

Université de Liège  
Faculté des Sciences Appliquées

**Development of non-linear  
Electro-Thermo-Mechanical Discontinuous  
Galerkin formulations**

Thèse présentée par

**Lina Homsy**

(Master en Sciences Appliquées) pour l'obtention du grade légal de

Docteur en Sciences de l'ingénieur  
Année académique 2016-2017

Université de Liège - Computational & Multiscale Mechanics of Materials (CM3)- Bât.  
B52/3

Quartier Polytech 1, Allée de la Découverte 9, B-4000 Liège 1, Belgique

Tél +32-4-3669125 - Fax +32-4-3669217

Email : lina.homsy@ulg.ac.be, eng.linahomsy@gmail.com



# Acknowledgment

This project has been funded with support of the European Commission. This publication reflects the view only of the author, and the Commission can not be held responsible for any use which may be made of the information contained therein.

*I gratefully acknowledge for the funding I received toward my PhD from EPIC (Erasmus Mundus)*

*I would like to express my gratitude to my thesis supervisor, Dr. L. Noels, an advisor that everyone would hope for. He provided me with an opportunity to work under his excellent guidance, I appreciate all the effort, teach and ideas throughout my PhD, which encouraged me to accomplish the goals of this research work. I am more than grateful.*

*Another big thanks goes to Dr. J. P. Ponthot, Dr. C. Geuzaine, Dr. E. Bechet, Dr. J. F. Remacle, and Dr. N. Chevaugeron for being in my thesis committee and for the time they gave to review and evaluate my thesis.*

*Special thanks to Nicolas de Hennin, for the trust that he gave me when he did the 'prise en charge, even though he doesn't know me.*

*I would like to give thank officemates Cristian, Gaetan, Philippe, and Dominik for the great atmosphere in the office and just for being such a nice guys. The presence of some people is gratuitously acknowledged, just for making my everyday life a bit nicer. In particular, I would like to thank Van Dung, Cristian, Christophe, Laura, Vladimir, Paulo, Isma , Kahdija, and Mouhamed for all the help, you are as sisters and brothers to me, I really appreciate. I am also thankful to the CM3 research group and all my colleagues who I shared with them very nice and valuable time. I would like to acknowledge Nema, Diana, Nina, Fadi, Iman, Joelle, Eyad for their share, help and support in various moments. Without you I would not be able to push myself to finish this work.*

*I would like to thank my family mom, dad, Dima (Jala and my adorable nieces Christa and Mierella), George (Dana), and Fadi for their encouragement and support. I love you so much and I feel very fortunate for having you in my life.*



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# Chapter 1

## Introduction

Shape Memory Polymers (SMP) are those unique materials that have the ability to memorize a macroscopic shape, in other words, to change shape and to recover the original shape. SMP can fix a temporary deformed configuration and recover their initial shape upon application of a stimulus such as temperature [36], light [38], electric field [18], magnetic field [65], water [31] and solvent [49]. Additional information about the different kinds of stimuli can be found in [9, 52]. These polymers take advantage of a property change at the glass transition temperature  $T_g$ . Below  $T_g$ , the movement of the polymer segments are frozen and the polymers are considered to be in a glassy state. Once they are heated above  $T_g$  the chains become weak and the polymers are considered to be in a rubbery state, such that the materials can be deformed with minimal force. Shape Memory Polymers are capable of large deformations (high recovery strain), which are essential for applications where storage space is critical. Structures can be folded in a compact phase and then they can recover their shape, because of an external stimulus. In addition they have other advantages such as low density, low cost, and easy processability.

However, SMP have the drawback of low strength and stiffness when they are used for structural applications. This drawback can be overcome by dispersing (distributing) continuous or discontinuous reinforcements throughout a polymer matrix, leading to Shape Memory Polymer Composites (SMPC). Meng et al. [53] have clarified that the aim of SMPC is to improve the shape memory recovery stress and the mechanical properties in addition to act as triggering mechanisms under light, moisture, electricity, or magnetic field, but also to tune the transition temperature. In particular, the kinds of reinforcement that we are interested in are nanowires, carbon nanotubes, and continuous carbon fibers dispersed throughout a shape memory polymer which results in composite materials with high stiffness and strength to weight ratios. The polymer matrix indeed avoids catastrophic failure due to fiber breaking, and the existence of the carbon fibers enhances strength and stiffness. Moreover, carbon fibers exhibit conductivity which can be exploited as a shape memory triggering mechanism. The range of composite material electrical conductivity can be controlled by the amount of carbon fibers, and the increase of temperature required to trigger the Shape Memory effect is obtained through Joule effect by applying an electric current, which makes them favorable and meet the particular requirements for many applications in which applying an external heat is difficult. Henceforth SMPC are the prime candidate materials for the area of deployable space structures (intelligent structures). A review con-

cerning polymer composites and conductive polymers under the scope of a thermoelectric application and the evaluation of their figure of merit along the last years have been reported by Culebras et al. [15], in which the improvement of the thermoelectric properties of polymers mixed with graphite/graphene, carbon nanotubes, or inorganic thermoelectric nanoparticles has been studied. Characterization, fabrication, and modeling of SMP and SMPC, in addition to their potential applications across a wide variety of fields from outer space to automobile actuators have been extensively described by Leng et al. [39], see Pilate et al. [59] as well for more applications. In particular, Yu et al. [78] have suggested to incorporate shape memory polymer with carbon nanotubes and short carbon fibers, because the existence of carbon nanotubes alone could decrease the elastic modulus and the stretch of the materials. They have shown experimentally the enhancement of the electrical, thermal, and shape memory properties of the conductive SMP composites, as the addition of the short carbon fibers has increased the electrical conductivity by 1000 times in comparison with carbon nanotubes alone when the same amount of the fillers are used. Besides, they have shown that this kind of SMPC is able to recover 98% in comparison to its original shape. It should be noted that continuous carbon fiber reinforced SMP shows an improvement in the mechanical properties related to stiffness and strength and this makes them good candidates for applications where structural stiffness is required, contrarily to particles or short fibers reinforced composites [35, 40].

The aforementioned studies and many other ones [19, 41, 53, 78] have shown the potential of SMP reinforced by fibers to be used for the spacecraft self-deployment devices such as antennas, hinge, trusses, boom, reflector, solar array, morphing skin, and vibration control devices. A good example is the prototype of solar array deployed by means of a SMPC hinge proposed by Lan et al. [35]. This panel can be compacted on earth, stored in a compacted shape, and then self deployed in space. The hinge is heated above glass transition temperature  $T_g$  by applying an electric potential of 20 [V], then it is bent to  $90^\circ$  by applying an external force at soft state, cooled while constrained to a room temperature, afterward reheated by applying the same electric potential again which causes the deployment of the prototype of the solar array, as shown in Fig. 1.1.

Many experimental studies for conductive shape memory polymer composites actuated by Joule heating have been explored by many researchers [18, 35, 42, 45, 46, 47, 48]. However, the Electro-Thermo-Mechanical coupled large deformation constitutive theory and numerical simulations for such behaviors are not wide spread, although it is useful to reduce the number of expensive experimental tests. In this work, a multi-field coupling resolution strategy is used for the resolution of electrical, energy, and momentum conservation equations by means of the Discontinuous Galerkin Finite Element Method (DGFEM) to solve the various interacting physics and coupled simulations.

The main idea of the Discontinuous Galerkin (DG) formalism is to constrain weakly the compatibility between elements, on the contrary to classical FEM. In this case, the solution is approximated by piece-wise continuous polynomial functions, which allows using discontinuous polynomial spaces of high degree and facilitate handling elements of different types and dynamic mesh modifications. Indeed, the possibility of using irregular and non conforming meshes in an algorithm makes it suitable for time dependent transient problems. They also allow having hanging nodes and different polynomial degrees at the interface, with a view to hp-adaptivity. In addition, since the DG method allows discontinuities of the physical unknowns within the interior of the problem domain, it is a natural approach

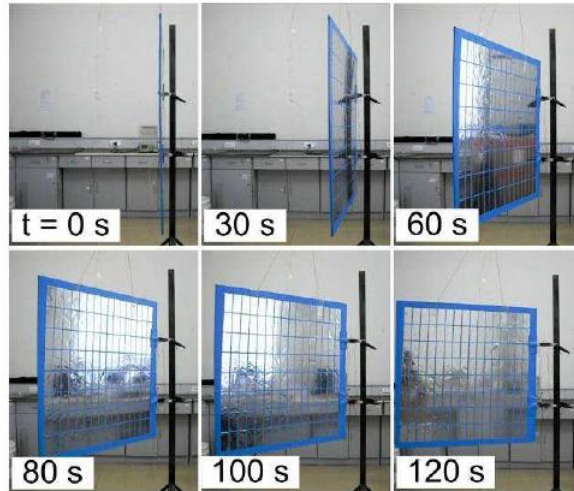


Figure 1.1: Shape recovery process of a prototype of solar array actuated by SMPC hinge [35]

to capture the jumps across the material interface in coupled problems. Above all, DG methods are also characterized by their flexibility in terms of mesh design while keeping their high order accuracy [29] and their high scalability in parallel simulations while optimal convergence rates are still achieved.

However, if not correctly formulated, discontinuous methods can exhibit instabilities, and the numerical results fail to approximate the exact solution. It is, therefore, important to have methods available which lead to reliable results for a wide variety of problems. By using an adequate inter element flux definition combined to stabilization techniques, the shortcomings of non-stabilized DG methods can be overcome [56, 60, 63].

Since the seminal work of Reed et al. [62], DG methods have been developed to solve hyperbolic, parabolic, and elliptic problems. The state of the art of DG methods and their developments can be found in [14]. Most of DG methods for elliptic and parabolic problems rely on the Interior Penalty (IP) method. The main principle of IP, as introduced in [16, 74], is to constrain weakly the compatibility instead of building it into the finite element which enables the use of discontinuous polynomial spaces of high degree. The interest in the symmetric interior penalty (SIPG) methods, which will be considered in this work, has been renewed by Wheeler [74] due to demands for optimality of convergence rates with the mesh size  $h_s$  (i.e., the rates of the convergence is  $k$  in the  $H^1$ -norm and  $k + 1$  in the  $L^2$ -norm, where  $k$  is the polynomial approximation degree). However there exist other possible choices of traces and numerical fluxes as discussed by Arnold et al. [5], who have provided an analysis of a large class of discontinuous methods for second order elliptic problems with different numerical fluxes, and demonstrated that correctly formulated IP, NIPG (Non-Symmetric Interior Penalty), LDG (Local discontinuous Galerkin), and other DG methods are consistent and stable methods. In particular Arnold et al. [5] have proposed a framework for dealing with linear elliptic problems by means of DG methods and demonstrated that DG methods which are completely consistent and stable achieve optimal error estimates, and that the inconsistent DG methods like the pure penalty methods can still achieve optimal error estimates provided they are super-penalized. Besides, Georgoulis [21] has derived

anisotropic hp-error bounds for linear second order elliptic diffusion convection reaction using Discontinuous Galerkin finite element method (SIPG and NIPG), on shape-regular and anisotropic elements, and for isotropic and anisotropic polynomial degrees for the element bases. He has also observed optimal order of convergence in the  $L^2$ -norm for the SIPG formulation when a uniform mesh size refinement for different values of  $k$  is employed. Moreover, he has shown that the solution of the adjoint problem suffers from sub-optimal rates of convergence when a NIPG formulation is used. Yadav et al. [76] have extended the DG methods from a linear self-adjoint elliptic problem to a second order nonlinear elliptic problem. The nonlinear system resulting from DG methods is then analyzed based on a fixed point argument. They have also shown that the error estimate in the  $L^2$ -norm for piece-wise polynomials of degree  $k \geq 1$  is  $k + 1$ . They have also provided numerical results to illustrate the theoretical results. Gudi [24] has proposed an analysis for the most popular DG schemes such as SIPG, NIPG, and LDG methods for one dimension linear and nonlinear elliptic problems, and the error estimate has been studied for each of these methods by reformulating the problems in a fixed point form. In addition, according to Gudi [24], optimal errors in the  $H^1$ -norm and in  $L^2$ -norm are proved for SIPG for polynomial degrees larger or equal to 2, and a loss in the optimality in the  $L^2$ -norm is observed for NIPG and LDG. In that work a deterioration in the order of convergence in the mesh size  $h_s$  is noted when linear polynomials are used.

Recently, DG has been used to solve coupled problems. For instance Wheeler and Sun [69] have proposed a primal DG method with interior penalty (IP) terms to solve coupled reactive transport in porous media. In that work, a cut-off operator is used in the DG scheme to treat the coupling and achieve convergence. They have declared that optimal convergence rates for both flow and transport terms can be achieved if the same polynomial degree of approximation is used. However if they are different, the behavior for the coupled system is controlled by the part with the lowest degree of approximation, and the error estimate in the  $L^2(H^1)$ -norm is nearly optimal in  $k$  with a loss of  $\frac{1}{2}$  when polynomials with different degrees are used. Furthermore, Zheng et al. [79] have proposed a DG method to solve thermo-elastic coupled problems due to temperature and pressure dependent thermal contact resistance. In that work the DG method is used to simulate the temperature jump, and the mechanical sub-problem is solved by the DG finite element method with a penalty function.

The main aim of this work is to derive a consistent and stable Discontinuous Galerkin (DG) method for Electro-Thermo-Mechanical coupling analyzes, which to the authors knowledge, has not been introduced yet. The constitutive equations governing Electro-Thermo-Mechanical coupling can be formulated as a function of the displacement  $\mathbf{u}$ , the electric potential  $V$  and the temperature  $T$ , in particular under the form  $f(\mathbf{u}, \frac{-V}{T}, \frac{1}{T})$ . Such a formulation for Electro-Thermal coupling, without the mechanical contribution has been considered in the literature, e.g. Mahan [51], Yang et al. [77], Liu [43], in order to obtain a conjugated pair of fluxes and fields gradient. Mahan [51] has provided a comparison between the different energy fluxes that have been developed and used by different researchers and concluded that all these different treatments result in the same equation. We have extended this energy consistent formulation to Electro-Thermo-Mechanics and by this way we are able to derive a consistent Discontinuous Galerkin (DG) method and its numerical properties for Electro-Thermo-Elasticity. The main advantage of this work is the aptitude to deal with arbitrary geometry and the capability of the formulation to capture the Electro-Thermo-Mechanical behavior for composite materials with high contrast: one phase has a

high electric conductivity (e.g., carbon fiber) and other is a resistible material (e.g., polymers). Moreover, another objective of this study is to investigate the response of carbon fiber reinforced shape memory polymer composites when an electric power is applied. For that a micromechanical model of unidirectional carbon fibers embedded in a shape memory polymer matrix is formulated considering the interaction of electrical, thermal, and mechanical fields. It is then solved using the DG method to determine the time dependent response of the Electro-Thermo-Mechanical shape memory polymer composites and to determine the effective properties and quantify the variation of the fields in the large deformation regime, when they are actuated by a low electric power.

This work is structured as follows

- Chapter 2, general properties of the finite element method and Hilbert spaces, describes the general properties that will be needed for deriving the numerical properties of DG formulation in the following three chapters, and defines the function spaces and the norms that will be considered.
- Chapter 3, a coupled Linear Thermo-Elasticity Discontinuous Galerkin method, focuses on the governing equations of Linear Thermo-Elasticity coupling and the derivation of a Discontinuous Galerkin (DG) finite element method. Next some theoretical results on the stability and uniqueness of the solution for this problem are presented, followed by the error analysis and numerical tests verification of the theoretical study.
- Chapter 4, a coupled Electro-Thermal Discontinuous Galerkin method, introduces Electro-Thermal coupling and its application. Then the chapter describes the governing equations of Electro-Thermal materials. An alternative weak form in terms of energetically conjugated fields gradients and fluxes is proposed. This weak form is then discretized using the Discontinuous Galerkin method, resulting in a particular choice of the test functions ( $\delta f_T = \delta(\frac{1}{T}), \delta f_V = \delta(\frac{-V}{T})$ ) and of the trial functions ( $f_T = \frac{1}{T}, f_V = \frac{-V}{T}$ ), where  $T$  is the temperature and  $V$  is the electric potential. This allows us to develop a DG formulation for nonlinear Electro-Thermo coupled problems. The numerical properties of the DG method are demonstrated, based on rewriting the nonlinear formulation in a fixed point form [34]. The numerical properties of the nonlinear elliptic problem, i.e. the consistency and the uniqueness of the solution are demonstrated, and the prior error estimates are shown to be optimal in the mesh size for polynomial approximation degrees  $k > 1$  for the energy-norm and  $L^2$ -norm (respectively in order  $k$  and  $k + 1$ ). Eventually several examples of applications in one, two, and three dimensions are provided for homogeneous and composite materials, in order to verify the accuracy and effectiveness of the Electro-Thermal DG formulation and to illustrate the algorithm properties.
- Chapter 5, a coupled Electro-Thermo-Mechanical Discontinuous Galerkin method, is developed considering the interaction of electrical, thermal, and mechanical fields. The DG method is formulated in finite deformations and finite fields variations, resulting into a set of non-linear equations. The DG method is implemented within a three-dimensional finite element code. Afterwards, the uniqueness and optimal numerical properties are derived for Electro-Thermo-Elasticity stated in a small deformation setting. In particular, the convergence rates of the error in both the energy and  $L^2$ -norms are shown to be optimal with respect to the mesh size in terms of the polynomial

degree approximation  $k$  (respectively in order  $k$  and  $k + 1$ ). This chapter concludes with some numerical tests supporting the developed theory. Moreover a unit cell of composite microstructures corresponding to periodically distributed carbon fibers in a polymer matrix is considered to clarify the Electro-Thermo-Mechanical behavior of composite materials.

- Chapter 6, the constitutive law of composite materials, presents details of two models that are used to describe the carbon fiber and shape memory polymer behaviors. A simple transversely isotropic hyperelastic formulation is used to model carbon fiber in the fully nonlinear range, and an Elasto-viscoplastic large deformation constitutive model is used for the shape memory polymers. These constitutive models are applied in simulating the behavior of SMPC unit cells in the large deformation regime, when it is actuated by a direct heat or low electric power.
- Chapter 7, the conclusions with future perspectives, contains some final comments regarding this work and some possible future directions of research.

The publications related to the thesis are

- L. Homsı, C. Geuzaine, L. Noels. Numerical properties of a discontinuous Galerkin fomulation for electro-thermal coupled problems. Proceedings of the 7th European Congress on Computational Methods in Applied Sciences and Engineering. Volume 2, 2016, 2558-2565.
- L. Homsı, C. Geuzaine, L. Noels, A coupled electro-thermal discontinuous Galerkin method. Journal of Computational Physics, 2017. (Minor revision)
- L. Homsı, L. Noels. A discontinuous Galerkin method for non-linear electro-thermo-mechanical problems; application to shape memory composite materials, *Meccanica*, submitted, 2017

## Chapter 2

# General properties of the finite element method and Hilbert spaces

### 2.1 Introduction

In this chapter, short introductions about the Sobolev space and Hilbert space in addition to the definitions of the norms and the main approximation properties, which will be used in the error analysis of the Discontinuous Galerkin Finite element method for linear and non-linear coupled problems, are presented without proofs.

### 2.2 Finite element partition

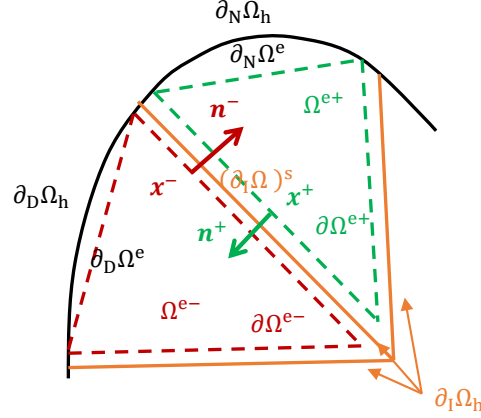
Let the body  $\Omega \in \mathbb{R}^d$ , with  $d = 2$  or  $3$  the space dimension, be approximated by a discretized body  $\Omega_h$  such that  $\Omega \approx \Omega_h = \cup_e \Omega^e$ , where a finite element in  $\Omega_h$  is denoted by  $\Omega^e$ . The boundary  $\partial\Omega_h$  is decomposed into a region of Dirichlet boundary  $\partial_D\Omega_h$ , and a region of Neumann boundary  $\partial_N\Omega_h$ . The intersecting boundary of the finite elements is denoted by  $\partial_I\Omega_h = \cup_e \partial\Omega^e \setminus \partial\Omega_h$  as shown in the Fig. 2.1, with  $\partial_N\Omega_h = \cup_e \partial_N\Omega^e$ ,  $\partial_D\Omega_h = \cup_e \partial_D\Omega^e$ ,  $\partial\Omega_h \cup \partial_I\Omega_h = \cup_e \partial\Omega^e$ , and  $\partial_I\Omega^e = \partial\Omega^e \cap \partial_I\Omega_h$ .

Within this finite element discretization, an interior face  $(\partial_I\Omega)^s = \partial\Omega^{e+} \cap \partial\Omega^{e-}$  is shared by elements  $\Omega^{e+}$  and  $\Omega^{e-}$ , and  $\mathbf{n}^-$  is the unit normal vector pointing from element  $\Omega^{e-}$  toward element  $\Omega^{e+}$ , see Fig. 2.1. Similarly, an exterior Neumann edge  $(\partial_N\Omega)^s = \partial\Omega^e \cap \partial_N\Omega_h$  is the intersection between the boundary of the element  $\Omega^e$ , an exterior Dirichlet edge  $(\partial_D\Omega)^s = \partial\Omega^e \cap \partial_D\Omega_h$  is the intersection between the boundary of the element  $\Omega^e$  and  $(\partial_{DI}\Omega)^s$  is a face either on  $\partial_I\Omega_h$  or on  $\partial_D\Omega_h$ , with  $\sum_s (\partial_{DI}\Omega)^s = \partial_I\Omega_h \cup \partial_D\Omega_h$ . Finally  $\mathbf{n}^- = \mathbf{n}$  is used to represent the outward unit normal vector of the external boundary  $\partial\Omega_h$ .

In this work, we assume a constant mesh size on the elements, but the theory can be generalized by considering bounded element sizes such as in [24]. We assume the discretization is shaped with a regular mesh of size  $h_s$  defined as  $\frac{|\Omega^e|}{|\partial\Omega^e|}$ . We also assume shape regularity of  $\Omega_h$  so that there exist constants  $c_1, c_2, c_3$  and  $c_4$ , independent of  $h_s$ , such that

$$\begin{aligned} c_1 \text{diam}((\partial_I\Omega)^s) &\leq h_s \leq c_2 \text{diam}((\partial_I\Omega)^s), \text{ and} \\ c_3 \text{diam}(\Omega^e) &\leq h_s \leq c_4 \text{diam}(\Omega^e), \end{aligned} \tag{2.1}$$

where  $(\partial_I\Omega)^s$  is a face between elements.

Figure 2.1: interface between two elements ( $\Omega^{e+}$ ) and ( $\Omega^{e-}$ )

### 2.3 Discontinuous Finite Element spaces

Let us define a vector  $\mathbf{O} = \begin{pmatrix} O_1 \\ \vdots \\ O_n \end{pmatrix}$  of size  $n$ , then let us now recall the Sobolev space

$W_r^s(\Omega)$ , with  $s$  a non-negative integer and  $r \in [1, \infty[$ , the subspace of all functions from the norm  $L^r(\Omega)$  whose generalized derivatives up to order  $s$  exist and belong to  $L^r(\Omega)$ , which is defined as

$$W_r^s(\Omega) = \{\mathbf{O} \in (L^r(\Omega))^n, \partial^\alpha \mathbf{O} \in (L^r(\Omega))^n; \forall |\alpha| \leq s, s \geq 1\}. \quad (2.2)$$

When  $r = 2$ , the spaces are Hilbert spaces:  $W_2^s(\Omega) = (H^s(\Omega))^n$ , and for  $s = 0$ , the space is the  $L^2$  space:  $(H^0(\Omega))^n = (L^2(\Omega))^n$ .

Furthermore in order to account for the discontinuity in  $\mathbf{O}$ , we can define the associated norm of the standard broken Sobolev space  $W_r^s(\Omega_h)$  of order  $s$  and exponent  $r$  with  $1 \leq r < \infty$ . Starting from the Sobolev space norm and semi norm

$$\begin{cases} \|\mathbf{O}\|_{W_r^s(\Omega^e)} &= \left( \sum_{|\alpha| \leq s} \int_{\Omega^e} \|\partial^\alpha O_1\|(\mathbf{x})\|^r d\mathbf{x} + \dots + \sum_{|\alpha| \leq s} \int_{\Omega^e} \|\partial^\alpha O_n\|(\mathbf{x})\|^r d\mathbf{x} \right)^{\frac{1}{r}}, \\ |\mathbf{O}|_{W_r^s(\Omega^e)} &= \left( \int_{\Omega^e} \|\partial^s O_1\|(\mathbf{x})\|^r d\mathbf{x} + \dots + \int_{\Omega^e} \|\partial^s O_n\|(\mathbf{x})\|^r d\mathbf{x} \right)^{\frac{1}{r}}, \end{cases} \quad (2.3)$$

the norm and semi norm of the broken Sobolev space read

$$\begin{cases} \|\mathbf{O}\|_{W_r^s(\Omega_h)} &= \left( \sum_e \|\mathbf{O}\|_{W_r^s(\Omega^e)}^r \right)^{\frac{1}{r}}, \\ |\mathbf{O}|_{W_r^s(\Omega_h)} &= \left( \sum_e |\mathbf{O}|_{W_r^s(\Omega^e)}^r \right)^{\frac{1}{r}}. \end{cases} \quad (2.4)$$

For the case  $r = \infty$ , the norm is defined as

$$\|\mathbf{O}\|_{W_\infty^s(\Omega_h)} = \max_e \|\mathbf{O}\|_{W_\infty^s(\Omega^e)}. \quad (2.5)$$



As the finite element space consists of discontinuous elements, the unknown field  $\mathbf{O}$  does not belong to  $H^s(\Omega_h)$  but in the following piecewise broken Sobolev space

$$X_s = \left\{ \mathbf{O} \in (L^2(\Omega_h))^n \mid \mathbf{O}|_{\Omega^e} \in (H^s(\Omega^e))^n \quad \forall \Omega^e \in \Omega_h \right\}. \quad (2.6)$$

We can now define the following broken Sobolev spaces  $X$ , particularized for  $s = 2$ , by

$$X = \left\{ \mathbf{O} \in (L^2(\Omega_h))^n \mid \mathbf{O}|_{\Omega^e} \in (H^2(\Omega^e))^n \quad \forall \Omega^e \in \Omega_h \right\}, \quad (2.7)$$

and

$$Y = \left\{ \nabla \mathbf{O} \in \left( (L^2(\Omega_h))^d \right)^n \mid \nabla \mathbf{O}|_{\Omega^e} \in (H^{s-1}(\Omega^e))^n \quad \forall \Omega^e \in \Omega_h \right\}. \quad (2.8)$$

We define the discontinuous manifolds on the polynomial approximation by

$$X^k = \left\{ \mathbf{O}_h \in (L^2(\Omega_h))^n \mid \mathbf{O}_h|_{\Omega^e} \in (\mathbb{P}^k(\Omega^e))^n \quad \forall \Omega^e \in \Omega_h \right\}, \quad (2.9)$$

where  $\mathbb{P}^k(\Omega^e)$  is the space of polynomial functions of order up to  $k$ .

At the interface between two elements, Fig. 2.1, each interior edge  $(\partial_1 \Omega)^s$  is shared by two elements  $-$  and  $+$ , where  $(\partial_1 \Omega)^s \subset \partial_1 \Omega^{e^-}$  and  $(\partial_1 \Omega)^s \subset \partial_1 \Omega^{e^+}$ . We can thus define two useful operators, the jump operator  $[[\cdot]] = [\bullet^+ - \bullet^-]$  that computes the discontinuity between the elements and the average operators  $\langle \cdot \rangle = \frac{1}{2}(\bullet^+ + \bullet^-)$  which is the mean between two element values. Those two operators can be extended on the Dirichlet boundary  $\partial_D \Omega_h$  as  $\langle \bullet \rangle = \bullet$ ,  $[[\bullet]] = (-\bullet)$ .

Let us define the mesh dependent norms, which will be considered in the following analysis, for  $\mathbf{O} \in X$

$$||| \mathbf{O} |||_*^2 = \sum_e \|\nabla \mathbf{O}\|_{L^2(\Omega^e)}^2 + \sum_e h_s^{-1} \|[[\mathbf{O}_n]]\|_{L^2(\partial \Omega^e)}^2, \quad (2.10)$$

$$||| \mathbf{O} |||^2 = \sum_e \|\mathbf{O}\|_{H^1(\Omega^e)}^2 + \sum_e h_s^{-1} \|[[\mathbf{O}_n]]\|_{L^2(\partial \Omega^e)}^2, \quad (2.11)$$

and

$$||| \mathbf{O} |||_1^2 = \sum_e \|\mathbf{O}\|_{H^1(\Omega^e)}^2 + \sum_e h_s \|\mathbf{O}\|_{H^1(\partial \Omega^e)}^2 + \sum_e h_s^{-1} \|[[\mathbf{O}_n]]\|_{L^2(\partial \Omega^e)}^2, \quad (2.12)$$

with  $\partial \Omega^e = \partial_1 \Omega^e \cup \partial_D \Omega^e$  and  $\mathbf{O}_n = \begin{pmatrix} \mathbf{n}^- & \mathbf{0} \dots \mathbf{0} \\ \vdots \\ \mathbf{0} & \mathbf{0} \dots \mathbf{n}^- \end{pmatrix}_{3n \times n} \mathbf{O}$ .

## 2.4 Finite element properties

First we discuss some inequalities for future use.

**Lemma 2.4.1** (Interpolant inequality). *For all  $\mathbf{O} \in (H^s(\Omega^e))^n$  there exists a sequence  $\mathbf{O}^h \in (\mathbb{P}^k(\Omega^e))^n$  and a positive constant  $C_{\mathcal{D}}^k$  depending on  $s$  and  $k$  but independent of  $\mathbf{O}$  and  $h_s$ , such that*

1. for any  $0 \leq n \leq s$

$$\| \mathbf{O} - \mathbf{O}^h \|_{H^n(\Omega^e)} \leq C_{\mathcal{D}}^k h_s^{\mu-n} \| \mathbf{O} \|_{H^s(\Omega^e)}, \quad (2.13)$$

2. for any  $0 \leq n \leq s - 1 + \frac{2}{r}$

$$\| \mathbf{O} - \mathbf{O}^h \|_{W_r^n(\Omega^e)} \leq C_{\mathcal{D}}^k h_s^{\mu-n-1+\frac{2}{r}} \| \mathbf{O} \|_{H^s(\Omega^e)} \text{ if } d = 2, \quad (2.14)$$

3. for any  $s > n + \frac{1}{2}$

$$\| \mathbf{O} - \mathbf{O}^h \|_{H^n(\partial\Omega^e)} \leq C_{\mathcal{D}}^k h_s^{\mu-n-\frac{1}{2}} \| \mathbf{O} \|_{H^s(\Omega^e)}, \quad (2.15)$$

where  $\mu = \min\{s, k+1\}$ .

The proof of the first and third properties can be found in [6], then by the use of the properties (1) and (3) in Lemma 1 of [2] and the scaling argument in [3], the second property can be derived in the particular case of  $d = 2$  as demonstrated in [24].

**Remarks**

i) The approximation property in (2) is still valid for  $r = \infty$ , see [50].

ii) For  $\mathbf{O} \in X_s$ , let us define the interpolant  $I_h \mathbf{O} \in X^k$  by  $I_h \mathbf{O}|_{\Omega^e} = \mathbf{O}^h(\mathbf{O}|_{\Omega^e})$ , which means  $I_h \mathbf{O}$  satisfies the interpolant inequality property provided in Lemma 2.4.1 on  $\Omega_h$ , see [30].

**Lemma 2.4.2** (Trace inequality). *For all  $\mathbf{O} \in (H^{s+1}(\Omega^e))^n$ , there exists a positive constant  $C_{\mathcal{T}}$ , such that*

$$\| \mathbf{O} \|_{W_r^s(\partial\Omega^e)}^r \leq C_{\mathcal{T}} \left( \frac{1}{h_s} \| \mathbf{O} \|_{W_r^s(\Omega^e)}^r + \| \mathbf{O} \|_{W_{2r-2}^s(\Omega^e)}^{r-1} \| \nabla^{s+1} \mathbf{O} \|_{L^2(\Omega^e)} \right), \quad (2.16)$$

where  $s = 0, 1$  and  $r = 2, 4$ , or in other words

$$\begin{aligned} \| \mathbf{O} \|_{L^2(\partial\Omega^e)}^2 &\leq C_{\mathcal{T}} \left( \frac{1}{h_s} \| \mathbf{O} \|_{L^2(\Omega^e)}^2 + \| \mathbf{O} \|_{L^2(\Omega^e)} \| \nabla \mathbf{O} \|_{L^2(\Omega^e)} \right), \\ \| \mathbf{O} \|_{L^4(\partial\Omega^e)}^4 &\leq C_{\mathcal{T}} \left( \frac{1}{h_s} \| \mathbf{O} \|_{L^4(\Omega^e)}^4 + \| \mathbf{O} \|_{L^6(\Omega^e)}^3 \| \nabla \mathbf{O} \|_{L^2(\Omega^e)} \right). \end{aligned} \quad (2.17)$$

The first equation,  $s = 0$  and  $r = 2$ , is proved in [60], and the second one,  $r = 4$  and  $s = 0$ , is proved in [24].

**Lemma 2.4.3** (Trace inequality on the finite element space). *For all  $\mathbf{O}_h \in (\mathbb{P}^k(\Omega^e))^n$  there exists a constant  $C_{\mathcal{K}}^k > 0$  depending on  $k$ , such that*

$$\| \nabla^l \mathbf{O}_h \|_{L^2(\partial\Omega^e)} \leq C_{\mathcal{K}}^k h_s^{-\frac{1}{2}} \| \nabla^l \mathbf{O}_h \|_{L^2(\Omega^e)} \quad l = 0, 1, \quad (2.18)$$

where  $C_{\mathcal{K}}^k = \sup_{\mathbf{v} \in P_K(\Omega^e)} \frac{h_s \| \nabla \mathbf{O}_h \|_{L^2(\partial\Omega^e)}^2}{\| \nabla \mathbf{O}_h \|_{L^2(\Omega^e)}^2}$  is a constant which depends on the degree of the polynomial approximation only with  $h_s = \frac{|\Omega^e|}{|\partial\Omega^e|}$ , see [27] for more details.

**Lemma 2.4.4** (Inverse inequality). *For  $\mathbf{O}_h \in (\mathbb{P}^k(\Omega^e))^n$  and  $r \geq 2$ , there exists  $C_{\mathcal{I}}^k > 0$ , such that*

$$\| \mathbf{O}_h \|_{L^r(\Omega^e)} \leq C_{\mathcal{I}}^k h_s^{\frac{d}{r} - \frac{d}{2}} \| \mathbf{O}_h \|_{L^2(\Omega^e)}, \quad (2.19)$$

$$\| \mathbf{O}_h \|_{L^r(\partial\Omega^e)} \leq C_{\mathcal{I}}^k h_s^{\frac{d-1}{r} - \frac{d-1}{2}} \| \mathbf{O}_h \|_{L^2(\partial\Omega^e)}, \quad (2.20)$$

$$\| \nabla \mathbf{O}_h \|_{L^2(\Omega^e)} \leq C_{\mathcal{I}}^k h_s^{-1} \| \mathbf{O}_h \|_{L^2(\Omega^e)}. \quad (2.21)$$

The proof of the first two properties can be found in [24] and the last one in [60]. Note that Eqs. (2.19, 2.20) involve the space dimension  $d = 2$

**Lemma 2.4.5** (Relation between energy norms on the finite element space). *From [74], for  $\mathbf{O}_h \in X^k$ , there exists a positive constant  $C^k$ , depending on  $k$ , such that*

$$\| \mathbf{O}_h \|_{1} \leq C^k \| \mathbf{O}_h \| . \quad (2.22)$$

The demonstration directly follows by bounding the extra terms  $\sum_e h_s \| \mathbf{O} \|_{H^1(\partial\Omega^e)}^2$  of the norm defined by Eq. (2.12), in comparison to the norm defined by Eq. (2.11), using successively the trace inequality, Eq. (2.17), and the inverse inequality, Eq. (2.21), for the first term, and the trace inequality on the finite element space, Eq. (2.18), for the second term. The demonstration is reported in Appendix A.1.

**Lemma 2.4.6** (Energy bound of interpolant error). *Let  $\mathbf{O}^e \in X_s$ ,  $s \geq 2$ , and let  $I_h \mathbf{O} \in X^k$ , be its interpolant. Therefore, there is a constant  $C^k > 0$  independent of  $h_s$ , such that*

$$\| \mathbf{O}^e - I_h \mathbf{O} \|_{1} \leq C^k h^{\mu-1} \| \mathbf{O}^e \|_{H^s(\Omega_h)}, \quad (2.23)$$

with  $\mu = \min\{s, k+1\}$ . The proof follows from Lemma 2.4.1, Eq. (2.13), and Eq. (2.15), applied on the mesh dependent norm (2.12) and is given in Appendix A.2.

**Lemma 2.4.7** ((Generalized) Hölder's Inequality). *Let  $1 \leq p, q, < \infty$  be such that  $\frac{1}{p} + \frac{1}{q} = 1$  and  $D \in \mathbb{R}^n$ . Suppose that  $\Phi \in L^p(D)$  and  $\Psi \in L^q(D)$ , then the Hölder's inequality reads [37],*

$$\left| \int_D \Psi \Phi dx \right| \leq \left( \int_D |\Psi|^p dx \right)^{\frac{1}{p}} \left( \int_D |\Phi|^q dx \right)^{\frac{1}{q}}. \quad (2.24)$$

Let  $1 \leq p, q, r < \infty$  be such that  $\frac{1}{p} + \frac{1}{q} + \frac{1}{r} = 1$  and  $D \in \mathbb{R}^n$ . Suppose that  $\Phi \in L^p(D)$ ,  $\Psi \in L^q(D)$  and  $\mu \in L^r(D)$ , then the generalized Hölder's inequality is stated as [37]

$$\left| \int_D \Psi \Phi \mu dx \right| \leq \left( \int_D |\Psi|^p dx \right)^{\frac{1}{p}} \left( \int_D |\Phi|^q dx \right)^{\frac{1}{q}} \left( \int_D |\mu|^r dx \right)^{\frac{1}{r}}. \quad (2.25)$$

**Lemma 2.4.8** ((Generalized) Cauchy-Schwarz' inequality). *Let  $1 \leq p, q < \infty$  be such that  $\frac{1}{p} + \frac{1}{q} = 1$ . Suppose that  $a_i$  and  $b_i$  are two sequences of  $n$  positive real numbers, then the Cauchy-Schwartz' inequality reads [60]*

$$\left( \sum_{i=1}^n a_i b_i \right) \leq \left( \sum_{i=1}^n a_i^p \right)^{\frac{1}{p}} \left( \sum_{i=1}^n b_i^q \right)^{\frac{1}{q}}. \quad (2.26)$$

Let  $1 \leq p, q, r < \infty$  be such that  $\frac{1}{p} + \frac{1}{q} + \frac{1}{r} = 1$ . Suppose that  $a_i, b_i,$  and  $c_i$  are three sequences of  $n$  positive real numbers, then the generalized Cauchy-Schwartz' inequality reads [60]

$$\left( \sum_{i=1}^n a_i b_i c_i \right) \leq \left( \sum_{i=1}^n a_i^p \right)^{\frac{1}{p}} \left( \sum_{i=1}^n b_i^q \right)^{\frac{1}{q}} \left( \sum_{i=1}^n c_i^r \right)^{\frac{1}{r}}. \quad (2.27)$$

## 2.5 Conclusions

Within this chapter, we have presented all the general definitions and space properties, that will be used in the following three chapters in the purpose of proving the uniqueness, the stability, and the optimal order of the convergence rate of the DG approximated solution for many kinds of non-linear coupled problems.

## Chapter 3

# A coupled Linear Thermo-Elasticity Discontinuous Galerkin method

### 3.1 Introduction

In this Chapter an illustration of DG for linear coupled problem is presented, such as linear Thermo-Elastic coupled problems. Many researchers have dealt with Thermo-Elasticity problems using different FE methods [1, 70], or Discontinuous Galerkin (DG) methods [28].

In the general cases of 2-way coupling between thermal loading and mechanical process, either a change of the stress causes a change on the temperature, or a change of the temperature causes a thermal stress. In the elasticity case, the effect of the mechanical deformation on the temperature variation can be neglected when not seeking the Thermo-Elastic damping. Henceforth, the thermal flux and temperature can be computed without the consideration of mechanical stresses, as it will be shown later.

This chapter consists of five sections after this introduction. The constitutive equations that govern Thermo-Elasticity are derived in Section 3.2. In Section 3.3 the DG formulation is developed. In Section 3.4 the numerical properties, such as the consistency, the upper and lower bounds, and the solution uniqueness are derived. The optimal error bounds are theoretically estimated and numerically verified in Section 3.5 using the Thermo-Elastic model. The conclusions is given in Section 3.6.

### 3.2 Governing equations for Thermo-Elasticity

In this section, the governing equations for linear Thermo-Elasticity with small displacements over the domain  $\Omega$  and its boundary  $d\Omega$ , are presented. First the conservation of the momentum balance is reduced into the following equation after neglecting the contribution of the body force and inertial forces as

$$\nabla \cdot \boldsymbol{\sigma} = 0, \text{ with } \boldsymbol{\sigma} = \boldsymbol{\mathcal{H}} : \boldsymbol{\varepsilon} - \boldsymbol{\mathcal{H}} : \boldsymbol{\alpha}_{\text{th}}(T - T_0), \quad (3.1)$$

where  $\boldsymbol{\sigma}$  [N/m<sup>2</sup>] is the Cauchy stress tensor,  $T_0$  [K] is the initial temperature,  $\boldsymbol{\alpha}_{\text{th}} = \alpha_{\text{th}}\mathbf{I}$  is the thermal expansion coefficient [1/K], with  $\mathbf{I}$  is the identity tensor,  $\boldsymbol{\mathcal{H}} = \frac{\partial^2 \psi}{\partial \boldsymbol{\varepsilon} \partial \boldsymbol{\varepsilon}}$  is the elasticity tensor [N/m<sup>2</sup>], with  $\psi$  is the strain energy density per unit volume and  $\boldsymbol{\varepsilon}$  is the strain tensor which is defined for small displacements as  $\boldsymbol{\varepsilon} = \frac{1}{2}(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)$ .

Furthermore, the second governing equation is the balance of energy, which is given by

$$-\nabla \cdot \mathbf{q} + \bar{f} = \rho c_v \dot{T}, \text{ with } \mathbf{q} = -\mathbf{k} \cdot \nabla T, \quad (3.2)$$

where the dot denotes the time derivative,  $\mathbf{q}$  [W/m<sup>2</sup>] is the thermal flux vector,  $\mathbf{k}$  [W/(K·m)] is the thermal conductivity tensor,  $c_v$  is the volumetric heat capacity per unit mass [J/(K·Kg)], and  $\bar{f}$  represents all the body sources of heat and could depend on both the space and time. Here for Thermo-Elasticity  $\bar{f}$  is defined as  $\bar{f} = -\boldsymbol{\mathcal{H}} : \boldsymbol{\alpha}_{\text{th}} T \frac{\partial \boldsymbol{\varepsilon}}{\partial t}$ .

These two equations are completed with the boundary conditions. First the natural (Neumann) boundary conditions, which constrain the secondary variables like forces and traction

$$\boldsymbol{\sigma} \cdot \mathbf{n} = \bar{\mathbf{t}}, \quad \mathbf{q} \cdot \mathbf{n} = \bar{q} \quad \forall \mathbf{x} \in \partial_N \Omega, \quad (3.3)$$

where  $\bar{\mathbf{t}}$  and  $\bar{q}$  are respectively the traction and heat flux per unit reference surface. Second the essential (Dirichlet) or geometric boundary conditions, which constrain the primary variables like displacements and temperature

$$\mathbf{u} = \bar{\mathbf{u}}, \quad T = \bar{T} \quad \forall \mathbf{x} \in \partial_D \Omega, \quad (3.4)$$

where  $\bar{\mathbf{u}}$  and  $\bar{T}$  are the prescribed displacement and temperature respectively.

Let us define a  $(d+1) \times 1$ -vector of the unknown fields  $\mathbf{E} = \begin{pmatrix} \mathbf{u} \\ T - T_0 \end{pmatrix}$ , where  $\mathbf{u}$  is the displacement vector,  $\mathbf{u} = \begin{pmatrix} u_x \\ u_y \\ u_z \end{pmatrix}$ . In addition, let us introduce a vector  $\mathbf{c}$  of size  $(4d-3) \times 1$

as  $\mathbf{c} = \mathbf{w} \nabla \mathbf{E}$ , where  $\mathbf{w}$  is a coefficients matrix of size  $(4d-3) \times (4d-3)$ ,  $\mathbf{w} = \begin{pmatrix} \mathbf{C} & \mathbf{0} \\ \mathbf{0} & \mathbf{k} \end{pmatrix}$ , with  $\mathbf{C}$  the matrix form of the material tensor  $\boldsymbol{\mathcal{H}}$ . Besides,  $\nabla \mathbf{E}$  is written using Voigt rules for the mechanical contribution, in other words the stress and strain are transformed into vectors, such that  $\nabla \mathbf{E}$  is a vector of size  $(4d-3) \times 1$  and defined for  $d=3$  as

$$\nabla \mathbf{E} = \begin{pmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \varepsilon_{zz} \\ 2\varepsilon_{xy} \\ 2\varepsilon_{xz} \\ 2\varepsilon_{yz} \\ \frac{\partial T}{\partial x} \\ \frac{\partial T}{\partial y} \\ \frac{\partial T}{\partial z} \end{pmatrix} = \begin{pmatrix} \frac{\partial}{\partial x} & 0 & 0 & 0 \\ 0 & \frac{\partial}{\partial y} & 0 & 0 \\ 0 & 0 & \frac{\partial}{\partial z} & 0 \\ \frac{\partial}{\partial y} & \frac{\partial}{\partial x} & 0 & 0 \\ \frac{\partial}{\partial z} & 0 & \frac{\partial}{\partial x} & 0 \\ 0 & \frac{\partial}{\partial z} & \frac{\partial}{\partial y} & 0 \\ 0 & 0 & 0 & \frac{\partial}{\partial x} \\ 0 & 0 & 0 & \frac{\partial}{\partial y} \\ 0 & 0 & 0 & \frac{\partial}{\partial z} \end{pmatrix} \begin{pmatrix} u_x \\ u_y \\ u_z \\ T - T_0 \end{pmatrix}. \quad (3.5)$$

Then the partial differential equations (3.1) and (3.2) of the linear Thermo-Elastic coupling problem, after neglecting the Thermo-Elastic damping, are rewritten under the form

$$\nabla^T(\mathbf{c}(\nabla \mathbf{E})) - \nabla^T(\mathbf{r}\mathbf{E}) = \mathbf{f}\dot{\mathbf{E}} \quad \text{in } \Omega, \quad (3.6)$$

where  $\mathbf{f}$  is of size  $(d+1) \times (d+1)$  with  $\mathbf{f} = \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \rho c_v \end{pmatrix}$  and  $\mathbf{r}$  is a matrix of size  $(4d-3) \times (d+1)$  with

$\mathbf{r} = \begin{pmatrix} \mathbf{0} & \mathbf{C}\boldsymbol{\alpha}_{\text{thc}} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}$ , with  $\boldsymbol{\alpha}_{\text{thc}}^T = (\alpha_{\text{th}} \alpha_{\text{th}} \alpha_{\text{th}} 0 0 0)$ , such that  $\mathbf{C}\boldsymbol{\alpha}_{\text{thc}}$  is a  $(3d-3) \times 1$  vector and given for  $d = 3$  by  $(\mathbf{C}\boldsymbol{\alpha}_{\text{thc}})^T = (3K\alpha_{\text{th}} \ 3K\alpha_{\text{th}} \ 3K\alpha_{\text{th}} \ 0 \ 0 \ 0)$  for isotropic materials, where  $K$  is the bulk modulus.

This equation is completed by the BCs

$$\bar{\mathbf{n}}^T(\mathbf{c} - \mathbf{r}\mathbf{E}) = \bar{\mathbf{c}} \quad \forall \mathbf{x} \in \partial_N\Omega, \quad (3.7)$$

$$\mathbf{E} = \bar{\mathbf{E}} \quad \forall \mathbf{x} \in \partial_D\Omega, \quad (3.8)$$

which result from the boundary condition Eqs. (3.3) and (3.4), and where

$$\bar{\mathbf{c}} = \begin{pmatrix} \bar{\mathbf{t}} \\ -\bar{q} \end{pmatrix}, \quad \bar{\mathbf{n}} = \begin{pmatrix} n_x & 0 & 0 & 0 \\ 0 & n_y & 0 & 0 \\ 0 & 0 & n_z & 0 \\ n_y & n_x & 0 & 0 \\ n_z & 0 & n_x & 0 \\ 0 & n_z & n_y & 0 \\ 0 & 0 & 0 & n_x \\ 0 & 0 & 0 & n_y \\ 0 & 0 & 0 & n_z \end{pmatrix}. \quad (3.9)$$

In this part, we assume that  $\partial_N\Omega$  and  $\partial_D\Omega$  are the same for both fields  $\mathbf{u}$  and  $T$ .

### 3.3 Discontinuous Galerkin formulation for linear Thermo-Elasticity

#### 3.3.1 Weak form

The DG weak formulation for linear Thermo-Elastic coupling is derived from the two governing equations (3.3) and (3.4) separately, then they are combined together in the matrix form.

Starting from the first governing Eq. (3.1) and multiplying it by the test function  $\delta\mathbf{u} \in [\Pi_c H^1(\Omega^e)]^d$  leads to

$$\sum_e \int_{\Omega^e} (\nabla \cdot \boldsymbol{\sigma}) \cdot \delta\mathbf{u} d\Omega = 0 \quad \forall \delta\mathbf{u} \in [\Pi_c H^1(\Omega^e)]^d. \quad (3.10)$$

Then by performing a volume integral and using the divergence theorem on each element  $\Omega^e$ , we reduce the order of the differential equation, so the weak form is stated as

$$\begin{aligned} & \sum_e \int_{\partial\Omega^e} \delta\mathbf{u} \cdot (\nabla\mathbf{u} : \boldsymbol{\mathcal{H}}) \cdot \mathbf{n} dS - \sum_e \int_{\partial\Omega^e} \delta\mathbf{u} \cdot (\boldsymbol{\mathcal{H}} : \boldsymbol{\alpha}_{\text{th}}(T - T_0)) \cdot \mathbf{n} dS \\ & = \sum_e \int_{\Omega^e} \nabla\mathbf{u} : \boldsymbol{\mathcal{H}} : \nabla\delta\mathbf{u} d\Omega - \sum_e \int_{\Omega^e} (\boldsymbol{\mathcal{H}} : \boldsymbol{\alpha}_{\text{th}}(T - T_0)) : \nabla\delta\mathbf{u} d\Omega, \end{aligned} \quad (3.11)$$

where

$$\int_{\partial\Omega^e} \delta\mathbf{u} \cdot \boldsymbol{\sigma} \cdot \mathbf{n} dS = \int_{\partial_N\Omega^e} \delta\mathbf{u} \cdot \boldsymbol{\sigma} \cdot \mathbf{n} dS + \int_{\partial_I\Omega^e \cup \partial_D\Omega^e} \delta\mathbf{u} \cdot \boldsymbol{\sigma} \cdot \mathbf{n} dS. \quad (3.12)$$

Different versions of the discontinuous Galerkin finite element methodology can be obtained by using different numerical flux coefficients [13]. In the present research, the arithmetic average of the two field gradient values at the boundary is employed. At the interface between two elements, Fig. 2.1, each interior edge  $(\partial_I\Omega)^s$ , shared by two elements  $-$  and  $+$ , is integrated over twice in Eq. (3.11), since  $(\partial_I\Omega)^s \subset \partial_I\Omega^{e^-}$  and  $(\partial_I\Omega)^s \subset \partial_I\Omega^{e^+}$ . By recalling the two useful operators, the jump  $[[\cdot]]$  and the average  $\langle \cdot \rangle$  operators, which are defined in Section 2.3, Eq. (3.12) can be rewritten using

$$\begin{aligned} \sum_e \int_{\partial_I\Omega^e} \delta\mathbf{u} \cdot \boldsymbol{\sigma} \cdot \mathbf{n} dS &= - \int_{\partial_I\Omega_h} (\delta\mathbf{u} \cdot \boldsymbol{\sigma}^+ - \delta\mathbf{u}^- \cdot \boldsymbol{\sigma}^-) \cdot \mathbf{n}^- dS \\ &= - \int_{\partial_I\Omega_h} [[\delta\mathbf{u} \cdot \boldsymbol{\sigma}]] \cdot \mathbf{n}^- dS, \end{aligned} \quad (3.13)$$

$$\sum_e \int_{\partial_D\Omega^e} \delta\mathbf{u} \cdot \boldsymbol{\sigma} \cdot \mathbf{n} dS = - \int_{\partial_D\Omega_h} [[\delta\mathbf{u} \cdot \boldsymbol{\sigma}]] \cdot \mathbf{n} dS \text{ and } \mathbf{n}^- = \mathbf{n}, \quad (3.14)$$

where  $\mathbf{n}^-$  is defined as the outward unit normal of the minus element  $\Omega^{e^-}$ , whereas  $\mathbf{n}^+$  is the outward unit normal of its neighboring element,  $\mathbf{n}^+ = -\mathbf{n}^-$ .

Eventually, using Eq. (3.3), Eq. (3.11) is rewritten

$$\int_{\partial_N\Omega_h} \delta\mathbf{u} \cdot \bar{\mathbf{t}} dS = \int_{\Omega_h} \boldsymbol{\sigma} : \nabla \delta\mathbf{u} d\Omega + \int_{\partial_I\Omega_h \cup \partial_D\Omega_h} [[\delta\mathbf{u} \cdot \boldsymbol{\sigma}]] \cdot \mathbf{n}^- dS \quad \forall \delta\mathbf{u} \in [\Pi_e H_c^1(\Omega^e)]^d. \quad (3.15)$$

For DG formulations, the jumps are commonly replaced by fluxes, which must be consistent. Thereafter, applying the mathematical identity  $[[ab]] = [[a]] \langle b \rangle + [[b]] \langle a \rangle$  on  $\partial_I\Omega_h$  and neglecting the second term because the exact stress is continuous, the flux related to Eq. (3.15) becomes  $[[\delta\mathbf{u} \cdot \boldsymbol{\sigma}]] = [[\delta\mathbf{u}]] \cdot \langle \boldsymbol{\sigma} \rangle$ .

Due to the discontinuous nature of the trial and test functions, in the DG weak form, the interelement discontinuity is allowed, so the continuity of unknown variables is enforced weakly by using symmetrization and stabilization terms at the interior elements boundary interfaces  $\partial_I\Omega_h$ . The BC (3.4) is also enforced weakly on the Dirichlet boundary. In order to remain general, and to ensure the optimal convergence rate, we consider the compatibility term as  $[[\mathbf{u}]] \cdot \langle \boldsymbol{\mathcal{H}} : \nabla \delta\mathbf{u} \rangle - \gamma [[\boldsymbol{\alpha}_{th} : \boldsymbol{\mathcal{H}}\mathbf{T}]] \cdot \langle \delta\mathbf{u} \rangle$ , where  $\gamma$  is a constant that will be determined later in order to achieve the optimal convergence rate.

Therefore, the SIPG formulation for the mechanical contribution is defined as finding



$\mathbf{u} \times \mathbf{T} \in [\Pi_e \mathbf{H}^1(\Omega^e)]^d \times \Pi_e \mathbf{H}^1(\Omega^e)$ , such that:

$$\begin{aligned}
& \int_{\partial_N \Omega_h} \delta \mathbf{u} \cdot \bar{\mathbf{t}} dS - \int_{\partial_D \Omega_h} \bar{\mathbf{u}} \cdot (\mathcal{H} : \nabla \delta \mathbf{u}) \cdot \mathbf{n} dS + \int_{\partial_D \Omega_h} \bar{\mathbf{u}} \otimes \mathbf{n} : \frac{\mathcal{H}\mathcal{B}}{h_s} : \delta \mathbf{u} \otimes \mathbf{n} dS \\
& + \gamma \int_{\partial_D \Omega_h} \delta \mathbf{u} \cdot (\boldsymbol{\alpha}_{\text{th}} : \mathcal{H}\bar{\mathbf{T}}) \cdot \mathbf{n} dS = \int_{\Omega_h} \boldsymbol{\sigma} : \nabla \delta \mathbf{u} d\Omega + \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} [[\delta \mathbf{u}]] \cdot \langle \boldsymbol{\sigma} \rangle \cdot \mathbf{n}^- dS \\
& + \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} [[\mathbf{u}]] \cdot \langle \mathcal{H} : \nabla \delta \mathbf{u} \rangle \cdot \mathbf{n}^- dS + \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} [[\mathbf{u}]] \otimes \mathbf{n}^- : \left\langle \frac{\mathcal{H}\mathcal{B}}{h_s} \right\rangle : [[\delta \mathbf{u}]] \otimes \mathbf{n}^- dS \\
& - \gamma \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \langle \delta \mathbf{u} \rangle \cdot [[\boldsymbol{\alpha}_{\text{th}} : \mathcal{H}\mathbf{T}]] \cdot \mathbf{n}^- dS \quad \forall \delta \mathbf{u} \in [\Pi_e \mathbf{H}^1(\Omega^e)]^d.
\end{aligned} \tag{3.16}$$

In this DG formulation  $\mathcal{B}$  is the stability parameter which has to be sufficiently high to guarantee stability as it will be shown later,  $\mathcal{H}$  is the constant elastic tensor and  $h_s$  is a measure of the mesh fineness.

In the same spirit, if Thermo-Elastic damping is neglected, the weak formulation for the second governing equation (3.2), can be derived by multiplying it with the test function  $\delta \mathbf{T} \in \Pi_e \mathbf{H}^1(\Omega^e)$ , leading to

$$- \sum_e \int_{\Omega^e} \nabla \cdot \mathbf{q} \delta \mathbf{T} d\Omega = \sum_e \int_{\Omega^e} \rho c_v \dot{\mathbf{T}} \delta \mathbf{T} d\Omega \quad \forall \delta \mathbf{T} \in \Pi_e \mathbf{H}^1(\Omega^e). \tag{3.17}$$

As for the mechanical equation, by using the divergence theorem, introducing the jump operator, and using the boundary condition Eqs. (3.3) and (3.4), this last equation becomes

$$\int_{\partial_N \Omega_h} \delta \mathbf{T} \mathbf{q} \cdot \mathbf{n} dS + \int_{\Omega_h} \rho c_v \dot{\mathbf{T}} \delta \mathbf{T} d\Omega = \int_{\Omega_h} \mathbf{q} \cdot \nabla \delta \mathbf{T} d\Omega + \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} [[\delta \mathbf{T} \mathbf{q}]] \cdot \mathbf{n}^- dS. \tag{3.18}$$

The consistent and stable weak form is obtained by considering the numerical thermal flux  $\langle \mathbf{q} \rangle = \frac{1}{2}(\mathbf{q}^+ + \mathbf{q}^-)$ , then using the virtual heat flux  $\delta \mathbf{q} = -\mathbf{k} \cdot \nabla \delta \mathbf{T}$ , and adding stability and symmetrization terms. The DG formulation of the thermal governing equation is then stated as finding  $\mathbf{T} \in \Pi_e \mathbf{H}^1(\Omega^e)$ , such that

$$\begin{aligned}
& - \int_{\partial_N \Omega_h} \delta \mathbf{T}_h \bar{\mathbf{q}} d\Omega - \int_{\Omega_h} \rho c_v \dot{\mathbf{T}} \delta \mathbf{T} d\Omega - \int_{\partial_D \Omega_h} (\mathbf{k} \cdot \nabla \delta \mathbf{T}) \cdot \mathbf{n} \bar{\mathbf{T}} dS \\
& + \int_{\partial_D \Omega_h} \delta \mathbf{T} \mathbf{n} \cdot \frac{\mathbf{k}\mathcal{B}}{h_s} \cdot \mathbf{n} \bar{\mathbf{T}} dS = \int_{\Omega_h} \nabla \mathbf{T} \cdot \mathbf{k} \cdot \nabla \delta \mathbf{T} d\Omega \\
& + \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} [[\delta \mathbf{T}]] \mathbf{n}^- \cdot \langle \mathbf{k} \cdot \nabla \mathbf{T} \rangle dS + \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} [[\mathbf{T}]] \mathbf{n}^- \cdot \langle \mathbf{k} \cdot \nabla \delta \mathbf{T} \rangle dS \\
& + \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} [[\delta \mathbf{T}]] \mathbf{n}^- \cdot \left\langle \frac{\mathcal{B}}{h_s} \mathbf{k} \right\rangle \cdot \mathbf{n}^- [[\mathbf{T}]] dS \quad \forall \delta \mathbf{T} \in \Pi_e \mathbf{H}^1(\Omega^e).
\end{aligned} \tag{3.19}$$

Thereafter, the two parts of the DG formulation can be combined in terms of the notations  $\mathbf{w}$ ,  $\mathbf{r}$ , and  $\mathbf{f}$  resulting in a stabilized DG formulation for linear Thermo-Elastic coupling.

The weak form is stated as finding  $\mathbf{E} \in [\Pi_e H^1(\Omega^e)]^3 \times \Pi_e H^1(\Omega^e)$  such that

$$\begin{aligned}
& \int_{\partial_N \Omega_h} \delta \mathbf{E}^T \bar{\mathbf{c}} dS - \int_{\Omega_h} \delta \mathbf{E}^T \mathbf{f} \dot{\mathbf{E}} d\Omega - \int_{\partial_D \Omega_h} \bar{\mathbf{E}}_n^T \mathbf{w} \nabla \delta \mathbf{E} dS + \int_{\partial_D \Omega_h} \bar{\mathbf{E}}_n^T \frac{\mathbf{w} \mathcal{B}}{h_s} \delta \mathbf{E}_n dS \\
& + \gamma \int_{\partial_D \Omega_h} \delta \mathbf{E}_n^T \mathbf{r} \bar{\mathbf{E}} dS = \int_{\Omega_h} (\nabla \delta \mathbf{E})^T \mathbf{w} \nabla \mathbf{E} d\Omega - \int_{\Omega_h} (\nabla \delta \mathbf{E})^T \mathbf{r} \mathbf{E} d\Omega \\
& + \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \llbracket \delta \mathbf{E}_n^T \rrbracket \langle \mathbf{w} \nabla \mathbf{E} \rangle dS - \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \llbracket \delta \mathbf{E}_n^T \rrbracket \langle \mathbf{r} \mathbf{E} \rangle dS \\
& + \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \llbracket \mathbf{E}_n^T \rrbracket \langle \mathbf{w} \nabla \delta \mathbf{E} \rangle dS - \gamma \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \langle \delta \mathbf{E}_n^T \rangle \llbracket \mathbf{r} \mathbf{E} \rrbracket dS \\
& + \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \llbracket \mathbf{E}_n^T \rrbracket \left\langle \frac{\mathbf{w} \mathcal{B}}{h_s} \right\rangle \llbracket \delta \mathbf{E}_n \rrbracket dS \quad \forall \delta \mathbf{E} \in [\Pi_e H^1(\Omega^e)]^d \times \Pi_e H^1(\Omega^e),
\end{aligned} \tag{3.20}$$

where  $\mathbf{E}_n$  is a  $9 \times 1$  vector

$$\mathbf{E}_n = \begin{pmatrix} u_x n_x^- \\ u_y n_y^- \\ u_z n_z^- \\ u_x n_y^- + u_y n_x^- \\ u_x n_z^- + u_z n_x^- \\ u_z n_y^- + u_y n_z^- \\ T n_x^- \\ T n_y^- \\ T n_z^- \end{pmatrix} = \begin{pmatrix} n_x^- & 0 & 0 & 0 \\ 0 & n_y^- & 0 & 0 \\ 0 & 0 & n_z^- & 0 \\ n_y^- & n_x^- & 0 & 0 \\ n_z^- & 0 & n_x^- & 0 \\ 0 & n_z^- & n_y^- & 0 \\ 0 & 0 & 0 & n_x^- \\ 0 & 0 & 0 & n_y^- \\ 0 & 0 & 0 & n_z^- \end{pmatrix} \begin{pmatrix} u_x \\ u_y \\ u_z \\ T - T_0 \end{pmatrix}, \tag{3.21}$$

and  $\bar{\mathbf{E}}_n$  is defined in the same way as  $\mathbf{E}_n$  after replacing  $\mathbf{n}^-$  by  $\mathbf{n}$  and  $\mathbf{E}$  by  $\bar{\mathbf{E}}$  in Eq. (3.21).

The last fifth terms presented in Eq. (3.20) are the interfaces terms, which correspond to:

1. The first two terms ensure consistency, they result directly from the discontinuity of the test function  $\delta \mathbf{E}$  between two elements, and involve the consistent numerical flux which is here the traditional average flux.
2. The third and fourth terms ensure compatibility of the weak form and the symmetry of the stiffness matrix after FE discretization. They also ensure the optimal convergence rate in the  $L^2$ -norm.
3. The last term ensures stability, as it is well known that the discontinuous formulation of elliptic problems requires quadratic terms. The stabilization terms depend on a stability parameter required to be large enough, which is independent of mesh size and material properties, as it will be shown in Section 3.4.
4. The contributions on  $\partial_D \Omega_h$  ensure that the Dirichlet boundary condition (3.8) is weakly enforced.

Let us recall the definition of the discontinuous FE space, Eq. (2.6), and rewrite it for the case of linear Thermo-Elasticity

$$X_s = \left\{ \mathbf{E} \in [L^2(\Omega_h)]^d \times L^2(\Omega_h) \mid \mathbf{E}|_{\Omega^e} \in [H^s(\Omega^e)]^d \times H^s(\Omega^e) \quad \forall \Omega^e \in \Omega_h \right\}, \tag{3.22}$$

we denote  $X_2$  by  $X$ . It should be noted that the test functions in the previous equations of the weak formulation belong to  $[H^1(\Omega^e)]^d \times H^1(\Omega^e)$ , however for the numerical analysis, we will need to be in  $[H^2(\Omega^e)]^d \times H^2(\Omega^e)$ . Therefore, Eq. (3.20) can be rewritten under the form of finding  $\mathbf{E} \in X$  such that

$$a(\mathbf{E}, \delta\mathbf{E}) = b(\delta\mathbf{E}) - \int_{\Omega_h} \delta\mathbf{E}^T \mathbf{f} \dot{\mathbf{E}} d\Omega, \quad \forall \delta\mathbf{E} \in X, \quad (3.23)$$

with

$$\begin{aligned} a(\mathbf{E}, \delta\mathbf{E}) &= \int_{\Omega_h} (\nabla \delta\mathbf{E})^T \mathbf{w} \nabla \mathbf{E} d\Omega - \int_{\Omega_h} (\nabla \delta\mathbf{E})^T \mathbf{r} \mathbf{E} d\Omega + \int_{\partial_T \Omega_h \cup \partial_D \Omega_h} \llbracket \delta\mathbf{E}_n^T \rrbracket \langle \mathbf{w} \nabla \mathbf{E} \rangle dS \\ &+ \int_{\partial_T \Omega_h \cup \partial_D \Omega_h} \llbracket \mathbf{E}_n^T \rrbracket \langle \mathbf{w} \nabla \delta\mathbf{E} \rangle dS + \int_{\partial_T \Omega_h \cup \partial_D \Omega_h} \llbracket \mathbf{E}_n^T \rrbracket \left\langle \frac{\mathbf{w} \mathcal{B}}{h_s} \right\rangle \llbracket \delta\mathbf{E}_n \rrbracket dS \\ &- \int_{\partial_T \Omega_h \cup \partial_D \Omega_h} \llbracket \delta\mathbf{E}_n^T \rrbracket \langle \mathbf{r} \mathbf{E} \rangle dS - \gamma \int_{\partial_T \Omega_h \cup \partial_D \Omega_h} \langle \delta\mathbf{E}_n^T \rangle \llbracket \mathbf{r} \mathbf{E} \rrbracket dS, \end{aligned} \quad (3.24)$$

$$\begin{aligned} b(\delta\mathbf{E}) &= \int_{\partial_N \Omega_h} \delta\mathbf{E}^T \bar{\mathbf{c}} dS - \int_{\partial_D \Omega_h} \bar{\mathbf{E}}_n^T \mathbf{w} \nabla \delta\mathbf{E} dS + \int_{\partial_D \Omega_h} \bar{\mathbf{E}}_n^T \frac{\mathbf{w} \mathcal{B}}{h_s} \delta\mathbf{E}_n dS \\ &+ \gamma \int_{\partial_D \Omega_h} \delta\mathbf{E}_n^T \mathbf{r} \bar{\mathbf{E}} dS. \end{aligned} \quad (3.25)$$

Note that

$$\begin{aligned} \int_{\Omega_h} (\nabla \delta\mathbf{E})^T \mathbf{r} \mathbf{E} d\Omega &= \sum_e \int_{\Omega^e} (\nabla \delta\mathbf{E})^T \mathbf{r} \mathbf{E} d\Omega \\ &= - \sum_e \int_{\Omega^e} \delta\mathbf{E}^T \nabla^T (\mathbf{r} \mathbf{E}) d\Omega + \sum_e \int_{\partial \Omega^e} \delta\mathbf{E}_n^T (\mathbf{r} \mathbf{E}) dS \\ &= - \int_{\Omega_h} \delta\mathbf{E}^T \nabla^T (\mathbf{r} \mathbf{E}) d\Omega - \int_{\partial_T \Omega_h} \llbracket \delta\mathbf{E}_n^T \mathbf{r} \mathbf{E} \rrbracket dS + \int_{\partial_N \Omega_h} \delta\mathbf{E}^T \bar{\mathbf{n}}^T \mathbf{r} \mathbf{E} dS + \int_{\partial_D \Omega_h} \delta\mathbf{E}_n^T \mathbf{r} \mathbf{E} dS \\ &= - \int_{\Omega_h} \delta\mathbf{E}^T \nabla^T (\mathbf{r} \mathbf{E}) d\Omega - \int_{\partial_T \Omega_h} \llbracket \delta\mathbf{E}_n^T \rrbracket \langle \mathbf{r} \mathbf{E} \rangle dS - \int_{\partial_T \Omega_h \cup \partial_D \Omega_h} \langle \delta\mathbf{E}_n^T \rangle \llbracket \mathbf{r} \mathbf{E} \rrbracket dS \\ &+ \int_{\partial_N \Omega_h} \delta\mathbf{E}^T \bar{\mathbf{n}}^T \mathbf{r} \mathbf{E} dS. \end{aligned} \quad (3.26)$$

For future use, it can be noted that the gradient of  $(\mathbf{r} \mathbf{E})$  consists of zero components and of the gradient of  $\boldsymbol{\alpha}_{th} : \mathcal{H} \mathbf{T}$ , which is  $\boldsymbol{\alpha}_{th} : \mathcal{H} \nabla \mathbf{T}$ . Henceforth the matrix  $\mathbf{r}$  can be rearranged in a new form  $\tilde{\mathbf{r}}$  of size  $(d+1) \times (4d-3)$  and by this way  $\nabla^T (\mathbf{r} \mathbf{E})$  can be replaced for  $d=3$  by  $\tilde{\mathbf{r}} \nabla \mathbf{E}$ , with

$$\tilde{\mathbf{r}}(\mathbf{E}) \nabla \mathbf{E} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 3K\alpha_{th} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3K\alpha_{th} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3K\alpha_{th} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \varepsilon_{zz} \\ 2\varepsilon_{xy} \\ 2\varepsilon_{xz} \\ 2\varepsilon_{yz} \\ \frac{\partial \Gamma}{\partial x} \\ \frac{\partial \Gamma}{\partial y} \\ \frac{\partial \Gamma}{\partial z} \end{pmatrix}. \quad (3.27)$$

Moreover, the following equality is also useful

$$\nabla^T(\tilde{\mathbf{r}}^T \delta \mathbf{E}) = \mathbf{r}^T \nabla \delta \mathbf{E} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 3K\alpha_{\text{th}}\delta\varepsilon_{xx} + 3K\alpha_{\text{th}}\delta\varepsilon_{yy} + 3K\alpha_{\text{th}}\delta\varepsilon_{zz} \end{pmatrix}. \quad (3.28)$$

Therefore, using Eq. (3.26), Eq. (3.23) can be rewritten as

$$\mathbf{a}'(\mathbf{E}, \delta \mathbf{E}) = \mathbf{b}'(\delta \mathbf{E}) - \int_{\Omega_h} \delta \mathbf{E}^T \mathbf{f} \dot{\mathbf{E}} d\Omega, \quad \forall \delta \mathbf{E} \in X, \quad (3.29)$$

with

$$\begin{aligned} \mathbf{a}'(\mathbf{E}, \delta \mathbf{E}) &= \int_{\Omega_h} (\nabla \delta \mathbf{E})^T \mathbf{w} \nabla \mathbf{E} d\Omega + \int_{\Omega_h} \delta \mathbf{E}^T \nabla^T(\mathbf{r} \mathbf{E}) d\Omega + \int_{\partial_1 \Omega_h \cup \partial_D \Omega_h} \llbracket \delta \mathbf{E}_n^T \rrbracket \langle \mathbf{w} \nabla \mathbf{E} \rangle dS \\ &+ \int_{\partial_1 \Omega_h \cup \partial_D \Omega_h} \llbracket \mathbf{E}_n^T \rrbracket \langle \mathbf{w} \nabla \delta \mathbf{E} \rangle dS + \int_{\partial_1 \Omega_h \cup \partial_D \Omega_h} \llbracket \mathbf{E}_n^T \rrbracket \left\langle \frac{\mathbf{w} \mathcal{B}}{h_s} \right\rangle \llbracket \delta \mathbf{E}_n \rrbracket dS \\ &+ (1 - \gamma) \int_{\partial_1 \Omega_h \cup \partial_D \Omega_h} \langle \delta \mathbf{E}_n^T \rangle \llbracket \mathbf{r} \mathbf{E} \rrbracket dS - \int_{\partial_N \Omega_h} \delta \mathbf{E}^T \bar{\mathbf{n}}^T(\mathbf{r} \mathbf{E}) dS - \int_{\partial_D \Omega_h} \llbracket \delta \mathbf{E}_n^T \rrbracket \langle \mathbf{r} \mathbf{E} \rangle dS, \end{aligned} \quad (3.30)$$

$$\begin{aligned} \mathbf{b}'(\delta \mathbf{E}) &= \int_{\partial_N \Omega_h} \delta \mathbf{E}^T \bar{\mathbf{c}} dS - \int_{\partial_D \Omega_h} \bar{\mathbf{E}}_n^T \mathbf{w} \nabla \delta \mathbf{E} dS + \int_{\partial_D \Omega_h} \bar{\mathbf{E}}_n^T \frac{\mathbf{w} \mathcal{B}}{h_s} \delta \mathbf{E}_n dS \\ &+ \gamma \int_{\partial_D \Omega_h} \delta \mathbf{E}_n^T \mathbf{r} \bar{\mathbf{E}} dS. \end{aligned} \quad (3.31)$$

In comparison with the 1D DG formulation proposed by Gudi et al. [24] for elliptic problems, Eq. (3.29) has additional terms on the Dirichlet and Neumann boundary parts related to the term  $\mathbf{r}$ . This is due to the fact that as the stress tensor is directly integrated in a FE model, we prefer to have the term in  $\int_{\Omega_h} (\nabla \delta \mathbf{E})^T \mathbf{r} \mathbf{E} d\Omega$  in Eq. (3.23) instead of the term  $\int_{\Omega_h} \delta \mathbf{E}^T \nabla^T(\mathbf{r} \mathbf{E}) d\Omega$  of Eq. (3.29), as dealt with by Gudi et al. [24]. Therefore, the integration by parts Eq. (3.26) yields these two extra terms.

### 3.3.2 Finite element discretization

Let us recall the polynomial space, Eq. (2.9), which becomes for the Linear Thermo-Elastic problems

$$X^k = \left\{ \mathbf{E}_h \in [L^2(\Omega_h)]^d \times L^2(\Omega_h) \mid \mathbf{E}_h|_{\Omega^e} \in [\mathbb{P}^k(\Omega^e)]^d \times \mathbb{P}^k(\Omega^e) \quad \forall \Omega^e \in \Omega_h \right\}, \quad (3.32)$$

where  $\mathbb{P}^k$  is a piecewise polynomial function of degree  $\leq k$ . Let  $\mathbf{E}_h = \begin{pmatrix} \mathbf{u}_h \\ T_h - T_0 \end{pmatrix}$  be the discrete approximation of  $\mathbf{E}$ , where the displacement vector  $\mathbf{u}_h$  and the temperature  $T_h$ , and the corresponding test functions  $\delta \mathbf{u}_h$  and  $\delta T_h$  respectively are approximated by the same shape functions  $N^a$  at node  $a$ , which are defined piecewise on the elements, we thus have

$$\delta \mathbf{u}_h = N_{\mathbf{u}}^a \delta \mathbf{u}^a, \quad \delta T_h = N_T^a \delta T^a, \quad \text{and} \quad (3.33)$$

$$\mathbf{u}_h = N_{\mathbf{u}}^a \mathbf{u}^a, \quad T_h = N_T^a T^a, \quad (3.34)$$

where  $\mathbf{u}^a$  denotes the nodal values of  $\mathbf{u}_h$  at node a and  $T^a$  denotes the nodal values of  $T_h$  at node a.

Likewise, the gradients of the fields can be deduced from

$$\nabla \delta \mathbf{u}_h = \delta \mathbf{u}^a \otimes \nabla N_{\mathbf{u}}^a, \quad \nabla \delta T_h = \nabla N_T^a \delta T^b, \quad \text{and} \quad (3.35)$$

$$\nabla \mathbf{u}_h = \mathbf{u}^a \otimes \nabla N_{\mathbf{u}}^a, \quad \nabla T_h = \nabla N_T^a T^a, \quad (3.36)$$

where  $\nabla N_{\mathbf{u}}^a$  and  $\nabla N_T^a$  are the gradients of the shape functions at node a.

The Discontinuous Galerkin Finite Element discretization of linear Thermo-Elastic coupled problems is stated as finding the approximated solution  $\mathbf{E}_h$  in  $X^k$ , such that

$$a(\mathbf{E}_h, \delta \mathbf{E}_h) = b(\delta \mathbf{E}_h) - \int_{\Omega_h} \delta \mathbf{E}_h^T \mathbf{f} \dot{\mathbf{E}}_h d\Omega, \quad \forall \delta \mathbf{E}_h \in X^k, \quad (3.37)$$

with  $a(\mathbf{E}_h, \delta \mathbf{E}_h)$  and  $b(\delta \mathbf{E}_h)$  defined by Eqs. (3.24, 3.25).

### 3.3.3 The system resolution

The set of Eqs. (3.16) and (3.19) can be rewritten under the form:

$$\mathbf{F}_{\text{ext}}^a(\mathbf{E}^b) = \mathbf{F}_{\text{int}}^a(\mathbf{E}^b) + \mathbf{F}_I^a(\mathbf{E}^b), \quad (3.38)$$

where  $\mathbf{E}^b$  is the  $(4 \times 1)$  vector of the unknown fields at node b.

The nonlinear Eqs. (3.38) are linearized by means of an implicit formulation and solved using the Newton Raphson scheme using an initial guess of the last solution. To this end, the forces are written in a residual form. The predictor at iteration 0, reads  $\mathbf{E}^b = \mathbf{E}^{b0}$ , and the residual at iteration i reads

$$\mathbf{F}_{\text{ext}}^a(\mathbf{E}^{bi}) - \mathbf{F}_{\text{int}}^a(\mathbf{E}^{bi}) - \mathbf{F}_I^a(\mathbf{E}^{bi}) = \mathbf{R}^a(\mathbf{E}^{bi}), \quad (3.39)$$

and at iteration i, the first order Taylor development yields the system to be solved, i.e.

$$\left( \frac{\partial \mathbf{F}_{\text{ext}}^a}{\partial \mathbf{E}^b} - \frac{\partial \mathbf{F}_{\text{int}}^a}{\partial \mathbf{E}^b} - \frac{\partial \mathbf{F}_I^a}{\partial \mathbf{E}^b} \right) \Big|_{\mathbf{E}=\mathbf{E}^{ci}} \Delta \mathbf{E}^b = -\mathbf{R}^a(\mathbf{E}^{ci}). \quad (3.40)$$

Let us define the tangent matrix of the coupled Thermo-Mechanical system  $\mathbf{K}_{\mathbf{E}}^{\text{ab}} = \frac{\partial \mathbf{F}_{\text{ext}}^a}{\partial \mathbf{E}^b} - \frac{\partial \mathbf{F}_{\text{int}}^a}{\partial \mathbf{E}^b} - \frac{\partial \mathbf{F}_I^a}{\partial \mathbf{E}^b}$ , and  $\Delta \mathbf{E}^b = (\mathbf{E}^b - \mathbf{E}^{bi})$ , then we have

$$\begin{pmatrix} \mathbf{K}_{\mathbf{uu}} & \mathbf{K}_{\mathbf{uT}} \\ \mathbf{K}_{\mathbf{Tu}} & \mathbf{K}_{\mathbf{TT}} \end{pmatrix} \begin{pmatrix} \Delta \mathbf{u} \\ \Delta T \end{pmatrix} = - \begin{pmatrix} \mathbf{R}_{\mathbf{u}}(\mathbf{u}, T) \\ \mathbf{R}_{\mathbf{T}}(\mathbf{u}, T) \end{pmatrix}. \quad (3.41)$$

The new solution is given by  $\mathbf{E}^{\mathbf{i}+1} = \mathbf{E}^{\mathbf{i}} + \Delta \mathbf{E}$ , and the iterations continue until the convergence is obtained, that is  $\|\mathbf{R}\| < \text{tol}$ .

The formula of the forces can be derived from Eqs. (3.16) and (3.19), which lead at each node a to:

$$\mathbf{F}_{\mathbf{u}\text{ext}}^{\mathbf{a}} = \mathbf{F}_{\mathbf{u}\text{int}}^{\mathbf{a}} + \mathbf{F}_{\mathbf{u}\text{I}}^{\mathbf{a}}, \quad (3.42)$$

$$F_{\text{T}\text{ext}}^{\mathbf{a}} = F_{\text{T}\text{int}}^{\mathbf{a}} + F_{\text{T}\text{I}}^{\mathbf{a}}. \quad (3.43)$$

First, the mechanical contribution, Eq. (3.42), reads

$$\begin{aligned} \mathbf{F}_{\mathbf{u}\text{ext}}^{\mathbf{a}} &= \int_{\partial_{\text{N}}\Omega_{\text{h}}} \mathbf{N}_{\mathbf{u}}^{\mathbf{a}} \bar{\mathbf{t}} \, \text{dS} - \int_{\partial_{\text{D}}\Omega_{\text{h}}} \bar{\mathbf{u}} \cdot (\mathcal{H} \cdot \nabla \mathbf{N}_{\mathbf{u}}^{\mathbf{a}}) \cdot \mathbf{n} \, \text{dS} + \int_{\partial_{\text{D}}\Omega_{\text{h}}} \bar{\mathbf{u}} \otimes \mathbf{n} : \left( \frac{\mathcal{H}\mathcal{B}}{h_{\text{s}}} \right) \cdot \mathbf{n} \mathbf{N}_{\mathbf{u}}^{\mathbf{a}} \, \text{dS} \\ &+ \gamma \int_{\partial_{\text{D}}\Omega_{\text{h}}} \mathbf{N}_{\mathbf{u}}^{\mathbf{a}} (\boldsymbol{\alpha}_{\text{th}} : \mathcal{H}\bar{\mathbf{T}}) \cdot \mathbf{n} \, \text{dS}, \end{aligned} \quad (3.44)$$

$$\mathbf{F}_{\mathbf{u}\text{int}}^{\mathbf{a}} = \sum_{\text{s}} \int_{\Omega^e} \boldsymbol{\sigma} \cdot \nabla \mathbf{N}_{\mathbf{u}}^{\mathbf{a}} \, \text{d}\Omega, \quad (3.45)$$

$$\mathbf{F}_{\mathbf{u}\text{I}}^{\mathbf{a}\pm} = \mathbf{F}_{\mathbf{u}\text{I}1}^{\mathbf{a}\pm} + \mathbf{F}_{\mathbf{u}\text{I}2}^{\mathbf{a}\pm} + \mathbf{F}_{\mathbf{u}\text{I}3}^{\mathbf{a}\pm}, \quad (3.46)$$

with the three mechanical contributions to the interface forces<sup>1</sup>

$$\mathbf{F}_{\mathbf{u}\text{I}1}^{\mathbf{a}\pm} = \sum_{\text{s}} \int_{(\partial_{\text{T}}\Omega)^{\text{s}}} (\pm \mathbf{N}_{\mathbf{u}}^{\mathbf{a}\pm}) \langle \boldsymbol{\sigma} \rangle \cdot \mathbf{n}^- \, \text{dS}, \quad (3.47)$$

$$\begin{aligned} \mathbf{F}_{\mathbf{u}\text{I}2}^{\mathbf{a}\pm} &= \frac{1}{2} \sum_{\text{s}} \int_{(\partial_{\text{T}}\Omega)^{\text{s}}} \llbracket \mathbf{u}_{\text{h}} \rrbracket \cdot (\mathcal{H}^{\pm} \cdot \nabla \mathbf{N}_{\mathbf{u}}^{\mathbf{a}\pm}) \cdot \mathbf{n}^- \, \text{dS} \\ &- \frac{\gamma}{2} \sum_{\text{s}} \int_{(\partial_{\text{T}}\Omega)^{\text{s}}} \mathbf{N}_{\mathbf{u}}^{\mathbf{a}\pm} \llbracket \boldsymbol{\alpha}_{\text{th}} : \mathcal{H}\mathbf{T}_{\text{h}} \rrbracket \cdot \mathbf{n}^- \, \text{dS}, \end{aligned} \quad (3.48)$$

$$\mathbf{F}_{\mathbf{u}\text{I}3}^{\mathbf{a}\pm} = \sum_{\text{s}} \int_{(\partial_{\text{T}}\Omega)^{\text{s}}} (\llbracket \mathbf{u}_{\text{h}} \rrbracket \otimes \mathbf{n}^-) : \left\langle \frac{\mathcal{H}\mathcal{B}}{h_{\text{s}}} \right\rangle \cdot \mathbf{n}^- (\pm \mathbf{N}_{\mathbf{u}}^{\mathbf{a}\pm}) \, \text{dS}. \quad (3.49)$$

In these equations the symbol  $\pm$  refers to the node  $\mathbf{a}^{\pm}$  (+ for node  $\mathbf{a}^+$  and  $-$  for node  $\mathbf{a}^-$ ). By the same way, the thermal contributions read

$$F_{\text{T}\text{ext}}^{\mathbf{a}} = - \int_{\partial_{\text{N}}\Omega_{\text{h}}} \mathbf{N}_{\text{T}}^{\mathbf{a}} \bar{q} \, \text{dS} - \int_{\partial_{\text{D}}\Omega_{\text{h}}} (\mathbf{k} \cdot \nabla \mathbf{N}_{\text{T}}^{\mathbf{a}}) \cdot \mathbf{n} \bar{\mathbf{T}} \, \text{dS} + \int_{\partial_{\text{D}}\Omega_{\text{h}}} \mathbf{N}_{\text{T}}^{\mathbf{a}} \mathbf{n} \cdot \frac{\mathbf{k}\mathcal{B}}{h_{\text{s}}} \cdot \mathbf{n} \bar{\mathbf{T}} \, \text{dS}, \quad (3.50)$$

$$F_{\text{T}\text{int}}^{\mathbf{a}} = - \sum_{\text{e}} \int_{\Omega^e} \mathbf{q} \cdot \nabla \mathbf{N}_{\text{T}}^{\mathbf{a}} \, \text{d}\Omega + \sum_{\text{e}} \int_{\Omega^e} \rho c_{\text{v}} \dot{\mathbf{T}} \mathbf{N}_{\text{T}}^{\mathbf{a}} \, \text{d}\Omega, \quad (3.51)$$

$$F_{\text{T}\text{I}}^{\mathbf{a}\pm} = F_{\text{T}\text{I}1}^{\mathbf{a}\pm} + F_{\text{T}\text{I}2}^{\mathbf{a}\pm} + F_{\text{T}\text{I}3}^{\mathbf{a}\pm}, \quad (3.52)$$

where the three thermal contributions to the interface forces read

$$F_{\text{T}\text{I}1}^{\mathbf{a}\pm} = \sum_{\text{s}} \int_{(\partial_{\text{T}}\Omega)^{\text{s}}} (\mp \mathbf{N}_{\text{T}}^{\mathbf{a}\pm}) \langle \mathbf{q} \rangle \cdot \mathbf{n}^- \, \text{dS}, \quad (3.53)$$

<sup>1</sup>The contributions on  $\partial_{\text{D}}\Omega_{\text{h}}$  can be directly deduced by removing the factor (1/2) accordingly to the definition of the average flux on the Dirichlet boundary.

$$F_{\text{TI}2}^{\text{a}\pm} = \frac{1}{2} \sum_s \int_{(\partial_1 \Omega)^s} \llbracket \text{T}_h \rrbracket (\mathbf{k}^\pm \cdot \nabla N_{\text{T}}^{\text{a}\pm}) \cdot \mathbf{n}^- \, dS, \quad (3.54)$$

$$F_{\text{TI}3}^{\text{a}\pm} = \sum_s \int_{(\partial_{\text{DI}} \Omega)^s} \llbracket \text{T}_h \rrbracket \mathbf{n}^- \cdot \left\langle \mathbf{k} \frac{\mathcal{B}}{h_s} \right\rangle \cdot \mathbf{n}^- (\pm N_{\text{T}}^{\text{a}\pm}) \, dS. \quad (3.55)$$

The stiffness matrix, has been decomposed into four sub-matrices with respect to the discretization of the four independent fields variables (3 for displacement  $\mathbf{u}$  and 1 for the temperature T), see Appendix B.1 for the details.

