulation of **conserving methods**.
4. **Temperature** can be used as a thermodynamical state variable allowing to handle with **Dirichlet's boundary conditions** and with naturally **temperature-based free-energy functions**.
5. The **internal variables** framework naturally contributes to the **irreversible operator** of the metriplectic structure. Although they can **break its symmetry**, this does not seem to be an impediment for the derivation of thermodynamically sound evolution equations and, accordingly, the discrete setting provided by EEM methods preserves all the preservation features.
6. The resulting EEM integration methods not only conserve angular, linear momentum and the laws of thermodynamics, but **considerably improves the stability and robustness** for large time steps.

Future works

Beyond the results contained in this dissertation, future lines of research are proposed next:

- For infinite-dimensional dissipative systems, exploring the use of multi-field variational for the treatment of the volumetric constraint of nearly or fully incompressible materials in such a way that the preservation features identified in the continuous equations remain ensured. This is of vital importance since, as has been introduced in this dissertation, the dissipative effects are usually associated with isochoric deformations while the thermal coupling is naturally associated with volumetric deformation via an thermal expansion coefficient. A departing point could be the work done in González (2000) for the formulation of an Energy-Momentum method in such context.
 - Extending the methodology to deal with the formulation of non-smooth dissipative systems, among which (thermo)plastic and (thermo)damage changes in the material are of great interest.
 - Related to the above, systematize the obtention of the reversible and irreversible operators of the GENERIC formalism for any set of state
-

variables and any source of dissipation in the line of the work due to Mielke (2011).

- An exploration of the performances of these methods for anisotropy material behavior in which the matrix and the fibers have different mechanical and thermal behaviors. In the aerospace industry there exist a bunch of demanding problems associated with composite materials that could be faced with this approach.
 - Comparison with the performances provided by variational integrators regarding time step sizes, order of accuracy, relative errors, computational cost, implementation issues, applicability, etc.
 - Despite the good performances of structure-preserving methods based on the discrete derivative operators, the fact that its implementation requires a full redefinition of the elements technology has so far prevented them to be embedded into commercial codes. In the same way that Energy-Momentum methods are not available in these codes, it is expectable that the EEM methods proposed in this dissertation have the same 'succeed'. Because of this, the search for alternatives for the discrete derivative operator that somehow makes the resulting EEM methods less intrusive, that is, they do not ideally require to change the standard element implementation, becomes a crucial issue. For Energy-Momentum methods, there have been several attempts towards this target, see for instance Romero (2001) or Krenk (2014), that could serve as a departing point for the here proposed EEM methods.
-

Discrete Derivative Operator

The design of the presented EEM integration methods relies crucially on a *discrete derivative operator* ($\mathbf{D}$). Such operator applies to scalar-valued functions defined in inner product spaces $(\mathcal{U}, \langle \cdot, \cdot \rangle_{\mathcal{U}})$ and satisfies two essential properties:

1. *Directionality*: the ability for the operator to relate univocally the function balance in an arbitrary set $[\mathbf{x}, \mathbf{y}]$ with the difference of such set, that is

$$f(\mathbf{x}) - f(\mathbf{y}) = \langle \mathbf{D}f(\mathbf{x}, \mathbf{y}), \mathbf{x} - \mathbf{y} \rangle_{\mathcal{U}} \quad (\text{A.1})$$

2. *Consistency*: the ability for the operator to render second order accuracy of the standard derivative at the set midpoint, that is

$$\mathbf{D}f(\mathbf{x}, \mathbf{y}) = Df\left(\frac{\mathbf{x} + \mathbf{y}}{2}\right) + \mathcal{O}(\|\mathbf{x} - \mathbf{y}\|^2). \quad (\text{A.2})$$

The concept of the *discrete derivative operator* dates at least back to the mid-seventies in LaBudde & Greenspan (1976a,b) (see also Maeda (1980, 1981), Gotusso (1985), Itoh & Abe (1988), McLachlan et al. (1999)). Later, González (1996) fully developed it in the context of geometric integration of Hamiltonian problems.

A.1 Mean value theorem

As a first approach to the discrete derivative operator, consider the theorem of the mean value which asserts that, given a scalar-valued function

$f(\mathbf{x}): C \rightarrow \mathbb{R}$, defined in $C \subset \mathbb{R}^d$, continuous on $[\mathbf{a}, \mathbf{b}]$ and differentiable on $(\mathbf{a}, \mathbf{b})$, where $\mathbf{a}, \mathbf{b} \in C$, then there exists at least a $\mathbf{c} \in (\mathbf{a}, \mathbf{b})$ such that

$$f(\mathbf{b}) - f(\mathbf{a}) = \nabla f(\mathbf{c}) \cdot (\mathbf{b} - \mathbf{a}) \quad (\text{A.3})$$

In view of this theorem, the existence of operators satisfying the directionality property is proved for scalar-valued functions under the conditions of continuity and derivability within the intervals of interest.

The mean value theorem for unidimensional scalar-valued functions, that is $C \subset \mathbb{R}$, is appealing because it is easily geometrically interpretable, see Figure A.1. Thus, given a smooth function $f: \mathbb{R} \rightarrow \mathbb{R}$ in an interval $[a, b]$ the secant joining the endpoints of the interval is parallel to the tangent at some point c within the interval.

Figure A.1. Geometrical interpretation of the mean value theorem

This geometrical interpretation readily provides an expression for the operator satisfying the directionality property of unidimensional functions, that is

$$Df(a, b) = f'(c) = \frac{f(b) - f(a)}{b - a} \quad (\text{A.4})$$

Moreover, the above formula turns out to be the only definition for this specific types of functions that furnishes such property. For more general types of function, however, there exists infinite formulae endowed with this property, as will be discussed in the next section.

On the other hand, the above definition of the operator collapses to the

continuous derivative as the interval becomes infinitesimal

$$\lim_{a \rightarrow b} Df(a, b) = f'(b) = f'(a), \quad (\text{A.5})$$

being hence well-defined.

Furthermore, this formula also results in a second order approximation to the standard derivative evaluated at interval midpoint so (A.4) is a valid discrete derivative operator for the formulation of structure-preserving methods according to the requirements introduced at the beginning of this Appendix.

A.2 The discrete derivative operator

For general scalar-valued functions there exist several definitions for the discrete derivative operator matching the directionality and consistency properties, as studied in Romero (2012). Therein, it is concluded that the optimal definition is the one introduced by González (1996) whose main features are discussed next.

Definition A.1. Let $f : \mathcal{U} \rightarrow \mathbb{R}$ be a smooth function, where $(\mathcal{U}, \langle \cdot, \cdot \rangle_{\mathcal{U}})$ is an inner product space, then the second-order discrete derivative operator is provided by

$$Df(\mathbf{x}, \mathbf{y}) = Df(\mathbf{v}) + \frac{f(\mathbf{x}) - f(\mathbf{y}) - \langle Df(\mathbf{v}), \mathbf{u} \rangle_{\mathcal{U}}}{\langle \mathbf{u}, \mathbf{u} \rangle_{\mathcal{U}}} \mathbf{u}, \quad (\text{A.6})$$

where $\mathbf{x}, \mathbf{y} \in \mathcal{U}$, $\mathbf{v} = (\mathbf{x} + \mathbf{y})/2$, $\mathbf{u} = \mathbf{x} - \mathbf{y}$ and D being standard derivative¹.

Remark A.1. As pointed out by Romero (2012), there exist as many second-order accurate operators as forms of defining the inner product appearing in (A.6) that verifies the directionality condition (A.1).

Definition A.2. If the inner product space has a partitioned structure $\mathcal{U} = U_1 \times \cdots \times U_k$ for some $k > 1$, and every $U_i, i = 1, \dots, k$ is endowed with an inner product $\langle \cdot, \cdot \rangle_{U_i}$, the partitioned discrete derivative operator for any smooth function $f : \mathcal{U} \rightarrow \mathbb{R}$, is provided by

$$\langle Df(\mathbf{x}, \mathbf{y}), \mathbf{u} \rangle_{\mathcal{U}} = \sum_{i=1}^k \langle D_i f(x_i, y_i), u_i \rangle_{U_i}, \quad (\text{A.7})$$

¹Note that the different notations used for the standard derivative operator D and the discrete derivative operator D .

for all $\mathbf{u} = (u_1, u_2, \dots, u_k) \in \mathcal{U}$, and with $\mathbf{x} = (x_1, x_2, \dots, x_k) \in \mathcal{U}$ and $\mathbf{y} = (y_1, y_2, \dots, y_k) \in \mathcal{U}$. The term $D_i f(x_i, y_i)$ might be interpreted as the i -th second order accurate discrete counterpart to the i -th partial derivative of the function f at midpoint and is provided by

$$D_i f(x_i, y_i) = \frac{1}{2} [D f_{xy}^i(x_i, y_i) + D f_{yx}^i(x_i, y_i)], \quad (\text{A.8})$$

where $f_{xy}^i, f_{yx}^i : U_i \rightarrow \mathbb{R}$ are defined by the relations

$$\begin{aligned} f_{xy}^i(\mathbf{w}) &= f(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_{i-1}, \mathbf{w}, \mathbf{y}_{i+1}, \dots, \mathbf{y}_k) \\ f_{yx}^i(\mathbf{w}) &= f(\mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_{i-1}, \mathbf{w}, \mathbf{x}_{i+1}, \dots, \mathbf{x}_k) \end{aligned} \quad (\text{A.9})$$

Properties. The above definitions automatically satisfy the two essential properties (A.1) and (A.2) required to discrete derivatives operators for the formulation of structure-preserving methods.

Proof. The verification of the directionality property is readily checked applying (A.6) to $\mathbf{u}$, yielding

$$\begin{aligned} \langle Df(\mathbf{x}, \mathbf{y}), \mathbf{u} \rangle_{\mathcal{U}} &= \langle Df(\mathbf{v}), \mathbf{u} \rangle_{\mathcal{U}} + \frac{f(\mathbf{x}) - f(\mathbf{y}) - \langle Df(\mathbf{v}), \mathbf{u} \rangle_{\mathcal{U}}}{\langle \mathbf{u}, \mathbf{u} \rangle_{\mathcal{U}}} \langle \mathbf{u}, \mathbf{u} \rangle_{\mathcal{U}} \\ &= f(\mathbf{x}) - f(\mathbf{y}) \end{aligned} \quad (\text{A.10})$$

□

Remark A.2. This proof would be valid for any $\mathbf{v}$ in (A.6), not necessarily at the midpoint, leading to as many discrete derivatives operator definitions as values of $\mathbf{v}$, although the second-order consistency condition (A.2) may be compromised.

Proof. The consistency property is verified by making $\mathbf{x} \rightarrow \mathbf{y}$ or $\mathbf{u} \rightarrow \mathbf{0}$ in (A.6). For that, consider the followings Taylor's expansions around the midpoint of both endpoints of the interval

$$\begin{aligned} f(\mathbf{x}) &= f(\mathbf{v}) + \langle \frac{1}{2} Df(\mathbf{v}), \mathbf{u} \rangle_{\mathcal{U}} \\ &\quad + \langle \frac{1}{4} D^2 f(\mathbf{v}), (\mathbf{u}, \mathbf{u}) \rangle_{\mathcal{U}} + \langle \frac{1}{8} D^3 f(\mathbf{v}), (\mathbf{u}, \mathbf{u}, \mathbf{u}) \rangle_{\mathcal{U}} \\ &\quad + \langle \frac{1}{16} D^4 f(\mathbf{v}), (\mathbf{u}, \mathbf{u}, \mathbf{u}, \mathbf{u}) \rangle_{\mathcal{U}} + \mathcal{O}(\|\mathbf{u}\|^5) \end{aligned} \quad (\text{A.11})$$

$$\begin{aligned}
f(\mathbf{y}) &= f(\mathbf{v}) - \langle \frac{1}{2} Df(\mathbf{v}), \mathbf{u} \rangle_{\mathcal{U}} \\
&+ \langle \frac{1}{4} D^2 f(\mathbf{v}), (\mathbf{u}, \mathbf{u}) \rangle_{\mathcal{U}} - \langle \frac{1}{8} D^3 f(\mathbf{v}), (\mathbf{u}, \mathbf{u}, \mathbf{u}) \rangle_{\mathcal{U}} \\
&+ \langle \frac{1}{16} D^4 f(\mathbf{v}), (\mathbf{u}, \mathbf{u}, \mathbf{u}, \mathbf{u}) \rangle_{\mathcal{U}} + \mathcal{O}(\|\mathbf{u}\|^5)
\end{aligned} \tag{A.12}$$

Combining now them yields the following crucial expansion

$$f(\mathbf{x}) = f(\mathbf{y}) + \langle Df(\mathbf{v}), \mathbf{u} \rangle_{\mathcal{U}} + \langle \frac{1}{4} D^3 f(\mathbf{v}), (\mathbf{u}, \mathbf{u}, \mathbf{u}) \rangle_{\mathcal{U}} + \mathcal{O}(\|\mathbf{u}\|^5) \tag{A.13}$$

This result can be used in the expression (A.6) to arrive at

$$Df(\mathbf{x}, \mathbf{y}) = Df(\mathbf{v}) + \frac{\langle \frac{1}{4} D^3 f(\mathbf{v}), (\mathbf{u}, \mathbf{u}, \mathbf{u}) \rangle_{\mathcal{U}} + \mathcal{O}(\|\mathbf{u}\|^5)}{\langle \mathbf{u}, \mathbf{u} \rangle_{\mathcal{U}}} \mathbf{u}, \tag{A.14}$$

Considering $\mathbf{u} = \alpha \mathbf{w}$ with $\alpha > 0$ and $\|\mathbf{w}\| = 1$, the last expression can be written as

$$Df(\mathbf{x}, \mathbf{y}) = Df(\mathbf{v}) + \langle \frac{1}{4} \alpha^3 D^3 f(\mathbf{v}), (\mathbf{w}, \mathbf{w}, \mathbf{w}) \rangle_{\mathcal{U}} + \mathcal{O}(\alpha^4), \tag{A.15}$$

proving the second order accuracy of the discrete derivative operator. This result also serves to verify that the discrete gradient operator is well-defined in the limit case of $\mathbf{u} \rightarrow 0$. $\square$

Definition A.3. A G-invariant function $f: \mathcal{U} \rightarrow \mathbb{R}$ is a function $f: \mathcal{U} \rightarrow \mathbb{R}$ that, given an action Φ of a Lie Group G on the space $\mathcal{U}$, satisfies

$$f(\Phi_g(\mathbf{z})) = f(\mathbf{z}) \quad \forall g \in G, \tag{A.16}$$

Definition A.4. A G-equivariant discrete derivative for a smooth G-invariant function $f: \mathcal{U} \rightarrow \mathbb{R}$ is a mapping $D^G f: \mathcal{U} \times \mathcal{U} \rightarrow T\mathcal{U}$ that satisfies two additional properties:

1. Equivariance:

$$D^G f(\Phi_g(\mathbf{x}), \Phi_g(\mathbf{y})) = \left[D\Phi_g \left(\frac{\mathbf{x} + \mathbf{y}}{2} \right) \right]^{-T} \cdot D^G f(\mathbf{x}, \mathbf{y}), \tag{A.17}$$

for all $g \in G$ and $\mathbf{x}, \mathbf{y} \in \mathcal{U}$.