### 3.4 Numerical properties of linear Thermo-Elastic DG formulation

In order to prove the consistency and the stability of the DG formulation for linear Thermo-Elastic formulations, we consider a steady state. Therefore the equation that governs the linear Thermo-Elastic coupling, Eq. (3.6), is rewritten in the following elliptic form

$$-\nabla^{\text{T}}(\mathbf{w}\nabla\mathbf{E}) + \nabla^{\text{T}}(\mathbf{r}\mathbf{E}) = 0, \quad \text{in } \Omega. \quad (3.56)$$

More details about the analysis of such linear elliptic problem formulation have been discussed in [74] for the case of one-field formulation. For the sake of completeness, we report the analysis for coupled problem here after. Henceforth, the weak DG formulation of the problem becomes, find  $\mathbf{E} \in X$  such that

$$a(\mathbf{E}, \delta\mathbf{E}) = b(\delta\mathbf{E}) \quad \forall \delta\mathbf{E} \in X, \quad (3.57)$$

with  $a(\mathbf{E}, \delta\mathbf{E})$  and  $b(\delta\mathbf{E})$  defined by Eq. (3.24) and Eq. (3.25) respectively.

It should be noted that the norms defined in Chapter 2, Eqs. (2.10 -2.12), are considered for the linear Thermo-Elastic coupling, with  $\mathbf{O} \equiv \mathbf{E}$ , which is a vector of size  $(d+1) \times 1$ .

Moreover, we have the following properties:

- The matrix  $\mathbf{w}$ , is a symmetric real matrix of size  $(4d-3) \times (4d-3)$  whose entries are bounded, piecewise continuous real-valued functions defined on  $\bar{\Omega}$ , and for every non-zero column vector  $\boldsymbol{\xi}$  of 9 real numbers, one has

$$\boldsymbol{\xi}^{\text{T}} \mathbf{w}(\mathbf{x}) \boldsymbol{\xi} > 0 \quad \forall \boldsymbol{\xi} \in \mathbb{R}^{4d-3}, \mathbf{x} \in \bar{\Omega}. \quad (3.58)$$

Let  $\lambda$  be the minimum eigenvalue of the matrix  $\mathbf{w}$ , then there is a positive constant  $C_\alpha$  such that

$$0 < C_\alpha < \lambda. \quad (3.59)$$

- There exists  $C_x$  such that

$$C_x = \max \{ \|\mathbf{w}\|_{L^\infty(\Omega)}, \|\mathbf{r}\|_{L^\infty(\Omega)} \}. \quad (3.60)$$

### 3.4.1 Consistency

To prove the consistency of the method, the exact solution  $\mathbf{E}^e \in [H^2(\Omega)]^d \times H^2(\Omega)$  of the problem is considered. This implies  $[[\mathbf{E}^e]] = 0$ ,  $\langle \mathbf{w} \nabla \mathbf{E}^e \rangle = \mathbf{w} \nabla \mathbf{E}^e$  on  $\partial_I \Omega_h$ , and  $[[\mathbf{E}^e]] = -\bar{\mathbf{E}}$  and  $\langle \mathbf{w} \nabla \mathbf{E}^e \rangle = \mathbf{w} \nabla \mathbf{E}^e$  on  $\partial_D \Omega_h$ . Therefore, Eq. (3.23) becomes:

$$\begin{aligned}
& \int_{\partial_N \Omega_h} \delta \mathbf{E}^T \bar{\mathbf{c}} dS - \int_{\partial_D \Omega_h} \bar{\mathbf{E}}_n^T \mathbf{w} \nabla \delta \mathbf{E} dS + \int_{\partial_D \Omega_h} \delta \mathbf{E}_n^T \left( \frac{\mathcal{B}}{h_s} \mathbf{w} \right) \bar{\mathbf{E}}_n dS \\
& + \gamma \int_{\partial_D \Omega_h} \delta \mathbf{E}_n^T \mathbf{r} \bar{\mathbf{E}} dS = \int_{\Omega_h} (\nabla \delta \mathbf{E})^T \mathbf{w} \nabla \mathbf{E}^e d\Omega - \int_{\Omega_h} (\nabla \delta \mathbf{E})^T \mathbf{r} \mathbf{E}^e d\Omega \\
& + \int_{\partial_I \Omega_h} [[\delta \mathbf{E}_n^T]] \mathbf{w} \nabla \mathbf{E}^e dS - \int_{\partial_I \Omega_h} [[\delta \mathbf{E}_n^T]] \mathbf{r} \mathbf{E}^e dS - \int_{\partial_D \Omega_h} \mathbf{E}_n^{eT} \mathbf{w} \nabla \delta \mathbf{E} dS \\
& - \int_{\partial_D \Omega_h} \delta \mathbf{E}_n^T \mathbf{w} \nabla \mathbf{E}^e dS + \int_{\partial_D \Omega_h} \delta \mathbf{E}_n^T \frac{\mathcal{B}}{h_s} \mathbf{w} \mathbf{E}_n^e dS + (1 + \gamma) \int_{\partial_D \Omega_h} \delta \mathbf{E}_n^T \mathbf{r} \mathbf{E}^e dS \quad \forall \delta \mathbf{E} \in X.
\end{aligned} \tag{3.61}$$

Integrating the first term of the right hand side by parts leads to

$$\sum_e \int_{\Omega^e} (\nabla \delta \mathbf{E})^T \mathbf{w} \nabla \mathbf{E}^e d\Omega = - \sum_e \int_{\Omega^e} \delta \mathbf{E}^T \nabla^T (\mathbf{w} \nabla \mathbf{E}^e) d\Omega + \sum_e \int_{\partial \Omega^e} \delta \mathbf{E}_n^T \mathbf{w} \nabla \mathbf{E}^e dS. \tag{3.62}$$

Similarly, we have

$$\sum_e \int_{\Omega^e} (\nabla \delta \mathbf{E})^T \mathbf{r} \mathbf{E}^e d\Omega = - \sum_e \int_{\Omega^e} \delta \mathbf{E}^T \nabla^T (\mathbf{r} \mathbf{E}^e) d\Omega + \sum_e \int_{\partial \Omega^e} \delta \mathbf{E}_n^T \mathbf{r} \mathbf{E}^e dS. \tag{3.63}$$

Substituting Eqs. (3.62) and (3.63) in Eq. (3.61), yields

$$\begin{aligned}
& \int_{\partial_N \Omega_h} \delta \mathbf{E}^T \bar{\mathbf{c}} dS - \int_{\partial_D \Omega_h} \bar{\mathbf{E}}_n^T (\mathbf{w} \nabla \delta \mathbf{E}) dS + \int_{\partial_D \Omega_h} \delta \mathbf{E}_n^T \left( \frac{\mathcal{B}}{h_s} \mathbf{w} \right) \bar{\mathbf{E}}_n dS \\
& + \gamma \int_{\partial_D \Omega_h} \delta \mathbf{E}_n^T \mathbf{r} \bar{\mathbf{E}} dS = - \int_{\Omega_h} \delta \mathbf{E}^T \nabla^T (\mathbf{w} \nabla \mathbf{E}^e) d\Omega + \int_{\partial_N \Omega_h} \delta \mathbf{E}_n^T (\mathbf{w} \nabla \mathbf{E}^e) dS \\
& + \int_{\Omega_h} \delta \mathbf{E}^T \nabla^T (\mathbf{r} \mathbf{E}^e) d\Omega - \int_{\partial_N \Omega_h} \delta \mathbf{E}_n^T \mathbf{r} \mathbf{E}^e dS - \int_{\partial_D \Omega_h} \mathbf{E}_n^{eT} \mathbf{w} \nabla \delta \mathbf{E} dS \\
& + \int_{\partial_D \Omega_h} \delta \mathbf{E}_n^T \frac{\mathcal{B}}{h_s} \mathbf{w} \mathbf{E}_n^e dS + \gamma \int_{\partial_D \Omega_h} \delta \mathbf{E}_n^T \mathbf{r} \mathbf{E}^e dS.
\end{aligned} \tag{3.64}$$

The arbitrary nature of the test functions  $\delta \mathbf{E}$  leads to recover the set of conservation laws, Eq. (3.6), and the boundary conditions, Eqs. (3.8) and (3.7).

### 3.4.2 Solution uniqueness

In this part and in the following sections, we assume that  $\partial_D \Omega_h = \partial \Omega_h$ . This assumption is not restrictive but simplifies the demonstrations.

**Lemma 3.4.1** (Lower bound). *For  $\mathcal{B}$  larger than a constant, which depends on the polynomial approximation only, there exist two positive constants  $C_1^k$  and  $C_2^k$ , such that*

$$a(\delta \mathbf{E}_h, \delta \mathbf{E}_h) \geq C_1^k \|\delta \mathbf{E}_h\|_*^2 - C_2^k \|\delta \mathbf{E}_h\|_{L^2(\Omega)}^2 \quad \forall \delta \mathbf{E}_h \in X^k, \tag{3.65}$$



$$a(\delta \mathbf{E}_h, \delta \mathbf{E}_h) \geq C_1^k \|\delta \mathbf{E}_h\|^2 - C_2^k \|\delta \mathbf{E}_h\|_{L^2(\Omega)}^2 \quad \forall \delta \mathbf{E}_h \in X^k, \quad (3.66)$$

where the norms have been defined by Eqs. (2.10, 2.11).

Proceeding by using the bounds (3.59) and (3.60), the Cauchy-Schwartz' inequality, Eq. (3.60), the trace inequality on the finite element space (2.18), the trace inequality, Eq. (2.16), and inverse inequality, Eq. (2.21), the  $\xi$ -inequality  $-\xi > 0 : |ab| \leq \frac{\xi}{4}a^2 + \frac{1}{\xi}b^2$ , as in Wheeler et al. [74] and Prudhomme et al. [60] analysis with some modifications, yields to prove this Lemma 3.4.1. The two positive constants  $C_1^k, C_2^k$  are independent of the mesh size, but do depend on  $k$  and  $\mathcal{B}$ , for details, see Appendix B.2. In particular, for  $C^k$  to be positive the following constrain on the stabilization parameter should be satisfied  $\mathcal{B} > \frac{C_\alpha^2}{C_\alpha} \max(4C_T(C_T^k+1), 4C_K^k)$ . Therefore for the method to be stable, the stabilization parameter should be large enough depending on the polynomial approximation under consideration for  $C_1^k$  to remain positive.

**Lemma 3.4.2** (Upper bound). *There exist  $C > 0$  and  $C^k > 0$  such that*

$$|a(\mathbf{m}, \delta \mathbf{E})| \leq C \|\mathbf{m}\|_1 \|\delta \mathbf{E}\|_1 \quad \forall \mathbf{m}, \delta \mathbf{E} \in X, \quad (3.67)$$

$$|a(\mathbf{m}, \delta \mathbf{E}_h)| \leq C^k \|\mathbf{m}\|_1 \|\delta \mathbf{E}_h\| \quad \forall \mathbf{m} \in X, \delta \mathbf{E}_h \in X^k, \quad (3.68)$$

$$|a(\mathbf{m}_h, \delta \mathbf{E}_h)| \leq C^k \|\mathbf{m}_h\| \|\delta \mathbf{E}_h\| \quad \forall \mathbf{m}_h, \delta \mathbf{E}_h \in X^k, \quad (3.69)$$

where the norms have been defined by Eqs. (2.10-2.12).

Applying the Hölder's inequality, Eq. (2.24), and the bound (3.60) on each term of  $a(\mathbf{m}, \delta \mathbf{E})$  and then applying the Cauchy-Schwartz' inequality, Eq. (2.27), lead to relation (3.67). Therefore relations (3.68) and (3.69) are easily deduced from the relation between energy norms on the finite element space, Eq. (2.22). The proof is presented in Appendix B.3.

Using Lemma 3.4.1 and Lemma 3.4.2, the stability of the method is demonstrated using the following Lemma.

**Lemma 3.4.3** (Auxiliary problem). *We consider the following auxiliary problem, with  $\phi \in [L^2(\Omega_h)]^d \times L^2(\Omega_h)$ :*

$$\begin{aligned} -\nabla^T(\mathbf{w}\nabla\psi) + \tilde{\mathbf{r}}\nabla\psi &= \phi \quad \text{on } \Omega_h, \\ \psi &= 0 \quad \text{on } \partial\Omega_h. \end{aligned} \quad (3.70)$$

Assuming regular ellipticity of the operator, there is a unique solution  $\psi \in [H^2(\Omega_h)]^d \times H^2(\Omega_h)$  to the problem stated by Eq. (3.70) satisfying the elliptic property

$$\|\psi\|_{H^2(\Omega_h)} \leq C \|\phi\|_{L^2(\Omega_h)}. \quad (3.71)$$

The proof for one field is given in [23], by combining [23, Theorem 8.3] to [23, Lemma 9.17].

Moreover, for a given  $\varphi \in [L^2(\Omega_h)]^d \times L^2(\Omega_h)$ . There exists a unique  $\phi_h \in X^k$  such that

$$a(\delta \mathbf{E}_h, \phi_h) = \sum_e \int_{\Omega^e} \varphi^T \delta \mathbf{E}_h d\Omega \quad \forall \delta \mathbf{E}_h \in X^k, \quad (3.72)$$

and there is a constant  $C^k$  such that:

$$\|\phi_h\| \leq C^k \|\varphi\|_{L^2(\Omega_h)}. \quad (3.73)$$

The proof follows from the use of Lemma 3.4.1 to bound  $\|\phi_h\|$  in terms of  $\|\varphi\|_{L^2(\Omega_h)}$  and  $\|\phi_h\|_{L^2(\Omega_h)}$ .  $\|\phi_h\|_{L^2(\Omega_h)}$  is then estimated by considering  $\phi = \phi_h \in X^k$  in Eq. (3.70), multiplying the result by  $\phi_h$  and integrating it by parts on  $\Omega_h$  yielding  $\|\phi_h\|_{L^2(\Omega_h)}^2 = a(\psi, \phi_h)$ . Inserting the interpolant  $I_h\phi$  in these last terms, making successive use of Lemmata 3.4.2 and 2.4.6, and using the regular ellipticity Eq. (3.71) allows deriving the bound  $\|\phi_h\|_{L^2(\Omega_h)} \leq C^k \|\varphi\|_{L^2(\Omega_h)}$ , which results into the proof of (3.73). The proof is derived in details in Appendix B.4.

The proof of the uniqueness can be derived directly using the auxiliary problem defined in Lemma 3.4.3. Let us assume there exist two solutions  $\mathbf{E}_{h_1}, \mathbf{E}_{h_2}$  for the problem stated in Eq. (3.57), such that we get

$$a(\mathbf{E}_{h_1} - \mathbf{E}_{h_2}, \delta\mathbf{E}_h) = 0 \quad \forall \delta\mathbf{E}_h \in X^k, \quad (3.74)$$

Let  $\boldsymbol{\nu} = \mathbf{E}_{h_1} - \mathbf{E}_{h_2}$ , then by recalling the auxiliary problem defined in Lemma Eq. (3.72), and setting  $\varphi = \boldsymbol{\nu}$  and  $\delta\mathbf{E}_h = \boldsymbol{\nu}$

$$\|\boldsymbol{\nu}\|_{L^2(\Omega_h)}^2 = a(\boldsymbol{\nu}, \phi_h) = a(\mathbf{E}_{h_1} - \mathbf{E}_{h_2}, \phi_h) = 0. \quad (3.75)$$

Hence  $\mathbf{E}_{h_1} = \mathbf{E}_{h_2}$  and there exist a unique solution  $\mathbf{E}_h$  for the problem Eq. (3.57).

### 3.4.3 Error in the energy norm

Let us decompose the global error which is the difference between the exact solution and the approximated solution  $\mathbf{e} = \mathbf{E}^e - \mathbf{E}_h$  by adding and subtracting the interpolation of the exact solution  $I_h\mathbf{E}$ , such that we get  $\mathbf{e} = \boldsymbol{\xi} - \boldsymbol{\eta}$ , with  $\boldsymbol{\xi} = I_h\mathbf{E} - \mathbf{E}_h \in X^k$  and  $\boldsymbol{\eta} = \mathbf{E}^e - I_h\mathbf{E} \in X$ , we thus obtain

$$\|\mathbf{e}\|_1 = \|\mathbf{E}^e - \mathbf{E}_h\|_1 = \|\boldsymbol{\xi} - \boldsymbol{\eta}\|_1 \leq \|\boldsymbol{\xi}\|_1 + \|\boldsymbol{\eta}\|_1. \quad (3.76)$$

By the use of the lower bound, Eq. (3.66), we have

$$C_1^k \|\boldsymbol{\xi}\|_1^2 - C_2^k \|\boldsymbol{\xi}\|_{L^2(\Omega_h)}^2 \leq a(\boldsymbol{\xi}, \boldsymbol{\xi}) = a((I_h\mathbf{E} - \mathbf{E}^e) + (\mathbf{E}^e - \mathbf{E}_h), \boldsymbol{\xi}). \quad (3.77)$$

From the Galerkin orthogonality property, i.e. as both  $\mathbf{E}^e$  and  $\mathbf{E}_h$  satisfy the weak form Eq. (3.23),  $a(\mathbf{E}^e - \mathbf{E}_h, \delta\mathbf{E}_h) = 0 \quad \forall \delta\mathbf{E}_h \in X^k$ , and

$$C_1^k \|\boldsymbol{\xi}\|_1^2 - C_2^k \|\boldsymbol{\xi}\|_{L^2(\Omega_h)}^2 \leq a(-\boldsymbol{\eta}, \boldsymbol{\xi}) \leq C^k \|\boldsymbol{\eta}\|_1 \|\boldsymbol{\xi}\|_1, \quad (3.78)$$

where we have used the upper bound Eq. (3.68). Moreover, as  $\|\boldsymbol{\xi}\|_{L^2(\Omega_h)} < \|\boldsymbol{\xi}\|_1$ , this last relation becomes

$$\|\boldsymbol{\xi}\|_1 \leq C^k \|\boldsymbol{\eta}\|_1 + C_2^k \|\boldsymbol{\xi}\|_{L^2(\Omega_h)}. \quad (3.79)$$

In order to bound  $\|\boldsymbol{\xi}\|_{L^2(\Omega_h)}$ , using the property of Lemma 3.4.3 and stating  $\boldsymbol{\varphi} = \boldsymbol{\xi}$ , the orthogonality relation,  $\delta\mathbf{E}_h = \boldsymbol{\xi}$ , and the upper bound Eq. (3.68), leads to

$$\|\boldsymbol{\xi}\|^2 = a(\boldsymbol{\xi}, \boldsymbol{\phi}_h) = a(-\boldsymbol{\eta}, \boldsymbol{\phi}_h) \leq C^k \|\boldsymbol{\eta}\|_1 \|\boldsymbol{\phi}_h\|. \quad (3.80)$$

Then using Eq. (3.73), Eq. (3.80) is rewritten as

$$\|\boldsymbol{\xi}\| \leq C^k \|\boldsymbol{\eta}\|_1. \quad (3.81)$$

Substituting this result in Eq. (3.79), yields

$$\|\boldsymbol{\xi}\| \leq C^k \|\boldsymbol{\eta}\|_1, \quad (3.82)$$

which leads to bound the error in term of  $\boldsymbol{\eta}$ , such that Eq. (3.76) becomes

$$\|\mathbf{e}\|_1 \leq C^k \|\boldsymbol{\eta}\|_1. \quad (3.83)$$

Using the energy norm bound of the interpolant error, Lemma 2.4.6, Eq. (2.23), for  $h_s$  small enough, there exists a constant  $C^k$  such that

$$\|\mathbf{e}\|_1 \leq C^k h_s^{\mu-1} \|\mathbf{E}^e\|_{H^s(\Omega_h)}, \quad (3.84)$$

with  $\mu = \min\{s, k+1\}$ .

#### 3.4.4 Error estimate in the $L^2$ -norm

Since the linear problem is adjoint consistent, an optimal order of convergence in the  $L^2$ -norm is obtained by applying the duality argument.

To this end, let us consider the following dual problem

$$\begin{aligned} -\nabla^T(\mathbf{w}\nabla\boldsymbol{\psi} + \tilde{\mathbf{r}}^T\boldsymbol{\psi}) &= \mathbf{e} \quad \text{on } \Omega_h, \\ \boldsymbol{\psi} &= \mathbf{g} \quad \text{on } \partial\Omega_h, \end{aligned} \quad (3.85)$$

which is assumed to satisfy the elliptic regularity condition as  $\mathbf{w}$  is positive definite with  $\boldsymbol{\psi} \in [H^{2m}(\Omega_h)]^d \times H^{2m}(\Omega_h)$  for  $p \geq 2m$  and

$$\|\boldsymbol{\psi}\|_{H^p(\Omega_h)} \leq C \left( \|\mathbf{e}\|_{H^{p-2m}(\Omega_h)} + \|\mathbf{g}\|_{H^{p-\frac{1}{2}}(\partial\Omega_h)} \right), \quad (3.86)$$

if  $\mathbf{e} \in [H^{p-2m}(\Omega_h)]^d \times H^{p-2m}(\Omega_h)$ .

Considering  $\mathbf{e} = \mathbf{E}^e - \mathbf{E}_h \in [L^2(\Omega_h)]^d \times L^2(\Omega_h)$  be the error and  $\mathbf{g} = 0$ , multiplying Eq. (3.85) by  $\mathbf{e}$ , and integrating over  $\Omega_h$

$$\int_{\Omega_h} [\mathbf{w}\nabla\boldsymbol{\psi}]^T \nabla\mathbf{e} d\Omega - \int_{\Omega_h} \mathbf{e}^T [\nabla^T(\tilde{\mathbf{r}}^T\boldsymbol{\psi})] d\Omega - \sum_e \int_{\partial\Omega^e} [\mathbf{w}\nabla\boldsymbol{\psi}]^T \mathbf{e}_n dS = \|\mathbf{e}\|_{L^2(\Omega_h)}^2, \quad (3.87)$$

with

$$\|\boldsymbol{\psi}\|_{H^2(\Omega_h)} \leq C \|\mathbf{e}\|_{L^2(\Omega_h)}. \quad (3.88)$$

However  $\nabla^T(\tilde{\mathbf{r}}^T \boldsymbol{\psi}) = \mathbf{r}^T \nabla \boldsymbol{\psi}$  as shown in Eq. (3.28) and Eq. (3.87) becomes

$$\begin{aligned} & \int_{\Omega_h} [\mathbf{w} \nabla \boldsymbol{\psi}]^T \nabla \mathbf{e} d\Omega + \int_{\partial_I \Omega_h} [\mathbf{w} \nabla \boldsymbol{\psi}]^T \llbracket \mathbf{e}_n \rrbracket dS - \int_{\partial_D \Omega_h} [\mathbf{w} \nabla \boldsymbol{\psi}]^T \mathbf{e}_n dS \\ & - \int_{\Omega_h} [\mathbf{r} \mathbf{e}]^T \nabla \boldsymbol{\psi} d\Omega = \|\mathbf{e}\|_{L^2(\Omega_h)}. \end{aligned} \quad (3.89)$$

Therefore since  $\llbracket \boldsymbol{\psi} \rrbracket = \llbracket \nabla \boldsymbol{\psi} \rrbracket = 0$  on  $\partial_I \Omega_h$  and  $\boldsymbol{\psi} = 0$  on  $\partial_D \Omega_h$ , and since  $\mathbf{w}$  is symmetric, by the comparison with Eq. (3.24), Eq. (3.89) reads for  $\gamma = 0$ ,

$$\|\mathbf{e}\|_{L^2(\Omega_h)}^2 = a(\mathbf{e}, \boldsymbol{\psi}). \quad (3.90)$$

Considering  $I_h \boldsymbol{\psi} \in X^k$ , and using the orthogonality relation, Eq. (3.90) is rewritten

$$\begin{aligned} \|\mathbf{e}\|_{L^2(\Omega_h)}^2 &= a(\mathbf{e}, \boldsymbol{\psi} - I_h \boldsymbol{\psi}) - a(\mathbf{e}, I_h \boldsymbol{\psi}) \\ &= a(\mathbf{e}, \boldsymbol{\psi} - I_h \boldsymbol{\psi}) - a(\mathbf{E}^e, I_h \boldsymbol{\psi}) + a(\mathbf{E}_h, I_h \boldsymbol{\psi}) \\ &= a(\mathbf{e}, \boldsymbol{\psi} - I_h \boldsymbol{\psi}). \end{aligned} \quad (3.91)$$

Using Lemma 3.4.2, Eq. (3.67), Lemma 2.4.6, Eq. (2.23), and Eq. (3.84), leads to

$$\begin{aligned} |a(\mathbf{e}, \boldsymbol{\psi} - I_h \boldsymbol{\psi})| &\leq C^k \|\mathbf{e}\|_1 \|\boldsymbol{\psi} - I_h \boldsymbol{\psi}\|_1 \\ &\leq C^k \|\mathbf{e}\|_1 h_s \|\boldsymbol{\psi}\|_{H^2(\Omega_h)} \\ &\leq C^k h_s \|\mathbf{E}^e - I_h \mathbf{E}\|_1 \|\boldsymbol{\psi}\|_{H^2(\Omega_h)} \\ &\leq C^k h_s^\mu \|\mathbf{E}^e\|_{H^s(\Omega_h)} \|\boldsymbol{\psi}\|_{H^2(\Omega_h)}, \end{aligned} \quad (3.92)$$

and using Eq. (3.88), this last result becomes

$$|a(\mathbf{e}, \boldsymbol{\psi} - I_h \boldsymbol{\psi})| \leq C^k h_s^\mu \|\mathbf{E}^e\|_{H^s(\Omega_h)} \|\mathbf{e}\|_{L^2(\Omega_h)}. \quad (3.93)$$

Therefore, by substituting this last result into Eq. (3.91), the final result of the  $L^2$ -norm error estimate is thus

$$\|\mathbf{e}\|_{L^2(\Omega_h)} \leq C^k h_s^\mu \|\mathbf{E}^e\|_{H^s(\Omega_h)}, \quad (3.94)$$

with  $\mu = \min\{s, k+1\}$ . This result demonstrates the optimal convergence rate in the  $L^2$ -norm of the method in terms of the mesh size  $h_s$ , providing  $\gamma$  is equal to 0 in relation (3.20). Indeed the convergence rate is  $k+1$  for  $s \geq k+1$ .

### 3.5 Numerical results

In this section, a numerical model for a pipe made of steel subjected to temperature differences is considered. Due to the symmetric nature of the problem, the study is restricted to a quarter of the pipe, whose planar model in plane strain is depicted in Fig. 3.1. The system's parameters are given in Table 3.1. An example of the mesh that is used for the numerical results is presented in Fig. 3.2.

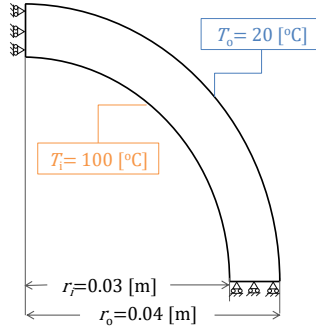


Figure 3.1: The boundary conditions for a quarter of a pipe

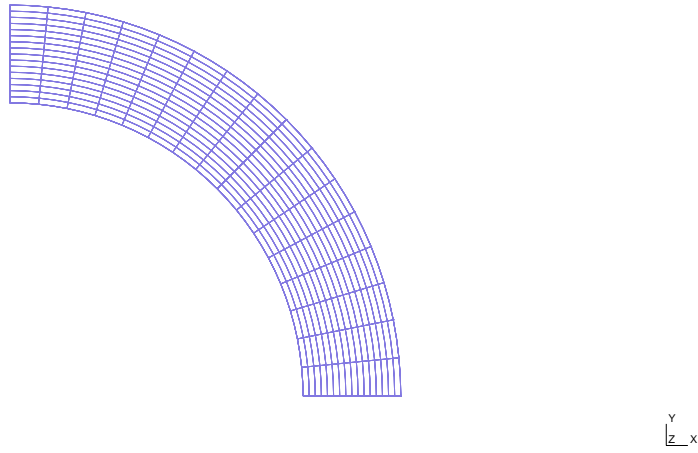


Figure 3.2: Mesh example

Table 3.1: Steel parameters

Parameter	Value
Density $\rho$ [Kg/m <sup>3</sup> ]	7850
Young's modulus E [Pa]	$2 \times 10^{11}$
Poisson ratio $\nu$ [-]	0.3
Thermal expansion $\alpha_{th}$ [1/K]	diag( $1.2 \times 10^{-5}$ )
Thermal conductivity $\mathbf{k}$ [W/(K · m)]	diag(51.9)

The analytical solutions for the pipe in a plane strain state are given as follows. Considering  $T_o$  is the temperature at the outer radius  $r_o$ , while  $T_i$  and  $r_i$  denote the same respective features, at the inner part, the analytical solution at any radius  $r$  is derived by following the approach proposed in [26], leading to

$$T(r) = C \left[ T_i + \frac{T_o - T_i}{\ln\left(\frac{r_o}{r_i}\right)} \ln\left(\frac{r}{r_i}\right) \right], \quad (3.95)$$

$$\sigma_r(r) = C \left[ \frac{\ln(\frac{r_o}{r})}{\ln(\frac{r_o}{r_i})} - \frac{\frac{r_o}{r} - 1}{\frac{r_o}{r_i} - 1} \right], \quad (3.96)$$

$$\sigma_\theta(r) = C \left[ \frac{\ln(\frac{r_o}{r} - 1)}{\ln(\frac{r_o}{r_i})} + \frac{\frac{r_o}{r} + 1}{\frac{r_o}{r_i} - 1} \right], \text{ and} \quad (3.97)$$

$$\sigma_z(r) = \nu(\sigma_r + \sigma_\theta) - \alpha_{th}TE, \quad (3.98)$$

where  $C = \frac{-E\alpha(T_i - T_o)}{2(1-\nu)}$ . The problem is solved numerically using the Finite Element implementation of the DG formulation Eq. (3.57), with  $\gamma = 0$ . Quadratic polynomial approximations and a stabilization parameter of value of 10 are considered. Figures 3.3, 3.4, 3.5, and 3.6 present the respective analytical and DGFEM solutions to our problem. It can be seen that the temperature distribution and the stress distribution agree very well with the analytical solution. The resulting dilatation of the outer radius is  $2.257 \times 10^{-3}$  [cm].

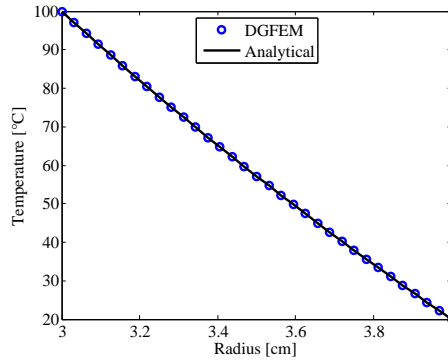


Figure 3.3: Analytical and numerical distributions of the temperature along the radius

The accuracy of the method is tested by analyzing the  $H^1$ -norm and  $L^2$ -norm. The error measured in the  $H^1$ -norm against the mesh size in the log-log scale is illustrated in Fig. 3.7(a), where the analytical solution is used as a reference solution. The optimal rate is observed and matches the theoretical order of convergence obtained in Section 3.4.3. In Fig. 3.7(b), as a uniform mesh refinement for polynomial of second degree is applied, a third order convergence rate in the  $L^2$ -norm is observed which agrees with the theorem derived in Section 3.4.4.

## 3.6 Conclusions

Throughout this chapter, the discontinuous Galerkin weak formulation for linear Thermo-Elasticity coupled problem has been derived. The stability of the bilinear weak form has been proved for stabilization parameter larger than a constant which depends on the polynomial order only. The error estimates in the  $H^1$ - and  $L^2$ -norms were derived as being optimal which has been verified through a numerical example.

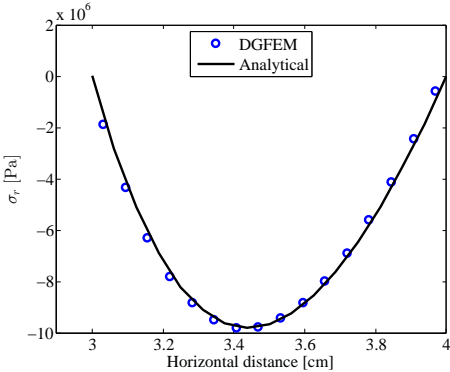


Figure 3.4: Analytical and numerical radial stress distributions

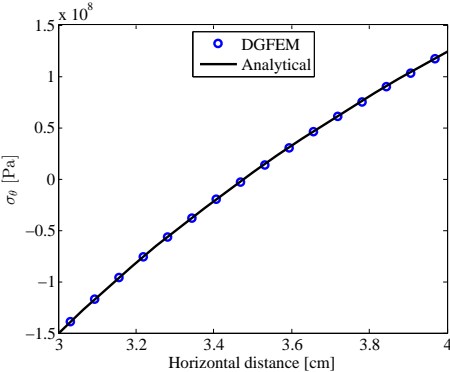


Figure 3.5: Analytical and numerical hoop stress distributions

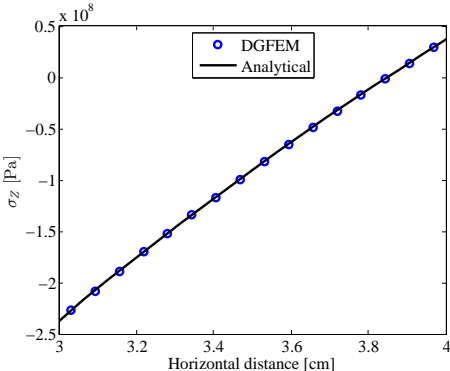


Figure 3.6: Analytical and numerical out of plane stress distributions

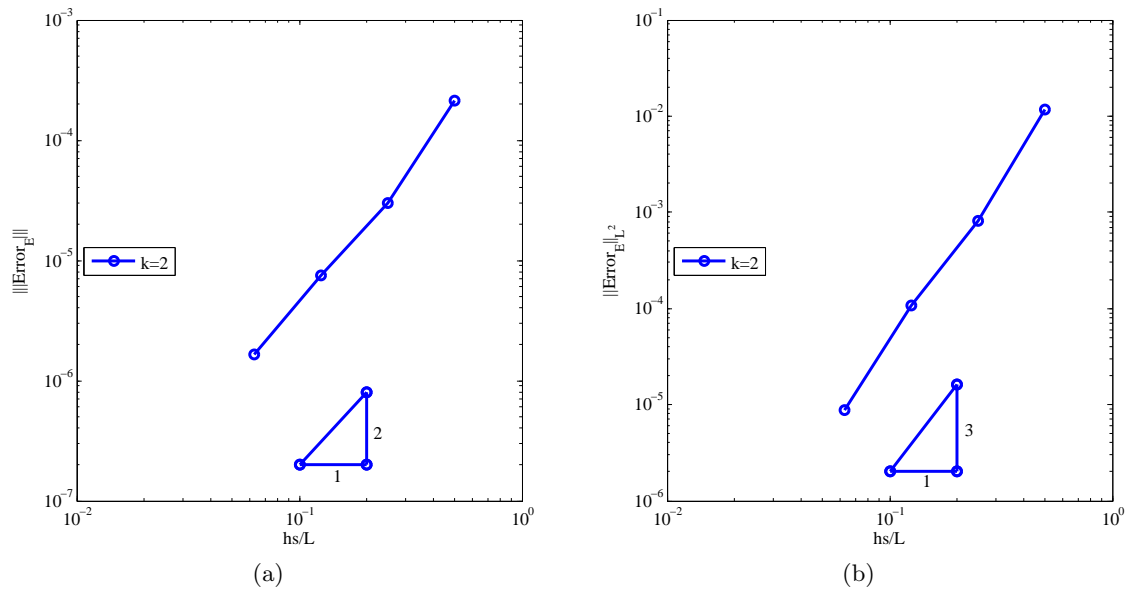


Figure 3.7: Error with respect to the mesh size. (a) The relative error in the energy-norm, and (b) the relative error in the  $L^2$ -norm



## Chapter 4

# A coupled Electro-Thermal Discontinuous Galerkin method

### 4.1 Introduction

Electro-Thermal materials received a significant interest in recent years due to their capability to convert electricity directly into heat and vice versa, which promises a wide range of applications in energy and environment fields.

The main interest of this chapter is to derive a consistent and stable Discontinuous Galerkin (DG) method for two-way Electro-Thermal coupling analyzes considering Electro-Thermal effects such as Seebeck and Peltier effects, and also Joule heating. These effects describe the direct conversion of the difference in electric potential into the temperature difference within the system (Peltier effect), which we are interested in, and vice versa (Seebeck effect). This is typical of thermo-electric cells which could work in two ways: electric generations [17] and heat pumps which operate in cool or heat modes [57].

Electro-Thermal continuum has extensively been developed in the literature [57, 51, 58, 43]. For example, as a non-exhaustive list, Ebling et al. [17] have implemented Thermo-Electric elements into the finite element method and have validated it by analytical and experimental results for the figure of merit values. Liu [43] has developed a continuum theory of Thermo-Electric bodies. He has applied it to predict the effective properties of thermo-electric composites. However he has considered that the temperature and voltage are constant on a homogeneous thermo-electric body as their variations are small, which leads to a linear system of partial differential equations. Pérez-Aparicio et al. [58] have proposed an Electro-Thermal formulation for simple configurations and have provided a comparison between analytical and numerical results.

The key point in being able to develop a stable DG method for Electro-Thermo coupling is to formulate the non-linear equations in terms of energetically conjugated pairs of fluxes and fields gradient. Indeed, the use of energetically consistent pairs allows writing the strong form in a matrix form suitable to the derivation of a SIPG weak form as it will be demonstrated in this chapter.

In this chapter we discuss the fundamental equations for the transport of electricity and heat, in terms of macroscopic variables such as temperature and electric potential. A fully coupled nonlinear weak formulation for Electro-Thermal problems is developed based

on continuum mechanics equations which are discretized using the Discontinuous Galerkin method.

The existence and uniqueness of the weak form solution are proved. The numerical properties of the nonlinear elliptic problem i.e., consistency and stability, are demonstrated under specific conditions, i.e. use of a high enough stabilization parameter and at least quadratic polynomial approximations. Moreover the prior error estimates in the  $H^1$ -norm and in the  $L^2$ -norm are shown to be optimal in the mesh size with the polynomial approximation degree.

This chapter is organized as follows. Section 4.2 describes the governing equations of Electro-Thermal materials. In order to develop the DG formulation, the weak form is formulated in terms of a conjugated pair of fluxes and fields gradients, resulting in a particular choice of the test functions ( $\delta f_T = \delta(\frac{1}{T}), \delta f_V = \delta(\frac{-V}{T})$ ) and of the trial functions ( $f_T = \frac{1}{T}, f_V = \frac{-V}{T}$ ), where  $T$  is the temperature and  $V$  is the electric potential, as proposed by Liu [43]. A complete nonlinear coupled finite element algorithm for Electro-Thermal materials is then developed in Section 4.3 using the DG method to derive the weak form. This results into a set of non-linear equations which is implemented within a three-dimensional finite element code. Section 4.4 focuses on the demonstration of the numerical properties of the DG method, based on rewriting the nonlinear formulation in a fixed point form [34]. The numerical properties of the nonlinear elliptic problem, i.e. consistency and the uniqueness of the solution, can then be demonstrated, and the prior error estimate is shown to be optimal in the mesh size for polynomial approximation degrees  $k > 1$ . In Section 4.5, several examples of applications in one, two and three dimensions are provided for single and composite materials, in order to validate the accuracy and effectiveness of the Electro-Thermal DG formulation and to illustrate the algorithmic properties. We end by some conclusions and remarks in Section 4.6.

## 4.2 Governing equations

In this section an overview of the basic equations that govern the Electro-Thermal phenomena is presented for a structure characterized by a volume  $\Omega$  whose external boundary is  $\partial\Omega$ . In particular we discuss the choice of the conjugated pair of fluxes and fields gradients that will be used to formulate the strong form in a matrix form.

### 4.2.1 Strong form

The first balance equation is the electrical charge conservation equation. When assuming a steady state, the solution of the electrical problem consists in solving the following Poisson type equation for the electrical potential

$$\nabla \cdot \mathbf{j}_e = 0 \quad \forall \mathbf{x} \in \Omega, \quad (4.1)$$

where  $\mathbf{j}_e$  [A/m<sup>2</sup>] denotes the flow of electrical current density vector, which is defined as the rate of charge carriers per unit area or the current per unit area. At zero temperature gradient, the current density  $\mathbf{j}_e$  is described by Ohm's law which is the relationship between the electric potential  $V$  [V] gradient and the electric current flux per unit area through the electric conductivity  $\mathbf{l}$  [S/m], with

$$\mathbf{j}_e = \mathbf{l} \cdot (-\nabla V). \quad (4.2)$$

However when  $T$  [K] varies inside the body, an electromotive force  $(\nabla V)^s$  per unit length appears, and reads

$$(\nabla V)^s = -\alpha \nabla T, \quad (4.3)$$

where  $\alpha$  [V/K] is the Seebeck coefficient which is in general temperature dependent and defined as the derivative of the electric potential with respect to the temperature. By taking in consideration the Seebeck effect, Eq. (4.3), and adding it to Ohm's Law, Eq.(4.2), for systems in which the particle density is homogeneous [51], the current density is rewritten as

$$\mathbf{j}_e = \mathbf{l} \cdot (-\nabla V) + \alpha \mathbf{l} \cdot (-\nabla T). \quad (4.4)$$

The second balance equation is the conservation of the energy flux, which is a combination of the inter exchanges between the thermal and electric energies:

$$\nabla \cdot \mathbf{j}_y = -\rho \partial_t y \quad \forall \mathbf{x} \in \Omega. \quad (4.5)$$

The right hand side of this equilibrium equation is the time derivative of the internal energy density  $y$  [J/Kg]

$$y = y_0 + c_v T, \quad (4.6)$$

which consists of the constant  $y_0$  independent of the temperature and of the electric potential, and of the volumetric heat capacity per unit mass [J/(K · Kg)] multiplied by the absolute temperature  $T$ . Moreover the energy flux  $\mathbf{j}_y$  is defined as

$$\mathbf{j}_y = \mathbf{q} + V \mathbf{j}_e, \quad (4.7)$$

where  $\mathbf{q}$  [W/m<sup>2</sup>] is the heat flux. On the one hand, at zero electric current density,  $\mathbf{j}_e = 0$  (open circuit), the heat flux is given by the Fourier's Law

$$\mathbf{q} = \mathbf{k} \cdot (-\nabla T), \quad (4.8)$$

in this equation  $\mathbf{k}$  [W/(K · m)] denotes the symmetric matrix of thermal conductivity coefficients, which may depend on the temperature. On the other hand, at zero temperature gradient, the heat flux is given by

$$\mathbf{q} = \beta_\alpha \mathbf{j}_e = \alpha T \mathbf{j}_e, \quad (4.9)$$

where the coupling between the heat flux  $\mathbf{q}$  and the electric current density  $\mathbf{j}_e$  is governed by the Peltier coefficient  $\beta_\alpha = \alpha T$ . By superimposing the previous terms to the Fourier's Law, Eq. (4.8), the thermal flux can be rewritten as:

$$\mathbf{q} = \mathbf{k} \cdot (-\nabla T) + \alpha T \mathbf{j}_e = (\mathbf{k} + \alpha^2 T \mathbf{l}) \cdot (-\nabla T) + \alpha T \mathbf{l} \cdot (-\nabla V). \quad (4.10)$$

The first term is due to the conduction and the second term corresponds to the joule heating effect.

Therefore the conservation laws are written as finding  $V, T \in H^2(\Omega) \times H^{2+}(\Omega)$  such that

$$\nabla \cdot \mathbf{j}_e = 0 \quad \forall \mathbf{x} \in \Omega, \quad (4.11)$$

$$\nabla \cdot \mathbf{j}_y = \nabla \cdot \mathbf{q} + \mathbf{j}_e \cdot \nabla V = -\rho \partial_t y \quad \forall \mathbf{x} \in \Omega, \quad (4.12)$$

where  $T$  belongs to the manifold  $H^{2+}$ , in which  $T$  is always strictly positive.

These equations are completed by suitable boundary, where the boundary  $\partial\Omega$  is decomposed into a region of Dirichlet boundary  $\partial_D\Omega$  and Neumann boundary  $\partial_N\Omega$  (i.e.,  $\partial_D\Omega \cup \partial_N\Omega = \partial\Omega$ , and  $\partial_D\Omega \cap \partial_N\Omega = \emptyset$ ). On the Dirichlet BC, one has

$$T = \bar{T} > 0, \quad V = \bar{V} \quad \forall \mathbf{x} \in \partial_D\Omega, \quad (4.13)$$

where  $\bar{T}$  and  $\bar{V}$  are the prescribed temperature and electric potential respectively. The natural Neumann boundary conditions are constraints on the secondary variables: the electric current for the electric charge equation and the energy flux for the energy equation, i.e.

$$\mathbf{q} \cdot \mathbf{n} = \bar{q}, \quad \mathbf{j}_e \cdot \mathbf{n} = \bar{j}_e, \quad \mathbf{j}_y \cdot \mathbf{n} = \bar{j}_y \quad \forall \mathbf{x} \in \partial_N\Omega, \quad (4.14)$$

with  $\mathbf{n}$  is the outward unit normal to the boundary  $\partial\Omega$ . For simplicity we consider the same boundary division into Neumann and Dirichlet parts for the both fields  $T$  and  $V$ . However in the general case this could be different.

The set of Eqs. (4.11, 4.12) can be rewritten under a matrix form. First we rewrite Eqs. (4.4, 4.7, 4.10) under the form

$$\mathbf{j} = \begin{pmatrix} \mathbf{j}_e \\ \mathbf{j}_y \end{pmatrix} = \begin{pmatrix} \mathbf{l} & \alpha \mathbf{l} \\ \mathbf{v} \mathbf{l} + \alpha T \mathbf{l} & \mathbf{k} + \alpha \mathbf{v} \mathbf{l} + \alpha^2 T \mathbf{l} \end{pmatrix} \begin{pmatrix} -\nabla V \\ -\nabla T \end{pmatrix}. \quad (4.15)$$

The set of governing Eqs. (4.11, 4.12) thus becomes finding  $V, T \in H^2(\Omega) \times H^{2+}(\Omega)$  such that

$$\text{div}(\mathbf{j}) = \begin{pmatrix} 0 \\ -\rho \partial_t y \end{pmatrix} = \mathbf{i}, \quad (4.16)$$

where we have introduced  $\mathbf{i} = \begin{pmatrix} 0 \\ -\rho \partial_t y \end{pmatrix}$  for a future use.

### 4.2.2 The conjugated driving forces

First the weak form of the conservation of electric charge carriers, Eq. (4.1), is obtained by taking the inner product of this equation with a suitable scalar test function  $\delta f_V \in H^1(\Omega')$  over a sub-domain  $\Omega' \subset \Omega$ , yielding

$$\int_{\Omega'} \nabla \cdot \mathbf{j}_e \delta f_V d\Omega' = 0 \quad \forall \delta f_V \in H^1(\Omega'). \quad (4.17)$$

After a simple formal integration by parts and using the divergence theorem, we obtain

$$-\int_{\Omega'} \mathbf{j}_e \cdot \nabla \delta f_V d\Omega' + \int_{\partial\Omega'} \mathbf{j}_e \cdot \mathbf{n} \delta f_V dS = 0 \quad \forall \delta f_V \in H^1(\Omega'). \quad (4.18)$$

Secondly, taking the inner product of the second balance equation, Eq. (4.12), with the test function  $\delta f_T \in H^1(\Omega')$ , over the sub-domain  $\Omega' \subset \Omega$  leads to

$$\int_{\Omega'} \nabla \cdot \mathbf{q} \delta f_T d\Omega' + \int_{\Omega'} \mathbf{j}_e \cdot \nabla V \delta f_T d\Omega' = -\int_{\Omega'} \rho \partial_t y \delta f_T d\Omega' \quad \forall \delta f_T \in H^1(\Omega'). \quad (4.19)$$

Moreover by applying the divergence theorem, one obtains

$$\int_{\Omega'} \mathbf{q} \cdot \nabla \delta f_T d\Omega' = \int_{\partial\Omega'} \mathbf{q} \cdot \mathbf{n} \delta f_T dS + \int_{\Omega'} \nabla V \cdot \mathbf{j}_e \delta f_T d\Omega' + \int_{\Omega'} \rho \partial_t y \delta f_T d\Omega' \quad \forall \delta f_T \in H^1(\Omega'). \quad (4.20)$$

By substituting the internal energy, Eq. (4.6), and the thermal flux, Eq. (4.10), this last equation reads

$$\begin{aligned} \int_{\Omega'} (\mathbf{k} \cdot (-\nabla T) + \alpha T \mathbf{j}_e) \cdot \nabla \delta f_T d\Omega' &= \int_{\Omega'} \rho c_v \partial_t T \delta f_T d\Omega' + \int_{\Omega'} \nabla V \cdot \mathbf{j}_e \delta f_T d\Omega' \\ &+ \int_{\partial\Omega'} (\mathbf{k} \cdot (-\nabla T) + \alpha T \mathbf{j}_e) \cdot \mathbf{n} \delta f_T dS. \end{aligned} \quad (4.21)$$

In order to define the conjugated forces, let us substitute  $\delta f_V$  by  $-\frac{V}{T}$  in Eq. (4.18). This results into

$$\int_{\partial\Omega'} \mathbf{j}_e \cdot \mathbf{n} \left(-\frac{V}{T}\right) dS = \int_{\Omega'} \mathbf{j}_e \cdot \left(-\frac{\nabla V}{T} + \frac{V}{T^2} \nabla T\right) d\Omega'. \quad (4.22)$$

Substituting  $\delta f_T$  by  $\frac{1}{T}$  in Eq. (4.21) leads to:

$$\begin{aligned} \int_{\Omega'} \left( (-\nabla T) \cdot \mathbf{k} \cdot \frac{(-\nabla T)}{T^2} - \alpha \frac{\mathbf{j}_e}{T} \cdot \nabla T \right) d\Omega' &= \int_{\Omega'} \left( \rho \frac{c_v}{T} \partial_t T \right) d\Omega' + \int_{\Omega'} \nabla V \cdot \frac{\mathbf{j}_e}{T} d\Omega' \\ &+ \int_{\partial\Omega'} \left( \mathbf{k} \cdot \left( \frac{-\nabla T}{T} \right) + \alpha \mathbf{j}_e \right) \cdot \mathbf{n} dS. \end{aligned} \quad (4.23)$$

By subtracting Eq. (4.22) from Eq. (4.23), one gets

$$\begin{aligned} &\int_{\Omega'} \frac{\rho c_v}{T} \partial_t T d\Omega' + \int_{\partial\Omega'} \left( \mathbf{k} \cdot \left( \frac{-\nabla T}{T} \right) + \alpha \mathbf{j}_e + \mathbf{j}_e \left( \frac{V}{T} \right) \right) \cdot \mathbf{n} dS \\ &= \int_{\Omega'} \left( -\mathbf{j}_e \cdot \frac{\nabla V}{T} + \mathbf{j}_e \cdot \frac{\nabla V}{T} - \mathbf{j}_e \frac{V}{T^2} \cdot \nabla T \right) d\Omega' \\ &+ \int_{\Omega'} \left( (-\nabla T) \cdot \mathbf{k} \cdot \frac{(-\nabla T)}{T^2} - \alpha \frac{\mathbf{j}_e}{T} \cdot \nabla T \right) d\Omega', \end{aligned} \quad (4.24)$$

or

$$\int_{\Omega'} \frac{1}{\Gamma} (\rho c_v \partial_t T) d\Omega' + \int_{\partial\Omega'} \frac{1}{\Gamma} (\mathbf{q} + \mathbf{j}_e V) \cdot \mathbf{n} dS = \int_{\Omega'} \frac{-\nabla T}{\Gamma^2} \cdot (\mathbf{j}_e V - \mathbf{k} \cdot \nabla T + \alpha \mathbf{j}_e T) d\Omega'. \quad (4.25)$$

Henceforth, as  $\mathbf{j}_y = \mathbf{q} + \mathbf{j}_e V$ , this last result is rewritten

$$\int_{\Omega'} \partial_t y \delta f_T d\Omega' + \int_{\partial\Omega'} \mathbf{j}_y \cdot \mathbf{n} \delta f_T dS = \int_{\Omega'} \mathbf{j}_y \cdot \nabla \delta f_T d\Omega'. \quad (4.26)$$

By this way we recover the conservation equation of the energy flux, Eq. (4.5), which shows that  $\mathbf{j}_e$ ,  $\mathbf{j}_y$  and  $\nabla(-\frac{V}{\Gamma})$ ,  $\nabla(\frac{1}{\Gamma})$  are conjugated pairs of fluxes and fields gradients as shown in [43].

subsection Strong form in terms of the conjugated pairs of fluxes and fields gradients

Let us define a  $2 \times 1$  vector of the unknown fields  $\mathbf{M} = \begin{pmatrix} f_V \\ f_T \end{pmatrix}$ , with  $f_V = -\frac{V}{\Gamma}$  and  $f_T = \frac{1}{\Gamma}$ , then the gradients of the fields vector  $\nabla \mathbf{M}$ , a  $2d \times 1$  vector in terms of  $(\nabla f_V, \nabla f_T)$ , is defined by

$$(\nabla \mathbf{M}) = \begin{pmatrix} \nabla f_V \\ \nabla f_T \end{pmatrix} = \begin{pmatrix} \nabla(-\frac{V}{\Gamma}) \\ \nabla(\frac{1}{\Gamma}) \end{pmatrix} = \begin{pmatrix} -\frac{1}{\Gamma} \mathbf{I} & \frac{V}{\Gamma^2} \mathbf{I} \\ \mathbf{0} & -\frac{1}{\Gamma^2} \mathbf{I} \end{pmatrix} \begin{pmatrix} \nabla V \\ \nabla T \end{pmatrix}, \quad (4.27)$$

where  $\mathbf{I}$  is the identity tensor. Hence, the fluxes defined by Eq. (4.15) can be expressed in terms of  $f_V, f_T$ , yielding

$$\mathbf{j} = \begin{pmatrix} \mathbf{j}_e \\ \mathbf{j}_y \end{pmatrix} = \begin{pmatrix} \mathbf{I} T & V T \mathbf{I} + \alpha T^2 \mathbf{1} \\ V T \mathbf{I} + \alpha T^2 \mathbf{1} & T^2 \mathbf{k} + 2\alpha T^2 V \mathbf{1} + \alpha^2 T^3 \mathbf{1} + T V^2 \mathbf{1} \end{pmatrix} \begin{pmatrix} \nabla f_V \\ \nabla f_T \end{pmatrix}. \quad (4.28)$$

The  $2d \times 1$  fluxes vector  $\mathbf{j}$  is the product of the fields gradients vector  $\nabla \mathbf{M}$ , which derived from the state variables  $(f_V, f_T)$ , by a coefficients matrix  $\mathbf{Z}(V, T)$  of size  $2d \times 2d$ , which is temperature and electric potential dependent. The conjugated pairs of fluxes and fields gradients stated by Eq. (4.28) were proposed by Liu [43]. This formulation of the conjugated forces leads to a symmetric coefficients matrix  $\mathbf{Z}(V, T)$  such that

$$\mathbf{j} = \mathbf{Z} \nabla \mathbf{M}. \quad (4.29)$$

From Eq. (4.28), the symmetric coefficients matrix  $\mathbf{Z}(V, T)$  is positive definite if  $\mathbf{Z}_{00}$  and  $\mathbf{Z}_{11} - \mathbf{Z}_{10}^T \mathbf{Z}_{00}^{-1} \mathbf{Z}_{01}$  are positive definite. As  $\mathbf{Z}_{00} = \mathbf{I} T$  is positive definite, and  $\mathbf{Z}_{11} - \mathbf{Z}_{10}^T \mathbf{Z}_{00}^{-1} \mathbf{Z}_{01} = \mathbf{k} T^2$  is also positive definite, then  $\mathbf{Z}(V, T)$  is a positive definite matrix.

The coefficient matrix  $\mathbf{Z}(V, T)$  in Eq. (4.28) could also be rewritten in term of  $(f_V, f_T) = (-\frac{V}{\Gamma}, \frac{1}{\Gamma})$ , as  $T = \frac{1}{f_T}$ ,  $V = -\frac{f_V}{f_T}$ :

$$\mathbf{Z}(f_V, f_T) = \begin{pmatrix} \frac{1}{f_T} \mathbf{1} & -\frac{f_V}{f_T^2} \mathbf{1} + \alpha \frac{1}{f_T^2} \mathbf{1} \\ -\frac{f_V}{f_T^2} \mathbf{1} + \alpha \frac{1}{f_T^2} \mathbf{1} & \frac{\mathbf{k}}{f_T^2} - 2\alpha \frac{f_V}{f_T^3} \mathbf{1} + \alpha^2 \frac{1}{f_T^3} \mathbf{1} + \frac{f_V^2}{f_T^3} \mathbf{1} \end{pmatrix}. \quad (4.30)$$

As the coefficients matrix is positive definite, the energy can be defined by

$$\begin{aligned} \nabla \mathbf{M}^T \mathbf{j} &= \nabla \mathbf{M}^T \mathbf{Z}(f_V, f_T) \nabla \mathbf{M} \\ &= (\nabla f_V \quad \nabla f_T) \begin{pmatrix} \frac{1}{f_T} \mathbf{1} & -\frac{f_V}{f_T^2} \mathbf{1} + \alpha \frac{1}{f_T^2} \mathbf{1} \\ -\frac{f_V}{f_T^2} \mathbf{1} + \alpha \frac{1}{f_T^2} \mathbf{1} & \frac{\mathbf{k}}{f_T^2} - 2\alpha \frac{f_V}{f_T^3} \mathbf{1} + \alpha^2 \frac{1}{f_T^3} \mathbf{1} + \frac{f_V^2}{f_T^3} \mathbf{1} \end{pmatrix} \begin{pmatrix} \nabla f_V \\ \nabla f_T \end{pmatrix} \geq 0. \end{aligned} \quad (4.31)$$

Finally, the strong form (4.15, 4.16) can be expressed as

$$\begin{cases} \operatorname{div}(\mathbf{j}) &= \mathbf{i} & \forall \mathbf{x} \in \Omega, \\ \mathbf{M} &= \bar{\mathbf{M}} & \forall \mathbf{x} \in \partial_D \Omega, \\ \bar{\mathbf{n}}^T \mathbf{j} &= \bar{\mathbf{j}} & \forall \mathbf{x} \in \partial_N \Omega, \end{cases} \quad (4.32)$$

where  $\bar{\mathbf{n}} = \begin{pmatrix} \mathbf{n} & 0 \\ 0 & \mathbf{n} \end{pmatrix}$ ,  $\bar{\mathbf{M}} \in L^2(\partial_D \Omega) \times L^{2+}(\partial_D \Omega)$ , and  $\bar{\mathbf{j}} = \begin{pmatrix} \bar{j}_e \\ \bar{j}_y \end{pmatrix}$ .

As explained by Liu [43], there is no unique choice of fluxes and fields gradients describing the transport process, such that an arbitrary additive constant in the electrical potential  $V$  should have no physical consequence. It can be shown that if  $(f_V, f_T)$  satisfies the conservation law Eq. (4.32)

$$\operatorname{div} \left( \mathbf{Z}(T, V + c) \nabla \mathbf{M}' \right) = \begin{pmatrix} 0 \\ -\partial_{t,y} \end{pmatrix}, \quad \nabla \mathbf{M}' = \begin{pmatrix} \nabla(f_V) - c \nabla(f_T) \\ \nabla(f_T) \end{pmatrix}, \quad (4.33)$$

showing that  $(f'_V = f_V - c f_T, f_T)$  also satisfies the conservation law.

### 4.3 Electro-Thermal analysis with the Discontinuous Galerkin (DG) finite element method

#### 4.3.1 Weak discontinuous form

The weak formulation of Eq. (4.11) is defined by multiplying it by a function  $\delta f_V \in \Pi_e H^1(\Omega^e)$ , performing a volume integral, and using the divergence theorem on each element  $\Omega^e$ . This leads to state the problem as finding  $f_V, f_T \in \Pi_e H^1(\Omega^e) \times \Pi_e H^{1+}(\Omega^e)$  such that

$$-\sum_e \int_{\Omega^e} \mathbf{j}_e(f_V, f_T) \cdot \nabla \delta f_V \, d\Omega + \sum_e \int_{\partial \Omega^e} \mathbf{j}_e(f_V, f_T) \cdot \mathbf{n} \delta f_V \, dS = 0 \quad \forall \delta f_V \in \Pi_e H^1(\Omega^e). \quad (4.34)$$

The surface integral of this last equation is rewritten as

$$\begin{aligned} \sum_e \int_{\partial \Omega^e} \mathbf{j}_e(f_V, f_T) \cdot \mathbf{n} \delta f_V \, dS &= \sum_e \int_{\partial_N \Omega^e} \mathbf{j}_e(f_V, f_T) \cdot \mathbf{n} \delta f_V \, dS \\ &+ \sum_e \int_{\partial_1 \Omega^e \cup \partial_D \Omega^e} \mathbf{j}_e(f_V, f_T) \cdot \mathbf{n} \delta f_V \, dS, \end{aligned} \quad (4.35)$$

where the subdivision  $\partial_1 \Omega^e$ ,  $\partial_D \Omega^e$ , and  $\partial_N \Omega^e$  have been defined in Section 2.2.

The second term of the right hand side of Eq. (4.35) can be rewritten using

$$\begin{aligned} \sum_e \int_{\partial_1 \Omega^e} \mathbf{j}_e(f_V, f_T) \cdot \mathbf{n} \delta f_V \, dS &= \int_{\partial_1 \Omega_h} (\mathbf{j}_e^-(f_V, f_T) \cdot \mathbf{n}^- \delta f_V^- + \mathbf{j}_e^+(f_V, f_T) \cdot \mathbf{n}^+ \delta f_V^+) \, dS \\ \sum_e \int_{\partial_D \Omega^e} \mathbf{j}_e(f_V, f_T) \cdot \mathbf{n} \delta f_V \, dS &= - \int_{\partial_D \Omega_h} (-\mathbf{j}_e(f_V, f_T) \cdot \mathbf{n}^- \delta f_V) \, dS, \end{aligned} \quad (4.36)$$

where  $\mathbf{n}^-$  is the outward unit normal of the minus element  $\Omega^{e^-}$ , whereas  $\mathbf{n}^+$  is the outward unit normal of its neighboring element,  $\mathbf{n}^+ = -\mathbf{n}^-$ , and  $\mathbf{n}^- = \mathbf{n}$  on  $\partial_D \Omega_h$ . We can use trace

operators introduced in Section 2.3 to manipulate the numerical flux and obtain the primal formulation. As a reminder on  $\partial_I\Omega_h$ , the average  $\langle \bullet \rangle$  and the jump  $\llbracket \bullet \rrbracket$  operators are defined as  $\langle \bullet \rangle = \frac{1}{2}(\bullet^+ + \bullet^-)$ ,  $\llbracket \bullet \rrbracket = (\bullet^+ - \bullet^-)$ . The definition of these two trace operators can be extended on the Dirichlet boundary  $\partial_D\Omega_h$  as  $\langle \bullet \rangle = \bullet$ ,  $\llbracket \bullet \rrbracket = (-\bullet)$ . Therefore, Eq. (4.35) becomes

$$\begin{aligned} \sum_e \int_{\partial\Omega^e} \mathbf{j}_e(f_V, f_{T_h}) \cdot \mathbf{n} \delta f_V dS &= \int_{\partial_N\Omega_h} \mathbf{j}_e(f_V, f_T) \cdot \mathbf{n} \delta f_V dS \\ &\quad - \int_{\partial_I\Omega_h \cup \partial_D\Omega_h} \llbracket \mathbf{j}_e(f_V, f_T) \delta f_V \rrbracket \cdot \mathbf{n}^- dS. \end{aligned} \quad (4.37)$$

Applying the boundary conditions specified in Eq. (4.14) and using this last result, allows Eq. (4.34) to be rewritten as finding  $f_V, f_T \in \Pi_e H^1(\Omega^e) \times \Pi_e H^{1+}(\Omega^e)$  such that

$$\begin{aligned} \int_{\partial_N\Omega_h} \bar{\mathbf{j}}_e \delta f_V dS &= \int_{\Omega_h} \mathbf{j}_e(f_V, f_T) \cdot \nabla \delta f_V d\Omega + \int_{\partial_I\Omega_h \cup \partial_D\Omega_h} \llbracket \mathbf{j}_e(f_V, f_T) \delta f_V \rrbracket \cdot \mathbf{n}^- dS \\ \forall \delta f_V &\in \Pi_e H^1(\Omega^e). \end{aligned} \quad (4.38)$$

Applying the mathematical identity  $\llbracket ab \rrbracket = \llbracket a \rrbracket \langle b \rangle + \llbracket b \rrbracket \langle a \rangle$ , and by neglecting the second term because only consistency of the test functions needs to be enforced, then the consistent flux related to Eq. (4.38) reads  $\llbracket \delta f_V \rrbracket \langle \mathbf{j}_e(f_V, f_T) \rangle \cdot \mathbf{n}^-$ .

Moreover, on the one hand, due to the discontinuous nature of the trial functions in the DG weak form, the inter-element discontinuity is allowed, so the continuity of unknown variables is enforced weakly by using symmetrization and stabilization terms at the interior elements boundary interface  $\partial_I\Omega_h$ . On the other hand, the Dirichlet boundary condition (4.13) is also enforced in a weak sense by considering the same symmetrization and stabilization terms at the Dirichlet elements boundary interface  $\partial_D\Omega_h$ . By using the definition of the electric current density, Eq. (4.4), the virtual electric current density  $\delta \mathbf{j}_e(f_V, f_T)$  reads

$$\delta \mathbf{j}_e = \mathbf{l} \cdot (-\nabla \delta V) - \alpha \mathbf{l} \cdot (-\nabla \delta T). \quad (4.39)$$

Using the definition of the conjugated force, Eq. (4.28), this last relation is rewritten

$$\delta \mathbf{j}_e(f_V, f_T) = \frac{\mathbf{l}}{f_T} \cdot \nabla \delta f_V + \left( -\frac{f_{V_h}}{f_T^2} + \alpha \frac{1}{f_T^2} \right) \mathbf{l} \cdot \nabla \delta f_T. \quad (4.40)$$

Eq. (4.40) is rewritten in terms of  $\mathbf{l}_1 = \frac{\mathbf{l}}{f_T}$  and  $\mathbf{l}_2 = \mathbf{l} \left( -\frac{f_V}{f_T^2} + \alpha \frac{1}{f_T^2} \right)$  as:

$$\delta \mathbf{j}_e(f_V, f_T) = \mathbf{l}_1(f_T) \cdot \nabla \delta f_V + \mathbf{l}_2(f_V, f_T) \cdot \nabla \delta f_T. \quad (4.41)$$

This last result allows formulating the symmetrization and quadratic stabilization terms so



the weak form Eq. (4.38) becomes finding  $f_V, f_T \in \Pi_e H^1(\Omega^e) \times \Pi_e H^{1+}(\Omega^e)$  such that:

$$\begin{aligned}
 & \int_{\partial_N \Omega_h} \bar{\mathbf{j}}_e \delta f_V \, dS - \int_{\partial_D \Omega_h} (\mathbf{l}_1(\bar{f}_T) \cdot \nabla \delta f_V + \mathbf{l}_2(\bar{f}_V, \bar{f}_T) \cdot \nabla \delta f_T) \cdot \mathbf{n} \bar{f}_V \, dS \\
 & + \int_{\partial_D \Omega_h} \left( \delta f_V \mathbf{n} \cdot \frac{\mathbf{l}_1(\bar{f}_T) \mathcal{B}}{h_s} + \delta f_T \mathbf{n} \cdot \frac{\mathbf{l}_2(\bar{f}_V, \bar{f}_T) \mathcal{B}}{h_s} \right) \cdot \mathbf{n} \bar{f}_V \, dS = \int_{\Omega_h} \mathbf{j}_e(f_V, f_T) \cdot \nabla \delta f_V \, d\Omega \\
 & + \int_{\partial_T \Omega_h \cup \partial_D \Omega_h} \llbracket \delta f_V \rrbracket \langle \mathbf{j}_e(f_V, f_T) \rangle \cdot \mathbf{n}^- \, dS + \int_{\partial_T \Omega_h} \llbracket f_V \rrbracket \langle \mathbf{l}_1(f_T) \cdot \nabla \delta f_V \rangle \cdot \mathbf{n}^- \, dS \\
 & + \int_{\partial_D \Omega_h} \llbracket f_V \rrbracket \langle \mathbf{l}_1(\bar{f}_T) \cdot \nabla \delta f_V \rangle \cdot \mathbf{n}^- \, dS \\
 & + \int_{\partial_T \Omega_h} \llbracket f_V \rrbracket \langle \mathbf{l}_2(f_V, f_T) \cdot \nabla \delta f_T \rangle \cdot \mathbf{n}^- \, dS \\
 & + \int_{\partial_D \Omega_h} \llbracket f_V \rrbracket \langle \mathbf{l}_2(\bar{f}_V, \bar{f}_T) \cdot \nabla \delta f_T \rangle \cdot \mathbf{n}^- \, dS \\
 & + \int_{\partial_T \Omega_h} \llbracket \delta f_V \rrbracket \mathbf{n}^- \cdot \left\langle \frac{\mathbf{l}_1(f_T) \mathcal{B}}{h_s} \right\rangle \cdot \mathbf{n}^- \llbracket f_V \rrbracket \, dS \\
 & + \int_{\partial_D \Omega_h} \llbracket \delta f_V \rrbracket \mathbf{n}^- \cdot \left\langle \frac{\mathbf{l}_1(\bar{f}_T) \mathcal{B}}{h_s} \right\rangle \cdot \mathbf{n}^- \llbracket f_V \rrbracket \, dS \\
 & + \int_{\partial_T \Omega_h} \llbracket \delta f_T \rrbracket \mathbf{n}^- \cdot \left\langle \frac{\mathbf{l}_2(f_V, f_T) \mathcal{B}}{h_s} \right\rangle \cdot \mathbf{n}^- \llbracket f_V \rrbracket \, dS \\
 & + \int_{\partial_D \Omega_h} \llbracket \delta f_T \rrbracket \mathbf{n}^- \cdot \left\langle \frac{\mathbf{l}_2(\bar{f}_V, \bar{f}_T) \mathcal{B}}{h_s} \right\rangle \cdot \mathbf{n}^- \llbracket f_V \rrbracket \, dS \\
 & \quad \forall \delta f_V, \delta f_T \in \Pi_e H^1(\Omega^e) \times \Pi_e H^1(\Omega^e).
 \end{aligned} \tag{4.42}$$

The last two terms of the left hand side of Eq. (4.42) make sure that the Dirichlet boundary condition (4.13) is weakly enforced, as it will be shown in Section 4.4. Moreover, in this equation  $\mathcal{B}$  is the stability parameter which has to be sufficiently high to guarantee stability as it will be shown in Section 4.4, and  $h_s$  is the characteristic length of the mesh, which will also be defined in Section 4.4.

In the same spirit, the weak formulation of the second governing Eq. (4.12) is derived by multiplying it by kinematically admissible function  $\delta f_T \in \Pi_e H^1(\Omega^e)$ , integrating over the whole domain, and applying the divergence theorem on each element, which lead to

$$\begin{aligned}
 & - \sum_e \int_{\Omega^e} \mathbf{j}_y(f_V, f_T) \cdot \nabla \delta f_T \, d\Omega + \sum_e \int_{\partial \Omega^e} \mathbf{j}_y(f_V, f_T) \cdot \mathbf{n} \delta f_T \, dS \\
 & = - \sum_e \int_{\Omega^e} \rho \partial_{ty} \delta f_T \, d\Omega \quad \forall \delta f_T \in \Pi_e H^1(\Omega^e).
 \end{aligned} \tag{4.43}$$

As for the electrical equation, by introducing the jump operator and the boundary condition Eq. (4.14), this equation becomes

$$\begin{aligned}
 & \int_{\partial_N \Omega_h} \delta f_T \bar{\mathbf{j}}_y \, dS = \int_{\Omega_h} \mathbf{j}_y(f_V, f_T) \cdot \nabla \delta f_T \, d\Omega + \int_{\partial_T \Omega_h \cup \partial_D \Omega_h} \llbracket \delta f_T \langle \mathbf{j}_y(f_V, f_T) \rangle \rrbracket \cdot \mathbf{n}^- \, dS \\
 & - \int_{\Omega_h} \rho \partial_{ty} \delta f_T \, d\Omega \quad \forall \delta f_T \in \Pi_e H^1(\Omega^e).
 \end{aligned} \tag{4.44}$$

The consistent and stable weak form is obtained by considering the numerical energy flux  $\langle \mathbf{j}_y(f_V, f_T) \rangle$ , and by adding stability and symmetrization terms in a weak sense. Using the definition of the conjugated force, Eq. (4.28), the virtual energy flux is expressed as

$$\begin{aligned} \delta \mathbf{j}_y(f_V, f_T) &= (\mathbf{k}T^2 + 2\alpha \mathbf{l}T^2V + \alpha^2 \mathbf{l}T^3 + \mathbf{l}TV^2) \cdot \nabla \delta f_T + (\alpha T^2 \mathbf{1} + \mathbf{l}TV) \cdot \nabla \delta f_V \\ &= \left( \frac{\mathbf{k}}{f_T^2} - 2\alpha \mathbf{l} \frac{f_V}{f_T^3} + \alpha^2 \mathbf{1} \frac{1}{f_T^3} + \mathbf{l} \frac{f_V^2}{f_T^3} \right) \cdot \nabla \delta f_T + \left( \alpha \mathbf{l} \frac{1}{f_T^2} - \mathbf{l} \frac{f_V}{f_T^2} \right) \cdot \nabla \delta f_V. \end{aligned} \quad (4.45)$$

Let us define  $\mathbf{j}_{y1}(f_V, f_T) = \frac{\mathbf{k}}{f_T^2} - 2\alpha \frac{f_V}{f_T^3} \mathbf{1} + \alpha^2 \frac{1}{f_T^3} \mathbf{1} + \frac{f_V^2}{f_T^3} \mathbf{1}$ , allowing Eq. (4.45) to be rewritten in terms of  $\mathbf{j}_{y1}, \mathbf{l}_2$  as:

$$\delta \mathbf{j}_y(f_V, f_T) = \mathbf{j}_{y1}(f_V, f_T) \cdot \nabla \delta f_T + \mathbf{l}_2(f_V, f_T) \cdot \nabla \delta f_V. \quad (4.46)$$

Eventually, considering the Dirichlet boundary condition (4.13), the stabilized form can be stated as finding  $f_V, f_T \in \Pi_e H^1(\Omega^e) \times \Pi_e H^{1+}(\Omega^e)$  such that

$$\begin{aligned} & \int_{\partial_N \Omega_h} \delta f_T \bar{\mathbf{j}}_y \cdot d\mathbf{S} - \int_{\partial_D \Omega_h} (\mathbf{j}_{y1}(\bar{f}_V, \bar{f}_T) \cdot \nabla \delta f_T + \mathbf{l}_2(\bar{f}_V, \bar{f}_T) \cdot \nabla \delta f_V) \cdot \mathbf{n} \bar{f}_T \, d\mathbf{S} \\ & + \int_{\partial_D \Omega_h} \left( \delta f_T \mathbf{n} \cdot \frac{\mathbf{j}_{y1}(\bar{f}_V, \bar{f}_T) \mathcal{B}}{h_s} + \delta f_V \mathbf{n} \cdot \frac{\mathbf{l}_2(\bar{f}_V, \bar{f}_T) \mathcal{B}}{h_s} \right) \cdot \mathbf{n} \bar{f}_T \, d\mathbf{S} \\ & = \int_{\Omega_h} \mathbf{j}_y(f_V, f_T) \cdot \nabla \delta f_T \, d\Omega - \int_{\Omega_h} \rho \partial_t y \delta f_T \, d\Omega \\ & + \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \llbracket \delta f_T \rrbracket \langle \mathbf{j}_y(f_V, f_T) \rangle \cdot \mathbf{n}^- \, d\mathbf{S} + \int_{\partial_I \Omega_h} \llbracket f_T \rrbracket \langle \mathbf{j}_{y1}(f_V, f_T) \cdot \nabla \delta f_T \rangle \cdot \mathbf{n}^- \, d\mathbf{S} \\ & + \int_{\partial_D \Omega_h} \llbracket f_T \rrbracket \langle \mathbf{j}_{y1}(\bar{f}_V, \bar{f}_T) \cdot \nabla \delta f_T \rangle \cdot \mathbf{n}^- \, d\mathbf{S} \\ & + \int_{\partial_I \Omega_h} \llbracket f_T \rrbracket \langle \mathbf{l}_2(f_V, f_T) \cdot \nabla \delta f_V \rangle \cdot \mathbf{n}^- \, d\mathbf{S} \\ & + \int_{\partial_D \Omega_h} \llbracket f_T \rrbracket \langle \mathbf{l}_2(\bar{f}_V, \bar{f}_T) \cdot \nabla \delta f_V \rangle \cdot \mathbf{n}^- \, d\mathbf{S} \\ & + \int_{\partial_I \Omega_h} \llbracket \delta f_T \rrbracket \mathbf{n}^- \cdot \left\langle \frac{\mathbf{j}_{y1}(f_V, f_T) \mathcal{B}}{h_s} \right\rangle \cdot \mathbf{n}^- \llbracket f_T \rrbracket \, d\mathbf{S} \\ & + \int_{\partial_D \Omega_h} \llbracket \delta f_T \rrbracket \mathbf{n}^- \cdot \left\langle \frac{\mathbf{j}_{y1}(\bar{f}_V, \bar{f}_T) \mathcal{B}}{h_s} \right\rangle \cdot \mathbf{n}^- \llbracket f_T \rrbracket \, d\mathbf{S} \\ & + \int_{\partial_I \Omega_h} \llbracket \delta f_V \rrbracket \mathbf{n}^- \cdot \left\langle \frac{\mathbf{l}_2(f_V, f_T) \mathcal{B}}{h_s} \right\rangle \cdot \mathbf{n}^- \llbracket f_T \rrbracket \, d\mathbf{S} \\ & + \int_{\partial_D \Omega_h} \llbracket \delta f_V \rrbracket \mathbf{n}^- \cdot \left\langle \frac{\mathbf{l}_2(\bar{f}_V, \bar{f}_T) \mathcal{B}}{h_s} \right\rangle \cdot \mathbf{n}^- \llbracket f_T \rrbracket \, d\mathbf{S} \\ & \quad \forall \delta f_V, \delta f_T \in \Pi_e H^1(\Omega^e) \times \Pi_e H^1(\Omega^e). \end{aligned} \quad (4.47)$$

The last nine terms presented in Eq. (4.42, 4.47) are the interfaces terms, which ensure the following characteristics and properties:

1. The consistency by the first term.

2. The compatibility by the second till fifth terms.
3. The stability by the last four terms, which is ensured by a stability parameter independent of mesh size and material properties, as it will be shown in Section 4.4.
4. The contributions on  $\partial_D \Omega_h$  ensure that the Dirichlet boundary condition (4.13) is weakly enforced.

The weak form (4.42, 4.47) is thus summarized as finding  $f_V, f_T \in \Pi_e H^1(\Omega^e) \times \Pi_e H^{1+}(\Omega^e)$  such that:

$$a_1(f_V, f_T, \delta f_V, \delta f_T) = b_1(\delta f_V, \delta f_T) \quad \forall \delta f_V, \delta f_T \in \Pi_e H^1(\Omega^e) \times \Pi_e H^1(\Omega^e), \quad (4.48)$$

$$a_2(f_V, f_T, \delta f_V, \delta f_T) = b_2(\delta f_V, \delta f_T) + \left(\rho \frac{\partial y}{\partial t}, \delta f_T\right) \quad \forall \delta f_V, \delta f_T \in \Pi_e H^1(\Omega^e) \times \Pi_e H^1(\Omega^e), \quad (4.49)$$

with

$$\begin{aligned} a_1(f_V, f_T, \delta f_V, \delta f_T) &= \int_{\Omega_h} \nabla f_V \cdot \mathbf{l}_1(f_T) \cdot \nabla \delta f_V d\Omega + \int_{\Omega_h} \nabla f_T \cdot \mathbf{l}_2(f_V, f_T) \cdot \nabla \delta f_V d\Omega \\ &+ \int_{\partial_T \Omega_h \cup \partial_D \Omega_h} [[\delta f_V]] \langle \mathbf{l}_1(f_T) \cdot \nabla f_V \rangle \cdot \mathbf{n}^- dS \\ &+ \int_{\partial_T \Omega_h \cup \partial_D \Omega_h} [[\delta f_V]] \langle \mathbf{l}_2(f_V, f_T) \cdot \nabla f_T \rangle \cdot \mathbf{n}^- dS \\ &+ \int_{\partial_T \Omega_h} [[f_V]] \langle \mathbf{l}_1(f_T) \cdot \nabla \delta f_V \rangle \cdot \mathbf{n}^- dS + \int_{\partial_D \Omega_h} [[f_V]] \langle \mathbf{l}_1(\bar{f}_T) \cdot \nabla \delta f_V \rangle \cdot \mathbf{n}^- dS \\ &+ \int_{\partial_T \Omega_h} [[f_V]] \langle \mathbf{l}_2(f_V, f_T) \cdot \nabla \delta f_T \rangle \cdot \mathbf{n}^- dS + \int_{\partial_D \Omega_h} [[f_V]] \langle \mathbf{l}_2(\bar{f}_V, \bar{f}_T) \cdot \nabla \delta f_T \rangle \cdot \mathbf{n}^- dS \\ &+ \int_{\partial_T \Omega_h} [[\delta f_V]] \mathbf{n}^- \cdot \left\langle \frac{\mathbf{l}_1(f_T) \mathcal{B}}{h_s} \right\rangle \cdot \mathbf{n}^- [[f_V]] dS \\ &+ \int_{\partial_D \Omega_h} [[\delta f_V]] \mathbf{n}^- \cdot \left\langle \frac{\mathbf{l}_1(\bar{f}_T) \mathcal{B}}{h_s} \right\rangle \cdot \mathbf{n}^- [[f_V]] dS \\ &+ \int_{\partial_T \Omega_h} [[\delta f_T]] \mathbf{n}^- \cdot \left\langle \frac{\mathbf{l}_2(f_V, f_T) \mathcal{B}}{h_s} \right\rangle \cdot \mathbf{n}^- [[f_V]] dS \\ &+ \int_{\partial_D \Omega_h} [[\delta f_T]] \mathbf{n}^- \cdot \left\langle \frac{\mathbf{l}_2(\bar{f}_V, \bar{f}_T) \mathcal{B}}{h_s} \right\rangle \cdot \mathbf{n}^- [[f_V]] dS, \end{aligned} \quad (4.50)$$

$$\begin{aligned}
a_2(f_V, f_T, \delta f_V, \delta f_T) &= \int_{\Omega_h} \nabla f_T \cdot \mathbf{j}_{y1}(f_V, f_T) \cdot \nabla \delta f_T d\Omega + \int_{\Omega_h} \nabla f_V \cdot \mathbf{l}_2(f_V, f_T) \cdot \nabla \delta f_T d\Omega \\
&+ \int_{\partial_T \Omega_h \cup \partial_D \Omega_h} [[\delta f_T]] \langle \mathbf{j}_{y1}(f_V, f_T) \cdot \nabla f_T \rangle \cdot \mathbf{n}^- dS \\
&+ \int_{\partial_T \Omega_h \cup \partial_D \Omega_h} [[\delta f_T]] \langle \mathbf{l}_2(f_V, f_T) \cdot \nabla f_V \rangle \cdot \mathbf{n}^- dS \\
&+ \int_{\partial_T \Omega_h} [[f_T]] \langle \mathbf{j}_{y1}(f_V, f_T) \cdot \nabla \delta f_T \rangle \cdot \mathbf{n}^- dS + \int_{\partial_D \Omega_h} [[f_T]] \langle \mathbf{j}_{y1}(\bar{f}_V, \bar{f}_T) \cdot \nabla \delta f_T \rangle \cdot \mathbf{n}^- dS \\
&+ \int_{\partial_T \Omega_h} [[f_T]] \langle \mathbf{l}_2(f_V, f_T) \cdot \nabla \delta f_V \rangle \cdot \mathbf{n}^- dS + \int_{\partial_D \Omega_h} [[f_T]] \langle \mathbf{l}_2(\bar{f}_V, \bar{f}_T) \cdot \nabla \delta f_V \rangle \cdot \mathbf{n}^- dS \\
&+ \int_{\partial_T \Omega_h} [[\delta f_T]] \mathbf{n}^- \cdot \left\langle \frac{\mathbf{j}_{y1}(f_V, f_T) \mathcal{B}}{h_s} \right\rangle \cdot \mathbf{n}^- [[f_T]] dS \\
&+ \int_{\partial_D \Omega_h} [[\delta f_T]] \mathbf{n}^- \cdot \left\langle \frac{\mathbf{j}_{y1}(\bar{f}_V, \bar{f}_T) \mathcal{B}}{h_s} \right\rangle \cdot \mathbf{n}^- [[f_T]] dS \\
&+ \int_{\partial_T \Omega_h} [[\delta f_V]] \mathbf{n}^- \cdot \left\langle \frac{\mathbf{l}_2(f_V, f_T) \mathcal{B}}{h_s} \right\rangle \cdot \mathbf{n}^- [[f_T]] dS \\
&+ \int_{\partial_D \Omega_h} [[\delta f_V]] \mathbf{n}^- \cdot \left\langle \frac{\mathbf{l}_2(\bar{f}_V, \bar{f}_T) \mathcal{B}}{h_s} \right\rangle \cdot \mathbf{n}^- [[f_T]] dS,
\end{aligned} \tag{4.51}$$

$$\begin{aligned}
b_1(\delta f_V, \delta f_T) &= \int_{\partial_N \Omega_h} \bar{j}_e \delta f_V dS \\
&- \int_{\partial_D \Omega_h} (\mathbf{l}_1(\bar{f}_T) \cdot \nabla \delta f_V + \mathbf{l}_2(\bar{f}_V, \bar{f}_T) \cdot \nabla \delta f_T) \cdot \mathbf{n} \bar{f}_V dS \\
&+ \int_{\partial_D \Omega_h} \left( \delta f_V \mathbf{n} \cdot \frac{\mathbf{l}_1(\bar{f}_T) \mathcal{B}}{h_s} + \delta f_T \mathbf{n} \cdot \frac{\mathbf{l}_2(\bar{f}_V, \bar{f}_T) \mathcal{B}}{h_s} \right) \cdot \mathbf{n} \bar{f}_V dS,
\end{aligned} \tag{4.52}$$

$$\begin{aligned}
b_2(\delta f_V, \delta f_T) &= \int_{\partial_N \Omega_h} \bar{j}_y \delta f_T dS \\
&- \int_{\partial_D \Omega_h} (\mathbf{j}_{y1}(\bar{f}_V, \bar{f}_T) \cdot \nabla \delta f_T + \mathbf{l}_2(\bar{f}_V, \bar{f}_T) \cdot \nabla \delta f_V) \cdot \mathbf{n} \bar{f}_T dS \\
&+ \int_{\partial_D \Omega_h} \left( \delta f_T \mathbf{n} \cdot \frac{\mathbf{j}_{y1}(\bar{f}_V, \bar{f}_T) \mathcal{B}}{h_s} + \delta f_V \mathbf{n} \cdot \frac{\mathbf{l}_2(\bar{f}_V, \bar{f}_T) \mathcal{B}}{h_s} \right) \cdot \mathbf{n} \bar{f}_T dS,
\end{aligned} \tag{4.53}$$

and

$$\left( \frac{\partial y}{\partial t}, \delta f_T \right) = \int_{\Omega_h} \rho \frac{\partial}{\partial t} (y_0 + c_v T) \delta f_T d\Omega. \tag{4.54}$$

The weak form stated by the set of Eqs. (4.48-4.49) can be rewritten in a matrix form by considering a two-field coupled problem as in Section 4.2.2. We can now recall the broken Sobolev spaces, Eq. (2.7), with<sup>1</sup>

$$X_s^{(+)} = \left\{ \mathbf{M} \in L^2(\Omega_h) \times L^{2^{(+)}}(\Omega_h) \mid_{\mathbf{M}|_{\Omega^e} \in H^s(\Omega^e) \times H^{s^{(+)}}(\Omega^e) \quad \forall \Omega^e \in \Omega_h} \right\}. \tag{4.55}$$

<sup>1</sup>By abuse of notations, the (+) superscript means either usual  $H^2$ -space or the space  $H^{2^+}$  of strictly positive values.

For future use, we define  $X^{(+)}$  as  $X_2^{(+)}$  and  $X^+$  the manifold such that  $f_T > 0$ , while  $X$  is the manifold for which  $f_T \geq 0$ , with  $X^+ \subset X$ .

Eq. (2.9) becomes

$$\mathbf{Y} = \left\{ \nabla \mathbf{M} \in (L^2(\Omega_h))^d \times (L^2(\Omega_h))^3 \mid \nabla \mathbf{M}|_{\Omega^e} \in H^1(\Omega^e) \times H^1(\Omega^e) \quad \forall \Omega^e \in \Omega_h \right\}. \quad (4.56)$$

It should be noted that the test functions in the previous equations of the weak formulation belong to  $H^1(\Omega^e) \times H^{1^+}(\Omega^e)$ , however for the numerical analysis, we will need to be in  $H^2(\Omega^e) \times H^{2^+}(\Omega^e)$ , in order to be able to consider  $s = 2$  in Eq. (2.7).

Using the notations considered to state the strong form (4.32), the weak form stated by Eqs. (4.48, 4.49) can be reformulated as finding  $\mathbf{M} \in X^+$  such that

$$a_3(\mathbf{M}, \delta \mathbf{M}) = b_3(\delta \mathbf{M}) - \int_{\Omega_h} \delta \mathbf{M}^T \text{id} \Omega \quad \forall \delta \mathbf{M} \in X. \quad (4.57)$$

For simplicity we introduce the vector  $\mathbf{M}_n = \begin{pmatrix} \mathbf{n}^- & 0 \\ 0 & \mathbf{n}^- \end{pmatrix} \mathbf{M}$  and  $\bar{\mathbf{M}}_n = \begin{pmatrix} \mathbf{n} & 0 \\ 0 & \mathbf{n} \end{pmatrix} \bar{\mathbf{M}}$ , which allows defining the different terms of the weak discontinuous formulation as

$$\begin{aligned} a_3(\mathbf{M}, \delta \mathbf{M}) &= \int_{\Omega_h} (\nabla \delta \mathbf{M})^T \mathbf{j}(\mathbf{M}, \nabla \mathbf{M}) d\Omega + \int_{\partial_1 \Omega_h \cup \partial_D \Omega_h} [[\delta \mathbf{M}_n^T]] \langle \mathbf{j}(\mathbf{M}, \nabla \mathbf{M}) \rangle dS \\ &+ \int_{\partial_1 \Omega_h} [[\mathbf{M}_n^T]] \langle \mathbf{Z}(\mathbf{M}) \nabla \delta \mathbf{M} \rangle dS + \int_{\partial_D \Omega_h} [[\mathbf{M}_n^T]] \langle \mathbf{Z}(\bar{\mathbf{M}}) \nabla \delta \mathbf{M} \rangle dS \\ &+ \int_{\partial_1 \Omega_h} [[\delta \mathbf{M}_n^T]] \left\langle \frac{\mathcal{B}}{h_s} \mathbf{Z}(\mathbf{M}) \right\rangle [[\mathbf{M}_n]] dS + \int_{\partial_D \Omega_h} [[\delta \mathbf{M}_n^T]] \left\langle \frac{\mathcal{B}}{h_s} \mathbf{Z}(\bar{\mathbf{M}}) \right\rangle [[\mathbf{M}_n]] dS, \end{aligned} \quad (4.58)$$

and

$$\begin{aligned} b_3(\delta \mathbf{M}) &= \int_{\partial_N \Omega_h} \delta \mathbf{M}^T \bar{\mathbf{j}} dS - \int_{\partial_D \Omega_h} \bar{\mathbf{M}}_n^T (\mathbf{Z}(\bar{\mathbf{M}}) \nabla \delta \mathbf{M}) dS \\ &+ \int_{\partial_D \Omega_h} \delta \mathbf{M}_n^T \left( \frac{\mathcal{B}}{h_s} \mathbf{Z}(\bar{\mathbf{M}}) \right) \bar{\mathbf{M}}_n dS. \end{aligned} \quad (4.59)$$

### 4.3.2 Finite element discretization

In the finite element method, the functions  $f_V$  and  $f_T$  are approximated by  $f_{V_h}$  and  $f_{T_h}$ , which are defined over a finite element  $\Omega^e$  using the interpolation concepts in terms of standard shape function  $N^a \in \mathbb{R}$  at node  $a$ , see [81], yielding

$$f_{V_h} = N_{f_V}^a f_V^a, \quad f_{T_h} = N_{f_T}^a f_T^a, \quad (4.60)$$

where  $f_V^a$  denotes the nodal value of  $f_{V_h}$  at node  $a$ . This directly leads to

$$\nabla f_{V_h} = \nabla N_{f_V}^a f_V^a, \quad \nabla f_{T_h} = \nabla N_{f_T}^a f_T^a, \quad (4.61)$$

where  $\nabla N^a$  is the gradient of the shape function at node  $a$ .

In order to obtain a Galerkin formulation, the test functions are approximated using the same interpolation, i.e.

$$\delta f_{V_h} = N_{f_V}^a \delta f_V^a, \quad \delta f_{T_h} = N_{f_T}^a \delta f_T^a. \quad (4.62)$$

$$\nabla \delta f_{V_h} = \nabla N_{f_V}^a \delta f_V^a, \quad \nabla \delta f_{T_h} = \nabla N_{f_T}^a \delta f_T^a, \quad (4.63)$$

The finite discontinuous polynomial approximation  $\mathbf{M}_h = \begin{pmatrix} f_{V_h} \\ f_{T_h} \end{pmatrix} \in X^{k^+}$  of the solution is thus defined in the following space according to Eq. (2.9)

$$X^{k^{(+)}} = \left\{ \mathbf{M}_h \in L^2(\Omega_h) \times L^{2^{(+)}}(\Omega_h) \mid \mathbf{M}_h|_{\Omega^e} \in \mathbb{P}^k(\Omega^e) \times \mathbb{P}^{k^{(+)}}(\Omega^e) \forall \Omega^e \in \Omega_h \right\}, \quad (4.64)$$

where  $\mathbb{P}^k(\Omega^e)$  is the space of polynomial functions of order up to  $k$  and  $\mathbb{P}^{k^+}$  means that the polynomial approximation remains positive. As a result, the problem becomes finding  $\mathbf{M}_h \in X^{k^+}$  such that

$$a_3(\mathbf{M}_h, \delta \mathbf{M}_h) = b_3(\delta \mathbf{M}_h) - \int_{\Omega_h} \delta \mathbf{M}^T \mathbf{id} \Omega \quad \forall \delta \mathbf{M}_h \in X^k. \quad (4.65)$$

The set of Eqs. (4.65) can be rewritten under the form:

$$\mathbf{F}_{\text{ext}}^a(\mathbf{M}^b) = \mathbf{F}_{\text{int}}^a(\mathbf{M}^b) + \mathbf{F}_I^a(\mathbf{M}^b), \quad (4.66)$$

where  $\mathbf{M}^b$  is the vector of the unknown fields at node  $b$

$$\mathbf{M}^b = \begin{pmatrix} f_V^b \\ f_T^b \end{pmatrix}. \quad (4.67)$$

The nonlinear Eqs. (4.66) are solved using the Newton Raphson scheme. To this end, the forces are written in a residual form. The predictor, iteration 0, reads  $\mathbf{M}^b = \mathbf{M}^{b0}$ , the residual at iteration  $i$  reads

$$\mathbf{F}_{\text{ext}}^a(\mathbf{M}^{bi}) - \mathbf{F}_{\text{int}}^a(\mathbf{M}^{bi}) - \mathbf{F}_I^a(\mathbf{M}^{bi}) = \mathbf{R}^a(\mathbf{M}^{bi}), \quad (4.68)$$

and at iteration  $i$ , the first order Taylor development yields the system to be solved, i.e.

$$\left( \frac{\partial \mathbf{F}_{\text{ext}}^a}{\partial \mathbf{M}^b} - \frac{\partial \mathbf{F}_{\text{int}}^a}{\partial \mathbf{M}^b} - \frac{\partial \mathbf{F}_I^a}{\partial \mathbf{M}^b} \right) \Big|_{\mathbf{M}=\mathbf{M}^{ci}} (\mathbf{M}^b - \mathbf{M}^{bi}) = -\mathbf{R}^a(\mathbf{M}^{ci}). \quad (4.69)$$

The formula of the forces can be derived from Eq. (4.48) and Eq. (4.49), after substituting Eq. (4.60-4.62), which leads at each node  $a$  to:

$$\mathbf{F}_{f_{V\text{ext}}}^a = \mathbf{F}_{f_{V\text{int}}}^a + \mathbf{F}_{f_{VI}}^a, \quad (4.70)$$

$$\mathbf{F}_{f_{T\text{ext}}}^a = \mathbf{F}_{f_{T\text{int}}}^a + \mathbf{F}_{f_{TI}}^a, \quad (4.71)$$

$$\begin{aligned}
 F_{f_{V\text{ext}}}^a &= \sum_s \int_{(\partial_N \Omega)^s} N_{f_V}^a \bar{\mathbf{j}}_e \, dS - \sum_s \int_{(\partial_D \Omega)^s} \bar{f}_V \mathbf{n} \cdot \mathbf{l}_1(\bar{f}_T) \cdot \nabla N_{f_V}^a \, dS \\
 &- \sum_s \int_{(\partial_D \Omega)^s} \bar{f}_T \mathbf{n} \cdot \mathbf{l}_2(\bar{f}_V, \bar{f}_T) \cdot \nabla N_{f_V}^a \, dS + \sum_s \int_{(\partial_D \Omega)^s} \bar{f}_V \mathbf{n} \cdot \left( \mathbf{l}_1(\bar{f}_T) \frac{\mathcal{B}}{h_s} \right) \cdot \mathbf{n} N_{f_V}^a \, dS \\
 &+ \sum_s \int_{(\partial_D \Omega)^s} \bar{f}_T \mathbf{n} \cdot \mathbf{l}_2(\bar{f}_V, \bar{f}_T) \frac{\mathcal{B}}{h_s} \cdot \mathbf{n} N_{f_V}^a \, dS,
 \end{aligned} \tag{4.72}$$

with

$$F_{f_{V\text{int}}}^a = \sum_e \int_{\Omega^e} \mathbf{j}_e(f_{V_h}, f_{T_h}) \cdot \nabla N_{f_V}^a \, d\Omega, \tag{4.73}$$

$$F_{f_{VI}}^{a\pm} = F_{f_{VI1}}^{a\pm} + F_{f_{VI2}}^{a\pm} + F_{f_{VI3}}^{a\pm}, \tag{4.74}$$

where the three contributions to the interface forces on  $\partial_I \Omega_h^2$  are respectively

$$F_{f_{VI1}}^{a\pm} = \sum_s \int_{(\partial_I \Omega)^s} \left( \pm N_{f_V}^{a\pm} \right) \langle \mathbf{j}_e(f_{V_h}, f_{T_h}) \rangle \cdot \mathbf{n}^- \, dS, \tag{4.75}$$

$$\begin{aligned}
 F_{f_{VI2}}^{a\pm} &= \frac{1}{2} \sum_s \int_{(\partial_I \Omega)^s} \llbracket f_{V_h} \rrbracket \left( \mathbf{l}_1^\pm(f_{T_h}) \cdot \nabla N_{f_V}^{a\pm} \right) \cdot \mathbf{n}^- \, dS \\
 &+ \frac{1}{2} \sum_s \int_{(\partial_I \Omega)^s} \llbracket f_{T_h} \rrbracket \left( \mathbf{l}_2^\pm(f_{V_h}, f_{T_h}) \cdot \nabla N_{f_V}^{a\pm} \right) \cdot \mathbf{n}^- \, dS,
 \end{aligned} \tag{4.76}$$

$$\begin{aligned}
 F_{f_{VI3}}^{a\pm} &= \sum_s \int_{(\partial_I \Omega)^s} \llbracket f_{V_h} \rrbracket \mathbf{n}^- \cdot \left\langle \mathbf{l}_1(f_{T_h}) \frac{\mathcal{B}}{h_s} \right\rangle \cdot \mathbf{n}^- \left( \pm N_{f_V}^{a\pm} \right) \, dS \\
 &+ \sum_s \int_{(\partial_I \Omega)^s} \llbracket f_{T_h} \rrbracket \mathbf{n}^- \cdot \left\langle \mathbf{l}_2(f_{V_h}, f_{T_h}) \frac{\mathcal{B}}{h_s} \right\rangle \cdot \mathbf{n}^- \left( \pm N_{f_V}^{a\pm} \right) \, dS.
 \end{aligned} \tag{4.77}$$

Similarly, the thermal contributions read

$$\begin{aligned}
 F_{f_{T\text{ext}}}^a &= \sum_s \int_{(\partial_N \Omega)^s} N_{f_T}^a \bar{\mathbf{j}}_y \, dS - \sum_s \int_{(\partial_D \Omega)^s} \bar{f}_T \mathbf{n} \cdot \mathbf{j}_{y1}(\bar{f}_V, \bar{f}_T) \cdot \nabla N_{f_T}^a \, dS \\
 &- \sum_s \int_{(\partial_D \Omega)^s} \bar{f}_V \mathbf{n} \cdot \mathbf{l}_2(\bar{f}_V, \bar{f}_T) \cdot \nabla N_{f_T}^a \, dS + \sum_s \int_{(\partial_D \Omega)^s} \bar{f}_T \mathbf{n} \cdot \mathbf{j}_{y1}(\bar{f}_V, \bar{f}_T) \frac{\mathcal{B}}{h_s} \cdot \mathbf{n} N_{f_T}^a \, dS \\
 &+ \sum_s \int_{(\partial_D \Omega)^s} \bar{f}_V \mathbf{n} \cdot \mathbf{l}_2(\bar{f}_V, \bar{f}_T) \frac{\mathcal{B}}{h_s} \cdot \mathbf{n} N_{f_T}^a \, dS,
 \end{aligned} \tag{4.78}$$

with

$$F_{f_{T\text{int}}}^a = \sum_e \int_{\Omega^e} \mathbf{j}_y(f_{V_h}, f_{T_h}) \cdot \nabla N_{f_T}^a \, d\Omega - \sum_e \int_{\Omega^e} \rho \partial_{ty} N_{f_T}^a \, d\Omega, \tag{4.79}$$

$$F_{f_{TI}}^{a\pm} = F_{f_{TI1}}^{a\pm} + F_{f_{TI2}}^{a\pm} + F_{f_{TI3}}^{a\pm}, \tag{4.80}$$

<sup>2</sup>The contributions on  $\partial_D \Omega_h$  can be directly deduced by removing the factor (1/2) accordingly to the definition of the average flux on the Dirichlet boundary and substituting  $\mathbf{l}_1(\bar{f}_T)$ ,  $\mathbf{l}_2(\bar{f}_V, \bar{f}_T)$  and  $\mathbf{j}_y(\bar{f}_V, \bar{f}_T)$ , which are constant with respect to  $f_{V_h}$ , and  $f_{T_h}$ , instead of  $\mathbf{l}_1(f_{T_h})$ ,  $\mathbf{l}_2(f_{V_h}, f_{T_h})$  and  $\mathbf{j}_y(f_{V_h}, f_{T_h})$ .

where the three contributions to the interface forces are respectively

$$\mathbf{F}_{f_{T11}}^{a\pm} = \sum_s \int_{(\partial_I \Omega)^s} \left( \pm N_{f_T}^{a\pm} \right) \langle \mathbf{j}_y(f_{V_h}, f_{T_h}) \rangle \cdot \mathbf{n}^- dS, \quad (4.81)$$

$$\begin{aligned} \mathbf{F}_{f_{T12}}^{a\pm} &= \frac{1}{2} \sum_s \int_{(\partial_I \Omega)^s} \llbracket f_{T_h} \rrbracket \left( \mathbf{j}_{y1}^\pm(f_{V_h}, f_{T_h}) \cdot \nabla N_{f_T}^{a\pm} \right) \cdot \mathbf{n}^- dS \\ &+ \frac{1}{2} \sum_s \int_{(\partial_I \Omega)^s} \llbracket f_{V_h} \rrbracket \left( \mathbf{l}_2^\pm(f_{V_h}, f_{T_h}) \cdot \nabla N_{f_T}^{a\pm} \right) \cdot \mathbf{n}^- dS, \end{aligned} \quad (4.82)$$

$$\begin{aligned} \mathbf{F}_{f_{T13}}^{a\pm} &= \sum_s \int_{(\partial_I \Omega)^s} \llbracket f_{T_h} \rrbracket \mathbf{n}^- \cdot \left\langle \mathbf{j}_{y1}(f_{V_h}, f_{T_h}) \frac{\mathcal{B}}{h_s} \right\rangle \cdot \mathbf{n}^- \left( \pm N_{f_T}^{a\pm} \right) dS \\ &+ \sum_s \int_{(\partial_I \Omega)^s} \llbracket f_{V_h} \rrbracket \mathbf{n}^- \cdot \left\langle \mathbf{l}_2(f_{V_h}, f_{T_h}) \frac{\mathcal{B}}{h_s} \right\rangle \cdot \mathbf{n}^- \left( \pm N_{f_T}^{a\pm} \right) dS. \end{aligned} \quad (4.83)$$

In these equations the symbol  $\pm$  refers to the node  $e^\pm$  (+ for node  $e^+$  and - for node  $e^-$ ).

This system is solved by means of a Newton-Raphson method with the stiffness matrix computed in Appendix C.1, where the iterations continue until the convergence to a specified tolerance is achieved.

## 4.4 Numerical properties

In this section, the numerical properties of the weak formulation stated by Eq. (4.57) are studied in steady state conditions ( $\mathbf{i} = 0$ ), and under the assumption that  $d = 2$ . It is demonstrated that the framework satisfies two fundamental properties of a numerical method: consistency and stability. Moreover we show that the method possesses the optimal convergence rate with respect to the mesh size.

### 4.4.1 Consistency

To prove the consistency of the method, the exact solution  $\mathbf{M}^e \in H^2(\Omega) \times H^{2^+}(\Omega)$  of the problem stated by Eq. (4.32) is considered. This implies  $\llbracket \mathbf{M}^e \rrbracket = 0$ ,  $\langle \mathbf{j} \rangle = \mathbf{j}$  on  $\partial_I \Omega_h$ , and  $\llbracket \mathbf{M}^e \rrbracket = -\bar{\mathbf{M}} = \mathbf{M}^e$ ,  $\langle \mathbf{j} \rangle = \mathbf{j} = \mathbf{Z}(\mathbf{M}^e) \nabla \mathbf{M}^e$ , and  $\mathbf{Z}(\mathbf{M}) = \mathbf{Z}(\bar{\mathbf{M}}) = \mathbf{Z}(\mathbf{M}^e)$  on  $\partial_D \Omega_h$ . Therefore, Eq. (4.57) becomes:

$$\begin{aligned} & \int_{\partial_N \Omega_h} \delta \mathbf{M}^T \bar{\mathbf{j}} dS - \int_{\partial_D \Omega_h} \bar{\mathbf{M}}_n^T (\mathbf{Z}(\bar{\mathbf{M}}) \nabla \delta \mathbf{M}) dS + \int_{\partial_D \Omega_h} \delta \mathbf{M}_n^T \left( \frac{\mathcal{B}}{h_s} \mathbf{Z}(\bar{\mathbf{M}}) \right) \bar{\mathbf{M}}_n dS \\ &= \int_{\Omega_h} (\nabla \delta \mathbf{M})^T \mathbf{j}(\mathbf{M}^e, \nabla \mathbf{M}^e) d\Omega + \int_{\partial_I \Omega_h} \llbracket \delta \mathbf{M}_n^T \rrbracket \mathbf{j}(\mathbf{M}^e, \nabla \mathbf{M}^e) dS \\ &- \int_{\partial_D \Omega_h} \delta \mathbf{M}_n^T \mathbf{j}(\mathbf{M}^e, \nabla \mathbf{M}^e) dS - \int_{\partial_D \Omega_h} \mathbf{M}_n^T \mathbf{Z}(\bar{\mathbf{M}}) \nabla \delta \mathbf{M} dS \\ &+ \int_{\partial_D \Omega_h} \delta \mathbf{M}_n^T \frac{\mathcal{B}}{h_s} \mathbf{Z}(\bar{\mathbf{M}}) \mathbf{M}_n^e dS \quad \forall \delta \mathbf{M} \in X. \end{aligned} \quad (4.84)$$



Integrating the first term of the right hand side by parts leads to

$$\begin{aligned} \sum_e \int_{\Omega^e} (\nabla \delta \mathbf{M})^T \mathbf{j}(\mathbf{M}^e, \nabla \mathbf{M}^e) d\Omega &= - \sum_e \int_{\Omega^e} \delta \mathbf{M}^T \nabla \mathbf{j}(\mathbf{M}^e, \nabla \mathbf{M}^e) d\Omega \\ &+ \sum_e \int_{\partial \Omega^e} \delta \mathbf{M}_n^T \mathbf{j}(\mathbf{M}^e, \nabla \mathbf{M}^e) dS, \end{aligned} \quad (4.85)$$

and Eq. (4.84) becomes

$$\begin{aligned} \int_{\partial_N \Omega_h} \delta \mathbf{M}^T \bar{\mathbf{j}} dS - \int_{\partial_D \Omega_h} \bar{\mathbf{M}}_n^T (\mathbf{Z}(\bar{\mathbf{M}}) \nabla \delta \mathbf{M}) dS + \int_{\partial_D \Omega_h} \delta \mathbf{M}_n^T \left( \frac{\mathcal{B}}{h_s} \mathbf{Z}(\bar{\mathbf{M}}) \right) \bar{\mathbf{M}}_n dS \\ = - \sum_e \int_{\Omega^e} \delta \mathbf{M}^T \nabla \mathbf{j}(\mathbf{M}^e, \nabla \mathbf{M}^e) d\Omega + \int_{\partial_N \Omega_h} \delta \mathbf{M}_n^T \mathbf{j}(\mathbf{M}^e, \nabla \mathbf{M}^e) dS \\ - \int_{\partial_D \Omega_h} \mathbf{M}_n^e{}^T \mathbf{Z}(\bar{\mathbf{M}}) \nabla \delta \mathbf{M} dS + \int_{\partial_D \Omega_h} \delta \mathbf{M}_n^T \frac{\mathcal{B}}{h_s} \mathbf{Z}(\bar{\mathbf{M}}) \mathbf{M}_n^e dS \quad \forall \delta \mathbf{M} \in X. \end{aligned} \quad (4.86)$$

The arbitrary nature of the test functions leads to recover the set of conservation laws, Eqs. (4.11-4.12), and the boundary conditions, Eqs. (4.13-4.14).

#### 4.4.2 Discontinuous space and finite element properties

In this part, we will assume that  $\partial_D \Omega_h = \partial \Omega_h$ . This assumption is not restrictive but simplifies the demonstrations.

The main approximation properties and norm definitions, which will be used in the error analysis of the Discontinuous Galerkin Finite element method, will first be recalled without proofs.

The norms which have been defined in Chapter 2, Eqs. (2.10-2.12), will also be considered for our subsequent analysis of Electro-Thermal coupling, with  $\mathbf{O} = \mathbf{M}$ , for  $\mathbf{M} \in X_2$ , where the norm  $\|\mathbf{M}\| = 0$  is defined in such a way that it will be equal to zero only when  $f_V = \text{cst}$  and  $f_T = \text{cst}$  on  $\Omega_h$  and are equal to 0 on  $\partial_D \Omega_h$ .

#### 4.4.3 Second order non-self-adjoint elliptic problem

The demonstration of the stability follows closely the approach developed by [25,60,74,76] for linear and nonlinear elliptic problems. As the problem is herein coupled, and as the elliptic operator is different, we report and modify the main steps of the demonstrations that were initially developed in [25,76] for  $d = 2$ .

The main idea to prove the solution uniqueness and to establish the prior error estimate is to reformulate the nonlinear problem in a fixed point form which is the solution of the linearized problem as proposed in [24,30,76].

Starting from the definition of matrix  $\mathbf{Z}(\mathbf{M})$ , Eq. (4.30), which is a symmetric and positive definite matrix, as we have proved in Section 4.2.2, let us define the minimum and maximum eigenvalues of the matrix  $\mathbf{Z}(\mathbf{M})$  as  $\lambda(\mathbf{M})$  and  $\Lambda(\mathbf{M})$ ; then for all  $\xi \in \mathbb{R}_0^{2d}$  one has

$$0 < \lambda(\mathbf{M}) |\xi|^2 \leq \xi_i \mathbf{Z}^{ij}(\mathbf{M}) \xi_j \leq \Lambda(\mathbf{M}) |\xi|^2. \quad (4.87)$$

Also by assuming that  $\|\mathbf{M}\|_{W_\infty^1} \leq \alpha$ , then there is a positive constant  $C_\alpha$  such that

$$0 < C_\alpha < \lambda(\mathbf{M}). \quad (4.88)$$

In the subsequent analysis, we use the following integral form of the Taylor's expansions of  $\mathbf{j}$ , defined in Eq. (4.29), for  $(\mathbf{V}, \nabla\mathbf{P}) \in X \times \mathbf{Y}$  in terms of  $(\mathbf{M}, \nabla\mathbf{M}) \in X \times \mathbf{Y}$ :

$$\begin{aligned} \mathbf{j}(\mathbf{V}, \nabla\mathbf{P}) - \mathbf{j}(\mathbf{M}, \nabla\mathbf{M}) &= -\mathbf{j}_\mathbf{M}(\mathbf{M}, \nabla\mathbf{M})(\mathbf{M} - \mathbf{V}) - \mathbf{j}_{\nabla\mathbf{M}}(\mathbf{M}, \nabla\mathbf{M})(\nabla\mathbf{M} - \nabla\mathbf{P}) \\ &\quad + \bar{\mathbf{R}}_\mathbf{j}(\mathbf{M} - \mathbf{V}, \nabla\mathbf{M} - \nabla\mathbf{P}) \\ &= -\bar{\mathbf{j}}_\mathbf{M}(\mathbf{M}, \nabla\mathbf{M})(\mathbf{M} - \mathbf{V}) - \bar{\mathbf{j}}_{\nabla\mathbf{M}}(\mathbf{M}, \nabla\mathbf{M})(\nabla\mathbf{M} - \nabla\mathbf{P}), \end{aligned} \quad (4.89)$$

where  $\mathbf{j}_\mathbf{M}$  is the partial derivative of  $\mathbf{j}$  with respect to  $\mathbf{M}$ ,  $\mathbf{j}_{\nabla\mathbf{M}}$  is the partial derivative of  $\mathbf{j}$  with respect to  $\nabla\mathbf{M}$  expressed in the matrix form, and  $\bar{\mathbf{R}}_\mathbf{j}$  is the residual. With  $\mathbf{V}^t = \mathbf{M} + t(\mathbf{V} - \mathbf{M})$ ,  $\nabla\mathbf{P}^t = \nabla\mathbf{M} + t(\nabla\mathbf{P} - \nabla\mathbf{M})$ , we have

$$\bar{\mathbf{j}}_\mathbf{M}(\mathbf{M}, \nabla\mathbf{M}) = \int_0^1 \mathbf{j}_\mathbf{M}(\mathbf{V}^t, \nabla\mathbf{P}^t) dt, \quad \bar{\mathbf{j}}_{\nabla\mathbf{M}}(\mathbf{M}, \nabla\mathbf{M}) = \int_0^1 \mathbf{j}_{\nabla\mathbf{M}}(\mathbf{V}^t, \nabla\mathbf{P}^t) dt, \quad (4.90)$$

$$\begin{aligned} \bar{\mathbf{R}}_\mathbf{j}(\mathbf{M} - \mathbf{V}, \nabla\mathbf{M} - \nabla\mathbf{P}) &= (\mathbf{M} - \mathbf{V})^T \bar{\mathbf{j}}_{\mathbf{M}\mathbf{M}}(\mathbf{V}, \nabla\mathbf{P})(\mathbf{M} - \mathbf{V}) \\ &\quad + (\nabla\mathbf{M} - \nabla\mathbf{P})^T \bar{\mathbf{j}}_{\nabla\mathbf{M}\nabla\mathbf{M}}(\mathbf{V}, \nabla\mathbf{P})(\nabla\mathbf{M} - \nabla\mathbf{P}) \\ &\quad + 2(\mathbf{M} - \mathbf{V})^T \bar{\mathbf{j}}_{\mathbf{M}\nabla\mathbf{M}}(\mathbf{V}, \nabla\mathbf{P})(\nabla\mathbf{M} - \nabla\mathbf{P}), \end{aligned} \quad (4.91)$$

and

$$\begin{aligned} \bar{\mathbf{j}}_{\mathbf{M}\mathbf{M}}(\mathbf{V}, \nabla\mathbf{P}) &= \int_0^1 (1-t) \mathbf{j}_{\mathbf{M}\mathbf{M}}(\mathbf{V}^t, \nabla\mathbf{P}^t) dt, \\ \bar{\mathbf{j}}_{\mathbf{M}\nabla\mathbf{M}}(\mathbf{V}, \nabla\mathbf{P}) &= \int_0^1 (1-t) \mathbf{j}_{\mathbf{M}\nabla\mathbf{M}}(\mathbf{V}^t, \nabla\mathbf{P}^t) dt, \\ \bar{\mathbf{j}}_{\nabla\mathbf{M}\nabla\mathbf{M}}(\mathbf{V}, \nabla\mathbf{P}) &= \int_0^1 (1-t) \mathbf{j}_{\nabla\mathbf{M}\nabla\mathbf{M}}(\mathbf{V}^t, \nabla\mathbf{P}^t) dt. \end{aligned} \quad (4.92)$$

Using the definition Eq. (4.29) of  $\mathbf{j}$ , we have  $\mathbf{j}_\mathbf{M} = \frac{\partial \mathbf{Z}}{\partial \mathbf{M}} \nabla\mathbf{M}$ ,  $\mathbf{j}_{\nabla\mathbf{M}} = \mathbf{Z}$ ,  $\mathbf{j}_{\mathbf{M}\mathbf{M}} = \frac{\partial^2 \mathbf{Z}}{\partial \mathbf{M}^2} \nabla\mathbf{M}$ ,  $\mathbf{j}_{\mathbf{M}\nabla\mathbf{M}} = \mathbf{j}_{\nabla\mathbf{M}\mathbf{M}} = \frac{\partial \mathbf{Z}}{\partial \mathbf{M}}$ ,  $\mathbf{j}_{\nabla\mathbf{M}\nabla\mathbf{M}} = 0$ . If  $f_T \geq f_{T0} > 0$ , then  $\bar{\mathbf{j}}_\mathbf{M}, \bar{\mathbf{j}}_{\mathbf{M}\mathbf{M}} \in \mathbf{L}^\infty(\Omega \times \mathbb{R} \times \mathbb{R}_0^+ \times \mathbb{R}^d \times \mathbb{R}^d)$  and  $\bar{\mathbf{j}}_{\nabla\mathbf{M}}, \bar{\mathbf{j}}_{\mathbf{M}\nabla\mathbf{M}}, \bar{\mathbf{j}}_{\nabla\mathbf{M}\mathbf{M}} \in \mathbf{L}^\infty(\Omega \times \mathbb{R} \times \mathbb{R}_0^+)$ . The expressions of the derivatives are given in C.2. Since  $\mathbf{j}$  is a twice continuously differential function with all the derivatives through the second order locally bounded in a ball around  $\mathbf{M} \in \mathbb{R} \times \mathbb{R}_0^+$  as it will be shown in Section 4.4.4, for  $d = 2$ , we denote by  $C_y$

$$C_y = \max \left\{ \|\mathbf{j}\|_{W_\infty^2(\Omega \times \mathbb{R} \times \mathbb{R}_0^+ \times \mathbb{R}^d \times \mathbb{R}^d)}, \|\bar{\mathbf{j}}_\mathbf{M}, \bar{\mathbf{j}}_{\nabla\mathbf{M}}, \bar{\mathbf{j}}_{\mathbf{M}\mathbf{M}}, \bar{\mathbf{j}}_{\mathbf{M}\nabla\mathbf{M}}, \bar{\mathbf{j}}_{\nabla\mathbf{M}\mathbf{M}}\|_{L^\infty(\Omega \times \mathbb{R} \times \mathbb{R}_0^+)} \right\}. \quad (4.93)$$

We can now study the weak form defined by Eq. (4.57) under the assumptions  $\mathbf{i} = 0$  and  $\bar{\mathbf{j}}$  independent of  $\mathbf{M}$ . The problem thus reads as finding  $\mathbf{M} \in X^+$  such that

$$a_3(\mathbf{M}, \delta\mathbf{M}) = b_3(\delta\mathbf{M}) \quad \forall \delta\mathbf{M} \in X, \quad (4.94)$$

with  $a_3(\mathbf{M}, \delta\mathbf{M})$  defined by Eq. (4.58) and  $b_3(\delta\mathbf{M})$  by Eq. (4.59).

#### 4.4.3.1 Derivation of the non-self-adjoint linear elliptic problem

Let us define  $\mathbf{M}^e \in H^2(\Omega) \times H^{2^+}(\Omega)$  the solution of the strong form stated by Eq. (4.32). Thus as  $[[\mathbf{M}^e]] = 0$  on  $\partial_I \Omega^e$  and as  $[[\mathbf{M}^e]] = -\mathbf{M}^e = -\bar{\mathbf{M}}$  on  $\partial_D \Omega^e$ , we have

$$\begin{aligned} a_3(\mathbf{M}^e, \delta \mathbf{M}^e) &= \int_{\Omega_h} (\nabla \delta \mathbf{M}^e)^T \mathbf{j}(\mathbf{M}^e, \nabla \mathbf{M}^e) d\Omega + \int_{\partial_I \Omega_h} [[\delta \mathbf{M}_{\mathbf{n}}^{eT}]] \langle \mathbf{j}(\mathbf{M}^e, \nabla \mathbf{M}^e) \rangle dS \\ &\quad - \int_{\partial_D \Omega_h} \delta \mathbf{M}_{\mathbf{n}}^{eT} \mathbf{j}(\mathbf{M}^e, \nabla \mathbf{M}^e) dS - \int_{\partial_D \Omega_h} \bar{\mathbf{M}}_{\mathbf{n}}^T \mathbf{Z}(\mathbf{M}^e) \nabla \delta \mathbf{M}^e dS \\ &\quad + \int_{\partial_D \Omega_h} \delta \mathbf{M}_{\mathbf{n}}^{eT} \frac{\mathcal{B}}{h_s} \mathbf{Z}(\mathbf{M}^e) \bar{\mathbf{M}}_{\mathbf{n}} dS = b_3(\delta \mathbf{M}^e) \quad \forall \delta \mathbf{M}^e \in X, \end{aligned} \quad (4.95)$$

as the weak form stated by Eq. (4.57) is consistent, see Section 4.4.1.

Using the weak formulation (4.94), we state the Discontinuous Galerkin finite element method for the problem as finding  $\mathbf{M}_h \in X^{k^+}$ , such that

$$a_3(\mathbf{M}_h, \delta \mathbf{M}_h) = b_3(\delta \mathbf{M}_h) \quad \forall \delta \mathbf{M}_h \in X^k \subset X. \quad (4.96)$$

Therefore, using  $\delta \mathbf{M}^e = \delta \mathbf{M}_h$  in Eq. (4.95) and subtracting it from the DG discretization (4.96) yields

$$\begin{aligned} 0 &= a_3(\mathbf{M}^e, \delta \mathbf{M}_h) - a_3(\mathbf{M}_h, \delta \mathbf{M}_h) = \int_{\Omega_h} (\nabla \delta \mathbf{M}_h)^T \mathbf{j}(\mathbf{M}^e, \nabla \mathbf{M}^e) d\Omega \\ &\quad - \int_{\Omega_h} (\nabla \delta \mathbf{M}_h)^T \mathbf{j}(\mathbf{M}_h, \nabla \mathbf{M}_h) d\Omega + \int_{\partial_I \Omega_h} [[\delta \mathbf{M}_{\mathbf{h}\mathbf{n}}^T]] \langle \mathbf{j}(\mathbf{M}^e, \nabla \mathbf{M}^e) \rangle dS \\ &\quad - \int_{\partial_D \Omega_h} \delta \mathbf{M}_{\mathbf{h}\mathbf{n}}^T \mathbf{j}(\mathbf{M}^e, \nabla \mathbf{M}^e) dS - \int_{\partial_D \Omega_h} \bar{\mathbf{M}}_{\mathbf{n}}^T \mathbf{j}_{\nabla \mathbf{M}}(\mathbf{M}^e) \nabla \delta \mathbf{M}_h dS \\ &\quad + \int_{\partial_D \Omega_h} \delta \mathbf{M}_{\mathbf{h}\mathbf{n}}^T \frac{\mathcal{B}}{h_s} \mathbf{j}_{\nabla \mathbf{M}}(\mathbf{M}^e) \bar{\mathbf{M}}_{\mathbf{n}} dS - \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} [[\mathbf{M}_{\mathbf{h}\mathbf{n}}^T]] \langle \mathbf{j}_{\nabla \mathbf{M}}(\mathbf{M}_h) \nabla \delta \mathbf{M}_h \rangle dS \\ &\quad - \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} [[\delta \mathbf{M}_{\mathbf{h}\mathbf{n}}^T]] \langle \mathbf{j}(\mathbf{M}_h, \nabla \mathbf{M}_h) \rangle dS \\ &\quad - \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} [[\mathbf{M}_{\mathbf{h}\mathbf{n}}^T]] \left\langle \frac{\mathcal{B}}{h_s} \mathbf{j}_{\nabla \mathbf{M}}(\mathbf{M}_h) \right\rangle [[\delta \mathbf{M}_{\mathbf{h}\mathbf{n}}]] dS, \quad \forall \delta \mathbf{M}_h \in X^k, \end{aligned} \quad (4.97)$$

where  $\mathbf{Z} = \mathbf{j}_{\nabla \mathbf{M}}$ .

By adding and subtracting successively  $\int_{\partial_I \Omega_h} [[\mathbf{M}_{\mathbf{n}}^{eT} - \mathbf{M}_{\mathbf{h}\mathbf{n}}^T]] \langle \mathbf{j}_{\nabla \mathbf{M}}(\mathbf{M}^e) \nabla \delta \mathbf{M}_h \rangle dS$

and  $\int_{\partial_I \Omega_h} [[\mathbf{M}_{\mathbf{n}}^{eT} - \mathbf{M}_{\mathbf{h}\mathbf{n}}^T]] \left\langle \frac{\mathcal{B}}{h_s} \mathbf{j}_{\nabla \mathbf{M}}(\mathbf{M}^e) \right\rangle [[\delta \mathbf{M}_{\mathbf{h}\mathbf{n}}]] dS$  to this last relation, and using  $[[\mathbf{M}_{\mathbf{n}}^e]] = 0$

on  $\partial_I\Omega_h$  and  $[[\mathbf{M}_n^e]] = -\mathbf{M}_n^e = -\bar{\mathbf{M}}_n$  on  $\partial_D\Omega_h$ , one gets

$$\begin{aligned}
0 &= \int_{\Omega_h} (\nabla\delta\mathbf{M}_h)^T (\mathbf{j}(\mathbf{M}^e, \nabla\mathbf{M}^e) - \mathbf{j}(\mathbf{M}_h, \nabla\mathbf{M}_h)) \, d\Omega \\
&+ \int_{\partial_I\Omega_h \cup \partial_D\Omega_h} [[\delta\mathbf{M}_{h_n}^T]] \langle \mathbf{j}(\mathbf{M}^e, \nabla\mathbf{M}^e) - \mathbf{j}(\mathbf{M}_h, \nabla\mathbf{M}_h) \rangle \, dS \\
&+ \int_{\partial_I\Omega_h \cup \partial_D\Omega_h} [[\mathbf{M}_n^{eT} - \mathbf{M}_{h_n}^T]] \langle \mathbf{j}_{\nabla\mathbf{M}}(\mathbf{M}^e) \nabla\delta\mathbf{M}_h \rangle \, dS \\
&- \int_{\partial_I\Omega_h} [[\mathbf{M}_n^{eT} - \mathbf{M}_{h_n}^T]] \langle (\mathbf{j}_{\nabla\mathbf{M}}(\mathbf{M}^e) - \mathbf{j}_{\nabla\mathbf{M}}(\mathbf{M}_h)) \nabla\delta\mathbf{M}_h \rangle \, dS \\
&+ \int_{\partial_I\Omega_h \cup \partial_D\Omega_h} [[\mathbf{M}_n^{eT} - \mathbf{M}_{h_n}^T]] \left\langle \frac{\mathcal{B}}{h_s} \mathbf{j}_{\nabla\mathbf{M}}(\mathbf{M}^e) \right\rangle [[\delta\mathbf{M}_{h_n}]] \, dS \\
&- \int_{\partial_I\Omega_h} [[\mathbf{M}_n^{eT} - \mathbf{M}_{h_n}^T]] \left\langle \frac{\mathcal{B}}{h_s} (\mathbf{j}_{\nabla\mathbf{M}}(\mathbf{M}^e) - \mathbf{j}_{\nabla\mathbf{M}}(\mathbf{M}_h)) \right\rangle [[\delta\mathbf{M}_{h_n}]] \, dS \quad \forall \delta\mathbf{M}_h \in X^k.
\end{aligned} \tag{4.98}$$

Using the Taylor series defined in Eq. (4.89) to rewrite the differences, we successively have:

$$\begin{aligned}
&\int_{\Omega_h} (\nabla\delta\mathbf{M}_h)^T (\mathbf{j}(\mathbf{M}^e, \nabla\mathbf{M}^e) - \mathbf{j}(\mathbf{M}_h, \nabla\mathbf{M}_h)) \, d\Omega \\
&= \int_{\Omega_h} (\nabla\delta\mathbf{M}_h)^T (\mathbf{j}_M(\mathbf{M}^e, \nabla\mathbf{M}^e)(\mathbf{M}^e - \mathbf{M}_h)) \, d\Omega \\
&+ \int_{\Omega_h} (\nabla\delta\mathbf{M}_h)^T (\mathbf{j}_{\nabla\mathbf{M}}(\mathbf{M}^e)(\nabla\mathbf{M}^e - \nabla\mathbf{M}_h)) \, d\Omega \\
&- \int_{\Omega_h} (\nabla\delta\mathbf{M}_h)^T (\bar{\mathbf{R}}_j(\mathbf{M}^e - \mathbf{M}_h, \nabla\mathbf{M}^e - \nabla\mathbf{M}_h)) \, d\Omega,
\end{aligned} \tag{4.99}$$

and

$$\begin{aligned}
&\int_{\partial_I\Omega_h \cup \partial_D\Omega_h} [[\delta\mathbf{M}_{h_n}^T]] \langle \mathbf{j}(\mathbf{M}^e, \nabla\mathbf{M}^e) - \mathbf{j}(\mathbf{M}_h, \nabla\mathbf{M}_h) \rangle \, dS \\
&= \int_{\partial_I\Omega_h \cup \partial_D\Omega_h} [[\delta\mathbf{M}_{h_n}^T]] \langle \mathbf{j}_M(\mathbf{M}^e, \nabla\mathbf{M}^e)(\mathbf{M}^e - \mathbf{M}_h) \rangle \, dS \\
&+ \int_{\partial_I\Omega_h \cup \partial_D\Omega_h} [[\delta\mathbf{M}_{h_n}^T]] \langle \mathbf{j}_{\nabla\mathbf{M}}(\mathbf{M}^e)(\nabla\mathbf{M}^e - \nabla\mathbf{M}_h) \rangle \, dS \\
&- \int_{\partial_I\Omega_h \cup \partial_D\Omega_h} [[\delta\mathbf{M}_{h_n}^T]] \langle \bar{\mathbf{R}}_j(\mathbf{M}^e - \mathbf{M}_h, \nabla\mathbf{M}^e - \nabla\mathbf{M}_h) \rangle \, dS.
\end{aligned} \tag{4.100}$$

We can now first define  $\mathcal{N}(\mathbf{M}^e, \mathbf{M}_h; \delta\mathbf{M}_h)$  as follows

$$\begin{aligned}
\mathcal{N}(\mathbf{M}^e, \mathbf{M}_h; \delta\mathbf{M}_h) &= \int_{\Omega_h} (\nabla \delta\mathbf{M}_h)^T (\bar{\mathbf{R}}_j(\mathbf{M}^e - \mathbf{M}_h, \nabla\mathbf{M}^e - \nabla\mathbf{M}_h)) d\Omega \\
&+ \int_{\partial_T\Omega_h \cup \partial_D\Omega_h} \llbracket \delta\mathbf{M}_{h_n}^T \rrbracket \langle \bar{\mathbf{R}}_j(\mathbf{M}^e - \mathbf{M}_h, \nabla\mathbf{M}^e - \nabla\mathbf{M}_h) \rangle dS \\
&+ \int_{\partial_T\Omega_h} \llbracket \mathbf{M}_n^{eT} - \mathbf{M}_{h_n}^T \rrbracket \langle (\mathbf{j}_{\nabla\mathbf{M}}(\mathbf{M}^e) - \mathbf{j}_{\nabla\mathbf{M}}(\mathbf{M}_h)) \nabla \delta\mathbf{M}_h \rangle dS \\
&+ \int_{\partial_T\Omega_h} \llbracket \mathbf{M}_n^{eT} - \mathbf{M}_{h_n}^T \rrbracket \left\langle \frac{\mathcal{B}}{h_s} (\mathbf{j}_{\nabla\mathbf{M}}(\mathbf{M}^e) - \mathbf{j}_{\nabla\mathbf{M}}(\mathbf{M}_h)) \right\rangle \llbracket \delta\mathbf{M}_{h_n} \rrbracket dS \\
&= \mathcal{I}_1 + \mathcal{I}_2 + \mathcal{I}_3 + \mathcal{I}_4.
\end{aligned} \tag{4.101}$$

Moreover, for given  $\boldsymbol{\psi} \in X^+$ ,  $\boldsymbol{\omega} \in X$  and  $\delta\boldsymbol{\omega} \in X$ , we define the following forms:

$$\begin{aligned}
\mathcal{A}(\boldsymbol{\psi}; \boldsymbol{\omega}, \delta\boldsymbol{\omega}) &= \int_{\Omega_h} (\nabla \delta\boldsymbol{\omega})^T \mathbf{j}_{\nabla\boldsymbol{\psi}}(\boldsymbol{\psi}) \nabla \boldsymbol{\omega} d\Omega + \int_{\partial_T\Omega_h \cup \partial_D\Omega_h} \llbracket \delta\boldsymbol{\omega}_n^T \rrbracket \langle \mathbf{j}_{\nabla\boldsymbol{\psi}}(\boldsymbol{\psi}) \nabla \boldsymbol{\omega} \rangle dS \\
&+ \int_{\partial_T\Omega_h \cup \partial_D\Omega_h} \llbracket \boldsymbol{\omega}_n^T \rrbracket \langle \mathbf{j}_{\nabla\boldsymbol{\psi}}(\boldsymbol{\psi}) \nabla \delta\boldsymbol{\omega} \rangle dS + \int_{\partial_T\Omega_h \cup \partial_D\Omega_h} \llbracket \boldsymbol{\omega}_n^T \rrbracket \left\langle \frac{\mathcal{B}}{h_s} \mathbf{j}_{\nabla\boldsymbol{\psi}}(\boldsymbol{\psi}) \right\rangle \llbracket \delta\boldsymbol{\omega}_n \rrbracket dS,
\end{aligned} \tag{4.102}$$

$$\mathcal{B}(\boldsymbol{\psi}; \boldsymbol{\omega}, \delta\boldsymbol{\omega}) = \int_{\Omega_h} (\nabla \delta\boldsymbol{\omega})^T \mathbf{j}_{\boldsymbol{\psi}}(\boldsymbol{\psi}, \nabla\boldsymbol{\psi}) \boldsymbol{\omega} d\Omega + \int_{\partial_T\Omega_h \cup \partial_D\Omega_h} \llbracket \delta\boldsymbol{\omega}_n^T \rrbracket \langle \mathbf{j}_{\boldsymbol{\psi}}(\boldsymbol{\psi}, \nabla\boldsymbol{\psi}) \boldsymbol{\omega} \rangle dS. \tag{4.103}$$

For fixed  $\boldsymbol{\psi}$ , the form  $\mathcal{A}(\boldsymbol{\psi}; \cdot, \cdot)$  and the form  $\mathcal{B}(\boldsymbol{\psi}; \cdot, \cdot)$  are bi-linear. Therefore, using the relations (4.99-4.100) and the definitions (4.101-4.103), the set of Eqs. (4.98) is rewritten as finding  $\mathbf{M}_h \in X^{k^+}$  such that:

$$\mathcal{A}(\mathbf{M}^e; \mathbf{M}^e - \mathbf{M}_h, \delta\mathbf{M}_h) + \mathcal{B}(\mathbf{M}^e; \mathbf{M}^e - \mathbf{M}_h, \delta\mathbf{M}_h) = \mathcal{N}(\mathbf{M}^e, \mathbf{M}_h; \delta\mathbf{M}_h) \quad \forall \delta\mathbf{M}_h \in X^k. \tag{4.104}$$

#### 4.4.4 Solution uniqueness

Let us first define  $\boldsymbol{\eta} = I_h\mathbf{M} - \mathbf{M}^e \in X$ , with  $I_h\mathbf{M} \in X^{k^+}$  the interpolant of  $\mathbf{M}^e$  in  $X^{k^+}$ . The last relation (4.104) thus becomes

$$\begin{aligned}
&\mathcal{A}(\mathbf{M}^e; I_h\mathbf{M} - \mathbf{M}_h, \delta\mathbf{M}_h) + \mathcal{B}(\mathbf{M}^e; I_h\mathbf{M} - \mathbf{M}_h, \delta\mathbf{M}_h) \\
&= \mathcal{A}(\mathbf{M}^e; \boldsymbol{\eta}, \delta\mathbf{M}_h) + \mathcal{B}(\mathbf{M}^e; \boldsymbol{\eta}, \delta\mathbf{M}_h) + \mathcal{N}(\mathbf{M}^e, \mathbf{M}_h; \delta\mathbf{M}_h) \quad \forall \delta\mathbf{M}_h \in X^k.
\end{aligned} \tag{4.105}$$

Now in order to prove the existence of a solution  $\mathbf{M}_h$  of the problem stated by Eq. (4.98), which corresponds to the DG finite element discretization (4.96), we state the problem in the fixed point formulation and we define a map  $S_h : X^{k^+} \rightarrow X^{k^+}$  as follows: for a given  $\mathbf{y} \in X^{k^+}$ , find  $S_h(\mathbf{y}) = \mathbf{M}_y \in X^{k^+}$ , such that

$$\begin{aligned}
&\mathcal{A}(\mathbf{M}^e; I_h\mathbf{M} - \mathbf{M}_y, \delta\mathbf{M}_h) + \mathcal{B}(\mathbf{M}^e; I_h\mathbf{M} - \mathbf{M}_y, \delta\mathbf{M}_h) \\
&= \mathcal{A}(\mathbf{M}^e; \boldsymbol{\eta}, \delta\mathbf{M}_h) + \mathcal{B}(\mathbf{M}^e; \boldsymbol{\eta}, \delta\mathbf{M}_h) + \mathcal{N}(\mathbf{M}^e, \mathbf{y}; \delta\mathbf{M}_h) \quad \forall \delta\mathbf{M}_h \in X^k.
\end{aligned} \tag{4.106}$$

The existence of a fixed point of the map  $S_h$  is equivalent to the existence of a solution  $\mathbf{M}_h$  of the discrete problem (4.96), see [24].

For the following analysis, we denote by  $C^k$ , a positive generic constant which is independent of the mesh size, but may depend on  $C_{\mathcal{T}}, C_{\mathcal{D}}^k, C_{\mathcal{I}}^k, C_{\mathcal{K}}^k$ , and on  $k$ , so it can take different values at different places.

To demonstrate the uniqueness, we have recourse to the following Lemmata.

**Lemma 4.4.1** (Lower bound). *For  $\mathcal{B}$  larger than a constant, which depends on the polynomial approximation only, there exist two constants  $C_1^k$  and  $C_2^k$ , such that*

$$\mathcal{A}(\mathbf{M}^e; \delta \mathbf{M}_h, \delta \mathbf{M}_h) + \mathcal{B}(\mathbf{M}^e; \delta \mathbf{M}_h, \delta \mathbf{M}_h) \geq C_1^k \|\delta \mathbf{M}_h\|_*^2 - C_2^k \|\delta \mathbf{M}_h\|_{L^2(\Omega)}^2 \quad \forall \delta \mathbf{M}_h \in X^k, \quad (4.107)$$

$$\mathcal{A}(\mathbf{M}^e; \delta \mathbf{M}_h, \delta \mathbf{M}_h) + \mathcal{B}(\mathbf{M}^e; \delta \mathbf{M}_h, \delta \mathbf{M}_h) \geq C_1^k \|\delta \mathbf{M}_h\|^2 - C_2^k \|\delta \mathbf{M}_h\|_{L^2(\Omega)}^2 \quad \forall \delta \mathbf{M}_h \in X^k, \quad (4.108)$$

where the norms have been defined by Eqs. (2.10) and (2.11). Proceeding by using the bounds (4.88) and (4.93), the Cauchy-Schwartz' inequality, Eq. (2.26), the trace inequality on the finite element space (2.18), the trace inequality, Eq. (2.16), and the inverse inequality, Eq. (2.21), the  $\xi$ -inequality  $-\xi > 0 : |ab| \leq \frac{\xi}{4}a^2 + \frac{1}{\xi}b^2$ , as in Wheeler et al. [74] and Prudhomme et al. [60] analysis with some modifications, yields to prove this Lemma 4.4.1. The two positive constants  $C_1^k, C_2^k$  are independent of the mesh size, but do depend on  $k$  and  $\mathcal{B}$ , for details, see Appendix C.3. In particular, for  $C_1^k$  to be positive the following constrain on the stabilization parameter should be satisfied  $\mathcal{B} > \frac{C_y^2}{C_\alpha^2} \max(C_{\mathcal{T}}(C_{\mathcal{I}}^k + 1), 4C_{\mathcal{K}}^{k^2})$ . Therefore for the method to be stable, the stabilization parameter should be large enough depending on the polynomial approximation.

**Lemma 4.4.2** (Upper bound). *There exist  $C > 0$  and  $C^k > 0$  such that*

$$|\mathcal{A}(\mathbf{M}^e; \mathbf{u}, \delta \mathbf{M}) + \mathcal{B}(\mathbf{M}^e; \mathbf{u}, \delta \mathbf{M})| \leq C \|\mathbf{u}\|_1 \|\delta \mathbf{M}\|_1 \quad \forall \mathbf{u}, \delta \mathbf{M} \in X, \quad (4.109)$$

$$|\mathcal{A}(\mathbf{M}^e; \mathbf{u}, \delta \mathbf{M}_h) + \mathcal{B}(\mathbf{M}^e; \mathbf{u}, \delta \mathbf{M}_h)| \leq C^k \|\mathbf{u}\|_1 \|\delta \mathbf{M}_h\| \quad \forall \mathbf{u} \in X, \delta \mathbf{M}_h \in X^k, \quad (4.110)$$

$$|\mathcal{A}(\mathbf{M}^e; \mathbf{u}_h, \delta \mathbf{M}_h) + \mathcal{B}(\mathbf{M}^e; \mathbf{u}_h, \delta \mathbf{M}_h)| \leq C^k \|\mathbf{u}_h\| \|\delta \mathbf{M}_h\| \quad \forall \mathbf{u}_h, \delta \mathbf{M}_h \in X^k, \quad (4.111)$$

where the norms have been defined by Eqs. (2.11) and (2.12). Applying the Hölder's inequality, Eq. (2.24), and the bound (4.93) on each term of  $\mathcal{A}(\mathbf{M}^e; \mathbf{u}, \delta \mathbf{M}) + \mathcal{B}(\mathbf{M}^e; \mathbf{u}, \delta \mathbf{M})$  and then applying the Cauchy-Schwartz' inequality, Eq. (2.27), lead to relation (4.109). Therefore relations (4.110) and (4.111) are easily deduced from the relation between energy norms on the finite element space, Eq. (2.22). The proof is presented in Appendix C.4.

**Lemma 4.4.3** (Auxiliary problem). *We consider the following auxiliary problem, with  $\phi \in L^2(\Omega)$ :*

$$\begin{aligned} -\nabla^T (\mathbf{j}_{\nabla \mathbf{M}}(\mathbf{M}^e) \nabla \psi + \mathbf{j}_{\mathbf{M}}(\mathbf{M}^e, \nabla \mathbf{M}^e) \psi) &= \phi \quad \text{on } \Omega, \\ \psi &= 0 \quad \text{on } \partial \Omega. \end{aligned} \quad (4.112)$$

Assuming regular ellipticity of the operator, there is a unique solution  $\psi \in H^2(\Omega) \times H^2(\Omega)$  to the problem stated by Eq. (4.112) satisfying the elliptic property

$$\|\psi\|_{H^2(\Omega_h)} \leq C \|\phi\|_{L^2(\Omega_h)}. \quad (4.113)$$

The proof is given in [23], by combining [23, Theorem 8.3] to [23, Lemma 9.17].

Moreover, for a given  $\boldsymbol{\varphi} \in L^2(\Omega_h) \times L^2(\Omega_h)$  there exists a unique  $\boldsymbol{\phi}_h \in X^k$  such that

$$\mathcal{A}(\mathbf{M}^e; \delta \mathbf{M}_h, \boldsymbol{\phi}_h) + \mathcal{B}(\mathbf{M}^e; \delta \mathbf{M}_h, \boldsymbol{\phi}_h) = \sum_e \int_{\Omega^e} \boldsymbol{\varphi}^T \delta \mathbf{M}_h d\Omega \quad \forall \delta \mathbf{M}_h \in X^k, \quad (4.114)$$

and there is a constant  $C^k$  such that :

$$\| \boldsymbol{\phi}_h \| \leq C^k \| \boldsymbol{\varphi} \|_{L^2(\Omega_h)}. \quad (4.115)$$

The proof follows from the use of Lemma 4.4.1 to bound  $\| \boldsymbol{\phi}_h \|$  in terms of  $\| \boldsymbol{\varphi} \|_{L^2(\Omega_h)}$  and  $\| \boldsymbol{\phi}_h \|_{L^2(\Omega_h)}$ .  $\| \boldsymbol{\phi}_h \|_{L^2(\Omega_h)}$  is then estimated by considering  $\boldsymbol{\phi} = \boldsymbol{\phi}_h \in X^k$  in Eq. (4.112), multiplying the result by  $\boldsymbol{\phi}_h$  and integrating it by parts on  $\Omega_h$  yielding  $\| \boldsymbol{\phi}_h \|_{L^2(\Omega_h)}^2 = \mathcal{A}(\mathbf{M}^e; \boldsymbol{\psi}, \boldsymbol{\phi}_h) + \mathcal{B}(\mathbf{M}^e; \boldsymbol{\psi}, \boldsymbol{\phi}_h)$ . Inserting the interpolant  $I_h \boldsymbol{\phi}$  in these last terms, making successive use of Lemmata 4.4.2 and 2.4.6, and using the regular ellipticity Eq. (4.113) allows deriving the bound  $\| \boldsymbol{\phi}_h \|_{L^2(\Omega_h)} \leq C^k \| \boldsymbol{\varphi} \|_{L^2(\Omega_h)}$ , which shows that  $\| \boldsymbol{\phi}_h \|$  is bounded by  $\| \boldsymbol{\varphi} \|_{L^2(\Omega_h)}$  and results into the proof of (4.115). The proof is derived in detail in Appendix C.5.

Now, to prove the existence of the solution of the discrete problem, it is enough to prove that the map  $S_h$  has a fixed point. So in order to prove that the solution  $\mathbf{M}_y$  is unique for a given  $\mathbf{y} \in X^{k+}$ , and that the solution is  $S_h(\mathbf{y}) = \mathbf{M}_y$ , let us assume that there are two distinct solutions  $\mathbf{M}_{y_1}, \mathbf{M}_{y_2}$  to the problem stated by Eq. (4.106), which results into

$$\begin{aligned} & \mathcal{A}(\mathbf{M}^e; I_h \mathbf{M} - \mathbf{M}_{y_1}, \delta \mathbf{M}_h) + \mathcal{B}(\mathbf{M}^e; I_h \mathbf{M} - \mathbf{M}_{y_1}, \delta \mathbf{M}_h) \\ & = \mathcal{A}(\mathbf{M}^e; I_h \mathbf{M} - \mathbf{M}_{y_2}, \delta \mathbf{M}_h) + \mathcal{B}(\mathbf{M}^e; I_h \mathbf{M} - \mathbf{M}_{y_2}, \delta \mathbf{M}_h) \quad \forall \delta \mathbf{M}_h \in X^k. \end{aligned} \quad (4.116)$$

For fixed  $\mathbf{M}^e$ ,  $\mathcal{A}$  and  $\mathcal{B}$  are bi-linear, therefore this last relation becomes

$$\mathcal{A}(\mathbf{M}^e; \mathbf{M}_{y_1} - \mathbf{M}_{y_2}, \delta \mathbf{M}_h) + \mathcal{B}(\mathbf{M}^e; \mathbf{M}_{y_1} - \mathbf{M}_{y_2}, \delta \mathbf{M}_h) = 0 \quad \forall \delta \mathbf{M}_h \in X^k. \quad (4.117)$$

Using Lemma 4.4.3, with  $\boldsymbol{\varphi} = \delta \mathbf{M}_h = \mathbf{M}_{y_1} - \mathbf{M}_{y_2} \in X^k$  results in stating that there is a unique  $\boldsymbol{\Phi}_h \in X^k$  solution of the problem Eq. (4.114), with for  $\delta \mathbf{M}_h = \mathbf{M}_{y_1} - \mathbf{M}_{y_2}$

$$\mathcal{A}(\mathbf{M}^e; \mathbf{M}_{y_1} - \mathbf{M}_{y_2}, \boldsymbol{\Phi}_h) + \mathcal{B}(\mathbf{M}^e; \mathbf{M}_{y_1} - \mathbf{M}_{y_2}, \boldsymbol{\Phi}_h) = \| \mathbf{M}_{y_1} - \mathbf{M}_{y_2} \|_{L^2(\Omega_h)}^2, \quad (4.118)$$

and that  $\| \boldsymbol{\Phi}_h \| \leq C^k \| \mathbf{M}_{y_1} - \mathbf{M}_{y_2} \|_{L^2(\Omega_h)}$ . Choosing  $\delta \mathbf{M}_h$  as  $\boldsymbol{\Phi}_h$  in Eq. (4.117), we have  $\| \mathbf{M}_{y_1} - \mathbf{M}_{y_2} \|_{L^2(\Omega_h)} = 0$ . Therefore, the solution  $S_h(\mathbf{y}) = \mathbf{M}_y$  is unique.

We will now show that  $S_h$  maps from a ball  $O_\sigma(I_h \mathbf{M}) \subset X^{k+}$  into itself and is continuous in the ball. We define the ball  $O_\sigma$  with radius  $\sigma$  and centered at the interpolant  $I_h \mathbf{M}$  of  $\mathbf{M}^e$  as

$$\begin{aligned} O_\sigma(I_h \mathbf{M}) &= \left\{ \mathbf{y} \in X^{k+} \text{ such that } \| I_h \mathbf{M} - \mathbf{y} \|_1 \leq \sigma \right\}, \\ & \text{with } \sigma = \frac{\| I_h \mathbf{M} - \mathbf{M}^e \|_1}{h_s^\varepsilon}, \quad 0 < \varepsilon < \frac{1}{4}. \end{aligned} \quad (4.119)$$

The idea is to work on a linearized problem in a ball  $O_\sigma(I_h\mathbf{M}) \subset X^{k+}$  around an interpolation  $I_h\mathbf{M}$  of  $\mathbf{M}^e$  so the nonlinear term  $\mathbf{j}$  and its derivatives are locally bounded in the ball  $O_\sigma(I_h\mathbf{M}) \subset X^{k+}$ . We note that from Lemma 2.4.6, Eq. (2.23), one has

$$\| \| I_h\mathbf{M} - \mathbf{M}^e \| \|_1 \leq C^k h_s^{\mu-1} \| \mathbf{M}^e \|_{H^s(\Omega_h)} \text{ and } \sigma \leq C^k C_M h_s^{\mu-1-\varepsilon} \| \mathbf{M}^e \|_{H^s(\Omega_h)} \quad \text{if } k \geq 2. \quad (4.120)$$

Assuming  $\mathbf{M}^e \in H^{\frac{5}{2}}(\Omega) \times H^{\frac{5}{2}+}(\Omega)$ , using the previous relation with  $s = \frac{5}{2}$ ,  $C_M = \| \mathbf{M}^e \|_{H^{\frac{5}{2}}(\Omega_h)}$ , and  $\mu = \frac{5}{2} = s$ , then we have

$$\| \| I_h\mathbf{M} - \mathbf{M}^e \| \|_1 \leq C^k h_s^{\frac{3}{2}} \| \mathbf{M}^e \|_{H^{\frac{5}{2}}(\Omega_h)} \text{ and } \sigma \leq C^k C_M h_s^{\frac{3}{2}-\varepsilon} \quad \text{if } k \geq 2. \quad (4.121)$$

It is shown in Appendix C.6, that  $\mathbf{j}(\mathbf{x}; \mathbf{y}, \nabla \mathbf{y})$ ,  $\mathbf{j}_M(\mathbf{x}; \mathbf{y}, \nabla \mathbf{y})$ ,  $\mathbf{j}_{MM}(\mathbf{x}; \mathbf{y}, \nabla \mathbf{y})$ ,  $\mathbf{j}_{\nabla M}(\mathbf{x}; \mathbf{y})$ ,  $\mathbf{j}_{M\nabla M}(\mathbf{x}; \mathbf{y})$  are bounded for  $\mathbf{x} \in \bar{\Omega}$ ,  $\mathbf{y} \in O_\sigma(I_h\mathbf{M})$ , by the same reasoning as in [76] for  $d = 2$ , which justify Eq. (4.93).

We can now bound the nonlinear term  $\mathcal{N}(\mathbf{M}^e; \mathbf{y}; \delta\mathbf{M}_h)$  of Eq. (4.108). Let  $\mathbf{y} \in O_\sigma(I_h\mathbf{M})$  and  $\zeta = \mathbf{M}^e - \mathbf{y}$  which can be expanded as  $\zeta = \boldsymbol{\eta} + \boldsymbol{\xi}$  with  $\boldsymbol{\eta} = \mathbf{M}^e - I_h\mathbf{M} \in X$  and  $\boldsymbol{\xi} = I_h\mathbf{M} - \mathbf{y} \in X^k$ , where  $I_h\mathbf{M}$  is the interpolant of  $\mathbf{M}^e$ . Toward this end, let us begin by computing the bounds of some terms which will be used in the following analysis.

**Lemma 4.4.4** (Intermediate bounds). *Let  $\boldsymbol{\xi} = I_h\mathbf{M} - \mathbf{y}$ ,  $\delta\mathbf{M}_h \in X^k$ ,  $\boldsymbol{\eta} = \mathbf{M}^e - I_h\mathbf{M} \in X$  and  $\zeta = \boldsymbol{\xi} + \boldsymbol{\eta}$ , then by bounding successively the two contributions, we can derive*

$$\begin{aligned} \left( \sum_e \| \zeta \|_{L^2(\Omega^e)}^2 \right)^{\frac{1}{2}} &\leq C^k \sigma \\ &\leq C^k h_s^{\mu-1-\varepsilon} \| \mathbf{M}^e \|_{H^s(\Omega_h)} = C^k h_s^{\frac{3}{2}-\varepsilon} \| \mathbf{M}^e \|_{H^{\frac{5}{2}}(\Omega_h)} \text{ if } k \geq 2, \end{aligned} \quad (4.122)$$

$$\begin{aligned} \left( \sum_e \| \zeta \|_{L^4(\Omega^e)}^4 \right)^{\frac{1}{4}} &\leq C^k h_s^{-\frac{1}{2}} \sigma \\ &\leq C^k h_s^{\mu-\frac{3}{2}-\varepsilon} \| \mathbf{M}^e \|_{H^s(\Omega_h)} = C^k h_s^{1-\varepsilon} \| \mathbf{M}^e \|_{H^{\frac{5}{2}}(\Omega_h)} \text{ if } k \geq 2, \end{aligned} \quad (4.123)$$

$$\begin{aligned} \left( \sum_e \| \nabla \zeta \|_{L^2(\Omega^e)}^2 \right)^{\frac{1}{2}} &\leq C^k \sigma \\ &\leq C^k h_s^{\mu-1-\varepsilon} \| \mathbf{M}^e \|_{H^s(\Omega_h)} = C^k h_s^{\frac{3}{2}-\varepsilon} \| \mathbf{M}^e \|_{H^{\frac{5}{2}}(\Omega_h)} \text{ if } k \geq 2, \end{aligned} \quad (4.124)$$

$$\| \boldsymbol{\eta} \|_{L^4(\partial\Omega^e)} \leq C_{\mathcal{T}}^{\frac{1}{4}} C_{\mathcal{D}}^k h_s^{\mu-\frac{3}{4}} \| \mathbf{M}^e \|_{H^s(\Omega^e)} = C_{\mathcal{T}}^{\frac{1}{4}} C_{\mathcal{D}}^k h_s^{\frac{7}{4}} \| \mathbf{M}^e \|_{H^{\frac{5}{2}}(\Omega^e)} \text{ if } k \geq 2, \quad (4.125)$$

$$\left( \sum_e \| [\boldsymbol{\eta}] \|_{L^4(\partial\Omega^e)}^4 \right)^{\frac{1}{4}} \leq C_{\mathcal{T}}^{\frac{1}{4}} C_{\mathcal{D}}^k h_s^{\mu-\frac{3}{4}} \| \mathbf{M}^e \|_{H^s(\Omega_h)} \leq C_{\mathcal{T}}^{\frac{1}{4}} C_{\mathcal{D}}^k h_s^{\frac{7}{4}} \| \mathbf{M}^e \|_{H^{\frac{5}{2}}(\Omega^e)} \text{ if } k \geq 2, \quad (4.126)$$

$$\| \nabla \boldsymbol{\eta} \|_{L^4(\partial\Omega^e)} \leq C_{\mathcal{T}}^{\frac{1}{4}} C_{\mathcal{D}}^k h_s^{\mu-\frac{7}{4}} \| \mathbf{M}^e \|_{H^s(\Omega^e)} = C_{\mathcal{T}}^{\frac{1}{4}} C_{\mathcal{D}}^k h_s^{\frac{3}{4}} \| \mathbf{M}^e \|_{H^{\frac{5}{2}}(\Omega^e)} \text{ if } k \geq 2, \quad (4.127)$$



$$\begin{aligned}
\left( \sum_e \|\boldsymbol{\xi}\|_{L^4(\partial\Omega^e)}^4 \right)^{\frac{1}{4}} &\leq C_{\mathcal{T}}^{\frac{1}{4}} C_{\mathcal{I}}^k C_{\mathcal{P}} h_s^{-\frac{3}{4}} \sigma \\
&\leq C_{\mathcal{T}}^{\frac{1}{4}} C_{\mathcal{I}}^k C_{\mathcal{P}} h_s^{\mu - \frac{7}{4} - \varepsilon} \|\mathbf{M}^e\|_{H^s(\Omega_h)} = C_{\mathcal{T}}^{\frac{1}{4}} C_{\mathcal{I}}^k C_{\mathcal{P}} h_s^{\frac{3}{4} - \varepsilon} \|\mathbf{M}^e\|_{H^{\frac{5}{2}}(\Omega_h)} \text{ if } k \geq 2,
\end{aligned} \tag{4.128}$$

$$\begin{aligned}
\left( \sum_e \|\llbracket \boldsymbol{\xi} \rrbracket\|_{L^4(\partial\Omega^e)}^4 \right)^{\frac{1}{4}} &\leq C_{\mathcal{I}}^k h_s^{\frac{1}{4}} \sigma \leq C_{\mathcal{I}}^k h_s^{\mu - \frac{3}{4} - \varepsilon} \|\mathbf{M}^e\|_{H^s(\Omega_h)} = C_{\mathcal{I}}^k h_s^{\frac{7}{4} - \varepsilon} \|\mathbf{M}^e\|_{H^{\frac{5}{2}}(\Omega_h)} \text{ if } k \geq 2,
\end{aligned} \tag{4.129}$$

$$\begin{aligned}
\left( \sum_e \|\nabla \boldsymbol{\xi}\|_{L^4(\partial\Omega^e)}^4 \right)^{\frac{1}{4}} &\leq C_{\mathcal{K}}^k C_{\mathcal{I}}^k h_s^{-\frac{3}{4}} \sigma \\
&\leq C_{\mathcal{K}}^k C_{\mathcal{I}}^k h_s^{\mu - \frac{7}{4} - \varepsilon} \|\mathbf{M}^e\|_{H^s(\Omega_h)} = C_{\mathcal{K}}^k C_{\mathcal{I}}^k h_s^{\frac{3}{4} - \varepsilon} \|\mathbf{M}^e\|_{H^{\frac{5}{2}}(\Omega_h)} \text{ if } k \geq 2,
\end{aligned} \tag{4.130}$$

$$\begin{aligned}
\left( \sum_e \|\boldsymbol{\zeta}\|_{L^4(\partial\Omega^e)}^4 \right)^{\frac{1}{4}} &\leq C^k h_s^{-\frac{3}{4}} \sigma \\
&\leq C^k h_s^{\mu - \frac{7}{4} - \varepsilon} \|\mathbf{M}^e\|_{H^s(\Omega_h)} = C^k h_s^{\frac{3}{4} - \varepsilon} \|\mathbf{M}^e\|_{H^{\frac{5}{2}}(\Omega_h)} \text{ if } k \geq 2,
\end{aligned} \tag{4.131}$$

$$\begin{aligned}
\left( \sum_e \|\llbracket \boldsymbol{\zeta} \rrbracket\|_{L^4(\partial\Omega^e)}^4 \right)^{\frac{1}{4}} &\leq C^k h_s^{\frac{1}{4}} \sigma \\
&\leq C^k h_s^{\mu - \frac{3}{4} - \varepsilon} \|\mathbf{M}^e\|_{H^s(\Omega_h)} = C^k h_s^{\frac{7}{4} - \varepsilon} \|\mathbf{M}^e\|_{H^{\frac{5}{2}}(\Omega_h)} \text{ if } k \geq 2.
\end{aligned} \tag{4.132}$$

$$\begin{aligned}
\left( \sum_e \|\nabla \boldsymbol{\zeta}\|_{L^4(\partial\Omega^e)}^4 \right)^{\frac{1}{4}} &\leq C^k h_s^{-\frac{3}{4}} \sigma \\
&\leq C^k h_s^{\mu - \frac{7}{4} - \varepsilon} \|\mathbf{M}^e\|_{H^s(\Omega_h)} = C^k h_s^{\frac{3}{4} - \varepsilon} \|\mathbf{M}^e\|_{H^{\frac{5}{2}}(\Omega_h)} \text{ if } k \geq 2,
\end{aligned} \tag{4.133}$$

$$\begin{cases} \|\delta \mathbf{M}_h\|_{W_4^1(\Omega^e)} &\leq C_{\mathcal{I}}^k h_s^{-\frac{1}{2}} \|\delta \mathbf{M}_h\|_{H^1(\Omega^e)}, \\ |\delta \mathbf{M}_h|_{W_4^1(\Omega^e)} &\leq C_{\mathcal{I}}^k h_s^{-\frac{1}{2}} |\delta \mathbf{M}_h|_{H^1(\Omega^e)}, \end{cases} \tag{4.134}$$

with  $\mu = \min\{s, k+1\}$ . These previous inequalities are derived in Appendix C.7 and only the final results are reported here.

We have now the tool to bound the nonlinear term  $\mathcal{N}(\mathbf{M}^e, \mathbf{y}; \delta \mathbf{M}_h)$  of Eq. (4.106).

**Lemma 4.4.5.** *Let  $\mathbf{y} \in O_\sigma(I_h \mathbf{M})$  and  $\delta \mathbf{M}_h \in X^k$ , then the nonlinear term  $\mathcal{N}(\mathbf{M}^e, \mathbf{y}; \delta \mathbf{M}_h)$  defined in Eq. (4.101), is bounded by*

$$\begin{aligned}
|\mathcal{N}(\mathbf{M}^e, \mathbf{y}; \delta \mathbf{M}_h)| &\leq C^k C_y \|\mathbf{M}^e\|_{H^s(\Omega_h)} h_s^{\mu - 2 - \varepsilon} \sigma \left[ |\delta \mathbf{M}_h|_{H^1(\Omega_h)} \right. \\
&\quad \left. + \left( \sum_e h_s |\delta \mathbf{M}_h|_{H^1(\partial\Omega^e)}^2 \right)^{\frac{1}{2}} + \left( \sum_e h_s^{-1} \|\llbracket \delta \mathbf{M}_{h_n} \rrbracket\|_{L^2(\partial\Omega^e)}^2 \right)^{\frac{1}{2}} \right].
\end{aligned} \tag{4.135}$$

The bound follows from the use of Lemma 4.4.4, Taylor's series (4.89-4.91), the generalized Hölder's inequality (2.25), the generalized Cauchy-Schwartz' inequality (2.27), the definition of  $C_y$  in Eq. (4.93), and is reported in Appendix C.8. Moreover, using the definition of the energy norm (2.12), this relation becomes

$$| \mathcal{N}(\mathbf{M}^e, \mathbf{y}; \delta \mathbf{M}_h) | \leq C^k C_y \| \mathbf{M}^e \|_{H^s(\Omega_h)} h_s^{\mu-2-\varepsilon} \sigma \| \delta \mathbf{M}_h \|_1, \quad (4.136)$$

which could be rewritten using Lemma 2.4.5 for the general case as

$$\begin{aligned} | \mathcal{N}(\mathbf{M}^e, \mathbf{y}; \delta \mathbf{M}_h) | &\leq C^k C_y \| \mathbf{M}^e \|_{H^s(\Omega_h)} h_s^{\mu-2-\varepsilon} \sigma \| \delta \mathbf{M}_h \| \\ &\leq C^k C_y C_M h_s^{\frac{1}{2}-\varepsilon} \sigma \| \delta \mathbf{M}_h \| \quad \text{if } k \geq 2. \end{aligned} \quad (4.137)$$

We now have the tools to demonstrate that  $S_h$  (i) maps from a ball  $O_\sigma(I_h \mathbf{M}) \subset X^k$  into itself and (ii) is continuous in the ball.

**Theorem 4.4.6** ( $S_h$  maps  $O_\sigma(I_h \mathbf{M})$  into itself). *Let  $0 < h_s < 1$  and  $\sigma$  be defined by Eq. (4.121). Then  $S_h$  maps the ball  $O_\sigma(I_h \mathbf{M})$  into itself.*

Let  $\mathbf{y} \in O_\sigma(I_h \mathbf{M}) \in X^k$  and  $S_h(\mathbf{y}) = \mathbf{M}_y$  be the solution of the problem given by Eq. (4.106). Then using Lemma 4.4.1, Eq. (4.108), Lemma 4.4.2, Eq. (4.110), Lemma 4.4.5, Eq. (4.136), and the definition of the ball (4.119), we successively find that

$$\begin{aligned} &C_1^k \| \| I_h \mathbf{M} - \mathbf{M}_y \| \|^2 - C_2^k \| I_h \mathbf{M} - \mathbf{M}_y \|_{L^2(\Omega_h)}^2 \\ &\leq \mathcal{A}(\mathbf{M}^e; I_h \mathbf{M} - \mathbf{M}_y, I_h \mathbf{M} - \mathbf{M}_y) + \mathcal{B}(\mathbf{M}^e; I_h \mathbf{M} - \mathbf{M}_y, I_h \mathbf{M} - \mathbf{M}_y) \\ &\leq \mathcal{A}(\mathbf{M}^e; I_h \mathbf{M} - \mathbf{M}^e, I_h \mathbf{M} - \mathbf{M}_y) + \mathcal{B}(\mathbf{M}^e; I_h \mathbf{M} - \mathbf{M}^e, I_h \mathbf{M} - \mathbf{M}_y) + \mathcal{N}(\mathbf{M}^e, \mathbf{y}, I_h \mathbf{M} - \mathbf{M}_y) \\ &\leq C^k \| \| I_h \mathbf{M} - \mathbf{M}^e \| \|_1 \| \| I_h \mathbf{M} - \mathbf{M}_y \| \| + C^k C_y \| \mathbf{M}^e \|_{H^s(\Omega_h)} h_s^{\mu-2-\varepsilon} \sigma \| \| I_h \mathbf{M} - \mathbf{M}_y \| \| \\ &\leq (C^k h_s^\varepsilon + C^k C_y \| \mathbf{M}^e \|_{H^s(\Omega_h)} h_s^{\mu-2-\varepsilon}) \sigma \| \| I_h \mathbf{M} - \mathbf{M}_y \| \| . \end{aligned} \quad (4.138)$$

Let us define  $C^{k'}$  ( $C^k, C_y, C_M$ ) a constant, that can depend on  $C^k, C_y$  and  $C_M$ , then, as  $0 < \varepsilon < \frac{1}{4}$ , the last expression can be rewritten for  $k \geq 2$ :

$$C_1^k \| \| I_h \mathbf{M} - \mathbf{M}_y \| \|^2 - C_2^k \| I_h \mathbf{M} - \mathbf{M}_y \|_{L^2(\Omega_h)}^2 \leq C^{k'} \sigma h_s^\varepsilon \| \| I_h \mathbf{M} - \mathbf{M}_y \| \| . \quad (4.139)$$

Then, in order to estimate  $\| I_h \mathbf{M} - \mathbf{M}_y \|_{L^2(\Omega_h)}$ , we consider the auxiliary problem defined in Lemma 4.4.3. Choosing  $\boldsymbol{\varphi} = \delta \mathbf{M}_h = I_h \mathbf{M} - \mathbf{M}_y$ , there exists  $\boldsymbol{\phi}_h$  such that,  $\| \boldsymbol{\phi}_h \| \leq C^k \| I_h \mathbf{M} - \mathbf{M}_y \|_{L^2(\Omega)}$  with

$$\begin{aligned} \| I_h \mathbf{M} - \mathbf{M}_y \|_{L^2(\Omega_h)}^2 &= \mathcal{A}(\mathbf{M}^e; I_h \mathbf{M} - \mathbf{M}_y, \boldsymbol{\phi}_h) + \mathcal{B}(\mathbf{M}^e; I_h \mathbf{M} - \mathbf{M}_y, \boldsymbol{\phi}_h) \\ &\leq \mathcal{A}(\mathbf{M}^e; I_h \mathbf{M} - \mathbf{M}^e, \boldsymbol{\phi}_h) + \mathcal{B}(\mathbf{M}^e; I_h \mathbf{M} - \mathbf{M}^e, \boldsymbol{\phi}_h) + \mathcal{N}(\mathbf{M}^e, \mathbf{y}; \boldsymbol{\phi}_h) \\ &\leq C^k \| \| I_h \mathbf{M} - \mathbf{M}^e \| \|_1 \| \| \boldsymbol{\phi}_h \| \| + C^k C_y \| \mathbf{M}^e \|_{H^s(\Omega_h)} h_s^{\mu-2-\varepsilon} \sigma \| \| \boldsymbol{\phi}_h \| \| \\ &\leq (C^k \sigma h_s^\varepsilon + C^k C_y \| \mathbf{M}^e \|_{H^s(\Omega_h)} \sigma h_s^{\mu-2-\varepsilon}) \| \| I_h \mathbf{M} - \mathbf{M}_y \| \|_{L^2(\Omega_h)} \\ &\leq C^{k'} \sigma h_s^\varepsilon \| \| I_h \mathbf{M} - \mathbf{M}_y \| \|_{L^2(\Omega_h)} \quad \text{if } k \geq 2, \end{aligned} \quad (4.140)$$

where we have used Lemma 4.4.2, Eq. (4.110), Lemma 4.4.5, Eq. (4.136), and the definition of the ball (4.119). Substituting Eq. (4.140) in Eq. (4.139) gives

$$\begin{aligned} C_1^k \|\| I_h \mathbf{M} - \mathbf{M}_y \|\|^2 &\leq C^{k'} \sigma h_s^\varepsilon \|\| I_h \mathbf{M} - \mathbf{M}_y \|\| + C_2^k \| I_h \mathbf{M} - \mathbf{M}_y \|_{L^2(\Omega_h)}^2 \\ &\leq C^{k'} \sigma h_s^\varepsilon \|\| I_h \mathbf{M} - \mathbf{M}_y \|\| + C_2^k C^{k'} \sigma h_s^\varepsilon \| I_h \mathbf{M} - \mathbf{M}_y \|_{L^2(\Omega_h)} \\ &\leq C^{k'} \sigma h_s^\varepsilon \|\| I_h \mathbf{M} - \mathbf{M}_y \|\| \quad \text{if } k \geq 2. \end{aligned} \quad (4.141)$$

Hence, we get

$$\|\| I_h \mathbf{M} - \mathbf{M}_y \|\| \leq C^{k'} \sigma h_s^\varepsilon \quad \text{if } k \geq 2, \quad (4.142)$$

and for a mesh size  $h_s$  small enough and a given ball size  $\sigma$ ,  $I_h \mathbf{M} - \mathbf{M}_y \rightarrow 0$ , hence  $S_h$  maps  $O_\sigma(I_h \mathbf{M})$  to itself.