2. Orthogonality:

$$D^G f(\mathbf{x}, \mathbf{y}) \cdot \boldsymbol{\xi}_{\mathcal{U}} \left(\frac{\mathbf{x} + \mathbf{y}}{2} \right) = 0 \quad \forall \boldsymbol{\xi} \in \mathfrak{g}^* \quad \text{and } \mathbf{x}, \mathbf{y} \in \mathcal{U}, \quad (\text{A.18})$$

where $\mathfrak{g}^*$ is the associated dual algebra of the Lie group G .

Proposition A.1. *Let $f : \mathcal{U} \rightarrow \mathbb{R}$ be a smooth G -invariant function, $\pi : \mathcal{U} \rightarrow \mathbb{R}^r$ be a set of invariant functions $\pi_i : \mathcal{U} \rightarrow \mathbb{R}$ which are invariant respect to an action Φ of a Lie group G . Let $\tilde{f} : \pi(\mathcal{U}) \rightarrow \mathbb{R}$ be the associated reduced function defined by $\tilde{f}(\pi(\mathbf{z})) = f(\mathbf{z})$, for all $\mathbf{z}$. If the invariant $\pi_i : \mathcal{U} \rightarrow \mathbb{R}$ is at most of degree two, then a G -equivariant discrete derivative for f is provided by*

$$D^G f(\mathbf{x}, \mathbf{y}) = D\tilde{f}(\pi(\mathbf{x}), \pi(\mathbf{y})) \circ D\pi(\mathbf{z}) = [D\pi(\mathbf{v})]^T D\tilde{f}(\pi(\mathbf{x}), \pi(\mathbf{y})), \quad (\text{A.19})$$

where for any $\mathbf{z} \in \mathcal{U}$, $D\pi(\mathbf{z}) \in \mathbb{R}^{r \times \dim(\mathcal{U})}$ and $r = \dim(\mathcal{U}) - o$, o being the number of orbits associated with the Lie group G .

Proof. The result is proved in González (1996) by direct verification of the properties which are summarized next.

1. The directionality property of G -equivariant discrete derivative operator establishes that

$$\begin{aligned} \langle D^G f(\mathbf{x}, \mathbf{y}), \mathbf{v} \rangle_{\mathcal{U}} &= \langle [D\pi(\mathbf{z})]^T D\tilde{f}(\pi(\mathbf{x}), \pi(\mathbf{y})), \mathbf{v} \rangle_{\mathcal{U}} \\ &= \langle D\tilde{f}(\pi(\mathbf{x}), \pi(\mathbf{y})), D\pi(\mathbf{z}) \cdot \mathbf{v} \rangle_{\mathcal{U}} \end{aligned} \quad (\text{A.20})$$

As, by assumption, the invariant function π is at most of degree two, it follows that

$$D\pi(\mathbf{z}) \cdot \mathbf{v} = \pi(\mathbf{y}) - \pi(\mathbf{x}) \quad (\text{A.21})$$

Then, the directionality property yields

$$\begin{aligned} \langle D^G f(\mathbf{x}, \mathbf{y}) \cdot \mathbf{v} &= D\tilde{f}(\pi(\mathbf{x}), \pi(\mathbf{y})) \cdot (\pi(\mathbf{y}) - \pi(\mathbf{x})) \\ &= \tilde{f}(\pi(\mathbf{x})) - \tilde{f}(\pi(\mathbf{y})) = f(\mathbf{y}) - f(\mathbf{x}) \end{aligned} \quad (\text{A.22})$$

2. The consistency property follows from the consistency of the standard discrete derivative operator (A.15).

3. The equivariance property is proved by using the invariability of the π function respect to the action Φ_g of a Lie group G , that is $\pi(\Phi_g(\mathbf{z})) = \pi(\mathbf{z})$, for all $\mathbf{z} \in \mathcal{U}$ and $g \in G$, which leads to

$$D\pi(\Phi_g(\mathbf{z})) = D\pi(\mathbf{z}) \circ [D\Phi_g(\mathbf{z})]^{-1} \quad (\text{A.23})$$

If the action satisfies $\frac{1}{2}[\Phi_g(\mathbf{x}) + \Phi_g(\mathbf{y})] = \Phi_g(\mathbf{z})$, that is the Lie Group is affine, then

$$\begin{aligned} D^G f(\Phi_g(\mathbf{x}), \Phi_g(\mathbf{y})) &= D\tilde{f}(\pi(\Phi_g(\mathbf{x})), \pi(\Phi_g(\mathbf{y}))) \circ D\pi(\Phi_g(\mathbf{z})) \\ &= D\tilde{f}(\pi(\mathbf{x}), \pi(\mathbf{y})) \circ D\pi(\Phi_g(\mathbf{z})) \\ &= D\tilde{f}(\pi(\mathbf{x}), \pi(\mathbf{y})) \circ D\pi(\mathbf{z}) \circ [D\Phi_g(\mathbf{z})]^{-1} \\ &= [D\Phi_g(\mathbf{z})]^{-T} \cdot \left(D\tilde{f}(\pi(\mathbf{x}), \pi(\mathbf{y})) \circ D\pi(\mathbf{z}) \right) \\ &= [D\Phi_g(\mathbf{z})]^{-T} \cdot D^G f(\mathbf{x}, \mathbf{y}) \end{aligned} \quad (\text{A.24})$$

4. The orthogonality property can also be proved by exploiting the invariability of the function π which allows to conclude that

$$D\pi(\mathbf{z}) \cdot \boldsymbol{\xi}_{\mathcal{U}}(\mathbf{z}) = 0, \quad \forall \boldsymbol{\xi} \in \mathfrak{g}^* \quad (\text{A.25})$$

and, hence,

$$D^G f(\mathbf{x}, \mathbf{y}) \cdot \boldsymbol{\xi}_{\mathcal{U}}(\mathbf{z}) = D\tilde{f}(\pi(\mathbf{x}), \pi(\mathbf{y})) \cdot (D\pi(\mathbf{z}) \cdot \boldsymbol{\xi}_{\mathcal{U}}(\mathbf{z})) = 0 \quad (\text{A.26})$$

□

A.3 Discrete derivative operator: Examples

• **Functions defined on a k -product-Cartesian space $\mathbb{R} \times \cdots \times \mathbb{R}$.** Given a function $f : \mathbb{R} \times \cdots \times \mathbb{R} \rightarrow \mathbb{R}$, the discrete derivative operator must be elaborated using the partitioned definition (5.3) in terms of k .

Thus, the case of $k = 1$ coincides with the mean value theorem (A.4).

For two-variable functions, $k = 2$, the first and the second partial discrete derivatives follow from (A.8) and (A.9) and are provided by

$$D_1 f(\mathbf{x}, \mathbf{y}) = \frac{f(x_1, x_2) - f(y_1, x_2) + f(x_1, y_2) - f(y_1, y_2)}{2(x_1 - y_1)} \quad (\text{A.27})$$

$$D_2 f(\mathbf{x}, \mathbf{y}) = \frac{f(x_1, x_2) - f(x_1, y_2) + f(y_1, x_2) - f(y_1, y_2)}{2(x_2 - y_2)} \quad (\text{A.28})$$

with $\mathbf{x} = (x_1, x_2)$ and $\mathbf{y} = (y_1, y_2)$.

The resulting expressions are required in the formulation of EEM for the Two thermo-spring system discussed in Section 5.3, as it is defined through potentials depending on two real variables.

For three-variable functions, $k = 3$, following (A.8) and (A.9), the partial discrete derivatives are provided by

$$D_1 f(\mathbf{x}, \mathbf{y}) = \frac{f(x_1, x_2, x_3) - f(y_1, x_2, x_3) + f(x_1, y_2, y_3) - f(y_1, y_2, y_3)}{2(x_1 - y_1)} \quad (\text{A.29})$$

$$D_2 f(\mathbf{x}, \mathbf{y}) = \frac{f(x_1, x_2, y_3) - f(x_1, y_2, y_3) + f(y_1, x_2, x_3) - f(y_1, y_2, x_3)}{2(x_2 - y_2)} \quad (\text{A.30})$$

$$D_3 f(\mathbf{x}, \mathbf{y}) = \frac{f(x_1, x_2, x_3) - f(x_1, x_2, y_3) + f(y_1, y_2, x_3) - f(y_1, y_2, y_3)}{2(x_3 - y_3)} \quad (\text{A.31})$$

with $\mathbf{x} = (x_1, x_2, x_3)$ and $\mathbf{y} = (y_1, y_2, y_3)$.

These discrete derivatives are involved in the formulation of the EEM methods for the Thermo-visco-elastic system presented in Section 5.4.

• **Functions defined on $\text{Sym}(\mathbb{T}_d^2)$.** Given a function $f : \text{Sym}(\mathbb{T}_d^2) \rightarrow \mathbb{R}$, the discrete derivative operator

$$Df(\mathbf{X}, \mathbf{Y}) = Df(\mathbf{V}) + \frac{f(\mathbf{X}) - f(\mathbf{Y}) - Df(\mathbf{V}) : \mathbf{U}}{\mathbf{U} : \mathbf{U}} \mathbf{U}, \quad (\text{A.32})$$

for all $\mathbf{X}, \mathbf{Y} \in \text{Sym}(\mathbb{T}_d^2)$, $\mathbf{U} = \mathbf{X} - \mathbf{Y}$ and $\mathbf{V} = \frac{1}{2}(\mathbf{X} + \mathbf{Y})$.

The free-energy functions defining nonlinear elastodynamics are of this type. Then, the stress formula that ensures the preservation of the Hamiltonian of such as systems is provided by the above formula for the discrete derivative operator. The interesting point in the above expression is on the fact that the standard derivatives are evaluated at the mean value of the tensor.

If f is at most quadratic, that is, the Saint-Venant Kirchhoff material model, the discrete gradient collapses to the standard derivative evaluated at midpoint so the midpoint methods becomes energy-preserving.

• **Functions defined on a k -product space of second-order tensors.** Given a function $f : (\mathbb{T}_d^2)^k \rightarrow \mathbb{R}$, the partitioned discrete derivative operator is elaborated in terms of k .

The case of $k = 1$ has just been introduced in (A.32).

For $k = 2$, two partial discrete derivative follows as

$$\begin{aligned} D_1 f(\mathbf{X}, \mathbf{Y}) &= \frac{1}{2} [D_1 f(\mathbf{V}_1, \mathbf{X}_2) + D_1 f(\mathbf{V}_1, \mathbf{Y}_2)] \\ &+ \frac{f(\mathbf{X}_1, \mathbf{X}_2) - f(\mathbf{Y}_1, \mathbf{X}_2) + f(\mathbf{X}_1, \mathbf{Y}_2) - f(\mathbf{Y}_1, \mathbf{Y}_2)}{2\mathbf{U}_1 : \mathbf{U}_1} \mathbf{U}_1 \\ &- \frac{[D_1 f(\mathbf{V}_1, \mathbf{X}_2) + D_1 f(\mathbf{V}_1, \mathbf{Y}_2)] : \mathbf{U}_1}{2\mathbf{U}_1 : \mathbf{U}_1} \mathbf{U}_1 \end{aligned} \quad (\text{A.33})$$

$$\begin{aligned} D_2 f(\mathbf{X}, \mathbf{Y}) &= \frac{1}{2} [D_2 f(\mathbf{X}_1, \mathbf{V}_2) + D_2 f(\mathbf{X}_1, \mathbf{Y}_2)] \\ &+ \frac{f(\mathbf{X}_1, \mathbf{X}_2) - f(\mathbf{X}_1, \mathbf{Y}_2) + f(\mathbf{Y}_1, \mathbf{X}_2) - f(\mathbf{Y}_1, \mathbf{Y}_2)}{2\mathbf{U}_2 : \mathbf{U}_2} \mathbf{U}_2 \\ &- \frac{[D_2 f(\mathbf{X}_1, \mathbf{V}_2) + D_2 f(\mathbf{X}_1, \mathbf{Y}_2)] : \mathbf{U}_2}{2\mathbf{U}_2 : \mathbf{U}_2} \mathbf{U}_2, \end{aligned} \quad (\text{A.34})$$

for all $\mathbf{X} = (\mathbf{X}_1, \mathbf{X}_2)$, $\mathbf{Y} = (\mathbf{Y}_1, \mathbf{Y}_2)$, $\mathbf{U} = \mathbf{X} - \mathbf{Y}$ and $\mathbf{V} = \frac{1}{2}(\mathbf{X} + \mathbf{Y})$.