**Theorem 4.4.7** (The continuity of the map  $S_h$  in the ball  $O_\sigma(I_h \mathbf{M})$ ). *For  $\mathbf{y}_1, \mathbf{y}_2 \in O_\sigma(I_h \mathbf{M})$ , let  $\mathbf{M}_{\mathbf{y}_1} = S_h(\mathbf{y}_1)$ ,  $\mathbf{M}_{\mathbf{y}_2} = S_h(\mathbf{y}_2)$  be solutions of Eq. (4.106). Then for  $0 < h_s < 1$*

$$\|\| \mathbf{M}_{\mathbf{y}_1} - \mathbf{M}_{\mathbf{y}_2} \|\| \leq C^k C_y \| \mathbf{M}^e \|_{H^s(\Omega_h)} h_s^{\mu-2-\varepsilon} \|\| \mathbf{y}_1 - \mathbf{y}_2 \|\|. \quad (4.143)$$

The solutions  $\mathbf{M}_{\mathbf{y}_1}$  and  $\mathbf{M}_{\mathbf{y}_2}$  of the linearized problem (4.106) satisfy

$$\begin{aligned} \mathcal{A}(\mathbf{M}^e; I_h \mathbf{M} - \mathbf{M}_{\mathbf{y}_1}, \delta \mathbf{M}_h) + \mathcal{B}(\mathbf{M}^e; I_h \mathbf{M} - \mathbf{M}_{\mathbf{y}_1}, \delta \mathbf{M}_h) \\ = \mathcal{A}(\mathbf{M}^e; \boldsymbol{\eta}, \delta \mathbf{M}_h) + \mathcal{B}(\mathbf{M}^e; \boldsymbol{\eta}, \delta \mathbf{M}_h) + \mathcal{N}(\mathbf{M}^e, \mathbf{y}_1; \delta \mathbf{M}_h) \quad \forall \delta \mathbf{M}_h \in X^k, \end{aligned} \quad (4.144)$$

and

$$\begin{aligned} \mathcal{A}(\mathbf{M}^e; I_h \mathbf{M} - \mathbf{M}_{\mathbf{y}_2}, \delta \mathbf{M}_h) + \mathcal{B}(\mathbf{M}^e; I_h \mathbf{M} - \mathbf{M}_{\mathbf{y}_2}, \delta \mathbf{M}_h) \\ = \mathcal{A}(\mathbf{M}^e; \boldsymbol{\eta}, \delta \mathbf{M}_h) + \mathcal{B}(\mathbf{M}^e; \boldsymbol{\eta}, \delta \mathbf{M}_h) + \mathcal{N}(\mathbf{M}^e, \mathbf{y}_2; \delta \mathbf{M}_h) \quad \forall \delta \mathbf{M}_h \in X^k, \end{aligned} \quad (4.145)$$

where  $\boldsymbol{\eta} = I_h \mathbf{M} - \mathbf{M}^e$ . By subtracting Eq. (4.144) from Eq. (4.145), we have

$$\begin{aligned} \mathcal{A}(\mathbf{M}^e; \mathbf{M}_{\mathbf{y}_2} - \mathbf{M}_{\mathbf{y}_1}, \delta \mathbf{M}_h) + \mathcal{B}(\mathbf{M}^e; \mathbf{M}_{\mathbf{y}_2} - \mathbf{M}_{\mathbf{y}_1}, \delta \mathbf{M}_h) \\ = \mathcal{N}(\mathbf{M}^e, \mathbf{y}_2; \delta \mathbf{M}_h) - \mathcal{N}(\mathbf{M}^e, \mathbf{y}_1; \delta \mathbf{M}_h). \end{aligned} \quad (4.146)$$

Choosing  $\boldsymbol{\zeta}_1 = \mathbf{M}^e - \mathbf{y}_1 \in X$  and  $\boldsymbol{\zeta}_2 = \mathbf{M}^e - \mathbf{y}_2 \in X$ , the right hand side of Eq. (4.146) can be rewritten as follows:

$$\begin{aligned} &\mathcal{N}(\mathbf{M}^e, \mathbf{y}_2; \delta \mathbf{M}_h) - \mathcal{N}(\mathbf{M}^e, \mathbf{y}_1; \delta \mathbf{M}_h) \\ &= \int_{\Omega_h} (\nabla \delta \mathbf{M}_h)^T (\bar{\mathbf{R}}_j(\boldsymbol{\zeta}_2, \nabla \boldsymbol{\zeta}_2) - \bar{\mathbf{R}}_j(\boldsymbol{\zeta}_1, \nabla \boldsymbol{\zeta}_1)) \, d\Omega \\ &+ \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \llbracket \delta \mathbf{M}_{h_n}^T \rrbracket \langle \bar{\mathbf{R}}_j(\boldsymbol{\zeta}_2, \nabla \boldsymbol{\zeta}_2) - \bar{\mathbf{R}}_j(\boldsymbol{\zeta}_1, \nabla \boldsymbol{\zeta}_1) \rangle \, dS \\ &+ \int_{\partial_I \Omega_h} \llbracket \mathbf{M}^{eT} - \mathbf{y}_{2_n}^T \rrbracket \langle (\mathbf{j}_{\nabla \mathbf{M}}(\mathbf{M}^e) - \mathbf{j}_{\nabla \mathbf{M}}(\mathbf{y}_2)) \nabla \delta \mathbf{M}_h \rangle \, dS \\ &- \int_{\partial_I \Omega_h} \llbracket \mathbf{M}^{eT} - \mathbf{y}_{1_n}^T \rrbracket \langle (\mathbf{j}_{\nabla \mathbf{M}}(\mathbf{M}^e) - \mathbf{j}_{\nabla \mathbf{M}}(\mathbf{y}_1)) \nabla \delta \mathbf{M}_h \rangle \, dS \\ &+ \int_{\partial_I \Omega_h} \llbracket \mathbf{M}^{eT} - \mathbf{y}_{2_n}^T \rrbracket \left\langle \frac{\mathcal{B}}{h_s} (\mathbf{j}_{\nabla \mathbf{M}}(\mathbf{M}^e) - \mathbf{j}_{\nabla \mathbf{M}}(\mathbf{y}_2)) \right\rangle \llbracket \delta \mathbf{M}_{h_n} \rrbracket \, dS \\ &- \int_{\partial_I \Omega_h} \llbracket \mathbf{M}^{eT} - \mathbf{y}_{1_n}^T \rrbracket \left\langle \frac{\mathcal{B}}{h_s} (\mathbf{j}_{\nabla \mathbf{M}}(\mathbf{M}^e) - \mathbf{j}_{\nabla \mathbf{M}}(\mathbf{y}_1)) \right\rangle \llbracket \delta \mathbf{M}_{h_n} \rrbracket \, dS. \end{aligned} \quad (4.147)$$

By applying Taylor series, Eqs. (4.89-4.92), to rewrite the right hand side, every term will be either in  $\mathbf{y}_1 - \mathbf{y}_2$  or in  $\nabla(\mathbf{y}_1 - \mathbf{y}_2)$ . For example, the bound of the first term is as follows

$$\begin{aligned}
& \int_{\Omega_h} (\nabla \delta \mathbf{M}_h)^T (\bar{\mathbf{R}}_{\mathbf{j}}(\boldsymbol{\zeta}_2, \nabla \boldsymbol{\zeta}_2) - \bar{\mathbf{R}}_{\mathbf{j}}(\boldsymbol{\zeta}_1, \nabla \boldsymbol{\zeta}_1)) \, d\Omega = \\
& \int_{\Omega_h} (\nabla \delta \mathbf{M}_h)^T (\mathbf{j}(\mathbf{y}_2, \nabla \mathbf{y}_2) - \mathbf{j}(\mathbf{M}^e, \nabla \mathbf{M}^e) + \mathbf{j}_{\mathbf{M}}(\mathbf{M}^e, \nabla \mathbf{M}^e)(\mathbf{M}^e - \mathbf{y}_2) \\
& + \mathbf{j}_{\nabla \mathbf{M}}(\mathbf{M}^e, \nabla \mathbf{M}^e)(\nabla \mathbf{M}^e - \nabla \mathbf{y}_2) - \mathbf{j}(\mathbf{y}_1, \nabla \mathbf{y}_1) + \mathbf{j}(\mathbf{M}^e, \nabla \mathbf{M}^e) \\
& - \mathbf{j}_{\mathbf{M}}(\mathbf{M}^e, \nabla \mathbf{M}^e)(\mathbf{M}^e - \mathbf{y}_1) - \mathbf{j}_{\nabla \mathbf{M}}(\mathbf{M}^e, \nabla \mathbf{M}^e)(\nabla \mathbf{M}^e - \nabla \mathbf{y}_1)) \, d\Omega \\
& = \int_{\Omega_h} (\nabla \delta \mathbf{M}_h)^T (\mathbf{j}(\mathbf{y}_2, \nabla \mathbf{y}_2) - \mathbf{j}(\mathbf{y}_1, \nabla \mathbf{y}_1) - \mathbf{j}_{\mathbf{M}}(\mathbf{M}^e, \nabla \mathbf{M}^e)(\mathbf{y}_2 - \mathbf{y}_1) \\
& - \mathbf{j}_{\nabla \mathbf{M}}(\mathbf{M}^e, \nabla \mathbf{M}^e)(\nabla \mathbf{y}_2 - \nabla \mathbf{y}_1)) \, d\Omega \tag{4.148} \\
& = \int_{\Omega_h} (\nabla \delta \mathbf{M}_h)^T ((\mathbf{j}_{\mathbf{M}}(\mathbf{y}_1, \nabla \mathbf{y}_1) - \mathbf{j}_{\mathbf{M}}(\mathbf{M}^e, \nabla \mathbf{M}^e)) (\mathbf{y}_2 - \mathbf{y}_1)) \, d\Omega \\
& + \int_{\Omega_h} (\nabla \delta \mathbf{M}_h)^T ((\mathbf{j}_{\nabla \mathbf{M}}(\mathbf{y}_1) - \mathbf{j}_{\nabla \mathbf{M}}(\mathbf{M}^e)) (\nabla \mathbf{y}_2 - \nabla \mathbf{y}_1)) \, d\Omega \\
& + \int_{\Omega_h} (\nabla \delta \mathbf{M}_h)^T (\bar{\mathbf{R}}_{\mathbf{j}}(\mathbf{y}_1 - \mathbf{y}_2, \nabla \mathbf{y}_1 - \nabla \mathbf{y}_2)) \, d\Omega.
\end{aligned}$$

The first term of the right hand side of Eq. (4.148) is bounded by using the generalized Hölder's inequality (2.25), the generalized Cauchy-Schwartz' inequality (2.27), the definition of  $C_y$  in Eq. (4.93), the inverse inequality (2.19), and the bounds (4.122, 4.124 and 4.134) as

$$\begin{aligned}
& \left| \int_{\Omega_h} (\nabla \delta \mathbf{M}_h)^T ((\mathbf{j}_{\mathbf{M}}(\mathbf{y}_1, \nabla \mathbf{y}_1) - \mathbf{j}_{\mathbf{M}}(\mathbf{M}^e, \nabla \mathbf{M}^e)) (\mathbf{y}_2 - \mathbf{y}_1)) \, d\Omega \right| \\
& \leq \left| \int_{\Omega_h} (\nabla \delta \mathbf{M}_h)^T ((\mathbf{y}_1 - \mathbf{y}_2)^T \bar{\mathbf{j}}_{\mathbf{M}\mathbf{M}}(\mathbf{y}_1, \nabla \mathbf{y}_1)(\mathbf{M}^e - \mathbf{y}_1)) \, d\Omega \right| \\
& + \left| \int_{\Omega_h} (\nabla \delta \mathbf{M}_h)^T ((\mathbf{y}_1 - \mathbf{y}_2)^T \bar{\mathbf{j}}_{\mathbf{M}\nabla \mathbf{M}}(\mathbf{y}_1)(\nabla \mathbf{M}^e - \nabla \mathbf{y}_1)) \, d\Omega \right| \\
& \leq C_y \sum_e \|\nabla \delta \mathbf{M}_h\|_{L^4(\Omega^e)} \|\mathbf{M}^e - \mathbf{y}_1\|_{L^2(\Omega^e)} \|\mathbf{y}_1 - \mathbf{y}_2\|_{L^4(\Omega^e)} \\
& + C_y \sum_e \|\nabla \delta \mathbf{M}_h\|_{L^4(\Omega^e)} \|\nabla \mathbf{M}^e - \nabla \mathbf{y}_1\|_{L^2(\Omega^e)} \|\mathbf{y}_1 - \mathbf{y}_2\|_{L^4(\Omega^e)} \tag{4.149} \\
& \leq C_y \left( \sum_e \|\nabla \delta \mathbf{M}_h\|_{W_4^1(\Omega^e)}^4 \right)^{\frac{1}{4}} \left( \sum_e \|\mathbf{y}_1 - \mathbf{y}_2\|_{L^4(\Omega^e)}^4 \right)^{\frac{1}{4}} \\
& \left[ \left( \sum_e \|\boldsymbol{\zeta}\|_{L^2(\Omega^e)}^2 \right)^{\frac{1}{2}} + \left( \sum_e \|\nabla \boldsymbol{\zeta}\|_{L^2(\Omega^e)}^2 \right)^{\frac{1}{2}} \right] \\
& \leq C^k C_y h_s^{\mu-2-\varepsilon} \|\delta \mathbf{M}_h\|_{H^1(\Omega_h)} \|\mathbf{y}_1 - \mathbf{y}_2\|_{L^2(\Omega_h)} \|\mathbf{M}^e\|_{H^s(\Omega_h)}.
\end{aligned}$$

Similarly, the second and third term are bounded using the generalized Hölder inequality (2.25), the generalized Cauchy-Schwartz' inequality (2.27), the definition of  $C_y$  in Eq. (4.93)

and other inequalities that are introduced in Lemma 4.4.4. Then the other terms in Eq. (4.147) can be rewritten in a similar way to Eq. (4.148), see [24]. Therefore, we have

$$| \mathcal{N}(\mathbf{M}^e, \mathbf{y}_2; \delta \mathbf{M}_h) - \mathcal{N}(\mathbf{M}^e, \mathbf{y}_1; \delta \mathbf{M}_h) | \leq C^k C_y \| \mathbf{M}^e \|_{H^s(\Omega_h)} h_s^{\mu-2-\varepsilon} \| \mathbf{y}_1 - \mathbf{y}_2 \| \| \delta \mathbf{M}_h \| . \quad (4.150)$$

Choosing  $\delta \mathbf{M}_h = \mathbf{M}_{\mathbf{y}_2} - \mathbf{M}_{\mathbf{y}_1}$ , and using Eq. (4.108), Eq. (4.146) becomes:

$$\begin{aligned} & C_1^k \| \mathbf{M}_{\mathbf{y}_2} - \mathbf{M}_{\mathbf{y}_1} \|^2 - C_2^k \| \mathbf{M}_{\mathbf{y}_2} - \mathbf{M}_{\mathbf{y}_1} \|_{L^2(\Omega_h)}^2 \\ & \leq \mathcal{A}(\mathbf{M}^e; \mathbf{M}_{\mathbf{y}_2} - \mathbf{M}_{\mathbf{y}_1}, \mathbf{M}_{\mathbf{y}_2} - \mathbf{M}_{\mathbf{y}_1}) \\ & \quad + \mathcal{B}(\mathbf{M}^e; \mathbf{M}_{\mathbf{y}_2} - \mathbf{M}_{\mathbf{y}_1}, \mathbf{M}_{\mathbf{y}_2} - \mathbf{M}_{\mathbf{y}_1}) \\ & \leq \mathcal{N}(\mathbf{M}^e, \mathbf{y}_2; \mathbf{M}_{\mathbf{y}_2} - \mathbf{M}_{\mathbf{y}_1}) - \mathcal{N}(\mathbf{M}^e, \mathbf{y}_1; \mathbf{M}_{\mathbf{y}_2} - \mathbf{M}_{\mathbf{y}_1}). \end{aligned} \quad (4.151)$$

Similarly, setting  $\delta \mathbf{M}_h = \mathbf{M}_{\mathbf{y}_2} - \mathbf{M}_{\mathbf{y}_1}$  in Eq. (4.150), Eq (4.151) becomes:

$$\begin{aligned} \| \mathbf{M}_{\mathbf{y}_2} - \mathbf{M}_{\mathbf{y}_1} \|^2 & \leq C_1^k C_y \| \mathbf{M}^e \|_{H^s(\Omega_h)} h_s^{\mu-2-\varepsilon} \| \mathbf{y}_2 - \mathbf{y}_1 \| \| \mathbf{M}_{\mathbf{y}_2} - \mathbf{M}_{\mathbf{y}_1} \| \\ & \quad + C_2^k \| \mathbf{M}_{\mathbf{y}_2} - \mathbf{M}_{\mathbf{y}_1} \|_{L^2(\Omega_h)}^2 . \end{aligned} \quad (4.152)$$

As  $\| \mathbf{M}_{\mathbf{y}_2} - \mathbf{M}_{\mathbf{y}_1} \|_{L^2(\Omega_h)}^2 \leq \| \mathbf{M}_{\mathbf{y}_2} - \mathbf{M}_{\mathbf{y}_1} \| \| \mathbf{M}_{\mathbf{y}_2} - \mathbf{M}_{\mathbf{y}_1} \|_{L^2(\Omega_h)}$ , this last relation becomes

$$\| \mathbf{M}_{\mathbf{y}_2} - \mathbf{M}_{\mathbf{y}_1} \| \leq C_1^k C_y \| \mathbf{M}^e \|_{H^s(\Omega_h)} h_s^{\mu-2-\varepsilon} \| \mathbf{y}_2 - \mathbf{y}_1 \| + C_2^k \| \mathbf{M}_{\mathbf{y}_2} - \mathbf{M}_{\mathbf{y}_1} \|_{L^2(\Omega_h)} . \quad (4.153)$$

In order to estimate  $\| \mathbf{M}_{\mathbf{y}_2} - \mathbf{M}_{\mathbf{y}_1} \|_{L^2(\Omega_h)}^2$ , we consider  $\boldsymbol{\varphi} = \mathbf{M}_{\mathbf{y}_2} - \mathbf{M}_{\mathbf{y}_1}$  in Lemma 4.4.3. Therefore, there exists a unique  $\boldsymbol{\phi}_h$  satisfying Eq. (4.114)  $\forall \delta \mathbf{M}_h \in X^k$ . In particular for  $\delta \mathbf{M}_h = \mathbf{M}_{\mathbf{y}_2} - \mathbf{M}_{\mathbf{y}_1}$ , this implies

$$\begin{aligned} \| \mathbf{M}_{\mathbf{y}_2} - \mathbf{M}_{\mathbf{y}_1} \|_{L^2(\Omega_h)}^2 & = \mathcal{A}(\mathbf{M}^e; \mathbf{M}_{\mathbf{y}_2} - \mathbf{M}_{\mathbf{y}_1}, \boldsymbol{\phi}_h) + \mathcal{B}(\mathbf{M}^e; \mathbf{M}_{\mathbf{y}_2} - \mathbf{M}_{\mathbf{y}_1}, \boldsymbol{\phi}_h) \\ & = \mathcal{N}(\mathbf{M}^e, \mathbf{y}_2; \boldsymbol{\phi}_h) - \mathcal{N}(\mathbf{M}^e, \mathbf{y}_1; \boldsymbol{\phi}_h) \\ & \leq C^k C_y \| \mathbf{M}^e \|_{H^s(\Omega_h)} h_s^{\mu-2-\varepsilon} \| \mathbf{y}_2 - \mathbf{y}_1 \| \| \boldsymbol{\phi}_h \| \\ & \leq C^k C_y \| \mathbf{M}^e \|_{H^s(\Omega_h)} h_s^{\mu-2-\varepsilon} \| \mathbf{y}_2 - \mathbf{y}_1 \| \| \mathbf{M}_{\mathbf{y}_2} - \mathbf{M}_{\mathbf{y}_1} \|_{L^2(\Omega_h)}, \end{aligned} \quad (4.154)$$

where we have used Eq (4.146), Eq. (4.150), and Eq. (4.115). Substituting Eq. (4.154) in Eq. (4.153) completes the proof of the theorem.

Using the Theorems 4.4.6 and 4.4.7 of the map  $S_h$ , we can conclude that for all  $0 < h_s < 1$ , the maps  $S_h$  has a fixed point  $\mathbf{M}_h$  of the ball  $O_\sigma(I_h \mathbf{M})$ , which is the solution of the nonlinear system of Eqs. (4.96).

#### 4.4.5 A priori error estimates

As  $S_h$  maps a ball into itself, we can use  $\mathbf{M}_h$  instead of  $\mathbf{M}_y$  in Eq. (4.142), hence we have

$$\| \| I_h \mathbf{M} - \mathbf{M}_h \| \| \leq C^{k'} \sigma h_s^\varepsilon = C^{k'} \| \| I_h \mathbf{M} - \mathbf{M}^e \| \|_1 . \quad (4.155)$$

Now using this last relation, Lemma 2.4.5, Eq. (2.22), Lemma 2.4.6, Eq. (2.23), and Eq. (4.155) lead to

$$\begin{aligned}
\| \mathbf{M}^e - \mathbf{M}_h \|_1 &\leq \| \mathbf{M}^e - \mathbf{I}_h \mathbf{M} \|_1 + \| \mathbf{I}_h \mathbf{M} - \mathbf{M}_h \|_1 \\
&\leq \| \mathbf{M}^e - \mathbf{I}_h \mathbf{M} \|_1 + C^{k'} \| \mathbf{I}_h \mathbf{M} - \mathbf{M}^e \|_1 \\
&\leq (1 + C^{k'}) \| \mathbf{M}^e - \mathbf{I}_h \mathbf{M} \|_1 \\
&\leq C^{k''} h_s^{\mu-1} \| \mathbf{M}^e \|_{H^s(\Omega_h)},
\end{aligned} \tag{4.156}$$

where  $\mu = \min \{s, k + 1\}$ , and  $C^{k''} = C^k(1 + C^{k'})$ . This shows that the error estimate is optimal in  $h_s$ .

#### 4.4.6 Error estimate in the $L^2$ -norm

Since the linearized problem (4.106) is adjoint consistent, an optimal order of convergence in the  $L^2$ -norm is obtained by applying the duality argument.

To this end, let us consider the following dual problem

$$\begin{aligned}
-\nabla^T (\mathbf{j}_{\nabla \mathbf{M}}(\mathbf{M}^e) \nabla \boldsymbol{\psi}) + \mathbf{j}_{\mathbf{M}}^T(\mathbf{M}^e, \nabla \mathbf{M}^e) \nabla \boldsymbol{\psi} &= \mathbf{e} \quad \text{on } \Omega, \\
\boldsymbol{\psi} &= \mathbf{g} \quad \text{on } \partial \Omega,
\end{aligned} \tag{4.157}$$

which is assumed to satisfy the elliptic regularity condition as  $\mathbf{j}_{\nabla \mathbf{M}}$  is positive definite with  $\boldsymbol{\psi} \in H^{2m}(\Omega_h) \times H^{2m}(\Omega_h)$  for  $p \geq 2m$  and

$$\| \boldsymbol{\psi} \|_{H^p(\Omega_h)} \leq C \left( \| \mathbf{e} \|_{H^{p-2m}(\Omega_h)} + \| \mathbf{g} \|_{H^{p-\frac{1}{2}}(\partial \Omega_h)} \right), \tag{4.158}$$

if  $\mathbf{e} \in H^{p-2m}(\Omega_h) \times H^{p-2m}(\Omega_h)$ .

Considering  $\mathbf{e} = \mathbf{M}^e - \mathbf{M}_h \in L^2(\Omega_h) \times L^2(\Omega_h)$  be the error and  $\mathbf{g} = 0$ , multiplying Eq. (4.157) by  $\mathbf{e}$ , and integrating over  $\Omega_h$ , result in

$$\begin{aligned}
\int_{\Omega_h} [\mathbf{j}_{\nabla \mathbf{M}}(\mathbf{M}^e) \nabla \boldsymbol{\psi}]^T \nabla \mathbf{e} d\Omega + \int_{\Omega_h} [\mathbf{j}_{\mathbf{M}}^T(\mathbf{M}^e, \nabla \mathbf{M}^e) \nabla \boldsymbol{\psi}]^T \mathbf{e} d\Omega \\
- \sum_e \int_{\partial \Omega^e} [\mathbf{j}_{\nabla \mathbf{M}}(\mathbf{M}^e) \nabla \boldsymbol{\psi}]^T \mathbf{e}_n dS = \| \mathbf{e} \|_{L^2(\Omega_h)}^2,
\end{aligned} \tag{4.159}$$

with

$$\| \boldsymbol{\psi} \|_{H^2(\Omega_h)} \leq C \| \mathbf{e} \|_{L^2(\Omega_h)}. \tag{4.160}$$

As  $[[\boldsymbol{\psi}]] = [[\nabla \boldsymbol{\psi}]] = 0$  on  $\partial_I \Omega_h$  and  $[[\boldsymbol{\psi}]] = -\boldsymbol{\psi} = 0$  on  $\partial_D \Omega_h$ , we have by comparison with Eqs. (4.102-4.103), that

$$\begin{cases} \int_{\Omega_h} [\mathbf{j}_{\nabla \mathbf{M}}(\mathbf{M}^e) \nabla \boldsymbol{\psi}]^T \nabla \mathbf{e} d\Omega + \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} [\mathbf{j}_{\nabla \mathbf{M}}(\mathbf{M}^e) \nabla \boldsymbol{\psi}]^T [[\mathbf{e}_n]] dS \\ \int_{\Omega_h} [\mathbf{j}_{\mathbf{M}}(\mathbf{M}^e, \nabla \mathbf{M}^e) \mathbf{e}]^T \nabla \boldsymbol{\psi} d\Omega \end{cases} = \begin{cases} \mathcal{A}(\mathbf{M}^e; \mathbf{e}, \boldsymbol{\psi}), \\ \mathcal{B}(\mathbf{M}^e; \mathbf{e}, \boldsymbol{\psi}), \end{cases} \tag{4.161}$$

as  $\mathbf{j}_{\mathbf{M}}$ ,  $\mathbf{j}_{\nabla \mathbf{M}}$  are symmetric. Therefore, Eq. (4.159) reads

$$\| \mathbf{e} \|_{L^2(\Omega_h)}^2 = \mathcal{A}(\mathbf{M}^e; \mathbf{e}, \boldsymbol{\psi}) + \mathcal{B}(\mathbf{M}^e; \mathbf{e}, \boldsymbol{\psi}). \tag{4.162}$$

From Eq. (4.104), one has

$$\mathcal{A}(\mathbf{M}^e; \mathbf{M}^e - \mathbf{M}_h, \mathbf{I}_h \boldsymbol{\psi}) + \mathcal{B}(\mathbf{M}^e; \mathbf{M}^e - \mathbf{M}_h, \mathbf{I}_h \boldsymbol{\psi}) = \mathcal{N}(\mathbf{M}^e, \mathbf{M}_h; \mathbf{I}_h \boldsymbol{\psi}), \quad (4.163)$$

as  $\mathbf{M}^e$  is the exact solution and  $\mathbf{I}_h \boldsymbol{\psi} \in \mathbf{X}^k$ , and Eq. (4.162) is rewritten

$$\| \mathbf{e} \|_{L^2(\Omega_h)}^2 = \mathcal{A}(\mathbf{M}^e; \mathbf{e}, \boldsymbol{\psi} - \mathbf{I}_h \boldsymbol{\psi}) + \mathcal{B}(\mathbf{M}^e; \mathbf{e}, \boldsymbol{\psi} - \mathbf{I}_h \boldsymbol{\psi}) + \mathcal{N}(\mathbf{M}^e, \mathbf{M}_h; \mathbf{I}_h \boldsymbol{\psi}). \quad (4.164)$$

First, using Lemma 4.4.2, Eq. (4.109), Lemma 2.4.6, Eq. (2.23), and Eq. (4.156), leads to

$$\begin{aligned} | \mathcal{A}(\mathbf{M}^e; \mathbf{e}, \boldsymbol{\psi} - \mathbf{I}_h \boldsymbol{\psi}) + \mathcal{B}(\mathbf{M}^e; \mathbf{e}, \boldsymbol{\psi} - \mathbf{I}_h \boldsymbol{\psi}) | &\leq C^k C_y \| \mathbf{e} \|_1 \| \boldsymbol{\psi} - \mathbf{I}_h \boldsymbol{\psi} \|_1 \\ &\leq C^k \| \mathbf{e} \|_1 h_s \| \boldsymbol{\psi} \|_{H^2(\Omega_h)} \\ &\leq C^{k''} h_s^\mu \| \mathbf{M}^e \|_{H^s(\Omega_h)} \| \boldsymbol{\psi} \|_{H^2(\Omega_h)}, \end{aligned} \quad (4.165)$$

with  $\mu = \min \{s, k + 1\}$ .

Then proceeding as for establishing Lemma 4.4.5 and using the a priori error estimate (4.155-4.156), we have

$$| \mathcal{N}(\mathbf{M}^e, \mathbf{M}_h; \mathbf{I}_h \boldsymbol{\psi}) | \leq C^{k''} C_y h_s^{2\mu-3} \| \mathbf{M}^e \|_{H^s(\Omega_h)}^2 \| \mathbf{I}_h \boldsymbol{\psi} \| . \quad (4.166)$$

The bound of  $| \mathcal{N}(\mathbf{M}^e, \mathbf{M}_h; \mathbf{I}_h \boldsymbol{\psi}) |$  is given in detail in Appendix C.9.

Finally, using Lemma 2.4.6, Eq. (2.23), remembering  $[[\boldsymbol{\psi}]] = 0$  in  $\Omega$ , we deduce that

$$\begin{aligned} \| \mathbf{I}_h \boldsymbol{\psi} \| &\leq \| \mathbf{I}_h \boldsymbol{\psi} - \boldsymbol{\psi} \|_1 + \| \boldsymbol{\psi} \|_1 \\ &\leq C^k h_s \| \boldsymbol{\psi} \|_{H^2(\Omega_h)} + \| \boldsymbol{\psi} \|_{H^1(\Omega_h)} \\ &\leq C^k (h_s + 1) \| \boldsymbol{\psi} \|_{H^2(\Omega_h)} . \end{aligned} \quad (4.167)$$

Combining Eqs. (4.165-4.167), Eq. (4.164) becomes, for  $\mu \geq 3$

$$\| \mathbf{e} \|_{L^2(\Omega_h)}^2 \leq C^{k''} h_s^\mu (1 + \| \mathbf{M}^e \|_{H^s(\Omega_h)}) \| \mathbf{M}^e \|_{H^s(\Omega_h)} \| \boldsymbol{\psi} \|_{H^2(\Omega_h)}, \quad (4.168)$$

with  $\mu = \min \{s, k + 1\}$ , or using Eq. (4.160), the final result for  $k \geq 2$

$$\| \mathbf{e} \|_{L^2(\Omega_h)} \leq C^{k''} C_M h_s^\mu \| \mathbf{M}^e \|_{H^s(\Omega_h)} . \quad (4.169)$$

This result demonstrates the optimal convergence rate of the method with the mesh-size for cases in which  $k \geq 2$  (so that  $\mu \geq 3$ ).

## 4.5 Numerical examples

We present 1-, 2-, and 3-dimensional simulations to verify the DG numerical properties for Electro-Thermal problems on shape regular and shape irregular meshes. First the method is compared to analytical results and a continuous Galerkin formulation on simple 1D-tests, then the method is applied on 2D-tests to verify the optimal convergence rates. Finally, a 3D unit cell model is presented. In the applications, the Dirichlet boundary conditions have been enforced strongly for simplicity.

### 4.5.1 1-D example with one material

The first test is inspired from [58], where the boundary condition induces an electric current density, with the temperature constrained on the two opposite faces, as shown in Fig. 4.1. The target of this test is to find the distribution of the temperature, electric potential and their corresponding fluxes, when considering the material properties, i.e.  $\mathbf{l}$ ,  $\mathbf{k}$ , and  $\alpha$ , as reported in Table 4.1. The simulation is performed using a quadratic polynomial approximation, with 12 elements, and the value of stabilization parameter is  $\mathcal{B} = 100$ .

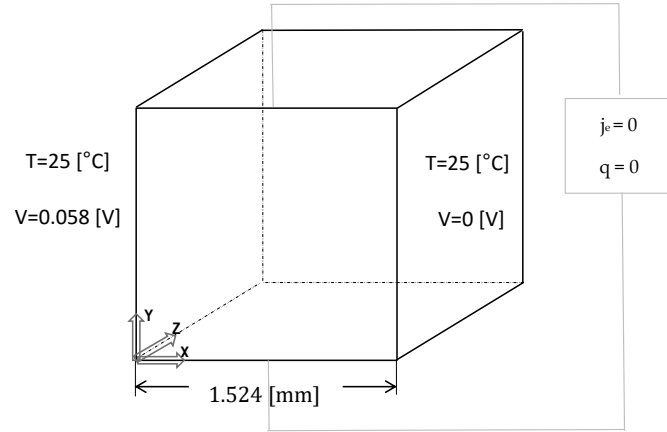


Figure 4.1: One-material Electro-Thermal problem and the boundary conditions

Table 4.1: Material parameter for Bismuth telluride

Parameter	Value
Electrical conductivity $\mathbf{l}$ [S/m]	diag( $8.422 \times 10^4$ )
Thermal conductivity $\mathbf{k}$ [W/(K · m)]	diag(1.612)
Seebeck coefficient $\alpha$ [V/K]	$1.941 \times 10^{-4}$

As it can be seen in Fig. 4.2(a), the electric potential distribution is close to linear but the temperature distribution is almost quadratic with a maximum value of 47 [°C] due to the volumetric Joule effect. This shows that this Electro-Thermal domain acts as a heat pump. Then Fig. 4.2(b) presents the distribution of thermal flux which is almost linear with an electric current of about  $3.2 \times 10^6$  [A/m<sup>2</sup>]. The results of the present DG method agree with the analytical approximation provided in [58] –the difference being due to the approximations required to derive the analytical solution.

Then the same test is simulated with the same boundary conditions, polynomial degree approximation, and value of  $\mathcal{B}$ , but with successively 3, 9, and 21 elements. Figure 4.3 presents the comparison of the results obtained with a Continuous Galerkin (CG) and the Discontinuous Galerkin (DG) formulations. As the distributions are almost parabolic, three elements already capture the solution, which does not make this test fit to study the convergence rate. Figure 4.4 illustrates the comparison of the thermal flux (one value per element



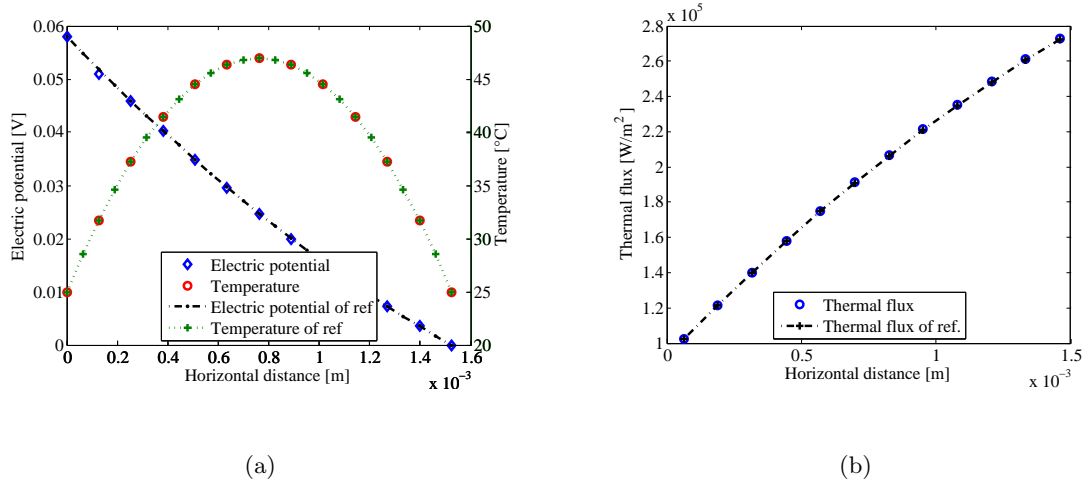


Figure 4.2: (a) The distributions of the electrical potential and temperature in the Electro-Thermal domain for one material, (b) the distribution of the thermal flux in the Electro-Thermal domain for one material. Ref.-curves are from [58]

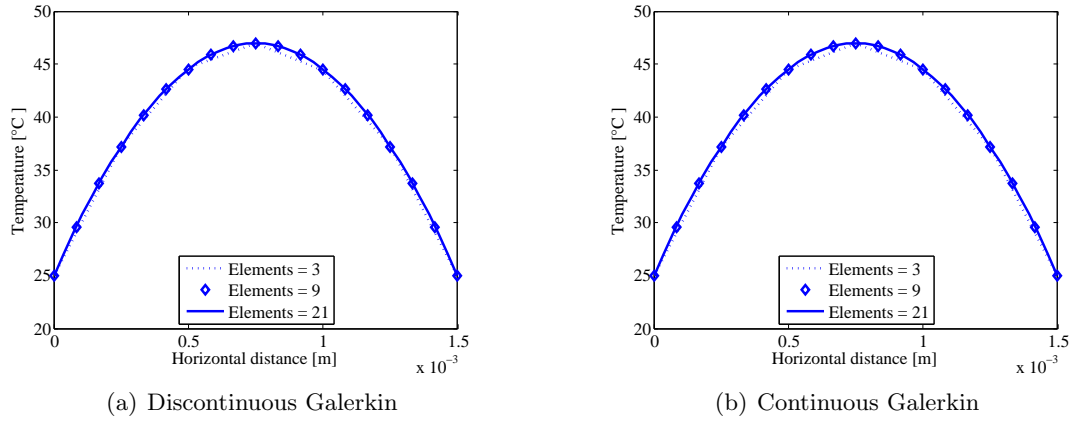


Figure 4.3: Comparison between the distributions of the temperature in the Electro-Thermal composite domain for different numbers of elements between (a) the DG formulation, and (b) the CG formulation

is reported) with different mesh sizes between the CG and DG formulations and shows that the same thermal flux distribution is recovered. We also note from Figs. 4.3(a and b) and Figs. 4.4(a and b), that the results of the present DG formulation are in agreement with those obtained by the CG method.

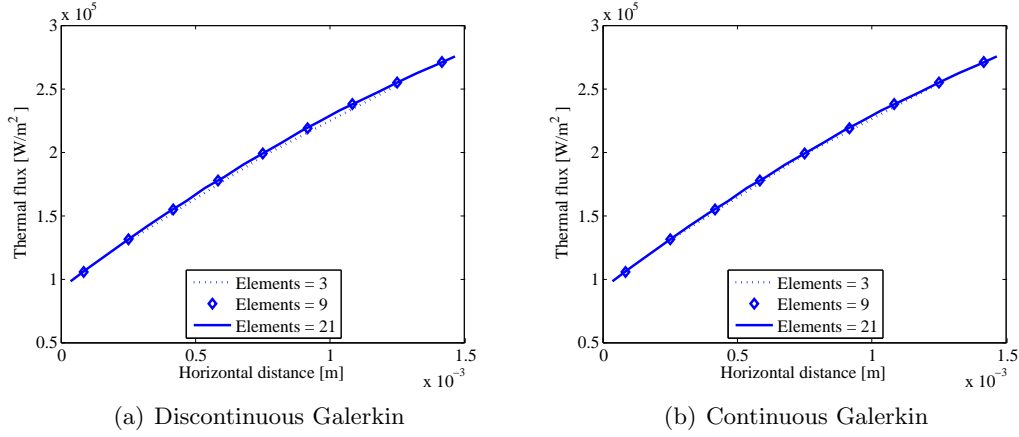


Figure 4.4: Comparison between the distributions of the thermal flux in the Electro-Thermal composite domain for different numbers of elements between (a) the DG formulation, and (b) the CG formulation

#### 4.5.2 1-D example with two materials

By applying the same kind of boundary conditions but for a combination of two materials –matrix (i.e., polymer) which is a non-conductive material and conductive fillers (i.e., carbon fiber)– as shown in Fig. 4.5, we can study the effect of the DG formulation in case of material interfaces. The electrical and thermal material properties considered for the verification are considered constant and reported in Table. 4.2, for the carbon fiber and the polymer matrix.

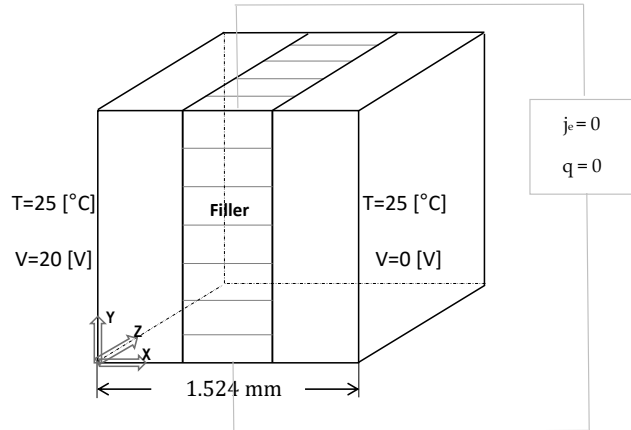


Figure 4.5: Electro-Thermal composite domain and the boundary conditions

Second order polynomial approximations, 12 elements, and the value of  $\mathcal{B} = 100$ , are still considered in this test. An electric potential difference of 20 [V] is applied, which is higher than in the previous test in order to reach a similar increase in temperature as for the previous test. Figure 4.6(a) shows the distribution of the voltage and the temperature in this Electro-Thermal composite domain, and Fig. 4.6(b) the distribution of the thermal

Table 4.2: Composite material phases parameters

Parameter	Carbon fiber	Polymer
Electrical conductivity $\mathbf{l}$ [S/m]	diag(100000)	diag(0.1)
Thermal conductivity $\mathbf{k}$ [W/(K · m)]	diag(40)	diag(0.2)
Seebeck coefficient $\alpha$ [V/K]	$3 \times 10^{-6}$	$3 \times 10^{-7}$

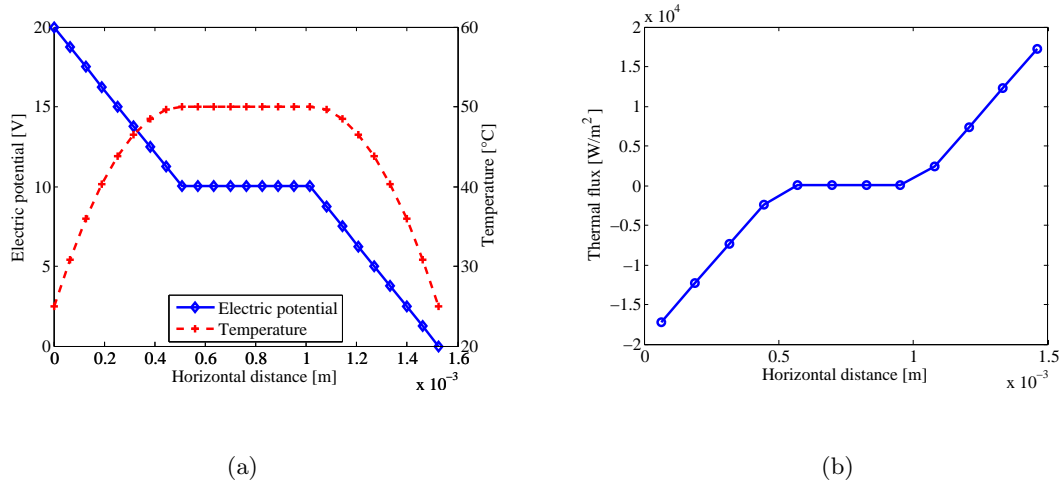


Figure 4.6: (a) The distributions of the electrical potential and temperature in the Electro-Thermal composite domain, and (b) the distribution of the thermal flux in the Electro-Thermal composite domain

flux. We can see that the temperature, electric potential, and thermal flux fields are almost constant in the filler (the conductive material), as its electrical conductivity is high, and transient gradually in the polymer matrix (non conductive material). The resulting electric current is of about  $1.96 \times 10^3$  [A/m<sup>2</sup>].

Then, we carry out the study of the stabilization parameter effect on the quality of the approximation in Fig. 4.7, where the internal energy per unit section is presented in terms of the stabilization parameter. The test is simulated with different values of the stabilization parameter  $\mathcal{B} = 1, 10, 25, 50, 100, 250, 500, 1000,$  and  $5000$ . Although for the lower value of the stability parameter, the energy is overestimated, sign of an instability, the energy converges from below for stabilization parameters  $\mathcal{B} \geq 10$ , which proves that if  $\mathcal{B}$  is large enough, the method is stable.

Figure 4.8 compares the results obtained on the composite domain for different electrical conductivity values of the matrix material, all the other parameters being the same as before. This figure shows the difference in the maximum temperature reached when different values of the electrical conductivity are applied. This result indicates that the present DG formulation can be used for composite materials with high or low contrast.

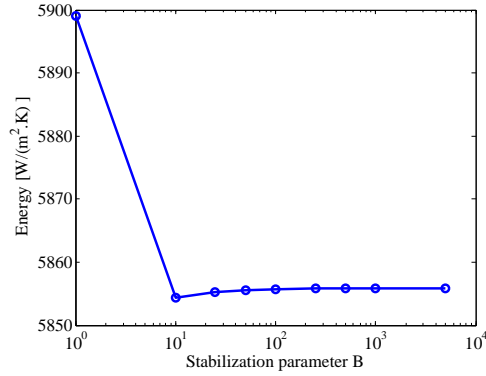


Figure 4.7: The internal energy of the Electro-Thermal composite domain for different values of the stabilization parameter  $\mathcal{B}$

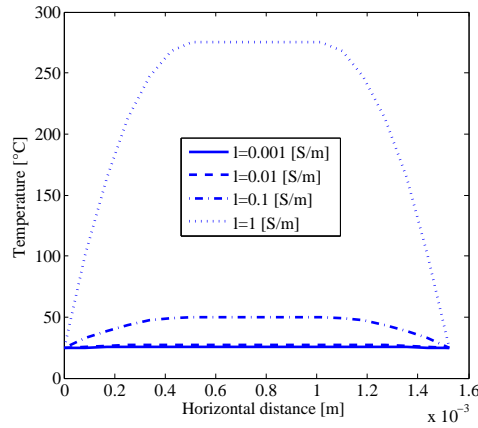


Figure 4.8: The temperature distributions in the Electro-Thermal composite domain for different values of electrical conductivity of the matrix material

### 4.5.3 1-D The variation of electric potential with temperature difference

The following test is motivated to convert heat energy into electricity, in the Bismuth Telluride with the material parameters as presented in Table 4.1 and with the boundary condition stated in Fig. 4.9

The result in Fig. 4.10 shows the relation between the electric potential and temperature difference. It can be seen that the output electric potential, according to Seebeck coefficient, increases as the temperature difference increases. This proves that our formulation is effective and works in the two directions, production of electricity from temperature difference, as showed on this test and production of temperature difference by applying electric current, as showed in the previous examples.

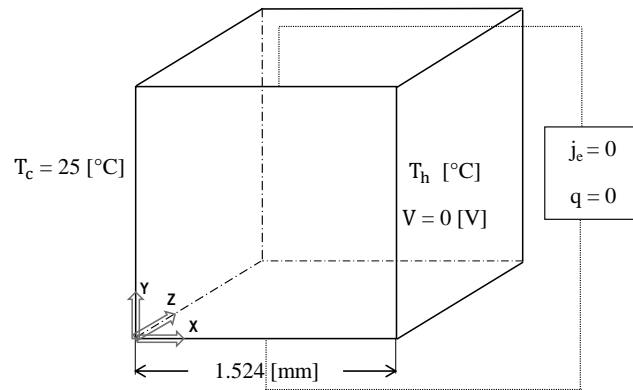


Figure 4.9: Electro-Thermal unit cell and boundary condition

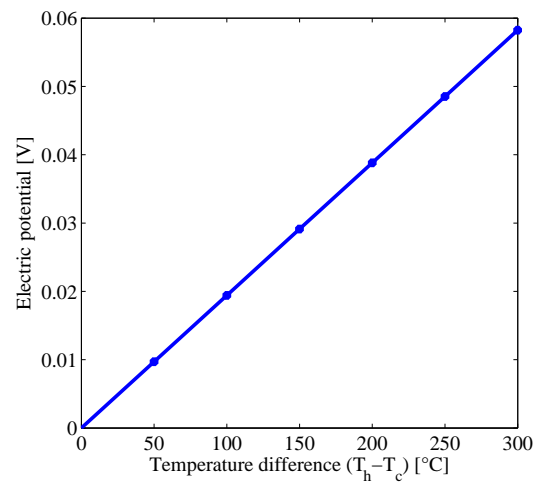


Figure 4.10: The variation of electric potential with temperature difference

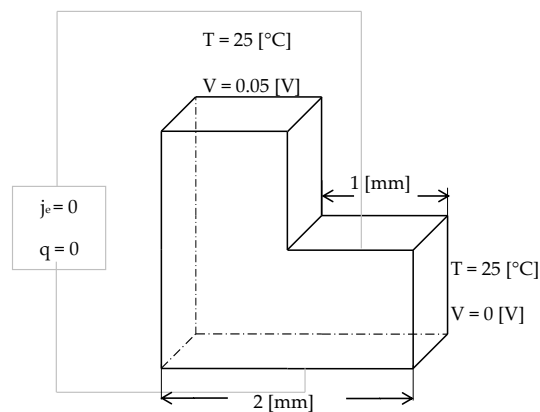


Figure 4.11: L-shaped Electro-Thermal problem and the boundary conditions

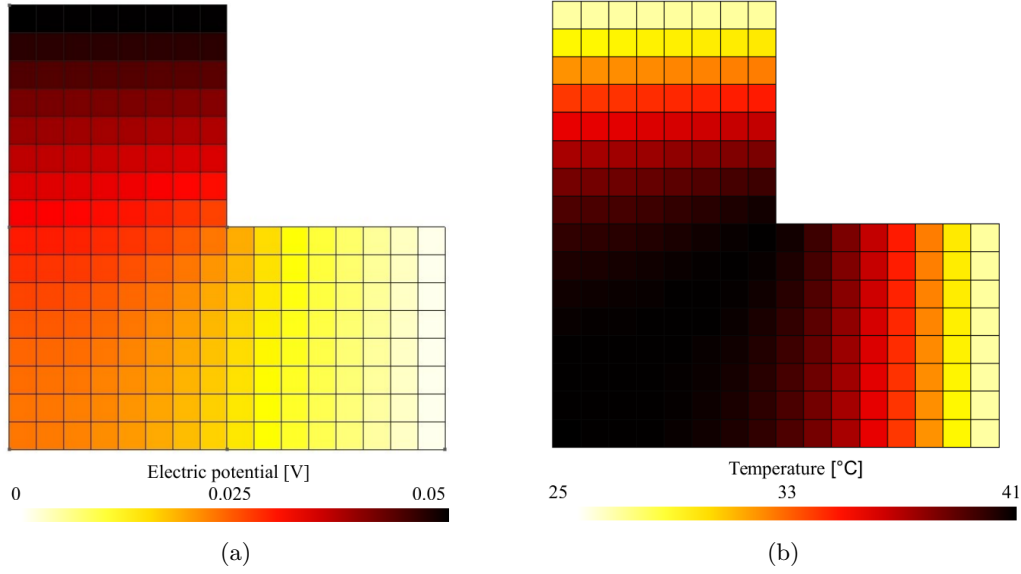


Figure 4.12: The distribution in the L-shaped Electro-Thermal problem of (a) the electrical potential, and (b) the temperature

#### 4.5.4 2-D study of convergence order

In order to generate 2D gradients, we consider an L-shaped domain with the boundary condition illustrated in Fig. 4.11, and with the material properties reported in Table. 4.1. To prove the optimal rate of convergence in the  $L^2$ -norm and  $H^1$ -norm, a uniform  $h_s$  refinement is considered. A second order polynomial approximation is considered with  $\mathcal{B} = 100$ . The resulting distributions of temperature and electrical potential are illustrated respectively in Fig. 4.12(a) and in Fig. 4.12(b).

First the convergence rate of the energy error  $\| \mathbf{M}^e - \mathbf{M}_h \|$  –error in the  $H^1$ -norm– with respect to the mesh size is reported in Fig. 4.13(a). The reference solution is obtained with a refined mesh of  $h_s/L = 1/32$ . It can be seen that as the mesh is refined, the error in the energy decreases quadratically for quadratic elements, once the mesh size is small enough. Thereby that confirms the prior error estimate derived in Section 4.4.5.

Second, the error in the  $L^2$ -norm in terms of the mesh size  $h_s$  is illustrated in Fig. 4.13(b). The computed order of convergence of order  $k + 1$  for  $k = 2$  is optimal, once the mesh size is small enough, in agreement with the theory predicted in Section 4.4.6.

#### 4.5.5 3-D unit cell simulation

The third test illustrates the electrical thermal behavior of a composite material i.e., carbon fiber reinforced polymer matrix, which is heated by electric current. The studied unit cell and the boundary conditions are illustrated in Fig. 4.14, and the materials properties are reported in Table 4.2. A finite element mesh of 90 quadratic bricks is considered (the test is thus run in 3D). The initial temperature of the cell is 25 [°C].

Figure 4.15 presents the distributions of the temperature and the electric potential in the unit cell. When the electric potential of 10 [V] is applied on one side, the temperature of

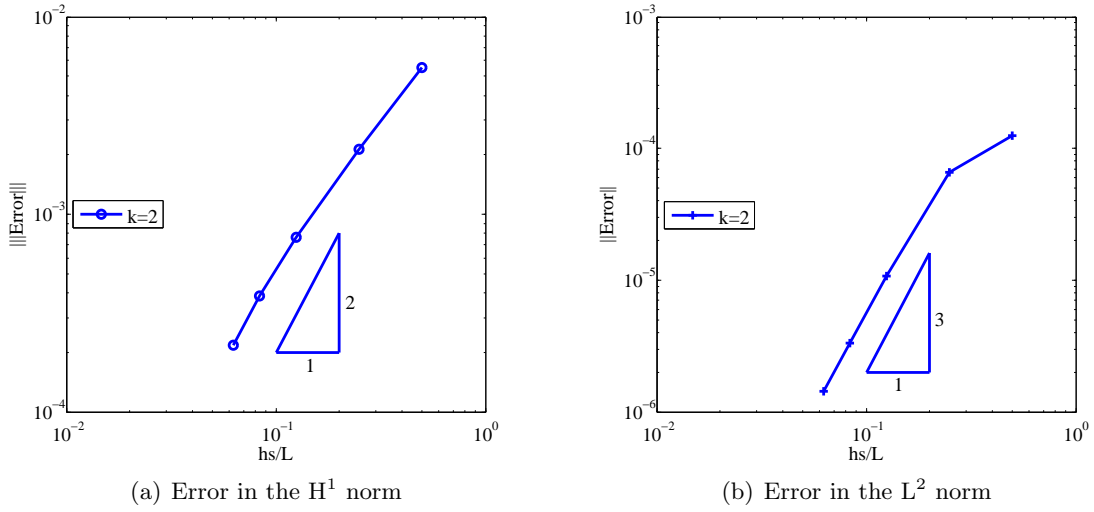


Figure 4.13: Error with respect to the mesh size. (a) Error in the  $H^1$  norm, (b) Error in the  $L^2$  norm

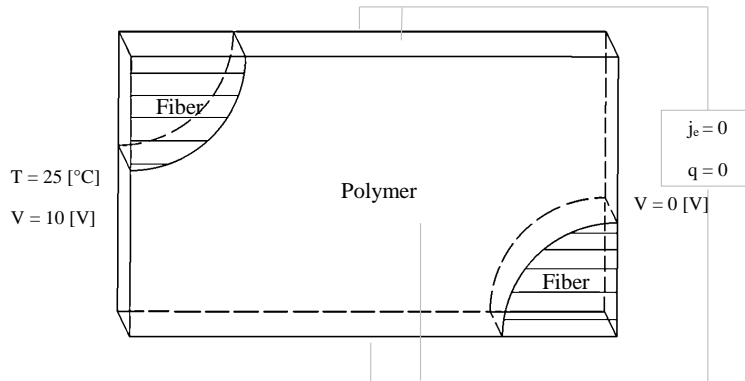


Figure 4.14: Electro-Thermal unit cell and boundary condition

the other side increases from 25 [°C] to 50 [°C]. This shows the applicability of the present formulation when different (irregular) mesh sizes are used simultaneously.

## 4.6 Conclusions

In this chapter, starting from the continuum theory for Electro-Thermal coupled problems, based on continuum mechanics and thermodynamic laws, a weak discontinuous Galerkin (DG) form has been formulated using conjugated fluxes and fields gradients.

As the weak discontinuous form is derived in terms of those energy conjugated fluxes and fields gradients, the resulting DG finite element method is consistent and stable. The numerical properties of the DG method for nonlinear elliptic problems, such as the consistency and uniqueness of the solution have been analyzed by reformulating the problem in a linearized fixed point form, following the methodology set by previous works [76, 25] for

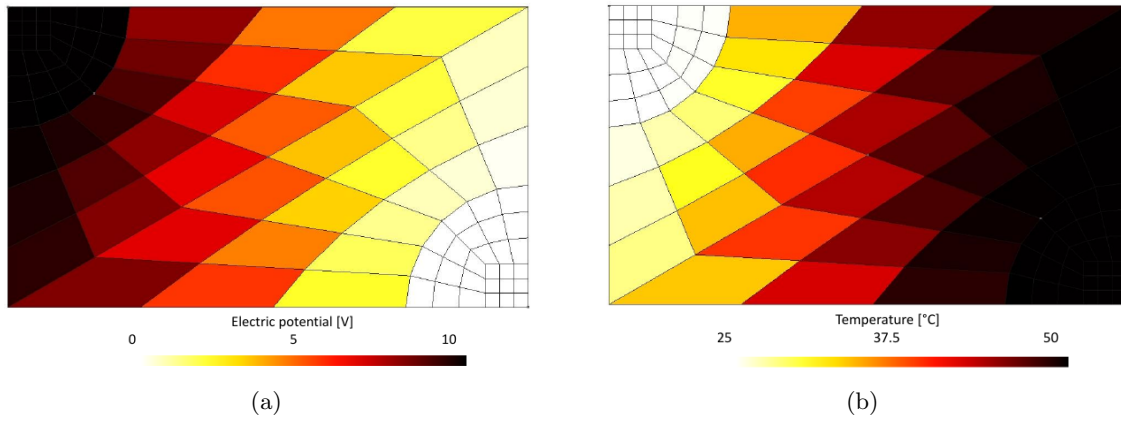


Figure 4.15: The distributions in the unit cell of (a) the electrical potential, and (b) the temperature

non-linear elliptic problems, but adapted for thermo-electrical problems.

The numerical verification has been undertaken to demonstrate the theoretical results. In particular, the convergence rates in the  $L^2$ -norm and the  $H^1$ -norm with respect to the mesh size are optimal and agree with the error analysis that was derived in the theory.

Finally, a unit cell problem has been solved numerically to illustrate the capability of the algorithm.



## Chapter 5

# A coupled Electro-Thermo-Mechanical Discontinuous Galerkin method

### 5.1 Introduction

When an electrically conducting phase is dispersed in sufficient quantity in a matrix of polymer, conductive polymer composites are formed.

Conductive polymer composites can be extended for application in various fields: heaters with distributed heat-emission and self-regulated heaters, shieldings for electromagnetic protection, contact buttons in computers and media technics, current-limiting devices, conductive adhesives, electronic applications, actuation of hybrid conductive shape memory polymers SMPs, and many others.

Carbon fiber reinforced polymer composites consist of at least two components, a polymer matrix (generally dielectric) and electrically conductive fillers. This combination results in multifunctional composites, both structural and conductive. The existence of the polymer matrix will avoid catastrophic failure due to fiber breaking because of its viscoelastic characteristic especially at high temperature, and the existence of the carbon fibers will enhance strength and stiffness on one hand, and will exhibit conductivity under an Electro-Thermal coupling effect on the other hand.

With a view to the modeling of such structures, a multi-field coupling resolution strategy is developed for the solution of electrical, energy, and momentum conservation equations by means of Discontinuous Galerkin finite element method. There have been many studies on Electro-Thermo-Mechanical coupling, e.g., Muliana et al. [55] have studied the time dependent response of active piezoelectric fiber and polymer composite. They have illustrated that time dependent response in the composites depends not only on the properties of the components but also on the prescribed boundary. In addition they have concluded that the study in a steady state of active composite fibers can lead to false detection of localized failure as the variation in field variables in the composite are not considered.

Rothe et al. [64] have considered the three-field problem of small strain for Electro-Thermal-Elasticity, where they have focused on the numerical treatment of the monolithic approach, with one dimensional analytical solution in the purpose of code verification. In

particular Zhupanska et al. [80] have discussed the governing equations describing electromagnetic, thermal, and mechanical field interactions. However the magnetic contribution was neglected for the current magnitude below 40 [A], this in turn results in solving Electro-Thermo-Mechanical coupling problem. In that paper, they have concluded that an application of an electric current to the unidirectional carbon fiber polymer matrix plates leads to 1D thermal field, which is constant in the direction transverse to the fiber direction.

A state of art report about Thermo-Electric polymers and figure of merits have been reviewed in [15]. Moreover the improvement of the thermoelectric efficiency has been discussed in that paper, and it was shown that it can be achieved by using materials either with high electrical conductivity or with high Seebeck coefficient.

In this chapter, a problem of electric current induced heating and the associated stresses in the conducting polymers composites are considered. When an electrical current is applied and heating is produced by the joule effect in conductive faces, and the material dilates.

This chapter is organized as follows. Section 5.2 describes the governing equations of Electro-Thermo-Mechanical materials. In this chapter the Electro-Mechanical coupling has been disregarded, as this coupling is out of the scope of our interest and the Thermo-Elastic damping has been disregarded as well, since the heating occurs slowly. The theory that is considered in the previous chapter has been extended for large deformation and the Discontinuous Galerkin formulation for Electro-Thermo-Mechanical bodies is developed in Section 5.3 with appropriate choice of trial functions ( $\mathbf{u}, f_V = \frac{-V}{T}, f_T = \frac{1}{T}$ ), where  $\mathbf{u}$  is the displacement,  $T$  is the temperature, and  $V$  is the electric potential, which results into a set of non-linear equations which is implemented within a three-dimensional finite element code. In Section 5.4 the stability, the uniqueness, and the convergence rate of the error in both the energy and  $L^2$ -norms have been derived in the particular case of small deformation. Afterwards, in Section 5.5 a volume element of carbon fibers embedded in a polymer matrix is considered to illustrate the Electro-Thermo-Mechanical behavior of composite materials, in addition to another numerical tests which support the theory that is developed in this chapter.

## 5.2 Governing equations for Electro-Thermo-Mechanical coupling

In this section an overview of the basic equations that govern the Electro-Thermo-Mechanical coupled phenomena is presented, where an Electro-Thermo-Mechanical body in its reference configuration  $\Omega_0 \in \mathbb{R}^d$  is considered, where  $d$  is the spatial dimension, whose Dirichlet boundary  $\partial_D \Omega_0$  and Neumann boundary  $\partial_N \Omega_0$  are the outer boundaries  $\partial \Omega_0$  of the domain.

The material properties may in general depend on the position. The first balance equation is the equation of motion which is the balance of linear momentum in the absence of body force with respect to the reference frame

$$\nabla_0 \cdot \mathbf{P}^T = 0 \quad \forall \mathbf{X} \in \Omega_0, \quad (5.1)$$

where  $\mathbf{P}$  is the first Piola-Kirchhoff tensor and  $\nabla_0 = \frac{\partial}{\partial \mathbf{X}}$  is the gradient with respect to the reference configuration.

The second balance equation is the electrical contribution which is the conservation of the electric current density flow with respect to the current frame  $\Omega$ . Recalling Eq. (4.1) from the second chapter and in order to transfer it into the reference configuration the formulation of Nanson is used such that

$$\int_S \mathbf{j}_e \cdot \mathbf{n} dS = \int_{S_0} (\mathbf{j}_e \cdot \mathbf{F}^{-T}) \cdot \mathbf{N} J dS_0, \quad (5.2)$$

where  $J = \det(\mathbf{F})$  is the determinate of the deformation tensor  $\mathbf{F} = \frac{\partial \mathbf{x}}{\partial \mathbf{X}}$ ,  $\mathbf{j}_e$  is the flow of electric current density,  $\mathbf{J}_e = \mathbf{j}_e \cdot \mathbf{F}^{-T} J$  is the current density with respect to the reference surface, and  $\mathbf{N}$  is the outward normal in the reference configuration. Hence the conservation of the electric current density flow with respect to the reference frame is

$$0 = \int_{\Omega} \nabla \cdot \mathbf{j}_e d\Omega = \int_{\Omega_0} \nabla_0 \cdot (\mathbf{j}_e \cdot \mathbf{F}^{-T} J) d\Omega_0 = \int_{\Omega_0} \nabla_0 \cdot \mathbf{J}_e d\Omega_0. \quad (5.3)$$

The flow of electric current density which is mapped into the reference configuration reads after recalling its definition from Eq. (4.4)

$$\mathbf{J}_e(\mathbf{F}, T, V) = \mathbf{j}_e \cdot \mathbf{F}^{-T} J = \mathbf{F}^{-1} \cdot \mathbf{l} \cdot \mathbf{F}^{-T} \cdot \left( -\frac{\partial V}{\partial \mathbf{X}} \right) J + \alpha \mathbf{F}^{-1} \cdot \mathbf{l} \cdot \mathbf{F}^{-T} \cdot \left( -\frac{\partial T}{\partial \mathbf{X}} \right) J. \quad (5.4)$$

Let us define the electrical conductivity in the reference configuration  $\mathbf{L}(\mathbf{F})$  as

$$\mathbf{L}(\mathbf{F}) = \mathbf{F}^{-1} \cdot \mathbf{l} \cdot \mathbf{F}^{-T} J. \quad (5.5)$$

Then Eq. (5.4) can be simplified as

$$\mathbf{J}_e(\mathbf{F}, T, V) = \mathbf{L}(\mathbf{F}) \cdot (-\nabla_0 V) + \alpha \mathbf{L}(\mathbf{F}) \cdot (-\nabla_0 T). \quad (5.6)$$

The third balance equation is the conservation of the energy flux Eq. (4.5). Let us first compute the divergence of the energy flux in the reference configuration using the formulation of Nanson which reads

$$\int_S \mathbf{j}_y \cdot \mathbf{n} dS = \int_{S_0} (\mathbf{j}_y \cdot \mathbf{F}^{-T}) \cdot \mathbf{N} J dS_0 = \int_{S_0} \mathbf{J}_y \cdot \mathbf{N} J dS_0, \quad (5.7)$$

and leads to

$$\int_{\Omega} \nabla \cdot \mathbf{j}_y d\Omega = \int_{\Omega_0} \nabla_0 \cdot (\mathbf{j}_y \cdot \mathbf{F}^{-T} J) d\Omega_0 = \int_{\Omega_0} \nabla_0 \cdot \mathbf{J}_y d\Omega_0, \quad (5.8)$$

where  $\mathbf{J}_y$  is the energy flux per unit surface in the reference configuration. Then the conservation of the energy flux in the reference configuration is stated as

$$\int_{\Omega_0} \nabla_0 \cdot \mathbf{J}_y d\Omega_0 = - \int_{\Omega_0} \rho_0 \frac{\partial y}{\partial t} d\Omega_0 + \int_{\Omega_0} \bar{F} d\Omega_0 \quad \forall \mathbf{X} \in \Omega_0. \quad (5.9)$$

The right hand side of this equilibrium equation is the time derivative of the internal energy density  $y$  and is given in Eq. (4.6) multiplied by the density  $\rho_0 = \rho J$  and  $\bar{F}$  represents all the body energy sources per unit reference volume.

Moreover, the left hand side of Eq. (5.9) involves the energy flux  $\mathbf{J}_y$  in the reference configuration, which is defined as

$$\mathbf{J}_y(\mathbf{F}, T, V) = \mathbf{j}_y \cdot \mathbf{F}^{-T} \mathbf{J} = \mathbf{Q} + V \mathbf{J}_e, \quad (5.10)$$

where  $\mathbf{Q}$  is the heat flux per unit surface in the reference configuration, which is defined after recalling Eq. (4.10) as

$$\mathbf{Q}(\mathbf{F}, T, V) = \mathbf{K} \cdot (-\nabla_0 T) + \alpha T \mathbf{J}_e. \quad (5.11)$$

In this last relation, we have defined the heat conductivity in the reference configuration  $\mathbf{K}(\mathbf{F})$  as

$$\mathbf{K}(\mathbf{F}) = \mathbf{F}^{-1} \cdot \mathbf{k} \cdot \mathbf{F}^{-T} \mathbf{J}, \quad (5.12)$$

and by substituting Eqs. (5.5, 5.11, and 5.12) in Eq. (5.10), we have

$$\mathbf{J}_y(\mathbf{F}, V, T) = (V \mathbf{L}(\mathbf{F}) + \alpha T \mathbf{L}(\mathbf{F})) \cdot (-\nabla_0 V) + (\mathbf{K}(\mathbf{F}) + \alpha V \mathbf{L}(\mathbf{F}) + \alpha^2 T \mathbf{L}(\mathbf{F})) \cdot (-\nabla_0 T). \quad (5.13)$$

The set of equations (5.6, 5.13) can be rewritten under a matrix form as

$$\mathbf{J} = \begin{pmatrix} \mathbf{J}_e \\ \mathbf{J}_y \end{pmatrix} = \begin{pmatrix} \mathbf{L}(\mathbf{F}) & \alpha \mathbf{L}(\mathbf{F}) \\ V \mathbf{L}(\mathbf{F}) + \alpha T \mathbf{L}(\mathbf{F}) & \mathbf{K}(\mathbf{F}) + \alpha V \mathbf{L}(\mathbf{F}) + \alpha^2 T \mathbf{L}(\mathbf{F}) \end{pmatrix} \begin{pmatrix} -\nabla_0 V \\ -\nabla_0 T \end{pmatrix}. \quad (5.14)$$

The set of governing equations (5.3, 5.9) thus becomes

$$\nabla_0^T(\mathbf{J}) = \begin{pmatrix} 0 \\ -\rho_0 \partial_{tY} + \bar{F} \end{pmatrix} = \mathbf{I}_i, \quad (5.15)$$

where  $\nabla_0$  is a vector operator in the reference configuration and  $\mathbf{I}_i$  represents the internal energy rate and the body energy sources.

Let us recall from Chapter 4 the vector of the unknown fields  $\mathbf{M} = \begin{pmatrix} f_V \\ f_T \end{pmatrix}$ , with  $f_V = -\frac{V}{T}$  and  $f_T = \frac{1}{T}$ , then the gradients of the fields vector in the reference frame  $\nabla_0 \mathbf{M}$ , a  $2d \times 1$  vector in terms of  $(\nabla_0 f_V, \nabla_0 f_T)$  are defined by

$$(\nabla_0 \mathbf{M}) = \begin{pmatrix} \nabla_0 f_V \\ \nabla_0 f_T \end{pmatrix} = \begin{pmatrix} \nabla_0(-\frac{V}{T}) \\ \nabla_0(\frac{1}{T}) \end{pmatrix} = \begin{pmatrix} -\frac{1}{T} \mathbf{I} & \frac{V}{T^2} \mathbf{I} \\ 0 & -\frac{1}{T^2} \mathbf{I} \end{pmatrix} \begin{pmatrix} \nabla_0 V \\ \nabla_0 T \end{pmatrix}. \quad (5.16)$$

Furthermore, the fluxes defined by Eq. (5.14) can be expressed in terms of  $f_V, f_T$ , and Eq. (5.14) is rewritten in terms of  $(f_V, f_T) = (-\frac{V}{T}, \frac{1}{T})$ , as  $T = \frac{1}{f_T}, V = -\frac{f_V}{f_T}$  in the reference configuration as:

$$\begin{aligned} \mathbf{J} &= \begin{pmatrix} \frac{1}{f_T} \mathbf{L}(\mathbf{F}) & -\frac{f_V}{f_T^2} \mathbf{L}(\mathbf{F}) + \alpha \frac{1}{f_T} \mathbf{L}(\mathbf{F}) \\ -\frac{f_V}{f_T^2} \mathbf{L}(\mathbf{F}) + \alpha \frac{1}{f_T} \mathbf{L}(\mathbf{F}) & \frac{1}{f_T} \mathbf{K}(\mathbf{F}) - 2\alpha \frac{f_V}{f_T^2} \mathbf{L}(\mathbf{F}) + \alpha^2 \frac{1}{f_T^2} \mathbf{L}(\mathbf{F}) + \frac{f_V^2}{f_T^3} \mathbf{L}(\mathbf{F}) \end{pmatrix} \begin{pmatrix} \nabla_0 f_V \\ \nabla_0 f_T \end{pmatrix} \\ &= \mathbf{Z}_0(\mathbf{F}, f_V, f_T) \nabla_0 \mathbf{M}. \end{aligned} \quad (5.17)$$

Similarly to Chapter 4, we have defined energetically conjugated pair of fluxes and field gradients in the reference configuration, in term of a symmetric and positive definite coefficient matrix  $\mathbf{Z}_0$ , whose its contents are in the reference configuration. By this way Eq. (5.17) has the new expression of the electric current density flow and energy flux in term of  $f_V, f_T$  in the reference configuration. For the future use, and from the last equations, one can define  $\mathbf{L}_1(\mathbf{F}, f_T), \mathbf{L}_2(\mathbf{F}, f_V, f_T)$  as

$$\mathbf{L}_1(\mathbf{F}, f_T) = \frac{1}{f_T} \mathbf{L}(\mathbf{F}), \quad \mathbf{L}_2(\mathbf{F}, f_V, f_T) = \left(-\frac{f_V}{f_T^2} + \alpha \frac{1}{f_T^2}\right) \mathbf{L}(\mathbf{F}), \quad (5.18)$$

and  $\mathbf{J}_{y_1}(\mathbf{F}, f_V, f_T)$  as

$$\mathbf{J}_{y_1}(\mathbf{F}, f_V, f_T) = \frac{1}{f_T^2} \mathbf{K}(\mathbf{F}) - 2\alpha \frac{f_V}{f_T^3} \mathbf{L}(\mathbf{F}) + \alpha^2 \frac{1}{f_T^3} \mathbf{L}(\mathbf{F}) + \frac{f_V^2}{f_T^3} \mathbf{L}(\mathbf{F}). \quad (5.19)$$

Therefore, Eq. (5.17) can be rewritten as

$$\mathbf{J} = \begin{pmatrix} \mathbf{L}_1(\mathbf{F}, f_T) & \mathbf{L}_2(\mathbf{F}, f_T, f_V) \\ \mathbf{L}_2(\mathbf{F}, f_T, f_V) & \mathbf{J}_{y_1}(\mathbf{F}, f_V, f_T) \end{pmatrix} \begin{pmatrix} \nabla_0 f_V \\ \nabla_0 f_T \end{pmatrix}. \quad (5.20)$$

To summarize, the conservation laws for Electro-Thermo-Mechanical coupling are rewritten in the reference configuration as finding  $\mathbf{u}, f_V, f_T \in [\mathbf{H}^2(\Omega_0)]^d \times \mathbf{H}^2(\Omega_0) \times \mathbf{H}^{2+}(\Omega_0)$  such that

$$\nabla_0 \cdot \mathbf{P}^T = 0, \quad \mathbf{P} = \mathbb{P}(\mathbf{F}, \dot{\mathbf{F}}, f_V, f_T, \boldsymbol{\xi}(\xi < t)) \quad \forall \mathbf{X} \in \Omega_0, \quad (5.21)$$

$$\nabla_0 \cdot \mathbf{J}_e = 0, \quad \mathbf{J}_e = \mathbb{J}_e(\mathbf{F}, f_V, f_T) \quad \forall \mathbf{X} \in \Omega_0, \quad (5.22)$$

$$\nabla_0 \cdot \mathbf{J}_y = -\rho_0 \partial_t y + \bar{F}, \quad \mathbf{J}_y = \mathbb{J}_y(\mathbf{F}, f_V, f_T) \quad \forall \mathbf{X} \in \Omega_0 \quad (5.23)$$

$$\mathbf{u} = \bar{\mathbf{u}}, \quad f_T = \bar{f}_T, \quad f_V = \bar{f}_V \quad \forall \mathbf{X} \in \partial_D \Omega_0, \quad (5.24)$$

$$\mathbf{P} \cdot \mathbf{N} = \bar{\mathbf{T}}, \quad \mathbf{J}_y \cdot \mathbf{N} = \bar{J}_y, \quad \mathbf{J}_e \cdot \mathbf{N} = \bar{J}_e \quad \forall \mathbf{X} \in \partial_N \Omega_0. \quad (5.25)$$

In these relations, we have expressed the governing equations  $\mathbb{P}, \mathbb{J}_e$ , and  $\mathbb{J}_y$  in a general way and in terms of the internal variables  $\boldsymbol{\xi}$ . The definition of  $\mathbb{P}$  will be specified in the next Chapter, while the definition of  $\mathbb{J}_e$  and  $\mathbb{J}_y$  follow Eq. (5.20).  $\mathbf{N}$  is the outward unit normal to the boundary  $\partial\Omega_0$  in the reference configuration, and  $\bar{\mathbf{T}}, \bar{J}_y, \bar{J}_e$  represent the outward traction, energy flux and electric current density respectively. Finally  $\bar{\mathbf{u}}, \bar{f}_T, \bar{f}_V$  are the prescribed  $\mathbf{u}, f_T, f_V$  respectively.

## 5.3 The Discontinuous Galerkin formulation for Electro-Thermo-Mechanical bodies

### 5.3.1 The Discontinuous Galerkin weak form

Let  $\Omega_{0h}$  be a shape regular family of triangulation of  $\Omega_0$ , such that  $\Omega_0 = \cup_e \Omega_0^e$ , with  $h_s = \max_{\Omega_0^e \in \Omega_{0h}} \text{diam}(\Omega_0^e)$  for  $\Omega_0^e \in \Omega_{0h}$  with  $\partial\Omega_0^e = \partial_N \Omega_0^e \cup \partial_D \Omega_0^e \cup \partial_I \Omega_0^e$ , and where  $\partial_I \Omega_{0h} = \cup_e \partial_I \Omega_0^e \setminus \partial\Omega_{0h}$ , is the intersecting boundary of the finite elements. Finally  $(\partial_{DI} \Omega_0)^s$  is a face either on  $\partial_I \Omega_{0h}$  or on  $\partial_D \Omega_{0h}$ , with  $\sum_s (\partial_{DI} \Omega_0)^s = \partial_I \Omega_{0h} \cup \partial_D \Omega_{0h}$ .

The discontinuous Galerkin finite element method results from the integration by parts on the finite element of the governing equations multiplied by discontinuous test functions. Let us multiply the first governing equation (5.21) by the virtual displacement  $\delta \mathbf{u}$ , and integrate on  $\Omega_{0h}$ , yielding

$$\sum_e \int_{\Omega_0^e} (\mathbf{P}(\mathbf{F}, f_V, f_T) \cdot \nabla_0) \cdot \delta \mathbf{u} d\Omega_0 = 0 \quad \forall \delta \mathbf{u} \in [H^1(\Omega_0^e)]^d. \quad (5.26)$$

Using the divergence theorem and integration by parts we reduce the order of the differential, and the weak form is then reduced to the following problem

$$\sum_e \int_{\partial \Omega_0^e} \delta \mathbf{u} \cdot \mathbf{P}(\mathbf{F}, f_V, f_T) \cdot \mathbf{N} dS_0 - \sum_e \int_{\Omega_0^e} \mathbf{P}(\mathbf{F}, f_V, f_T) : \nabla_0 \delta \mathbf{u} d\Omega_0 = 0, \quad (5.27)$$

where

$$\begin{aligned} \int_{\partial \Omega_0^e} \delta \mathbf{u} \cdot \mathbf{P}(\mathbf{F}, f_V, f_T) \cdot \mathbf{N} dS_0 &= \int_{\partial_N \Omega_0^e} \delta \mathbf{u} \cdot \mathbf{P}(\mathbf{F}, f_V, f_T) \cdot \mathbf{N} dS_0 \\ &+ \int_{\partial_I \Omega_0^e \cup \partial_D \Omega_{0h}} \delta \mathbf{u} \cdot \mathbf{P}(\mathbf{F}, f_V, f_T) \cdot \mathbf{N} dS_0, \end{aligned} \quad (5.28)$$

and

$$\begin{aligned} \sum_e \int_{\partial_I \Omega_0^e} \delta \mathbf{u} \cdot \mathbf{P}(\mathbf{F}, f_V, f_T) \cdot \mathbf{N} dS_0 &= \int_{\partial_I \Omega_{0h}} (\delta \mathbf{u}^- \cdot \mathbf{P}^-(\mathbf{F}, f_V, f_T) \cdot \mathbf{N}^- dS_0 \\ &+ \delta \mathbf{u}^+ \cdot \mathbf{P}^+(\mathbf{F}, f_V, f_T) \cdot \mathbf{N}^+ dS_0), \end{aligned} \quad (5.29)$$

where  $\mathbf{N}^-$  is defined as the reference outward unit normal of the minus element  $\Omega_0^e^-$ , whereas  $\mathbf{N}^+$  is the reference outward unit normal of its neighboring element,  $\mathbf{N}^+ = -\mathbf{N}^-$ .

Using the two useful operators defined previously in Chapter 3, the jump and average operators, at the interface terms and at the Dirichlet boundary as it will be enforced weakly as well, we have

$$\begin{aligned} \sum_e \int_{\partial_I \Omega_0^e} \delta \mathbf{u} \cdot \mathbf{P}(\mathbf{F}, f_V, f_T) \cdot \mathbf{N} dS_0 &= - \int_{\partial_I \Omega_{0h}} (\delta \mathbf{u}^+ \cdot \mathbf{P}^+(\mathbf{F}, f_V, f_T) - \delta \mathbf{u}^- \cdot \mathbf{P}^-(\mathbf{F}, f_V, f_T)) \cdot \mathbf{N}^- dS_0 \\ &= - \int_{\partial_I \Omega_{0h}} [[\delta \mathbf{u} \cdot \mathbf{P}(\mathbf{F}, f_V, f_T)]] \cdot \mathbf{N}^- dS_0, \text{ and} \end{aligned} \quad (5.30)$$

$$\sum_e \int_{\partial_D \Omega_0^e} \delta \mathbf{u} \cdot \mathbf{P}(\mathbf{F}, f_V, f_T) \cdot \mathbf{N} dS_0 = - \int_{\partial_D \Omega_{0h}} [[\delta \mathbf{u} \cdot \mathbf{P}(\mathbf{F}, f_V, f_T)]] \cdot \mathbf{N}^- dS_0 \text{ and } \mathbf{N}^- = \mathbf{N}. \quad (5.31)$$

Eventually using Eq. (5.25), Eq. (5.27) is rewritten

$$\begin{aligned} \int_{\partial_N \Omega_{0h}} \delta \mathbf{u} \cdot \bar{\mathbf{T}} dS_0 &= \int_{\Omega_{0h}} \mathbf{P}(\mathbf{F}, f_V, f_T) : \nabla_0 \delta \mathbf{u} d\Omega_0 + \int_{\partial_I \Omega_{0h} \cup \partial_D \Omega_{0h}} [[\delta \mathbf{u} \cdot \mathbf{P}(\mathbf{F}, f_V, f_T)]] \cdot \mathbf{N}^- dS_0 \\ &\forall \delta \mathbf{u} \in [H^1(\Omega_0^e)]^d. \end{aligned} \quad (5.32)$$

As the consistency due to the jump of the test functions needs to be enforced, then the flux related to Eq. (5.32) becomes  $[[\delta\mathbf{u} \cdot \mathbf{P}(\mathbf{F}, f_V, f_T)]] = [[\delta\mathbf{u}]] \cdot \langle \mathbf{P}(\mathbf{F}, f_V, f_T) \rangle$

Then by considering the virtual Piola stress for a linearized problem expressed as  $\delta\mathbf{P} = \mathcal{H} : \nabla\delta\mathbf{u}$ , where for simplicity we consider  $\mathcal{H}$  as constant, we can add the compatibility and stabilization terms at the interior elements boundary interfaces  $\partial_I\Omega_{0h}$  and at the Dirichlet elements boundary interface  $\partial_D\Omega_h$  in a similar way to what has done in Chapters 3 and 4. Note that when writing the SIPG, we do not have a contribution on  $\delta f_T$  to ensure optimal convergence rate in  $L^2$ -norm as discussed in Chapter 3. Altogether, we seek to find  $\mathbf{u}, f_T \in \Pi_e [H^1(\Omega_0^e)]^d \times \Pi_e H^{1+}(\Omega_0^e)$ , such that:

$$\begin{aligned}
 & \int_{\partial_N\Omega_{0h}} \delta\mathbf{u} \cdot \bar{\mathbf{T}} dS_0 - \int_{\partial_D\Omega_{0h}} \bar{\mathbf{u}} \cdot (\mathcal{H} : \nabla_0\delta\mathbf{u}) \cdot \mathbf{N} dS_0 \\
 & + \int_{\partial_D\Omega_{0h}} \bar{\mathbf{u}} \otimes \mathbf{N} : \left( \frac{\mathcal{H}\mathcal{B}}{h_s} \right) : \delta\mathbf{u} \otimes \mathbf{N} dS_0 + \int_{\partial_D\Omega_{0h}} \delta\mathbf{u} \cdot \left( -\frac{\boldsymbol{\alpha}_{th} : \mathcal{H}}{f_T^2} \bar{f}_T + \frac{\boldsymbol{\alpha}_{th} : \mathcal{H}}{f_{T_0}^2} f_{T_0} \right) \cdot \mathbf{N} dS_0 \\
 & = \int_{\Omega_{0h}} \mathbf{P}(\mathbf{F}, f_V, f_T) : \nabla_0\delta\mathbf{u} d\Omega_0 + \int_{\partial_I\Omega_{0h} \cup \partial_D\Omega_{0h}} [[\delta\mathbf{u}]] \cdot \langle \mathbf{P}(\mathbf{F}, f_V, f_T) \rangle \cdot \mathbf{N}^- dS_0 \\
 & + \int_{\partial_I\Omega_{0h} \cup \partial_D\Omega_{0h}} [[\mathbf{u}]] \cdot \langle \mathcal{H} : \nabla_0\delta\mathbf{u} \rangle \cdot \mathbf{N}^- dS_0 \\
 & + \int_{\partial_I\Omega_{0h} \cup \partial_D\Omega_{0h}} [[\mathbf{u}]] \otimes \mathbf{N}^- : \left\langle \frac{\mathcal{H}\mathcal{B}}{h_s} \right\rangle : [[\delta\mathbf{u}]] \otimes \mathbf{N}^- dS_0 \\
 & - \int_{\partial_D\Omega_{0h}} [[\delta\mathbf{u}]] \cdot \left( -\frac{\boldsymbol{\alpha}_{th} : \mathcal{H}}{f_T^2} \bar{f}_T + \frac{\boldsymbol{\alpha}_{th} : \mathcal{H}}{f_{T_0}^2} f_{T_0} \right) \cdot \mathbf{N}^- dS_0 \quad \forall \delta\mathbf{u} \in [\Pi_e H^1(\Omega_0^e)]^d,
 \end{aligned} \tag{5.33}$$

where  $f_{T_0}$  is the initial value of  $f_T$ , which is extracted from  $f_{T_0} = \frac{1}{T_0}$ ,  $\mathcal{B}$  is the stability parameter which has to be sufficiently high to guarantee stability,  $\mathcal{H}$  is a constant tangent and  $h_s$  is a measure of the mesh fineness. The term in  $\boldsymbol{\alpha}_{th} : \mathcal{H}$  on  $\partial_D\Omega_{0h}$  is used to constrain weakly the variable  $f_T$  on the Dirichlet BC.

Secondly let us multiply the second balance electrical equation Eq. (5.22) by a virtual potential  $\delta f_V = \delta \left( \frac{-V}{T} \right)$  and let us integrate over  $\Omega_0$ , yielding

$$\sum_e \int_{\Omega_0^e} \nabla_0 \cdot \mathbf{J}_e(\mathbf{F}, f_V, f_T) \delta f_V d\Omega_0 = 0 \quad \forall \delta f_V \in \Pi_e H^1(\Omega_0^e), \tag{5.34}$$

where  $\mathbf{J}_e$  is the electric current density in the reference configuration. Using the divergence theorem and the notations introduced before for the average and the jump operators, since the test function  $\delta f_V$  is discontinuous, Eq. (5.34) becomes

$$\begin{aligned}
 \sum_e \int_{\Omega_0^e} \mathbf{J}_e(\mathbf{F}, f_V, f_{T_h}) \cdot \nabla_0 \delta f_V dS_0 & = \int_{\partial_N\Omega_{0h}} \bar{\mathbf{J}}_e \delta f_V dS_0 \\
 & - \int_{\partial_I\Omega_{0h} \cup \partial_D\Omega_{0h}} [[\mathbf{J}_e(\mathbf{F}, f_V, f_T) \delta f_V]] \cdot \mathbf{N}^- dS_0.
 \end{aligned} \tag{5.35}$$

Similar to what has been done for the mechanical equation, a consistent interface flux related to Eq. (5.35) is considered and we choose  $[[\delta f_V]] \langle \mathbf{J}_e(\mathbf{F}, f_V, f_T) \rangle \cdot \mathbf{N}^-$ . According to

the definitions of  $\mathbf{L}_1(\mathbf{F}, f_T)$ ,  $\mathbf{L}_2(\mathbf{F}, f_V, f_T)$ , in Eq. (5.18), the virtual electric current density  $\delta \mathbf{J}_e(\mathbf{F}, f_V, f_T)$  is written as

$$\delta \mathbf{J}_e(\mathbf{F}, f_V, f_T) = \mathbf{L}_1(\mathbf{F}, f_T) \cdot \nabla_0 \delta f_V + \mathbf{L}_2(\mathbf{F}, f_V, f_T) \cdot \nabla_0 \delta f_T. \quad (5.36)$$

This last result allows formulating the compatibility and quadratic stabilization terms so the weak form Eq. (5.35) is stated as finding  $\mathbf{u}, f_V, f_T \in \Pi_e [H^1(\Omega_0^e)]^d \times \Pi_e H^1(\Omega_0^e) \times \Pi_e H^{1+}(\Omega_0^e)$  such that:

$$\begin{aligned} & \int_{\partial_N \Omega_{0h}} \bar{\mathbf{J}}_e \delta f_V \, dS_0 - \int_{\partial_D \Omega_{0h}} (\mathbf{L}_1(\mathbf{F}, \bar{f}_T) \cdot \nabla_0 \delta f_V + \mathbf{L}_2(\mathbf{F}, \bar{f}_V, \bar{f}_T) \cdot \nabla_0 \delta f_T) \cdot \mathbf{N} \bar{f}_V \, dS_0 \\ & + \int_{\partial_D \Omega_{0h}} \left( \delta f_{V\mathbf{n}} \cdot \frac{\mathbf{L}_1(\mathbf{F}, \bar{f}_T) \mathcal{B}}{h_s} + \delta f_{T\mathbf{n}} \cdot \frac{\mathbf{L}_2(\mathbf{F}, \bar{f}_V, \bar{f}_T) \mathcal{B}}{h_s} \right) \cdot \mathbf{N} \bar{f}_V \, dS_0 \\ & = \int_{\Omega_{0h}} \mathbf{J}_e(\mathbf{F}, f_V, f_T) \cdot \nabla_0 \delta f_V \, d\Omega_0 + \int_{\partial_I \Omega_{0h} \cup \partial_D \Omega_{0h}} [[\delta f_V]] \langle \mathbf{J}_e(\mathbf{F}, f_V, f_T) \rangle \cdot \mathbf{N}^- \, dS_0 \\ & + \int_{\partial_I \Omega_{0h}} [[f_V]] \langle \mathbf{L}_1(\mathbf{F}, f_T) \cdot \nabla_0 \delta f_V \rangle \cdot \mathbf{N}^- \, dS_0 \\ & + \int_{\partial_D \Omega_{0h}} [[f_V]] \langle \mathbf{L}_1(\mathbf{F}, \bar{f}_T) \cdot \nabla_0 \delta f_V \rangle \cdot \mathbf{N}^- \, dS_0 \\ & + \int_{\partial_I \Omega_{0h}} [[f_V]] \langle \mathbf{L}_2(\mathbf{F}, f_V, f_T) \cdot \nabla_0 \delta f_T \rangle \cdot \mathbf{N}^- \, dS_0 \\ & + \int_{\partial_D \Omega_{0h}} [[f_V]] \langle \mathbf{L}_2(\mathbf{F}, \bar{f}_V, \bar{f}_T) \cdot \nabla_0 \delta f_T \rangle \cdot \mathbf{N}^- \, dS_0 \\ & + \int_{\partial_I \Omega_{0h}} [[\delta f_V]] \mathbf{N}^- \cdot \left\langle \frac{\mathbf{L}_1(\mathbf{F}, f_T) \mathcal{B}}{h_s} \right\rangle \cdot \mathbf{N}^- [[f_V]] \, dS_0 \\ & + \int_{\partial_D \Omega_{0h}} [[\delta f_V]] \mathbf{N}^- \cdot \left\langle \frac{\mathbf{L}_1(\mathbf{F}, \bar{f}_T) \mathcal{B}}{h_s} \right\rangle \cdot \mathbf{N}^- [[f_V]] \, dS_0 \\ & + \int_{\partial_I \Omega_{0h}} [[\delta f_T]] \mathbf{N}^- \cdot \left\langle \frac{\mathbf{L}_2(\mathbf{F}, f_V, f_T) \mathcal{B}}{h_s} \right\rangle \cdot \mathbf{N}^- [[f_V]] \, dS_0 \\ & + \int_{\partial_D \Omega_{0h}} [[\delta f_T]] \mathbf{N}^- \cdot \left\langle \frac{\mathbf{L}_2(\mathbf{F}, \bar{f}_V, \bar{f}_T) \mathcal{B}}{h_s} \right\rangle \cdot \mathbf{N}^- [[f_V]] \, dS_0 \\ & \quad \forall \delta f_V, \delta f_T \in \Pi_e H^1(\Omega_0^e) \times \Pi_e H^1(\Omega_0^e). \end{aligned} \quad (5.37)$$

Thirdly, like for the electrical solution, an IP discontinuous Galerkin finite element formulation is used to discretize the thermal equation. Let us multiply the third balance thermal equation Eq. (5.23), by the test function  $\delta f_T = \delta(\frac{1}{T})$ , and integrate over  $\Omega_0$ , yielding

$$\begin{aligned} \sum_e \int_{\Omega_0^e} \nabla_0 \cdot \mathbf{J}_y(\mathbf{F}, f_V, f_T) \delta f_T \, d\Omega_0 & = - \sum_e \int_{\Omega_0^e} \rho_0 \partial_{ty} \delta f_T \, d\Omega_0 + \sum_e \int_{\Omega_0^e} \bar{F} \delta f_T \, d\Omega_0 \\ & \quad \forall \delta f_T \in \Pi_e H^1(\Omega_0^e). \end{aligned} \quad (5.38)$$

As for the electrical equation, by using the divergence theorem and introducing the jump



operator and the boundary condition Eqs. (5.24, 5.25), this last equation becomes

$$\begin{aligned} \int_{\partial_N \Omega_{0h}} \delta f_T \bar{J}_y \, dS_0 &= \int_{\Omega_{0h}} \mathbf{J}_y(\mathbf{F}, f_V, f_T) \cdot \nabla_0 \delta f_T \, d\Omega_0 - \int_{\Omega_{0h}} \rho_0 \partial_t y \delta f_T \, d\Omega_0 \\ &+ \int_{\partial_T \Omega_{0h} \cup \partial_D \Omega_{0h}} \llbracket \delta f_T \mathbf{J}_y(\mathbf{F}, f_V, f_T) \rrbracket \cdot \mathbf{N}^- \, dS_0 + \int_{\Omega_{0h}} \bar{F} \delta f_T \, d\Omega_0 \quad \forall \delta f_T \in \Pi_e H^1(\Omega_0^e). \end{aligned} \quad (5.39)$$

The consistent and stable weak form is obtained by considering the numerical energy flux, and by adding stability and compatibility terms.