These formulas are symmetric respect to the first and the second variables so they can be exchangeable leading to the same expression for the discrete derivative operator. They are involved in the formulation of the EEM method for isothermal dissipative dynamics defined in (5.249) and based on an internal variable. The first variable is then identified with the right Cauchy-Green deformation tensor and the second with the internal variable.

For $k = 3$, the corresponding three partial discrete derivatives are provided by

$$\begin{aligned} D_1 f(\mathbf{X}, \mathbf{Y}) &= \frac{1}{2} [D_1 f(\mathbf{V}_1, \mathbf{X}_2, \mathbf{X}_3) + D_1 f(\mathbf{V}_1, \mathbf{Y}_2, \mathbf{Y}_3)] \\ &+ \frac{f(\mathbf{X}_1, \mathbf{X}_2, \mathbf{X}_3) - f(\mathbf{Y}_1, \mathbf{X}_2, \mathbf{X}_3) + f(\mathbf{X}_1, \mathbf{Y}_2, \mathbf{Y}_3) - f(\mathbf{Y}_1, \mathbf{Y}_2, \mathbf{Y}_3)}{2\mathbf{U}_1 : \mathbf{U}_1} \mathbf{U}_1 \\ &- \frac{[D_1 f(\mathbf{V}_1, \mathbf{X}_2, \mathbf{X}_3) + D_1 f(\mathbf{V}_1, \mathbf{Y}_2, \mathbf{Y}_3)] : \mathbf{U}_1}{2\mathbf{U}_1 : \mathbf{U}_1} \mathbf{U}_1 \end{aligned} \quad (\text{A.35})$$

$$\begin{aligned} D_2 f(\mathbf{X}, \mathbf{Y}) &= \frac{1}{2} [D_2 f(\mathbf{X}_1, \mathbf{V}_2, \mathbf{X}_3) + D_2 f(\mathbf{Y}_1, \mathbf{V}_2, \mathbf{Y}_3)] \\ &+ \frac{f(\mathbf{X}_1, \mathbf{X}_2, \mathbf{Y}_3) - f(\mathbf{X}_1, \mathbf{Y}_2, \mathbf{Y}_3) + f(\mathbf{Y}_1, \mathbf{X}_2, \mathbf{X}_3) - f(\mathbf{Y}_1, \mathbf{Y}_2, \mathbf{X}_3)}{2\mathbf{U}_2 : \mathbf{U}_2} \mathbf{U}_2 \\ &- \frac{[D_2 f(\mathbf{X}_1, \mathbf{V}_2, \mathbf{X}_3) + D_2 f(\mathbf{Y}_1, \mathbf{V}_2, \mathbf{Y}_3)] : \mathbf{U}_2}{2\mathbf{U}_2 : \mathbf{U}_2} \mathbf{U}_2 \end{aligned} \quad (\text{A.36})$$

$$\begin{aligned}
D_3 f(\mathbf{X}, \mathbf{Y}) = & \frac{1}{2} [D_3 f(\mathbf{X}_1, \mathbf{X}_2, \mathbf{V}_3) + D_3 f(\mathbf{Y}_1, \mathbf{Y}_2, \mathbf{V}_3)] \\
& + \frac{f(\mathbf{X}_1, \mathbf{X}_2, \mathbf{X}_3) - f(\mathbf{X}_1, \mathbf{X}_2, \mathbf{Y}_3) + f(\mathbf{Y}_1, \mathbf{Y}_2, \mathbf{X}_3) - f(\mathbf{Y}_1, \mathbf{Y}_2, \mathbf{Y}_3)}{2\mathbf{U}_3 : \mathbf{U}_3} \mathbf{U}_3 \\
& - \frac{[D_3 f(\mathbf{X}_1, \mathbf{X}_2, \mathbf{V}_3) + D_3 f(\mathbf{Y}_1, \mathbf{Y}_2, \mathbf{V}_3)] : \mathbf{U}_3}{2\mathbf{U}_3 : \mathbf{U}_3} \mathbf{U}_3,
\end{aligned} \tag{A.37}$$

for all $\mathbf{X} = (\mathbf{X}_1, \mathbf{X}_2, \mathbf{X}_3)$, $\mathbf{Y} = (\mathbf{Y}_1, \mathbf{Y}_2, \mathbf{Y}_3)$, $\mathbf{U} = \mathbf{X} - \mathbf{Y}$ and $\mathbf{V} = \frac{1}{2}(\mathbf{X} + \mathbf{Y})$.

In this case, the formulas is not symmetric respect to three variables, although the crucial properties of the operator is ensured for any combination of them. Then, the EEM method for isothermal dissipative dynamics based on two internal variables requires the use of these expressions.

The appealing differences between the elaborated discrete derivatives for different value of k lead the formulation of EEM methods to depend substantially on this issue, as was remarked in 5.5 for the number of internal variables chosen to model the viscoelastic effects.

• **Functions defined on a k -product space of real numbers and second order tensors.** Among all possible combinations, two choices are of interest since they are involved in the formulation of EEM methods for coupled thermoelastic and thermo dissipative dynamics.

Thus, consider a function defined on a product space of a real number and a symmetric second order tensor, that is $f : \text{Sym}(\mathbb{T}_d^2) \times \mathbb{R} \rightarrow \mathbb{R}$, then, the partial discrete derivative result in

$$\begin{aligned}
D_1 f(X, Y) = & \frac{1}{2} [D_1 f(\mathbf{V}, x) + D_1 f(\mathbf{V}, y)] \\
& + \frac{f(\mathbf{X}, x) - f(\mathbf{Y}, x) + f(\mathbf{X}, y) - f(\mathbf{Y}, y)}{2\mathbf{U} : \mathbf{U}} \mathbf{U} \\
& - \frac{[D_1 f(\mathbf{V}, x) + D_1 f(\mathbf{V}, y)] : \mathbf{U}}{2\mathbf{U} : \mathbf{U}} \mathbf{U}
\end{aligned} \tag{A.38}$$

$$D_2 f(X, Y) = \frac{f(\mathbf{X}, x) - f(\mathbf{X}, y) + f(\mathbf{Y}, x) - f(\mathbf{Y}, y)}{2u} \tag{A.39}$$

with $X = (\mathbf{X}, x) \in \text{Sym}(\mathbb{T}_d^2) \times \mathbb{R}$, $Y = (\mathbf{Y}, y) \in \text{Sym}(\mathbb{T}_d^2) \times \mathbb{R}$, $U = X - Y$ and $V = \frac{1}{2}(X + Y)$.

The above formulas are necessary for the formulation of EEM methods for thermo-elastic continuum dynamics. In particular, the above partial discrete derivatives are directly identified with the algorithmic stress tensor and the algorithmic temperature of the entropy-based EEM method. For the

temperature-based EEM method, however, these expressions are involved in its formulation but are not directly identified with algorithmic quantities.

Finally, consider a function defined on a product space of a real number and more than one second order tensors, that is $f : \text{Sym}(\mathbb{T}_d^2) \times \mathbb{R} \times \text{Sym}(\mathbb{T}_d^2) \times \cdots \times \text{Sym}(\mathbb{T}_d^2) \rightarrow \mathbb{R}$. These types of functions are involved in thermo dissipative potential so its partial discrete derivatives are needed for the formulation of EEM method for such a problem.

For the particular case of just one internal variable, the partial discrete derivative arising from the definitions (A.8) and (A.9) are

$$\begin{aligned} D_1 f(X, Y) = & \frac{1}{2} [D_1 f(\mathbf{V}_1, x, \mathbf{X}_3) + D_1 f(\mathbf{V}_1, y, \mathbf{Y}_3)] \\ & + \frac{f(\mathbf{X}_1, x, \mathbf{X}_3) - f(\mathbf{Y}_1, x, \mathbf{X}_3) + f(\mathbf{X}_1, y, \mathbf{Y}_3) - f(\mathbf{Y}_1, y, \mathbf{Y}_3)}{2\mathbf{U}_1 : \mathbf{U}_1} \mathbf{U}_1 \\ & - \frac{[D_1 f(\mathbf{V}_1, x, \mathbf{X}_3) + D_1 f(\mathbf{V}_1, y, \mathbf{Y}_3)] : \mathbf{U}_1}{2\mathbf{U}_1 : \mathbf{U}_1} \mathbf{U}_1 \end{aligned} \quad (\text{A.40})$$

$$D_2 f(X, Y) = \frac{f(\mathbf{X}_1, x, \mathbf{Y}_3) - f(\mathbf{X}_1, y, \mathbf{Y}_3) + f(\mathbf{Y}_1, x, \mathbf{X}_3) - f(\mathbf{Y}_1, y, \mathbf{X}_3)}{2u} \quad (\text{A.41})$$

$$\begin{aligned} D_3 f(X, Y) = & \frac{1}{2} [D_3 f(\mathbf{X}_1, x, \mathbf{V}_3) + D_3 f(\mathbf{Y}_1, y, \mathbf{V}_3)] \\ & + \frac{f(\mathbf{X}_1, x, \mathbf{X}_3) - f(\mathbf{X}_1, x, \mathbf{Y}_3) + f(\mathbf{Y}_1, y, \mathbf{X}_3) - f(\mathbf{Y}_1, y, \mathbf{Y}_3)}{2\mathbf{U}_3 : \mathbf{U}_3} \mathbf{U}_3 \\ & - \frac{[D_3 f(\mathbf{X}_1, x, \mathbf{V}_3) + D_3 f(\mathbf{Y}_1, y, \mathbf{V}_3)] : \mathbf{U}_3}{2\mathbf{U}_3 : \mathbf{U}_3} \mathbf{U}_3, \end{aligned} \quad (\text{A.42})$$

with $X = (\mathbf{X}_1, x, \mathbf{X}_3) \in \text{Sym}(\mathbb{T}_d^2) \times \mathbb{R} \times \text{Sym}(\mathbb{T}_d^2)$, $Y = (\mathbf{Y}_1, y, \mathbf{Y}_3) \in \text{Sym}(\mathbb{T}_d^2) \times \mathbb{R} \times \text{Sym}(\mathbb{T}_d^2)$, $U = X - Y$ and $V = \frac{1}{2}(X + Y)$.

The resulting expressions enable the formulation of EEM methods for the thermo dissipative continuum dynamics presented in Section 5.6 based on just one internal variables, which is besides the most common choice.

A.4 Linearization of the discrete derivative operator

All the proposed EEM methods are implicit and lie at the discrete derivative operator. Therefore, in the required linearization process the linearized

discrete derivative operator will be involved. For this reason, it is elaborated next with the help of the directional (Fréchet) derivative defined as follows

$$\left. \frac{d}{d\epsilon} [Df(\mathbf{x} + \epsilon \mathbf{w}, \mathbf{y})] \right|_{\epsilon=0} = D_{\mathbf{x}}(Df(\mathbf{x}, \mathbf{y}))[\mathbf{w}] = \frac{\partial Df(\mathbf{x}, \mathbf{y})}{\partial \mathbf{x}} \cdot \mathbf{w} \quad (\text{A.43})$$

Using the definition (A.6) together with the associative property and the chain product rule of the directional derivative the linearized discrete derivative can be demonstrated to be

$$\begin{aligned} D_{\mathbf{x}}(Df(\mathbf{x}, \mathbf{y}))[\mathbf{w}] &= \\ &= \frac{1}{2} D^2 f(\mathbf{v}) \cdot \mathbf{w} + D_{\mathbf{x}} \left(\frac{f(\mathbf{x}) - f(\mathbf{y}) - \langle Df(\mathbf{v}), \mathbf{u} \rangle_{\mathcal{U}}}{\langle \mathbf{u}, \mathbf{u} \rangle_{\mathcal{U}}} \right) [\mathbf{w}] \mathbf{u} \\ &\quad + \frac{f(\mathbf{x}) - f(\mathbf{y}) - \langle Df(\mathbf{v}), \mathbf{u} \rangle_{\mathcal{U}}}{\langle \mathbf{u}, \mathbf{u} \rangle_{\mathcal{U}}} \mathbf{I} \cdot \mathbf{w} \end{aligned} \quad (\text{A.44})$$

with $\mathbf{I}$ being the identity in the tangent space $T\mathcal{U}$.