The virtual energy flux is expressed from Eq. (5.17) in terms of  $\mathbf{J}_{y1}(\mathbf{F}, f_V, f_T)$ ,  $\mathbf{L}_2(\mathbf{F}, f_V, f_T)$  from Eqs. (5.19, 5.18), leading to

$$\delta \mathbf{J}_y(\mathbf{F}, f_V, f_T) = \mathbf{J}_{y1}(\mathbf{F}, f_V, f_T) \cdot \nabla_0 \delta f_T + \mathbf{L}_2(\mathbf{F}, f_V, f_T) \cdot \nabla_0 \delta f_V. \quad (5.40)$$

Eventually the stabilized form of Eq. (5.38) can be stated as finding  $\mathbf{u}, f_V, f_T \in \Pi_e [\mathbf{H}^1(\Omega_0^e)]^d \times \Pi_e H^1(\Omega_0^e) \times \Pi_e H^{1+}(\Omega_0^e)$  such that

$$\begin{aligned} &\int_{\partial_N \Omega_{0h}} \delta f_T \bar{J}_y \, dS_0 - \int_{\partial_D \Omega_{0h}} (\mathbf{J}_{y1}(\mathbf{F}, \bar{f}_V, \bar{f}_T) \cdot \nabla_0 \delta f_T + \mathbf{L}_2(\mathbf{F}, \bar{f}_V, \bar{f}_T) \cdot \nabla_0 \delta f_V) \cdot \mathbf{N} \bar{f}_T \, dS_0 \\ &+ \int_{\partial_D \Omega_{0h}} \left( \delta f_T \mathbf{N} \cdot \frac{\mathbf{J}_{y1}(\mathbf{F}, \bar{f}_V, \bar{f}_T) \mathcal{B}}{h_s} + \delta f_V \mathbf{N} \cdot \frac{\mathbf{L}_2(\mathbf{F}, \bar{f}_V, \bar{f}_T) \mathcal{B}}{h_s} \right) \cdot \mathbf{N} \bar{f}_T \, dS_0 \\ &= \int_{\Omega_{0h}} \mathbf{J}_y(\mathbf{F}, f_V, f_T) \cdot \nabla_0 \delta f_T \, d\Omega_0 - \int_{\Omega_{0h}} \rho_0 \partial_t y \delta f_T \, d\Omega_0 + \int_{\Omega_{0h}} \bar{F} \delta f_T \, d\Omega_0 \\ &+ \int_{\partial_T \Omega_{0h} \cup \partial_D \Omega_{0h}} \llbracket \delta f_T \rrbracket \langle \mathbf{J}_y(\mathbf{F}, f_V, f_T) \rangle \cdot \mathbf{N}^- \, dS_0 \\ &+ \int_{\partial_T \Omega_{0h}} \llbracket f_T \rrbracket \langle \mathbf{J}_{y1}(\mathbf{F}, f_V, f_T) \cdot \nabla_0 \delta f_T \rangle \cdot \mathbf{N}^- \, dS_0 \\ &+ \int_{\partial_D \Omega_{0h}} \llbracket f_T \rrbracket \langle \mathbf{J}_{y1}(\mathbf{F}, \bar{f}_V, \bar{f}_T) \cdot \nabla_0 \delta f_T \rangle \cdot \mathbf{N}^- \, dS_0 \\ &+ \int_{\partial_T \Omega_{0h}} \llbracket f_T \rrbracket \langle \mathbf{L}_2(\mathbf{F}, f_V, f_T) \cdot \nabla_0 \delta f_V \rangle \cdot \mathbf{N}^- \, dS_0 \\ &+ \int_{\partial_D \Omega_{0h}} \llbracket f_T \rrbracket \langle \mathbf{L}_2(\mathbf{F}, \bar{f}_V, \bar{f}_T) \cdot \nabla_0 \delta f_V \rangle \cdot \mathbf{N}^- \, dS_0 \\ &+ \int_{\partial_T \Omega_{0h}} \llbracket \delta f_T \rrbracket \mathbf{N}^- \cdot \left\langle \frac{\mathbf{J}_{y1}(\mathbf{F}, f_V, f_T) \mathcal{B}}{h_s} \right\rangle \cdot \mathbf{N}^- \llbracket f_T \rrbracket \, dS_0 \\ &+ \int_{\partial_D \Omega_{0h}} \llbracket \delta f_T \rrbracket \mathbf{N}^- \cdot \left\langle \frac{\mathbf{J}_{y1}(\mathbf{F}, \bar{f}_V, \bar{f}_T) \mathcal{B}}{h_s} \right\rangle \cdot \mathbf{N}^- \llbracket f_T \rrbracket \, dS_0 \\ &+ \int_{\partial_T \Omega_{0h}} \llbracket \delta f_V \rrbracket \mathbf{N}^- \cdot \left\langle \frac{\mathbf{L}_2(\mathbf{F}, f_V, f_T) \mathcal{B}}{h_s} \right\rangle \cdot \mathbf{N}^- \llbracket f_T \rrbracket \, dS_0 \\ &+ \int_{\partial_D \Omega_{0h}} \llbracket \delta f_V \rrbracket \mathbf{N}^- \cdot \left\langle \frac{\mathbf{L}_2(\mathbf{F}, \bar{f}_V, \bar{f}_T) \mathcal{B}}{h_s} \right\rangle \cdot \mathbf{N}^- \llbracket f_T \rrbracket \, dS_0 \\ &\forall \delta f_V, \delta f_T \in \Pi_e H^1(\Omega_0^e) \times \Pi_e H^1(\Omega_0^e). \end{aligned} \quad (5.41)$$

Using the notations considered to state the strong form, Eq. (5.17), the weak forms stated by Eqs. (5.37, 5.41) can be combined and reformulated as finding  $\mathbf{u}, \mathbf{M} \in [\Pi_e H^1(\Omega_0^e)]^d \times$

$\Pi_e H^1(\Omega_0^e) \times \Pi_e H^{1+}(\Omega_0^e)$  such that

$$\begin{aligned}
& \int_{\partial_N \Omega_{0h}} \delta \mathbf{M}^T \bar{\mathbf{J}} d\Omega_0 - \int_{\partial_D \Omega_{0h}} \bar{\mathbf{M}}_N^T (\mathbf{Z}_0(\mathbf{F}, \bar{\mathbf{M}}) \nabla_0 \delta \mathbf{M}) dS_0 \\
& + \int_{\partial_D \Omega_{0h}} \delta \mathbf{M}_N^T \left( \frac{\mathcal{B}}{h_s} \mathbf{Z}_0(\mathbf{F}, \bar{\mathbf{M}}) \right) \bar{\mathbf{M}}_N dS_0 = \int_{\Omega_{0h}} \nabla_0 \delta \mathbf{M}^T \mathbf{J}(\mathbf{F}, \mathbf{M}, \nabla_0 \mathbf{M}) d\Omega_0 \\
& + \int_{\Omega_{0h}} \delta \mathbf{M}^T \mathbf{I}_i d\Omega_0 + \int_{\partial_I \Omega_{0h} \cup \partial_D \Omega_{0h}} \llbracket \delta \mathbf{M}_N^T \rrbracket \langle \mathbf{J}(\mathbf{F}, \mathbf{M}, \nabla_0 \mathbf{M}) \rangle dS_0 \\
& + \int_{\partial_I \Omega_{0h}} \llbracket \mathbf{M}_N^T \rrbracket \langle \mathbf{Z}_0(\mathbf{F}, \mathbf{M}) \nabla_0 \delta \mathbf{M} \rangle dS_0 \tag{5.42} \\
& + \int_{\partial_D \Omega_{0h}} \llbracket \mathbf{M}_N^T \rrbracket \langle \mathbf{Z}_0(\mathbf{F}, \bar{\mathbf{M}}) \nabla_0 \delta \mathbf{M} \rangle dS_0 \\
& + \int_{\partial_I \Omega_{0h}} \llbracket \delta \mathbf{M}_N^T \rrbracket \left\langle \frac{\mathcal{B}}{h_s} \mathbf{Z}_0(\mathbf{F}, \mathbf{M}) \right\rangle \llbracket \mathbf{M}_N \rrbracket dS_0 \\
& + \int_{\partial_D \Omega_{0h}} \llbracket \delta \mathbf{M}_N^T \rrbracket \left\langle \frac{\mathcal{B}}{h_s} \mathbf{Z}_0(\mathbf{F}, \bar{\mathbf{M}}) \right\rangle \llbracket \mathbf{M}_N \rrbracket dS_0 \quad \forall \delta \mathbf{M} \in \Pi_e H^1(\Omega_0^e) \times \Pi_e H^1(\Omega_0^e),
\end{aligned}$$

where  $\bar{\mathbf{J}} = \begin{pmatrix} \bar{J}_e \\ \bar{J}_y \end{pmatrix}$  and  $\bar{\mathbf{M}} = \begin{pmatrix} \bar{f}_V \\ \bar{f}_T \end{pmatrix}$ , and where the vector  $\mathbf{M}_N = \begin{pmatrix} \mathbf{N}^- & 0 \\ 0 & \mathbf{N}^- \end{pmatrix} \mathbf{M}$  and  $\bar{\mathbf{M}}_N = \begin{pmatrix} \mathbf{N} & 0 \\ 0 & \mathbf{N} \end{pmatrix} \bar{\mathbf{M}}$  are introduced for simplicity.

It should be noted that the test functions in the previous equations of the weak formulation belong to  $[H^1(\Omega^e)]^d \times H^1(\Omega^e) \times H^{1+}(\Omega^e)$ , however for the numerical analysis, we will need to be in  $[H^2(\Omega^e)]^d \times H^2(\Omega^e) \times H^{2+}(\Omega^e)$ , as shown in the following sections. The equivalent manifold to Eq. (2.6)<sup>1</sup>, is rewritten as

$$X_s^{(+)} = \left\{ \mathbf{G} \in [L^2(\Omega_h)]^d \times L^2(\Omega_h) \times L^{2(+)}(\Omega_h) \mid \text{such that } \mathbf{G}|_{\Omega^e} \in [H^s(\Omega^e)]^d \times H^s(\Omega^e) \times H^{s(+)}(\Omega^e) \quad \forall \Omega^e \in \Omega_h \right\}. \tag{5.43}$$

For the future use, we define  $X^{(+)}$  as  $X_2^{(+)}$  and  $X^+$  the manifold such that  $f_T > 0$ , while  $X$  is the manifold for which  $f_T \lesseqgtr 0$ , with  $X^+ \subset X$ . Moreover, using Eq. (2.9), we have

$$\mathbf{Y} = \left\{ \nabla \mathbf{G} \in \left( (L^2(\Omega_h))^d \right)^{(d+2)} \mid \nabla \mathbf{G}|_{\Omega^e} \in (H^1(\Omega^e))^{d+2} \quad \forall \Omega^e \in \Omega_h \right\}. \tag{5.44}$$

Thereafter, the problem is formulated as finding  $\mathbf{u}, \mathbf{M} \in X^+$  such that

$$A(\mathbf{F}, \mathbf{M}, \delta \mathbf{u}) = B(\delta \mathbf{u}), \quad \forall \delta \mathbf{u} \in X, \text{ and} \tag{5.45}$$

$$C(\mathbf{F}, \mathbf{M}, \delta \mathbf{M}) = D(\mathbf{F}, \delta \mathbf{M}) - \int_{\Omega_{0h}} \delta \mathbf{M}^T \mathbf{I}_i d\Omega_0 \quad \forall \delta \mathbf{M} \in X. \tag{5.46}$$

<sup>1</sup>One more time, by abuse of notations, the (+) superscript means either usual  $H^s$ -space or the space  $H^{s+}$  of strictly positive values.

In these last two equations, the nonlinear forms read

$$\begin{aligned}
 A(\mathbf{F}, \mathbf{M}, \delta \mathbf{u}) &= \int_{\Omega_{0h}} \mathbf{P}(\mathbf{F}, \mathbf{M}) : \nabla_0 \delta \mathbf{u} \, d\Omega_0 + \int_{\partial_I \Omega_{0h} \cup \partial_D \Omega_{0h}} [[\delta \mathbf{u}]] \cdot \langle \mathbf{P}(\mathbf{F}, \mathbf{M}) \rangle \cdot \mathbf{N}^- \, dS_0 \\
 &+ \int_{\partial_I \Omega_{0h} \cup \partial_D \Omega_{0h}} [[\mathbf{u}]] \cdot \langle \mathcal{H} : \nabla_0 \delta \mathbf{u} \rangle \cdot \mathbf{N}^- \, dS_0 + \int_{\partial_I \Omega_{0h} \cup \partial_D \Omega_{0h}} [[\mathbf{u}]] \otimes \mathbf{N}^- : \left\langle \frac{\mathcal{H}\mathcal{B}}{h_s} \right\rangle : [[\delta \mathbf{u}]] \otimes \mathbf{N}^- \, dS_0 \\
 &- \int_{\partial_D \Omega_{0h}} [[\delta \mathbf{u}]] \cdot \langle -\mathcal{Y}(\mathbf{M})\mathbf{M} + \mathcal{Y}_0 \mathbf{M}_0 \rangle \cdot \mathbf{N}^- \, dS_0,
 \end{aligned} \tag{5.47}$$

where  $\mathcal{Y}(f_T)$ ,  $\mathcal{Y}_0(f_{T_0})$  are a matrices of size  $d \times d \times 2$  such that  $\mathcal{Y}(\mathbf{M})\mathbf{M} = \alpha_{th} : \mathcal{H} \frac{1}{f_T^2} f_T$  and  $\mathcal{Y}_0(\mathbf{M}_0)\mathbf{M}_0 = \alpha_{th} : \mathcal{H} \frac{1}{f_{T_0}^2} f_{T_0}$ ,

$$\begin{aligned}
 B(\delta \mathbf{u}) &= \int_{\partial_N \Omega_{0h}} \delta \mathbf{u} \cdot \bar{\mathbf{T}} \, dS_0 - \int_{\partial_D \Omega_{0h}} \bar{\mathbf{u}} \cdot (\mathcal{H} : \nabla_0 \delta \mathbf{u}) \cdot \mathbf{N} \, dS_0 \\
 &+ \int_{\partial_D \Omega_{0h}} \bar{\mathbf{u}} \otimes \mathbf{N} : \left( \frac{\mathcal{H}\mathcal{B}}{h_s} \right) : \delta \mathbf{u} \otimes \mathbf{N} \, dS_0 + \int_{\partial_D \Omega_{0h}} \delta \mathbf{u} \cdot \langle -\mathcal{Y}(\bar{\mathbf{M}})\bar{\mathbf{M}} + \mathcal{Y}_0 \mathbf{M}_0 \rangle \cdot \mathbf{N} \, dS_0
 \end{aligned} \tag{5.48}$$

$$\begin{aligned}
 C(\mathbf{F}, \mathbf{M}, \delta \mathbf{M}) &= \int_{\Omega_{0h}} (\nabla_0 \delta \mathbf{M})^T \mathbf{J}(\mathbf{F}, \mathbf{M}, \nabla_0 \mathbf{M}) \, d\Omega_0 \\
 &+ \int_{\partial_I \Omega_{0h} \cup \partial_D \Omega_{0h}} [[\delta \mathbf{M}_N^T]] \langle \mathbf{J}(\mathbf{F}, \mathbf{M}, \nabla_0 \mathbf{M}) \rangle \, dS_0 \\
 &+ \int_{\partial_I \Omega_{0h}} [[\mathbf{M}_N^T]] \langle \mathbf{Z}_0(\mathbf{F}, \mathbf{M}) \nabla_0 \delta \mathbf{M} \rangle \, dS_0 \\
 &+ \int_{\partial_D \Omega_{0h}} [[\mathbf{M}_N^T]] \langle \mathbf{Z}_0(\mathbf{F}, \bar{\mathbf{M}}) \nabla_0 \delta \mathbf{M} \rangle \, dS_0 \\
 &+ \int_{\partial_I \Omega_{0h}} [[\delta \mathbf{M}_N^T]] \left\langle \frac{\mathcal{B}}{h_s} \mathbf{Z}_0(\mathbf{F}, \mathbf{M}) \right\rangle [[\mathbf{M}_N]] \, dS_0 \\
 &+ \int_{\partial_D \Omega_{0h}} [[\delta \mathbf{M}_N^T]] \left\langle \frac{\mathcal{B}}{h_s} \mathbf{Z}_0(\mathbf{F}, \bar{\mathbf{M}}) \right\rangle [[\mathbf{M}_N]] \, dS_0, \text{ and}
 \end{aligned} \tag{5.49}$$

$$\begin{aligned}
 D(\mathbf{F}, \delta \mathbf{M}) &= \int_{\partial_N \Omega_{0h}} \delta \mathbf{M}^T \bar{\mathbf{J}} \, d\Omega_0 - \int_{\partial_D \Omega_{0h}} \bar{\mathbf{M}}_N^T (\mathbf{Z}_0(\mathbf{F}, \bar{\mathbf{M}}) \nabla_0 \delta \mathbf{M}) \, dS_0 \\
 &+ \int_{\partial_D \Omega_{0h}} \delta \mathbf{M}_N^T \left( \frac{\mathcal{B}}{h_s} \mathbf{Z}_0(\mathbf{F}, \bar{\mathbf{M}}) \right) \bar{\mathbf{M}}_N \, dS_0.
 \end{aligned} \tag{5.50}$$

### 5.3.2 The Finite element discretization of the coupled problem

In the computational model, a finite dimensional space of real valued piecewise polynomial functions is introduced such that

$$X^{k(+)} = \left\{ \begin{array}{l} (\mathbf{u}_h, f_{V_h}, f_{T_h}) \in [L^2(\Omega_{0h})]^d \times L^2(\Omega_{0h}) \times L^{2(+)}(\Omega_{0h}) \\ \text{such that } (\mathbf{u}_h, f_{V_h}, f_{T_h})|_{\Omega_0^e} \in [\mathbb{P}^k(\Omega_0^e)]^d \times \mathbb{P}^k(\Omega_0^e) \times \mathbb{P}^{k(+)}(\Omega_0^e) \forall \Omega_0^e \in \Omega_{0h} \end{array} \right\}, \tag{5.51}$$

where  $\mathbb{P}^k(\Omega_0^e)$  is the space of polynomial functions of order up to  $k$  and  $\mathbb{P}^{k^+}$  means that the polynomial approximation remains positive. The discretization of the system is carried out using the discontinuous Galerkin Finite element (DGFE) method. Accordingly, we introduce the shape functions for the trial functions  $\mathbf{u}$ ,  $f_V$ , and  $f_T$  and test functions  $\delta\mathbf{u}$ ,  $\delta f_V$ , and  $\delta f_T$  which are thus interpolated as

$$\mathbf{u}_h = N_{\mathbf{u}}^a \mathbf{u}^a, \quad f_{V_h} = N_{f_V}^a f_V^a, \quad f_{T_h} = N_{f_T}^a f_T^a, \quad (5.52)$$

where  $\mathbf{u}^a$ ,  $f_V^a$ , and  $f_T^a$  denote the nodal values of respectively  $\mathbf{u}_h$ ,  $f_{V_h}$ , and  $f_{T_h}$  at node  $a$ . Similarly, we have

$$\delta\mathbf{u}_h = N_{\mathbf{u}}^a \delta\mathbf{u}^a, \quad \delta f_{V_h} = N_{f_V}^a \delta f_V^a, \quad \delta f_{T_h} = N_{f_T}^a \delta f_T^a, \quad (5.53)$$

The gradients are computed by:

$$\nabla_0 \mathbf{u}_h = \nabla_0 N_{\mathbf{u}}^a \otimes \mathbf{u}^a, \quad \nabla_0 f_{V_h} = \nabla_0 N_{f_V}^a f_V^a, \quad \nabla_0 f_{T_h} = \nabla_0 N_{f_T}^a f_T^a, \quad (5.54)$$

where  $\nabla_0 N_{\mathbf{u}}^a$ ,  $\nabla_0 N_{f_V}^a$ , and  $\nabla_0 N_{f_T}^a$  are the gradients of the shape functions at node  $a$ . Similarly, we have

$$\nabla_0 \delta\mathbf{u}_h = \nabla_0 N_{\mathbf{u}}^a \otimes \delta\mathbf{u}^a, \quad \nabla_0 \delta f_{V_h} = \nabla_0 N_{f_V}^a \delta f_V^a, \quad \nabla_0 \delta f_{T_h} = \nabla_0 N_{f_T}^a \delta f_T^a. \quad (5.55)$$

A solution approximation  $\mathbf{M}_h = \begin{pmatrix} f_{V_h} \\ f_{T_h} \end{pmatrix}$ ,  $\mathbf{u}_h$  of respectively  $\mathbf{M}$ ,  $\mathbf{u}$ , is sought as the solution of the discrete coupled problem, is stated as finding  $\mathbf{u}_h, \mathbf{M}_h \in X^{k^+}$  such that

$$A(\mathbf{F}_h, \mathbf{M}_h, \delta\mathbf{u}_h) = B(\delta\mathbf{u}_h) \quad \forall \delta\mathbf{u}_h \in X^k, \text{ and} \quad (5.56)$$

$$C(\mathbf{F}_h, \mathbf{M}_h, \delta\mathbf{M}_h) = D(\mathbf{F}_h, \delta\mathbf{M}_h) - \int_{\Omega_{0h}} \delta\mathbf{M}_h^T \mathbf{I}_i d\Omega_0 \quad \forall \delta\mathbf{M}_h \in X^k. \quad (5.57)$$

### 5.3.3 The system resolution

The set of Eqs. (5.56, 5.57) can be rewritten under the form:

$$\mathbf{F}_{\text{ext}}^a(\mathbf{G}^b) = \mathbf{F}_{\text{int}}^a(\mathbf{G}^b) + \mathbf{F}_I^a(\mathbf{G}^b), \quad (5.58)$$

where  $\mathbf{G}^b$  is a  $5 \times 1$  vector of the unknown fields at node  $b$

$$\mathbf{G}^b = \begin{pmatrix} \mathbf{u}^b \\ f_V^b \\ f_T^b \end{pmatrix}, \text{ with } \mathbf{u}^b = \begin{pmatrix} u_x^b \\ u_y^b \\ u_z^b \end{pmatrix}. \quad (5.59)$$

The nonlinear Eqs. (5.58) are linearized by means of an implicit formulation and solved using the Newton Raphson scheme using an initial guess of the last solution. To this end, the forces are written in a residual form. The predictor at iteration 0, reads  $\mathbf{G}^c = \mathbf{G}^{c0}$ , and the residual at iteration  $i$  reads

$$\mathbf{F}_{\text{ext}}^a(\mathbf{G}^c) - \mathbf{F}_{\text{int}}^a(\mathbf{G}^c) - \mathbf{F}_I^a(\mathbf{G}^c) = \mathbf{R}^a(\mathbf{G}^{ci}), \quad (5.60)$$

and at iteration  $i$ , the first order Taylor development yields the system to be solved, i.e.

$$\left( \frac{\partial \mathbf{F}_{\text{ext}}^{\mathbf{a}}}{\partial \mathbf{G}^{\mathbf{b}}} - \frac{\partial \mathbf{F}_{\text{int}}^{\mathbf{a}}}{\partial \mathbf{G}^{\mathbf{b}}} - \frac{\partial \mathbf{F}_{\text{I}}^{\mathbf{a}}}{\partial \mathbf{G}^{\mathbf{b}}} \right) \Big|_{\mathbf{G}=\mathbf{G}^{\text{ci}}} \Delta \mathbf{G}^{\mathbf{b}} = -\mathbf{R}^{\mathbf{a}}(\mathbf{G}^{\text{ci}}). \quad (5.61)$$

Let us define the tangent matrix of the coupled Electro-Thermo-Mechanical system  $\mathbb{K}_{\mathbf{G}}^{\text{ab}} = \frac{\partial \mathbf{F}_{\text{ext}}^{\mathbf{a}}}{\partial \mathbf{G}^{\mathbf{b}}} - \frac{\partial \mathbf{F}_{\text{int}}^{\mathbf{a}}}{\partial \mathbf{G}^{\mathbf{b}}} - \frac{\partial \mathbf{F}_{\text{I}}^{\mathbf{a}}}{\partial \mathbf{G}^{\mathbf{b}}}$ , and  $\Delta \mathbf{G}^{\mathbf{b}} = (\mathbf{G}^{\mathbf{b}} - \mathbf{G}^{\text{bi}})$ , then we have

$$\begin{pmatrix} \mathbb{K}_{\mathbf{uu}} & \mathbb{K}_{\mathbf{uf}_V} & \mathbb{K}_{\mathbf{uf}_T} \\ \mathbb{K}_{\mathbf{f}_V \mathbf{u}} & \mathbb{K}_{\mathbf{f}_V \mathbf{f}_V} & \mathbb{K}_{\mathbf{f}_V \mathbf{f}_T} \\ \mathbb{K}_{\mathbf{f}_T \mathbf{u}} & \mathbb{K}_{\mathbf{f}_T \mathbf{f}_V} & \mathbb{K}_{\mathbf{f}_T \mathbf{f}_T} \end{pmatrix} \begin{pmatrix} \Delta \mathbf{u} \\ \Delta \mathbf{f}_V \\ \Delta \mathbf{f}_T \end{pmatrix} = - \begin{pmatrix} \mathbf{R}_{\mathbf{u}}(\mathbf{u}, \mathbf{f}_V, \mathbf{f}_T) \\ \mathbf{R}_{\mathbf{f}_V}(\mathbf{u}, \mathbf{f}_V, \mathbf{f}_T) \\ \mathbf{R}_{\mathbf{f}_T}(\mathbf{u}, \mathbf{f}_V, \mathbf{f}_T) \end{pmatrix}. \quad (5.62)$$

The new solution is given by  $\mathbf{G}^{\mathbf{i}+1} = \mathbf{G}^{\mathbf{i}} + \Delta \mathbf{G}$ , and the iterations continue until the convergence is obtained, that is until  $\|\mathbf{R}\| < \text{tol}$ .

The formula of the forces can be derived from Eqs. (5.56, 5.57), which leads at each node  $a$  to:

$$\mathbf{F}_{\mathbf{u}/\mathbf{f}_V/\mathbf{f}_T \text{ext}}^{\mathbf{a}} = \mathbf{F}_{\mathbf{u}/\mathbf{f}_V/\mathbf{f}_T \text{int}}^{\mathbf{a}} + \mathbf{F}_{\mathbf{u}/\mathbf{f}_V/\mathbf{f}_T \text{I}}^{\mathbf{a}}. \quad (5.63)$$

First the mechanical contribution reads

$$\begin{aligned} \mathbf{F}_{\mathbf{u} \text{ext}}^{\mathbf{a}} &= \sum_{\mathbf{s}} \int_{(\partial_{\mathbf{N}} \Omega_0)^{\mathbf{s}}} N_{\mathbf{u}}^{\mathbf{a}} \bar{\mathbf{T}} dS_0 - \sum_{\mathbf{s}} \int_{(\partial_{\mathbf{D}} \Omega_0)^{\mathbf{s}}} (\bar{\mathbf{u}} \otimes \mathbf{N} : \mathcal{H}) \cdot \nabla_0 N_{\mathbf{u}}^{\mathbf{a}} dS_0 \\ &+ \sum_{\mathbf{s}} \int_{(\partial_{\mathbf{D}} \Omega_0)^{\mathbf{s}}} \left( \bar{\mathbf{u}} \otimes \mathbf{N} : \frac{\mathcal{H}\mathcal{B}}{h_{\mathbf{s}}} \right) \cdot \mathbf{N} N_{\mathbf{u}}^{\mathbf{a}} dS_0 \\ &+ \int_{\partial_{\mathbf{D}} \Omega_{0\text{h}}} \left( -\frac{\alpha_{\text{th}} : \mathcal{H}}{f_{\text{T}}^2} \bar{f}_{\text{T}} + \frac{\alpha_{\text{th}} : \mathcal{H}}{f_{\text{T}_0}^2} f_{\text{T}_0} \right) \cdot \mathbf{N} N_{\mathbf{u}}^{\mathbf{a}} dS_0, \end{aligned} \quad (5.64)$$

$$\mathbf{F}_{\mathbf{u} \text{int}}^{\mathbf{a}} = \sum_{\mathbf{e}} \int_{\Omega_0^{\mathbf{e}}} \mathbf{P}(\mathbf{F}_{\text{h}}, \mathbf{f}_{V_{\text{h}}}, \mathbf{f}_{T_{\text{h}}}) \cdot \nabla_0 N_{\mathbf{u}}^{\mathbf{a}} d\Omega_0, \text{ and} \quad (5.65)$$

$$\mathbf{F}_{\mathbf{u} \text{I}}^{\mathbf{a}\pm} = \mathbf{F}_{\mathbf{u} \text{I}1}^{\mathbf{a}\pm} + \mathbf{F}_{\mathbf{u} \text{I}2}^{\mathbf{a}\pm} + \mathbf{F}_{\mathbf{u} \text{I}3}^{\mathbf{a}\pm}, \quad (5.66)$$

with the three mechanical contributions to the interface forces <sup>2</sup>

$$\mathbf{F}_{\mathbf{u} \text{I}1}^{\mathbf{a}\pm} = \sum_{\mathbf{s}} \int_{(\partial_{\text{T}} \Omega_0)^{\mathbf{s}}} (\pm N_{\mathbf{u}}^{\mathbf{a}\pm}) \langle \mathbf{P}(\mathbf{F}_{\text{h}}, \mathbf{f}_{V_{\text{h}}}, \mathbf{f}_{T_{\text{h}}}) \rangle \cdot \mathbf{N}^- dS_0, \quad (5.67)$$

$$\mathbf{F}_{\mathbf{u} \text{I}2}^{\mathbf{a}\pm} = \frac{1}{2} \sum_{\mathbf{s}} \int_{(\partial_{\text{T}} \Omega_0)^{\mathbf{s}}} [\mathbf{u}_{\text{h}}] \otimes \mathbf{N}^- : \mathcal{H}^{\pm} \cdot \nabla_0 N_{\mathbf{u}}^{\mathbf{a}\pm} dS_0, \quad (5.68)$$

$$\mathbf{F}_{\mathbf{u} \text{I}3}^{\mathbf{a}\pm} = \sum_{\mathbf{s}} \int_{(\partial_{\text{T}} \Omega_0)^{\mathbf{s}}} ([\mathbf{u}_{\text{h}}] \otimes \mathbf{N}^-) : \left\langle \frac{\mathcal{H}\mathcal{B}}{h_{\mathbf{s}}} \right\rangle \cdot \mathbf{N}^- (\pm N_{\mathbf{u}}^{\mathbf{a}\pm}) dS_0. \quad (5.69)$$

<sup>2</sup>The contributions on  $\partial_{\mathbf{D}} \Omega_{0\text{h}}$  can be directly deduced by removing the factor  $(1/2)$  accordingly to the definition of the average flux on the Dirichlet boundary and by using  $\mathbf{L}_1(\mathbf{F}_{\text{h}}, \bar{f}_{\text{T}})$ ,  $\mathbf{L}_2(\mathbf{F}_{\text{h}}, \bar{f}_V, \bar{f}_{\text{T}})$ , and  $\mathbf{J}_{y_1}(\mathbf{F}_{\text{h}}, \bar{f}_V, \bar{f}_{\text{T}})$  instead of  $\mathbf{L}_1(\mathbf{F}_{\text{h}}, \mathbf{f}_{T_{\text{h}}})$ ,  $\mathbf{L}_2(\mathbf{F}_{\text{h}}, \mathbf{f}_{V_{\text{h}}}, \mathbf{f}_{T_{\text{h}}})$ , and  $\mathbf{J}_{y_1}(\mathbf{F}_{\text{h}}, \mathbf{f}_{V_{\text{h}}}, \mathbf{f}_{T_{\text{h}}})$ . However, there is one more additional term in  $\mathbf{F}_{\mathbf{u} \text{I}1}^{\mathbf{a}\pm}$  in the Dirichlet boundary, which is  $\sum_{\mathbf{s}} \int_{(\partial_{\mathbf{D}} \Omega_0)^{\mathbf{s}}} (N_{\mathbf{u}}^{\mathbf{a}}) \left( -\frac{\alpha_{\text{th}} : \mathcal{H}}{f_{\text{T}}^2} f_{\text{T}} + \frac{\alpha_{\text{th}} : \mathcal{H}}{f_{\text{T}_0}^2} f_{\text{T}_0} \right) \cdot \mathbf{N}^- dS_0$ .

Secondly, the electrical contributions read

$$\begin{aligned}
\mathbf{F}_{\text{fVext}}^{\text{a}} &= \sum_{\text{s}} \int_{(\partial_{\text{N}}\Omega_0)^{\text{s}}} \mathbf{N}_{\text{fV}}^{\text{a}} \bar{\mathbf{J}}_{\text{e}} \text{dS}_0 - \sum_{\text{s}} \int_{(\partial_{\text{D}}\Omega_0)^{\text{s}}} \bar{\mathbf{f}}_{\text{V}} \mathbf{N} \cdot \mathbf{L}_1(\mathbf{F}_{\text{h}}, \bar{\mathbf{f}}_{\text{T}}) \cdot \nabla_0 \mathbf{N}_{\text{fV}}^{\text{a}} \text{dS}_0 \\
&- \sum_{\text{s}} \int_{(\partial_{\text{D}}\Omega_0)^{\text{s}}} \bar{\mathbf{f}}_{\text{T}} \mathbf{N} \cdot \mathbf{L}_2(\mathbf{F}_{\text{h}}, \bar{\mathbf{f}}_{\text{V}}, \bar{\mathbf{f}}_{\text{T}}) \cdot \nabla_0 \mathbf{N}_{\text{fV}}^{\text{a}\pm} \text{dS}_0 \\
&+ \sum_{\text{s}} \int_{(\partial_{\text{D}}\Omega_0)^{\text{s}}} \bar{\mathbf{f}}_{\text{V}} \mathbf{N} \cdot \mathbf{L}_1(\mathbf{F}_{\text{h}}, \bar{\mathbf{f}}_{\text{T}}) \frac{\mathcal{B}}{h_{\text{s}}} \cdot \mathbf{N} \mathbf{N}_{\text{fV}}^{\text{a}} \text{dS}_0 \\
&+ \sum_{\text{s}} \int_{(\partial_{\text{D}}\Omega_0)^{\text{s}}} \bar{\mathbf{f}}_{\text{T}} \mathbf{N} \cdot \mathbf{L}_2(\mathbf{F}_{\text{h}}, \bar{\mathbf{f}}_{\text{V}}, \bar{\mathbf{f}}_{\text{T}}) \frac{\mathcal{B}}{h_{\text{s}}} \cdot \mathbf{N} \mathbf{N}_{\text{fV}}^{\text{a}} \text{dS}_0,
\end{aligned} \tag{5.70}$$

$$\mathbf{F}_{\text{fVint}}^{\text{a}} = \sum_{\text{e}} \int_{\Omega_0^{\text{e}}} \mathbf{J}_{\text{e}}(\mathbf{F}_{\text{h}}, f_{\text{Vh}}, f_{\text{Th}}) \cdot \nabla_0 \mathbf{N}_{\text{fV}}^{\text{a}} \text{d}\Omega_0, \text{ and} \tag{5.71}$$

$$\mathbf{F}_{\text{fV1}}^{\text{a}\pm} = \mathbf{F}_{\text{fV11}}^{\text{a}\pm} + \mathbf{F}_{\text{fV12}}^{\text{a}\pm} + \mathbf{F}_{\text{fV13}}^{\text{a}\pm}, \tag{5.72}$$

with the three electric contributions to the interface forces

$$\mathbf{F}_{\text{fV11}}^{\text{a}\pm} = \sum_{\text{s}} \int_{(\partial_{\text{T}}\Omega_0)^{\text{s}}} (\pm \mathbf{N}_{\text{fV}}^{\text{a}\pm}) \langle \mathbf{J}_{\text{e}}(\mathbf{F}_{\text{h}}, f_{\text{Vh}}, f_{\text{Th}}) \rangle \cdot \mathbf{N}^- \text{dS}_0, \tag{5.73}$$

$$\begin{aligned}
\mathbf{F}_{\text{fV12}}^{\text{a}\pm} &= \frac{1}{2} \sum_{\text{s}} \int_{(\partial_{\text{T}}\Omega_0)^{\text{s}}} \llbracket f_{\text{Vh}} \rrbracket \left( \mathbf{L}_1^{\pm}(\mathbf{F}_{\text{h}}, f_{\text{Th}}) \cdot \nabla_0 \mathbf{N}_{\text{fV}}^{\text{a}\pm} \right) \cdot \mathbf{N}^- \text{dS}_0 \\
&+ \frac{1}{2} \sum_{\text{s}} \int_{(\partial_{\text{T}}\Omega_0)^{\text{s}}} \llbracket f_{\text{Th}} \rrbracket \left( \mathbf{L}_2^{\pm}(\mathbf{F}_{\text{h}}, f_{\text{Vh}}, f_{\text{Th}}) \cdot \nabla_0 \mathbf{N}_{\text{fV}}^{\text{a}\pm} \right) \cdot \mathbf{N}^- \text{dS}_0,
\end{aligned} \tag{5.74}$$

$$\begin{aligned}
\mathbf{F}_{\text{fV13}}^{\text{a}\pm} &= \sum_{\text{s}} \int_{(\partial_{\text{T}}\Omega_0)^{\text{s}}} \llbracket f_{\text{Vh}} \rrbracket \mathbf{N}^- \cdot \left\langle \mathbf{L}_1(\mathbf{F}_{\text{h}}, f_{\text{Th}}) \frac{\mathcal{B}}{h_{\text{s}}} \right\rangle \cdot \mathbf{N}^- (\pm \mathbf{N}_{\text{fV}}^{\text{a}\pm}) \text{dS}_0 \\
&+ \sum_{\text{s}} \int_{(\partial_{\text{T}}\Omega_0)^{\text{s}}} \llbracket f_{\text{Th}} \rrbracket \mathbf{N}^- \cdot \left\langle \mathbf{L}_2(\mathbf{F}_{\text{h}}, f_{\text{Vh}}, f_{\text{Th}}) \frac{\mathcal{B}}{h_{\text{s}}} \right\rangle \cdot \mathbf{N}^- (\pm \mathbf{N}_{\text{fV}}^{\text{a}\pm}) \text{dS}_0.
\end{aligned} \tag{5.75}$$

Similarly, the thermal contributions read

$$\begin{aligned}
\mathbf{F}_{\text{fTtext}}^{\text{a}} &= \sum_{\text{s}} \int_{(\partial_{\text{N}}\Omega_0)^{\text{s}}} \mathbf{N}^{\text{a}} \bar{\mathbf{J}}_{\text{y}} \text{dS}_0 - \sum_{\text{s}} \int_{(\partial_{\text{D}}\Omega_0)^{\text{s}}} \bar{\mathbf{f}}_{\text{T}} \mathbf{N} \cdot \mathbf{J}_{\text{y1}}(\mathbf{F}_{\text{h}}, \bar{\mathbf{f}}_{\text{V}}, \bar{\mathbf{f}}_{\text{T}}) \cdot \nabla_0 \mathbf{N}_{\text{fT}}^{\text{a}} \text{dS}_0 \\
&- \sum_{\text{s}} \int_{(\partial_{\text{D}}\Omega_0)^{\text{s}}} \bar{\mathbf{f}}_{\text{V}} \mathbf{N} \cdot \mathbf{L}_2(\mathbf{F}_{\text{h}}, \bar{\mathbf{f}}_{\text{V}}, \bar{\mathbf{f}}_{\text{T}}) \cdot \nabla_0 \mathbf{N}_{\text{fT}}^{\text{a}} \text{dS}_0 \\
&+ \sum_{\text{s}} \int_{(\partial_{\text{D}}\Omega_0)^{\text{s}}} \bar{\mathbf{f}}_{\text{T}} \mathbf{N} \cdot \mathbf{J}_{\text{y1}}(\mathbf{F}_{\text{h}}, \bar{\mathbf{f}}_{\text{V}}, \bar{\mathbf{f}}_{\text{T}}) \frac{\mathcal{B}}{h_{\text{s}}} \cdot \mathbf{N} \mathbf{N}_{\text{fT}}^{\text{a}} \text{dS}_0 \\
&+ \sum_{\text{s}} \int_{(\partial_{\text{D}}\Omega_0)^{\text{s}}} \bar{\mathbf{f}}_{\text{V}} \mathbf{N} \cdot \mathbf{L}_2(\mathbf{F}_{\text{h}}, \bar{\mathbf{f}}_{\text{V}}, \bar{\mathbf{f}}_{\text{T}}) \frac{\mathcal{B}}{h_{\text{s}}} \cdot \mathbf{N} \mathbf{N}_{\text{fT}}^{\text{a}} \text{dS}_0,
\end{aligned} \tag{5.76}$$

$$\begin{aligned}
\mathbf{F}_{\text{fTint}} &= \sum_{\text{e}} \int_{\Omega_0^{\text{e}}} \mathbf{J}_{\text{y}}(\mathbf{F}_{\text{h}}, f_{\text{Vh}}, f_{\text{Th}}) \cdot \nabla_0 \mathbf{N}_{\text{fT}}^{\text{a}} \text{d}\Omega_0 - \sum_{\text{e}} \int_{\Omega_0^{\text{e}}} \rho_0 \partial_{\text{t}} \mathbf{y} \mathbf{N}_{\text{fT}}^{\text{a}} \text{d}\Omega_0 \\
&+ \sum_{\text{e}} \int_{\Omega_0^{\text{e}}} \bar{\mathbf{F}} \mathbf{N}_{\text{fT}}^{\text{a}} \text{d}\Omega_0,
\end{aligned} \tag{5.77}$$

and

$$\mathbf{F}_{f_{\text{Tl}}}^{\text{a}\pm} = \mathbf{F}_{f_{\text{Tl1}}}^{\text{a}\pm} + \mathbf{F}_{f_{\text{Tl2}}}^{\text{a}\pm} + \mathbf{F}_{f_{\text{Tl3}}}^{\text{a}\pm}, \quad (5.78)$$

where the three thermal contributions to the interface forces read

$$\mathbf{F}_{f_{\text{Tl1}}}^{\text{a}\pm} = \sum_{\text{s}} \int_{(\partial_{\text{T}}\Omega_0)^{\text{s}}} (\pm N_{f_{\text{T}}}^{\text{a}\pm}) \langle \mathbf{J}_{\text{y}}(\mathbf{F}_{\text{h}}, f_{\text{V}_{\text{h}}}, f_{\text{T}_{\text{h}}}) \rangle \cdot \mathbf{N}^- \text{dS}_0, \quad (5.79)$$

$$\begin{aligned} \mathbf{F}_{f_{\text{Tl2}}}^{\text{a}\pm} &= \frac{1}{2} \sum_{\text{s}} \int_{(\partial_{\text{T}}\Omega_0)^{\text{s}}} \llbracket f_{\text{T}_{\text{h}}} \rrbracket \left( \mathbf{J}_{\text{y}_1}^{\pm}(\mathbf{F}_{\text{h}}, f_{\text{V}_{\text{h}}}, f_{\text{T}_{\text{h}}}) \cdot \nabla_0 N_{f_{\text{T}}}^{\text{a}\pm} \right) \cdot \mathbf{N}^- \text{dS}_0 \\ &+ \frac{1}{2} \sum_{\text{s}} \int_{(\partial_{\text{T}}\Omega_0)^{\text{s}}} \llbracket f_{\text{V}_{\text{h}}} \rrbracket \left( \mathbf{L}_2^{\pm}(\mathbf{F}_{\text{h}}, f_{\text{V}_{\text{h}}}, f_{\text{T}_{\text{h}}}) \cdot \nabla_0 N_{f_{\text{T}}}^{\text{a}\pm} \right) \cdot \mathbf{N}^- \text{dS}_0, \end{aligned} \quad (5.80)$$

$$\begin{aligned} \mathbf{F}_{f_{\text{Tl3}}}^{\text{a}\pm} &= \sum_{\text{s}} \int_{(\partial_{\text{T}}\Omega_0)^{\text{s}}} \llbracket f_{\text{T}_{\text{h}}} \rrbracket \mathbf{N}^- \cdot \left\langle \mathbf{J}_{\text{y}_1}(\mathbf{F}_{\text{h}}, f_{\text{V}_{\text{h}}}, f_{\text{T}_{\text{h}}}) \frac{\mathcal{B}}{h_{\text{s}}} \right\rangle \cdot \mathbf{N}^- (\pm N_{f_{\text{T}}}^{\text{a}\pm}) \text{dS}_0 \\ &+ \sum_{\text{s}} \int_{(\partial_{\text{T}}\Omega_0)^{\text{s}}} \llbracket f_{\text{V}_{\text{h}}} \rrbracket \mathbf{N}^- \cdot \left\langle \mathbf{L}_2(\mathbf{F}_{\text{h}}, f_{\text{V}_{\text{h}}}, f_{\text{T}_{\text{h}}}) \frac{\mathcal{B}}{h_{\text{s}}} \right\rangle \cdot \mathbf{N}^- (\pm N_{f_{\text{T}}}^{\text{a}\pm}) \text{dS}_0. \end{aligned} \quad (5.81)$$

The stiffness matrix has been decomposed into nine sub-matrices as shown in Eq. (5.62) with respect to the discretization of the five independent field variables (3 for displacement  $\mathbf{u}$ ,  $f_{\text{V}}$ , and  $f_{\text{T}}$ ). The stiffness derivation is detailed in Appendix D.1.

## 5.4 Numerical properties in a small deformation setting

The demonstration of the numerical properties for Electro-Thermo-Mechanical coupled problems is derived in the same spirit as in Chapter 4, under the assumption  $d = 2$ , under the assumptions of temperature independent material properties, (however  $\mathbf{J}_{\text{y}}$ ,  $\mathbf{L}_1$ ,  $\mathbf{L}_2$  remain temperature and electric potential dependent but  $\mathcal{C}$  (the matrix form of the material constant tensor  $\mathcal{H}$ ),  $\alpha_{\text{th}}$  are temperature and electric potential in-dependent), and in the absence of the heat source, such that the term  $\bar{F}$  in Eq. (5.23) is equal to zero. We also require a framework in small deformation and linear elasticity in order to demonstrate the stability and convergence rates.

Let us consider the vector of the unknown fields  $\mathbf{G}$  defined as in Eq. (5.59). In addition, by recalling Eqs. (3.1, 4.39, and 4.45), we can introduce the matrix  $\mathbf{w}$  of size  $(5d - 3) \times 1$  as  $\mathbf{w}(\mathbf{G}, \nabla \mathbf{G}) = \mathbf{v}(\mathbf{G}) \nabla \mathbf{G}$ , with  $\mathbf{v}$  the coefficient matrix of size  $(5d - 3) \times (5d - 3)$

such that  $\mathbf{v} = \begin{pmatrix} \mathcal{C} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{l}_1 & \mathbf{l}_2 \\ \mathbf{0} & \mathbf{l}_2 & \mathbf{j}_{\text{y}_1} \end{pmatrix}$ , where  $\mathcal{C}$  is the constant material tensor corresponding to  $\mathcal{H}$  written using Voigt's notations. By the use of Eq. (4.30),  $\mathbf{v}$  can also be written as

$\mathbf{v} = \begin{pmatrix} \mathcal{C} & \mathbf{0} \\ \mathbf{0} & \mathbf{Z} \end{pmatrix}$ . Moreover, we define the matrices  $\mathbf{o} = \begin{pmatrix} \mathbf{0} & \mathbf{0} & \frac{-\mathcal{C}}{f_{\text{T}}^2} \alpha_{\text{thc}} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \end{pmatrix}$  and

$\mathbf{o}_0 = \begin{pmatrix} \mathbf{0} & \mathbf{0} & \frac{-\mathcal{C}}{f_{\text{T}_0}^2} \alpha_{\text{thc}} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \end{pmatrix}$  of size  $(5d - 3) \times (d + 2)$ ,  $\alpha_{\text{thc}}$  is a vector of size  $(3d - 3) \times 1$  with

$\boldsymbol{\alpha}_{\text{thc}}^T = (\alpha_{\text{th}} \alpha_{\text{th}} \alpha_{\text{th}} 0 0 0)$ , and  $\mathbf{C}\boldsymbol{\alpha}_{\text{thc}}$  a vector of size  $(3d - 3) \times 1$  and given for  $d = 3$  by  $(\mathbf{C}\boldsymbol{\alpha}_{\text{thc}})^T = (3K\alpha_{\text{th}} 3K\alpha_{\text{th}} 3K\alpha_{\text{th}} 0 0 0)$  for isotropic materials. Finally we define  $\mathbf{h}$  a matrix of size  $(d + 2) \times (d + 2)$  with  $\mathbf{h} = \begin{pmatrix} \mathbf{0} & \mathbf{0} & \mathbf{0} \\ 0 & 0 & 0 \\ 0 & 0 & \rho c_v \end{pmatrix}$ . In these relations  $\nabla \mathbf{G}$  is a  $(5d - 3) \times 1$  vector of the gradient of the unknown fields, which is defined as  $\nabla \mathbf{G} = (\nabla) \mathbf{G}$  and is written for  $d = 3$  using Voigt's rules for the mechanical contribution as

$$(\nabla \mathbf{G}) = \begin{pmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \varepsilon_{zz} \\ 2\varepsilon_{xy} \\ 2\varepsilon_{xz} \\ 2\varepsilon_{yz} \\ \frac{\partial f_V}{\partial x} \\ \frac{\partial f_V}{\partial y} \\ \frac{\partial f_V}{\partial z} \\ \frac{\partial f_T}{\partial x} \\ \frac{\partial f_T}{\partial y} \\ \frac{\partial f_T}{\partial z} \end{pmatrix} = \begin{pmatrix} \frac{\partial}{\partial x} & 0 & 0 & 0 & 0 \\ 0 & \frac{\partial}{\partial y} & 0 & 0 & 0 \\ 0 & 0 & \frac{\partial}{\partial z} & 0 & 0 \\ \frac{\partial}{\partial y} & \frac{\partial}{\partial x} & 0 & 0 & 0 \\ \frac{\partial}{\partial z} & 0 & \frac{\partial}{\partial x} & 0 & 0 \\ 0 & \frac{\partial}{\partial z} & \frac{\partial}{\partial y} & 0 & 0 \\ 0 & 0 & 0 & \frac{\partial}{\partial x} & 0 \\ 0 & 0 & 0 & \frac{\partial}{\partial y} & 0 \\ 0 & 0 & 0 & \frac{\partial}{\partial z} & 0 \\ 0 & 0 & 0 & 0 & \frac{\partial}{\partial x} \\ 0 & 0 & 0 & 0 & \frac{\partial}{\partial y} \\ 0 & 0 & 0 & 0 & \frac{\partial}{\partial z} \end{pmatrix} \begin{pmatrix} u_x \\ u_y \\ u_z \\ f_V \\ f_T \end{pmatrix}. \quad (5.82)$$

From these definitions and using Voigt's notation, the energy conjugated stress for small deformation can be written under the form

$$\begin{pmatrix} \boldsymbol{\sigma}_{xx} \\ \boldsymbol{\sigma}_{yy} \\ \boldsymbol{\sigma}_{zz} \\ \boldsymbol{\tau}_{xy} \\ \boldsymbol{\tau}_{xz} \\ \boldsymbol{\tau}_{yz} \\ \mathbf{j}_{e_x} \\ \mathbf{j}_{e_y} \\ \mathbf{j}_{e_z} \\ \mathbf{j}_{y_x} \\ \mathbf{j}_{y_y} \\ \mathbf{j}_{y_z} \end{pmatrix} = \mathbf{v}(\mathbf{G}) \nabla \mathbf{G} + \boldsymbol{\alpha}(\mathbf{G}) \mathbf{G} - \mathbf{o}_0 \mathbf{G}_0. \quad (5.83)$$

Therefore, the boundary value problem for Electro-Thermo-Elasticity coupled Eqs. (5.21-5.25) is written under small deformation assumption under the form

$$-\nabla^T [\mathbf{w}(\mathbf{G}, \nabla \mathbf{G}) + \boldsymbol{\alpha}(\mathbf{G}) \mathbf{G} - \mathbf{o}_0 \mathbf{G}_0] = \mathbf{h} \dot{\mathbf{G}} \quad \text{in } \Omega, \quad (5.84)$$

with

$$\mathbf{G} = \bar{\mathbf{G}} \quad \forall \mathbf{x} \in \partial_D \Omega, \quad (5.85)$$

$$\bar{\mathbf{n}}^T (\mathbf{w} + \boldsymbol{\alpha} \mathbf{G} - \mathbf{o}_0 \mathbf{G}_0) = \bar{\mathbf{w}} \quad \forall \mathbf{x} \in \partial_N \Omega, \quad (5.86)$$



where for  $d = 3$   $\bar{\mathbf{n}} =$  
$$\begin{pmatrix} n_x & 0 & 0 & 0 & 0 \\ 0 & n_y & 0 & 0 & 0 \\ 0 & 0 & n_z & 0 & 0 \\ n_y & n_x & 0 & 0 & 0 \\ n_z & 0 & n_x & 0 & 0 \\ 0 & n_z & n_y & 0 & 0 \\ 0 & 0 & 0 & n_x & 0 \\ 0 & 0 & 0 & n_y & 0 \\ 0 & 0 & 0 & n_z & 0 \\ 0 & 0 & 0 & 0 & n_x \\ 0 & 0 & 0 & 0 & n_y \\ 0 & 0 & 0 & 0 & n_z \end{pmatrix}, \mathbf{G}_0$$
 is a vector of the initial values  $\mathbf{G}_0 =$  
$$\begin{pmatrix} u_{x_0} \\ u_{y_0} \\ u_{z_0} \\ f_{V_0} \\ f_{T_0} \end{pmatrix},$$

$\bar{\mathbf{G}}$  gathers the constrained fields  $\bar{\mathbf{u}}$ ,  $\bar{f}_V$ ,  $\bar{f}_T$  and  $\bar{\mathbf{w}}$  gathers the constrained fluxes  $\bar{\mathbf{t}}$ ,  $\bar{j}_y$ , and  $\bar{j}_e$ .

For the following analysis we will consider a steady state, such that the time derivative term is neglected,  $\mathbf{h}\mathbf{G} = 0$ , then Eq. (5.84) becomes

$$-\nabla^T(\mathbf{w}(\mathbf{G}, \nabla\mathbf{G})) - \nabla^T(\mathbf{o}(\mathbf{G})\mathbf{G}) = 0 \quad \text{in } \Omega. \quad (5.87)$$

It can be noticed that the gradient of  $(\mathbf{o}(\mathbf{G})\mathbf{G})$  consists of zero components and of the gradient of  $(-\frac{\alpha_{th}\mathcal{H}}{f_T^2}f_T)$ , such that  $\nabla(-\frac{\alpha_{th}\mathcal{H}}{f_T^2}f_T) = \frac{\alpha_{th}\mathcal{H}}{f_T^2}\nabla f_T$ . Henceforth the matrix  $\mathbf{o}(\mathbf{G})$  can be rearranged in a new form  $\tilde{\mathbf{o}}(\mathbf{G})$  of size  $(d+2) \times (5d-3)$ , such that  $-\nabla^T(\mathbf{o}(\mathbf{G})\mathbf{G})$  can be replaced by  $\tilde{\mathbf{o}}(\mathbf{G})\nabla\mathbf{G}$ , with

$$\tilde{\mathbf{o}}(\mathbf{G})\nabla\mathbf{G} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{3K\alpha_{th}}{f_T^2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{3K\alpha_{th}}{f_T^2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{3K\alpha_{th}}{f_T^2} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \varepsilon_{zz} \\ 2\varepsilon_{xy} \\ 2\varepsilon_{xz} \\ 2\varepsilon_{yz} \\ \frac{\partial f_V}{\partial f_T} \\ \frac{\partial x}{\partial f_T} \\ \frac{\partial y}{\partial f_T} \\ \frac{\partial f_V}{\partial z} \\ \frac{\partial x}{\partial f_T} \\ \frac{\partial y}{\partial f_T} \\ \frac{\partial f_T}{\partial z} \end{pmatrix}. \quad (5.88)$$

The operator  $\tilde{\mathbf{o}}$  can be seen as the transpose operator which accounts for the definition of the  $\nabla$  operator.

Therefore Eq. (5.87) becomes

$$-\nabla^T(\mathbf{w}(\mathbf{G}, \nabla\mathbf{G})) + \tilde{\mathbf{o}}(\mathbf{G})\nabla\mathbf{G} = 0 \quad \text{in } \Omega. \quad (5.89)$$

By comparing this formulation for Electro-Thermo-Elasticity with the formulation of Thermo-Elasticity in Chapter 3, it can be seen that the two formulations Eq. (3.6) and Eq. (5.89) are similar, however, it is nonlinear in this Chapter, while in Chapter 3 it is linear. The weak form can be derived straightforwardly in a similar way as for Eqs. (5.33, 5.37, 5.41) under the matrices form defined in Eq. (5.89), with the assumptions  $\mathbf{h}\bar{\mathbf{G}} = 0$  and  $\bar{\mathbf{w}}$  independent of  $\mathbf{G}$ .

The associated DG form for the Electro-Thermo-Elasticity problem is now defined as finding  $\mathbf{G} \in X^+$  such that

$$\mathbf{a}(\mathbf{G}, \delta\mathbf{G}) = \mathbf{b}(\delta\mathbf{G}), \quad \forall \delta\mathbf{G} \in X, \quad (5.90)$$

with

$$\begin{aligned} \mathbf{a}(\mathbf{G}, \delta\mathbf{G}) &= \int_{\Omega_h} (\nabla\delta\mathbf{G})^T \mathbf{w}(\mathbf{G}, \nabla\mathbf{G}) d\Omega + \int_{\Omega_h} \delta\mathbf{G}^T \bar{\mathbf{o}}(\mathbf{G}) \nabla\mathbf{G} d\Omega \\ &+ \int_{\partial_T\Omega_h \cup \partial_D\Omega_h} \llbracket \delta\mathbf{G}_n^T \rrbracket \langle \mathbf{w}(\mathbf{G}, \nabla\mathbf{G}) \rangle dS + \int_{\partial_T\Omega_h} \llbracket \mathbf{G}_n^T \rrbracket \langle \mathbf{v}(\mathbf{G}) \nabla\delta\mathbf{G} \rangle dS \\ &+ \int_{\partial_D\Omega_h} \llbracket \mathbf{G}_n^T \rrbracket \langle \mathbf{v}(\bar{\mathbf{G}}) \nabla\delta\mathbf{G} \rangle dS + \int_{\partial_T\Omega_h} \llbracket \mathbf{G}_n^T \rrbracket \left\langle \frac{\mathbf{v}(\mathbf{G})\mathcal{B}}{h_s} \right\rangle \llbracket \delta\mathbf{G}_n \rrbracket dS \\ &+ \int_{\partial_D\Omega_h} \llbracket \mathbf{G}_n^T \rrbracket \left\langle \frac{\mathbf{v}(\bar{\mathbf{G}})\mathcal{B}}{h_s} \right\rangle \llbracket \delta\mathbf{G}_n \rrbracket dS - \int_{\partial_T\Omega_h \cup \partial_D\Omega_h} \langle \delta\mathbf{G}_n^T \rangle \llbracket \mathbf{o}(\mathbf{G})\mathbf{G} - \mathbf{o}_0\mathbf{G}_0 \rrbracket dS \\ &+ \int_{\partial_N\Omega_h} \delta\mathbf{G}^T \bar{\mathbf{n}}^T (\mathbf{o}(\mathbf{G})\mathbf{G} - \mathbf{o}_0\mathbf{G}_0) dS, \end{aligned} \quad (5.91)$$

and

$$\begin{aligned} \mathbf{b}(\delta\mathbf{G}) &= \int_{\partial_N\Omega_h} \delta\mathbf{G}^T \bar{\mathbf{w}} dS - \int_{\partial_D\Omega_h} \bar{\mathbf{G}}_n^T \mathbf{v}(\bar{\mathbf{G}}) \nabla\delta\mathbf{G} dS \\ &+ \int_{\partial_D\Omega_h} \delta\mathbf{G}_n^T \frac{\mathbf{v}(\bar{\mathbf{G}})\mathcal{B}}{h_s} \bar{\mathbf{G}}_n dS + \int_{\partial_D\Omega_h} \delta\mathbf{G}_n^T (\mathbf{o}(\bar{\mathbf{G}})\bar{\mathbf{G}} - \mathbf{o}_0\mathbf{G}_0) dS, \end{aligned} \quad (5.92)$$

where  $\mathbf{G}_n$  is a  $12 \times 1$  vector, which is defined as

$$\mathbf{G}_n = \begin{pmatrix} u_x n_x \\ u_y n_y^- \\ u_z n_z^- \\ u_x n_y^- + u_y n_x^- \\ u_x n_z^- + u_z n_x^- \\ u_z n_y^- + u_y n_z^- \\ f_V n_x^- \\ f_V n_y^- \\ f_V n_z^- \\ f_T n_x^- \\ f_T n_y^- \\ f_T n_z^- \end{pmatrix} = \begin{pmatrix} n_x^- & 0 & 0 & 0 & 0 \\ 0 & n_y^- & 0 & 0 & 0 \\ 0 & 0 & n_z^- & 0 & 0 \\ n_y^- & n_x^- & 0 & 0 & 0 \\ n_z^- & 0 & n_x^- & 0 & 0 \\ 0 & n_z^- & n_y^- & 0 & 0 \\ 0 & 0 & 0 & n_x^- & 0 \\ 0 & 0 & 0 & n_y^- & 0 \\ 0 & 0 & 0 & n_z^- & 0 \\ 0 & 0 & 0 & 0 & n_x^- \\ 0 & 0 & 0 & 0 & n_y^- \\ 0 & 0 & 0 & 0 & n_z^- \end{pmatrix} \begin{pmatrix} u_x \\ u_y \\ u_z \\ f_V \\ f_T \end{pmatrix}. \quad (5.93)$$

Note that, using the identity  $\llbracket ab \rrbracket = \llbracket a \rrbracket \langle b \rangle + \langle a \rangle \llbracket b \rrbracket$  on  $\partial_1 \Omega_h$ , we have

$$\begin{aligned}
& \int_{\Omega_h} \delta \mathbf{G}^T \tilde{\mathbf{o}}(\mathbf{G}) \nabla \mathbf{G} d\Omega = - \int_{\Omega_h} \delta \mathbf{G}^T \nabla^T (\mathbf{o}(\mathbf{G}) \mathbf{G} - \mathbf{o}_0 \mathbf{G}_0) d\Omega \\
& = \sum_e \int_{\Omega^e} (\nabla \delta \mathbf{G})^T (\mathbf{o}(\mathbf{G}) \mathbf{G} - \mathbf{o}_0 \mathbf{G}_0) d\Omega - \sum_e \int_{\partial \Omega^e} \delta \mathbf{G}_n^T (\mathbf{o}(\mathbf{G}) \mathbf{G} - \mathbf{o}_0 \mathbf{G}_0) dS \\
& = \int_{\Omega_h} (\nabla \delta \mathbf{G})^T (\mathbf{o}(\mathbf{G}) \mathbf{G} - \mathbf{o}_0 \mathbf{G}_0) d\Omega - \int_{\partial_N \Omega_h} \delta \mathbf{G}_n^T \bar{\mathbf{n}}^T (\mathbf{o}(\mathbf{G}) \mathbf{G} - \mathbf{o}_0 \mathbf{G}_0) dS \\
& \quad - \int_{\partial_D \Omega_h} \delta \mathbf{G}_n^T (\mathbf{o}(\mathbf{G}) \mathbf{G} - \mathbf{o}_0 \mathbf{G}_0) dS + \int_{\partial_1 \Omega_h} \llbracket \delta \mathbf{G}_n^T \rrbracket \langle (\mathbf{o}(\mathbf{G}) \mathbf{G} - \mathbf{o}_0 \mathbf{G}_0) \rangle dS \\
& \quad + \int_{\partial_1 \Omega_h} \langle \delta \mathbf{G}_n^T \rangle \llbracket \mathbf{o}(\mathbf{G}) \mathbf{G} - \mathbf{o}_0 \mathbf{G}_0 \rrbracket dS.
\end{aligned} \tag{5.94}$$

Therefore, Eq. (5.90) can be rewritten as

$$a'(\mathbf{G}, \delta \mathbf{G}) = b'(\delta \mathbf{G}), \quad \forall \delta \mathbf{G} \in X, \tag{5.95}$$

with

$$\begin{aligned}
a'(\mathbf{G}, \delta \mathbf{G}) & = \int_{\Omega_h} (\nabla \delta \mathbf{G})^T \mathbf{w}(\mathbf{G}, \nabla \mathbf{G}) d\Omega + \int_{\Omega_h} (\nabla \delta \mathbf{G})^T (\mathbf{o}(\mathbf{G}) \mathbf{G} - \mathbf{o}_0 \mathbf{G}_0) d\Omega \\
& \quad + \int_{\partial_1 \Omega_h \cup \partial_D \Omega_h} \llbracket \delta \mathbf{G}_n^T \rrbracket \langle \mathbf{w}(\mathbf{G}, \nabla \mathbf{G}) \rangle dS + \int_{\partial_1 \Omega_h} \llbracket \mathbf{G}_n^T \rrbracket \langle \mathbf{v}(\mathbf{G}) \nabla \delta \mathbf{G} \rangle dS \\
& \quad + \int_{\partial_D \Omega_h} \llbracket \mathbf{G}_n^T \rrbracket \langle \mathbf{v}(\bar{\mathbf{G}}) \nabla \delta \mathbf{G} \rangle dS + \int_{\partial_1 \Omega_h} \llbracket \mathbf{G}_n^T \rrbracket \left\langle \frac{\mathbf{v}(\mathbf{G}) \mathcal{B}}{h_s} \right\rangle \llbracket \delta \mathbf{G}_n \rrbracket dS \\
& \quad + \int_{\partial_D \Omega_h} \llbracket \mathbf{G}_n^T \rrbracket \left\langle \frac{\mathbf{v}(\bar{\mathbf{G}}) \mathcal{B}}{h_s} \right\rangle \llbracket \delta \mathbf{G}_n \rrbracket dS + \int_{\partial_1 \Omega_h \cup \partial_D \Omega_h} \llbracket \delta \mathbf{G}_n^T \rrbracket \langle \mathbf{o}(\mathbf{G}) \mathbf{G} - \mathbf{o}_0 \mathbf{G}_0 \rangle dS \\
& \quad - \int_{\partial_D \Omega_h} \langle \delta \mathbf{G}_n^T \rangle \llbracket \mathbf{o}(\mathbf{G}) \mathbf{G} - \mathbf{o}_0 \mathbf{G}_0 \rrbracket dS,
\end{aligned} \tag{5.96}$$

$$\begin{aligned}
b'(\delta \mathbf{E}) & = \int_{\partial_N \Omega_h} \delta \mathbf{G}^T \bar{\mathbf{w}} dS - \int_{\partial_D \Omega_h} \bar{\mathbf{G}}_n^T \mathbf{v}(\bar{\mathbf{G}}) \nabla \delta \mathbf{G} dS \\
& \quad + \int_{\partial_D \Omega_h} \delta \mathbf{G}_n^T \frac{\mathbf{v}(\bar{\mathbf{G}}) \mathcal{B}}{h_s} \bar{\mathbf{G}}_n dS + \int_{\partial_D \Omega_h} \delta \mathbf{G}_n^T (\mathbf{o}(\bar{\mathbf{G}}) \bar{\mathbf{G}} - \mathbf{o}_0 \mathbf{G}_0) dS.
\end{aligned} \tag{5.97}$$

Henceforth, using Eq. (5.83), it is shown that Eq. (5.95), which is derived from Eq. (5.90), corresponds to the weak form Eqs. (5.45, 5.46).

Unlike the usual case in DG, where the interface term involves  $\mathbf{o}$  in the average operator  $\langle \cdot \rangle$ , Eq. (5.91) shows that  $\mathbf{o}$  is rather involved in the jump  $\llbracket \cdot \rrbracket$ . This comes from the integration by parts in Eq. (5.94), in which  $\mathbf{o}$  is  $\mathbf{G}$  dependent. However, this allows the volume and consistency terms in Eq. (5.95) to be directly expressed in terms of the stress  $\mathbf{w} \nabla \mathbf{G} - (\mathbf{o} \mathbf{G} - \mathbf{o}_0 \mathbf{G}_0)$ , which is convenient when dealing with a non-linear formulation as in Eqs. (5.45, 5.46).

### 5.4.1 Consistency

To prove the consistency of the method, the exact solution  $\mathbf{G}^e \in [\mathbf{H}^2(\Omega)]^d \times \mathbf{H}^2(\Omega) \times \mathbf{H}^{2^+}(\Omega)$  of the problem stated by Eq. (5.89) is considered. This implies  $[[\mathbf{G}^e]] = 0$ ,  $\langle \mathbf{w} \rangle = \mathbf{w}$ ,  $[[\mathbf{o}(\mathbf{G}^e)\mathbf{G}^e - \mathbf{o}_0\mathbf{G}_0]] = 0$  on  $\partial_I\Omega_h$ , and  $[[\mathbf{G}^e]] = -\bar{\mathbf{G}} = -\mathbf{G}^e$ ,  $[[\mathbf{o}(\mathbf{G}^e)\mathbf{G}^e - \mathbf{o}_0\mathbf{G}_0]] = -\mathbf{o}(\bar{\mathbf{G}})\bar{\mathbf{G}} + \mathbf{o}_0\mathbf{G}_0$ ,  $\langle \mathbf{w} \rangle = \mathbf{v}(\bar{\mathbf{G}})\nabla\bar{\mathbf{G}} = \mathbf{v}(\mathbf{G}^e)\nabla\mathbf{G}^e$ , and  $\mathbf{v}(\mathbf{G}) = \mathbf{v}(\bar{\mathbf{G}}) = \mathbf{v}(\mathbf{G}^e)$  on  $\partial_D\Omega_h$ . Therefore, Eq. (5.90) becomes:

$$\begin{aligned}
& \int_{\partial_N\Omega_h} \delta\mathbf{G}^T \bar{\mathbf{w}} dS - \int_{\partial_D\Omega_h} \bar{\mathbf{G}}_n^T \mathbf{v}(\bar{\mathbf{G}}) \nabla \delta\mathbf{G} dS + \int_{\partial_D\Omega_h} \delta\mathbf{G}_n^T (\mathbf{o}(\bar{\mathbf{G}})\bar{\mathbf{G}} - \mathbf{o}_0\mathbf{G}_0) dS \\
& + \int_{\partial_D\Omega_h} \delta\mathbf{G}_n^T \frac{\mathbf{v}(\bar{\mathbf{G}})\mathcal{B}}{h_s} \bar{\mathbf{G}}_n dS = \int_{\Omega_h} (\nabla \delta\mathbf{G})^T \mathbf{w}(\mathbf{G}^e, \nabla\mathbf{G}^e) d\Omega \\
& + \int_{\Omega_h} \delta\mathbf{G}^T \tilde{\mathbf{o}}(\mathbf{G}^e) \nabla\mathbf{G}^e d\Omega + \int_{\partial_I\Omega_h} [[\delta\mathbf{G}_n^T]] \langle \mathbf{w}(\mathbf{G}^e, \nabla\mathbf{G}^e) \rangle dS \\
& - \int_{\partial_D\Omega_h} \delta\mathbf{G}_n^T \mathbf{w}(\mathbf{G}^e, \nabla\mathbf{G}^e) dS - \int_{\partial_D\Omega_h} \mathbf{G}_n^{eT} \mathbf{v}(\bar{\mathbf{G}}) \nabla \delta\mathbf{G} dS + \int_{\partial_D\Omega_h} \delta\mathbf{G}_n^T \frac{\mathcal{B}}{h_s} \mathbf{v}(\bar{\mathbf{G}}) \mathbf{G}_n^e dS \\
& + \int_{\partial_D\Omega_h} \delta\mathbf{G}_n^T (\mathbf{o}(\mathbf{G}^e)\mathbf{G}^e - \mathbf{o}_0\mathbf{G}_0) dS + \int_{\partial_N\Omega_h} \delta\mathbf{G}^T \bar{\mathbf{n}}^T (\mathbf{o}(\mathbf{G}^e)\mathbf{G}^e - \mathbf{o}_0\mathbf{G}_0) dS \quad \forall \delta\mathbf{G} \in \mathbf{X}.
\end{aligned} \tag{5.98}$$

Integrating the first term of the right hand side by parts leads to

$$\begin{aligned}
\sum_e \int_{\Omega^e} (\nabla \delta\mathbf{G})^T \mathbf{w}(\mathbf{G}^e, \nabla\mathbf{G}^e) d\Omega &= - \sum_e \int_{\Omega^e} \delta\mathbf{G}^T \nabla^T \mathbf{w}(\mathbf{G}^e, \nabla\mathbf{G}^e) d\Omega \\
&+ \sum_e \int_{\partial\Omega^e} \delta\mathbf{G}_n^T \mathbf{w}(\mathbf{G}^e, \nabla\mathbf{G}^e) dS,
\end{aligned} \tag{5.99}$$

and Eq.(5.98) becomes

$$\begin{aligned}
& \int_{\partial_N\Omega_h} \delta\mathbf{G}^T \bar{\mathbf{w}} dS - \int_{\partial_D\Omega_h} \bar{\mathbf{G}}_n^T (\mathbf{v}(\bar{\mathbf{G}})\nabla\delta\mathbf{G}) dS + \int_{\partial_D\Omega_h} \delta\mathbf{G}_n^T (\mathbf{o}(\bar{\mathbf{G}})\bar{\mathbf{G}} - \mathbf{o}_0\mathbf{G}_0) dS \\
& + \int_{\partial_D\Omega_h} \delta\mathbf{G}_n^T \left( \frac{\mathcal{B}}{h_s} \mathbf{v}(\bar{\mathbf{G}}) \right) \bar{\mathbf{G}}_n dS = - \int_{\Omega_h} \delta\mathbf{G}^T \nabla^T \mathbf{w}(\mathbf{G}^e, \nabla\mathbf{G}^e) d\Omega \\
& + \int_{\partial_N\Omega_h} \delta\mathbf{G}_n^T \mathbf{w}(\mathbf{G}^e, \nabla\mathbf{G}^e) dS + \int_{\Omega_h} \delta\mathbf{G}^T \tilde{\mathbf{o}}(\mathbf{G}^e) \nabla\mathbf{G}^e d\Omega \\
& - \int_{\partial_D\Omega_h} \mathbf{G}_n^{eT} \mathbf{v}(\bar{\mathbf{G}}) \nabla \delta\mathbf{G} dS + \int_{\partial_D\Omega_h} \delta\mathbf{G}_n^T \frac{\mathcal{B}}{h_s} \mathbf{v}(\bar{\mathbf{G}}) \mathbf{G}_n^e dS \\
& + \int_{\partial_D\Omega_h} \delta\mathbf{G}_n^T (\mathbf{o}(\mathbf{G}^e)\mathbf{G}^e - \mathbf{o}_0\mathbf{G}_0) dS + \int_{\partial_N\Omega_h} \delta\mathbf{G}^T \bar{\mathbf{n}}^T (\mathbf{o}(\mathbf{G}^e)\mathbf{G}^e - \mathbf{o}_0\mathbf{G}_0) dS \quad \forall \delta\mathbf{G} \in \mathbf{X}.
\end{aligned} \tag{5.100}$$

The arbitrary nature of the test functions leads to recover the set of conservation laws, Eqs. (5.84), and the boundary conditions, Eqs. (5.85-5.86).

### 5.4.2 Second order non-self-adjoint elliptic problem

In this part, we will assume that  $\partial_D\Omega_h = \partial\Omega_h$ . This assumption is not restrictive but simplifies the demonstrations.

Our subsequent analysis will be derived similar to the one in Section 4.2.2.

Starting from the definition of matrix  $\mathbf{v}(\mathbf{G})$ , which is a symmetric and positive definite matrix, as its components  $\mathbf{C}$  and  $\mathbf{Z}$  are positive definite matrix. Let us define the minimum and maximum eigenvalues of the matrix  $\mathbf{v}(\mathbf{G})$  as  $\lambda(\mathbf{G})$  and  $\Lambda(\mathbf{G})$ , then for all  $\xi \in \mathbb{R}_0^{5d-3}$

$$0 < \lambda(\mathbf{G})|\xi|^2 \leq \xi_i \mathbf{v}^{ij}(\mathbf{G}) \xi_j \leq \Lambda(\mathbf{G})|\xi|^2. \quad (5.101)$$

Also by assuming that  $\|\mathbf{G}\|_{W_\infty^1} \leq \alpha$ , then there is a positive constant  $C_\alpha$  such that

$$0 < C_\alpha < \lambda(\mathbf{G}). \quad (5.102)$$

In the following analysis, we use the integral form of the Taylor's expansions of  $\mathbf{w}$ , introduced in Eqs. (4.89- 4.92).

For the future use, let us introduce for  $d = 3$ ,  $\mathbf{d}(\mathbf{G}, \nabla \mathbf{G}) = \tilde{\mathbf{o}}(\mathbf{G}) \nabla \mathbf{G}$  a  $(d+2) \times 1$  vector,  $\mathbf{d}_{\nabla \mathbf{G}}(\mathbf{G}) = \tilde{\mathbf{o}}(\mathbf{G})$  of size  $(d+2) \times (5d-3)$ ,  $\mathbf{d}_{\mathbf{G}}(\mathbf{G}, \nabla \mathbf{G}) = \tilde{\mathbf{o}}_{\mathbf{G}}(\mathbf{G}) \nabla \mathbf{G}$  a  $(d+2) \times (d+2)$  matrix,  $\mathbf{d}_{\mathbf{G}\mathbf{G}}(\mathbf{G}, \nabla \mathbf{G}) = \tilde{\mathbf{o}}_{\mathbf{G}\mathbf{G}}(\mathbf{G}) \nabla \mathbf{G}$  a  $(d+2) \times (d+2) \times (d+2)$  matrix,  $\mathbf{d}_{\nabla \mathbf{G}\mathbf{G}}(\mathbf{G}) = \tilde{\mathbf{o}}_{\mathbf{G}}(\mathbf{G})$  a  $(d+2) \times (5d-3) \times (5d-3)$  matrix, the  $(5d-3) \times 1$  vector  $\mathbf{p}(\mathbf{G}) = \mathbf{o}(\mathbf{G})\mathbf{G}$  and its first and second derivatives  $\mathbf{p}_{\mathbf{G}}(\mathbf{G})$  of size  $(5d-3) \times (d+2)$  and  $\mathbf{p}_{\mathbf{G}\mathbf{G}}(\mathbf{G})$  of size  $(5d-3) \times (d+2) \times (d+2)$  respectively, which will be computed later. Those matrices will be needed for the further derivation of Taylor series as in Eq. (4.91). By recalling the definition  $\mathbf{w}(\mathbf{G}, \nabla \mathbf{G}) = \mathbf{v}(\mathbf{G}) \nabla \mathbf{G}$ , then the expression of the derivatives  $\mathbf{w}_{\mathbf{G}}(\mathbf{G}, \nabla \mathbf{G}) = \mathbf{v}_{\mathbf{G}}(\mathbf{G}) \nabla \mathbf{G}$ ,  $\mathbf{w}_{\nabla \mathbf{G}}(\mathbf{G}) = \mathbf{v}(\mathbf{G})$ ,  $\mathbf{w}_{\mathbf{G}\mathbf{G}}(\mathbf{G}, \nabla \mathbf{G}) = \mathbf{v}_{\mathbf{G}\mathbf{G}}(\mathbf{G}) \nabla \mathbf{G}$ , and  $\mathbf{w}_{\mathbf{G}\nabla \mathbf{G}}(\mathbf{G}) = \mathbf{v}_{\mathbf{G}}(\mathbf{G})$  of  $\mathbf{w}(\mathbf{G}, \nabla \mathbf{G})$  can be extracted directly from Appendix C.2, as  $\mathbf{C}$  for all the derivation is a constant matrix.

Let us define the solution  $\mathbf{G}^e \in [H^2(\Omega)]^d \times H^2(\Omega) \times H^{2+}(\Omega)$  of the strong form stated by Eqs. (5.84-5.86). Thus since  $[\mathbf{G}^e] = 0$  on  $\partial_I \Omega^e$  and  $[\mathbf{G}^e] = -\mathbf{G}^e = -\bar{\mathbf{G}}$  on  $\partial_D \Omega^e$ , and since Eq. (5.90) satisfies the consistency, we have

$$\begin{aligned} a(\mathbf{G}^e, \delta \mathbf{G}^e) &= \int_{\Omega_h} (\nabla \delta \mathbf{G}^e)^T \mathbf{w}(\mathbf{G}^e, \nabla \mathbf{G}^e) d\Omega + \int_{\Omega_h} \delta \mathbf{G}^{eT} \tilde{\mathbf{o}}(\mathbf{G}^e) \nabla \mathbf{G}^e d\Omega \\ &+ \int_{\partial_I \Omega_h} \left[ \delta \mathbf{G}_{\mathbf{n}}^{eT} \right] \langle \mathbf{w}(\mathbf{G}^e, \nabla \mathbf{G}^e) \rangle dS - \int_{\partial_D \Omega_h} \delta \mathbf{G}_{\mathbf{n}}^{eT} \mathbf{w}(\mathbf{G}^e, \nabla \mathbf{G}^e) dS \\ &- \int_{\partial_D \Omega_h} \mathbf{G}_{\mathbf{n}}^{eT} \mathbf{v}(\mathbf{G}^e) \nabla \delta \mathbf{G}^e dS + \int_{\partial_D \Omega_h} \mathbf{G}_{\mathbf{n}}^{eT} \frac{\mathbf{v}(\mathbf{G}^e) \mathcal{B}}{h_s} \delta \mathbf{G}_{\mathbf{n}}^e dS \\ &+ \int_{\partial_D \Omega_h} \delta \mathbf{G}_{\mathbf{n}}^{eT} (\mathbf{o}(\mathbf{G}^e) \mathbf{G}^e - \mathbf{o}_0 \mathbf{G}_0) dS = b(\delta \mathbf{G}^e) \quad \forall \delta \mathbf{G}^e \in X, \end{aligned} \quad (5.103)$$

with

$$\begin{aligned} b(\delta \mathbf{G}^e) &= - \int_{\partial_D \Omega_h} \bar{\mathbf{G}}_{\mathbf{n}}^T (\mathbf{v}(\bar{\mathbf{G}}) \nabla \delta \mathbf{G}^e) dS + \int_{\partial_D \Omega_h} \delta \mathbf{G}_{\mathbf{n}}^{eT} (\mathbf{o}(\bar{\mathbf{G}}) \bar{\mathbf{G}} - \mathbf{o}_0 \mathbf{G}_0) dS \\ &+ \int_{\partial_D \Omega_h} \delta \mathbf{G}_{\mathbf{n}}^{eT} \left( \frac{\mathcal{B}}{h_s} \mathbf{v}(\bar{\mathbf{G}}) \right) \bar{\mathbf{G}}_{\mathbf{n}} dS. \end{aligned} \quad (5.104)$$

Therefore, using  $\delta \mathbf{G}^e = \delta \mathbf{G}_h$  in Eq. (5.103) and subtracting the DG discretization (5.90) from Eq. (5.103), then adding and subtracting successively  $\int_{\partial_I \Omega_h} \left[ \mathbf{G}_{\mathbf{n}}^{eT} - \mathbf{G}_{h\mathbf{n}}^T \right] \langle \mathbf{w}_{\nabla \mathbf{G}}(\mathbf{G}^e) \nabla \delta \mathbf{G}_h \rangle dS$ ,

$\int_{\partial_I \Omega_h} \llbracket \mathbf{G}_n^{eT} - \mathbf{G}_{hn}^T \rrbracket \left\langle \frac{\mathcal{B}}{h_s} \mathbf{w}_{\nabla \mathbf{G}}(\mathbf{G}^e) \right\rangle \llbracket \delta \mathbf{G}_{hn} \rrbracket dS$  to this last relation, and using  $\llbracket \mathbf{G}_n^e \rrbracket = 0$ ,  $\llbracket \mathbf{o}(\mathbf{G}^e) \mathbf{G}^e - \mathbf{o}_0 \mathbf{G}_0 \rrbracket = 0$  on  $\partial_I \Omega_h$  and  $\llbracket \mathbf{G}_n^e \rrbracket = -\mathbf{G}_n^e = -\bar{\mathbf{G}}_n$ ,  $\llbracket \mathbf{o}(\mathbf{G}^e) \mathbf{G}^e - \mathbf{o}_0 \mathbf{G}_0 \rrbracket = -\mathbf{o}(\bar{\mathbf{G}}) \bar{\mathbf{G}} + \mathbf{o}_0 \mathbf{G}_0$  on  $\partial_D \Omega_h$ , one gets

$$\begin{aligned}
0 &= \int_{\Omega_h} (\nabla \delta \mathbf{G}_h)^T (\mathbf{w}(\mathbf{G}^e, \nabla \mathbf{G}^e) - \mathbf{w}(\mathbf{G}_h, \nabla \mathbf{G}_h)) d\Omega \\
&+ \int_{\Omega_h} \delta \mathbf{G}_h^T (\tilde{\mathbf{o}}(\mathbf{G}^e) \nabla \mathbf{G}^e - \tilde{\mathbf{o}}(\mathbf{G}_h) \nabla \mathbf{G}_h) d\Omega \\
&+ \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \llbracket \delta \mathbf{G}_{hn}^T \rrbracket \langle \mathbf{w}(\mathbf{G}^e, \nabla \mathbf{G}^e) - \mathbf{w}(\mathbf{G}_h, \nabla \mathbf{G}_h) \rangle dS \\
&+ \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \llbracket \mathbf{G}_n^{eT} - \mathbf{G}_{hn}^T \rrbracket \langle \mathbf{w}_{\nabla \mathbf{G}}(\mathbf{G}^e) \nabla \delta \mathbf{G}_h \rangle dS \\
&- \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \llbracket \mathbf{G}^{eT} \mathbf{o}^T(\mathbf{G}^e) - \mathbf{G}_h^T \mathbf{o}^T(\mathbf{G}_h) \rrbracket \langle \delta \mathbf{G}_{hn} \rangle dS \\
&- \int_{\partial_I \Omega_h} \llbracket \mathbf{G}_n^{eT} - \mathbf{G}_{hn}^T \rrbracket \langle (\mathbf{w}_{\nabla \mathbf{G}}(\mathbf{G}^e) - \mathbf{w}_{\nabla \mathbf{G}}(\mathbf{G}_h)) \nabla \delta \mathbf{G}_h \rangle dS \\
&+ \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \llbracket \mathbf{G}_n^{eT} - \mathbf{G}_{hn}^T \rrbracket \left\langle \frac{\mathcal{B}}{h_s} \mathbf{w}_{\nabla \mathbf{G}}(\mathbf{G}^e) \right\rangle \llbracket \delta \mathbf{G}_{hn} \rrbracket dS \\
&- \int_{\partial_I \Omega_h} \llbracket \mathbf{G}_n^{eT} - \mathbf{G}_{hn}^T \rrbracket \left\langle \frac{\mathcal{B}}{h_s} (\mathbf{w}_{\nabla \mathbf{G}}(\mathbf{G}^e) - \mathbf{w}_{\nabla \mathbf{G}}(\mathbf{G}_h)) \right\rangle \llbracket \delta \mathbf{G}_{hn} \rrbracket dS \quad \forall \delta \mathbf{G}_h \in X^k.
\end{aligned} \tag{5.105}$$

Using the Taylor series defined in Eq. (4.89) the first three terms of the previous equation can be successively rewritten as following. The first term of Eq. (5.105) can be rewritten as

$$\begin{aligned}
&\int_{\Omega_h} (\nabla \delta \mathbf{G}_h)^T (\mathbf{w}(\mathbf{G}^e, \nabla \mathbf{G}^e) - \mathbf{w}(\mathbf{G}_h, \nabla \mathbf{G}_h)) d\Omega \\
&= \int_{\Omega_h} (\nabla \delta \mathbf{G}_h)^T (\mathbf{w}_{\mathbf{G}}(\mathbf{G}^e, \nabla \mathbf{G}^e) (\mathbf{G}^e - \mathbf{G}_h)) d\Omega \\
&+ \int_{\Omega_h} (\nabla \delta \mathbf{G}_h)^T (\mathbf{w}_{\nabla \mathbf{G}}(\mathbf{G}^e) (\nabla \mathbf{G}^e - \nabla \mathbf{G}_h)) d\Omega \\
&- \int_{\Omega_h} (\nabla \delta \mathbf{G}_h)^T (\bar{\mathbf{R}}_{\mathbf{w}} (\mathbf{G}^e - \mathbf{G}_h, \nabla \mathbf{G}^e - \nabla \mathbf{G}_h)) d\Omega,
\end{aligned} \tag{5.106}$$

with

$$\begin{aligned}
\bar{\mathbf{R}}_{\mathbf{w}} (\mathbf{G}^e - \mathbf{G}_h, \nabla \mathbf{G}^e - \nabla \mathbf{G}_h) &= (\mathbf{G}^e - \mathbf{G}_h)^T \bar{\mathbf{w}}_{\mathbf{G}\mathbf{G}}^T (\mathbf{G}_h) (\mathbf{G}_h - \mathbf{G}_h) \\
&+ 2(\mathbf{G}^e - \mathbf{G}_h)^T \bar{\mathbf{w}}_{\nabla \mathbf{G}\mathbf{G}}^T (\mathbf{G}_h) (\nabla \mathbf{G}^e - \nabla \mathbf{G}_h),
\end{aligned} \tag{5.107}$$

where  $\bar{\mathbf{w}}_{\mathbf{G}\mathbf{G}}$  is  $(5d - 3) \times (d + 2) \times (d + 2)$  matrix and  $\bar{\mathbf{w}}_{\nabla \mathbf{G}\mathbf{G}}$  is  $(5d - 3) \times (5d - 3) \times (d + 2)$

matrix. Similarly, the second term of Eq. (5.105) can be rewritten as

$$\begin{aligned}
\int_{\Omega_h} \delta \mathbf{G}_h^T (\tilde{\mathbf{o}}(\mathbf{G}^e) \nabla \mathbf{G}^e - \tilde{\mathbf{o}}(\mathbf{G}_h) \nabla \mathbf{G}_h) d\Omega &= \int_{\Omega_h} \delta \mathbf{G}_h^T (\mathbf{d}(\mathbf{G}^e, \nabla \mathbf{G}^e) - \mathbf{d}(\mathbf{G}_h, \nabla \mathbf{G}_h)) d\Omega \\
&= \int_{\Omega_h} \delta \mathbf{G}_h^T \mathbf{d}_G(\mathbf{G}^e, \nabla \mathbf{G}^e)(\mathbf{G}^e - \mathbf{G}_h) d\Omega \\
&\quad + \int_{\Omega_h} \delta \mathbf{G}_h^T \mathbf{d}_{\nabla G}(\mathbf{G}^e)(\nabla \mathbf{G}^e - \nabla \mathbf{G}_h) d\Omega \\
&\quad - \int_{\Omega_h} \delta \mathbf{G}_h^T \bar{\mathbf{R}}_d(\mathbf{G}^e - \mathbf{G}_h, \nabla \mathbf{G}^e - \nabla \mathbf{G}_h) d\Omega,
\end{aligned} \tag{5.108}$$

where  $\bar{\mathbf{R}}_d(\mathbf{G}^e - \mathbf{G}_h)$  can be derived from Eq. (4.91) as

$$\begin{aligned}
\bar{\mathbf{R}}_d(\mathbf{G}^e - \mathbf{G}_h, \nabla \mathbf{G}^e - \nabla \mathbf{G}_h) &= (\mathbf{G}^e - \mathbf{G}_h)^T \bar{\mathbf{d}}_{GG}(\mathbf{G}_h, \nabla \mathbf{G}_h)(\mathbf{G}^e - \mathbf{G}_h) \\
&\quad + 2(\mathbf{G}^e - \mathbf{G}_h)^T \bar{\mathbf{d}}_{\nabla GG}(\mathbf{G}_h)(\nabla \mathbf{G}^e - \nabla \mathbf{G}_h).
\end{aligned} \tag{5.109}$$

Likewise, the third term is rewritten as

$$\begin{aligned}
&\int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \llbracket \delta \mathbf{G}_{h_n}^T \rrbracket \langle \mathbf{w}(\mathbf{G}^e, \nabla \mathbf{G}^e) - \mathbf{w}(\mathbf{G}_h, \nabla \mathbf{G}_h) \rangle dS \\
&= \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \llbracket \delta \mathbf{G}_{h_n}^T \rrbracket \langle \mathbf{w}_G(\mathbf{G}^e, \nabla \mathbf{G}^e)(\mathbf{G}^e - \mathbf{G}_h) \rangle dS \\
&\quad + \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \llbracket \delta \mathbf{G}_{h_n}^T \rrbracket \langle \mathbf{w}_{\nabla G}(\mathbf{G}^e)(\nabla \mathbf{G}^e - \nabla \mathbf{G}_h) \rangle dS \\
&\quad - \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \llbracket \delta \mathbf{G}_{h_n}^T \rrbracket \langle \bar{\mathbf{R}}_w(\mathbf{G}^e - \mathbf{G}_h, \nabla \mathbf{G}^e - \nabla \mathbf{G}_h) \rangle dS.
\end{aligned} \tag{5.110}$$

The fifth term is developed by using the definition of  $\mathbf{p}^T(\mathbf{G}) = \mathbf{G}^T \mathbf{o}^T(\mathbf{G})$  and using the Taylor's series as in Eq. (4.89), but written on  $\mathbf{p}(\mathbf{G})$ :  $\mathbf{p}^T(\mathbf{G}^e) - \mathbf{p}^T(\mathbf{G}_h) = (\mathbf{G}^e - \mathbf{G}_h)^T \mathbf{p}_G^T(\mathbf{G}^e) - \bar{\mathbf{R}}_p(\mathbf{G}^e - \mathbf{G}_h)$ , where  $\bar{\mathbf{R}}_p(\mathbf{G}^e - \mathbf{G}_h) = (\mathbf{G}^e - \mathbf{G}_h)^T \bar{\mathbf{p}}_{GG}^T(\mathbf{G}_h)(\mathbf{G}^e - \mathbf{G}_h)$ .

Therefore, the fifth term of Eq. (5.105) becomes

$$\begin{aligned}
&- \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \llbracket \mathbf{G}^{eT} \mathbf{o}^T(\mathbf{G}^e) - \mathbf{G}_h^T \mathbf{o}^T(\mathbf{G}_h) \rrbracket \langle \delta \mathbf{G}_{h_n} \rangle dS \\
&= - \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \llbracket (\mathbf{G}^{eT} - \mathbf{G}_h^T) \mathbf{p}_G^T(\mathbf{G}^e) \rrbracket \langle \delta \mathbf{G}_{h_n} \rangle dS \\
&\quad + \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \llbracket \bar{\mathbf{R}}_p(\mathbf{G}^e - \mathbf{G}_h) \rrbracket \langle \delta \mathbf{G}_{h_n} \rangle dS.
\end{aligned} \tag{5.111}$$

However, one has  $\mathbf{p}_G^T = \frac{\partial(\mathbf{G}^T \mathbf{o}^T(\mathbf{G}))}{\partial \mathbf{G}} = \mathbf{G}^T \frac{\partial \mathbf{o}^T(\mathbf{G})}{\partial \mathbf{G}} + \mathbf{o}^T(\mathbf{G})$ , which once computed explicitly as to derive Eq. (5.94) gives  $\mathbf{p}_G^T = -\mathbf{o}^T(\mathbf{G})$ . Moreover  $\bar{\mathbf{R}}_p(\mathbf{G}^e - \mathbf{G}_h) = -(\mathbf{G}^e - \mathbf{G}_h)^T \bar{\mathbf{o}}_G^T(\mathbf{G}_h)(\mathbf{G}^e - \mathbf{G}_h)$ , and the previous equation can also be written as

$$\begin{aligned}
&- \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \llbracket \mathbf{G}^{eT} \mathbf{o}^T(\mathbf{G}^e) - \mathbf{G}_h^T \mathbf{o}^T(\mathbf{G}_h) \rrbracket \langle \delta \mathbf{G}_{h_n} \rangle dS \\
&= \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \llbracket (\mathbf{G}^{eT} - \mathbf{G}_h^T) \mathbf{o}^T(\mathbf{G}^e) \rrbracket \langle \delta \mathbf{G}_{h_n} \rangle dS \\
&\quad - \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \llbracket (\mathbf{G}^e - \mathbf{G}_h)^T \bar{\mathbf{o}}_G^T(\mathbf{G}_h)(\mathbf{G}^e - \mathbf{G}_h) \rrbracket \langle \delta \mathbf{G}_{h_n} \rangle dS.
\end{aligned} \tag{5.112}$$

Finally since  $\mathbf{G}^T \mathbf{o}^T(\mathbf{G}') \delta \mathbf{G}_n = \mathbf{G}_n^T \tilde{\mathbf{o}}^T(\mathbf{G}') \delta \mathbf{G} = -\frac{3K}{f_T^2} f_T \alpha_{th} n_x^- \delta u_x - \frac{3K}{f_T^2} f_T \alpha_{th} n_y^- \delta u_y - \frac{3K}{f_T^2} f_T \alpha_{th} n_z^- \delta u_z$ , then Eq. (5.112) is rewritten as

$$\begin{aligned} & - \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \left[ \mathbf{G}^{eT} \mathbf{o}^T(\mathbf{G}^e) - \mathbf{G}_h^T \mathbf{o}^T(\mathbf{G}_h) \right] \langle \delta \mathbf{G}_{h_n} \rangle dS \\ & = \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \left[ (\mathbf{G}_n^{eT} - \mathbf{G}_{h_n}^T) \tilde{\mathbf{o}}^T(\mathbf{G}^e) \right] \langle \delta \mathbf{G}_h \rangle dS \\ & - \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \left[ (\mathbf{G}^e - \mathbf{G}_h)^T \tilde{\mathbf{o}}_G^T(\mathbf{G}_h) (\mathbf{G}^e - \mathbf{G}_h) \right] \langle \delta \mathbf{G}_{h_n} \rangle dS. \end{aligned} \quad (5.113)$$

We can now first define  $\mathcal{N}(\mathbf{G}^e, \mathbf{G}_h; \delta \mathbf{G}_h)$  as follows

$$\begin{aligned} \mathcal{N}(\mathbf{G}^e, \mathbf{G}_h; \delta \mathbf{G}_h) & = \int_{\Omega_h} (\nabla \delta \mathbf{G}_h)^T (\bar{\mathbf{R}}_w(\mathbf{G}^e - \mathbf{G}_h, \nabla \mathbf{G}^e - \nabla \mathbf{G}_h)) d\Omega \\ & + \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \left[ \delta \mathbf{G}_{h_n}^T \right] \langle \bar{\mathbf{R}}_w(\mathbf{G}^e - \mathbf{G}_h, \nabla \mathbf{G}^e - \nabla \mathbf{G}_h) \rangle dS \\ & + \int_{\partial_I \Omega_h} \left[ \mathbf{G}_n^{eT} - \mathbf{G}_{h_n}^T \right] \langle (\mathbf{w}_{\nabla \mathbf{G}}(\mathbf{G}^e) - \mathbf{w}_{\nabla \mathbf{G}}(\mathbf{G}_h)) \nabla \delta \mathbf{G}_h \rangle dS \\ & + \int_{\partial_I \Omega_h} \left[ \mathbf{G}_n^{eT} - \mathbf{G}_{h_n}^T \right] \left\langle \frac{\mathcal{B}}{h_s} (\mathbf{w}_{\nabla \mathbf{G}}(\mathbf{G}^e) - \mathbf{w}_{\nabla \mathbf{G}}(\mathbf{G}_h)) \right\rangle \left[ \delta \mathbf{G}_{h_n} \right] dS \\ & + \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \left[ (\mathbf{G}^e - \mathbf{G}_h)^T \tilde{\mathbf{o}}_G^T(\mathbf{G}_h) (\mathbf{G}^e - \mathbf{G}_h) \right] \langle \delta \mathbf{G}_{h_n} \rangle dS \\ & + \int_{\Omega_h} \delta \mathbf{G}_n^T \bar{\mathbf{R}}_d(\mathbf{G}^e - \mathbf{G}_h, \nabla \mathbf{G}^e - \nabla \mathbf{G}_h) d\Omega \\ & = \mathcal{I}_1 + \mathcal{I}_2 + \mathcal{I}_3 + \mathcal{I}_4 + \mathcal{I}_5 + \mathcal{I}_6. \end{aligned} \quad (5.114)$$

Moreover, for given  $\boldsymbol{\psi} \in X^+$ ,  $\boldsymbol{\omega} \in X$  and  $\delta \boldsymbol{\omega} \in X$ , we define the following forms:

$$\begin{aligned} \mathcal{A}(\boldsymbol{\psi}; \boldsymbol{\omega}, \delta \boldsymbol{\omega}) & = \int_{\Omega_h} \nabla \delta \boldsymbol{\omega}^T \mathbf{w}_{\nabla \boldsymbol{\psi}}(\boldsymbol{\psi}) \nabla \boldsymbol{\omega} d\Omega + \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \left[ \delta \boldsymbol{\omega}_n^T \right] \langle \mathbf{w}_{\nabla \boldsymbol{\psi}}(\boldsymbol{\psi}) \nabla \boldsymbol{\omega} \rangle dS \\ & + \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \left[ \boldsymbol{\omega}_n^T \right] \langle \mathbf{w}_{\nabla \boldsymbol{\psi}}(\boldsymbol{\psi}) \nabla \delta \boldsymbol{\omega} \rangle dS + \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \left[ \boldsymbol{\omega}_n^T \right] \left\langle \frac{\mathcal{B}}{h_s} \mathbf{w}_{\nabla \boldsymbol{\psi}}(\boldsymbol{\psi}) \right\rangle \left[ \delta \boldsymbol{\omega}_n \right] dS, \end{aligned} \quad (5.115)$$

$$\begin{aligned} \mathcal{B}(\boldsymbol{\psi}; \boldsymbol{\omega}, \delta \boldsymbol{\omega}) & = \int_{\Omega_h} \nabla \delta \boldsymbol{\omega}^T (\mathbf{w}_{\boldsymbol{\psi}}(\boldsymbol{\psi}, \nabla \boldsymbol{\psi}) \boldsymbol{\omega}) d\Omega + \int_{\Omega_h} \delta \boldsymbol{\omega}^T \mathbf{d}_{\nabla \boldsymbol{\psi}}(\boldsymbol{\psi}) \nabla \boldsymbol{\omega} d\Omega \\ & + \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \left[ \delta \boldsymbol{\omega}_n^T \right] \langle \mathbf{w}_{\boldsymbol{\psi}}^T(\boldsymbol{\psi}) \boldsymbol{\omega} \rangle dS + \int_{\Omega_h} \delta \boldsymbol{\omega}^T \mathbf{d}_{\boldsymbol{\psi}}(\boldsymbol{\psi}, \nabla \boldsymbol{\psi}) \boldsymbol{\omega} d\Omega \\ & + \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \left[ \boldsymbol{\omega}_n^T \mathbf{d}_{\nabla \boldsymbol{\psi}}^T(\boldsymbol{\psi}) \right] \langle \delta \boldsymbol{\omega} \rangle dS. \end{aligned} \quad (5.116)$$

For fixed  $\boldsymbol{\psi}$ , the form  $\mathcal{A}(\boldsymbol{\psi}; \cdot, \cdot)$  and the form  $\mathcal{B}(\boldsymbol{\psi}; \cdot, \cdot)$  are bi-linear. Comparing with the fixed form from Gudi et al. [24] for non-linear elliptic problems, the formulations  $\mathcal{A}$  and  $\mathcal{B}$  are similar, except the last term of  $\mathcal{B}(\boldsymbol{\psi}; \cdot, \cdot)$  in which  $\mathbf{d}_{\nabla \boldsymbol{\psi}}(\boldsymbol{\psi})$  appears in the  $\llbracket \cdot \rrbracket$  operator instead of the  $\langle \cdot \rangle$  operator. Nevertheless, this term becomes identical with the one in Gudi



et al. [24] for fixed  $\boldsymbol{\psi}$ . However the  $\mathcal{N}$  is different in the fifth and sixth term, so they will require a different treatment.

Therefore, using the relations (5.114-5.116) and the definitions (5.106-5.110), the set of Eqs. (5.105) is rewritten as finding  $\mathbf{G}_h \in X^{k^+}$  such that:

$$\mathcal{A}(\mathbf{G}^e; \mathbf{G}^e - \mathbf{G}_h, \delta \mathbf{G}_h) + \mathcal{B}(\mathbf{G}^e; \mathbf{G}^e - \mathbf{G}_h, \delta \mathbf{G}_h) = \mathcal{N}(\mathbf{G}^e, \mathbf{G}_h; \delta \mathbf{G}_h) \quad \forall \delta \mathbf{G}_h \in X^k. \quad (5.117)$$

When comparing the Electro-Thermo-Elasticity coupling formulation of this Chapter, and the Electro-Thermal coupling formulation of Chapter 4, it can be seen that both of them are nonlinear formulations. However, additional terms appear in the Electro-Thermo-Elasticity coupled formulation, which are related to the expansion term (the term in  $\mathbf{o}$ ).

If  $f_T \geq f_{T0} > 0$ , then  $\bar{\mathbf{w}}_{\mathbf{G}}, \bar{\mathbf{w}}_{\nabla \mathbf{G}}, \bar{\mathbf{w}}_{\mathbf{G}\mathbf{G}}, \bar{\mathbf{w}}_{\mathbf{G}\nabla \mathbf{G}}, \bar{\mathbf{w}}_{\nabla \mathbf{G}\mathbf{G}}, \bar{\mathbf{o}}_{\mathbf{G}}, \bar{\mathbf{d}}, \bar{\mathbf{d}}_{\mathbf{G}}, \bar{\mathbf{d}}_{\nabla \mathbf{G}}, \bar{\mathbf{d}}_{\mathbf{G}\mathbf{G}}, \bar{\mathbf{d}}_{\nabla \mathbf{G}\mathbf{G}} \in \mathbf{L}^\infty(\Omega \times \mathbb{R}^{(d+1)} \times \mathbb{R}_0^+)$ . These matrices with  $(\bar{\cdot})$  are related to the remainder term of Taylor's expansion formulation, similar to Eq. (4.89), as will be shown later. Since  $\mathbf{w}, \mathbf{o}$ , and  $\mathbf{d}$  are twice continuously differentiable function with all the derivatives through the second order locally bounded in a ball around  $\mathbf{G} \in [\mathbb{R}]^3 \times \mathbb{R} \times \mathbb{R}_0^+$  as it will be shown in Section 5.4.3, and we denote by  $C_y$

$$C_y = \max \left\{ \|\mathbf{w}, \mathbf{d}\|_{W_\infty^2(\Omega \times \mathbb{R}^{d+1} \times \mathbb{R}_0^+ \times \mathbb{R}^{(5d-3)}), \right. \\ \left. \|\bar{\mathbf{w}}_{\mathbf{G}}, \bar{\mathbf{w}}_{\nabla \mathbf{G}}, \bar{\mathbf{w}}_{\mathbf{G}\mathbf{G}}, \bar{\mathbf{w}}_{\mathbf{G}\nabla \mathbf{G}}, \bar{\mathbf{w}}_{\nabla \mathbf{G}\mathbf{G}}, \bar{\mathbf{o}}_{\mathbf{G}}, \bar{\mathbf{d}}_{\mathbf{G}}, \bar{\mathbf{d}}_{\nabla \mathbf{G}}, \bar{\mathbf{d}}_{\mathbf{G}\mathbf{G}}, \bar{\mathbf{d}}_{\nabla \mathbf{G}\mathbf{G}}\|_{L^\infty(\Omega \times \mathbb{R}^d \times \mathbb{R}_0^+)} \right\}. \quad (5.118)$$

### 5.4.3 Solution uniqueness

Let us first assume  $\boldsymbol{\eta} = I_h \mathbf{G} - \mathbf{G}^e \in X$ , with  $I_h \mathbf{G} \in X^{k^+}$  the interpolant of  $\mathbf{G}^e$  in  $X^{k^+}$ . The last relation (5.117) thus becomes

$$\mathcal{A}(\mathbf{G}^e; I_h \mathbf{G} - \mathbf{G}_h, \delta \mathbf{G}_h) + \mathcal{B}(\mathbf{G}^e; I_h \mathbf{G} - \mathbf{G}_h, \delta \mathbf{G}_h) = \mathcal{A}(\mathbf{G}^e; \boldsymbol{\eta}, \delta \mathbf{G}_h) + \mathcal{B}(\mathbf{G}^e; \boldsymbol{\eta}, \delta \mathbf{G}_h) \\ + \mathcal{N}(\mathbf{G}^e, \mathbf{G}_h; \delta \mathbf{G}_h) \quad \forall \delta \mathbf{G}_h \in X^k. \quad (5.119)$$

Now in order to prove the existence of a solution  $\mathbf{G}_h$  of the problem stated by Eq. (5.105), which corresponds to the DG finite element discretization (5.90), we state the problem in the fixed point formulation and we define a map  $S_h : X^{k^+} \rightarrow X^{k^+}$  as follows: for a given  $\mathbf{y} \in X^{k^+}$ , find  $S_h(\mathbf{y}) = \mathbf{G}_y \in X^{k^+}$ , such that

$$\mathcal{A}(\mathbf{G}^e; I_h \mathbf{G} - \mathbf{G}_y, \delta \mathbf{G}_h) + \mathcal{B}(\mathbf{G}^e; I_h \mathbf{G} - \mathbf{G}_y, \delta \mathbf{G}_h) = \mathcal{A}(\mathbf{G}^e; \boldsymbol{\eta}, \delta \mathbf{G}_h) + \mathcal{B}(\mathbf{G}^e; \boldsymbol{\eta}, \delta \mathbf{G}_h) \\ + \mathcal{N}(\mathbf{G}^e, \mathbf{y}; \delta \mathbf{G}_h) \quad \forall \delta \mathbf{G}_h \in X^k. \quad (5.120)$$

The existence of a unique solution  $\mathbf{G}_h$  of the discrete problem (5.90) is equivalent to the existence of a fixed point of the map  $S_h$ , see [25].

For the subsequent analysis, we denote by  $C^k$ , a positive generic constant which is independent of the mesh size, but does depend on the polynomial approximation degree  $k$ .

**Lemma 5.4.1** (Lower bound). *For  $\mathcal{B}$  larger than a constant, which depends on the polynomial approximation only, there exist two constants  $C_1^k$  and  $C_2^k$ , such that*

$$\mathcal{A}(\mathbf{G}^e; \delta \mathbf{G}_h, \delta \mathbf{G}_h) + \mathcal{B}(\mathbf{G}^e; \delta \mathbf{G}_h, \delta \mathbf{G}_h) \geq C_1^k \|\delta \mathbf{G}_h\|_*^2 - C_2^k \|\delta \mathbf{G}_h\|_{L^2(\Omega)}^2 \quad \forall \delta \mathbf{G}_h \in X^k, \quad (5.121)$$

$$\mathcal{A}(\mathbf{G}^e; \delta \mathbf{G}_h, \delta \mathbf{G}_h) + \mathcal{B}(\mathbf{G}^e; \delta \mathbf{G}_h, \delta \mathbf{G}_h) \geq C_1^k \|\delta \mathbf{G}_h\|^2 - C_2^k \|\delta \mathbf{G}_h\|_{L^2(\Omega)}^2 \quad \forall \delta \mathbf{G}_h \in X^k. \quad (5.122)$$

The two positive constants  $C_1^k, C_2^k$  are independent of the mesh size, but do depend on  $k$  and  $\mathcal{B}$ . These bounds are estimated by proceeding in a similar way as for Lemmata 3.4.1 and 4.4.1 in Chapters 3 and 4 respectively, and the stability of the method is conditioned by the constant  $\mathcal{B} > \frac{C_y^2}{C_\alpha^2} \max(4C_T(C_T^k + 1), 4C_K^k)$  under consideration for  $C_1^k$  to remain positive, for details see Appendix D.2.

**Lemma 5.4.2** (Upper bound). *There exist  $C > 0$  and  $C^k > 0$  such that*

$$|\mathcal{A}(\mathbf{G}^e; \mathbf{m}, \delta \mathbf{G}) + \mathcal{B}(\mathbf{G}^e; \mathbf{m}, \delta \mathbf{G})| \leq C \|\mathbf{m}\|_1 \|\delta \mathbf{G}\|_1 \quad \forall \mathbf{m}, \delta \mathbf{G} \in X, \quad (5.123)$$

$$|\mathcal{A}(\mathbf{G}^e; \mathbf{m}, \delta \mathbf{G}_h) + \mathcal{B}(\mathbf{G}^e; \mathbf{m}, \delta \mathbf{G}_h)| \leq C^k \|\mathbf{m}\|_1 \|\delta \mathbf{G}_h\| \quad \forall \mathbf{m} \in X, \delta \mathbf{G}_h \in X^k, \quad (5.124)$$

$$|\mathcal{A}(\mathbf{G}^e; \mathbf{m}_h, \delta \mathbf{G}_h) + \mathcal{B}(\mathbf{G}^e; \mathbf{m}_h, \delta \mathbf{G}_h)| \leq C^k \|\mathbf{m}_h\| \|\delta \mathbf{G}_h\| \quad \forall \mathbf{m}_h, \delta \mathbf{G}_h \in X^k. \quad (5.125)$$

The upper bounds are established similarly to the demonstration of Lemmata 3.4.2, 4.4.2 in the previous two chapters. The proof is presented in Appendix D.3.

Using Lemma 5.4.1 and Lemma 5.4.2, the stability of the method is demonstrated through the following Lemmata.

**Lemma 5.4.3** (Auxiliary problem). *We consider the following auxiliary problem, with  $\phi \in L^2(\Omega)$ :*

$$\begin{aligned} -\nabla^T(\mathbf{w}_{\nabla \mathbf{G}}(\mathbf{G}^e)\nabla \psi + \mathbf{w}_{\mathbf{G}}(\mathbf{G}^e, \nabla \mathbf{G}^e)\psi) + \mathbf{d}_{\nabla \mathbf{G}}(\mathbf{G}^e)\nabla \psi + \mathbf{d}_{\mathbf{G}}(\mathbf{G}^e, \nabla \mathbf{G}^e)\psi &= \phi \quad \text{on } \Omega, \\ \psi &= 0 \quad \text{on } \partial\Omega. \end{aligned} \quad (5.126)$$

Assuming regular ellipticity of the operators and that  $\mathbf{w}_{\mathbf{G}}$  and  $\mathbf{d}_{\mathbf{G}}$  satisfy the weak minimum principle [23, Theorem 8.3], there is a unique solution  $\psi \in [H^2(\Omega)]^d \times H^2(\Omega) \times H^2(\Omega)$  to the problem stated by Eq. (5.126) satisfying the elliptic property

$$\|\psi\|_{H^2(\Omega_h)} \leq C \|\phi\|_{L^2(\Omega_h)}. \quad (5.127)$$

The proof is given in [23], by combining [23, Theorem 8.3] to [23, Lemma 9.17].

Moreover, for a given  $\varphi \in [L^2(\Omega_h)]^d \times L^2(\Omega_h) \times L^2(\Omega_h)$  there exists a unique  $\phi_h \in X^k$  such that

$$\mathcal{A}(\mathbf{G}^e; \delta \mathbf{G}_h, \phi_h) + \mathcal{B}(\mathbf{G}^e; \delta \mathbf{G}_h, \phi_h) = \sum_e \int_{\Omega^e} \varphi^T \delta \mathbf{G}_h d\Omega \quad \forall \delta \mathbf{G}_h \in X^k, \quad (5.128)$$

and there is a constant  $C^k$  such that :

$$\|\phi_h\| \leq C^k \|\varphi\|_{L^2(\Omega_h)}. \quad (5.129)$$

The proof follows from the use of Lemma 5.4.1 to bound  $\|\phi_h\|$  in terms of  $\|\varphi\|_{L^2(\Omega_h)}$  and  $\|\phi_h\|_{L^2(\Omega_h)}$ .  $\|\phi_h\|_{L^2(\Omega_h)}$  is then estimated by considering  $\phi = \phi_h \in X^k$  in Eq. (5.126), multiplying the result by  $\phi_h$  and integrating it by parts on  $\Omega_h$  yielding  $\|\phi_h\|_{L^2(\Omega_h)}^2 = \mathcal{A}(\mathbf{G}^e; \psi, \phi_h) + \mathcal{B}(\mathbf{G}^e; \psi, \phi_h)$ . Inserting the interpolant  $I_h \phi$  in these last terms, making successive use of Lemmata 5.4.2 and 2.4.6, and using the regular ellipticity Eq. (5.127) allows deriving the bound  $\|\phi_h\|_{L^2(\Omega_h)} \leq C^k \|\varphi\|_{L^2(\Omega_h)}$ , which results into the proof of the solution uniqueness. The proof is derived in details in Appendix D.4.

In order to prove that the solution  $\mathbf{G}_y$  is unique for a given  $\mathbf{y} \in X^{k+}$ , and that the solution is  $S_h(\mathbf{y}) = \mathbf{G}_y$ , let us assume that there are two distinct solutions  $\mathbf{G}_{y_1}, \mathbf{G}_{y_2}$  to the problem stated by Eq. (5.120), which results into

$$\begin{aligned} & \mathcal{A}(\mathbf{G}^e; \mathbf{I}_h \mathbf{G} - \mathbf{G}_{y_1}, \delta \mathbf{G}_h) + \mathcal{B}(\mathbf{G}^e; \mathbf{I}_h \mathbf{G} - \mathbf{G}_{y_1}, \delta \mathbf{G}_h) \\ &= \mathcal{A}(\mathbf{G}^e; \mathbf{I}_h \mathbf{G} - \mathbf{G}_{y_2}, \delta \mathbf{G}_h) + \mathcal{B}(\mathbf{G}^e; \mathbf{I}_h \mathbf{G} - \mathbf{G}_{y_2}, \delta \mathbf{G}_h) \quad \forall \delta \mathbf{G}_h \in X^k. \end{aligned} \quad (5.130)$$

For fixed  $\mathbf{G}^e$ ,  $\mathcal{A}$  and  $\mathcal{B}$  are bi-linear, therefore this last relation becomes

$$\mathcal{A}(\mathbf{G}^e; \mathbf{G}_{y_1} - \mathbf{G}_{y_2}, \delta \mathbf{G}_h) + \mathcal{B}(\mathbf{G}^e; \mathbf{G}_{y_1} - \mathbf{G}_{y_2}, \delta \mathbf{G}_h) = 0 \quad \forall \delta \mathbf{G}_h \in X^k. \quad (5.131)$$

Using Lemma 5.4.3, with  $\varphi = \delta \mathbf{G}_h = \mathbf{G}_{y_1} - \mathbf{G}_{y_2} \in X^k$  results in stating that there is a unique  $\Phi_h \in X^k$  solution of the problem Eq. (5.128), with for  $\delta \mathbf{G}_h = \mathbf{G}_{y_1} - \mathbf{G}_{y_2}$

$$\mathcal{A}(\mathbf{G}^e; \mathbf{G}_{y_1} - \mathbf{G}_{y_2}, \Phi_h) + \mathcal{B}(\mathbf{G}^e; \mathbf{G}_{y_1} - \mathbf{G}_{y_2}, \Phi_h) = \|\mathbf{G}_{y_1} - \mathbf{G}_{y_2}\|_{L^2(\Omega_h)}^2, \quad (5.132)$$

and with  $\|\|\Phi_h\|\| \leq C^k \|\mathbf{G}_{y_1} - \mathbf{G}_{y_2}\|_{L^2(\Omega_h)}$ . Choosing  $\delta \mathbf{G}_h$  as  $\Phi_h$  in Eq. (5.131), we have  $\|\mathbf{G}_{y_1} - \mathbf{G}_{y_2}\|_{L^2(\Omega_h)} = 0$ . Therefore, the solution  $S_h(\mathbf{y}) = \mathbf{G}_y$  is unique.

We will now show that  $S_h$  maps from a ball  $O_\sigma(\mathbf{I}_h \mathbf{G}) \subset X^{k+}$  into itself and is continuous in the ball. Therefore we define the ball  $O_\sigma$  with radius  $\sigma$  and centered at the interpolant  $\mathbf{I}_h \mathbf{G}$  of  $\mathbf{G}^e$  as

$$\begin{aligned} O_\sigma(\mathbf{I}_h \mathbf{G}) &= \left\{ \mathbf{y} \in X^{k+} \text{ such that } \|\|\mathbf{I}_h \mathbf{G} - \mathbf{y}\|\|_1 \leq \sigma \right\}, \\ &\text{with } \sigma = \frac{\|\|\mathbf{I}_h \mathbf{G} - \mathbf{G}^e\|\|_1}{h_s^\varepsilon}, \quad 0 < \varepsilon < \frac{1}{4}. \end{aligned} \quad (5.133)$$

The idea proposed in [25] is to work on a linearized problem in a ball  $O_\sigma(\mathbf{I}_h \mathbf{G}) \subset X^{k+}$  around an interpolant  $\mathbf{I}_h \mathbf{G}$  of  $\mathbf{G}^e$  so the nonlinear terms  $\mathbf{w}$  and  $\mathbf{d}$  and their derivatives are locally bounded in the ball  $O_\sigma(\mathbf{I}_h \mathbf{G}) \subset X^{k+}$ . Assuming  $\mathbf{G}^e \in \left[ H^{\frac{5}{2}}(\Omega) \right]^d \times H^{\frac{5}{2}}(\Omega) \times H^{\frac{5}{2}+}(\Omega)$ , and applying Lemma 2.4.6, Eq. (2.23) with  $s = \frac{5}{2}$ ,  $C_G = \|\mathbf{G}^e\|_{H^{\frac{5}{2}}(\Omega_h)}$ , and  $\mu = \frac{5}{2} = s$ , it follows that

$$\|\|\mathbf{I}_h \mathbf{G} - \mathbf{G}^e\|\|_1 \leq C^k h_s^{\frac{3}{2}} \|\mathbf{G}^e\|_{H^{\frac{5}{2}}(\Omega_h)} \quad \text{and} \quad \sigma \leq C^k C_G h_s^{\frac{3}{2}-\varepsilon} \quad \text{if } k \geq 2. \quad (5.134)$$

We can show that  $\mathbf{w}(\mathbf{x}; \mathbf{y}, \nabla \mathbf{y})$ ,  $\mathbf{w}_G(\mathbf{x}; \mathbf{y}, \nabla \mathbf{y})$ ,  $\mathbf{w}_{GG}(\mathbf{x}; \mathbf{y}, \nabla \mathbf{y})$ ,  $\mathbf{w}_{\nabla G}(\mathbf{x}; \mathbf{y})$ ,  $\mathbf{w}_{G\nabla G}(\mathbf{x}; \mathbf{y})$ ,  $\mathbf{o}(\mathbf{x}; \mathbf{y})$ ,  $\mathbf{o}_G(\mathbf{x}; \mathbf{y})$ ,  $\mathbf{d}(\mathbf{x}; \mathbf{y}, \nabla \mathbf{y})$ ,  $\mathbf{d}_G(\mathbf{x}; \mathbf{y}, \nabla \mathbf{y})$ ,  $\mathbf{d}_{GG}(\mathbf{x}; \mathbf{y}, \nabla \mathbf{y})$ ,  $\mathbf{d}_{\nabla G}(\mathbf{x}; \mathbf{y})$ ,  $\mathbf{d}_{G\nabla G}(\mathbf{x}; \mathbf{y})$  are bounded for  $\mathbf{x} \in \Omega$ ,  $\mathbf{y} \in O_\sigma(\mathbf{I}_h \mathbf{G})$ , by the same reasoning as in [76] and as explained in Chapter 4, which justifies Eq. (5.118).

**Lemma 5.4.4.** *Let  $\mathbf{y} \in O_\sigma(\mathbf{I}_h \mathbf{G})$  and  $\delta \mathbf{G}_h \in X^k$ , then the bound of the nonlinear term  $\mathcal{N}(\mathbf{G}^e, \mathbf{y}; \delta \mathbf{G}_h)$  defined in Eq. (5.114) reads*

$$\begin{aligned} |\mathcal{N}(\mathbf{G}^e, \mathbf{y}; \delta \mathbf{G}_h)| &\leq C^k C_y \|\mathbf{G}^e\|_{H^s(\Omega_h)} h_s^{\mu-2-\varepsilon} \sigma \left[ \|\delta \mathbf{G}_h\|_{H^1(\Omega_h)} + \left( \sum_e h_s \|\delta \mathbf{G}_h\|_{H^1(\partial\Omega^e)}^2 \right)^{\frac{1}{2}} + \right. \\ &\quad \left. \left( \sum_e h_s^{-1} \|\|\delta \mathbf{G}_{h_n}\|\|_{L^2(\partial\Omega^e)}^2 \right)^{\frac{1}{2}} \right]. \end{aligned} \quad (5.135)$$

This bound of the nonlinear term  $\mathcal{N}(\mathbf{G}^e, \mathbf{y}; \delta \mathbf{G}_h)$  defined Eq. (5.120) is derived in Appendix D.5 by bounding every term separately using Taylor series (5.107 and 5.109), the generalized Hölder inequality, the generalized Cauchy-Schwartz' inequality, the definition of  $C_y$  in Eq. (5.118), the definition of the ball, Eqs. (5.133, 5.134) and some other inequalities which are reported in Chapter 2, such as trace inequalities, Eqs. (2.16-2.18), inverse inequalities, Eqs. (2.19-2.21) for  $d = 2$ , and interpolation inequalities for  $d = 2$ , Eqs. (2.13-2.15). The proof follows from the argumentation reported in [25] and the bound of the nonlinear term  $\mathcal{N}(\mathbf{G}^e, \mathbf{y}; \delta \mathbf{G}_h)$  is nominated by the term with the largest bound, see Appendix D.5 for details.

Moreover, using the definition of the energy norm (2.12), this relation becomes

$$|\mathcal{N}(\mathbf{G}^e, \mathbf{y}; \delta \mathbf{G}_h)| \leq C^k C_y \|\mathbf{G}^e\|_{H^s(\Omega_h)} h_s^{\mu-2-\varepsilon} \sigma \|\delta \mathbf{G}_h\|_1, \quad (5.136)$$

which could be rewritten using Lemma 2.4.5 for the general case as

$$\begin{aligned} |\mathcal{N}(\mathbf{G}^e, \mathbf{y}; \delta \mathbf{G}_h)| &\leq C^k C_y \|\mathbf{G}^e\|_{H^s(\Omega_h)} h_s^{\mu-2-\varepsilon} \sigma \|\delta \mathbf{G}_h\| \\ &\leq C^k C_y C_G h_s^{\frac{1}{2}-\varepsilon} \sigma \|\delta \mathbf{G}_h\| \quad \text{if } k \geq 2. \end{aligned} \quad (5.137)$$

We now have the tools to demonstrate that  $S_h$  (i) maps from a ball  $O_\sigma(I_h \mathbf{G}) \subset X^{k+}$  into itself and (ii) is continuous in the ball.

**Theorem 5.4.5** ( $S_h$  maps  $O_\sigma(I_h \mathbf{G})$  into itself). *Let  $0 < h_s < 1$  and  $\sigma$  be defined by Eq. (5.134). Then  $S_h$  maps the ball  $O_\sigma(I_h \mathbf{G})$  into itself.*

$$\|\| I_h \mathbf{G} - \mathbf{G}_y \|\| \leq C^{k'} \sigma h_s^\varepsilon \text{ if } k \geq 2, \quad (5.138)$$

and for a mesh size  $h_s$  small enough and a given ball size  $\sigma$ ,  $I_h \mathbf{G} - \mathbf{G}_y \rightarrow 0$ , hence  $S_h$  maps  $O_\sigma(I_h \mathbf{G})$  to itself. The demonstration follows the same procedure as in the Theorem 4.4.6.

**Theorem 5.4.6** (The continuity of the map  $S_h$  in the ball  $O_\sigma(I_h \mathbf{G})$ ). *For  $\mathbf{y}_1, \mathbf{y}_2 \in O_\sigma(I_h \mathbf{G})$ , let  $\mathbf{G}_{y_1} = S_h(\mathbf{y}_1)$ ,  $\mathbf{G}_{y_2} = S_h(\mathbf{y}_2)$  be solutions of Eq. (5.120). Then for  $0 < h_s < 1$*

$$\|\| \mathbf{G}_{y_1} - \mathbf{G}_{y_2} \|\| \leq C^k C_y \|\mathbf{G}^e\|_{H^s(\Omega_h)} h_s^{\mu-2-\varepsilon} \|\| \mathbf{y}_1 - \mathbf{y}_2 \|\|. \quad (5.139)$$

Repeating the same argument as in Theorem 4.4.7, one can easily obtain the proof.

Using the Theorems 5.4.5, 5.4.6 of the map  $S_h$ , we can deduced that for all  $0 < h_s < 1$ , the maps  $S_h$  has a fixed point  $\mathbf{G}_h$  of the ball  $O_\sigma(I_h \mathbf{G})$ , and this fixed point is the solution of the nonlinear system of Eqs. (5.90).

#### 5.4.4 A priori error estimates

As  $S_h$  has a fixed point  $\mathbf{G}_h$ , we can use  $\mathbf{G}_h$  instead of  $\mathbf{G}_y$  in Eq. (5.138), hence we have

$$\|\| I_h \mathbf{G} - \mathbf{G}_h \|\| \leq C^{k'} \sigma h_s^\varepsilon = C^{k'} \|\| I_h \mathbf{G} - \mathbf{G}^e \|\|. \quad (5.140)$$

Now using this last relation, Lemma 2.4.5, Eq. (2.22), Lemma 2.4.6, Eq. (2.23), and Eq. (4.155) lead to

$$\begin{aligned} \|\| \mathbf{G}^e - \mathbf{G}_h \|\|_1 &\leq \|\| \mathbf{G}^e - I_h \mathbf{G} \|\|_1 + \|\| I_h \mathbf{G} - \mathbf{G}_h \|\|_1 \leq \|\| \mathbf{G}^e - I_h \mathbf{G} \|\|_1 + C^{k'} \|\| I_h \mathbf{G} - \mathbf{G}^e \|\|_1 \\ &\leq (1 + C^{k'}) \|\| \mathbf{G}^e - I_h \mathbf{G} \|\|_1 \leq C^{k''} h_s^{\mu-1} \|\mathbf{G}^e\|_{H^s(\Omega_h)}, \end{aligned} \quad (5.141)$$

where  $\mu = \min \{s, k + 1\}$ , and  $C^{k''} = C^k(1 + C^{k'})$ . This shows that the error estimate is optimal in  $h_s$ .

#### 5.4.5 Error estimate in the $L^2$ -norm

The optimal order of convergence in the  $L^2$ -norm is obtained by applying the duality argument. Thereby, let us consider the following dual problem

$$\begin{aligned} -\nabla^T(\mathbf{w}_{\nabla\mathbf{G}}(\mathbf{G}^e)\nabla\boldsymbol{\psi} + \mathbf{d}_{\nabla\mathbf{G}}^T(\mathbf{G}^e)\boldsymbol{\psi}) + \mathbf{w}_{\mathbf{G}}^T(\mathbf{G}^e, \nabla\mathbf{G}^e)\nabla\boldsymbol{\psi} + \mathbf{d}_{\mathbf{G}}(\mathbf{G}^e, \nabla\mathbf{G}^e)\boldsymbol{\psi} &= \mathbf{e} \text{ on } \Omega, \\ \boldsymbol{\psi} &= \mathbf{g} \text{ on } \partial\Omega, \end{aligned} \quad (5.142)$$

which is assumed to satisfy the elliptic regularity condition as  $\mathbf{w}_{\nabla\mathbf{G}}$  is positive definite and that  $\mathbf{d}_{\nabla\mathbf{G}}^T$  and  $\mathbf{d}_{\mathbf{G}}$  satisfy the weak minimum principle [23, Theorem 8.3], with  $\boldsymbol{\psi} \in [H^{2m}(\Omega_h)]^d \times H^{2m}(\Omega_h) \times H^{2m}(\Omega_h)$  for  $p \geq 2m$  and

$$\|\boldsymbol{\psi}\|_{\mathbf{H}^p(\Omega_h)} \leq C \left( \|\mathbf{e}\|_{\mathbf{H}^{p-2m}(\Omega_h)} + \|\mathbf{g}\|_{\mathbf{H}^{p-\frac{1}{2}}(\partial\Omega_h)} \right), \quad (5.143)$$

if  $\mathbf{e} \in [H^{p-2m}(\Omega_h)]^d \times H^{p-2m}(\Omega_h) \times H^{p-2m}(\Omega_h)$ .

Considering  $\mathbf{e} = \mathbf{G}^e - \mathbf{G}_h \subset [L^2(\Omega_h)]^d \times L^2(\Omega_h) \times L^2(\Omega_h)$  be the error and  $\mathbf{g} = 0$ , multiplying Eq. (5.142) by  $\mathbf{e}$ , and integrating over  $\Omega_h$ , yields

$$\begin{aligned} &\int_{\Omega_h} [\mathbf{w}_{\nabla\mathbf{G}}(\mathbf{G}^e)\nabla\boldsymbol{\psi}]^T \nabla\mathbf{e} d\Omega + \int_{\Omega_h} [\mathbf{d}_{\nabla\mathbf{G}}^T(\mathbf{G}^e)\boldsymbol{\psi}]^T \nabla\mathbf{e} d\Omega + \int_{\Omega_h} [\mathbf{w}_{\mathbf{G}}^T(\mathbf{G}^e, \nabla\mathbf{G}^e)\nabla\boldsymbol{\psi}]^T \mathbf{e} d\Omega \\ &+ \int_{\Omega_h} [\mathbf{d}_{\mathbf{G}}(\mathbf{G}^e, \nabla\mathbf{G}^e)\boldsymbol{\psi}]^T \mathbf{e} d\Omega - \sum_e \int_{\partial\Omega^e} [\mathbf{w}_{\nabla\mathbf{G}}(\mathbf{G}^e)\nabla\boldsymbol{\psi}]^T \mathbf{e}_n dS \\ &- \sum_e \int_{\partial\Omega^e} [\mathbf{e}_n^T \mathbf{d}_{\nabla\mathbf{G}}^T(\mathbf{G}^e)] \boldsymbol{\psi} dS = \|\mathbf{e}\|_{L^2(\Omega_h)}^2, \end{aligned} \quad (5.144)$$

with

$$\|\boldsymbol{\psi}\|_{H^2(\Omega_h)} \leq C \|\mathbf{e}\|_{L^2(\Omega_h)}. \quad (5.145)$$

As  $[\boldsymbol{\psi}] = [\nabla\boldsymbol{\psi}] = 0$  on  $\partial_I\Omega_h$  and  $\boldsymbol{\psi} = 0$  on  $\partial_D\Omega_h$ , we have by comparison with Eqs. (5.115-5.116), that

$$\begin{cases} \int_{\Omega_h} [\mathbf{w}_{\nabla\mathbf{G}}(\mathbf{G}^e)\nabla\boldsymbol{\psi}]^T \nabla\mathbf{e} d\Omega + \int_{\partial_I\Omega_h} [\mathbf{w}_{\nabla\mathbf{G}}(\mathbf{G}^e)\nabla\boldsymbol{\psi}]^T [\mathbf{e}_n] dS \\ - \int_{\partial_D\Omega_h} [\mathbf{w}_{\nabla\mathbf{G}}(\mathbf{G}^e)\nabla\boldsymbol{\psi}]^T \mathbf{e}_n dS = \mathcal{A}(\mathbf{G}^e; \mathbf{e}, \boldsymbol{\psi}), \\ \int_{\Omega_h} [\mathbf{w}_{\mathbf{G}}(\mathbf{G}^e, \nabla\mathbf{G}^e)\mathbf{e}]^T \nabla\boldsymbol{\psi} d\Omega + \int_{\Omega_h} [\mathbf{d}_{\mathbf{G}}(\mathbf{G}^e, \nabla\mathbf{G}^e)\boldsymbol{\psi}]^T \mathbf{e} d\Omega \\ + \int_{\Omega_h} [\mathbf{d}_{\nabla\mathbf{G}}^T(\mathbf{G}^e)\boldsymbol{\psi}]^T \nabla\mathbf{e} d\Omega + \int_{\partial_I\Omega_h} [\mathbf{e}_n^T \mathbf{d}_{\nabla\mathbf{G}}^T(\mathbf{G}^e)] \boldsymbol{\psi} dS \\ - \int_{\partial_D\Omega_h} \mathbf{e}_n^T \mathbf{d}_{\nabla\mathbf{G}}^T(\mathbf{G}^e)\boldsymbol{\psi} dS = \mathcal{B}(\mathbf{G}^e; \mathbf{e}, \boldsymbol{\psi}), \end{cases} \quad (5.146)$$

as  $\mathbf{w}_{\mathbf{G}}$ ,  $\mathbf{w}_{\nabla\mathbf{G}}$  are symmetric. Therefore, Eq. (5.144) reads

$$\|\mathbf{e}\|_{L^2(\Omega_h)}^2 = \mathcal{A}(\mathbf{G}^e; \mathbf{e}, \boldsymbol{\psi}) + \mathcal{B}(\mathbf{G}^e; \mathbf{e}, \boldsymbol{\psi}). \quad (5.147)$$

From Eq. (5.117), one has

$$\mathcal{A}(\mathbf{G}^e; \mathbf{G}^e - \mathbf{G}_h, \mathbf{I}_h \boldsymbol{\psi}) + \mathcal{B}(\mathbf{G}^e; \mathbf{G}^e - \mathbf{G}_h, \mathbf{I}_h \boldsymbol{\psi}) = \mathcal{N}(\mathbf{G}^e, \mathbf{G}_h; \mathbf{I}_h \boldsymbol{\psi}), \quad (5.148)$$

since  $\mathbf{G}^e$  is the exact solution and  $\mathbf{I}_h \boldsymbol{\psi} \in \mathbf{X}^k$ , and Eq. (5.147) is rewritten

$$\| \mathbf{e} \|_{\mathbf{L}^2(\Omega_h)}^2 = \mathcal{A}(\mathbf{G}^e; \mathbf{e}, \boldsymbol{\psi} - \mathbf{I}_h \boldsymbol{\psi}) + \mathcal{B}(\mathbf{G}^e; \mathbf{e}, \boldsymbol{\psi} - \mathbf{I}_h \boldsymbol{\psi}) + \mathcal{N}(\mathbf{G}^e, \mathbf{G}_h; \mathbf{I}_h \boldsymbol{\psi}). \quad (5.149)$$

First, using Lemma 5.4.2, Eq. (5.123), Lemma 2.4.6, Eq. (2.23), and Eq. (5.141), leads to

$$\begin{aligned} | \mathcal{A}(\mathbf{G}^e; \mathbf{e}, \boldsymbol{\psi} - \mathbf{I}_h \boldsymbol{\psi}) + \mathcal{B}(\mathbf{G}^e; \mathbf{e}, \boldsymbol{\psi} - \mathbf{I}_h \boldsymbol{\psi}) | &\leq C^k \| \mathbf{e} \|_1 \| \boldsymbol{\psi} - \mathbf{I}_h \boldsymbol{\psi} \|_1 \\ &\leq C^k \| \mathbf{e} \|_1 h_s \| \boldsymbol{\psi} \|_{\mathbf{H}^2(\Omega_h)} \\ &\leq C^{k''} h_s^\mu \| \mathbf{G}^e \|_{\mathbf{H}^s(\Omega_h)} \| \boldsymbol{\psi} \|_{\mathbf{H}^2(\Omega_h)}, \end{aligned} \quad (5.150)$$

with  $\mu = \min \{s, k + 1\}$ .

Then proceeding as for establishing Lemma 5.4.4 and using the a priori error estimate (5.140-5.141), we have

$$| \mathcal{N}(\mathbf{G}^e, \mathbf{G}_h; \mathbf{I}_h \boldsymbol{\psi}) | \leq C^{k''} C_y h_s^{2\mu-3} \| \mathbf{G}^e \|_{\mathbf{H}^s(\Omega_h)}^2 \| \mathbf{I}_h \boldsymbol{\psi} \|_1. \quad (5.151)$$

The bound of  $| \mathcal{N}(\mathbf{G}^e, \mathbf{G}_h; \mathbf{I}_h \boldsymbol{\psi}) |$  can be derived in the same way as Eq. (4.166) as reported in Appendix C.9.

Finally, using Lemma 2.4.6, Eq. (2.23), remembering  $[[\boldsymbol{\psi}]] = 0$  in  $\Omega$ , we deduce that

$$\begin{aligned} \| \mathbf{I}_h \boldsymbol{\psi} \|_1 &\leq \| \mathbf{I}_h \boldsymbol{\psi} - \boldsymbol{\psi} \|_1 + \| \boldsymbol{\psi} \|_1 \\ &\leq C^k h_s \| \boldsymbol{\psi} \|_{\mathbf{H}^2(\Omega_h)} + \| \boldsymbol{\psi} \|_{\mathbf{H}^1(\Omega_h)} \\ &\leq C^k (h_s + 1) \| \boldsymbol{\psi} \|_{\mathbf{H}^2(\Omega_h)}. \end{aligned} \quad (5.152)$$

Combining Eqs. (5.150-5.152), Eq. (5.149) becomes, for  $\mu \geq 3$

$$\| \mathbf{e} \|_{\mathbf{L}^2(\Omega_h)}^2 \leq C^{k''} h_s^\mu (1 + \| \mathbf{G}^e \|_{\mathbf{H}^s(\Omega_h)}) \| \mathbf{G}^e \|_{\mathbf{H}^s(\Omega_h)} \| \boldsymbol{\psi} \|_{\mathbf{H}^2(\Omega_h)}, \quad (5.153)$$

with  $\mu = \min \{s, k + 1\}$ , or using Eq. (5.145), the final result for  $k \geq 2$

$$\| \mathbf{e} \|_{\mathbf{L}^2(\Omega_h)} \leq C^{k''} C_G h_s^\mu \| \mathbf{G}^e \|_{\mathbf{H}^s(\Omega_h)}. \quad (5.154)$$

This result demonstrates the optimal convergence rate of the method with the mesh-size for cases in which  $k \geq 2$ , (so that  $\mu \geq 3$ ).

## 5.5 Numerical results

In this section the following numerical tests are performed: the 2D pipe for the convergence verification of Electro-Thermo-Elasticity problem, and the 3D cell of polymer reinforced by carbon fibers, where the behavior of that composite material is studied when it is driven by applying electric current. All the simulations are performed using polynomial of second degree and stabilization parameter of value  $\beta = 100$ .

### 5.5.1 2-D study of convergence order

The same quarter of the pipe as in Chapter 3 is considered for the convergence study. The material parameters are reported in Table 5.1 and the boundary conditions are presented in Fig. 5.1 and completed by a plane strain condition. The initial value for the temperature is  $T_0 = 20$  [°C] and  $V_0 = 0$  [V] for the electric potential. The same mesh as shown in Fig. 3.2 is considered. At the inner boundary, the value of the electric potential is 0.05 [V], Fig. 5.1. The resulting electric potential distribution is shown in Fig. 5.2(a) and causes a gradual increase in temperature from 20 [°C] at the inner face to 145.7 [°C] at the outer face, as shown in Fig. 5.2(b). Consequently, an expansion of the pipe of  $6.35 \times 10^{-4}$  [cm] at the outer radius is observed.

Table 5.1: Material parameters

Parameter	Value
Poisson ratio[-]	0.33
Young's modulus E [Pa]	$50 \times 10^9$
Thermal expansion $\alpha_{\text{th}}$ [1/K]	diag( $2 \times 10^{-6}$ )
Thermal conductivity $\mathbf{k}$ [W/(K · m)]	diag(1.612)
Seebeck coefficient $\alpha$ [S/m]	$1.941 \times 10^{-4}$
Electrical conductivity $\mathbf{l}$ [V/K]	diag( $8.422 \times 10^4$ )

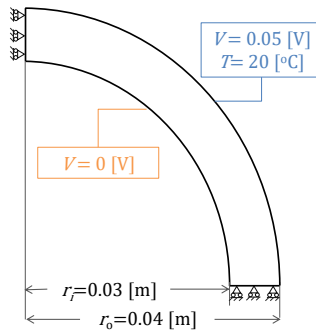


Figure 5.1: The boundary conditions for a quarter of a pipe

The convergence of the DGFEM has been investigated on uniform meshes for the quadratic polynomial degree  $k = 2$ . In Fig. 5.3(a) the error measured in the energy norm  $\| \mathbf{e} \|$  is plotted against the mesh size  $h_s$ . The observed rate is quadratic. This optimal result agrees with our theoretical estimate in Section 5.4.4.

A refinement of the mesh, together with the use of second order-degree polynomial, leads to the  $L^2$ -norm to converge with a rate  $h_s^3$  as this can be seen in Fig. 5.3(b). The theoretical result of Section 5.4.5 is consequently validated.

### 5.5.2 3-D unit cell simulation

The same test as in Chapter 4 is applied. The boundary conditions are illustrated in Fig. 5.4, where the electric potential difference is applied on the transverse direction (a)

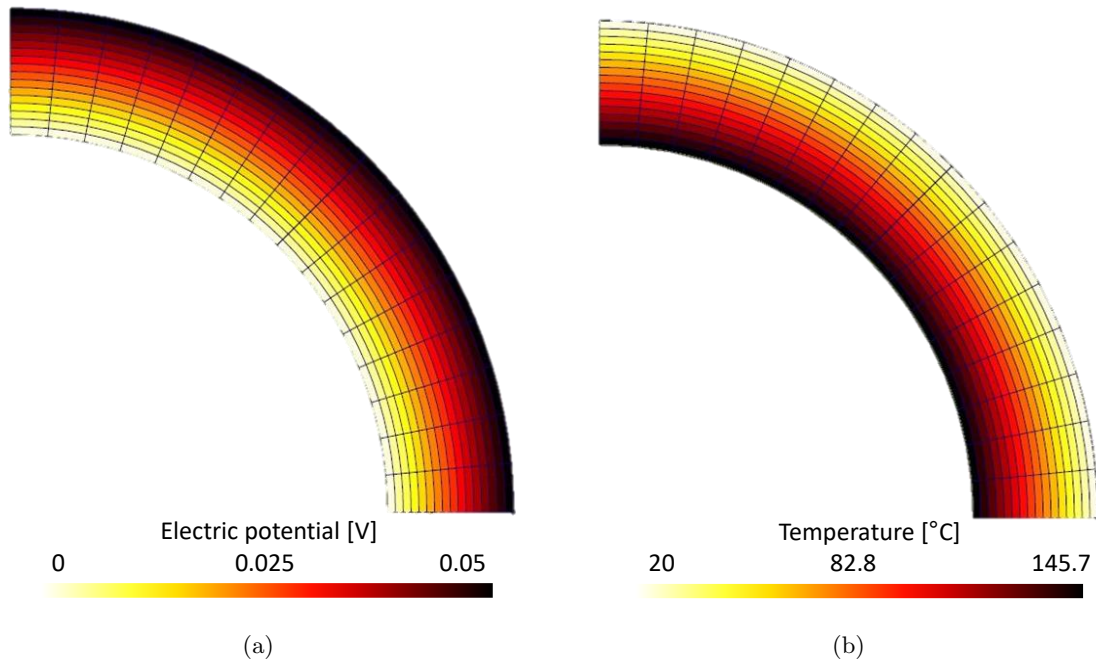


Figure 5.2: The distribution along the radius of (a) the electric potential and (b) the temperature

and on the longitudinal direction (b). The displacement is constrained along three faces as follows: the nodes in the XY-plane are fixed in the Z-direction, the nodes in the YZ-plane are fixed in the X-direction, and the nodes in the XZ-plane are fixed in the Y-direction, while the other three faces are restrained in order to get a uniform deformation, the top face is restrained in the Z direction, the infront face is restrained in the Y direction and the right face is restrained in the X direction. Finally the initial values for the temperature and electric potential are  $T_0 = 5$  [°C] and  $V_0 = 0$  [V] respectively. The material properties of the polymers and carbon fibers are presented respectively in Tables 6.1 and 6.2. It should be noted that the considered constitutive equations of the carbon fiber and shape memory polymer, are presented in the following Chapter. The temperatures for the tests presented in this Chapter remain lower than the glass transition temperature. However more tests that involve SMP behavior above and below glass transition temperature will be presented in the next Chapter.

For the transverse case, Fig. 5.4(a), the distribution of electric potential and temperature are given in Figs. 5.5. When an electric potential of 11 [V] is applied the temperature increases from 5 [°C] to 35 [°C] on the unconstrained face, where the temperature is restrained on this right face to get uniform distribution for the temperature. The displacement is measured with respect to the right side of the cell, and the cell expansion due to the electric potential increase is plotted in Fig. 5.7(a).

The same test is performed with an electric potential applied in the longitudinal direction. The boundary conditions are shown in Fig. 5.4(b). It can be seen that in order to get an increase in temperature close to the one of the previous test, from 5 [°C] to 36.4 [°C], an electric potential of 0.16 [V] has been applied, as shown in Fig. 5.6, where a constrain is



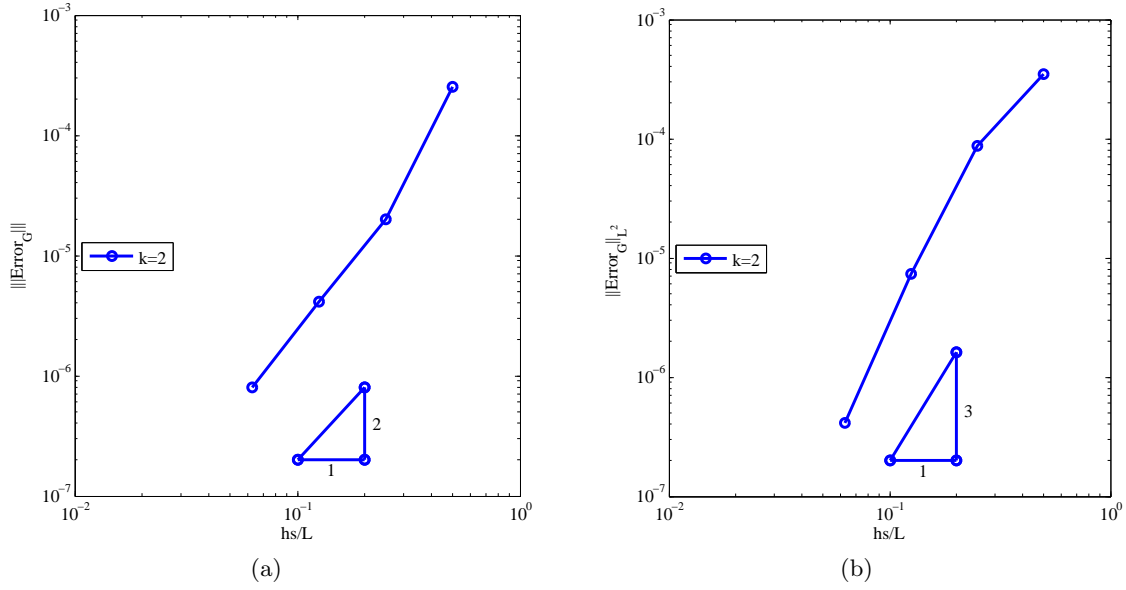


Figure 5.3: Error with respect to the mesh size. (a) The energy error, and (b) The error of the fields

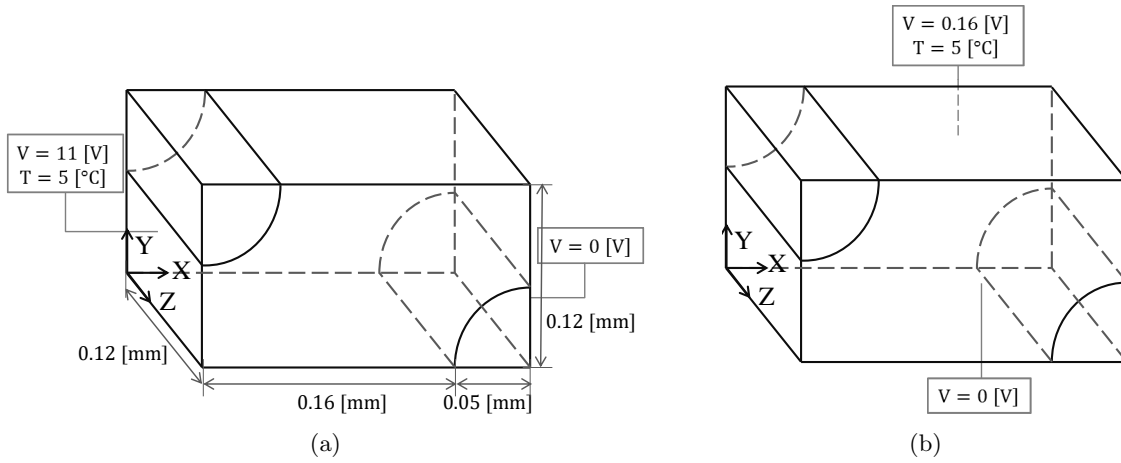


Figure 5.4: Boundary conditions applied in (a) the transversal direction, and (b) the longitudinal direction

applied on the infront face to get a uniform temperature distribution on that face. This is lower than the previous test. The strain/electric potential dependency is depicted in Fig. 5.7(b).

## 5.6 Conclusions

Throughout this chapter, the DG method has been studied for a coupled Electro-Thermo-Mechanical problem. We have established the stability and uniqueness of the DG analytical

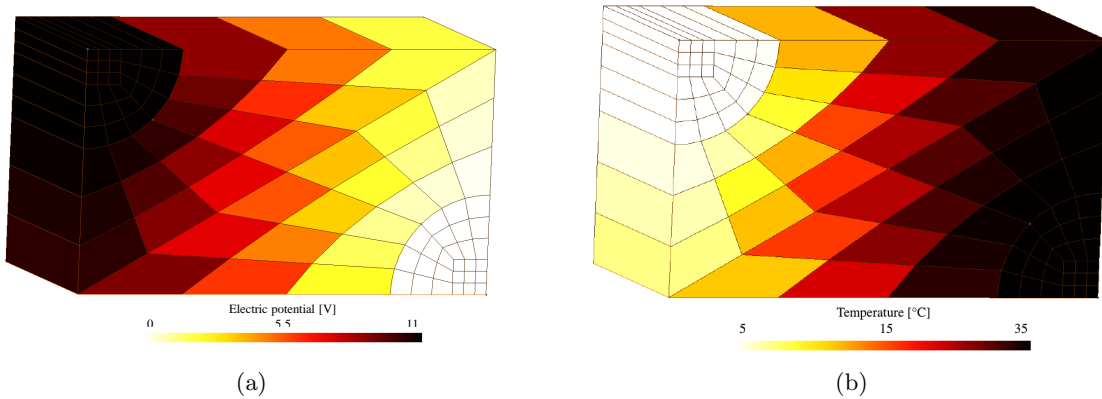


Figure 5.5: The distribution of the unit cell of (a) the electric potential, and (b) the temperature, for an electric potential difference applied on the transversal direction

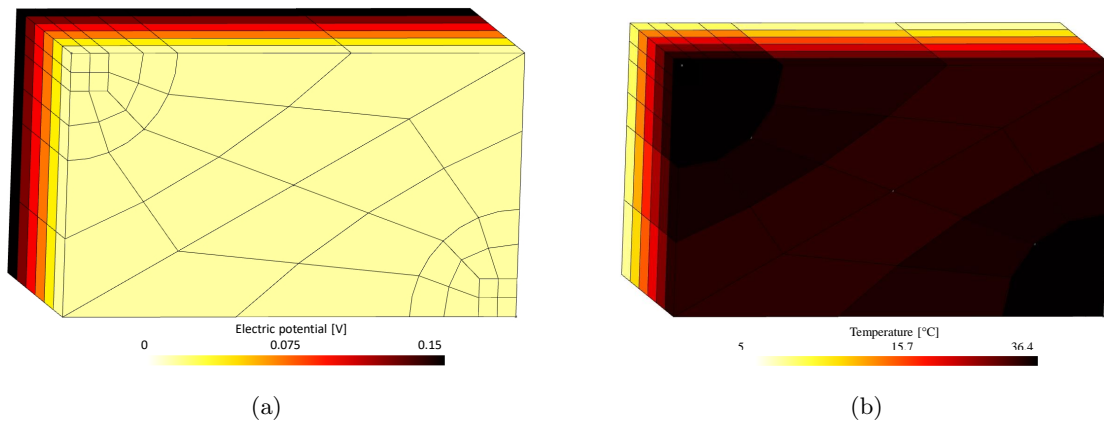
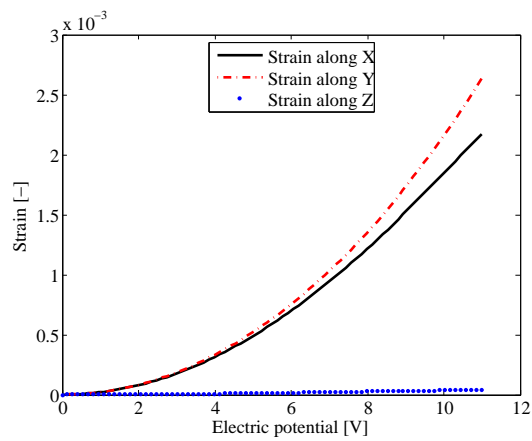
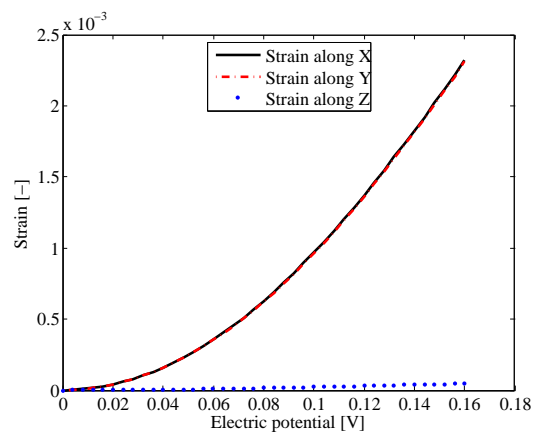


Figure 5.6: The distribution of the unit cell of (a) the electric potential, and (b) the temperature, for an electric potential difference applied on the longitudinal direction

approximated solution, as well as the optimal convergence order in both  $H^1$ - and  $L^2$ -norms for small deformation problems and have verified these properties through numerical simulations. A micromechanical model of unidirectional carbon fibers embedded in a polymer matrix is formulated considering the interaction of electrical, thermal, and mechanical fields. The applicability of the DG method to coupled ETM problems is therefore verified, thus making possible to predict the carbon fiber reinforced polymers behavior.



(a)



(b)

Figure 5.7: The engineering strain versus electric potential difference applied in the (a) transversal direction, and (b) longitudinal directions (the strain along x superposes the strain along y)



## Chapter 6

# The constitutive laws of smart composite materials

### 6.1 Introduction

Nowadays, most of the material surrounding us are made of different components to improve the physical properties of the resulting material, for example carbon fiber reinforced polymer composites which have increasingly become important due to their unique properties, as they combine the favorite characteristics of the both materials. In the construction of fiber reinforced composite material, the high strength and stiffness of the carbon fibers are combined with a low density stable matrix to create a combined material with desirable material properties. Our choice for the fiber and the polymers, as discussed in Chapter 1, is shape memory polymers reinforced by carbon fiber (SMPC).

The two most common uses for carbon fiber are in applications where high strength to weight and high stiffness to weight ratios are desirable. These include aerospace structures, wind turbines, military structures, robotics, manufacturing fixtures, sports equipment, and many others. Certain applications also exploit carbon fiber electrical conductivity, as well as their high thermal conductivity in the case of specialized carbon fiber.

Shape memory polymer is polymer having the ability to return from a deformed state to its original shape, in other word, to remember the original shape. Starting from its primary shape, deforming it into a temporary shape, it memorizes a macroscopic shape and returns into its primary shape upon applying a particular stimulus such as temperature, electric field, magnetic field, light, water or solvent. This ability of the material reverting back from its temporary shape to its permanent shape is known as shape memory effect (SME). In this work, we are interested in the thermal activation mechanism. These polymers take advantage of a property change at the glass transition temperature  $T_g$ , such that the material can be deformed with minimal force at temperatures above their  $T_g$  (hysteretic rubber state), where the polymers are considered as viscous materials. Once cooled below the  $T_g$  (glassy state) the SMPs become rigid again and the polymers are considered as elastic materials. As a result they can maintain the shape that were given to them in their viscous states as long as the temperature remains lower than their glass transition. The typical Thermo-Mechanical cycle for SMP consists of the following steps as shown in Fig. 6.1

1. Deforming the polymer at temperature above the glass transition  $T_g$ .

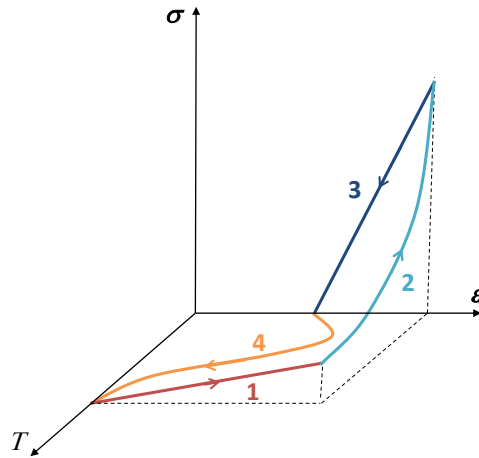


Figure 6.1: Thermo-Mechanical cycle of a Shape Memory Polymer

2. Fixing the polymer at constant deformation by cooling it to a temperature below  $T_g$
3. Releasing the constraint upon the completion of cooling, to obtain the temporary pre-deformed shape. The polymer will hold this temporary shape as long as the temperature remains lower than the glass transition temperature.
4. Heating back the deformed structure above  $T_g$ , to recover the original shape

The objective of this chapter is to implement, modify and develop large deformation constitutive theories and a numerical FE model able to model the response of Shape Memory Polymers (SMPs) and Shape Memory Polymers composites (SMPC) subjected to a variety of Thermo-Mechanical and Electro-Thermo-Mechanical histories.

The composite material system is obtained by defining two separate models, one for carbon fiber and another one for shape memory polymers. For carbon fiber the transversely isotropic hyperelastic model is considered while an elasto-visco-plastic model is considered for the shape memory polymers.

The Thermo-Mechanical behaviors of shape memory polymer depend on the temperature and time rate. Auxiliary studies have examined the numerical Thermo-Mechanical constitutive modeling [7, 8, 10, 44, 61, 68, 71] of shape memory polymers. The aforementioned fundamental studies have been instrumental in understanding and quantifying the response of unreinforced shape memory polymers. The constitutive model proposed by Srivastava et al. [68] is based on the glass transition concept. The material is assumed to be softer in the rubber regime above  $T_g$  and to be harder in the glassy polymer regime below  $T_g$ . During the phase transition, part of the material is in the glassy state and the other is in the rubbery state. Internal variables and constraints have been used to prescribe the transition between the two phases. This constitutive theory is discussed for application to amorphous polymers which are called amorphous thermosets that are chemically crosslinked shape memory polymers, which have more desirable properties in comparison with thermoplastic when they are physically crosslinked. This constitutive model is able to reproduce the fundamental features of the macroscopic stress-strain response of the material in the two phases.

In addition this formulation is able to predict the nonlinear history and strain rate dependence at large strain.

The current chapter is organized in the following sections. In Section 6.2 the constitutive equation proposed in [11] of carbon fiber is presented and extended to Thermo-Elasticity, and in Section 6.3 the constitutive equation for SMP is derived following the model of Srivastava et al. [68]. Afterward, numerical tests are carried out in Section 6.4 to show the capabilities of the constitutive laws in predicting the shape memory polymers and shape memory polymer composites behaviors. The two uniaxial compression tests of shape memory polymer are performed, one with free recovery and the other with constrained recovery. Then the third uniaxial compression test shows the different responses of SMP in terms of temperature and strain rate changes, and the model predictions are compared with the available numerical and experimental results. Finally, other compression and bending tests are applied to simulate the behavior of a structure made of conductive SMPC behavior in the large-deformation regime, in which the shape memory effect is triggered by applying an indirect heat (by means of a low electric field).

## 6.2 Material model of carbon fiber

Carbon fiber is a transversely isotropic material and subsequently the number of mechanical constants are reduced to 5 because of the in-plane isotropy.

$$\begin{aligned} E^T &= E_1 = E_2 \neq E_3 = E^L, & \nu^{TT} &= \nu_{12} = \nu_{21} \neq \nu_{13} = \nu_{23} = \nu^{TL} \\ G^{LT} &= G_{13} = G_{23} = G_3 = G^L. \end{aligned} \quad (6.1)$$

The missing in-plane shear modulus  $G^{TT}$  is obtained from  $\nu^{TT}$  and  $E^T$ , with

$$G^{TT} = G_{12} = \frac{E^T}{2(1 + \nu^{TT})}. \quad (6.2)$$

In the previous relation, the subscript 3 or the superscript L refers to the fiber direction and 1, 2, or T is a direction transverse to the fiber direction. Along the longitudinal direction the Poisson ratios are not symmetric but instead satisfy  $\frac{\nu_{ij}}{E_i} = \frac{\nu_{ji}}{E_j}$ .

In order to model the carbon fiber, we have considered the equation proposed by Bonet et al. [11], which describes the isotropic hyperelastic solids in the large strain regime. In addition, we have added the thermal contribution, characterized by the thermal expansion term  $\alpha_{th}$ . In this formulation, the strain energy density  $\psi$  consists of an isotropic component  $\psi^{is}$  and of an orthotropic transversely isotropic component  $\psi^{tr}$  such that  $\psi = \psi^{is} + \psi^{tr}$ . The Neo-Hookean equation is used to model the isotropic part, such that

$$\psi^{is} = \frac{1}{2}G^{TT}(\text{tr}\mathbf{C} - 3) - G^{TT}(\ln J - 3\alpha_{th}(T - T_0)) + \frac{1}{2}\lambda(\ln J - 3\alpha_{th}(T - T_0))^2, \quad (6.3)$$

where this energy density function has been defined by C. Miehe in [54]. In this equation, the deformation gradient  $\mathbf{F}$ , with  $J = \det\mathbf{F} = \sqrt{\det\mathbf{C}}$ , its Jaccobian.

The orthotropic transversely isotropic component is obtained from a generalization of the model proposed by Bonet et al. [11], with some modifications proposed by Wu et al. [75],

as the original formulation considered that  $\nu^{\text{TL}} = \nu^{\text{TT}}$ , which is wrong for carbon fibers. After the addition of the thermal contribution, one thus has

$$\psi^{\text{tr}} = [\alpha^{\text{trn}} + 2\beta^{\text{trn}}(\ln J - 3\alpha_{\text{th}}(T - T_0)) + \gamma^{\text{trn}}(I_4 - 1)](I_4 - 1) - \frac{1}{2}\alpha^{\text{trn}}(I_5 - 1), \quad (6.4)$$

where  $I_4$  and  $I_5$  denote the two new pseudo invariants of  $\mathbf{C}$  expressed as [66, 67],

$$I_4 = \mathbf{A} \cdot \mathbf{C} \cdot \mathbf{A} \quad \text{and} \quad I_5 = \mathbf{A} \cdot \mathbf{C}^2 \cdot \mathbf{A}, \quad (6.5)$$

where the unit vector  $\mathbf{A}$  defines the main direction of orthotropy (fiber direction) in the undeformed configuration.

The parameters of the model Eq. (6.4),  $\lambda$ ,  $\mathbf{G}^{\text{TT}}$ ,  $\alpha^{\text{tr}}$ ,  $\beta^{\text{tr}}$  and  $\gamma^{\text{tr}}$  are obtained from the measured properties Eqs. (6.1, 6.2) as

$$\begin{aligned} \lambda &= \frac{\mathbf{E}^{\text{T}}(\nu^{\text{TT}} + n\nu^{\text{TL}^2})}{m(1 + \nu^{\text{TT}})}, \quad \mathbf{G}^{\text{TT}} = \frac{\mathbf{E}^{\text{T}}}{2(1 + \nu^{\text{TT}})}, \\ \alpha^{\text{tr}} &= \mathbf{G}^{\text{TT}} - \mathbf{G}^{\text{LT}} \\ \beta^{\text{tr}} &= \frac{\mathbf{E}^{\text{T}} [n\nu^{\text{TL}}(1 + \nu^{\text{TT}} - \nu^{\text{TL}}) - \nu^{\text{TT}}]}{4m(1 + \nu^{\text{TT}})}, \\ \gamma^{\text{tr}} &= \frac{\mathbf{E}^{\text{T}}(1 - \nu^{\text{TT}})}{8m} - \frac{\lambda + 2\mathbf{G}^{\text{TT}}}{8} + \frac{\alpha^{\text{tr}}}{2} - \beta^{\text{tr}}, \\ m &= 1 - \nu^{\text{TT}} - 2n\nu^{\text{TT}^2}, \quad n = \frac{\mathbf{E}^{\text{L}}}{\mathbf{E}^{\text{T}}}. \end{aligned} \quad (6.6)$$

The second Piola-Kirchhoff stress tensor can be obtained by differentiating the free energy in terms of the right Cauchy-Green strain tensor  $\mathbf{S} = 2\frac{\partial\psi}{\partial\mathbf{C}}$  leading to

$$\mathbf{S} = \mathbf{S}^{\text{is}} + \mathbf{S}^{\text{tr}}, \quad (6.7)$$

$$\mathbf{S}^{\text{is}} = \lambda \ln J \mathbf{C}^{-1} + \mathbf{G}^{\text{TT}}(\mathbf{I} - \mathbf{C}^{-1}) - 3\lambda\alpha_{\text{th}}(T - T_0)\mathbf{C}^{-1}, \quad (6.8)$$

where  $\mathbf{I}$  is the identity tensor, and with

$$\begin{aligned} \mathbf{S}^{\text{tr}} &= 2\beta^{\text{tr}}(I_4 - 1)\mathbf{C}^{-1} + 2[\alpha^{\text{tr}} + 2\beta^{\text{tr}}(\ln J - 3\alpha_{\text{th}}(T - T_0)) + 2\gamma^{\text{tr}}(I_4 - 1)]\mathbf{A} \otimes \mathbf{A} \\ &\quad - \alpha^{\text{tr}}(\mathbf{C} \cdot \mathbf{A} \otimes \mathbf{A} + \mathbf{A} \otimes \mathbf{C} \cdot \mathbf{A}). \end{aligned} \quad (6.9)$$

Then the first Piola-Kirchhoff stress tensor is evaluated from the second Piola-Kirchhoff stress tensor as

$$\mathbf{P} = \mathbf{F}\mathbf{S}. \quad (6.10)$$

The stiffness is computed in detail in Appendix E.1.

### 6.3 Constitutive equations of shape memory polymer

In this Section, we summarize the work of Srivastava et al. [68] to model the shape memory polymer behavior above and below glass transition.



### 6.3.1 Kinematics

We consider a homogeneous body  $\Omega_0$  identified by the region of space it occupies in a fixed reference configuration, and denote by  $\mathbf{X}$  an arbitrary material point of  $\Omega_0$ . A motion of  $\Omega_0$  is then a smooth one-to-one mapping

$$\mathbf{x} = \mathbf{x}(\mathbf{X}, t), \quad (6.11)$$

with the deformation gradient

$$\mathbf{F} = \nabla_0 \mathbf{x}. \quad (6.12)$$

To model the inelastic response of the amorphous polymeric materials, we assume that the deformation gradient  $\mathbf{F}$  may be multiplicatively decomposed into elastic and plastic parts

$$\mathbf{F} = \mathbf{F}^{e(\alpha)} \cdot \mathbf{F}^{p(\alpha)} \text{ with } \det \mathbf{F}^{e(\alpha)} > 0 \text{ and } \det \mathbf{F}^{p(\alpha)} > 0, \quad (6.13)$$

where  $\mathbf{F}^{e(\alpha)}$  is the elastic distortion with

$$J^{e(\alpha)} = \det \mathbf{F}^{e(\alpha)} = J > 0, \quad (6.14)$$

and  $\mathbf{F}^{p(\alpha)}$  is the inelastic distortion with

$$J^{p(\alpha)} = \det \mathbf{F}^{p(\alpha)} = 1 \text{ with initial value } \mathbf{F}^{p(\alpha)}(\mathbf{X}, 0) = \mathbf{I}. \quad (6.15)$$

In these equations we have considered the possibility to account for several mechanisms  $\alpha = 1, 2, 3$ . Moreover, the elastic decomposition of the deformation gradient can be written as

$$\mathbf{F}^{e(\alpha)} = \mathbf{R}^{e(\alpha)} \cdot \mathbf{U}^{e(\alpha)}, \quad (6.16)$$

leading to

$$\mathbf{C}^{e(\alpha)} = \mathbf{U}^{e(\alpha)2} = \mathbf{F}^{e(\alpha)T} \cdot \mathbf{F}^{e(\alpha)}, \quad (6.17)$$

where  $\mathbf{C}^{e(\alpha)}$  is the elastic right Cauchy-Green strain tensor, and to

$$\mathbf{B}^{e(\alpha)} = \mathbf{F}^{e(\alpha)} \cdot \mathbf{F}^{e(\alpha)T}, \quad (6.18)$$

where  $\mathbf{B}^{e(\alpha)}$  is the elastic left Cauchy-Green strain tensor.

### 6.3.2 Elasto-visco-plasticity

The material may be idealized to be isotropic. Accordingly, all constitutive functions are presumed to be isotropic in character.