Applying the chain rule to the second term on the right hand side of the above equation leads to

$$\begin{aligned} &D_{\mathbf{x}} \left(\frac{f(\mathbf{x}) - f(\mathbf{y}) - \langle Df(\mathbf{v}), \mathbf{u} \rangle_{\mathcal{U}}}{\langle \mathbf{u}, \mathbf{u} \rangle_{\mathcal{U}}} \right) [\mathbf{w}] \\ &= \frac{D_{\mathbf{x}}(f(\mathbf{x}) - f(\mathbf{y}) - \langle Df(\mathbf{v}), \mathbf{u} \rangle_{\mathcal{U}})[\mathbf{w}]}{\langle \mathbf{u}, \mathbf{u} \rangle_{\mathcal{U}}} \\ &\quad - \frac{(f(\mathbf{x}) - f(\mathbf{y}) - \langle Df(\mathbf{v}), \mathbf{u} \rangle_{\mathcal{U}}) D_{\mathbf{x}}(\langle \mathbf{u}, \mathbf{u} \rangle_{\mathcal{U}})[\mathbf{w}]}{(\langle \mathbf{u}, \mathbf{u} \rangle_{\mathcal{U}})^2} \\ &= \frac{\langle Df(\mathbf{x}), \mathbf{w} \rangle_{\mathcal{U}} - \langle \langle D^2 f(\mathbf{v}), \frac{1}{2} \mathbf{w} \rangle_{\mathcal{U}}, \mathbf{u} \rangle_{\mathcal{U}} - \langle Df(\mathbf{v}), \mathbf{w} \rangle_{\mathcal{U}}}{\langle \mathbf{u}, \mathbf{u} \rangle_{\mathcal{U}}} \\ &\quad - \frac{2(f(\mathbf{x}) - f(\mathbf{y}) - \langle Df(\mathbf{v}), \mathbf{u} \rangle_{\mathcal{U}}) \langle \mathbf{u}, \mathbf{w} \rangle_{\mathcal{U}}}{(\langle \mathbf{u}, \mathbf{u} \rangle_{\mathcal{U}})^2} \end{aligned} \quad (\text{A.45})$$

Finally, all these terms can be rearranged so that the linearization can be expressed as follows

$$\begin{aligned} \frac{\partial Df(\mathbf{x}, \mathbf{y})}{\partial \mathbf{x}} &= \frac{1}{2} D^2 f(\mathbf{v}) \\ &\quad + \frac{\mathbf{u} \otimes Df(\mathbf{x}) - \mathbf{u} \otimes (\frac{1}{2} D^2 f(\mathbf{v}) \cdot \mathbf{u}) - \mathbf{u} \otimes Df(\mathbf{v})}{\langle \mathbf{u}, \mathbf{u} \rangle_{\mathcal{U}}} \\ &\quad + 2 \frac{f(\mathbf{x}) - f(\mathbf{y}) - \langle Df(\mathbf{v}), \mathbf{u} \rangle_{\mathcal{U}}}{\langle \mathbf{u}, \mathbf{u} \rangle_{\mathcal{U}}} \left(\frac{1}{2} \mathbf{I} - \frac{\mathbf{u} \otimes \mathbf{u}}{\langle \mathbf{u}, \mathbf{u} \rangle_{\mathcal{U}}} \right) \end{aligned} \quad (\text{A.46})$$

This result leads to non-symmetric tangents which tends to disappear as the time step size is reduced or $\mathbf{u} \rightarrow 0$

$$\lim_{\mathbf{u} \rightarrow 0} \frac{\partial \mathbf{D}f(\mathbf{x}, \mathbf{y})}{\partial \mathbf{x}} = \frac{1}{2} D^2 f(\mathbf{x}) = \frac{1}{2} D^2 f(\mathbf{y}) \quad (\text{A.47})$$

Linearized balance laws and spatial discretization

APPENDIX B

B.1 Linearization and Newton-Raphson process

The weak formulation of the thermo-dissipative continuum dynamics presented in Chapter 3 and recovered by the GENERIC framework in Chapter 4 is nonlinear respect to both the geometry and the material. Therefore, for a given instant time, there exist a state of thermodynamic equilibrium given by a deformed configuration and a thermodynamic variable: temperature, entropy or others. As a result, this nonlinear formulation must be linearized in order to obtain such thermodynamic equilibrium states by using the Newton-Raphson iterative process.

This linearization can be performed in either the Lagrangian or Eulerian descriptions, leading both to the same quantities. For convenience, all the balance laws have been elaborated in the Lagrangian description where every volume integral is performed over the same fixed initial volume: V_0 .

Unlike other approaches found in the literature, all the methods dealt with in this dissertation are monolithic in the sense that the mechanic and thermal coupling is solved at once. Thereby, each term in the weak formulation must be linearized respect to both the mechanic and thermal configurations.

Based on the mechanical context, the notation of the virtual work principle for the linear momentum weak form (3.148)₂ is assumed by choosing $\mathbf{w}_p = \delta \mathbf{p} / \rho_0 = \delta \mathbf{v}$, and accordingly define the inertial, internal and external

virtual work terms

$$\delta W(\boldsymbol{\varphi}, \mathbf{p}, s, \boldsymbol{\Lambda}^\alpha, \delta \mathbf{v}) = \delta W_{\text{ine}}(\mathbf{p}, \delta \mathbf{v}) + \delta W_{\text{int}}(\boldsymbol{\varphi}, s, \boldsymbol{\Lambda}^\alpha, \delta \mathbf{v}) - \delta W_{\text{ext}}(\boldsymbol{\varphi}, \delta \mathbf{v}) \quad (\text{B.1})$$

with s representing the thermodynamic variable and

$$\begin{aligned} \delta W_{\text{ine}}(\mathbf{p}, \delta \mathbf{v}) &= \int_{\mathcal{B}_0} \delta \mathbf{v} \cdot \dot{\mathbf{p}} dV_0 \\ \delta W_{\text{int}}(\boldsymbol{\varphi}, s, \boldsymbol{\Lambda}^\alpha, \delta \mathbf{v}) &= \int_{\mathcal{B}_0} \nabla_0 \delta \mathbf{v} : \mathbf{F} \mathbf{S} dV_0 \\ \delta W_{\text{ext}}(\boldsymbol{\varphi}, \delta \mathbf{v}) &= \int_{\mathcal{B}_0} \delta \mathbf{v} \cdot \mathbf{B}_0 dV_0 + \int_{\partial \mathcal{B}_0} \delta \mathbf{v} \cdot \mathbf{T}_0 dA_0 \end{aligned} \quad (\text{B.2})$$

In analogy with the virtual work principle, the weak form of the energy balance, formulated either in entropy form (3.146), with $w_\eta = \delta \eta$, or in temperature form (3.147), with $w_\Theta = \delta \Theta$, is expressed as follows

$$\begin{aligned} \delta Q^s(\boldsymbol{\varphi}, \mathbf{p}, s, \boldsymbol{\Lambda}^\alpha, \delta s) &= \delta Q_{\text{ine}}^s(s, \delta s) + \delta Q_{\text{int}}^s(\boldsymbol{\varphi}, \mathbf{p}, s, \boldsymbol{\Lambda}^\alpha, \delta s) \\ &\quad + \delta Q_{\text{dis}}^s(\boldsymbol{\varphi}, s, \boldsymbol{\Lambda}^\alpha, \delta s) - \delta Q_{\text{ext}}^s(s, \delta s), \end{aligned} \quad (\text{B.3})$$

where the inertial-like term is

$$\delta Q_{\text{ine}}^s(s, \delta s) = \int_{\mathcal{B}_0} \delta s \dot{s} dV_0, \quad (\text{B.4})$$

with s playing the role of either entropy or temperature.

The rest of the terms needs differentiated definitions for the entropy or the temperature formulation. Thus, in the entropy formulation the term called *internal* considers the heat conduction phenomenon, that is

$$\begin{aligned} \delta Q_{\text{int}}^\eta(\boldsymbol{\varphi}, \eta, \boldsymbol{\Lambda}^\alpha, \delta \eta) &= - \int_{\mathcal{B}_0} \nabla_0 \left[\frac{\delta \eta}{\Theta} \right] \cdot \mathbf{H} dV_0 \\ &= - \int_{\mathcal{B}_0} \frac{\nabla_0 \delta \eta \Theta - \delta \eta \nabla_0 \Theta}{\Theta^2} \cdot \mathbf{H} dV_0 \end{aligned} \quad (\text{B.5})$$

whereas in the temperature formulation, in addition to it, the term accounting for the thermoelastic heating is also encompassed to be

$$\begin{aligned} \delta Q_{\text{int}}^\Theta(\boldsymbol{\varphi}, \mathbf{p}, \Theta, \boldsymbol{\Lambda}^\alpha, \delta \Theta) &= - \int_{\mathcal{B}_0} \frac{1}{c} \nabla_0 \delta \Theta \cdot \mathbf{H} dV_0 \\ &\quad + \int_{\mathcal{B}_0} \frac{1}{c} \delta \Theta \mathbf{F} \mathbf{V} : \nabla_0 \left[\frac{\mathbf{p}}{\rho_0} \right] dV_0 \end{aligned} \quad (\text{B.6})$$

The same happens to the *dissipation* term, which, in the entropy formulation, only accounts for the rate of dissipation

$$\delta Q_{\text{dis}}^\eta(\boldsymbol{\varphi}, \eta, \boldsymbol{\Lambda}^\alpha, \delta\eta) = \int_{\mathcal{B}_0} \frac{\delta\eta}{\Theta} \dot{\mathcal{D}} dV_0 = \int_{\mathcal{B}_0} \frac{\delta\eta}{\Theta} \sum_{\alpha=1}^m \mathbf{Q}^\alpha : \mathcal{K}(\mathbf{Q}^\alpha) dV_0, \quad (\text{B.7})$$

whereas, in the temperature formulation, it also collects the thermodissipative heating to be

$$\delta Q_{\text{dis}}^\Theta(\boldsymbol{\varphi}, \Theta, \boldsymbol{\Lambda}^\alpha, \delta\Theta) = \int_{\mathcal{B}_0} \frac{\delta\Theta}{c} \dot{\mathcal{D}} dV_0 + \int_{\mathcal{B}_0} \frac{\delta\Theta}{c} \mathcal{H}_d dV_0 \quad (\text{B.8})$$

Finally, the *external* term in the entropy case is provided by

$$\delta Q_{\text{ext}}^\eta(\eta, \delta\eta) = \int_{\mathcal{B}_0} \frac{\delta\eta}{\Theta} \mathcal{R} dV_0 + \int_{\partial\mathcal{B}_0} \frac{\delta\eta}{\Theta} H_N dA_0, \quad (\text{B.9})$$

whereas, in the temperature one, is provided by

$$\delta Q_{\text{ext}}^\Theta(\Theta, \delta\Theta) = \int_{\mathcal{B}_0} \frac{\delta\Theta}{c} \mathcal{R} dV_0 + \int_{\partial\mathcal{B}_0} \frac{\delta\Theta}{c} H_N dA_0 \quad (\text{B.10})$$

So far, the thermo-dissipative continuum evolution equations have been presented as a first order partial differential equation (3.148). However, in order to simplify the linearization process, the density linear momentum and internal variables will be eliminated by using (3.148)₁ and (3.148)₄, thus transforming the original 1st order PDE system into a 2nd order PDE one, typically handled in continuum dynamics. The second elimination agrees with a condensation strategy for the internal variables. Thereby, the thermodynamic state is fully defined by the configuration $\boldsymbol{\varphi}$, which somehow retains the information stored by the density linear momentum and the internal variables, and the chosen thermodynamic state variable s .

Then, the Newton-Rapshon departs from a trial solution $(\boldsymbol{\varphi}_k, s_k)$ so that the thermodynamic *equilibrium* can be achieved by the linearization of the above equations in the direction of an increment $\mathbf{u}$ in $\boldsymbol{\varphi}_k$, henceforth referred to as *configurational linearization*, by using the directional derivative $D(\cdot)[\cdot]$, as

$$\begin{aligned} \delta W(\boldsymbol{\varphi}_k, \mathbf{p}, s, \boldsymbol{\Lambda}^\alpha, \delta\mathbf{v}) + D\delta W(\boldsymbol{\varphi}_k, \mathbf{p}, s, \boldsymbol{\Lambda}^\alpha, \delta\mathbf{v})[\mathbf{u}] &= 0 \\ \delta Q(\boldsymbol{\varphi}_k, \mathbf{p}, s, \boldsymbol{\Lambda}^\alpha, \delta s) + D\delta Q(\boldsymbol{\varphi}_k, \mathbf{p}, s, \boldsymbol{\Lambda}^\alpha, \delta s)[\mathbf{u}] &= 0 \end{aligned} \quad (\text{B.11})$$

and in the direction of an increment t in s_k , hereafter referred to as *thermal linearization*, as

$$\begin{aligned} \delta W(\boldsymbol{\varphi}, \mathbf{p}, s_k, \boldsymbol{\Lambda}^\alpha, \delta\mathbf{v}) + D\delta W(\boldsymbol{\varphi}, \mathbf{p}, s_k, \boldsymbol{\Lambda}^\alpha, \delta\mathbf{v})[t] &= 0 \\ \delta Q(\boldsymbol{\varphi}, \mathbf{p}, s_k, \boldsymbol{\Lambda}^\alpha, \delta s) + D\delta Q(\boldsymbol{\varphi}, \mathbf{p}, s_k, \boldsymbol{\Lambda}^\alpha, \delta s)[t] &= 0 \end{aligned} \quad (\text{B.12})$$

B.2 Lagrangian linearization of the IBVP weak form

The directional derivative is applied to each term defined in the previous section to obtain the linearized form of the problem's weak form. According to the Newton-Rapshon process (B.11) - (B.12), each term requires the elaboration of two types of directional derivatives, one that accounts for changes in the configuration and another that measures the changes due to a perturbation on the thermodynamical state variable.