Let us assume that the free energy has the separable form

$$\psi_R = \sum_{\alpha} \psi^{(\alpha)}(\Phi_{\mathbf{C}^{e(\alpha)}}, T), \quad (6.19)$$

where  $\Phi_{\mathbf{C}^{e(\alpha)}}$  represents a list of the principle invariants of  $\mathbf{C}^{e(\alpha)}$  and  $T$  is the temperature. The Cauchy stress is decomposed in terms of the mechanisms

$$\boldsymbol{\sigma} = \sum_{(\alpha)} \boldsymbol{\sigma}^{(\alpha)} \quad , \quad \boldsymbol{\sigma}^{(\alpha)} = \boldsymbol{\sigma}^{(\alpha)T}, \quad (6.20)$$

with

$$\begin{aligned}
\boldsymbol{\sigma}^{(\alpha)} &= \frac{1}{J} \mathbf{F} \mathbf{S}^{(\alpha)} \mathbf{F}^T \\
&= \frac{1}{J} \mathbf{F} \left( 2 \frac{\partial \psi^{(\alpha)}(\Phi_{\mathbf{C}^{e(\alpha)}}, \mathbf{T})}{\partial \mathbf{C}} \right) \mathbf{F}^T \\
&= \frac{1}{J} \mathbf{F} \left( 2 \frac{\partial \psi^{(\alpha)}(\Phi_{\mathbf{C}^{e(\alpha)}}, \mathbf{T})}{\partial \mathbf{C}^e} : \frac{\partial \mathbf{C}^e}{\partial \mathbf{C}} \right) \mathbf{F}^T \\
&= \frac{1}{J} \mathbf{F} \mathbf{F}^{\mathbf{p}(\alpha)-1} \left( 2 \frac{\partial \psi^{e(\alpha)}(\Phi_{\mathbf{C}^{e(\alpha)}}, \mathbf{T})}{\partial \mathbf{C}^e} \right) \mathbf{F}^{\mathbf{p}(\alpha)-T} \mathbf{F}^T \\
&= \frac{1}{J} \mathbf{F}^{e(\alpha)} \mathbf{S}^{e(\alpha)} \mathbf{F}^{e(\alpha)T},
\end{aligned} \tag{6.21}$$

where  $\mathbf{S}^{e(\alpha)}$  is the symmetric elastic second Piola-Kirchhoff stress

$$\mathbf{S}^{e(\alpha)} = 2 \frac{\partial \psi^{(\alpha)}(\Phi_{\mathbf{C}^{e(\alpha)}}, \mathbf{T})}{\partial \mathbf{C}^{e(\alpha)}}. \tag{6.22}$$

Moreover, the first Piola-Kirchhoff stress tensor can be computed from the following equation

$$\begin{aligned}
\mathbf{P}^{(\alpha)} &= J \boldsymbol{\sigma}^{(\alpha)} \mathbf{F}^{-T} = J \frac{1}{J} \mathbf{F}^{e(\alpha)} \mathbf{S}^{e(\alpha)} \mathbf{F}^{e(\alpha)T} \mathbf{F}^{-T} \\
&= \mathbf{F}^{e(\alpha)} \mathbf{S}^{e(\alpha)} \mathbf{F}^{\mathbf{p}(\alpha)-T} = \mathbf{F} \mathbf{F}^{\mathbf{p}(\alpha)-1} \mathbf{S}^{e(\alpha)} \mathbf{F}^{\mathbf{p}(\alpha)-T}.
\end{aligned} \tag{6.23}$$

The driving stress of the plastic flow is the symmetric Mandel stress, which is defined as

$$\begin{aligned}
\mathbf{M}^{e(\alpha)} &= J \mathbf{R}^{e(\alpha)T} \boldsymbol{\sigma}^{(\alpha)} \mathbf{R}^{e(\alpha)} \\
&= J \mathbf{R}^{e(\alpha)T} \mathbf{F}^{e(\alpha)} \mathbf{F}^{e(\alpha)-1} \boldsymbol{\sigma}^{(\alpha)} \mathbf{F}^{e(\alpha)-T} \mathbf{F}^{e(\alpha)T} \mathbf{R}^{e(\alpha)} \\
&= \mathbf{U}^{e(\alpha)} \mathbf{S}^{e(\alpha)} \mathbf{U}^{e(\alpha)} = \mathbf{C}^{e(\alpha)} \mathbf{S}^{e(\alpha)},
\end{aligned} \tag{6.24}$$

where  $\mathbf{M}^{e(\alpha)}$  is the elastic Mandel stress,  $\mathbf{R}^{e(\alpha)}$  is the rotation matrix, if  $\mathbf{C}^{e(\alpha)}$  and  $\mathbf{S}^{e(\alpha)}$  permute. The corresponding equivalent shear stress is given by

$$\bar{\tau}^{(\alpha)} = \frac{1}{\sqrt{2}} |\mathbf{M}_0^{e(\alpha)}|, \tag{6.25}$$

where  $\mathbf{M}_0^{e(\alpha)}$  is the deviatoric part of the Mandel stress

$$\mathbf{M}_0^{e(\alpha)} = \mathbf{M}^{e(\alpha)} + \bar{p} \mathbf{I} \quad , \quad \bar{p} = -\frac{1}{3} \text{tr} \mathbf{M}^{e(\alpha)}. \tag{6.26}$$

Moreover  $|\mathbf{M}_0^{e(\alpha)}|$  is the norm of the deviatoric part of the Mandel stress with

$$|\mathbf{M}_0^{e(\alpha)}| = \sqrt{\mathbf{M}_0^{e(\alpha)} : \mathbf{M}_0^{e(\alpha)}}. \tag{6.27}$$

The plastic flow reads

$$\dot{\mathbf{F}}^{\mathbf{p}(\alpha)} = \mathbf{D}^{\mathbf{p}(\alpha)} \mathbf{F}^{\mathbf{p}(\alpha)}, \tag{6.28}$$

where each  $\mathbf{F}^{p(\alpha)}$  is to be regarded as an internal variable of the theory and which is defined as a solution of the differential equation

$$\mathbf{D}^{p(\alpha)} = \dot{\epsilon}^{p(\alpha)} \left( \frac{\mathbf{M}_0^{e(\alpha)}}{2\bar{\tau}^\alpha} \right), \quad (6.29)$$

where  $\mathbf{D}^p$  is the plastic stretching tensor, and  $\dot{\epsilon}^{p(\alpha)}$  is an equivalent plastic shear strain rate

$$\dot{\epsilon}^{p(\alpha)} = \sqrt{2} |\mathbf{D}^{p(\alpha)}|. \quad (6.30)$$

In order to account for the major strain-hardening and softening characteristics of polymeric materials observed during visco-plastic deformation, we introduce macroscopic internal variables to represent important aspects of the microstructural resistance to plastic flow. The list of  $m$  scalar internal state-variables reads

$$\boldsymbol{\xi}^{(\alpha)} = (\boldsymbol{\xi}_1^{(\alpha)}, \boldsymbol{\xi}_2^{(\alpha)}, \boldsymbol{\xi}_3^{(\alpha)}, \dots, \boldsymbol{\xi}_m^{(\alpha)}). \quad (6.31)$$

Besides, let

$$\boldsymbol{\Lambda}^{(\alpha)} = (\mathbf{C}^{e(\alpha)}, \mathbf{B}^{p(\alpha)}, \boldsymbol{\xi}^{(\alpha)}, \mathbf{T}), \quad (6.32)$$

denotes a list of constitutive variables. Then for a given  $\bar{\tau}^{(\alpha)}$  and  $\boldsymbol{\Lambda}^{(\alpha)}$ , the equivalent plastic shear strain rate  $\dot{\epsilon}^{p(\alpha)}$  is obtained by solving a scalar strength relation such as

$$\bar{\tau}^{(\alpha)} = \Upsilon^{(\alpha)}(\boldsymbol{\Lambda}^{(\alpha)}, \dot{\epsilon}^{p(\alpha)}), \quad (6.33)$$

where the strength function  $\Upsilon^{(\alpha)}(\boldsymbol{\Lambda}^{(\alpha)}, \dot{\epsilon}^{p(\alpha)})$  is an isotropic function of its arguments.

### 6.3.3 Partial differential governing equations

The partial differential equation for the deformation is obtained in the absence of body force, as shown in Chapter 5, Eq. (5.1), from the following expression,

$$\nabla_0 \cdot \mathbf{P}^T = 0, \quad (6.34)$$

where  $\mathbf{P}$  denotes the first Piola Kirchhoff stress, which is defined as

$$\mathbf{P} = \mathbf{J} \boldsymbol{\sigma} \mathbf{F}^{-T}. \quad (6.35)$$

The partial differential equation for the temperature is obtained by the balance on energy, from Eq. (5.9) after neglecting the electrical contribution, as

$$\nabla_0 \cdot \mathbf{Q} = -\rho_0 c_v \dot{T} + \bar{F}, \quad (6.36)$$

where the thermal flux is governed by the Fourier law  $\mathbf{Q} = -\mathbf{K} \cdot \nabla_0 T$  and  $\bar{F}$  denotes all the body sources of heat and is expressed as

$$\bar{F} = Q_r + \sum_{\alpha} \bar{\tau}^{(\alpha)} \dot{\epsilon}^{p(\alpha)} + \mathbf{T} \frac{\partial^2 \psi^{e(\alpha)}}{\partial \mathbf{C}^{e(\alpha)} \partial T} : \dot{\mathbf{C}}^{e(\alpha)}, \quad (6.37)$$

where  $Q_r$  is the scalar heat supply measured per unit reference volume and the last term of the right hand side is the thermo-elastic damping term which is neglected. Instead we assume

that only a fraction  $v$  of the rate of the plastic dissipation contributes to the temperature change

$$\bar{F} = Q_r + v \sum_{\alpha} \bar{\tau}^{(\alpha)} \dot{\epsilon}^{p(\alpha)}, \quad (6.38)$$

where  $0 \leq v \leq 1$  is fraction of the rate of plastic dissipation contribution to the temperature change. The volumetric heat capacity per unit mass is a function of the glass transition temperature, and is defined as follows

$$c_v = \begin{cases} c_0 - c_1(T - T_g) & \text{if } T \leq T_g \\ c_0 & \text{if } T > T_g. \end{cases} \quad (6.39)$$

The theory with three micromechanisms  $M=3$  as shown in Fig. 6.2 is considered. These three micromechanisms are intended to represent the following underlying physical phenomena:

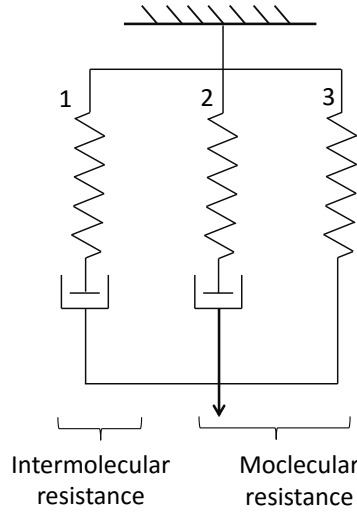


Figure 6.2: A spring-dashpot schematic of the constitutive law

1. The first micromechanism ( $\alpha = 1$ ) represents an elastic resistance due to intermolecular energetic bond-stretching. The dashpot represents thermally-activated plastic flow due to inelastic mechanisms, such as chain segment rotation and relative slippage of the polymer chains between neighboring cross-linkage points.
2. The second micromechanism ( $\alpha = 2$ ) represents the molecular chains between mechanical crosslinks. At temperatures below  $T_g$  the polymer exhibits a significant amount of mechanical crosslinking which disintegrates when the temperature is increased above  $T_g$ .
3. The third micromechanism ( $\alpha = 3$ ) introduces the molecular chains between chemical crosslinks. The nonlinear springs represent resistances due to changes in the free energy upon stretching of the molecular chains between the crosslinks.

The used strategy to model the response of the material as the temperature traverses  $T_g$  (glass transition) is as follows

- For  $T < T_g$  we do not allow any plastic flow in the dashpot associated with micromechanism  $\alpha = 2$ . Thus since the springs in  $\alpha = 2$  and  $\alpha = 3$  are in parallel, the three micromechanism model reduces to a simpler two micromechanism model.
- For  $T > T_g$  only mechanisms  $\alpha = 1$  and  $\alpha = 3$  contribute to the macroscopic stress.

The glass transition in amorphous polymers depends on the strain rate to which the material is subjected.

$$\dot{\epsilon} = \sqrt{2}|\mathbf{D}_0|, \quad (6.40)$$

where  $\dot{\epsilon}$  is the equivalent shear strain rate, and  $\mathbf{D}_0$  denotes the total deviatoric stretching tensor

$$\mathbf{D}_0 = \text{sym}_0(\dot{\mathbf{F}}\mathbf{F}^{-1}). \quad (6.41)$$

In this equation,  $\text{sym}_0$  denotes the symmetric deviatoric part. This symmetric part is obtained as  $\mathbf{D}$  computed by the following equation

$$\mathbf{D} = \frac{1}{2}(\dot{\mathbf{F}}\mathbf{F}^{-1} + \mathbf{F}^{-T}\dot{\mathbf{F}}^T), \quad (6.42)$$

and the symmetric deviatoric stretching tensor thus reads

$$\mathbf{D}_0 = \mathbf{D} - \frac{1}{3}\text{tr}\mathbf{D}\mathbf{I}. \quad (6.43)$$

Eventually, the glass transition  $T_g$  is calculated from the following expression

$$T_g = \begin{cases} T_r & \text{if } \dot{\epsilon} \leq \epsilon_r, \\ T_r + n \log\left(\frac{\dot{\epsilon}}{\epsilon_r}\right) & \text{if } \dot{\epsilon} > \epsilon_r, \end{cases} \quad (6.44)$$

where  $T_r$  is the reference glass transition temperature at low strain rate,  $\dot{\epsilon}$  is the shear strain rate, and  $\epsilon_r$  is the reference strain rate.

### 6.3.4 Definition of the micromechanisms

#### 6.3.4.1 The first micromechanism ( $\alpha = 1$ ) of Shape-Memory Polymers (SMP)

The non-linear spring represents an elastic resistance due to intermolecular energetic bond-stretching. The dashpot represents thermally activated plastic flow due to inelastic mechanisms.

At the first we need to calculate the Cauchy stress  $\boldsymbol{\sigma}^{(1)}$  using

$$\boldsymbol{\sigma}^{(1)} = J^{-1}\mathbf{R}^{e(1)}\mathbf{M}^{e(1)}\mathbf{R}^{e(1)T}, \quad (6.45)$$

where  $\mathbf{M}^{e(1)}$  is the symmetric Mandel stress which is symmetric by definition, and  $\mathbf{R}^{e(1)}$  is the rotation matrix. The Mandel stress reads

$$\mathbf{M}^{e(1)} = \frac{\partial \psi^{e(1)}(\mathbf{E}^{e(1)}, T)}{\partial \mathbf{E}^{e(1)}}. \quad (6.46)$$

$\mathbf{E}^{e(1)}$  denotes the logarithmic elastic strain, which is evaluated using the eigenvalue decomposition of  $\mathbf{C}^{e(1)}$  with

$$\mathbf{C}^{e(1)} = \sum_{i=1}^3 (\lambda_i^e)^2 \mathbf{r}_i^e \otimes \mathbf{r}_i^e, \quad \mathbf{E}^{e(1)} = \sum_{i=1}^3 \ln \lambda_i^e \mathbf{r}_i^e \otimes \mathbf{r}_i^e, \quad (6.47)$$

where  $\lambda_1^e, \lambda_2^e, \lambda_3^e$  are the positive eigenvalues of  $\mathbf{U}^e$ , and  $\mathbf{r}_1^e, \mathbf{r}_2^e, \mathbf{r}_3^e$  are the orthonormal eigenvectors of  $\mathbf{C}^e$  and  $\mathbf{U}^e$ . The relation (6.46) is derived from Eq. (6.24) as

$$\begin{aligned} \mathbf{M}^{e(1)} &= 2\mathbf{C}^{e(1)} \frac{\partial \psi^{e(1)}(\mathbf{E}^{e(1)}, \mathbf{T})}{\partial \mathbf{C}^{e(1)}} = 2\mathbf{C}^{e(1)} \frac{\partial \psi^{e(1)}(\mathbf{E}^{e(1)}, \mathbf{T})}{\partial \mathbf{E}^{e(1)}} \frac{\partial \mathbf{E}^{e(1)}}{\partial \mathbf{C}^{e(1)}} \\ &= \mathbf{C}^{e(1)-1} \mathbf{M}^{e(1)} \mathbf{C}^{e(1)} = \mathbf{M}^{e(1)}, \end{aligned} \quad (6.48)$$

if  $\mathbf{C}^{e(1)}$  and  $\mathbf{M}^{e(1)}$  permute. Permutation of  $\mathbf{C}^{e(1)}$  and  $\mathbf{M}^{e(1)}$  is directly obtained from the eigenvectors decomposition Eq. (6.47), as  $\mathbf{C}^{e(1)}, \mathbf{E}^{e(1)}$  and  $\mathbf{M}^{e(1)}$  have the same basis  $\mathbf{r}_i^e \otimes \mathbf{r}_i^e$ .

It should be noted that in this work  $\mathbf{E}^{e(1)}$  is computed by using a Taylor series approximation of Eq. (6.47), and not through the eigenvalue decomposition.

The following simple generalization of the classical strain energy function of infinitesimal isotropic elasticity is considered, which uses a logarithmic measure of finite strain [4]<sup>1</sup>, then the form of the elastic free energy is

$$\psi^{e(1)} = G |\mathbf{E}_0^{e(1)}|^2 + \frac{1}{2} K \left( \text{tr} \mathbf{E}^{e(1)} \right)^2 - 3K \left( \text{tr} \mathbf{E}^{e(1)} \right) \alpha_{\text{th}} (\mathbf{T} - \mathbf{T}_0) + \tilde{f}(\mathbf{T}). \quad (6.49)$$

This relation of free energy allows the stress to be determined via the strain relation, where the deviatoric part of strain is denoted by  $\mathbf{E}_0^e$ , and  $\tilde{f}(\mathbf{T})$  is an entropic contribution to the free energy related to the temperature dependent specific heat of the material, and where the temperature dependent parameters  $G(\mathbf{T}), K(\mathbf{T}), \alpha_{\text{th}}(\mathbf{T})$  are respectively the shear modulus, bulk modulus, and the coefficient of thermal expansion. Substituting Eq. (6.49) in Eq. (6.46), as  $|\mathbf{E}_0^{e(1)}| = \mathbf{E}_0^{e(1)} : \mathbf{E}_0^{e(1)}$  one can get directly  $\mathbf{M}^{e(1)}$  as

$$\mathbf{M}^{e(1)} = 2G \mathbf{E}_0^{e(1)} + K \left( \text{tr} \mathbf{E}^{e(1)} \right) \mathbf{I} - 3K \alpha_{\text{th}} (\mathbf{T} - \mathbf{T}_0) \mathbf{I}. \quad (6.50)$$

Moreover, one can get

$$\bar{\tau}^{(1)} = \frac{1}{\sqrt{2}} |\mathbf{M}_0^{e(1)}|, \quad \bar{p} = -\frac{1}{3} \text{tr} \mathbf{M}^{e(1)}, \quad \mathbf{M}_0^{e(1)} = \mathbf{M}^{e(1)} + \bar{p} \mathbf{I}, \quad (6.51)$$

where  $\bar{p}$  is the normal pressure which has negative value for hydrostatic stress,  $\bar{\tau}^{(1)}$  is the equivalent shear stress, and  $\mathbf{M}_0^{e(1)}$  is the deviatoric part of the Mandel stress. The temperature dependence of the shear modulus may be approximated by the following function, where it decrease significantly for polymers as the temperature increases through the glass transition temperature of the material:

$$G(\mathbf{T}) = \frac{1}{2} (G_{\text{gl}} + G_{\text{r}}) - \frac{1}{2} (G_{\text{gl}} - G_{\text{r}}) \tanh \left( \frac{1}{\Delta} (\mathbf{T} - \mathbf{T}_{\text{g}}) \right) - M(\mathbf{T} - \mathbf{T}_{\text{g}}), \quad (6.52)$$

<sup>1</sup>This free energy function is used for moderately large elastic stretches parameters

where  $M = M_{gl}$  if  $T \leq T_g$ ,  $M = M_r$  if  $T > T_g$ ,  $G_{gl}$ ,  $G_r$  are the values of the shear modulus in the glassy and rubbery regions,  $\Delta$  is a parameter related to the temperature range across which the glass transition occurs, and the parameter  $M$  represents the slope of the temperature variation of  $G$  outside the transition region.

The coefficient of thermal expansion is taken to have a bilinear temperature dependence, with the following contribution to the thermal expansion term  $\alpha_{th}(T - T_0)$  in the free energy relation. Four cases are considered for the coefficient of thermal expansion in terms of the initial temperature  $T_0$

$$\alpha_{th}(T - T_0) = \begin{cases} \alpha_{gl}(T - T_0) & \text{if } T \leq T_g \text{ and } T_0 \leq T_g, \\ \alpha_r(T - T_0) + (\alpha_{gl} - \alpha_r)(T - T_g) & \text{if } T \leq T_g \text{ and } T_0 > T_g, \\ \alpha_{gl}(T - T_0) + (\alpha_r - \alpha_{gl})(T - T_g) & \text{if } T > T_g \text{ and } T_0 \leq T_g, \\ \alpha_r(T - T_0) & \text{if } T > T_g \text{ and } T_0 > T_g. \end{cases} \quad (6.53)$$

The temperature dependence of Poisson ratio  $\nu(T)$  is given by

$$\nu(T) = \frac{1}{2}(\nu_{gl} + \nu_r) - \frac{1}{2}(\nu_{gl} - \nu_r) \tanh\left(\frac{1}{\Delta}(T - T_g)\right). \quad (6.54)$$

The temperature dependence of the bulk modulus  $K(T)$  is then obtained by using the standard relation for isotropic materials

$$K(T) = G(T) \frac{2(1 + \nu(T))}{3(1 - 2\nu(T))}. \quad (6.55)$$

Moreover, the evaluation equation for  $\mathbf{F}^{p(1)}$  follows Eqs. (6.28-6.30) which are rewritten

$$\dot{\mathbf{F}}^{p(1)} = \mathbf{D}^{p(1)} \mathbf{F}^{p(1)}, \quad (6.56)$$

with

$$\mathbf{D}^{p(1)} = \dot{\epsilon}^{p(1)} \frac{\mathbf{M}_0^{e(1)}}{2\bar{\tau}^{(1)}}. \quad (6.57)$$

The thermally-activated relation for the equivalent plastic strain rate in the specific form reads

$$\dot{\epsilon}^{p(1)} = \begin{cases} 0 & \text{if } \tau_e \leq 0, \\ \dot{\epsilon}_0^{(1)} \exp\left(-\frac{1}{\xi}\right) \exp\left(-\frac{Q(T)}{K_B T}\right) \left[\sinh\left(\frac{\tau^{e(1)} * V}{2K_B T}\right)\right]^{1/m^{(1)}} & \text{if } \tau_e > 0, \end{cases} \quad (6.58)$$

where  $\dot{\epsilon}^{p(1)}$  is the plastic strain rate, the parameter  $\dot{\epsilon}_0^{(1)}$  is a pre-exponential factor with units of 1/time,  $K_B$  is Boltzmann's constant,  $V$  is an activation volume,  $m^{(1)}$  is the sensitive parameter for the strain rate and  $\tau^{e(1)}$  denotes a net shear stress for the thermally activated flow

$$\tau^{e(1)} = \bar{\tau}^{(1)} - (S_a + S_b + \alpha_p \bar{p}), \quad (6.59)$$

with  $\alpha_p \geq 0$  a parameter introduced to account for the pressure sensitivity. The term  $\exp\left(-\frac{1}{\xi}\right)$  in Eq. (6.58) represents a concentration of flow defects, with

$$\xi = \begin{cases} \xi_{gl} & \text{if } T \leq T_g, \\ \xi_{gl} + d(T - T_g) & \text{if } T > T_g. \end{cases} \quad (6.60)$$

Finally  $Q(T)$  is the temperature dependence of the activation energy with

$$Q(T) = \frac{1}{2} (Q_{gl} + Q_r) - \frac{1}{2} (Q_{gl} - Q_r) \tanh\left(\frac{1}{\Delta}(T - T_g)\right), \quad (6.61)$$

which takes the value,  $Q_{gl}$  in the glassy regime and  $Q_r$  in the rubbery regime.

#### 6.3.4.2 Equations for internal variables

Typical initial conditions presume that the body is initially (at time  $t=0$ ) in a virgin state, leading to

$$\mathbf{F}^{(\alpha)}(\mathbf{X}, 0) = \mathbf{F}^{p(\alpha)}(\mathbf{X}, 0) = \mathbf{I} \Rightarrow \mathbf{F}^{e(\alpha)}(\mathbf{X}, 0) = \mathbf{I}, \quad (6.62)$$

$$\xi_i^{(\alpha)}(\mathbf{X}, 0) = \xi_i^{(\alpha)} (= \text{constant}). \quad (6.63)$$

For the first micromechanism, the list  $\xi^1$  of internal variables consists of three positive scalars, such that

$$\xi^1 = (\varphi, S_a, S_b), \quad (6.64)$$

where the variable  $\varphi \geq 0$  and  $S_a \geq 0$  are introduced to model the yield peak which is observed in the intrinsic stress-strain response of glassy polymers and  $S_b \geq 0$  is introduced to model the isotropic hardening at high strain. In details, the three internal variables correspond to

- The high order parameter  $\varphi$  is introduced to represent material disorder with the microscale dilatation induced by plastic deformation;
- The resistance  $S_a$  represents the disorder of the material which causes a transient change in the stress as the a result of plastic deformation proceeding;
- The resistance  $S_b \geq 0$  is introduced to model a dissipative resistance to the plastic flow;

The evolutions of  $\dot{S}_a$  and  $\dot{\varphi}$  are governed by

$$\dot{S}_a = h_a(S_a^* - S_a)\dot{\epsilon}^{p(1)} \quad \text{with initial value } S_a = S_{a0}, \quad (6.65)$$

$$\dot{\varphi} = g(\varphi^* - \varphi)\dot{\epsilon}^{p(1)} \quad \text{with initial value } \varphi = \varphi_0. \quad (6.66)$$

In these equations, we have introduced

$$S_a^* = b(\varphi^* - \varphi), \quad (6.67)$$

which controls the extent of the stress, and  $\varphi^*$  as

$$\varphi^*(\dot{\epsilon}^{p(1)}, T) = \begin{cases} z \left( \left(1 - \frac{T}{T_g}\right)^r + h_g \right) \left( \frac{\dot{\epsilon}^{p(1)}}{\epsilon_r} \right)^s & \text{if } (T \leq T_g) \text{ and } (\dot{\epsilon}^{p(1)} > 0), \\ zh_g \left( \frac{\dot{\epsilon}^{p(1)}}{\epsilon_r} \right)^s & \text{if } (T > T_g) \text{ and } (\dot{\epsilon}^{p(1)} > 0), \end{cases} \quad (6.68)$$

which represents the temperature and strain rate dependency of  $\varphi$ , where  $z$ ,  $r$ ,  $h_g$ , and  $s$  are taken to be constants. In particular  $h_g$  is introduced to get a small value for  $\varphi^*$  when



$T > T_g$ , instead of 0 in order to improve the convergence of numerical model. Then the evolution of  $S_b$  is governed by

$$S_b = S_{b0} + H_b(\bar{\lambda} - 1)^a, \quad \bar{\lambda} = \sqrt{\text{tr}\mathbf{C}/3}, \quad (6.69)$$

where  $\bar{\lambda}$  is an effective stretch which increases or decreases as the overall stretch increases or decreases, and the hardening parameter  $H_b$  is temperature dependent, with

$$H_b(T) = \frac{1}{2}(H_{gl} + H_r) - \frac{1}{2}(H_{gl} - H_r) \tanh\left(\frac{1}{\Delta}(T - T_g)\right) - L(T - T_g), \quad (6.70)$$

where  $H_{gl}$  and  $H_r$  are the values in glassy and rubbery regions, and where  $L$  represents the slope of the temperature variation of  $H_b$ , and takes the value of  $L = L_{gl}$  if  $T \leq T_g$  and  $L = L_r$  if  $T > T_g$ .

### 6.3.4.3 The second micromechanism ( $\alpha = 2$ ) of Shape-Memory Polymers (SMP)

The second mechanism represents the molecular chains between mechanical-crosslinks. The nonlinear spring in this mechanism represents resistances due to changes in the free energy upon stretching of the molecular chains between the crosslinks and the dashpot corresponds to the thermally-activated plastic flow resulting from a phenomenon of disintegrating of the mechanical cross-links for  $T > T_g$ .

Defining

$$\bar{\mathbf{F}}^{e(2)} = J^{-\frac{1}{3}}\mathbf{F}^{e(2)}, \quad \det\bar{\mathbf{F}}^{e(2)} = 1, \quad (6.71)$$

$$\bar{\mathbf{C}}^{e(2)} = \bar{\mathbf{F}}^{e(2)T}\bar{\mathbf{F}}^{e(2)} = J^{-\frac{2}{3}}\mathbf{C}^{e(2)}, \quad (6.72)$$

where  $\bar{\mathbf{C}}^{e(2)}$  denotes the distortional (or volume preserving) right Cauchy strain tensor, we can define a free energy function in form

$$\psi^{(2)} = \bar{\psi}^{(2)}(\bar{\mathbf{C}}^{e(2)}, T) \quad (6.73)$$

which is an isotropic function of its argument, the volumetric elastic energies for  $\psi^{(2)}$  or  $\psi^{(3)}$  are not needed as it has been already accounted for a volumetric elastic energy in  $\psi^{(1)}$ . Employing the simple phenomenological form for the free energy function  $\psi^{(2)}$  proposed by Gent [20], one has

$$\bar{\psi}^{(2)} = -\frac{1}{2} \mu^{(2)} I_m^{(2)} \ln\left(1 - \frac{\text{tr}\bar{\mathbf{C}}^{e(2)} - 3}{I_m^{(2)}}\right), \quad (6.74)$$

where  $\mu^{(2)}$  is the rubbery shear modulus. The experimental results indicate that it is temperature dependent and decreases with increasing temperature such as

$$\mu^{(2)} = \mu_g \exp(-N(T - T_g)), \quad (6.75)$$

where  $\mu_g$  is the value of  $\mu^{(2)}$  at the glass transition temperature, and  $N$  is a parameter that represents the slope of temperature variation on a logarithmic scale. The parameter  $I_m^{(2)}$  is taken to be temperature constant.

Using the free energy Eq. (6.74) yields the corresponding second Piola stress  $\mathbf{S}^{e(2)}$  as

$$\begin{aligned}\mathbf{S}^{e(2)} &= 2 \frac{\partial \bar{\psi}^{(2)}}{\partial \mathbf{C}^{e(2)}} = 2 \frac{\partial \bar{\psi}^{(2)}}{\partial \bar{\mathbf{C}}^{e(2)}} : \frac{\partial \bar{\mathbf{C}}^{e(2)}}{\partial \mathbf{C}^{e(2)}} \\ &= J^{-\frac{2}{3}} \mu^{(2)} \left(1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)} - 3}{I_m^{(2)}}\right)^{-1} \left[\mathbf{I} - \frac{1}{3} (\text{tr} \bar{\mathbf{C}}^{e(2)}) \bar{\mathbf{C}}^{e(2)-1}\right].\end{aligned}\quad (6.76)$$

Then Eq. (6.21) gives the contribution to the Cauchy stress  $\boldsymbol{\sigma}^{(2)}$  as

$$\begin{aligned}\boldsymbol{\sigma}^{(2)} &= \mathbf{J}^{-1} \mathbf{F}^{e(2)} \mathbf{S}^{e(2)} \mathbf{F}^{e(2)\text{T}} \\ &= \mathbf{J}^{-1} \left[ \mu^{(2)} \left(1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)} - 3}{I_m^{(2)}}\right)^{-1} \bar{\mathbf{B}}_0^{e(2)} \right],\end{aligned}\quad (6.77)$$

with

$$\bar{\mathbf{B}}^{e(2)} = \bar{\mathbf{F}}^{e(2)} \bar{\mathbf{F}}^{e(2)\text{T}} = \mathbf{J}^{-\frac{2}{3}} \mathbf{B}^{e(2)}, \quad (6.78)$$

where  $\bar{\mathbf{B}}_0^{e(2)} = \mathbf{B}^{e(2)} - \frac{1}{3} \text{tr} \mathbf{C}^{e(2)} \mathbf{I}$  is the deviatoric part of  $\mathbf{B}^{e(2)}$  the left Cauchy Green strain tensor, and where  $\text{tr} \mathbf{C} = \text{tr} \mathbf{B}$ .

Also from Eq. (6.24) and Eq. (6.76) the corresponding Mandel stress reads

$$\mathbf{M}^{e(2)} = \mathbf{C}^{e(2)} \mathbf{S}^{e(2)} = \mu^{(2)} \left(1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)} - 3}{I_m^{(2)}}\right)^{-1} \bar{\mathbf{C}}_0^{e(2)}, \quad (6.79)$$

where  $\bar{\mathbf{C}}_0^{e(2)} = \bar{\mathbf{C}}^{e(2)} - \frac{1}{3} \text{tr} \bar{\mathbf{C}}^{e(2)} \mathbf{I}$  is the deviatoric part of  $\bar{\mathbf{C}}^{e(2)}$  the right Cauchy Green tensor. Clearly, as  $\bar{\mathbf{C}}^{e(2)}$  and  $\mathbf{C}^{e(2)}$  permute,  $\mathbf{M}^{e(2)}$  and  $\bar{\mathbf{C}}^{e(2)}$  permute as well.

The equivalent shear stress of the plastic flow is given by

$$\bar{\tau}^{(2)} = \frac{1}{\sqrt{2}} |\mathbf{M}^{e(2)}|. \quad (6.80)$$

The plastic flow is based on

$$\dot{\mathbf{F}}^{\text{p}(2)} = \mathbf{D}^{\text{p}(2)} \mathbf{F}^{\text{p}(2)}, \quad (6.81)$$

with the plastic stretching  $\mathbf{D}^{\text{p}(2)}$  obtained by

$$\mathbf{D}^{\text{p}(2)} = \dot{\epsilon}^{\text{p}(2)} \frac{\mathbf{M}^{e(2)}}{2\bar{\tau}^{(2)}}, \quad (6.82)$$

where the equivalent shear strain rate reads:

$$\dot{\epsilon}^{\text{p}(2)} = \sqrt{2} |\mathbf{D}^{\text{p}(2)}|. \quad (6.83)$$

For the second mechanism, we consider the equivalent plastic strain rate

$$\dot{\epsilon}^{\text{p}(2)} = \dot{\epsilon}_0^{(2)} \left( \frac{\bar{\tau}^{(2)}}{S^{(2)}} \right)^{\frac{1}{m^{(2)}}}, \quad (6.84)$$

where  $\dot{\epsilon}_0^{(2)}$  is a reference plastic shear strain rate,  $m^{(2)}$  is the positive valued strain rate sensitivity parameter,  $S^{(2)}$  is a temperature dependent parameter, which can be determined by

$$S^{(2)}(T) = \frac{1}{2} (S_{\text{gl}}^{(2)} + S_{\text{r}}^{(2)}) - \frac{1}{2} (S_{\text{gl}}^{(2)} - S_{\text{r}}^{(2)}) \tanh\left(\frac{1}{\Delta_2} (T - T_{\text{g}})\right), \quad (6.85)$$

where  $S_{\text{gl}}^{(2)}$  and  $S_{\text{r}}^{(2)}$  denote respectively the glass and rubbery sensitivities and  $\Delta_2$  is a parameter related to the temperature range across which the glass transition occurs.

#### 6.3.4.4 The third micromechanism ( $\alpha = 3$ ) of Shape Memory Polymers (SMP)

The micromechanism  $\alpha = 3$  represents chemically-crosslinked backbone of the thermoset polymer in which the crosslinks do not slip. The nonlinear spring in this mechanism represents resistances due to changes in the free energy upon stretching of the molecular chains between the crosslinks.

Accordingly we do not use a dashpot for this micromechanism, and we set  $\mathbf{F}^{p(3)} = \mathbf{I}$ , so that  $\mathbf{F}^{e(3)} = \mathbf{F}$ , with

$$\bar{\mathbf{F}} = \mathbf{J}^{-\frac{1}{3}} \mathbf{F}, \det \bar{\mathbf{F}} = 1. \quad (6.86)$$

Then right Cauchy Green strain tensor is defined as follows

$$\bar{\mathbf{C}} = \bar{\mathbf{F}}^T \bar{\mathbf{F}} = \mathbf{J}^{-\frac{2}{3}} \mathbf{C}. \quad (6.87)$$

The free energy is a function of  $\bar{\mathbf{C}}$ , and is defined similar to mechanisms  $\alpha = 2$ , and is given by a deviatoric Gent form [20]

$$\psi^{(3)} = \bar{\psi}^{(3)}(\bar{\mathbf{C}}) = -\frac{1}{2} \mu^{(3)} \mathbf{I}_m^{(3)} \ln\left(1 - \frac{\text{tr} \bar{\mathbf{C}} - 3}{\mathbf{I}_m^{(3)}}\right), \quad (6.88)$$

where the material constant  $\mu^{(3)} > 0$  is assumed to be temperature-independent.

Using

$$\frac{\partial \bar{\mathbf{C}}}{\partial \mathbf{C}} = \frac{1}{\mathbf{J}^{\frac{2}{3}}} \left( \mathbf{I} - \frac{1}{3} \bar{\mathbf{C}} \otimes \bar{\mathbf{C}}^{-1} \right), \quad (6.89)$$

the free energy Eq. (6.87) yields the corresponding second Piola stress  $\mathbf{S}^{(3)}$  as

$$\begin{aligned} \mathbf{S}^{(3)} &= 2 \frac{\partial \bar{\psi}^{(3)}}{\partial \bar{\mathbf{C}}} : \frac{\partial \bar{\mathbf{C}}}{\partial \mathbf{C}} \\ &= \mathbf{J}^{-\frac{2}{3}} \mu^{(3)} \left(1 - \frac{\text{tr} \bar{\mathbf{C}} - 3}{\mathbf{I}_m^{(3)}}\right)^{-1} \left[ \mathbf{I} - \frac{1}{3} (\text{tr} \bar{\mathbf{C}}) \bar{\mathbf{C}}^{-1} \right]. \end{aligned} \quad (6.90)$$

Furthermore, by the use of Eq. (6.21), the contribution to the Cauchy stress  $\boldsymbol{\sigma}^{(3)}$  reads

$$\begin{aligned} \boldsymbol{\sigma}^{(3)} &= \mathbf{J}^{-1} \mathbf{F} \mathbf{S}^{(3)} \mathbf{F}^T \\ &= \mathbf{J}^{-1} \left[ \mu^{(3)} \left(1 - \frac{\text{tr} \bar{\mathbf{C}} - 3}{\mathbf{I}_m^{(3)}}\right)^{-1} \bar{\mathbf{B}}_0 \right], \end{aligned} \quad (6.91)$$

where  $\bar{\mathbf{B}}_0 = \bar{\mathbf{B}} - \frac{1}{3} \text{tr} \bar{\mathbf{C}} \mathbf{I}$  is the deviatoric part of left Cauchy Green strain tensor

$$\bar{\mathbf{B}} = \bar{\mathbf{F}} \bar{\mathbf{F}}^T = \mathbf{J}^{-\frac{2}{3}} \mathbf{B}, \quad (6.92)$$

with  $\mathbf{B}$  the left Cauchy Green strain tensor.

#### 6.3.5 Finite increment form of the Shape Memory Polymer constitutive law

In this section we present the finite increment form of the theory developed previously. The resolution of the system follows the predictor-corrector scheme during the time interval  $[t_n; t_{n+1}]$ , where we use the subscript  $n$  for the previous time  $t_n$  and  $n + 1$  for the current time  $t_{n+1}$ . The formulation can be summarized as follows:

- Prediction step: The plastic deformation gradient is initialized to the value at the previous step  $\mathbf{F}_{(\text{pr})}^{\text{p}(\alpha)} = \mathbf{F}_{(\text{n})}^{\text{p}(\alpha)}$ , and the elastic deformation follows

$$\mathbf{F}_{(\text{n}+1)}^{\text{e}(\alpha)} = \mathbf{F}_{(\text{n}+1)} \mathbf{F}_{(\text{n})}^{\text{p}(\alpha)-1}, \quad (6.93)$$

leading to the right Cauchy strain elastic predictor

$$\mathbf{C}_{(\text{pr})}^{\text{e}(\alpha)} = \mathbf{F}_{(\text{pr})}^{\text{p}(\alpha)-\text{T}} \mathbf{F}_{(\text{n}+1)}^{\text{T}} \mathbf{F}_{(\text{n}+1)} \mathbf{F}_{(\text{pr})}^{\text{p}(\alpha)-1}. \quad (6.94)$$

- Correction step: In this step we solve the system of equations that has been developed in Section 6.3.4, to extract the plastic increment using the evaluation equation of the plastic deformation gradient during the time step between the configurations n and n+1, with

$$\mathbf{F}_{(\text{n}+1)}^{\text{p}(\alpha)} = \exp(\Delta \mathbf{D}^{\text{p}(\alpha)}) \mathbf{F}_{(\text{n})}^{\text{p}(\alpha)}. \quad (6.95)$$

Then the elastic deformation tensor is obtained from

$$\mathbf{F}_{(\text{n}+1)}^{\text{e}(\alpha)} = \mathbf{F}_{(\text{n}+1)} \mathbf{F}_{(\text{n})}^{\text{p}(\alpha)-1} (\exp(\Delta \mathbf{D}^{\text{p}(\alpha)}))^{-1}. \quad (6.96)$$

By Eq. (6.82), one can have

$$\Delta \mathbf{D}^{\text{p}(\alpha)} = (\epsilon_{(\text{n}+1)}^{\text{p}(\alpha)} - \epsilon_{(\text{n})}^{\text{p}(\alpha)}) \frac{\mathbf{M}^{\text{e}(\alpha)}}{2\bar{\tau}(\alpha)} = \Delta \epsilon^{\text{p}(\alpha)} \left( \frac{\mathbf{M}^{\text{e}(\alpha)}}{2\bar{\tau}(\alpha)} \right), \quad (6.97)$$

and the expression of the elastic deformation tensor can be rewritten under the form

$$\mathbf{F}_{(\text{n}+1)}^{\text{e}(\alpha)} = \mathbf{F}_{(\text{n}+1)} \mathbf{F}_{(\text{n})}^{\text{p}(\alpha)-1} \exp\left[ (\Delta \epsilon^{\text{p}(\alpha)}) \frac{(\mathbf{M}^{\text{e}(\alpha)})}{2\bar{\tau}(\alpha)} \right]^{-1}. \quad (6.98)$$

As the plastic flow is independent from the rotation tensor, the plastic correction can be computed in an unrotated configuration.

More details about the predictor-corrector algorithm and the stiffness computation can be found in Appendix E.2.

## 6.4 Numerical simulations

The constitutive equations for SMP and carbon fiber that were presented in the previous sections have been implemented in a DGFEM software, i.e. GMSH [22], to model Shape Memory Polymer and Shape Memory Polymer composite behaviors. The numerical results are compared with some experimental tests performed by [68].

All material parameters of the SMP which have been used in the simulations are reported in Table 6.1, where the thermo-mechanical parameters have been calibrated by Srivastava et al. [68] to fit the experimental data of tert-butyl acrylate (90% by weight) with crosslinking

Table 6.1: Shape memory polymers parameters

Parameter	Value	Parameter	Value
$\dot{\epsilon}_0^{(1)}$ [1/s]	$1.73 \times 10^{13}$	$\rho$ [Kg/m <sup>3</sup> ]	1020
$\epsilon_r$	$5.2 \times 10^{-4}$	$\dot{\epsilon}_0^{(2)}$ [1/s]	$5.2 \times 10^{-4}$
$\alpha_{gl}$ [1/K]	$13 \times 10^{-5}$	$\alpha_r$ [1/K]	$25 \times 10^{-5}$
$T_r$ [K]	310	n [K]	2.1
$G_{gl}$ [Pa]	$156 \times 10^6$	$G_r$ [Pa]	$13.4 \times 10^6$
$M_{gl}$ [Pa/K]	$7.4 \times 10^6$	$M_r$ [Pa/K]	$0.168 \times 10^6$
$Q_{gl}$ [J]	$1.4 \times 10^{-19}$	$Q_r$ [J]	$0.2 \times 10^{-21}$
$H_{gl}$ [Pa/K]	$1.56 \times 10^6$	$H_r$ [Pa/K]	$0.76 \times 10^6$
$L_{gl}$ [Pa/K]	$0.44 \times 10^6$	$L_r$ [Pa/K]	$0.006 \times 10^6$
$\nu_{gl}$	0.35	$\nu_r$	0.49
$\Delta$	2.6	$m^{(1)}$	0.17
$h_a$	230	g	5.8
z	0.083	r	1.3
s	0.005	a	0.5
d [1/K]	0.015	$\zeta_{gl}$	0.14
$S_{a0}$ [Pa]	0	$S_{b0}$ [Pa]	0
V [m <sup>3</sup> ]	$2.16 \times 10^{-27}$	$I_m^{(2)}$	6.3
$\alpha_p$	0.058	$\varphi_0$	0
$\beta$	0.5	$h_a$	230
$S_{gl}$ [Pa]	$58 \times 10^6$	$S_r$ [Pa]	$3 \times 10^2$
N [1/K]	0.045	$\mu_g$ [Pa]	$1.38 \times 10^6$
$I_m^{(3)}$	5	$m^{(2)}$	0.19
$\mu^{(3)}$ [Pa]	$0.75 \times 10^6$	w	0.7
$c_0$ [J/(Kg · K)]	1710	$c_1$ [J/Kg]	4.
$h_g$	$10^{-6}$	$\alpha$ [V/K] [s/m]	$3 \times 10^{-7}$
b [Pa]	$5850 \times 10^6$		
$\mathbf{k}$ [W/(K · m)]	diag(0.2)	$\mathbf{l}$ [V/K]	diag(0.1)

agent poly (ethylene glycol) dimethacrylate (10% by weight). The parameters related to the conductivity are assumed to correspond to nano-composites and consist of values of the order of magnitude that can be found in [72].

The composite cell models of carbon fiber reinforced SMP are studied using the carbon fiber material parameters reported in Table 6.2, which are given in Wu et al. paper [75], while the approximated electrical and thermal parameters are taken from [32, 33, 12, 73].

#### 6.4.1 3-D Shape memory polymers tests

Three tests have been considered to show the ability of the model to recover SMP behavior on a cube of size  $1 \times 1 \times 1$  [mm<sup>3</sup>], meshed with quadratic elements, and using a stabilization parameter of value  $\beta=100$ . In the first one, the different responses of SMP at different temperatures are extracted and compared to experimental data, then in the sec-

Table 6.2: Carbon fiber properties

Parameter	Value
Density $\rho$ [Kg/m <sup>3</sup> ]	1750
Longitudinal Young's modulus $E_L$ [GPa]	230
Transverse Young's modulus $E_T$ [GPa]	40
Transverse Poisson ratio $\nu_{TT}$ [-]	0.2
Longitudinal-transverse Poisson ratio $\nu_{LT}$ [-]	0.256
Transverse shear modulus $G_{TT}$ [GPa]	16.7
Longitudinal shear modulus $G_{LT}$ [GPa]	24
Thermal expansion $\alpha_{th}$ [1/K]	$2 \times 10^{-6}$
Thermal conductivity $\mathbf{k}$ [W/(K · m)]	diag(40)
Seebeck coefficient $\alpha$ [V/K]	$3 \times 10^{-6}$
Electrical conductivity $\mathbf{1} \alpha$ [S/m]	diag(10) $\times 10^4$
Heat capacity $c_v$ [J/(kg · K)]	712

ond one the sample is subjected to constrained recovery, and in the third one the sample is subjected to free recovery.

#### 6.4.1.1 Uniaxial compression tests

In these tests, we consider a single quadratic element. The tests are performed at constant temperatures of 22 [°C], 40 [°C], and 50 [°C], and are subjected to strain control up to true strain  $\simeq 100$  % at a rates of 0.1 [s<sup>-1</sup>], and 0.001 [s<sup>-1</sup>]. Fig. 6.3 shows the different behaviors of the SMP above and below glass transition temperature and at different strain rates. At temperature below glass transition,  $T = 22$  [°C], Fig. 6.3(a), the yield peak appears followed by strain softening, then strain hardening. Since the temperature is lower than  $T_g$ , permanent plastic deformation can be seen. At temperature above glass transition, at  $T = 65$  [°C], Fig. 6.3(c), the stiffness is clearly lower and as the constrain is removed, SMP recovers its original shape. A distinct behavior is observed near glass transition temperature,  $T = 40$  [°C], Fig. 6.3(b), where at high strain rate 0.1 [s<sup>-1</sup>], it behaves as a glassy polymer, while at low strain rate 0.001 [s<sup>-1</sup>] it behaves as hysteretic rubber. In these figures, it can be noted that at high strain rates the generated stress is higher and the glass transition temperature is not constant, it increases with the increase of the strain rate. Our results agree with the experimental results reported by Srivastava et al. [68].

#### 6.4.1.2 A shape memory polymer constrained recovery tests

In these tests, the mesh is composed of 8 quadratic bricks. The cube is subjected to the following Thermo-Mechanical cycle under a constrained recovery

- At temperature above glass transition a compressive strain of 15 % is applied.
- The temperature is decreased below the glass transition to room temperature 25 [°C] under a constrained strain.

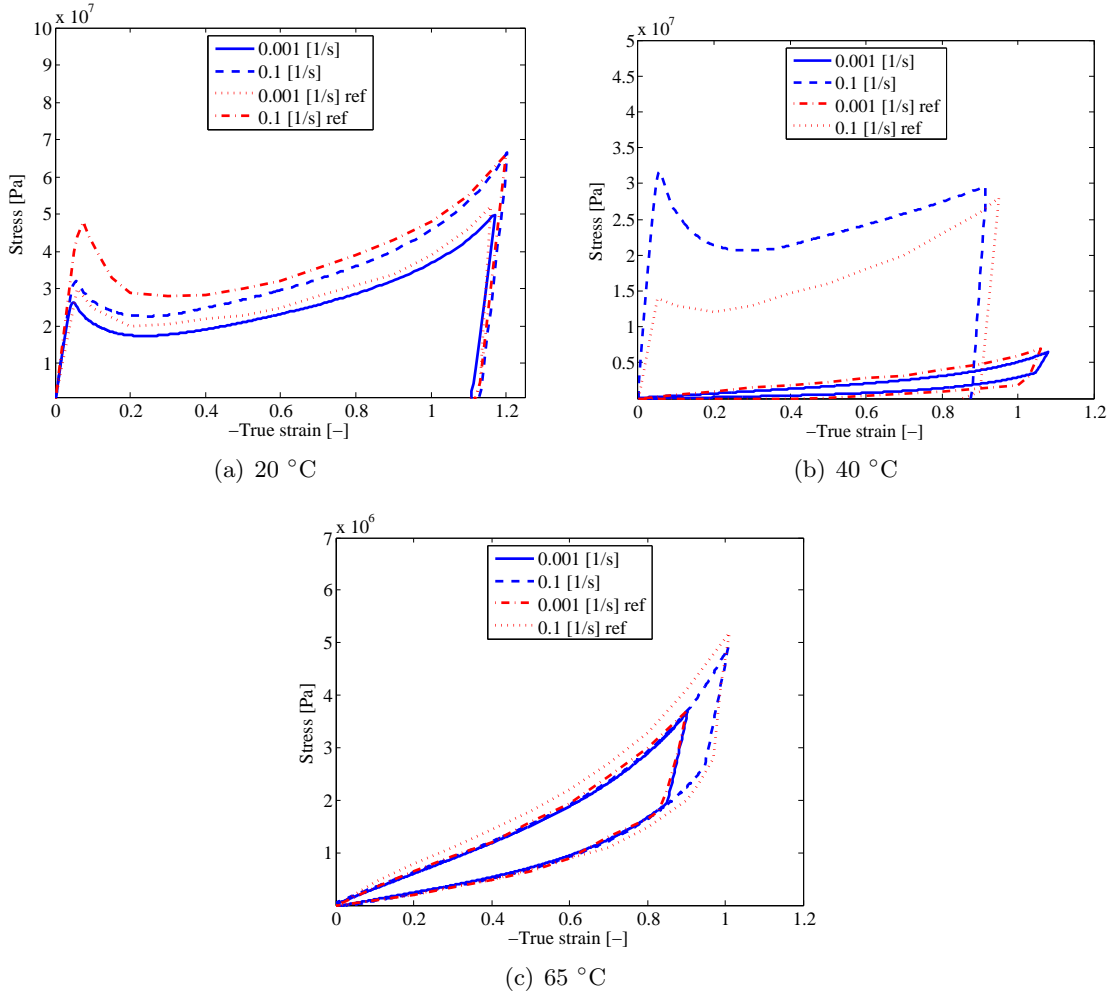


Figure 6.3: Stress-strain curves at strain rates  $0.1 \text{ [s}^{-1}\text{]}$  and  $0.001 \text{ [s}^{-1}\text{]}$ , and at different temperatures  $22 \text{ [}^\circ\text{C]}$ ,  $40 \text{ [}^\circ\text{C]}$ , and  $65 \text{ [}^\circ\text{C]}$  and experimental results reported in [68]

- The temperature is increased back above glass transition  $58 \text{ [}^\circ\text{C]}$  under the compression constrain.

The engineering strain and temperature histories are plotted in Fig. 6.4 and the force versus time curve is plotted in Fig. 6.5, where the effect of material hardening in the force during the deformation above  $T_g$  is shown, then during the cooling the effect of material softening is also seen. In the same figure the same test is performed a second time but without considering mechanism 2, and it is clear that the two curves agree well.

In order to highlight the time dependency behavior of SMP, the same test is performed with an increase in the strain rate from  $0.0015 \text{ s}^{-1}$  of the previous test to  $0.015 \text{ s}^{-1}$  as presented in Fig. 6.6. The resulting curve when the 3 mechanisms are used still agrees very well with the curve with two mechanisms, i.e. when the second mechanisms is not considered.

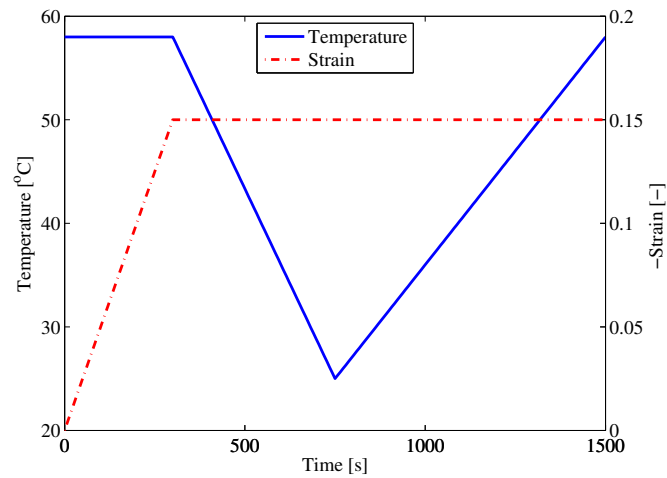


Figure 6.4: The temperature and displacement histories of the constrained recovery test

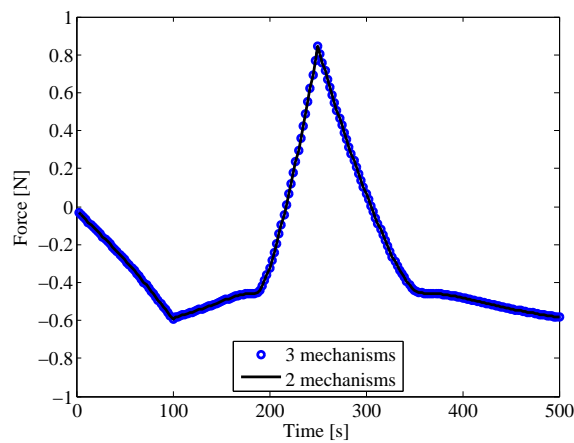


Figure 6.5: The force versus time curve for small strain rate of the constrained recovery test

#### 6.4.1.3 A shape memory polymer free recovery tests

In these tests, the mesh is composed of 8 quadratic bricks. The applied pressure and heating-cooling cycle for the free recovery test are presented in Fig. 6.7, the specimen was subjected to the following Thermo-Mechanical cycle

- Apply a pressure of  $9 \times 10^5$  [N/m<sup>2</sup>] on the cube at temperature above glass transition 60 [°C].
- Cool it down to 21 [°C] under the compression pressure.
- Remove the constrain at 21 [°C].
- Reheat it again above glass transition to 60 [°C] allowing to recover freely the original shape.



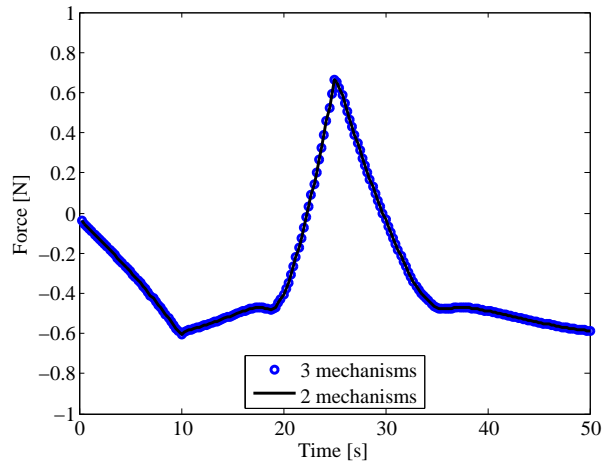


Figure 6.6: The force versus time curve for high strain rate of the constrained recovery test

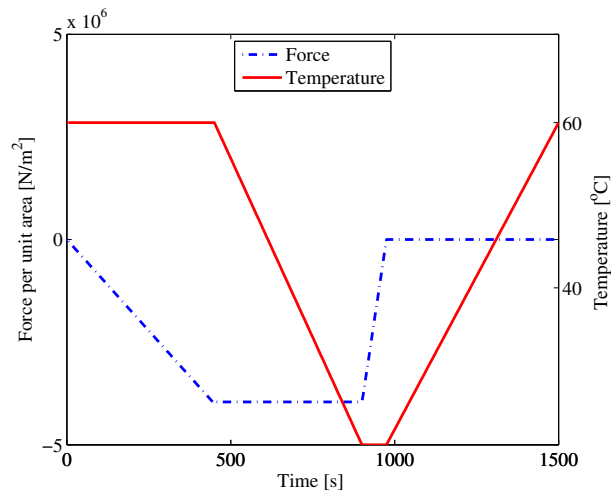


Figure 6.7: The pressure and temperature versus time of the free recovery test

The engineering strain versus temperature histories are plotted in Fig. 6.8, and the shape recovery is showed. We have the same result when the same test is applied without considering the second mechanism, as displayed in the same figure. Henceforth from the previous two tests, the constrained and the free recovery tests, we can conclude that the Thermo-Mechanical properties of SMP can be reproduced without considering the second mechanism. Eventually the following tests will be performed without considering the second mechanism, since the resolution of mechanism 2 is time consuming as compared to the other two ones.

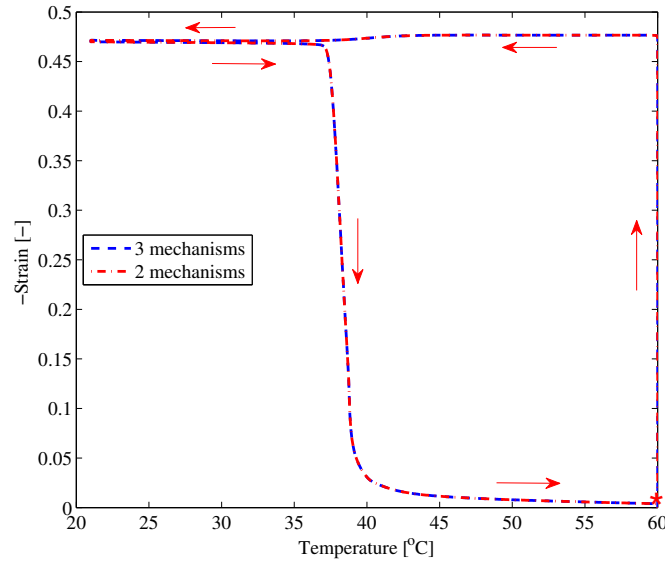


Figure 6.8: The strain versus temperature curve of the free recovery test

#### 6.4.2 3-D Electro-Thermo-Mechanical coupling compression test applied on Shape memory polymers reinforced by carbon fibers (SMPC)

The following test focuses in applying the proposed composite model to simulate the conductive SMPC behavior at large-deformation regime, when triggered by Joule effect. The geometry is illustrated in Fig. 6.9 and the applied boundary conditions are the following: the displacement is constrained along three perpendicular faces as follows: the nodes in the XY-plane are fixed along the Z-direction, the nodes in the YZ-plane are fixed along the X-direction, and the nodes in the XZ-plane are fixed along the Y-direction, while the other three faces are restrained in order to get a uniform deformation, the top face is restrained in the Z-direction, the infront face is restrained in the Y-direction and the right face is restrained in the X-direction. It should be noted that the temperature is restrained on the Shape Memory Polymer volume to get a uniform distribution of the temperature. The initial value of the electric potential is 0 [V] and the initial value of the temperature is 21 [°C]. The material parameters are provided in Tables 6.1 and 6.2. A finite element mesh of 79 quadratic bricks is considered and the value of stabilization parameter is  $\beta=100$ . The test is implemented with displacement control as shown in Fig. 6.11, and the applied electric potential on the back face is given in the same figure, while on the infront face is 0 [V].

The unit cell of SMPC is subjected to indirect heating by applying electric potential with the following Electro-Thermo-Mechanical history:

- Apply an electric field of 0.28 [V] in order to heat the cell above the glass transition temperature of 37 [°C].
- Compress the sample above glass transition.
- Reduce the electric field to 0 [V], in order to cool the cell down to room temperature, while the cell is still under a constrained strain.

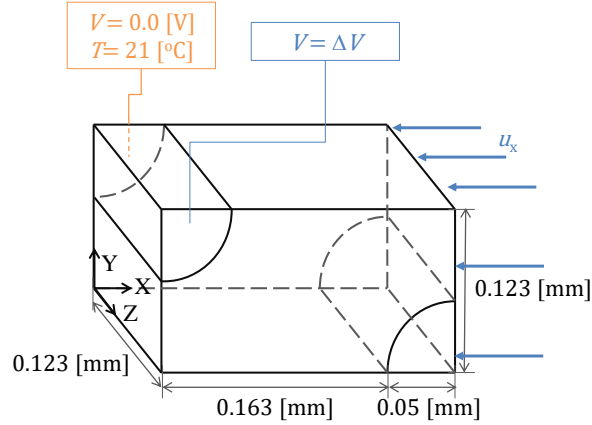


Figure 6.9: Unit cell of SMPC used for the compression test

- Increase the electric field back to 0.28 [V], which causes increase in the temperature of the sample to a temperature above the glass transition, and maintain the deformation constant until the cell reaches a value above the glass transition temperature of 37 [°C], then unload the material in order to recover the original shape.

The resulting temperature of the SMP volume versus time is plotted in Fig. 6.12.

The particular behavior of SMPC is illustrated through the average stress shown in Fig. 6.13. Deformed shapes of the SMPC unit cell and the corresponding stress distribution along the compression direction are illustrated in Fig. 6.10. It appears that the force starts to increase (in absolute value) during the heating by Joule effect due to thermal dilation, and a sudden drop can be observed once the temperature reaches the glass transition temperature  $T_g$ . Then the force increases due to the cell deformation above the glass transition temperature  $T_g$ . Afterward, there is an increase of the force during the constrained cooling as the deformation constraint is still applied. When the temperature is minimal, the force has almost vanished, which represent a fixation of the deformation, see also the limited stress distribution in Fig. 6.10(b). Then, the force decreases dramatically and changes the sign when it reaches the glass transition temperature  $T_g$ , which means that it tends to recover the original shape, see the important stress distribution in Fig. 6.10(c). once the displacement constrain is removed above  $T_g$ , the force reaches a zero value as the cell recover its original shape above the glass transition temperature  $T_g$  around 1200 [s], see Fig. 6.10(d).

### 6.4.3 3-D Electro-Thermo-Mechanical coupling bending test applied on Shape memory polymers reinforced by carbon fibers (SMPC)

The aim of the following test is to apply the free recovery test on carbon fiber reinforced shape memory polymer.

The unit cell of SMPC is subjected to indirect heating by applying electric potential. This cell is similar to the one illustrated in Fig. 6.9, but with different dimensions: the length of the unit cell is 1.7 [mm], the width is 0.0425 [mm], the height is 0.0614 [mm], and the CF radius is 0.01 [mm], as shown in Fig. 6.14, to achieve proper bending conditions. The back side of the cell is fixed along all the directions, the temperature is fixed on that

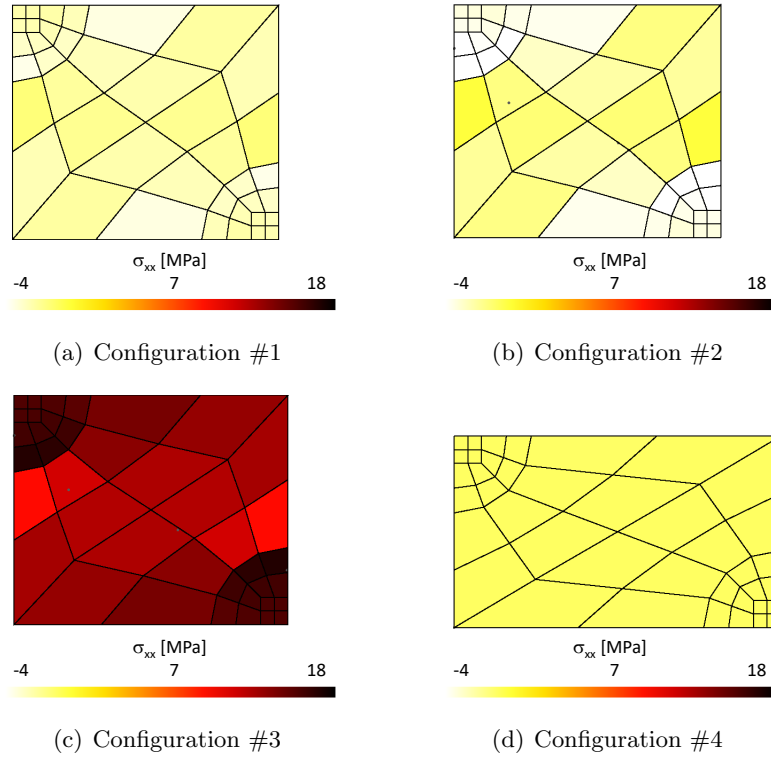


Figure 6.10: Snapshots of the SMPC unit-cell under compression test during the Electro-Thermo-Mechanical cycle. #1 ( $t = 750$  s): after compression above the glass transition temperature. #2 ( $t = 900$  s): after having released the voltage difference. #3 ( $t = 1135$  s): after having applied again a voltage difference to reheat above the glass transition temperature with partial compression. #4 ( $t = 1500$  s): after having removed the compression above the glass transition temperature.

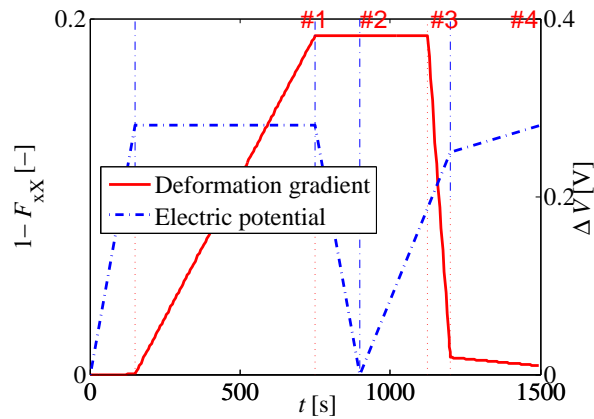


Figure 6.11: The displacement and temperature versus time of SMPC unit cell

face and on the infront side as well, while differences in the electric potentials are applied on those faces, see Fig. 6.15. One more condition is to restrain the side faces along the

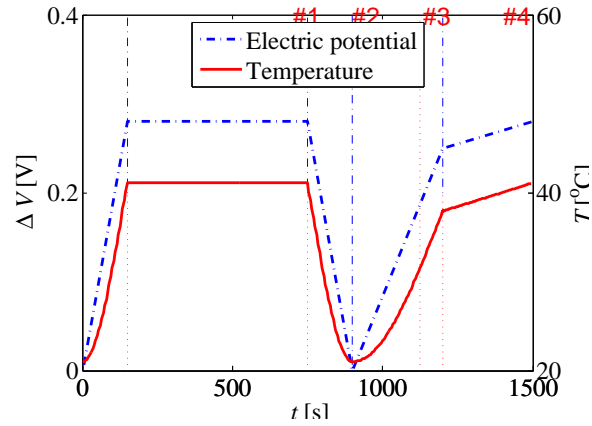


Figure 6.12: The distributions of the electric potential and the resulting SMP temperature versus time

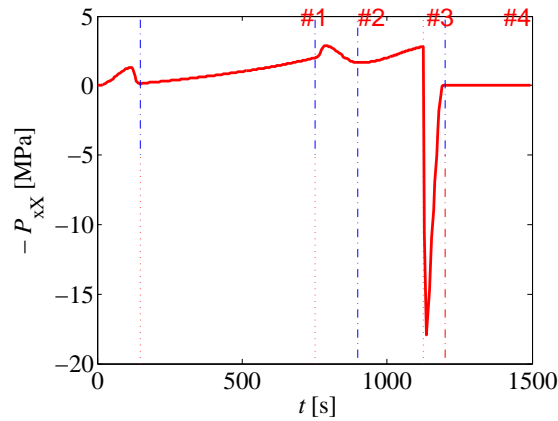


Figure 6.13: The force versus time

X-direction, in order to get a uniform deformation. The initial value of the temperature is 25 [°C] and the initial value of the electric potential is 0 [V]. A finite element mesh of 90 linear bricks is considered, and the value of the stabilization parameter is  $\beta = 100$ .

The applied boundary condition for the force and electric potential versus time are illustrated in Fig .6.15, with the following Electro-Thermo-Mechanical history

- Apply an electric field of 0.35 [V], which generates heat and increases the temperature.
- Apply perpendicular force on the free infront face.
- Reduce the electric field to 0 [V], in order to cool the cell down under a constrained strain.
- Remove the force at 25 [°C].
- Increase the electric field back to 0.35 [V], which causes an increase in the temperature of the composite cell to recover freely the original shape.

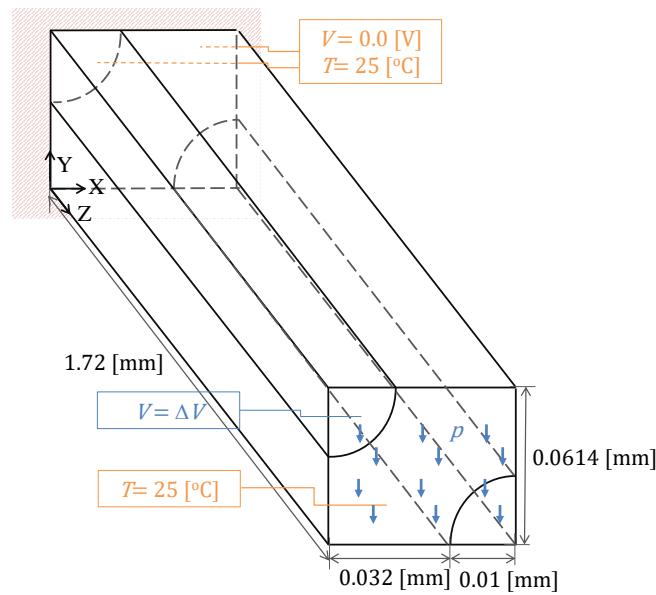


Figure 6.14: Unit cell of SMPC beam for the bending test

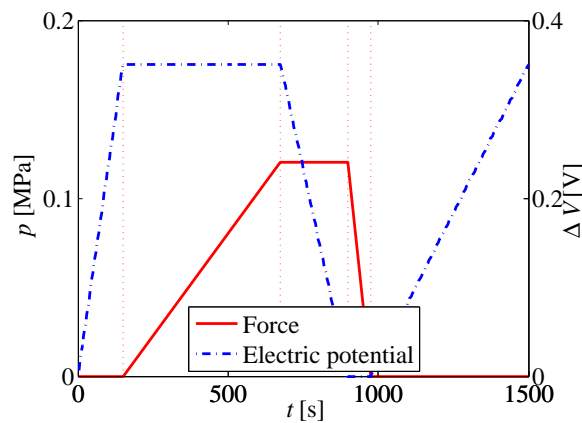


Figure 6.15: Boundary condition of SMPC beam for the bending test

The resulting temperature history is evaluated at the mid-length of the beam and is shown in Fig. 6.16, and the electric potential and temperature distribution along the beam length at time  $t=500$  [s] are illustrated in Fig. 6.17. When an electric potential of 0.35 [V] is applied, the temperature increases inside the beam and reaches 59.7 [°C], which is above the glass transition temperature, at the beam mid-length. The distribution of the electric potential is close to linear but the distribution of the temperature is almost quadratic with a maximum value of 59.7 [°C]. Therefore, only a part of the beam has a shape memory effect that can be triggered during the test.

The displacement history of the beam extremity is illustrated in Fig. 6.18, and the successive configurations are reported in Fig. 6.19. It can be noticed that the cell recovers part of the deformation as the force is removed. Indeed, only part of the deformation can be recovered since, on the one hand the carbon fibers remain elastic, and on the other hand

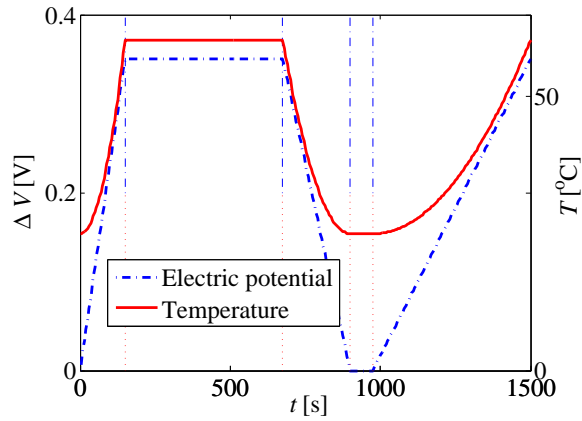


Figure 6.16: The evolution of the applied electric potential difference on the beam extremities and the evolution of the resulting temperature at the beam mid-length

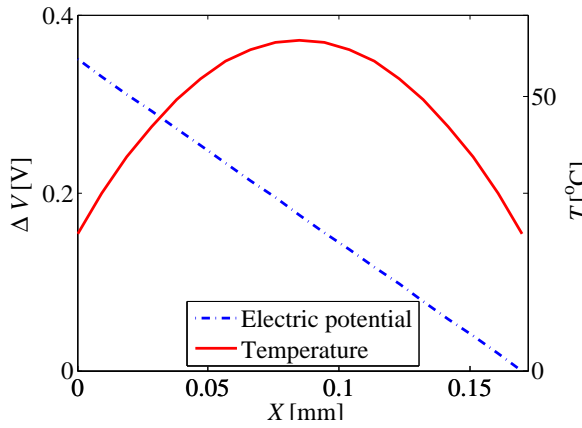


Figure 6.17: The distributions of the temperature and electric potential along the beam length at time 500 [s]

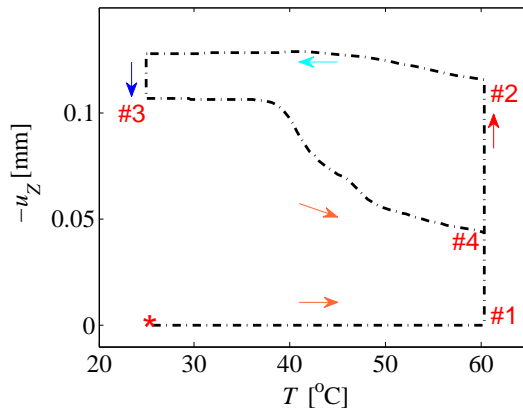


Figure 6.18: Shape Memory recovery via the temperature generated by Joule effect

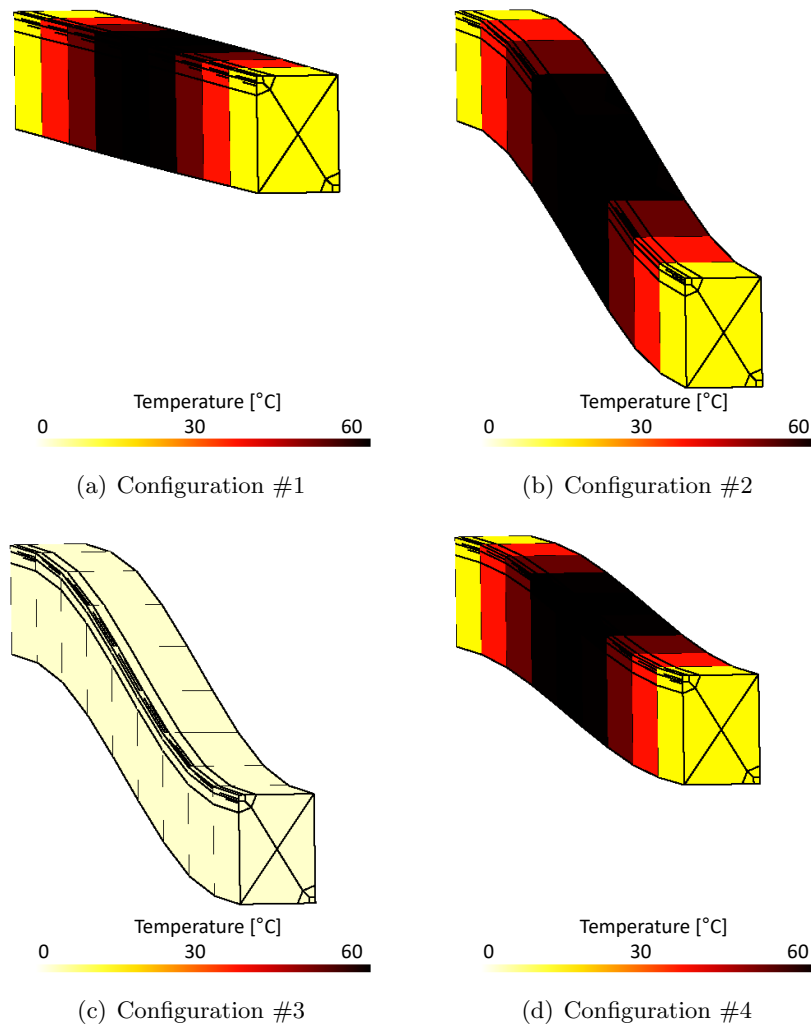


Figure 6.19: Snapshots of the SMPC beam simulation during the Electro-Thermo-Mechanical cycle of the free recovery bending test. #1: after applying an electric potential of 0.35 [V] to heat the beam above the glass transition temperature. #2: after applying the load to bend the beam. #3: after removing the load at 0 [V] of electric potential. #4: after reapplying an electric potential of 0.35 [V] to recover the initial configuration.

only one part of the beam reaches a value higher than the glass transition.

## 6.5 Conclusions

The main focus of this chapter is to apply the presented constitutive models in simulating the conductive SMPC behavior in the large-deformation regime, when it is actuated by joule effect, in addition to simulate non conductive SMP. Several numerical simulations are reported for simple and complicated geometries in the large-deformation regime. The presented models are able to predict the behavior of carbon fiber reinforced Shape Memory



Polymers for free recovery and constrained recovery.



## Chapter 7

# Conclusions and perspectives

In this thesis the DG method has been extended to simulate linear and nonlinear coupled problems, in particular Thermo-Elastic, Electro-Thermal, and Electro-Thermo-Mechanical coupled problems. Starting from the first principles of solid mechanics, and electrical and thermal field theories as the basic tools, the DG method has been derived as a consistent and stable weak form to solve the various interacting physics in the coupled simulations for non-composite and composite materials, in particular, for carbon fiber reinforced Shape Memory Polymer Composites (SMPC).

In Chapter 3, the DG for Thermo-Elastic problems has been analyzed, then it has been extended to nonlinear Electro-Thermal elliptic problems in Chapter 4, and to Electro-Thermo-Mechanics in Chapter 5. The Electro-Thermal coupling equations were formulated in terms of energetically conjugated pairs of fluxes and fields gradient. Indeed, the use of energetically consistent pairs allowed us writing the strong form in a matrix form suitable to the derivation of a stable SIPG weak form. Particular attention was paid in proving the uniqueness, consistency, and stability of the discrete solution for the Thermo-Elasticity, Electro-Thermal, and Electro-Thermo-Elasticity coupling problems (the latter one being formulated in a small deformation setting). In addition, the optimal error estimate in the  $L^2$ - and  $H^1$ -norms were proved under the assumption of the use of a polynomial degree of approximation  $k \geq 2$ . Moreover, numerical simulations were carried out to illustrate the performance of the DGFEM applied on linear elliptic problems and non-linear elliptic problems in order to confirm the theoretical results.

In Chapter 6, the constitutive equations that govern the behaviors of carbon fiber and shape memory polymer have been presented. Numerical simulations were performed for composite and non-composite SMP. It was shown that the constitutive model of SMP is able to predict the characteristic behavior of SMPs above and below the glass transition temperature. The numerical results were compared with some experimental results presented in the literature, showing good agreements. A micromechanical model of unidirectional carbon fibers embedded in a shape memory polymer matrix was formulated by considering the interaction of electrical, thermal, and mechanical fields. When the mechanical and electrical loads were applied, the heat induced due to the Joule effect triggered the shape memory behavior.

In this work the DG method was used to solve linear and nonlinear elliptic coupled problems and the theoretical results were derived. It would be worthwhile to extend the

study of DG methods to time dependent problems. Moreover, in the future, the multiphysics framework will serve as a basis toward the formulation of multi-scale analyzes for smart composite materials.

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# Appendix A

## Annexes related to chapter 2

### A.1 Bounds of the norms

For  $\mathbf{O}_h \in X^k$ , the two extra terms of the norm defined by Eq. (2.12) in comparison to the norm defined by Eq. (2.11) can be linked with the other terms. First, using the trace inequality, Eq. (2.17) and the inverse inequality, Eq. (2.21), we have

$$\begin{aligned} \sum_e h^s \|\mathbf{O}_h\|_{L^2(\partial\Omega^e)}^2 &\leq \sum_e C_{\mathcal{T}} \left( \|\mathbf{O}_h\|_{L^2(\Omega^e)}^2 + h^s \|\mathbf{O}_h\|_{L^2(\Omega^e)} \|\nabla \mathbf{O}_h\|_{L^2(\Omega^e)} \right) \\ &\leq \sum_e C_{\mathcal{T}} (C_{\mathcal{I}}^k + 1) \|\mathbf{O}_h\|_{L^2(\Omega^e)}^2. \end{aligned} \quad (\text{A.1})$$

Then by Eq. (2.18), we have

$$\sum_e h^s \|\nabla \mathbf{O}_h\|_{L^2(\partial\Omega^e)}^2 \leq \sum_e C_{\mathcal{K}}^k \|\nabla \mathbf{O}_h\|_{L^2(\Omega^e)}^2. \quad (\text{A.2})$$

Therefore the norm  $\|\|\mathbf{O}_h\|\|_1$ , Eq. (2.12), can be bounded by

$$\begin{aligned} \|\|\mathbf{O}_h\|\|_1 &\leq \sum_e \left( (1 + C_{\mathcal{T}}(C_{\mathcal{I}}^k + 1)) \|\mathbf{O}_h\|_{L^2(\Omega^e)}^2 + (C_{\mathcal{K}}^k + 1) \|\nabla \mathbf{O}_h\|_{L^2(\Omega^e)}^2 \right. \\ &\quad \left. + h_s^{-1} \|\llbracket \mathbf{O}_{\mathbf{n}_h} \rrbracket\|_{L^2(\partial\Omega^e)}^2 \right). \end{aligned} \quad (\text{A.3})$$

This leads to complete the proof of Lemma 2.4.5, that

$$\|\|\mathbf{O}_h\|\|_1 \leq C^k \|\|\mathbf{O}_h\|\|, \quad (\text{A.4})$$

with  $C^k = \max(1 + C_{\mathcal{T}}(C_{\mathcal{I}}^k + 1), (C_{\mathcal{K}}^k + 1))$ .

### A.2 Energy bound

Using the definition of the mesh dependent norm, Eq. (2.12), with  $\boldsymbol{\eta} = \mathbf{O}^e - I_h \mathbf{O} \in X$  in  $X_2$ , where  $I_h \mathbf{O}$  is the interpolant of  $\mathbf{O}^e$  in  $X^k$  we have

$$\|\|\boldsymbol{\eta}\|\|_1^2 = \sum_e \|\boldsymbol{\eta}\|_{H^1(\Omega^e)}^2 + \sum_e h_s \|\boldsymbol{\eta}\|_{H^1(\partial\Omega^e)}^2 + \sum_e h_s^{-1} \|\llbracket \boldsymbol{\eta}_{\mathbf{n}} \rrbracket\|_{L^2(\partial\Omega^e)}^2. \quad (\text{A.5})$$

For the first term of the right hand side, using the interpolation inequality, Eq. (2.13), leads to

$$\sum_e \|\boldsymbol{\eta}\|_{H^1(\Omega^e)}^2 \leq C_{\mathcal{D}}^{k^2} h_s^{2\mu-2} \sum_e \|\mathbf{O}^e\|_{H^s(\Omega^e)}^2, \quad (\text{A.6})$$

with  $\mu = \min(s, k+1)$ ,  $s > 1$ . Then, applying Lemma 2.4.1, Eq. (2.15), yields

$$\sum_e h_s \|\boldsymbol{\eta}\|_{H^1(\partial\Omega^e)}^2 \leq C_{\mathcal{D}}^{k^2} (h_s^{2\mu-2}) \sum_e \|\mathbf{O}^e\|_{H^s(\Omega^e)}^2. \quad (\text{A.7})$$

Now for the last interface term in Eq. (A.5), as the interior edge  $(\partial_I\Omega)^s$  is shared by the element  $+$  and  $-$ , using  $(a-b)^2 \leq 2a^2 + 2b^2$ , we have

$$\begin{aligned} & \sum_e \int_{\partial\Omega^e} h_s^{-1} \|\llbracket \boldsymbol{\eta}_{\mathbf{n}} \rrbracket\|^2 dS \\ & \leq h_s^{-1} \sum_e \left( 2 \int_{\partial_I\Omega^e} \|\boldsymbol{\eta}_{\mathbf{n}}^+\|^2 dS + 2 \int_{\partial_I\Omega^e} \|\boldsymbol{\eta}_{\mathbf{n}}^-\|^2 dS + \int_{\partial_D\Omega^e} \|\boldsymbol{\eta}_{\mathbf{n}}\|^2 dS \right) \\ & \leq 4 \sum_e \int_{\partial\Omega^e} h_s^{-1} \|\boldsymbol{\eta}_{\mathbf{n}}\|^2 dS. \end{aligned} \quad (\text{A.8})$$

Therefore, using Lemma 1, Eq. (2.15) leads to

$$\sum_e h_s^{-1} \|\llbracket \boldsymbol{\eta}_{\mathbf{n}} \rrbracket\|_{L^2(\partial\Omega^e)}^2 \leq 4 \sum_e h_s^{-1} \|\boldsymbol{\eta}_{\mathbf{n}}\|_{H^0(\partial\Omega^e)}^2 \leq 4C_{\mathcal{D}}^{k^2} \sum_e h_s^{2\mu-2} \|\mathbf{O}^e\|_{H^s(\Omega^e)}^2. \quad (\text{A.9})$$

By combining the above results, the proof of Lemma 2.4.6 is completed as

$$\|\boldsymbol{\eta}\|_1 \leq C^k h_s^{\mu-1} \left( \sum_e \|\mathbf{O}^e\|_{H^s(\Omega^e)}^2 \right)^{\frac{1}{2}} = C^k h_s^{\mu-1} \|\mathbf{O}^e\|_{H^s(\Omega_h)}, \quad (\text{A.10})$$

with  $\mu = \min(s, k+1)$ .

## Appendix B

# Annexes related to chapter 3

### B.1 Stiffness matrix for Thermo-Elastic coupling

First  $\mathbf{K}_{\mathbf{uu}}$ , the derivative of the displacement contributions with respect to  $\mathbf{u}$ , is computed using Eq. (3.45)

$$\frac{\partial \mathbf{F}_{\mathbf{u}^{\text{int}}}^{\mathbf{a}}}{\partial \mathbf{u}^{\mathbf{b}}} = \sum_e \int_{\Omega^e} \frac{\partial \boldsymbol{\sigma}}{\partial \mathbf{u}^{\mathbf{b}}} \cdot \nabla N_{\mathbf{u}}^{\mathbf{a}} d\Omega = \sum_e \int_{\Omega^e} \nabla N_{\mathbf{u}}^{\mathbf{a}} \cdot \boldsymbol{\mathcal{H}} \cdot \nabla N_{\mathbf{u}}^{\mathbf{b}} d\Omega. \quad (\text{B.1})$$

Similarly, for the interface contribution<sup>1</sup>, Eqs. (4.75, 4.76, and 4.77), from Eqs. (3.47), (3.48), and (3.49) one can get

$$\frac{\partial \mathbf{F}_{\mathbf{u}^{\text{I1}}}^{\mathbf{a}\pm}}{\partial \mathbf{u}^{\mathbf{b}\pm}} = \frac{1}{2} \sum_s \int_{(\partial\Gamma)^s} (\pm N_{\mathbf{u}}^{\mathbf{a}\pm}) \mathbf{n}^- \cdot \boldsymbol{\mathcal{H}}^{\pm} \cdot \nabla N_{\mathbf{u}}^{\mathbf{b}\pm} dS, \quad (\text{B.2})$$

$$\frac{\partial \mathbf{F}_{\mathbf{u}^{\text{I2}}}^{\mathbf{a}\pm}}{\partial \mathbf{u}^{\mathbf{b}\pm}} = \frac{1}{2} \sum_s \int_{(\partial\Gamma)^s} (\pm N_{\mathbf{u}}^{\mathbf{b}\pm}) \nabla N_{\mathbf{u}}^{\mathbf{a}\pm} \cdot \boldsymbol{\mathcal{H}}^{\pm} \cdot \mathbf{n}^- dS, \quad (\text{B.3})$$

$$\frac{\partial \mathbf{F}_{\mathbf{u}^{\text{I3}}}^{\mathbf{a}\pm}}{\partial \mathbf{u}^{\mathbf{b}\pm}} = \frac{1}{2} \sum_s \int_{(\partial\Gamma)^s} (\pm N_{\mathbf{u}}^{\mathbf{b}\pm}) \mathbf{n}^- \cdot \frac{\boldsymbol{\mathcal{H}}^{\pm} \boldsymbol{\beta}}{2h_s} \cdot \mathbf{n}^- (\pm N_{\mathbf{u}}^{\mathbf{a}\pm}) dS, \quad (\text{B.4})$$

where the symbol  $\pm$  refers to the node  $\mathbf{a}^{\pm}$  (+ for node  $\mathbf{a}^+$  and - for node  $\mathbf{a}^-$ ).