Linearization of the inertial virtual work. Considering the relation between the motion and the density linear momentum (3.148)₁ the linearization with respect to the configuration of the inertial term results in

$$D\delta W_{\text{ine}}(\mathbf{p}, \delta \mathbf{v})[\mathbf{u}] = \int_{\mathcal{B}_0} \delta \mathbf{v} \cdot D\dot{\mathbf{p}}[\mathbf{u}] dV_0 = \int_{\mathcal{B}_0} \delta \mathbf{v} \cdot \rho_0 \ddot{\mathbf{u}} dV_0 \quad (\text{B.13})$$

This term does not contribute to the linearization with respect to the thermodynamical variable.

Linearization of the internal virtual work. Using the product rule for directional derivatives and the definition of the material elasticity tensor, the directional derivative in the direction of an increment of $\mathbf{u}$ is obtained as

$$\begin{aligned} D\delta W_{\text{int}}(\boldsymbol{\varphi}, s, \boldsymbol{\Lambda}^\alpha, \delta \mathbf{v})[\mathbf{u}] &= \int_{\mathcal{B}_0} D(\nabla_0 \delta \mathbf{v} : \mathbf{FS})[\mathbf{u}] dV_0 \\ &= \int_{\mathcal{B}_0} \frac{1}{2} D\delta \dot{\mathbf{C}}[\mathbf{u}] : \mathbf{S} dV_0 + \int_{\mathcal{B}_0} \frac{1}{2} \delta \dot{\mathbf{C}} : D\mathbf{S}[\mathbf{u}] dV_0 \\ &= \int_{\mathcal{B}_0} \mathbf{S} : (\nabla_0 \delta \mathbf{v}^T \nabla_0 \mathbf{u}) dV_0 + \int_{\mathcal{B}_0} \frac{1}{4} D\mathbf{C}[\delta \mathbf{v}] : \mathbb{C} : D\mathbf{C}[\mathbf{u}] dV_0 \\ &= \int_{\mathcal{B}_0} \mathbf{S} : (\nabla_0 \delta \mathbf{v}^T \nabla_0 \mathbf{u}) dV_0 + \int_{\mathcal{B}_0} \frac{1}{4} D\mathbf{C}[\delta \mathbf{v}] : \mathbb{C} : D\mathbf{C}[\mathbf{u}] dV_0, \end{aligned} \quad (\text{B.14})$$

where use has been made of the crucial relation

$$D\mathbf{C}[\delta \mathbf{v}] = \nabla_0 \delta \mathbf{v}^T \mathbf{F} + \mathbf{F}^T \nabla_0 \delta \mathbf{v} = \delta \dot{\mathbf{F}}^T \mathbf{F} + \mathbf{F}^T \delta \dot{\mathbf{F}} = \delta \dot{\mathbf{C}}, \quad (\text{B.15})$$

and the linearized material fourth order tensor $\mathbb{C} : \mathcal{B}_0 \times [0, T] \mapsto \text{Sym}(\mathbb{T}_d^4)$ has been introduced as

$$\mathbb{C}(\mathbf{X}, t) := 2 \frac{\partial \mathbf{S}(\mathbf{C}, s, \boldsymbol{\Lambda}^\alpha)}{\partial \mathbf{C}}, \quad (\text{B.16})$$

with $\mathbf{S}(\mathbf{C}, s, \boldsymbol{\Lambda}^\alpha)$ being provided either by (3.36) or (3.18) according to the election of the thermodynamical variable.

The resulting linearized term (B.14) is a classical result in nonlinear continuum mechanics. In fact, its terms are normally referred to as *geometrical* and *material* tangents.

On the other hand, the thermodynamically-linearized term is elaborated as follows

$$\begin{aligned} D\delta W_{\text{int}}(\boldsymbol{\varphi}, s, \boldsymbol{\Lambda}^\alpha, \delta \mathbf{v})[t] &= \int_{\mathcal{B}_0} D(\nabla_0 \delta \mathbf{v} : \mathbf{FS})[t] dV_0 \\ &= \int_{\mathcal{B}_0} \frac{1}{2} \delta \dot{\mathbf{C}} : D\mathbf{S}[t] dV_0 = \int_{\mathcal{B}_0} \frac{1}{2} \delta \dot{\mathbf{C}} : \frac{\partial \mathbf{S}}{\partial s} t dV_0 \quad (\text{B.17}) \\ &= \int_{\mathcal{B}_0} \frac{1}{2} D\mathbf{C}[\delta \mathbf{v}] : \mathbf{T} t dV_0, \end{aligned}$$

where $\mathbf{T} : \mathcal{B}_0 \times [0, T] \mapsto \text{Sym}(\mathbb{T}_d^2)$ the referential stress-temperature tensor.

Linearization of the external virtual work. In some applications the external actions may be motion-dependent, i.e $\mathbf{B}_0(\boldsymbol{\varphi})$ or $\mathbf{T}_0(\boldsymbol{\varphi})$, so that they would contribute to the linearized equations as follows

$$\begin{aligned} D\delta W_{\text{ext}}(\boldsymbol{\varphi}, \delta \mathbf{v})[\mathbf{u}] &= \int_{\mathcal{B}_0} \delta \mathbf{v} \cdot D\mathbf{B}_0[\mathbf{u}] dV_0 + \int_{\partial \mathcal{B}_0} \delta \mathbf{v} \cdot D\mathbf{T}_0[\mathbf{u}] dA_0 \\ &= \int_{\mathcal{B}_0} \delta \mathbf{v} \cdot \frac{\partial \mathbf{B}_0}{\partial \boldsymbol{\varphi}} \mathbf{u} dV_0 + \int_{\partial \mathcal{B}_0} \delta \mathbf{v} \cdot \frac{\partial \mathbf{T}_0}{\partial \boldsymbol{\varphi}} \mathbf{u} dA_0 \quad (\text{B.18}) \end{aligned}$$

For the energy balance weak form, the distinction for the entropy and the temperature formulations must be made.

B.2.1 Linearization of the entropy formulation

Linearization of the inertial-like virtual energy. The application of the directional derivative with respect the thermodynamical variable in the direction of s to (B.4), $s = \eta$, yields

$$D\delta Q_{\text{ine}}^\eta(\eta, \delta \eta)[s] = \int_{\mathcal{B}_0} \delta \eta D\dot{\eta}[s] dV_0 = \int_{\mathcal{B}_0} \delta \eta \dot{s} dV_0 \quad (\text{B.19})$$

As this term does not depend on the configuration $\boldsymbol{\varphi}$, it has no contribution to the configurational linearized equations.

Linearization of the internal virtual energy. This term contributes to both the configurational and thermal linearized equations.

Then, the linearization respect to the thermal variable entropy is elaborated by using the chain rule of the directional derivative in (B.5) to yield

$$\begin{aligned} D\delta Q_{\text{int}}^\eta(\boldsymbol{\varphi}, \eta, \boldsymbol{\Lambda}^\alpha, \delta\eta)[s] = & - \int_{\mathcal{B}_0} \nabla_0 \left[D \left(\frac{\delta\eta}{\Theta} \right) [s] \right] \cdot \mathbf{H} dV_0 \\ & - \int_{\mathcal{B}_0} \nabla_0 \left[\frac{\delta\eta}{\Theta} \right] \cdot D\mathbf{H}[s] dV_0 \end{aligned} \quad (\text{B.20})$$

The first directional derivative is developed by the product rule to be

$$D \left(\frac{\delta\eta}{\Theta} \right) [s] = -\frac{\delta\eta}{\Theta^2} D\Theta[s] = -\frac{\delta\eta}{\Theta^2} \frac{\partial\Theta}{\partial\eta} s, \quad (\text{B.21})$$

while the second one results in

$$\begin{aligned} D\mathbf{H}[s] &= D(-J\mathbf{F}^{-1}\boldsymbol{\kappa}\mathbf{F}^{-\text{T}}\nabla_0\Theta)[s] \\ &= -J\mathbf{F}^{-1}D\boldsymbol{\kappa}[s]\mathbf{F}^{-\text{T}}\nabla_0\Theta - J\mathbf{F}^{-1}\boldsymbol{\kappa}\mathbf{F}^{-\text{T}}\nabla_0D\Theta[s] \\ &= -J\mathbf{F}^{-1}\frac{\partial\boldsymbol{\kappa}}{\partial\Theta}D\Theta[s]\mathbf{F}^{-\text{T}}\nabla_0\Theta - J\mathbf{F}^{-1}\boldsymbol{\kappa}\mathbf{F}^{-\text{T}}\nabla_0\left[\frac{\partial\Theta}{\partial\eta}\right]_s \end{aligned} \quad (\text{B.22})$$

In the common case of thermal isotropy the above term can be simplified to be

$$D\mathbf{H}[s] = -k'(\Theta)\frac{\partial\Theta}{\partial\eta}sJ\mathbf{C}^{-1}\nabla_0\Theta - k(\Theta)J\mathbf{C}^{-1}\nabla_0\left[\frac{\partial\Theta}{\partial\eta}\right]_s \quad (\text{B.23})$$

Thereby, the full thermally-linearized internal term can be rearranged as

$$\begin{aligned} D\delta Q_{\text{int}}^\eta(\boldsymbol{\varphi}, \eta, \boldsymbol{\Lambda}^\alpha, \delta\eta)[s] &= \int_{\mathcal{B}_0} \nabla_0 \left[\frac{\delta\eta}{\Theta^2} \frac{\partial\Theta}{\partial\eta} s \right] \cdot \mathbf{H} dV_0 \\ &+ \int_{\mathcal{B}_0} \nabla_0 \left[\frac{\delta\eta}{\Theta} \right] \cdot k'(\Theta) \frac{\partial\Theta}{\partial\eta} s J\mathbf{C}^{-1} \nabla_0 \Theta dV_0 \\ &+ \int_{\mathcal{B}_0} \nabla_0 \left[\frac{\delta\eta}{\Theta} \right] \cdot k(\Theta) J\mathbf{C}^{-1} \nabla_0 \left[\frac{\partial\Theta}{\partial\eta} \right]_s dV_0 \end{aligned} \quad (\text{B.24})$$

The linearization respect to the configuration is provided by the following

directional derivative

$$\begin{aligned}
D\delta Q_{\text{int}}^\eta(\boldsymbol{\varphi}, \eta, \delta\eta)[\mathbf{u}] &= - \int_{\mathcal{B}_0} \nabla_0 \left[D \left(\frac{\delta\eta}{\Theta} \right) [\mathbf{u}] \right] \cdot \mathbf{H} dV_0 \\
&\quad - \int_{\mathcal{B}_0} \nabla_0 \left[\frac{\delta\eta}{\Theta} \right] \cdot D\mathbf{H}[\mathbf{u}] dV_0 \\
&= \int_{\mathcal{B}_0} \nabla_0 \left[\frac{\delta\eta}{\Theta^2} D\Theta[\mathbf{u}] \right] \cdot \mathbf{H} dV_0 \\
&\quad + \int_{\mathcal{B}_0} \nabla_0 \left[\frac{\delta\eta}{\Theta} \right] \cdot D(J\mathbf{F}^{-1}\boldsymbol{\kappa}\mathbf{F}^{-T})[\mathbf{u}] \nabla_0 \Theta dV_0 \\
&\quad + \int_{\mathcal{B}_0} \nabla_0 \left[\frac{\delta\eta}{\Theta} \right] \cdot J\mathbf{F}^{-1}\boldsymbol{\kappa}\mathbf{F}^{-T} \nabla_0 D\Theta[\mathbf{u}] dV_0
\end{aligned} \tag{B.25}$$

To proceed further, the ensuing directional derivative needs to be elaborated

$$\begin{aligned}
D(J\mathbf{F}^{-1}\boldsymbol{\kappa}\mathbf{F}^{-T})[\mathbf{u}] &= DJ[\mathbf{u}]\mathbf{F}^{-1}\boldsymbol{\kappa}\mathbf{F}^{-T} + J\mathbf{F}^{-1}D\boldsymbol{\kappa}[\mathbf{u}]\mathbf{F}^{-T} \\
&\quad + JD\mathbf{F}^{-1}[\mathbf{u}]\boldsymbol{\kappa}\mathbf{F}^{-T} + J\mathbf{F}^{-1}\boldsymbol{\kappa}D\mathbf{F}^{-T}[\mathbf{u}],
\end{aligned} \tag{B.26}$$

where the resulting directional derivatives are classic in nonlinear mechanics, see Bonet & Wood (2008), and are provided by

$$\begin{aligned}
DJ[\mathbf{u}] &= D \det \mathbf{F} [D\mathbf{F}[\mathbf{u}]] = J\mathbf{F}^{-T} : \nabla_0 \mathbf{u} \\
D\mathbf{F}^{-1}[\mathbf{u}] &= D\mathbf{F}^{-1} [D\mathbf{F}[\mathbf{u}]] = -\mathbf{F}^{-1} \nabla_0 \mathbf{u} \mathbf{F}^{-1} \\
D\mathbf{F}^{-T}[\mathbf{u}] &= D\mathbf{F}^{-T} [D\mathbf{F}[\mathbf{u}]] = -\mathbf{F}^{-T} \nabla_0 \mathbf{u}^T \mathbf{F}^{-T}
\end{aligned} \tag{B.27}$$

In addition, the spatial conductivity tensor is linearized as

$$D\boldsymbol{\kappa}[\mathbf{u}] = D\boldsymbol{\kappa}[D\Theta[\mathbf{u}]] = \frac{\partial \boldsymbol{\kappa}}{\partial \Theta} D\Theta[\mathbf{u}] \tag{B.28}$$

Finally, both (B.25) and (B.28) can be fully elaborated by using

$$D\Theta[\mathbf{u}] = D\Theta[D\mathbf{C}[\mathbf{u}]] = 2 \frac{\partial \Theta}{\partial \mathbf{C}} : \mathbf{F}^T \nabla_0 \mathbf{u}, \tag{B.29}$$

where use has been made of (B.15) and the symmetry of the tensor $\frac{\partial \Theta}{\partial \mathbf{C}}$.

Linearization of the dissipated virtual energy. As the above term, the dissipated virtual energy one has contributions to both the configurational and thermal linearized equations.

On the one hand, the thermal linearization yields

$$\begin{aligned}
D\delta Q_{\text{dis}}^\eta[s] &= \int_{\mathcal{B}_0} D\left(\frac{\delta\eta}{\Theta}\right)[s] \sum_{\alpha=1}^m \mathbf{Q}^\alpha : \mathcal{K}(\mathbf{Q}^\alpha) dV_0 \\
&+ \int_{\mathcal{B}_0} \frac{\delta\eta}{\Theta} \sum_{\alpha=1}^m D\mathbf{Q}^\alpha[s] : \mathcal{K}(\mathbf{Q}^\alpha) dV_0 \\
&+ \int_{\mathcal{B}_0} \frac{\delta\eta}{\Theta} \sum_{\alpha=1}^m \mathbf{Q}^\alpha : D\mathcal{K}(\mathbf{Q}^\alpha)[s] dV_0 \\
&= - \int_{\mathcal{B}_0} \frac{\delta\eta}{\Theta^2} \frac{\partial\Theta}{\partial\eta} s \dot{\mathcal{D}} dV_0 + \int_{\mathcal{B}_0} \frac{\delta\eta}{\Theta} \sum_{\alpha=1}^m \frac{\partial\mathbf{Q}^\alpha}{\partial\eta} s : \mathcal{K}(\mathbf{Q}^\alpha) dV_0 \\
&+ \int_{\mathcal{B}_0} \frac{\delta\eta}{\Theta} \sum_{\alpha=1}^m \mathbf{Q}^\alpha : \left(\frac{d\mathcal{K}}{d\mathbf{Q}^\alpha} : \frac{\partial\mathbf{Q}^\alpha}{\partial\eta} \right) s dV_0
\end{aligned} \tag{B.30}$$

On the other hand, the configurational linearized contribution results in

$$\begin{aligned}
D\delta Q_{\text{dis}}^\eta[\mathbf{u}] &= \int_{\mathcal{B}_0} D\left(\frac{\delta\eta}{\Theta}\right)[\mathbf{u}] \sum_{\alpha=1}^m \mathbf{Q}^\alpha : \mathcal{K}(\mathbf{Q}^\alpha) dV_0 \\
&+ \int_{\mathcal{B}_0} \frac{\delta\eta}{\Theta} \sum_{\alpha=1}^m D\mathbf{Q}^\alpha[\mathbf{u}] : \mathcal{K}(\mathbf{Q}^\alpha) dV_0 \\
&+ \int_{\mathcal{B}_0} \frac{\delta\eta}{\Theta} \sum_{\alpha=1}^m \mathbf{Q}^\alpha : D\mathcal{K}[D\mathbf{Q}^\alpha[\mathbf{u}]] dV_0
\end{aligned} \tag{B.31}$$

where the first term is fully elaborated using the chain rule together with (B.29) while the rest ones lie at the following directional derivative

$$D\mathbf{Q}^\alpha[\mathbf{u}] = D\mathbf{Q}^\alpha[DC[\mathbf{u}]] = \mathbb{Q}^\alpha : \mathbf{F}^T \nabla_0 \mathbf{u}, \tag{B.32}$$

with $\mathbb{Q}^\alpha : \mathcal{B}_0 \times [0, T] \mapsto \text{Sym}(\mathbb{T}_d^4)$ being the linearized material-dissipative fourth order tensor provided by

$$\mathbb{Q}^\alpha := 2 \frac{\partial \mathbf{Q}^\alpha(\mathbf{C}, \eta, \mathbf{\Lambda}^\alpha)}{\partial \mathbf{C}} \tag{B.33}$$

Rearranging terms the contribution to the configurational linearized equa-

tions yields

$$\begin{aligned}
D\delta Q_{\text{dis}}^\eta[\mathbf{u}] &= - \int_{\mathcal{B}_0} 2\dot{D} \frac{\delta\eta}{\Theta^2} \frac{\partial\Theta}{\partial\mathbf{C}} : \mathbf{F}^T \nabla_0 \mathbf{u} dV_0 \\
&+ \int_{\mathcal{B}_0} \frac{\delta\eta}{\Theta} \sum_{\alpha=1}^m \mathbb{Q}^\alpha : \mathbf{F}^T \nabla_0 \mathbf{u} : \dot{\mathbf{\Lambda}}^\alpha dV_0 \\
&+ \int_{\mathcal{B}_0} \frac{\delta\eta}{\Theta} \sum_{\alpha=1}^m \mathbf{Q}^\alpha : \left(\frac{d\mathcal{K}}{d\mathbf{Q}^\alpha} : \mathbb{Q}^\alpha : \mathbf{F}^T \nabla_0 \mathbf{u} \right) dV_0
\end{aligned} \tag{B.34}$$

B.2.2 Linearization of the temperature formulation

Linearization of the inertial-like virtual energy. This term only contributes to the thermal linearized equations, that is

$$D\delta Q_{\text{ine}}^\Theta(\Theta, \delta\Theta)[t] = \int_{\mathcal{B}_0} \delta\Theta D\dot{\Theta}[t] dV_0 = \int_{\mathcal{B}_0} \delta\Theta \dot{t} dV_0 \tag{B.35}$$

Linearization of the internal virtual energy. As was defined in (B.6), it has two terms that will hereafter be indicated by the subscript 1 and 2, respectively.

Thus, the first term is thermally linearized as follows

$$D\delta Q_{\text{int},1}^\Theta(\boldsymbol{\varphi}, \Theta, \delta\Theta)[t] = - \int_{\mathcal{B}_0} \frac{1}{c} \nabla_0 \delta\Theta \cdot D\mathbf{H}[t] dV_0 \tag{B.36}$$

where the directional derivative applied to the heat vector $\mathbf{H}$ nearly resembles the expression (B.22), this time considering the temperature as state variable to give

$$D\mathbf{H}[t] = -J\mathbf{F}^{-1} \frac{\partial\boldsymbol{\kappa}}{\partial\Theta} t \mathbf{F}^{-T} \nabla_0 \Theta - J\mathbf{F}\boldsymbol{\kappa}(\Theta) \mathbf{F}^{-T} \nabla_0 t \tag{B.37}$$

The second term is conveniently expressed in terms of the rate of the Cauchy-Green deformation tensor, using (3.83) to be linearized as follows

$$\begin{aligned}
D\delta Q_{\text{int},2}^\Theta(\boldsymbol{\varphi}, \Theta, \delta\Theta)[t] &= \int_{\mathcal{B}_0} D \left(\frac{\delta\Theta}{c} \frac{1}{2} \dot{\mathbf{C}} : \mathbf{V} \right) [t] dV_0 \\
&= \int_{\mathcal{B}_0} \frac{\delta\Theta}{c} \frac{1}{2} \dot{\mathbf{C}} : D\mathbf{V}[t] dV_0 = \int_{\mathcal{B}_0} \frac{\delta\Theta}{c} \frac{1}{2} \dot{\mathbf{C}} : \frac{\partial\mathbf{V}}{\partial\Theta} t dV_0 \\
&= \int_{\mathcal{B}_0} \frac{\delta\Theta}{c} \frac{1}{2} \dot{\mathbf{C}} : D\mathbf{V}[t] dV_0 = \int_{\mathcal{B}_0} \frac{\delta\Theta}{c} \frac{1}{2} D\mathbf{C}[\mathbf{v}] : \frac{\partial\mathbf{V}}{\partial\Theta} t dV_0
\end{aligned} \tag{B.38}$$

On the other hand, the first term contributes to the configurational linearized equations in the following way

$$D\delta Q_{\text{int},1}^{\Theta}(\boldsymbol{\varphi}, \Theta, \delta\Theta)[\mathbf{u}] = - \int_{\mathcal{B}_0} \frac{1}{c} \nabla_0 \delta\Theta \cdot D\mathbf{H}[\mathbf{u}] dV_0 \quad (\text{B.39})$$

The linearization of the heat vector then follows the expression (B.26) except for the term derived from the conductivity tensor as, in the temperature formulation, it does not depend any longer on the configuration, that is

$$D\mathbf{H}[\mathbf{u}] = -(DJ[\mathbf{u}]\mathbf{F}^{-1}\boldsymbol{\kappa}\mathbf{F}^{-\text{T}} + J D\mathbf{F}^{-1}[\mathbf{u}]\boldsymbol{\kappa}\mathbf{F}^{-\text{T}} + J\mathbf{F}^{-1}\boldsymbol{\kappa} D\mathbf{F}^{-\text{T}}[\mathbf{u}])\nabla_0\Theta, \quad (\text{B.40})$$

with the appearing directional derivatives being again provided by (B.27).

In analogy with (B.14), the second term can be demonstrated to contribute to the configurational linearization as follows

$$\begin{aligned} D\delta Q_{\text{int},2}^{\Theta}(\boldsymbol{\varphi}, \Theta, \delta\Theta)[\mathbf{u}] &= \int_{\mathcal{B}_0} \frac{\delta\Theta}{c} D\left(\frac{1}{2}\dot{\mathbf{C}} : \mathbf{V}\right)[\mathbf{u}] dV_0 \\ &= \int_{\mathcal{B}_0} \frac{1}{c} \delta\Theta \left(\frac{1}{2} D\dot{\mathbf{C}}[\mathbf{u}] : \mathbf{V} + \frac{1}{2} \dot{\mathbf{C}} : D\mathbf{V}[\mathbf{u}]\right) dV_0 \\ &= \int_{\mathcal{B}_0} \frac{1}{c} \delta\Theta \left(\frac{1}{2} D\dot{\mathbf{C}}[\mathbf{u}] : \mathbf{V} + \frac{1}{4} D\mathbf{C}[\mathbf{v}] : \mathbb{D} : D\mathbf{C}[\mathbf{u}]\right) dV_0 \\ &= \int_{\mathcal{B}_0} \frac{1}{c} \delta\Theta \left(\mathbf{V} : (\nabla_0 \mathbf{v}^{\text{T}} \nabla_0 \mathbf{u}) + \frac{1}{4} D\mathbf{C}[\mathbf{v}] : \mathbb{D} : D\mathbf{C}[\mathbf{u}]\right) dV_0, \end{aligned} \quad (\text{B.41})$$

where following the definition of the material tensor (B.16), the fourth order tensor $\mathbb{D} : \mathcal{B}_0 \times [0, T] \mapsto \text{Sym}(\mathbb{T}_d^4)$ has been introduced as

$$\mathbb{D} := 2 \frac{\partial \mathbf{V}(\mathbf{C}, \Theta, \boldsymbol{\Lambda}^{\alpha})}{\partial \mathbf{C}} \quad (\text{B.42})$$

Linearization of the dissipated virtual energy. This term was also introduced as sum of two contributions, the first accounting for the rate of dissipation and the second for the thermo-dissipative heating, which will be hereafter referred to 1 and 2, respectively.

Then, the linearization of the first term respect to the temperature is

$$\begin{aligned} D\delta Q_{\text{dis},1}^{\Theta}[t] &= \int_{\mathcal{B}_0} \frac{\delta\Theta}{c} \sum_{\alpha=1}^m D\mathbf{Q}^{\alpha}[t] : \mathcal{K}(\mathbf{Q}^{\alpha}) dV_0 \\ &\quad + \int_{\mathcal{B}_0} \frac{\delta\Theta}{c} \sum_{\alpha=1}^m \mathbf{Q}^{\alpha} : D\mathcal{K}[D\mathbf{Q}^{\alpha}[t]] dV_0 \end{aligned} \quad (\text{B.43})$$

whereas the second term counterpart similarly yields

$$\begin{aligned}
D\delta Q_{\text{dis},2}^{\Theta}[t] &= \int_{\mathcal{B}_0} \frac{\delta\Theta}{c} D\mathcal{H}_d[t] dV_0 \\
&= \int_{\mathcal{B}_0} \frac{\delta\Theta}{c} \sum_{\alpha=1}^m D\mathbf{W}^{\alpha}[t] : \mathcal{K}(\mathbf{Q}^{\alpha}) dV_0 \\
&\quad + \int_{\mathcal{B}_0} \frac{\delta\Theta}{c} \sum_{\alpha=1}^m \mathbf{W}^{\alpha} : D\mathcal{K}[D\mathbf{Q}^{\alpha}[t]] dV_0
\end{aligned} \tag{B.44}$$

These last expressions are completed by the following directional derivatives

$$\begin{aligned}
D\mathbf{Q}^{\alpha}[t] &= \frac{\partial \mathbf{Q}^{\alpha}}{\partial \Theta} t \\
D\mathbf{W}^{\alpha}[t] &= \frac{\partial \mathbf{W}^{\alpha}}{\partial \Theta} t \\
D\mathcal{K}[D\mathbf{Q}^{\alpha}[t]] &= \frac{d\mathcal{K}}{d\mathbf{Q}^{\alpha}} : \frac{\partial \mathbf{Q}^{\alpha}}{\partial \Theta} t
\end{aligned} \tag{B.45}$$

Likewise, the resulting linearization of the first term is alike (B.31), that is

$$\begin{aligned}
D\delta Q_{\text{dis},1}^{\Theta}[\mathbf{u}] &= \int_{\mathcal{B}_0} \frac{1}{c} \delta\Theta \sum_{\alpha=1}^m D\mathbf{Q}^{\alpha}[D\mathbf{C}[\mathbf{u}]] : \mathcal{K}(\mathbf{Q}^{\alpha}) dV_0 \\
&\quad + \int_{\mathcal{B}_0} \frac{1}{c} \delta\Theta \sum_{\alpha=1}^m \mathbf{Q}^{\alpha} : D\mathcal{K}[D\mathbf{Q}^{\alpha}[D\mathbf{C}[\mathbf{u}]]] dV_0 \\
&= \int_{\mathcal{B}_0} \frac{1}{c} \delta\Theta \sum_{\alpha=1}^m \mathbf{Q}^{\alpha} : \mathbf{F}^T \nabla_0 \mathbf{u} : \mathcal{K}(\mathbf{Q}^{\alpha}) dV_0 \\
&\quad + \int_{\mathcal{B}_0} \frac{1}{c} \delta\Theta \sum_{\alpha=1}^m \mathbf{Q}^{\alpha} : \frac{d\mathcal{K}}{d\mathbf{Q}^{\alpha}} : \mathbf{Q}^{\alpha} : \mathbf{F}^T \nabla_0 \mathbf{u} dV_0,
\end{aligned} \tag{B.46}$$

now $\mathbf{Q}^{\alpha} : \mathcal{B}_0 \mapsto \text{Sym}(\mathbb{T}_d^4)$ being provided by

$$\mathbf{Q}^{\alpha} := 2 \frac{\partial \mathbf{Q}^{\alpha}(\mathbf{C}, \Theta, \mathbf{\Lambda}^{\alpha})}{\partial \mathbf{C}} \tag{B.47}$$

Finally, similarly proceeding with the second term, its configurationally

linearized counterpart results in

$$\begin{aligned}
D\delta Q_{\text{dis},2}^{\Theta}[\mathbf{u}] &= \int_{\mathcal{B}_0} \frac{\delta\Theta}{c} D\mathcal{H}_d[\mathbf{u}] dV_0 \\
&= \int_{\mathcal{B}_0} \frac{\delta\Theta}{c} \sum_{\alpha=1}^m D\mathbf{W}^{\alpha}[D\mathbf{C}[\mathbf{u}]] : \mathcal{K}(\mathbf{Q}^{\alpha}) dV_0 \\
&\quad + \int_{\mathcal{B}_0} \frac{\delta\Theta}{c} \sum_{\alpha=1}^m \mathbf{W}^{\alpha} : D\mathcal{K}[D\mathbf{Q}^{\alpha}[D\mathbf{C}[\mathbf{u}]]] dV_0 \\
&= \int_{\mathcal{B}_0} \frac{\delta\Theta}{c} \sum_{\alpha=1}^m \mathbb{W}^{\alpha} : \mathbf{F}^T \nabla_0 \mathbf{u} : \mathcal{K}(\mathbf{Q}^{\alpha}) dV_0 \\
&\quad + \int_{\mathcal{B}_0} \frac{\delta\Theta}{c} \sum_{\alpha=1}^m \mathbf{W}^{\alpha} : \frac{d\mathcal{K}}{d\mathbf{Q}^{\alpha}} : \mathbf{Q}^{\alpha} : \mathbf{F}^T \nabla_0 \mathbf{u} dV_0,
\end{aligned} \tag{B.48}$$

where, in analogy with (B.33), the resulting symmetric fourth order tensor $\mathbb{W}^{\alpha} : \mathcal{B}_0 \mapsto \text{Sym}(\mathbb{T}_d^4)$ has been introduced as

$$\mathbb{W}^{\alpha} := 2 \frac{\partial \mathbf{W}^{\alpha}(\mathbf{C}, \Theta, \mathbf{\Lambda}^{\alpha})}{\partial \mathbf{C}} \tag{B.49}$$

B.2.3 Spatially discretized evolution equations

The discretization is performed in the undeformed configuration using isoparametric elements defined by nodal particles $\mathbf{X}_a$

$$\mathbf{X}^e = \sum_{a=1}^p N_a(\xi, \eta, \zeta) \mathbf{X}_a, \tag{B.50}$$

with N_a being the a -th standard element shape function and p being the number of nodes of the element.

Discretized state variables. In the isoparametric approach, the state variables are approximated using the same standard shape functions, such that

$$\boldsymbol{\varphi}^e = \sum_{a=1}^p N_a \mathbf{x}_a(t), \quad s^e = \sum_{a=1}^p N_a s_a(t), \quad \mathbf{\Lambda}^{\alpha,e} = \sum_{a=1}^p N_a \mathbf{\Lambda}_a^{\alpha}(t), \tag{B.51}$$

with $\mathbf{x}_a$ being the current position of the nodal particles.

Discretized kinematics. All the kinematic quantities are discretized based on the discretization of the motion function. Thus, the discretized deformation gradient tensor results from applying the material gradient to it as follows

$$\mathbf{F}^e = \sum_{a=1}^p \mathbf{x}_a(t) \otimes \nabla_0 N_a, \quad (\text{B.52})$$

and, consequently, the discretized right Cauchy-Green deformation tensor is

$$\mathbf{C}^e = \sum_{a=1}^p \sum_{b=1}^p \mathbf{x}_a(t) \cdot \mathbf{x}_b(t) \nabla_0 N_a \otimes \nabla_0 N_b, \quad (\text{B.53})$$

The material gradient of the shape functions can be obtained from the gradient in the isoparametric space ($\nabla_{\boldsymbol{\xi}}$), where they are naturally defined, as follows

$$\nabla_0 N_a = \left(\frac{\partial \mathbf{X}}{\partial \boldsymbol{\xi}} \right)^{-T} \nabla_{\boldsymbol{\xi}} N_a, \quad \text{with} \quad \frac{\partial \mathbf{X}}{\partial \boldsymbol{\xi}} = \sum_{a=1}^p \mathbf{X}_a \otimes \nabla_{\boldsymbol{\xi}} N_a \quad (\text{B.54})$$

On the other hand, the discretized material velocity, or the linear momentum density, results from time differentiating the discretized motion to give

$$\mathbf{v}^e = \mathbf{p}^e / \rho_0^e = \sum_{a=1}^p N_a \dot{\mathbf{x}}_a(t), \quad (\text{B.55})$$

Discretized linear momentum equation. Consider the contribution to δW caused by a single virtual nodal velocity $\delta \mathbf{v}_a$ occurring at a typical node i of element e . Following the format provided by (B.1), the contribution due to the inertial term is elaborated as follows

$$\delta W_{\text{ine}}^e(\dot{\mathbf{p}}, N_a \delta \mathbf{v}_a) = \delta \mathbf{v}_a \cdot \int_{\mathcal{B}_0^e} N_a \dot{\mathbf{p}} dV_0^e \quad (\text{B.56})$$

Similarly, the contribution due to the internal forces results in

$$\begin{aligned} \delta W_{\text{int}}^e(\boldsymbol{\varphi}^e, s^e, \boldsymbol{\Lambda}^{\alpha,e}, N_a \delta \mathbf{v}_a) &= \int_{\mathcal{B}_0^e} (\delta \mathbf{v}_a \otimes \nabla_0 N_a) : \mathbf{F}^e \mathbf{S}^e dV_0^e \\ &= \delta \mathbf{v}_a \cdot \int_{\mathcal{B}_0^e} \mathbf{F}^e \mathbf{S}^e \nabla_0 N_a dV_0^e \end{aligned} \quad (\text{B.57})$$

And, finally, the contribution due to the external forces yields

$$\delta W_{\text{ext}}^e(\boldsymbol{\varphi}^e, N_a \delta \mathbf{v}_a) = \delta \mathbf{v}_a \cdot \int_{\mathcal{B}_0^e} N_a \mathbf{B}_0 dV_0^e + \delta \mathbf{v}_a \cdot \int_{\partial \mathcal{B}_0^e} N_a \mathbf{T}_0 dA_0^e \quad (\text{B.58})$$

Arranging each of the above contribution, the searched contribution caused by a single virtual velocity at a node e is provided by

$$\begin{aligned} \delta W^e(\boldsymbol{\varphi}, s, \boldsymbol{\Lambda}^\alpha, N_a \delta \mathbf{v}_a) = \delta \mathbf{v}_a \cdot & \left(\int_{\mathcal{B}_0^e} N_a \dot{\mathbf{p}} dV_0^e + \int_{\mathcal{B}_0^e} \mathbf{F}^e \mathbf{S}^e \nabla_0 N_a dV_0^e \right. \\ & \left. - \int_{\mathcal{B}_0^e} N_a \mathbf{B}_0 dV_0^e - \int_{\partial \mathcal{B}_0^e} N_a \mathbf{T}_0 dA_0^e \right) \end{aligned} \quad (\text{B.59})$$

It only remains to assemble each of the element contribution concurring in a node to obtain the discretized linear momentum equation

$$\delta W(\boldsymbol{\varphi}, s, \boldsymbol{\Lambda}^\alpha, N_a \delta \mathbf{v}_a) = \sum_{\substack{e=1 \\ e \ni a}}^{m_a} \delta W^e(\boldsymbol{\varphi}, s, \boldsymbol{\Lambda}^\alpha, N_a \delta \mathbf{v}_a) = \sum_{\substack{e=1 \\ e \ni a}}^{m_a} \delta \mathbf{v}_a \cdot (\mathbf{I}_a^e + \mathbf{T}_a^e - \mathbf{F}_a^e) \quad (\text{B.60})$$

Discretized energy equation. Analogously, consider the contribution to δQ caused by a single variation of the thermal variable δs_a occurring at a typical node i of element e . Then, the contribution of each of the term in (B.1) is elaborated next according to the choice for the thermal variable. First, the inertial-like term contributes as follows

$$\delta Q_{\text{ine}}^{s,e}(s^e, N_a \delta s_a) = \delta s_a \int_{\mathcal{B}_0^e} N_a \dot{s}^e dV_0^e, \quad (\text{B.61})$$

with s playing the role of either entropy or temperature.

The rest of the terms needs differentiated elaborations for the entropy or the temperature formulation. Thus, in the entropy formulation the contribution due to the internal term (B.5) results in

$$\begin{aligned} \delta Q_{\text{int}}^{\eta,e}(\boldsymbol{\varphi}^e, \eta^e, \boldsymbol{\Lambda}^{\alpha,e}, N_a \delta \eta_a) &= - \int_{\mathcal{B}_0^e} \nabla_0 \left[\frac{N_a \delta \eta_a}{\Theta^e} \right] \cdot \mathbf{H}^e dV_0^e \\ &= \delta \eta_a \left(- \int_{\mathcal{B}_0^e} \frac{1}{\Theta^e} \nabla_0 N_a \cdot \mathbf{H}^e dV_0^e + \int_{\mathcal{B}_0^e} \frac{N_a}{(\Theta^e)^2} \nabla_0 \Theta^e \cdot \mathbf{H}^e dV_0^e \right) \end{aligned} \quad (\text{B.62})$$

with

$$\mathbf{H}^e = -\mathbf{K}^e \nabla_0 \Theta^e \quad (\text{B.63})$$

The entropy formulation requires further elaboration of the gradient of temperature to express it in terms of the state variables. To this end, the chain rule is applied to give

$$\nabla_0 \Theta^e = \frac{\partial \Theta}{\partial \mathbf{C}} : \nabla_0 \mathbf{C}^e + \frac{\partial \Theta}{\partial \eta} \nabla_0 \eta^e + \frac{\partial \Theta}{\partial \boldsymbol{\Lambda}^\alpha} : \nabla_0 \boldsymbol{\Lambda}^{\alpha,e}, \quad (\text{B.64})$$

where the gradients applied to state variables are easily computed through the gradient of the shape functions. However, the gradient of the right Cauchy-Green deformation tensor needs further elaboration to relate it with the discretized motion state variable. The directional derivative is used to arrive at the identity

$$\begin{aligned} DC^e[\mathbf{U}] &= \nabla_0 \mathbf{C} : \mathbf{U} = \mathbf{F}^T \nabla_0 \mathbf{F} \mathbf{U} + \nabla_0 \mathbf{F} \mathbf{U}^T \mathbf{F} \\ &= \mathbf{F}^T \nabla_0 \mathbf{F} : \mathbf{U} + \nabla_0 \mathbf{F}^T \mathbf{F} : \mathbf{U} \\ &= (\mathbf{F}^T \nabla_0 \mathbf{F} + \nabla_0 \mathbf{F}^T \mathbf{F}) : \mathbf{U} \end{aligned} \quad (\text{B.65})$$

Therefore, the problem is translated to compute the gradient of the discretized deformation gradient (B.52). The application of the material gradient to it leads to

$$\begin{aligned} \nabla_0 \mathbf{F}^e &= \sum_{a=1}^p \mathbf{x}_a \otimes \nabla_0^2 N_a \\ &= \sum_{a=1}^p \mathbf{x}_a \otimes \left[\frac{\partial^2 N_a}{\partial \boldsymbol{\xi}^2} : \left(\frac{\partial \boldsymbol{\xi}}{\partial \mathbf{X}} \otimes \frac{\partial \boldsymbol{\xi}}{\partial \mathbf{X}} \right) + \frac{\partial N_a}{\partial \boldsymbol{\xi}} : \frac{\partial^2 \boldsymbol{\xi}}{\partial \mathbf{X}^2} \right] \\ &= \sum_{a=1}^p \mathbf{x}_a \otimes \left[\left(\frac{\partial \mathbf{X}}{\partial \boldsymbol{\xi}} \otimes \frac{\partial \mathbf{X}}{\partial \boldsymbol{\xi}} \right)^{-T} : \frac{\partial^2 N_a}{\partial \boldsymbol{\xi}^2} + \frac{\partial N_a}{\partial \boldsymbol{\xi}} : \frac{\partial^2 \boldsymbol{\xi}}{\partial \mathbf{X}^2} \right], \end{aligned} \quad (\text{B.66})$$

where use has been made of (B.54)₂.

The main implication of the above expression is that second derivatives of the standard shape functions are required, imposing an extra requirement over the definition of shape functions, that is, they must have non-trivial second derivatives. This issue was pointed out in Section 3.8.1.

Summarizing, the gradient of the discretized right Cauchy-Green defor-

mation tensor results in

$$\begin{aligned}\nabla_0 \mathbf{C} &= (\mathbf{F}^e)^T \nabla_0 \mathbf{F}^e + \mathbf{F}^e (\nabla_0 \mathbf{F}^e)^T = \sum_{a=1}^p (\nabla_0 N_a \otimes \mathbf{x}_a) (\mathbf{x}_a \otimes \nabla_0^2 N_a) \\ &\quad + \sum_{a=1}^p (\mathbf{x}_a \otimes \nabla_0 N_a) (\nabla_0^2 N_a \otimes \mathbf{x}_a) \quad (\text{B.67}) \\ &= 2 \sum_{a=1}^p (\mathbf{x}_a \cdot \mathbf{x}_a) (\nabla_0 N_a \otimes \nabla_0^2 N_a)\end{aligned}$$

On the other hand, for the temperature formulation, the contribution of the internal term (B.6) is

$$\begin{aligned}\delta Q_{\text{int}}^{\Theta,e}(\boldsymbol{\varphi}^e, \mathbf{p}^e, \Theta^e, \boldsymbol{\Lambda}^{\alpha,e}, N_a \delta \Theta_a) &= -\delta \Theta_a \int_{\mathcal{B}_0^e} \frac{1}{c} \nabla_0 N_a \cdot \mathbf{H}^e dV_0^e \\ &\quad + \delta \Theta_a \int_{\mathcal{B}_0^e} \frac{1}{c} \mathbf{F}^e \mathbf{V}^e : \nabla_0 \left[\frac{\mathbf{p}^e}{\rho_0^e} \right] N_a dV_0^e \quad (\text{B.68})\end{aligned}$$

The *dissipation* term also adopts different definitions for each of the formulations considered. In the entropy one provided by (B.7), its contribution is

$$\begin{aligned}\delta Q_{\text{dis}}^{\eta,e}(\boldsymbol{\varphi}^e, \eta^e, \boldsymbol{\Lambda}^{\alpha,e}, N_a \delta \eta_a) &= \delta \eta_a \int_{\mathcal{B}_0^e} \frac{1}{\Theta^e} \dot{\mathcal{D}}^e N_a dV_0^e \\ &= \delta \eta_a \int_{\mathcal{B}_0^e} \frac{1}{\Theta^e} \sum_{\alpha=1}^m \mathbf{Q}^{\alpha,e} : \mathcal{K}(\mathbf{Q}^{\alpha,e}) N_a dV_0^e, \quad (\text{B.69})\end{aligned}$$

whereas, in the temperature formulation (B.8), it becomes

$$\begin{aligned}\delta Q_{\text{dis}}^{\Theta,e}(\boldsymbol{\varphi}^e, \Theta^e, \boldsymbol{\Lambda}^{\alpha,e}, N_a \delta \Theta_a) &= \delta \Theta_a \int_{\mathcal{B}_0^e} \frac{1}{c} \dot{\mathcal{D}}^e N_a dV_0^e \\ &\quad + \delta \Theta_a \int_{\mathcal{B}_0^e} \frac{1}{c} \mathcal{H}_d^e N_a dV_0^e \quad (\text{B.70})\end{aligned}$$

with

$$\mathcal{H}_d^e = \sum_{\alpha=1}^m \mathbf{W}^{\alpha,e} : \mathcal{K}(\mathbf{Q}^{\alpha,e}) \quad (\text{B.71})$$

Finally, the external term in the entropy case (B.9) is discretized as follows

$$\delta Q_{\text{ext}}^{\eta,e}(\eta^e, N_a \delta \eta_a) = \delta \eta_a \int_{\mathcal{B}_0^e} \frac{1}{\Theta^e} \mathcal{R} N_a dV_0^e + \delta \eta_a \int_{\partial \mathcal{B}_0^e} \frac{1}{\Theta^e} H_N N_a dA_0^e, \quad (\text{B.72})$$

whereas, in the temperature one (B.10), is

$$\delta Q_{\text{ext}}^{\Theta,e}(\Theta^e, N_a \delta \Theta_a) = \delta \Theta_a \int_{\mathcal{B}_0^e} \frac{1}{c} \mathcal{R} N_a dV_0^e + \delta \Theta_a \int_{\partial \mathcal{B}_0^e} \frac{1}{c} H_N N_a dA_0^e \quad (\text{B.73})$$

Then, each of the above contributions are regrouped and assembled in the same way as was performed for the linear momentum balance to arrive at the discretized energy balance formulated either in entropy or in temperatures variables

$$\begin{aligned} \delta Q^s(\boldsymbol{\varphi}, \mathbf{p}, \eta, \boldsymbol{\Lambda}^\alpha, N_a \delta \eta_a) &= \sum_{\substack{e=1 \\ e \ni a}}^{m_a} \delta Q^s(\boldsymbol{\varphi}^e, \mathbf{p}^e, s^e, \boldsymbol{\Lambda}^{\alpha,e}, N_a \delta \eta_a) \\ &= \sum_{\substack{e=1 \\ e \ni a}}^{m_a} \delta s_a (\mathbf{J}_a^e + \mathbf{Q}_a^e + \mathbf{D}_a^e - \mathbf{G}_a^e), \end{aligned} \quad (\text{B.74})$$

where $\mathbf{J}_a^e$ is the inertial-like equivalent nodal heat, $\mathbf{Q}_a^e$ is the equivalent nodal heat, $\mathbf{D}_a^e$ is the dissipated equivalent nodal heat and $\mathbf{G}_a^e$ is the external equivalent nodal heat.

B.2.4 Discretization of the linearized evolution equations

The linearization of discretized evolution equation of linear momentum and energy can be derived from the discretized form of the evolution equations presented in the previous subsection and following (B.11) and (B.12), such that

$$\begin{aligned} D\delta W^e(\boldsymbol{\varphi}, \mathbf{p}, s, \boldsymbol{\Lambda}^\alpha, N_a \delta \mathbf{v}_a)[N_b \mathbf{u}_b] &= D(\delta \mathbf{v}_a \cdot (\mathbf{I}_a^e + \mathbf{T}_a^e - \mathbf{F}_a^e))[N_b \mathbf{u}_b] \\ &= \delta \mathbf{v}_a \cdot D(\mathbf{I}_a^e + \mathbf{T}_a^e - \mathbf{F}_a^e)[N_b \mathbf{u}_b] \quad (\text{B.75}) \\ &= \delta \mathbf{v}_a \cdot \mathbf{M}_{ab}^e \ddot{\mathbf{u}}_b + \delta \mathbf{v}_a \cdot \mathbf{K}_{ab}^e \mathbf{u}_b \end{aligned}$$

$$\begin{aligned} D\delta W^e(\boldsymbol{\varphi}, \mathbf{p}, s, \boldsymbol{\Lambda}^\alpha, N_a \delta s_a)[N_b t_b] &= D(\delta s_a (\mathbf{I}_a^e + \mathbf{T}_a^e - \mathbf{F}_a^e))[N_b t_b] \\ &= \delta s_a D(\mathbf{T}_a^e)[N_b t_b] \quad (\text{B.76}) \\ &= \delta s_a \mathbf{S}_{ab}^e t_b \end{aligned}$$

$$\begin{aligned} D\delta Q^e(\boldsymbol{\varphi}, \mathbf{p}, s, \boldsymbol{\Lambda}^\alpha, N_a \delta s_a)[N_b t_b] &= D(\delta s_a (\mathbf{J}_a^e + \mathbf{Q}_a^e + \mathbf{D}_a^e - \mathbf{G}_a^e))[N_b t_b] \\ &= \delta s_a D(\mathbf{J}_a^e + \mathbf{Q}_a^e + \mathbf{D}_a^e - \mathbf{G}_a^e)[N_b t_b] \\ &= \delta s_a \mathbf{C}_{ab}^e \dot{t}_b + \delta s_a \mathbf{Q}_{ab}^e t_b + \delta s_a \mathbf{D}_{ab}^e t_b \quad (\text{B.77}) \end{aligned}$$

$$\begin{aligned}
D\delta Q^e(\boldsymbol{\varphi}, \mathbf{p}, s, \boldsymbol{\Lambda}^\alpha, N_a \delta s_a)[N_b \mathbf{u}_b] &= D(\delta s_a(\mathbf{J}_a^e + \mathbf{Q}_a^e + \mathbf{D}_a^e - \mathbf{G}_a^e))[N_b \mathbf{u}_b] \\
&= \delta s_a D(\mathbf{J}_a^e + \mathbf{Q}_a^e + \mathbf{D}_a^e - \mathbf{G}_a^e)[N_b \mathbf{u}_b] \\
&= \delta s_a \mathbf{C}_{ab}^e \cdot \mathbf{u}_b + \delta s_a \mathbf{P}^e \cdot \mathbf{u}_b + \delta s_a \mathbf{L}^e \cdot \mathbf{u}_b
\end{aligned} \tag{B.78}$$

Similar procedures as those carried out in the previous subsection allow to obtain the expressions for the arising quantities. Then, the classical example of the linearization of the inertial terms leads to the definition of the mass matrix according to

$$\begin{aligned}
D\delta W_{\text{ine}}^e(\mathbf{p}, N_a \delta \mathbf{v}_a)[N_b \mathbf{u}_b] &= \int_{\mathcal{B}_0} N_a \delta \mathbf{v}_a \cdot \rho_0 N_b \ddot{\mathbf{u}}_b dV_0 \\
&= \delta \mathbf{v}_a \cdot \int_{\mathcal{B}_0} \rho_0 N_a N_b dV_0 \ddot{\mathbf{u}}_b
\end{aligned} \tag{B.79}$$

Similarly, the expression for the stiffness matrix can be obtained. For the inertial-like term of the energy balance, a similar matrix arose, that is

$$D\delta Q_{\text{ine}}^{s,e}(N_a \delta s_a)[N_b s_b] = \int_{\mathcal{B}_0} N_a \delta s_a N_b \dot{s}_b dV_0^e = \delta s_a \int_{\mathcal{B}_0} N_a N_b dV_0^e \dot{s}_b \tag{B.80}$$

Finally, as an example, the matrix $\mathbf{Q}^e$ is derived for the entropy formulation

$$\begin{aligned}
D\delta Q_{\text{int}}^{\eta,e}(\boldsymbol{\varphi}^e, \eta^e, N_a \delta \eta_a)[N_b s_b] &= \delta \eta_a \int_{\mathcal{B}_0} \nabla_0 N_a \cdot \mathbf{K}^e \nabla_0 \left[\frac{\partial \Theta}{\partial \eta} \right] N_b dV_0 s_b \\
&+ \delta \eta_a \int_{\mathcal{B}_0} k'(\Theta^e) \frac{\partial \Theta^e}{\partial \eta^e} \nabla_0 N_a \cdot [J \mathbf{C}^{e,-1} \nabla_0 \Theta^e] dN_b V_0 s_b
\end{aligned} \tag{B.81}$$

where, as in the discretized energy balance, the appearing material gradients must be computed according to (B.65) - (B.67) with

$$\nabla_0 \left[\frac{\partial \Theta}{\partial \eta} \right] = \frac{\partial^2 \Theta}{\partial \eta \partial \mathbf{C}} : \nabla_0 \mathbf{C} + \frac{\partial^2 \Theta}{\partial \eta^2} \nabla_0 \eta + \frac{\partial^2 \Theta}{\partial \eta \partial \boldsymbol{\Lambda}^\alpha} : \nabla_0 \boldsymbol{\Lambda}^\alpha \tag{B.82}$$

Once each of the contributions has been computed, the global matrices are obtained by performing the classical assembly.

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