The stiffness matrix of the mechanical forces with respect to T,  $\mathbf{K}_{\mathbf{uT}}$  is evaluated from

$$\frac{\partial \mathbf{F}_{\mathbf{u}^{\text{int}}}^{\mathbf{a}}}{\partial T^{\mathbf{b}}} = - \sum_e \int_{\Omega^e} N_{\mathbf{T}}^{\mathbf{b}} \boldsymbol{\alpha}_{\text{th}} : \boldsymbol{\mathcal{H}} \cdot \nabla N_{\mathbf{u}}^{\mathbf{a}} d\Omega, \quad (\text{B.5})$$

$$\frac{\partial \mathbf{F}_{\mathbf{u}^{\text{I1}}}^{\mathbf{a}}}{\partial T^{\mathbf{b}\pm}} = \frac{1}{2} \sum_s \int_{(\partial\Gamma)^s} (\mp N_{\mathbf{u}}^{\mathbf{a}\pm}) \boldsymbol{\alpha}_{\text{th}}^{\pm} : \boldsymbol{\mathcal{H}}^{\mp} \cdot \mathbf{n}^- N_{\mathbf{T}}^{\mathbf{b}\pm} dS. \quad (\text{B.6})$$

$$\frac{\partial \mathbf{F}_{\mathbf{u}^{\text{I2}}}^{\mathbf{a}\pm}}{\partial T^{\mathbf{b}\pm}} = - \frac{\gamma}{2} \sum_s \int_{(\partial\Gamma)^s} N_{\mathbf{u}}^{\mathbf{a}\pm} \boldsymbol{\alpha}_{\text{th}}^{\pm} : \boldsymbol{\mathcal{H}}^{\pm} (\mp N_{\mathbf{T}}^{\mathbf{b}\pm}) \cdot \mathbf{n}^- dS, \quad (\text{B.7})$$

<sup>1</sup>The contributions on  $\partial_D \Omega_h$  can be directly deduced by removing the factor (1/2) accordingly to the definition of the average flux on the Dirichlet boundary.

The derivatives of the thermal contributions with respect to  $f_T$ ,  $\mathbf{K}_{TT}$ , for the volume term is obtained from Eq. (3.51)

$$\begin{aligned} \frac{\partial F_{Tint}^a}{\partial T^b} &= - \sum_e \int_{\Omega^e} \frac{\partial \mathbf{q}}{\partial T} \cdot \nabla N_T^a N_T^b d\Omega - \sum_e \int_{\Omega^e} \nabla N_T^a \cdot \frac{\partial \mathbf{q}}{\partial \nabla T} \cdot \nabla N_T^b d\Omega \\ &+ \sum_e \int_{\Omega^e} \frac{\partial \dot{T}}{\partial T} \rho_{c_v} N_T^b N_T^a d\Omega = \sum_e \int_{\Omega^e} \nabla N_T^a \cdot \mathbf{k} \cdot \nabla N_T^b d\Omega \\ &+ \sum_e \int_{\Omega^e} \frac{\partial \dot{T}}{\partial T} \rho_{c_v} N_T^b N_T^a d\Omega, \end{aligned} \quad (B.8)$$

and the derivatives of the interface forces are computed by calling Eqs. (3.53), (3.54), and (3.55) leading to

$$\begin{aligned} \frac{\partial F_{TI1}^{a\pm}}{\partial T^{b\pm}} &= \frac{1}{2} \sum_s \int_{(\partial_I \Omega)^s} (\mp N_T^{a\pm}) \frac{\partial \mathbf{q}^\pm}{\partial T^\pm} N_T^{b\pm} \cdot \mathbf{n}^- dS_0 \\ &+ \frac{1}{2} \sum_s \int_{(\partial_I \Omega)^s} (\mp N_T^{a\pm}) \left( \frac{\partial \mathbf{q}^\pm}{\partial \nabla T^\pm} \cdot \nabla N_T^{b\pm} \right) \cdot \mathbf{n}^- dS \\ &= \frac{1}{2} \sum_s \int_{(\partial_I \Omega)^s} (\pm N_T^{a\pm}) (\mathbf{k}^\pm \cdot \nabla N_T^{b\pm}) \cdot \mathbf{n}^- dS, \end{aligned} \quad (B.9)$$

$$\frac{\partial F_{TI2}^{a\pm}}{\partial T^{b\pm}} = \frac{1}{2} \sum_s \int_{(\partial_I \Omega)^s} (\pm N_T^{b\pm}) \mathbf{k}^\pm \cdot \nabla N_T^{a\pm} \cdot \mathbf{n}^- dS, \text{ and} \quad (B.10)$$

$$\frac{\partial F_{TI3}^{a\pm}}{\partial T^{b\pm}} = \frac{1}{2} \sum_s \int_{(\partial_I \Omega)^s} (\pm N_T^{a\pm}) \mathbf{n}^- \cdot \frac{\mathbf{k}^\pm \mathcal{B}}{h_s} \cdot \mathbf{n}^- (\pm N_T^{b\pm}) dS. \quad (B.11)$$

## B.2 Lower bound for Thermo-Elastic coupling

In order to derive the lower bound of the Thermo-Elastic DG formulation, let us first use  $\delta \mathbf{E}_h$  as  $\mathbf{E}_h$  in Eq. (3.24), yielding

$$\begin{aligned} a(\delta \mathbf{E}_h, \delta \mathbf{E}_h) &= \int_{\Omega_h} (\nabla \delta \mathbf{E})_h^T \mathbf{w} \nabla \delta \mathbf{E}_h d\Omega - \int_{\Omega_h} \delta \mathbf{E}_h^T \mathbf{r}^T \nabla \delta \mathbf{E}_h d\Omega \\ &+ 2 \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \llbracket \delta \mathbf{E}_h^T \rrbracket \langle \mathbf{w} \nabla \delta \mathbf{E}_{h_n} \rangle dS + \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \llbracket \delta \mathbf{E}_{h_n}^T \rrbracket \left\langle \frac{\mathbf{w} \mathcal{B}}{h_s} \right\rangle \llbracket \delta \mathbf{E}_{h_n} \rrbracket dS \\ &- \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \llbracket \delta \mathbf{E}_{h_n}^T \rrbracket \langle \mathbf{r} \delta \mathbf{E}_h \rangle dS - \gamma \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \langle \delta \mathbf{E}_{h_n}^T \rangle \llbracket \mathbf{r} \delta \mathbf{E}_h \rrbracket dS. \end{aligned} \quad (B.12)$$

Using Eqs. (3.59) and (3.60), Eq. (B.12) becomes

$$\begin{aligned}
a(\delta \mathbf{E}_h, \delta \mathbf{E}_h) &\geq \sum_e \left( C_\alpha \|\nabla \delta \mathbf{E}_h\|_{L^2(\Omega^e)}^2 - C_x \|\nabla \delta \mathbf{E}_h\|_{L^2(\Omega^e)} \|\delta \mathbf{E}_h\|_{L^2(\Omega^e)} \right) \\
&\quad - 2 \sum_s C_x \left| \int_{(\partial_{DI}\Omega)^s} \llbracket \delta \mathbf{E}_{h_n} \rrbracket \langle \nabla \delta \mathbf{E}_h \rangle \, dS \right| \\
&\quad - (1 + \gamma) \sum_s C_x \left| \int_{(\partial_{DI}\Omega)^s} \llbracket \delta \mathbf{E}_{h_n} \rrbracket \langle \delta \mathbf{E}_h \rangle \, dS \right| \\
&\quad + \sum_s C_\alpha \frac{\mathcal{B}}{h_s} \|\llbracket \delta \mathbf{E}_{h_n} \rrbracket\|_{L^2((\partial_{DI}\Omega)^s)}^2.
\end{aligned} \tag{B.13}$$

The third and fourth terms of the right hand side in Eq. (B.13) can be bounded using Cauchy-Schwartz' inequality, Eq. (2.26),

$$\begin{aligned}
&2C_x \sum_s \left| \int_{(\partial_{DI}\Omega)^s} \llbracket \delta \mathbf{E}_{h_n} \rrbracket \langle \nabla \delta \mathbf{E}_h \rangle \, dS \right| + (1 + \gamma) C_x \sum_s \left| \int_{(\partial_{DI}\Omega)^s} \llbracket \delta \mathbf{E}_{h_n} \rrbracket \langle \delta \mathbf{E}_h \rangle \, dS \right| \\
&\leq 2C_x \left( \sum_s \frac{1}{h_s} \|\llbracket \delta \mathbf{E}_{h_n} \rrbracket\|_{L^2((\partial_{DI}\Omega)^s)}^2 \right)^{\frac{1}{2}} \left( \sum_s h_s \|\langle \nabla \delta \mathbf{E}_h \rangle\|_{L^2((\partial_{DI}\Omega)^s)}^2 \right)^{\frac{1}{2}} \\
&\quad + (1 + \gamma) C_x \left( \sum_s \frac{1}{h_s} \|\llbracket \delta \mathbf{E}_{h_n} \rrbracket\|_{L^2((\partial_{DI}\Omega)^s)}^2 \right)^{\frac{1}{2}} \left( \sum_s h_s \|\langle \delta \mathbf{E}_h \rangle\|_{L^2((\partial_{DI}\Omega)^s)}^2 \right)^{\frac{1}{2}} \\
&\leq 2C_x \left( \sum_s \frac{1}{h_s} \|\llbracket \delta \mathbf{E}_{h_n} \rrbracket\|_{L^2((\partial_{DI}\Omega)^s)}^2 \right)^{\frac{1}{2}} \left[ \left( \sum_s h_s \|\langle \nabla \delta \mathbf{E}_h \rangle\|_{L^2((\partial_{DI}\Omega)^s)}^2 \right)^{\frac{1}{2}} \right. \\
&\quad \left. + \left( \sum_s h_s \|\langle \delta \mathbf{E}_h \rangle\|_{L^2((\partial_{DI}\Omega)^s)}^2 \right)^{\frac{1}{2}} \right],
\end{aligned} \tag{B.14}$$

assuming  $\gamma \leq 1$ .

First, the term  $h_s \|\langle \nabla \delta \mathbf{E}_h \rangle\|_{L^2((\partial_{DI}\Omega)^s)}^2$  can be bounded using the trace inequality on the finite element space (2.18), with

$$\begin{aligned}
\sum_s h_s \|\langle \nabla \delta \mathbf{E}_h \rangle\|_{L^2((\partial_{DI}\Omega)^s)}^2 &= \frac{1}{2} \sum_e h_s \|\langle \nabla \delta \mathbf{E}_h \rangle\|_{L^2(\partial_t \Omega^e)}^2 + \sum_e h_s \|\langle \nabla \delta \mathbf{E}_h \rangle\|_{L^2(\partial_D \Omega^e)}^2 \\
&\leq \sum_e h_s \|\nabla \delta \mathbf{E}_h\|_{L^2(\partial \Omega^e)}^2 \leq C_{\mathcal{K}}^{k^2} \sum_e \|\nabla \delta \mathbf{E}_h\|_{L^2(\Omega^e)}^2.
\end{aligned} \tag{B.15}$$

Then using the trace inequality, Eq. (2.16), and inverse inequality, Eq. (2.21), we have

$$\begin{aligned}
\sum_s h_s \|\langle \delta \mathbf{E}_h \rangle\|_{L^2((\partial_{\text{DI}}\Omega)^s)}^2 &= \frac{1}{2} \sum_e h_s \|\langle \delta \mathbf{E}_h \rangle\|_{L^2(\partial_1 \Omega^e)}^2 + \sum_e h_s \|\langle \delta \mathbf{E}_h \rangle\|_{L^2(\partial_{\text{D}} \Omega^e)}^2 \\
&\leq \sum_e h_s \|\delta \mathbf{E}_h\|_{L^2(\partial \Omega^e)}^2 \\
&\leq C_{\mathcal{T}} \sum_e \left( \|\delta \mathbf{E}_h\|_{L^2(\Omega^e)}^2 + h_s \|\delta \mathbf{E}_h\|_{L^2(\Omega^e)} \|\nabla \delta \mathbf{E}_h\|_{L^2(\Omega^e)} \right) \\
&\leq \sum_e C_{\mathcal{T}} (C_{\mathcal{I}}^k + 1) \|\delta \mathbf{E}_h\|_{L^2(\Omega^e)}^2.
\end{aligned} \tag{B.16}$$

Therefore Eq. (B.14) is rewritten as

$$\begin{aligned}
&2C_x \sum_s \left| \int_{(\partial_{\text{DI}}\Omega)^s} \llbracket \delta \mathbf{E}_{h_n} \rrbracket \langle \nabla \delta \mathbf{E}_h \rangle \, dS \right| + (1 + \gamma) C_x \sum_s \left| \int_{(\partial_{\text{DI}}\Omega)^s} \llbracket \delta \mathbf{E}_{h_n} \rrbracket \langle \delta \mathbf{E}_h \rangle \, dS \right| \\
&\leq C_x \left( \sum_s \frac{1}{h_s} \|\llbracket \delta \mathbf{E}_{h_n} \rrbracket\|_{L^2((\partial_1 \Omega)^s)}^2 \right)^{\frac{1}{2}} \left( \sum_e \max(4C_{\mathcal{T}}(C_{\mathcal{I}}^k + 1), 4C_{\mathcal{K}}^{k^2}) (\|\delta \mathbf{E}_h\|_{H^1(\Omega^e)}^2) \right)^{\frac{1}{2}}.
\end{aligned} \tag{B.17}$$

Finally, by the use of the  $\xi$ -inequality  $-\xi > 0 : |ab| \leq \frac{\xi}{4} a^2 + \frac{1}{\xi} b^2$  with  $\xi = \frac{C_\alpha}{C_x \max(4C_{\mathcal{T}}(C_{\mathcal{I}}^k + 1), 4C_{\mathcal{K}}^{k^2})}$ , we arrive at

$$\begin{aligned}
&2C_x \sum_s \left| \int_{(\partial_{\text{DI}}\Omega)^s} \llbracket \delta \mathbf{E}_{h_n} \rrbracket \langle \nabla \delta \mathbf{E}_h \rangle \, dS \right| + (1 + \gamma) C_x \sum_s \left| \int_{(\partial_{\text{DI}}\Omega)^s} \llbracket \delta \mathbf{E}_{h_n} \rrbracket \langle \delta \mathbf{E}_h \rangle \, dS \right| \\
&\leq \frac{C_\alpha}{4} \sum_e \|\delta \mathbf{E}_h\|_{H^1(\Omega^e)}^2 + \frac{C_x^2}{C_\alpha} \max(4C_{\mathcal{T}}(C_{\mathcal{I}}^k + 1), 4C_{\mathcal{K}}^{k^2}) \sum_s \frac{1}{h_s} \|\llbracket \delta \mathbf{E}_{h_n} \rrbracket\|_{L^2((\partial_1 \Omega)^s)}^2.
\end{aligned} \tag{B.18}$$

For the second term of the right hand side of Eq. (B.13), by choosing  $\xi = \frac{C_\alpha}{C_x}$  and applying the  $\xi$ -inequality, we find

$$\begin{aligned}
\sum_e C_x \|\nabla \delta \mathbf{E}_h\|_{L^2(\Omega^e)} \|\delta \mathbf{E}_h\|_{L^2(\Omega^e)} &\leq \frac{C_x}{\xi} \sum_e \|\delta \mathbf{E}_h\|_{L^2(\Omega^e)}^2 + \frac{C_x \xi}{4} \sum_e \|\nabla \delta \mathbf{E}_h\|_{L^2(\Omega^e)}^2 \\
&\leq \frac{C_x^2}{C_\alpha} \sum_e \|\delta \mathbf{E}_h\|_{L^2(\Omega^e)}^2 + \frac{C_\alpha}{4} \sum_e \|\nabla \delta \mathbf{E}_h\|_{L^2(\Omega^e)}^2.
\end{aligned} \tag{B.19}$$

If we substitute Eqs. (B.18) and (B.19) in Eq. (B.13), we thus obtain the following result:

$$\begin{aligned}
a(\delta \mathbf{E}_h, \delta \mathbf{E}_h) &\geq \frac{C_\alpha}{2} \sum_e \|\nabla \delta \mathbf{E}_h\|_{L^2(\Omega^e)}^2 - \left( \frac{C_x^2}{C_\alpha} + \frac{C_\alpha}{4} \right) \sum_e \|\delta \mathbf{E}_h\|_{L^2(\Omega^e)}^2 \\
&\quad + \left[ \mathcal{B}C_\alpha - \frac{C_x^2}{C_\alpha} \max(4C_{\mathcal{T}}(C_{\mathcal{I}}^k + 1), 4C_{\mathcal{K}}^{k^2}) \right] h_s^{-1} \sum_e \|\llbracket \delta \mathbf{E}_{h_n} \rrbracket\|_{L^2(\partial \Omega^e)}^2.
\end{aligned} \tag{B.20}$$



This last relation can be rewritten as

$$\begin{aligned} a(\delta\mathbf{E}_h, \delta\mathbf{E}_h) &\geq C_1^k \left[ \sum_e \|\nabla\delta\mathbf{E}_h\|_{L^2(\Omega^e)}^2 + h_s^{-1} \sum_e \|\llbracket\delta\mathbf{E}_{h_n}\rrbracket\|_{L^2(\partial\Omega^e)}^2 \right] \\ &\quad - C_2^k \|\delta\mathbf{E}_h\|_{L^2(\Omega_h)}^2 \quad \forall \delta\mathbf{E}_h \in X^k, \end{aligned} \quad (\text{B.21})$$

where  $C_1^k = \min\left(\frac{C_\alpha}{2}, \mathcal{B}C_\alpha - \frac{C_x^2}{C_\alpha} \max(4C_{\mathcal{T}}(C_{\mathcal{I}}^k + 1), 4C_{\mathcal{K}}^{k^2})\right)$ , which is positive when  $\mathcal{B} > \frac{C_x^2}{C_\alpha} \max(4C_{\mathcal{T}}(C_{\mathcal{I}}^k + 1), 4C_{\mathcal{K}}^{k^2})$ , and  $C_2^k = \frac{C_x^2}{C_\alpha} + \frac{C_\alpha}{4} > 0$ .

Therefore, comparing with the definition of the mesh dependent norm, Eq. (2.10), we have

$$a(\delta\mathbf{E}_h, \delta\mathbf{E}_h) \geq C_1^k \|\delta\mathbf{E}_h\|_*^2 - C_2^k \|\delta\mathbf{E}_h\|_{L^2(\Omega_h)}^2 \quad \forall \delta\mathbf{E}_h \in X^k. \quad (\text{B.22})$$

Moreover, starting from Eq. (B.20) and choosing  $C_2^k = \frac{C_x^2}{C_\alpha} + \frac{3C_\alpha}{4}$ , we rewrite the expression in terms of the norm (2.11) as

$$a(\delta\mathbf{E}_h, \delta\mathbf{E}_h) \geq C_1^k \|\delta\mathbf{E}_h\|^2 - C_2^k \|\delta\mathbf{E}_h\|_{L^2(\Omega_h)}^2 \quad \forall \delta\mathbf{E}_h \in X^k. \quad (\text{B.23})$$

Hence, this shows that the stability of the method is conditioned by the constant  $\mathcal{B}$ , which should be large enough.

### B.3 Upper bound for Thermo-Elastic coupling

We prove herein that our DG formulation for Thermo-Elastic is upper bounded. First the upper bound of the bi-linear form Eq. (3.24), for  $\mathbf{E}, \delta\mathbf{E} \in X$  is obtained by

$$\begin{aligned} |a(\mathbf{E}, \delta\mathbf{E})| &\leq \left| \int_{\Omega_h} (\nabla\mathbf{E})^T \mathbf{w} \nabla\delta\mathbf{E} d\Omega \right| + \left| \int_{\Omega_h} \mathbf{E}^T \mathbf{r}^T \nabla\delta\mathbf{E} d\Omega \right| \\ &\quad + \left| \int_{\partial\Gamma\Omega_h \cup \partial_D\Omega_h} \llbracket\delta\mathbf{E}_n^T\rrbracket \langle \mathbf{w} \nabla\mathbf{E} \rangle dS \right| + \left| \int_{\partial\Gamma\Omega_h \cup \partial_D\Omega_h} \llbracket\mathbf{E}_n^T\rrbracket \langle \mathbf{w} \nabla\delta\mathbf{E} \rangle dS \right| \\ &\quad + \left| \int_{\partial\Gamma\Omega_h \cup \partial_D\Omega_h} \llbracket\mathbf{E}_n^T\rrbracket \left\langle \frac{\mathbf{w}\mathcal{B}}{h_s} \right\rangle \llbracket\delta\mathbf{E}_n\rrbracket dS \right| + \left| \gamma \int_{\partial\Gamma\Omega_h \cup \partial_D\Omega_h} \langle \delta\mathbf{E}_n^T \rangle \llbracket\mathbf{r}\mathbf{E}\rrbracket dS \right| \\ &\quad + \left| \int_{\partial\Gamma\Omega_h \cup \partial_D\Omega_h} \llbracket\delta\mathbf{E}_n^T\rrbracket \langle \mathbf{r}\mathbf{E} \rangle dS \right|. \end{aligned} \quad (\text{B.24})$$

Then let us bound every term in the right hand side using the Hölder's inequality, Eq. (2.24), and the bound Eq. (3.60). The bound of the first term reads

$$\begin{aligned} \left| \int_{\Omega_h} \nabla\mathbf{E}^T \mathbf{w} \nabla\delta\mathbf{E} d\Omega \right| &\leq \sum_e \left( \int_{\Omega^e} |\nabla\mathbf{E}^T \mathbf{w} \nabla\delta\mathbf{E}| d\Omega \right) \\ &\leq C_x \sum_e \|\nabla\delta\mathbf{E}\|_{L^2(\Omega^e)} \|\nabla\mathbf{E}\|_{L^2(\Omega^e)}, \end{aligned} \quad (\text{B.25})$$

likewise, for the second term, we have

$$\begin{aligned} \left| \int_{\Omega_h} \mathbf{E}^T \mathbf{r}^T \nabla\delta\mathbf{E} d\Omega \right| &\leq \sum_e \left( \int_{\Omega^e} |\mathbf{E}^T \mathbf{r}^T \nabla\delta\mathbf{E}| d\Omega \right) \\ &\leq C_x \sum_e \|\nabla\delta\mathbf{E}\|_{L^2(\Omega^e)} \|\mathbf{E}\|_{L^2(\Omega^e)}, \end{aligned} \quad (\text{B.26})$$

and for the third term we have

$$\begin{aligned}
& \left| \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \llbracket \delta \mathbf{E}_n^T \rrbracket \langle \mathbf{w} \nabla \mathbf{E} \rangle dS \right| \leq \frac{1}{2} \sum_e \int_{\partial_I \Omega^e} \llbracket \delta \mathbf{E}_n^T \rrbracket \langle \mathbf{w} \nabla \mathbf{E} \rangle dS \\
& + \sum_e \int_{\partial_D \Omega^e} \llbracket \delta \mathbf{E}_n^T \rrbracket \langle \mathbf{w} \nabla \mathbf{E} \rangle dS \leq \sum_e \left\| h_s^{\frac{1}{2}} \mathbf{w} \nabla \mathbf{E} \right\|_{L^2(\partial \Omega^e)} \left\| h_s^{-\frac{1}{2}} \llbracket \delta \mathbf{E}_n \rrbracket \right\|_{L^2(\partial \Omega^e)} \quad (\text{B.27}) \\
& \leq C_x \sum_e \left\| h_s^{\frac{1}{2}} \nabla \mathbf{E} \right\|_{L^2(\partial \Omega^e)} \left\| h_s^{-\frac{1}{2}} \llbracket \delta \mathbf{E}_n \rrbracket \right\|_{L^2(\partial \Omega^e)}.
\end{aligned}$$

The same argument goes for the fourth, sixth, and seventh terms as follow

$$\left| \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \llbracket \mathbf{E}_n^T \rrbracket \langle \mathbf{w} \nabla \delta \mathbf{E} \rangle dS \right| \leq C_x \sum_e \left\| h_s^{\frac{1}{2}} \nabla \delta \mathbf{E} \right\|_{L^2(\partial \Omega^e)} \left\| h_s^{-\frac{1}{2}} \llbracket \mathbf{E}_n \rrbracket \right\|_{L^2(\partial \Omega^e)}, \quad (\text{B.28})$$

$$\begin{aligned}
& \left| \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \langle \delta \mathbf{E}_n^T \rangle \llbracket \mathbf{r} \mathbf{E} \rrbracket dS \right| \leq \frac{1}{2} \sum_e \int_{\partial_I \Omega^e} \langle \delta \mathbf{E}_n^T \rangle \llbracket \mathbf{r} \mathbf{E} \rrbracket dS \\
& + \sum_e \int_{\partial_D \Omega^e} \langle \delta \mathbf{E}_n^T \rangle \llbracket \mathbf{r} \mathbf{E} \rrbracket dS \leq C_x \sum_e \left\| h_s^{\frac{1}{2}} \delta \mathbf{E} \right\|_{L^2(\partial \Omega^e)} \left\| h_s^{-\frac{1}{2}} \llbracket \mathbf{E}_n \rrbracket \right\|_{L^2(\partial \Omega^e)}, \quad (\text{B.29})
\end{aligned}$$

$$\begin{aligned}
& \left| \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \llbracket \delta \mathbf{E}_n^T \rrbracket \langle \mathbf{r} \mathbf{E} \rangle dS \right| \leq \frac{1}{2} \sum_e \int_{\partial_I \Omega^e} \llbracket \delta \mathbf{E}_n^T \rrbracket \langle \mathbf{r} \mathbf{E} \rangle dS \\
& + \sum_e \int_{\partial_D \Omega^e} \llbracket \delta \mathbf{E}_n^T \rrbracket \langle \mathbf{r} \mathbf{E} \rangle dS \leq C_x \sum_e \left\| h_s^{\frac{1}{2}} \mathbf{E} \right\|_{L^2(\partial \Omega^e)} \left\| h_s^{-\frac{1}{2}} \llbracket \delta \mathbf{E}_n \rrbracket \right\|_{L^2(\partial \Omega^e)}. \quad (\text{B.30})
\end{aligned}$$

In the same way, the fifth term becomes

$$\begin{aligned}
& \left| \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \llbracket \mathbf{E}_n^T \rrbracket \left\langle \frac{\mathbf{w} \mathcal{B}}{h_s} \right\rangle \llbracket \delta \mathbf{E}_n \rrbracket dS \right| \leq \frac{1}{2} \sum_e \int_{\partial_I \Omega^e} \llbracket \mathbf{E}_n^T \rrbracket \left\langle \frac{\mathbf{w} \mathcal{B}}{h_s} \right\rangle \llbracket \delta \mathbf{E}_n \rrbracket dS \\
& + \sum_e \int_{\partial_D \Omega^e} \llbracket \mathbf{E}_n^T \rrbracket \left\langle \frac{\mathbf{w} \mathcal{B}}{h_s} \right\rangle \llbracket \delta \mathbf{E}_n \rrbracket dS \quad (\text{B.31}) \\
& \leq \mathcal{B} C_x \sum_e \left\| h_s^{-\frac{1}{2}} \llbracket \delta \mathbf{E}_n \rrbracket \right\|_{L^2(\partial \Omega^e)} \left\| h_s^{-\frac{1}{2}} \llbracket \mathbf{E}_n \rrbracket \right\|_{L^2(\partial \Omega^e)}.
\end{aligned}$$

Therefore by combining the above results and assuming  $|\gamma| \leq 1$ , we can rewrite Eq. (B.24) as follows

$$\begin{aligned}
|a(\mathbf{E}, \delta\mathbf{E})| &\leq C_x \sum_e \|\nabla\mathbf{E}\|_{L^2(\Omega^e)} \|\nabla\delta\mathbf{E}\|_{L^2(\Omega^e)} \\
&+ C_x \sum_e \|\mathbf{E}\|_{L^2(\Omega^e)} \|\nabla\delta\mathbf{E}\|_{L^2(\Omega^e)} \\
&+ \mathcal{B}C_x \sum_e \|\mathbf{h}_s^{-\frac{1}{2}} \llbracket \mathbf{E}_n \rrbracket\|_{L^2(\partial\Omega^e)} \|\mathbf{h}_s^{-\frac{1}{2}} \llbracket \delta\mathbf{E}_n \rrbracket\|_{L^2(\partial\Omega^e)} \\
&+ C_x \sum_e \|\mathbf{h}_s^{\frac{1}{2}} \nabla\mathbf{E}\|_{L^2(\partial\Omega^e)} \|\mathbf{h}_s^{-\frac{1}{2}} \llbracket \delta\mathbf{E}_n \rrbracket\|_{L^2(\partial\Omega^e)} \\
&+ C_x \sum_e \|\mathbf{h}_s^{-\frac{1}{2}} \llbracket \mathbf{E}_n \rrbracket\|_{L^2(\partial\Omega^e)} \|\mathbf{h}_s^{\frac{1}{2}} \nabla\delta\mathbf{E}\|_{L^2(\partial\Omega^e)} \\
&+ C_x \sum_e \|\mathbf{h}_s^{\frac{1}{2}} \mathbf{E}\|_{L^2(\partial\Omega^e)} \|\mathbf{h}_s^{-\frac{1}{2}} \llbracket \delta\mathbf{E}_n \rrbracket\|_{L^2(\partial\Omega^e)} \\
&+ C_x \sum_e \|\mathbf{h}_s^{\frac{1}{2}} \delta\mathbf{E}\|_{L^2(\partial\Omega^e)} \|\mathbf{h}_s^{-\frac{1}{2}} \llbracket \mathbf{E}_n \rrbracket\|_{L^2(\partial\Omega^e)}.
\end{aligned} \tag{B.32}$$

Choosing  $C = \max(C_x, C_x\mathcal{B})$ , the previous equation is rewritten as:

$$\begin{aligned}
|a(\mathbf{E}, \delta\mathbf{E})| &\leq C \sum_e \|\nabla\mathbf{E}\|_{L^2(\Omega^e)} \|\nabla\delta\mathbf{E}\|_{L^2(\Omega^e)} \\
&+ C \sum_e \|\mathbf{E}\|_{L^2(\Omega^e)} \|\nabla\delta\mathbf{E}\|_{L^2(\Omega^e)} \\
&+ C \sum_e \|\mathbf{h}_s^{-\frac{1}{2}} \llbracket \mathbf{E}_n \rrbracket\|_{L^2(\partial\Omega^e)} \|\mathbf{h}_s^{-\frac{1}{2}} \llbracket \delta\mathbf{E}_n \rrbracket\|_{L^2(\partial\Omega^e)} \\
&+ C \sum_e \|\mathbf{h}_s^{\frac{1}{2}} \nabla\mathbf{E}\|_{L^2(\partial\Omega^e)} \|\mathbf{h}_s^{-\frac{1}{2}} \llbracket \delta\mathbf{E}_n \rrbracket\|_{L^2(\partial\Omega^e)} \\
&+ C \sum_e \|\mathbf{h}_s^{-\frac{1}{2}} \llbracket \mathbf{E}_n \rrbracket\|_{L^2(\partial\Omega^e)} \|\mathbf{h}_s^{\frac{1}{2}} \nabla\delta\mathbf{E}\|_{L^2(\partial\Omega^e)} \\
&+ C \sum_e \|\mathbf{h}_s^{\frac{1}{2}} \mathbf{E}\|_{L^2(\partial\Omega^e)} \|\mathbf{h}_s^{-\frac{1}{2}} \llbracket \delta\mathbf{E}_n \rrbracket\|_{L^2(\partial\Omega^e)} \\
&+ C \sum_e \|\mathbf{h}_s^{\frac{1}{2}} \delta\mathbf{E}\|_{L^2(\partial\Omega^e)} \|\mathbf{h}_s^{-\frac{1}{2}} \llbracket \mathbf{E}_n \rrbracket\|_{L^2(\partial\Omega^e)}.
\end{aligned} \tag{B.33}$$

After some maths, this becomes

$$\begin{aligned}
|a(\mathbf{E}, \delta\mathbf{E})| &\leq C \sum_e \left[ \|\nabla\mathbf{E}\|_{L^2(\Omega^e)} + \|\mathbf{E}\|_{L^2(\Omega^e)} + (\mathbf{h}_s)^{\frac{1}{2}} \|\mathbf{E}\|_{L^2(\partial\Omega^e)} \right. \\
&\quad \left. + (\mathbf{h}_s)^{\frac{1}{2}} \|\nabla\mathbf{E}\|_{L^2(\partial\Omega^e)} + \left(\frac{1}{\mathbf{h}_s}\right)^{\frac{1}{2}} \|\llbracket \mathbf{E}_n \rrbracket\|_{L^2(\partial\Omega^e)} \right] \\
&\quad \times \left[ \|\nabla\delta\mathbf{E}\|_{L^2(\Omega^e)} + \|\delta\mathbf{E}\|_{L^2(\Omega^e)} + (\mathbf{h}_s)^{\frac{1}{2}} \|\delta\mathbf{E}\|_{L^2(\partial\Omega^e)} \right. \\
&\quad \left. + (\mathbf{h}_s)^{\frac{1}{2}} \|\nabla\delta\mathbf{E}\|_{L^2(\partial\Omega^e)} + \left(\frac{1}{\mathbf{h}_s}\right)^{\frac{1}{2}} \|\llbracket \delta\mathbf{E}_n \rrbracket\|_{L^2(\partial\Omega^e)} \right].
\end{aligned} \tag{B.34}$$

Using the Cauchy-Schwartz' inequality, Eq. (2.26), and the property  $2ab \leq a^2 + b^2$ , this last equation becomes

$$\begin{aligned}
|a(\mathbf{E}, \delta\mathbf{E})|^2 &\leq C^2 \sum_e \left[ \|\nabla\mathbf{E}\|_{L^2(\Omega^e)} + \|\mathbf{E}\|_{L^2(\Omega^e)} + (h_s)^{\frac{1}{2}} \|\mathbf{E}\|_{L^2(\partial\Omega^e)} \right. \\
&\quad \left. + (h_s)^{\frac{1}{2}} \|\nabla\mathbf{E}\|_{L^2(\partial\Omega^e)} + \left(\frac{1}{h_s}\right)^{\frac{1}{2}} \|\llbracket\mathbf{E}_n\rrbracket\|_{L^2(\partial\Omega^e)} \right]^2 \\
&\quad \times \sum_{e'} \left[ \|\nabla\delta\mathbf{E}\|_{L^2(\Omega^{e'})} + \|\delta\mathbf{E}\|_{L^2(\Omega^{e'})} + (h_s)^{\frac{1}{2}} \|\delta\mathbf{E}\|_{L^2(\partial\Omega^{e'})} \right. \\
&\quad \left. + (h_s)^{\frac{1}{2}} \|\nabla\delta\mathbf{E}\|_{L^2(\partial\Omega^{e'})} + \left(\frac{1}{h_s}\right)^{\frac{1}{2}} \|\llbracket\delta\mathbf{E}_n\rrbracket\|_{L^2(\partial\Omega^{e'})} \right]^2 \\
&\leq 4C^2 \sum_e \left[ \|\nabla\mathbf{E}\|_{L^2(\Omega^e)}^2 + \|\mathbf{E}\|_{L^2(\Omega^e)}^2 + h_s \|\mathbf{E}\|_{L^2(\partial\Omega^e)}^2 + \right. \\
&\quad \left. h_s \|\nabla\mathbf{E}\|_{L^2(\partial\Omega^e)}^2 + h_s^{-1} \|\llbracket\mathbf{E}_n\rrbracket\|_{L^2(\partial\Omega^e)}^2 \right] \times \\
&\quad \sum_{e'} \left[ \|\nabla\delta\mathbf{E}\|_{L^2(\Omega^{e'})}^2 + \|\delta\mathbf{E}\|_{L^2(\Omega^{e'})}^2 + h_s \|\delta\mathbf{E}\|_{L^2(\partial\Omega^{e'})}^2 \right. \\
&\quad \left. + h_s \|\nabla\delta\mathbf{E}\|_{L^2(\partial\Omega^{e'})}^2 + h_s^{-1} \|\llbracket\delta\mathbf{E}_n\rrbracket\|_{L^2(\partial\Omega^{e'})}^2 \right]. \tag{B.35}
\end{aligned}$$

Considering 4 in  $C^2$ , and using the definition of the mesh dependent norm, (2.12), we get:

$$|a(\mathbf{E}, \delta\mathbf{E})| \leq C \|\mathbf{E}\|_1 \|\delta\mathbf{E}\|_1 \quad \forall \mathbf{E}, \delta\mathbf{E} \in X. \tag{B.36}$$

Moreover, using Eq. (2.22), we obtain directly

$$|a(\mathbf{E}, \delta\mathbf{E}_h)| \leq C^k \|\mathbf{E}\|_1 \|\delta\mathbf{E}_h\|_1 \quad \forall \mathbf{E} \in X, \delta\mathbf{E}_h \in X^k, \tag{B.37}$$

and again, using Eq. (2.22), we have

$$|a(\mathbf{E}_h, \delta\mathbf{E}_h)| \leq C^k \|\mathbf{E}_h\|_1 \|\delta\mathbf{E}_h\|_1 \quad \forall \mathbf{E}_h, \delta\mathbf{E}_h \in X^k. \tag{B.38}$$

## B.4 Uniqueness of the solution for Thermo-Elastic coupling

Let us first show that for a given  $\boldsymbol{\xi} \in [L^2(\Omega)]^d \times L^2(\Omega)$ , there is a unique  $\boldsymbol{\phi}_h \in X^k$  such that

$$a(\delta\mathbf{E}_h, \boldsymbol{\phi}_h) = \sum_e \int_{\Omega_e} \boldsymbol{\xi}^T \delta\mathbf{E}_h d\Omega \quad \forall \delta\mathbf{E}_h \in X^k. \tag{B.39}$$

From Lemma 3.4.1, Eq. (3.66), with  $\delta\mathbf{E}_h = \boldsymbol{\phi}_h \in X^k$ ,  $\exists C_1^k, C_2^k$ , such that:

$$a(\boldsymbol{\phi}_h, \boldsymbol{\phi}_h) \geq C_1^k \|\boldsymbol{\phi}_h\|_1^2 - C_2^k \|\boldsymbol{\phi}_h\|_{L^2(\Omega_h)}^2. \tag{B.40}$$

Using  $\delta\mathbf{E}_h = \boldsymbol{\phi}_h$  in Eq. (B.39) thus yields

$$\begin{aligned}
C_1^k \|\boldsymbol{\phi}_h\|_1^2 - C_2^k \|\boldsymbol{\phi}_h\|_{L^2(\Omega_h)}^2 &\leq \sum_e \int_{\Omega} \boldsymbol{\xi}^T \boldsymbol{\phi}_h d\Omega \\
&\leq \|\boldsymbol{\xi}\|_{L^2(\Omega_h)} \|\boldsymbol{\phi}_h\|_{L^2(\Omega_h)}, \tag{B.41}
\end{aligned}$$

or again

$$C_1^k ||| \boldsymbol{\phi}_h |||^2 \leq \| \boldsymbol{\xi} \|_{L^2(\Omega_h)} \| \boldsymbol{\phi}_h \|_{L^2(\Omega_h)} + C_2^k \| \boldsymbol{\phi}_h \|_{L^2(\Omega_h)}^2. \quad (\text{B.42})$$

Using the definition (2.11) of the energy norm, we have that  $\| \boldsymbol{\phi}_h \|_{L^2(\Omega_h)} \leq ||| \boldsymbol{\phi}_h |||$ , and Eq. (B.42) becomes

$$C_1^k ||| \boldsymbol{\phi}_h |||^2 \leq \| \boldsymbol{\xi} \|_{L^2(\Omega_h)} ||| \boldsymbol{\phi}_h ||| + C_2^k ||| \boldsymbol{\phi}_h ||| \| \boldsymbol{\phi}_h \|_{L^2(\Omega_h)}. \quad (\text{B.43})$$

Hence, we have

$$||| \boldsymbol{\phi}_h ||| \leq C_3^k \| \boldsymbol{\xi} \|_{L^2(\Omega_h)} + C_4^k \| \boldsymbol{\phi}_h \|_{L^2(\Omega_h)}. \quad (\text{B.44})$$

In order to estimate  $\| \boldsymbol{\phi}_h \|_{L^2(\Omega_h)}$ , we use the auxiliary problem stated by Eq. (3.70), with  $\boldsymbol{\phi} = \boldsymbol{\phi}_h$ . Then it follows from [23, Theorem 8.3 and Lemma 9.17] that there exists a unique solution  $\boldsymbol{\psi} \in [H^2(\Omega)]^d \times H^2(\Omega)$  to the problem stated by Eq. (3.70), and the solution satisfies the elliptic property stated by Eq. (3.71). Multiplying Eq. (3.70) by  $\boldsymbol{\phi}_h$ , integrating on  $\Omega_h$ , and integrating by parts yield

$$\begin{aligned} & \sum_e \int_{\Omega^e} [\mathbf{w} \nabla \boldsymbol{\psi}]^T \nabla \boldsymbol{\phi}_h d\Omega - \sum_e \int_{\partial \Omega^e} [\mathbf{w} \nabla \boldsymbol{\psi}]^T \boldsymbol{\phi}_{h_n} dS \\ & - \sum_e \int_{\Omega^e} [\mathbf{r} \boldsymbol{\psi}]^T \nabla \boldsymbol{\phi}_h d\Omega + \sum_e \int_{\partial \Omega^e} [\mathbf{r} \boldsymbol{\psi}]^T \boldsymbol{\phi}_{h_n} dS = \int_{\Omega_h} \boldsymbol{\phi}_h^T \boldsymbol{\phi}_h d\Omega = \| \boldsymbol{\phi}_h \|_{L^2(\Omega_h)}^2. \end{aligned} \quad (\text{B.45})$$

As  $\boldsymbol{\psi} \in [H^2(\Omega)]^d \times H^2(\Omega)$  implies  $[[\boldsymbol{\psi}]] = [[\nabla \boldsymbol{\psi}]] = 0$  on  $\partial_I \Omega_h$  and  $[[\boldsymbol{\psi}]] = -\boldsymbol{\psi} = 0$  on  $\partial_D \Omega_h$ , we conclude that

$$\begin{cases} \int_{\Omega_h} [\mathbf{w} \nabla \boldsymbol{\psi}]^T \nabla \boldsymbol{\phi}_h + \int_{\partial_I \Omega_h} [\mathbf{w} \nabla \boldsymbol{\psi}]^T [[\boldsymbol{\phi}_{h_n}]] dS + \int_{\partial_D \Omega_h} [\mathbf{w} \nabla \boldsymbol{\psi}]^T [[\boldsymbol{\phi}_{h_n}]] dS \\ - \int_{\Omega_h} [\mathbf{r} \boldsymbol{\psi}]^T \nabla \boldsymbol{\phi}_h d\Omega - \int_{\partial_I \Omega_h} [\mathbf{r} \boldsymbol{\psi}]^T [[\boldsymbol{\phi}_{h_n}]] dS - \int_{\partial_D \Omega_h} [\mathbf{r} \boldsymbol{\psi}]^T [[\boldsymbol{\phi}_{h_n}]] dS = a(\boldsymbol{\psi}, \boldsymbol{\phi}_h), \end{cases} \quad (\text{B.46})$$

leading to

$$\| \boldsymbol{\phi}_h \|_{L^2(\Omega_h)}^2 = a(\boldsymbol{\psi}, \boldsymbol{\phi}_h). \quad (\text{B.47})$$

Inserting  $I_h \boldsymbol{\psi}$  the interpolant of  $\boldsymbol{\psi}$  in  $X^k$ , as  $a(\boldsymbol{\psi}, \boldsymbol{\phi}_h)$  is a bilinear form, this can be rewritten as

$$\| \boldsymbol{\phi}_h \|_{L^2(\Omega_h)}^2 = a(\boldsymbol{\psi} - I_h \boldsymbol{\psi}, \boldsymbol{\phi}_h) + a(I_h \boldsymbol{\psi}, \boldsymbol{\phi}_h). \quad (\text{B.48})$$

From Eq. (B.39), in the particular case of  $\delta \mathbf{E}_h = I_h \boldsymbol{\psi}$ , we have for one solution  $\boldsymbol{\phi}_h$

$$a(I_h \boldsymbol{\psi}, \boldsymbol{\phi}_h) = \int_{\Omega_h} \boldsymbol{\xi} I_h \boldsymbol{\psi} d\Omega \leq \| \boldsymbol{\xi} \|_{L^2(\Omega_h)} \| I_h \boldsymbol{\psi} \|_{L^2(\Omega_h)}. \quad (\text{B.49})$$

Using Lemma 3.4.2, Eq. (3.68), and Lemma 2.4.6, Eq. (2.23), we get

$$\begin{aligned} | a(\boldsymbol{\psi} - I_h \boldsymbol{\psi}, \boldsymbol{\phi}_h) | & \leq C^k ||| \boldsymbol{\psi} - I_h \boldsymbol{\psi} |||_1 ||| \boldsymbol{\phi}_h ||| \\ & \leq C^k I_h^{\mu-1} \| \boldsymbol{\psi} \|_{H^s(\Omega_h)} ||| \boldsymbol{\phi}_h |||, \end{aligned} \quad (\text{B.50})$$

with  $\mu = \min \{s, k + 1\}$ .

Substituting Eq. (B.49) and Eq. (B.50), for  $s = 2$ , in Eq. (B.48), yields

$$\| \phi_h \|_{L^2(\Omega_h)}^2 \leq C^k h_s \| \psi \|_{H^2(\Omega_h)} \| | \phi_h | \| + \| \xi \|_{L^2(\Omega_h)} \| I_h \psi \|_{L^2(\Omega_h)}, \quad (\text{B.51})$$

whereas, for  $h_s$  sufficient small, the term  $\| I_h \psi \|_{L^2(\Omega)}$  can be bounded using Lemma 2.4.6, Eq. (2.23)

$$\begin{aligned} \| I_h \psi \|_{L^2(\Omega_h)} &\leq \| I_h \psi - \psi + \psi \|_{L^2(\Omega_h)} \\ &\leq \| I_h \psi - \psi \|_{L^2(\Omega_h)} + \| \psi \|_{L^2(\Omega_h)} \leq \| | I_h \psi - \psi | \|_1 + \| \psi \|_{H^2(\Omega_h)} \\ &\leq C^k h_s \| \psi \|_{H^2(\Omega_h)} + \| \psi \|_{H^2(\Omega_h)} \leq C^k \| \psi \|_{H^2(\Omega_h)}. \end{aligned} \quad (\text{B.52})$$

Eq. (B.51) is thus rewritten for small  $h_s$  as

$$\| \phi_h \|_{L^2(\Omega_h)}^2 \leq C^k \| \psi \|_{H^2(\Omega_h)} \left( h_s \| | \phi_h | \| + \| \xi \|_{L^2(\Omega_h)} \right). \quad (\text{B.53})$$

By using the regular ellipticity Eq. (3.71), we obtain

$$\| \phi_h \|_{L^2(\Omega_h)} \leq C^k h_s \| | \phi_h | \| + C^k \| \xi \|_{L^2(\Omega_h)} \leq C^k \| \xi \|_{L^2(\Omega_h)}, \quad (\text{B.54})$$

for small  $h_s$ . Hence we complete the proof of Lemma 3.4.3 by substituting Eq. (B.54) in Eq. (B.44)

$$\| | \phi_h | \| \leq C^k \| \xi \|_{L^2(\Omega_h)}. \quad (\text{B.55})$$

## Appendix C

# Annexes related to chapter 4

### C.1 Stiffness matrix for Electro-Thermal coupling

For the stiffness matrix, we have four sub matrices with respect to the discretization with the two independent variables. First part is the derivative of the electrical contributions with respect to  $f_V$ . From Eq. (4.73), we have

$$\begin{aligned} \frac{\partial F_{f_{Vint}}^a}{\partial f_V^b} &= \sum_e \int_{\Omega^e} \frac{\partial \mathbf{j}_e}{\partial f_V} \cdot \nabla N_{f_V}^a N_{f_V}^b d\Omega \\ &+ \sum_e \int_{\Omega^e} \nabla N_{f_V}^a \cdot \frac{\partial \mathbf{j}_e}{\partial \nabla f_V} \cdot \nabla N_{f_V}^b d\Omega, \end{aligned} \quad (C.1)$$

and for the interface terms  $\partial_I \Omega_h^1$ , Eqs. (4.75, 4.76, and 4.77), we have

$$\begin{aligned} \frac{\partial F_{f_{VI1}}^{a\pm}}{\partial f_V^{b\pm}} &= \frac{1}{2} \sum_s \int_{(\partial_I \Omega)^s} \left( \pm N_{f_V}^{a\pm} \right) \frac{\partial \mathbf{j}_e^\pm}{\partial f_V^\pm} \cdot \mathbf{n}^- N_{f_V}^{b\pm} dS \\ &+ \frac{1}{2} \sum_s \int_{(\partial_I \Omega)^s} \left( \pm N_{f_V}^{a\pm} \right) \mathbf{n}^- \cdot \frac{\partial \mathbf{j}_e^\pm}{\partial \nabla f_V^\pm} \cdot \nabla N_{f_V}^{b\pm} dS, \end{aligned} \quad (C.2)$$

$$\begin{aligned} \frac{\partial F_{f_{VI2}}^{a\pm}}{\partial f_V^{b\pm}} &= \frac{1}{2} \sum_s \int_{(\partial_I \Omega)^s} \left( \pm N_{f_V}^{b\pm} \right) \left( \mathbf{l}_1^\pm \cdot \nabla N_{f_V}^{a\pm} \right) \cdot \mathbf{n}^- dS \\ &+ \frac{1}{2} \sum_s \int_{(\partial_I \Omega)^s} \llbracket f_{T_h} \rrbracket \mathbf{n}^- \cdot \frac{\partial \mathbf{l}_2^\pm}{\partial f_V^\pm} \cdot \nabla N_{f_V}^{a\pm} N_{f_V}^{b\pm} dS, \end{aligned} \quad (C.3)$$

$$\begin{aligned} \frac{\partial F_{f_{VI3}}^{a\pm}}{\partial f_V^{b\pm}} &= \sum_s \int_{(\partial_I \Omega)^s} \left( \pm N_{f_V}^{a\pm} \right) \mathbf{n}^- \cdot \left\langle \frac{\mathbf{l}_1 \mathcal{B}}{h_s} \right\rangle \cdot \mathbf{n}^- \left( \pm N_{f_V}^{b\pm} \right) dS \\ &+ \frac{1}{2} \sum_s \int_{(\partial_I \Omega)^s} \left( \pm N_{f_V}^{a\pm} \right) \mathbf{n}^- \cdot \frac{\partial \mathbf{l}_2^\pm}{\partial f_V^\pm} \frac{\mathcal{B}}{h_s} \cdot \mathbf{n}^- N_{f_V}^{b\pm} \llbracket f_{T_h} \rrbracket dS. \end{aligned} \quad (C.4)$$

<sup>1</sup>The contributions on  $\partial_D \Omega_h$  can be directly deduced by removing the factor (1/2) accordingly to the definition of the average flux on the Dirichlet boundary and  $\mathbf{l}_1(f_T)$ ,  $\mathbf{l}_2(f_V, f_T)$  and  $\mathbf{j}_y(f_V, f_T)$ , which are constant with respect to  $f_{V_h}$ , and  $f_{T_h}$ , instead of  $\mathbf{l}_1(f_{T_h})$ ,  $\mathbf{l}_2(f_{V_h}, f_{T_h})$  and  $\mathbf{j}_y(f_{V_h}, f_{T_h})$ .

Similarly, the derivatives of the forces for the electrical contribution with respect to  $f_T$  are

$$\begin{aligned} \frac{\partial F_{f_{\text{vint}}}^a}{\partial f_T^b} &= \sum_e \int_{\Omega^e} \frac{\partial \mathbf{j}_e}{\partial f_T} \cdot \nabla N_{f_V}^a N_{f_T}^b d\Omega \\ &+ \sum_e \int_{\Omega^e} \nabla N_{f_V}^a \cdot \frac{\partial \mathbf{j}_e}{\partial \nabla f_T} \cdot \nabla N_{f_T}^b d\Omega, \end{aligned} \quad (\text{C.5})$$

$$\begin{aligned} \frac{\partial F_{f_{\text{VI1}}}^{a\pm}}{\partial f_T^{b\pm}} &= \frac{1}{2} \sum_s \int_{(\partial_1 \Omega)^s} \left( \pm N_{f_V}^{a\pm} \right) \frac{\partial \mathbf{j}_e^\pm}{\partial f_T} N_{f_T}^{b\pm} \cdot \mathbf{n}^- dS \\ &+ \frac{1}{2} \sum_s \int_{(\partial_1 \Omega)^s} \left( \pm N_{f_V}^{a\pm} \right) \frac{\partial \mathbf{j}_e^\pm}{\partial \nabla f_T} \cdot \nabla N_{f_T}^{b\pm} \cdot \mathbf{n}^- dS, \end{aligned} \quad (\text{C.6})$$

$$\begin{aligned} \frac{\partial F_{f_{\text{VI2}}}^{a\pm}}{\partial f_T^{b\pm}} &= \frac{1}{2} \sum_s \int_{(\partial_1 \Omega)^s} \left( \pm N_{f_T}^{b\pm} \right) \left( \mathbf{l}_2^\pm \cdot \nabla N_{f_V}^{a\pm} \right) \cdot \mathbf{n}^- dS \\ &+ \frac{1}{2} \sum_s \int_{(\partial_1 \Omega)^s} \llbracket f_{V_h} \rrbracket \left( \frac{\partial \mathbf{l}_1^\pm}{\partial f_T} \cdot \nabla N_{f_V}^{a\pm} N_{f_T}^{b\pm} \right) \cdot \mathbf{n}^- dS \\ &+ \frac{1}{2} \sum_s \int_{(\partial_1 \Omega)^s} \llbracket f_{T_h} \rrbracket \left( \frac{\partial \mathbf{l}_2^\pm}{\partial f_T} \cdot \nabla N_{f_T}^{a\pm} N_{f_T}^{b\pm} \right) \cdot \mathbf{n}^- dS, \end{aligned} \quad (\text{C.7})$$

$$\begin{aligned} \frac{\partial F_{f_{\text{VI3}}}^{a\pm}}{\partial f_T^{b\pm}} &= \sum_s \int_{(\partial_1 \Omega)^s} \left( \pm N_{f_V}^{a\pm} \right) \mathbf{n}^- \cdot \left\langle \frac{\mathbf{l}_2 \mathcal{B}}{h_s} \right\rangle \cdot \mathbf{n}^- \left( \pm N_{f_T}^{b\pm} \right) dS \\ &+ \frac{1}{2} \sum_s \int_{(\partial_1 \Omega)^s} \llbracket f_{V_h} \rrbracket \mathbf{n}^- \cdot \frac{\partial \mathbf{l}_1^\pm}{\partial f_T} \frac{\mathcal{B}}{h_s} \cdot \mathbf{n}^- N_{f_T}^{b\pm} \left( \pm N_{f_V}^{a\pm} \right) dS \\ &+ \frac{1}{2} \sum_s \int_{(\partial_1 \Omega)^s} \left( \pm N_{f_V}^{a\pm} \right) \mathbf{n}^- \cdot \frac{\partial \mathbf{l}_2^\pm}{\partial f_T} \frac{\mathcal{B}}{h_s} \cdot \mathbf{n}^- N_{f_T}^{b\pm} \llbracket f_{T_h} \rrbracket dS. \end{aligned} \quad (\text{C.8})$$

The derivatives of the thermal contributions with respect to  $f_T$  read, for the volume term Eq. (4.79)

$$\begin{aligned} \frac{\partial F_{f_{\text{Tint}}}^a}{\partial f_T^b} &= \sum_e \int_{\Omega^e} \rho \frac{\partial \mathbf{j}_y}{\partial f_T} \cdot \nabla N_{f_T}^a N^b d\Omega + \sum_e \int_{\Omega^e} \nabla N_{f_T}^a \cdot \frac{\partial \mathbf{j}_y}{\partial \nabla f_T} \cdot \nabla N_{f_T}^b d\Omega \\ &- \sum_e \int_{\Omega^e} \frac{\partial_t y}{\partial f_T} N_{f_T}^b N_{f_T}^a d\Omega, \end{aligned} \quad (\text{C.9})$$

and for the interface forces Eq. (4.81, 4.82 and 4.83)

$$\begin{aligned} \frac{\partial F_{f_{\text{TI1}}}^{a\pm}}{\partial f_T^{b\pm}} &= \frac{1}{2} \sum_s \int_{(\partial_1 \Omega)^s} \left( \pm N_{f_T}^{a\pm} \right) \frac{\partial \mathbf{j}_y^\pm}{\partial f_T} \cdot \mathbf{n}^- N_{f_T}^{b\pm} dS \\ &+ \frac{1}{2} \sum_s \int_{(\partial_1 \Omega)^s} \left( \pm N_{f_T}^{a\pm} \right) \left( \frac{\partial \mathbf{j}_y^\pm}{\partial \nabla f_T} \cdot \nabla N_{f_T}^{b\pm} \right) \cdot \mathbf{n}^- dS, \end{aligned} \quad (\text{C.10})$$



$$\begin{aligned}
\frac{\partial F_{f_{T12}}^{a\pm}}{\partial f_T^{b\pm}} &= \frac{1}{2} \sum_s \int_{(\partial_1\Omega)^s} \left( \pm N_{f_T}^{b\pm} \right) \left( \mathbf{j}_{y1}^{\pm} \cdot \nabla N_{f_T}^{a\pm} \right) \cdot \mathbf{n}^- dS \\
&+ \frac{1}{2} \sum_s \int_{(\partial_1\Omega)^s} \llbracket f_{T_h} \rrbracket \left( \frac{\mathbf{j}_{y1}^{\pm}}{\partial f_T^{\pm}} \cdot \nabla N_{f_T}^{a\pm} N_{f_T}^{b\pm} \right) \cdot \mathbf{n}^- dS \\
&+ \frac{1}{2} \sum_s \int_{(\partial_1\Omega)^s} \llbracket f_{V_h} \rrbracket \left( \frac{\partial_2^{\pm}}{\partial f_T^{\pm}} \cdot \nabla N_{f_T}^{a\pm} N_{f_T}^{b\pm} \right) \cdot \mathbf{n}^- dS,
\end{aligned} \tag{C.11}$$

$$\begin{aligned}
\frac{\partial F_{f_{T13}}^{a\pm}}{\partial f_T^{b\pm}} &= \sum_s \int_{(\partial_1\Omega)^s} \left( \pm N_{f_T}^{a\pm} \right) \mathbf{n}^- \cdot \left\langle \frac{\mathbf{j}_{y1} \mathcal{B}}{h_s} \right\rangle \cdot \mathbf{n}^- \left( \pm N_{f_T}^{b\pm} \right) dS \\
&+ \frac{1}{2} \sum_s \int_{(\partial_1\Omega)^s} \left( \pm N_{f_T}^{a\pm} \right) \mathbf{n}^- \cdot \frac{\partial \mathbf{j}_{y1}^{\pm}}{\partial f_T^{\pm}} \frac{\mathcal{B}}{h_s} \cdot \mathbf{n}^- N_{f_T}^{b\pm} \llbracket f_{T_h} \rrbracket dS \\
&+ \frac{1}{2} \sum_s \int_{(\partial_1\Omega)^s} \llbracket f_{V_h} \rrbracket \mathbf{n}^- \cdot \frac{\partial_2^{\pm}}{\partial f_T^{\pm}} \frac{\mathcal{B}}{h_s} \cdot \mathbf{n}^- N_{f_T}^{b\pm} \left( \pm N_{f_T}^{a\pm} \right) dS.
\end{aligned} \tag{C.12}$$

The last part is the derivatives of the thermal contribution forces with respect to  $f_V$

$$\begin{aligned}
\frac{\partial F_{f_{Tint}}^a}{\partial f_V^b} &= \sum_e \int_{\Omega^e} \rho \frac{\partial \mathbf{j}_y}{\partial f_V} \cdot \nabla N_{f_T}^a N_{f_V}^b d\Omega + \sum_e \int_{\Omega^e} \nabla N_{f_T}^a \cdot \frac{\partial \mathbf{j}_y}{\partial \nabla f_V} \cdot \nabla N_{f_V}^b d\Omega \\
&- \sum_e \int_{\Omega^e} \frac{\partial_t \mathbf{j}_y}{\partial f_V} N_{f_V}^b N_{f_T}^a d\Omega,
\end{aligned} \tag{C.13}$$

$$\begin{aligned}
\frac{\partial F_{f_{T11}}^{a\pm}}{\partial f_V^{b\pm}} &= \frac{1}{2} \sum_s \int_{(\partial_1\Omega)^s} \left( \pm N_{f_T}^{a\pm} \right) \frac{\partial \mathbf{j}_y^{\pm}}{\partial f_V^{\pm}} \cdot \mathbf{n}^- N_{f_V}^{b\pm} dS \\
&+ \frac{1}{2} \sum_s \int_{(\partial_1\Omega)^s} \left( \pm N_{f_T}^{a\pm} \right) \mathbf{n}^- \cdot \frac{\partial \mathbf{j}_y^{\pm}}{\partial \nabla f_V^{\pm}} \cdot \nabla N_{f_V}^{b\pm} dS,
\end{aligned} \tag{C.14}$$

$$\begin{aligned}
\frac{\partial F_{f_{T12}}^{a\pm}}{\partial f_V^{b\pm}} &= \frac{1}{2} \sum_s \int_{(\partial_1\Omega)^s} \left( \pm N_{f_V}^{b\pm} \right) \left( \mathbf{l}_2^{\pm} \cdot \nabla N_{f_T}^{a\pm} \right) \cdot \mathbf{n}^- dS \\
&+ \frac{1}{2} \sum_s \int_{(\partial_1\Omega)^s} \llbracket f_{T_h} \rrbracket \left( \frac{\partial \mathbf{j}_{y1}^{\pm}}{\partial f_V^{\pm}} \cdot \nabla N_{f_T}^{a\pm} N_{f_V}^{b\pm} \right) \cdot \mathbf{n}^- dS \\
&+ \frac{1}{2} \sum_s \int_{(\partial_1\Omega)^s} \llbracket f_{V_h} \rrbracket \left( \frac{\partial_2^{\pm}}{\partial f_V^{\pm}} \cdot \nabla N_{f_T}^{a\pm} N_{f_V}^{b\pm} \right) \cdot \mathbf{n}^- dS,
\end{aligned} \tag{C.15}$$

$$\begin{aligned}
\frac{\partial F_{f_{T13}}^{a\pm}}{\partial f_V^{b\pm}} &= \sum_s \int_{(\partial_1\Omega)^s} \left( \pm N_{f_V}^{b\pm} \right) \mathbf{n}^- \cdot \left\langle \frac{\mathbf{l}_2 \mathcal{B}}{h_s} \right\rangle \cdot \mathbf{n}^- \left( \pm N_{f_T}^{a\pm} \right) dS \\
&+ \frac{1}{2} \sum_s \int_{(\partial_1\Omega)^s} \llbracket f_{T_h} \rrbracket \mathbf{n}^- \cdot \frac{\partial \mathbf{j}_{y1}^{\pm}}{\partial f_V^{\pm}} \frac{\mathcal{B}}{h_s} \cdot \mathbf{n}^- N_{f_V}^{b\pm} \left( \pm N_{f_T}^{a\pm} \right) dS \\
&+ \frac{1}{2} \sum_s \int_{(\partial_1\Omega)^s} \llbracket f_{V_h} \rrbracket \mathbf{n}^- \cdot \frac{\partial_2^{\pm}}{\partial f_V^{\pm}} \frac{\mathcal{B}}{h_s} \cdot \mathbf{n}^- N_{f_V}^{b\pm} \left( \pm N_{f_T}^{a\pm} \right) dS.
\end{aligned} \tag{C.16}$$

All the tensor derivatives are explicitly given in Appendix D.1.2.

## C.2 Derivatives

Let the derivative of the fluxes  $\mathbf{j}(6 \times 1)$  defined in Eq. (4.29, 5.17) with respect to the fields vector  $\mathbf{M}(2 \times 1)$  be  $\mathbf{j}_{\mathbf{M}}$ , which could be split into

$$\mathbf{j}_{f_V} = \begin{pmatrix} 0 & -\frac{1}{f_T^2} \mathbf{1} \\ -\frac{1}{f_T^2} \mathbf{1} & -2\alpha \frac{1}{f_T^3} \mathbf{1} + 2 \frac{f_V}{f_T^3} \mathbf{1} \end{pmatrix} \begin{pmatrix} \nabla f_V \\ \nabla f_T \end{pmatrix}, \text{ and} \quad (\text{C.17})$$

$$\mathbf{j}_{f_T} = \begin{pmatrix} -\frac{1}{f_T^2} \mathbf{1} & +2 \frac{f_V}{f_T^3} \mathbf{1} - 2\alpha \frac{1}{f_T^3} \mathbf{1} \\ +2 \frac{f_V}{f_T^3} \mathbf{1} - 2\alpha \frac{1}{f_T^3} \mathbf{1} & -2 \frac{\mathbf{k}}{f_T^3} + 6\alpha \frac{f_V}{f_T^4} \mathbf{1} - 3\alpha^2 \frac{1}{f_T^4} \mathbf{1} - 3 \frac{f_V^2}{f_T^4} \mathbf{1} \end{pmatrix} \begin{pmatrix} \nabla f_V \\ \nabla f_T \end{pmatrix}, \quad (\text{C.18})$$

and let the derivatives of the previous matrices with respect to the gradient of the unknown fields be  $\mathbf{j}_{\mathbf{M}\nabla\mathbf{M}}$  which could be split into

$$\mathbf{j}_{f_V\nabla\mathbf{M}} = \begin{pmatrix} 0 & -\frac{1}{f_T^2} \mathbf{1} \\ -\frac{1}{f_T^2} \mathbf{1} & -2\alpha \frac{1}{f_T^3} \mathbf{1} + 2 \frac{f_V}{f_T^3} \mathbf{1} \end{pmatrix}, \quad (\text{C.19})$$

$$\mathbf{j}_{f_T\nabla\mathbf{M}} = \begin{pmatrix} -\frac{1}{f_T^2} \mathbf{1} & +2 \frac{f_V}{f_T^3} \mathbf{1} - 2\alpha \frac{1}{f_T^3} \mathbf{1} \\ +2 \frac{f_V}{f_T^3} \mathbf{1} - 2\alpha \frac{1}{f_T^3} \mathbf{1} & -2 \frac{\mathbf{k}}{f_T^3} + 6\alpha \frac{f_V}{f_T^4} \mathbf{1} - 3\alpha^2 \frac{1}{f_T^4} \mathbf{1} - 3 \frac{f_V^2}{f_T^4} \mathbf{1} \end{pmatrix}. \quad (\text{C.20})$$

Then let  $\mathbf{j}_{\mathbf{M}\mathbf{M}}$  be the derivative of  $\mathbf{j}_{\mathbf{M}}$ , with respect to  $\mathbf{M}$ , this consists of the four following matrices

$$\mathbf{j}_{f_V f_V} = \begin{pmatrix} 0 & 0 \\ 0 & +\frac{2}{f_T^3} \mathbf{1} \end{pmatrix} \begin{pmatrix} \nabla f_V \\ \nabla f_T \end{pmatrix}, \quad (\text{C.21})$$

$$\mathbf{j}_{f_V f_T} = \begin{pmatrix} 0 & +2 \frac{1}{f_T^3} \mathbf{1} \\ +2 \frac{1}{f_T^3} \mathbf{1} & +6 \frac{\alpha}{f_T^4} \mathbf{1} - 6 \frac{f_V}{f_T^4} \mathbf{1} \end{pmatrix} \begin{pmatrix} \nabla f_V \\ \nabla f_T \end{pmatrix}, \quad (\text{C.22})$$

$$\mathbf{j}_{f_T f_V} = \begin{pmatrix} 0 & +2 \frac{1}{f_T^3} \mathbf{1} \\ +2 \frac{1}{f_T^3} \mathbf{1} & +6\alpha \frac{1}{f_T^4} \mathbf{1} + 6 \frac{f_V}{f_T^4} \mathbf{1} \end{pmatrix} \begin{pmatrix} \nabla f_V \\ \nabla f_T \end{pmatrix} = \mathbf{j}_{f_V f_T}, \text{ and} \quad (\text{C.23})$$

$$\mathbf{j}_{f_T f_T} = \begin{pmatrix} 2 \frac{1}{f_T^3} \mathbf{1} & -6 \frac{f_V}{f_T^4} \mathbf{1} + 6\alpha \frac{1}{f_T^4} \mathbf{1} \\ -6 \frac{f_V}{f_T^4} \mathbf{1} + 6\alpha \frac{1}{f_T^4} \mathbf{1} & +6 \frac{\mathbf{k}}{f_T^4} - 24\alpha \frac{f_V}{f_T^5} \mathbf{1} + 12\alpha^2 \frac{1}{f_T^5} \mathbf{1} + 12 \frac{f_V^2}{f_T^5} \mathbf{1} \end{pmatrix} \begin{pmatrix} \nabla f_V \\ \nabla f_T \end{pmatrix}. \quad (\text{C.24})$$

### C.3 Lower bound for Electro-Thermal coupling

In order to prove Lemma 4.4.1, let us first use Eq. (4.102) and Eq. (4.103), yielding

$$\begin{aligned}
& \mathcal{A}(\mathbf{M}^e; \delta\mathbf{M}_h, \delta\mathbf{M}_h) + \mathcal{B}(\mathbf{M}^e; \delta\mathbf{M}_h, \delta\mathbf{M}_h) \\
&= \int_{\Omega_h} (\nabla \delta\mathbf{M}_h)^T \mathbf{j}_{\nabla\mathbf{M}}(\mathbf{M}^e) \nabla \delta\mathbf{M}_h \, d\Omega \\
&+ \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \llbracket \delta\mathbf{M}_{h_n}^T \rrbracket \langle \mathbf{j}_{\nabla\mathbf{M}}(\mathbf{M}^e) \nabla \delta\mathbf{M}_h \rangle \, dS \\
&+ \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \llbracket \delta\mathbf{M}_{h_n}^T \rrbracket \langle \mathbf{j}_{\nabla\mathbf{M}}(\mathbf{M}^e) \nabla \delta\mathbf{M}_h \rangle \, dS \\
&+ \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \llbracket \delta\mathbf{M}_{h_n}^T \rrbracket \left\langle \frac{\mathcal{B}}{h_s} \mathbf{j}_{\nabla\mathbf{M}}(\mathbf{M}^e) \right\rangle \llbracket \delta\mathbf{M}_{h_n} \rrbracket \, dS \\
&+ \int_{\Omega_h} (\nabla \delta\mathbf{M}_h)^T \mathbf{j}_{\mathbf{M}}(\mathbf{M}^e, \nabla\mathbf{M}^e) \delta\mathbf{M}_h \, d\Omega \\
&+ \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \llbracket \delta\mathbf{M}_{h_n}^T \rrbracket \langle \mathbf{j}_{\mathbf{M}}(\mathbf{M}^e, \nabla\mathbf{M}^e) \delta\mathbf{M}_h \rangle \, dS \quad \forall \delta\mathbf{M}_h \in X^k.
\end{aligned} \tag{C.25}$$

This equation can be rewritten as

$$\begin{aligned}
& \mathcal{A}(\mathbf{M}^e; \delta\mathbf{M}_h, \delta\mathbf{M}_h) + \mathcal{B}(\mathbf{M}^e; \delta\mathbf{M}_h, \delta\mathbf{M}_h) \\
&= \int_{\Omega_h} (\nabla \delta\mathbf{M}_h)^T \mathbf{j}_{\nabla\mathbf{M}}(\mathbf{M}^e) \nabla \delta\mathbf{M}_h \, d\Omega \\
&+ \int_{\Omega_h} (\nabla \delta\mathbf{M}_h)^T \mathbf{j}_{\mathbf{M}}(\mathbf{M}^e, \nabla\mathbf{M}^e) \delta\mathbf{M}_h \, d\Omega \\
&+ 2 \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \llbracket \delta\mathbf{M}_{h_n}^T \rrbracket \langle \mathbf{j}_{\nabla\mathbf{M}}(\mathbf{M}^e) \nabla \delta\mathbf{M}_h \rangle \, dS \\
&+ \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \llbracket \delta\mathbf{M}_{h_n}^T \rrbracket \langle \mathbf{j}_{\mathbf{M}}(\mathbf{M}^e, \nabla\mathbf{M}^e) \delta\mathbf{M}_h \rangle \, dS \\
&+ \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \llbracket \delta\mathbf{M}_{h_n}^T \rrbracket \left\langle \frac{\mathcal{B}}{h_s} \mathbf{j}_{\nabla\mathbf{M}}(\mathbf{M}^e) \right\rangle \llbracket \delta\mathbf{M}_{h_n} \rrbracket \, dS.
\end{aligned} \tag{C.26}$$

Using Eqs. (4.88) and (4.93), Eq. (C.26) becomes

$$\begin{aligned}
& \mathcal{A}(\mathbf{M}^e; \delta\mathbf{M}_h, \delta\mathbf{M}_h) + \mathcal{B}(\mathbf{M}^e; \delta\mathbf{M}_h, \delta\mathbf{M}_h) \\
&\geq \sum_e \left( C_\alpha \|\nabla \delta\mathbf{M}_h\|_{L^2(\Omega^e)}^2 - C_y \|\nabla \delta\mathbf{M}_h\|_{L^2(\Omega^e)} \|\delta\mathbf{M}_h\|_{L^2(\Omega^e)} \right) \\
&- 2 \sum_s C_y \left| \int_{(\partial_{DI}\Omega)^s} \llbracket \delta\mathbf{M}_{h_n} \rrbracket \langle \nabla \delta\mathbf{M}_h \rangle \, dS \right| \\
&- \sum_s C_y \left| \int_{(\partial_{DI}\Omega)^s} \llbracket \delta\mathbf{M}_{h_n} \rrbracket \langle \delta\mathbf{M}_h \rangle \, dS \right| + \sum_s C_\alpha \frac{\mathcal{B}}{h_s} \|\llbracket \delta\mathbf{M}_{h_n} \rrbracket\|_{L^2((\partial_{DI}\Omega)^s)}^2,
\end{aligned} \tag{C.27}$$

where  $\int_{\partial_I \Omega_h} + \int_{\partial_D \Omega_h} = \sum_s \int_{(\partial_{DI}\Omega)^s}$ .

The third and fourth terms of the right hand side in Eq. (C.27) can be bounded using Cauchy-Schwartz' inequality, Eq. (2.26),

$$\begin{aligned}
& 2C_y \sum_s \left| \int_{(\partial_{\text{DI}}\Omega)^s} \llbracket \delta \mathbf{M}_{\text{hn}} \rrbracket \langle \nabla \delta \mathbf{M}_{\text{h}} \rangle \, \text{dS} \right| + C_y \sum_s \left| \int_{(\partial_{\text{DI}}\Omega)^s} \llbracket \delta \mathbf{M}_{\text{hn}} \rrbracket \langle \delta \mathbf{M}_{\text{h}} \rangle \, \text{dS} \right| \\
& \leq 2C_y \left( \sum_s \frac{1}{h_s} \left\| \llbracket \delta \mathbf{M}_{\text{hn}} \rrbracket \right\|_{L^2((\partial_{\text{DI}}\Omega)^s)}^2 \right)^{\frac{1}{2}} \left( \sum_s h_s \left\| \langle \nabla \delta \mathbf{M}_{\text{h}} \rangle \right\|_{L^2((\partial_{\text{DI}}\Omega)^s)}^2 \right)^{\frac{1}{2}} \\
& + C_y \left( \sum_s \frac{1}{h_s} \left\| \llbracket \delta \mathbf{M}_{\text{hn}} \rrbracket \right\|_{L^2((\partial_{\text{DI}}\Omega)^s)}^2 \right)^{\frac{1}{2}} \left( \sum_s h_s \left\| \langle \delta \mathbf{M}_{\text{h}} \rangle \right\|_{L^2((\partial_{\text{DI}}\Omega)^s)}^2 \right)^{\frac{1}{2}} \\
& \leq 2C_y \left( \sum_s \frac{1}{h_s} \left\| \llbracket \delta \mathbf{M}_{\text{hn}} \rrbracket \right\|_{L^2((\partial_{\text{DI}}\Omega)^s)}^2 \right)^{\frac{1}{2}} \left[ \left( \sum_s h_s \left\| \langle \nabla \delta \mathbf{M}_{\text{h}} \rangle \right\|_{L^2((\partial_{\text{DI}}\Omega)^s)}^2 \right)^{\frac{1}{2}} \right. \\
& \left. + \frac{1}{2} \left( \sum_s h_s \left\| \langle \delta \mathbf{M}_{\text{h}} \rangle \right\|_{L^2((\partial_{\text{DI}}\Omega)^s)}^2 \right)^{\frac{1}{2}} \right], \tag{C.28}
\end{aligned}$$

where the term  $h_s \left\| \langle \nabla \delta \mathbf{M}_{\text{h}} \rangle \right\|_{L^2((\partial_{\text{DI}}\Omega)^s)}^2$  can be bounded using the trace inequality on the finite element space (2.18), with

$$\begin{aligned}
\sum_s h_s \left\| \langle \nabla \delta \mathbf{M}_{\text{h}} \rangle \right\|_{L^2((\partial_{\text{DI}}\Omega)^s)}^2 & = \frac{1}{2} \sum_e h_s \left\| \langle \nabla \delta \mathbf{M}_{\text{h}} \rangle \right\|_{L^2(\partial_1 \Omega^e)}^2 + \sum_e h_s \left\| \nabla \delta \mathbf{M}_{\text{h}} \right\|_{L^2(\partial_{\text{D}} \Omega^e)}^2 \\
& \leq \sum_e h_s \left\| \nabla \delta \mathbf{M}_{\text{h}} \right\|_{L^2(\partial \Omega^e)}^2 \leq C_{\mathcal{K}}^{k^2} \sum_e \left\| \nabla \delta \mathbf{M}_{\text{h}} \right\|_{L^2(\Omega^e)}^2. \tag{C.29}
\end{aligned}$$

Then using the trace inequality, Eq. (2.16), and inverse inequality, Eq. (2.21), we have

$$\begin{aligned}
\frac{1}{4} \sum_s h_s \left\| \langle \delta \mathbf{M}_{\text{h}} \rangle \right\|_{L^2((\partial_{\text{DI}}\Omega)^s)}^2 & = \frac{1}{8} \sum_e h_s \left\| \langle \delta \mathbf{M}_{\text{h}} \rangle \right\|_{L^2(\partial_1 \Omega^e)}^2 + \frac{1}{4} \sum_e h_s \left\| \delta \mathbf{M}_{\text{h}} \right\|_{L^2(\partial_{\text{D}} \Omega^e)}^2 \\
& \leq \frac{1}{4} \sum_e h_s \left\| \delta \mathbf{M}_{\text{h}} \right\|_{L^2(\partial \Omega^e)}^2 \\
& \leq \frac{1}{4} C_{\mathcal{T}} \sum_e \left( \left\| \delta \mathbf{M}_{\text{h}} \right\|_{L^2(\Omega^e)}^2 + h_s \left\| \delta \mathbf{M}_{\text{h}} \right\|_{L^2(\Omega^e)} \left\| \nabla \delta \mathbf{M}_{\text{h}} \right\|_{L^2(\Omega^e)} \right) \\
& \leq \sum_e \frac{C_{\mathcal{T}}(C_{\mathcal{I}}^k + 1)}{4} \left\| \delta \mathbf{M}_{\text{h}} \right\|_{L^2(\Omega^e)}^2. \tag{C.30}
\end{aligned}$$

Therefore Eq. (C.28) is rewritten as

$$\begin{aligned}
& 2C_y \sum_s \left| \int_{(\partial_{\text{DI}}\Omega)^s} \llbracket \delta \mathbf{M}_{\text{hn}} \rrbracket \langle \nabla \delta \mathbf{M}_{\text{h}} \rangle \, \text{dS} \right| + C_y \sum_s \left| \int_{(\partial_{\text{DI}}\Omega)^s} \llbracket \delta \mathbf{M}_{\text{hn}} \rrbracket \langle \delta \mathbf{M}_{\text{h}} \rangle \, \text{dS} \right| \\
& \leq C_y \left( \sum_s \frac{1}{h_s} \left\| \llbracket \delta \mathbf{M}_{\text{hn}} \rrbracket \right\|_{L^2((\partial_{\text{DI}}\Omega)^s)}^2 \right)^{\frac{1}{2}} \left( \sum_e \max(C_{\mathcal{T}}(C_{\mathcal{I}}^k + 1), 4C_{\mathcal{K}}^{k^2}) \left\| \delta \mathbf{M}_{\text{h}} \right\|_{H^1(\Omega^e)}^2 \right)^{\frac{1}{2}}. \tag{C.31}
\end{aligned}$$

Finally, by the use of the  $\xi$ -inequality  $-\xi > 0 : |ab| \leq \frac{\xi}{4}a^2 + \frac{1}{\xi}b^2$  with  $\xi = \frac{C_\alpha}{C_y \max(C_{\mathcal{T}}(C_{\mathcal{I}}^k + 1), 4C_{\mathcal{K}}^{k^2})}$ , we arrive at

$$\begin{aligned} & 2C_y \sum_s \left| \int_{(\partial_{\text{DI}}\Omega)^s} [[\delta\mathbf{M}_{\text{hn}}]] \langle \nabla \delta\mathbf{M}_h \rangle \, dS \right| + C_y \sum_s \left| \int_{(\partial_{\text{DI}}\Omega)^s} [[\delta\mathbf{M}_{\text{hn}}]] \langle \delta\mathbf{M}_h \rangle \, dS \right| \\ & \leq \frac{C_\alpha}{4} \sum_e \|\delta\mathbf{M}_h\|_{H^1(\Omega^e)}^2 + \frac{C_y^2}{C_\alpha} \max(C_{\mathcal{T}}(C_{\mathcal{I}}^k + 1), 4C_{\mathcal{K}}^{k^2}) \sum_s \frac{1}{h_s} \|[ [\delta\mathbf{M}_{\text{hn}}]] ]\|_{L^2((\partial_{\text{DI}}\Omega)^s)}^2. \end{aligned} \quad (\text{C.32})$$

For the second term of the right hand side of Eq. (C.27), choosing  $\xi = \frac{C_\alpha}{C_y}$  and applying the  $\xi$ -inequality, we find

$$\begin{aligned} \sum_e C_y \|\nabla \delta\mathbf{M}_h\|_{L^2(\Omega^e)} \|\delta\mathbf{M}_h\|_{L^2(\Omega^e)} & \leq \frac{C_y}{\xi} \sum_e \|\delta\mathbf{M}_h\|_{L^2(\Omega^e)}^2 + \frac{C_y \xi}{4} \sum_e \|\delta \nabla \mathbf{M}_h\|_{L^2(\Omega^e)}^2 \\ & \leq \frac{C_y^2}{C_\alpha} \sum_e \|\delta\mathbf{M}_h\|_{L^2(\Omega^e)}^2 + \frac{C_\alpha}{4} \sum_e \|\nabla \delta\mathbf{M}_h\|_{L^2(\Omega^e)}^2. \end{aligned} \quad (\text{C.33})$$

If we substitute Eqs. (C.32) and (C.33) in Eq. (C.27), we thus obtain the following result:

$$\begin{aligned} & \mathcal{A}(\mathbf{M}^e; \delta\mathbf{M}_h, \delta\mathbf{M}_h) + \mathcal{B}(\mathbf{M}^e; \delta\mathbf{M}_h, \delta\mathbf{M}_h) \\ & \geq \frac{C_\alpha}{2} \sum_e \|\nabla \delta\mathbf{M}_h\|_{L^2(\Omega^e)}^2 - \left( \frac{C_y^2}{C_\alpha} + \frac{C_\alpha}{4} \right) \sum_e \|\delta\mathbf{M}_h\|_{L^2(\Omega^e)}^2 \\ & \quad + \left[ \mathcal{B}C_\alpha - \frac{C_y^2}{C_\alpha} \max(C_{\mathcal{T}}(C_{\mathcal{I}}^k + 1), 4C_{\mathcal{K}}^{k^2}) \right] h_s^{-1} \sum_e \|[ [\delta\mathbf{M}_{\text{hn}}]] ]\|_{L^2(\partial\Omega^e)}^2. \end{aligned} \quad (\text{C.34})$$

This last relation can be rewritten as

$$\begin{aligned} \mathcal{A}(\mathbf{M}^e; \delta\mathbf{M}_h, \delta\mathbf{M}_h) + \mathcal{B}(\mathbf{M}^e; \delta\mathbf{M}_h, \delta\mathbf{M}_h) & \geq C_1^k \left[ \sum_e \|\nabla \delta\mathbf{M}_h\|_{L^2(\Omega^e)}^2 + h_s^{-1} \sum_e \|[ [\delta\mathbf{M}_{\text{hn}}]] ]\|_{L^2(\partial\Omega^e)}^2 \right] \\ & \quad - C_2^k \|\delta\mathbf{M}_h\|_{L^2(\Omega_h)}^2 \quad \forall \delta\mathbf{M}_h \in X^k. \end{aligned} \quad (\text{C.35})$$

where  $C_1^k = \min\left(\frac{C_\alpha}{2}, \mathcal{B}C_\alpha - \frac{C_y^2}{C_\alpha} \max(C_{\mathcal{T}}(C_{\mathcal{I}}^k + 1), 4C_{\mathcal{K}}^{k^2})\right)$ , which is positive when  $\mathcal{B} > \frac{C_y^2}{C_\alpha} \max(C_{\mathcal{T}}(C_{\mathcal{I}}^k + 1), 4C_{\mathcal{K}}^{k^2})$ , and  $C_2^k = \frac{C_y^2}{C_\alpha} + \frac{C_\alpha}{4} > 0$ .

Therefore, comparing with the definition of the mesh dependent norm, Eq. (2.10), we have

$$\mathcal{A}(\mathbf{M}^e; \delta\mathbf{M}_h, \delta\mathbf{M}_h) + \mathcal{B}(\mathbf{M}^e; \delta\mathbf{M}_h, \delta\mathbf{M}_h) \geq C_1^k \|\delta\mathbf{M}_h\|_*^2 - C_2^k \|\delta\mathbf{M}_h\|_{L^2(\Omega_h)}^2 \quad \forall \delta\mathbf{M}_h \in X^k. \quad (\text{C.36})$$

Moreover, starting from Eq. (C.34) and choosing  $C_2^k = \frac{C_y^2}{C_\alpha} + \frac{3C_\alpha}{4}$ , we rewrite the expression in terms of the norm (2.11) as

$$\mathcal{A}(\mathbf{M}^e; \delta\mathbf{M}_h, \delta\mathbf{M}_h) + \mathcal{B}(\mathbf{M}^e; \delta\mathbf{M}_h, \delta\mathbf{M}_h) \geq C_1^k \|\delta\mathbf{M}_h\|^2 - C_2^k \|\delta\mathbf{M}_h\|_{L^2(\Omega_h)}^2 \quad \forall \delta\mathbf{M}_h \in X^k. \quad (\text{C.37})$$

Hence, this shows that the stability of the method is conditioned by the constant  $\mathcal{B}$ , which should be large enough.

## C.4 Upper bound for Electro-Thermal coupling

The upper bound of the bi-linear form is determined by recalling Eq. (4.102) and Eq. (4.103), for  $\mathbf{u}, \delta\mathbf{M} \in X$

$$\begin{aligned}
\mathcal{A}(\mathbf{M}^e; \mathbf{u}, \delta\mathbf{M}) + \mathcal{B}(\mathbf{M}^e; \mathbf{u}, \delta\mathbf{M}) &= \int_{\Omega_h} (\nabla\delta\mathbf{M})^T \mathbf{j}_{\nabla\mathbf{M}}(\mathbf{M}^e) \nabla\mathbf{u} d\Omega \\
&+ \int_{\partial_I\Omega_h \cup \partial_D\Omega_h} \llbracket \delta\mathbf{M}_n^T \rrbracket \langle \mathbf{j}_{\nabla\mathbf{M}}(\mathbf{M}^e) \nabla\mathbf{u} \rangle dS + \int_{\partial_I\Omega_h \cup \partial_D\Omega_h} \llbracket \mathbf{u}_n^T \rrbracket \langle \mathbf{j}_{\nabla\mathbf{M}}(\mathbf{M}^e) \nabla\delta\mathbf{M} \rangle dS \\
&+ \int_{\partial_I\Omega_h \cup \partial_D\Omega_h} \llbracket \delta\mathbf{M}_n^T \rrbracket \left\langle \frac{\mathcal{B}}{h_s} \mathbf{j}_{\nabla\mathbf{M}}(\mathbf{M}^e) \right\rangle \llbracket \mathbf{u}_n \rrbracket dS + \int_{\Omega_h} (\nabla\delta\mathbf{M})^T \mathbf{j}_{\mathbf{M}}(\mathbf{M}^e, \nabla\mathbf{M}^e) \mathbf{u} d\Omega \\
&+ \int_{\partial_I\Omega_h \cup \partial_D\Omega_h} \llbracket \delta\mathbf{M}_n^T \rrbracket \langle \mathbf{j}_{\mathbf{M}}(\mathbf{M}^e, \nabla\mathbf{M}^e) \mathbf{u} \rangle dS.
\end{aligned} \tag{C.38}$$

Every term in the right hand side of Eq. (C.38) is bounded using the Hölder's inequality, Eq. (2.24), and the bound (4.93). This successively results in

$$\begin{aligned}
\left| \int_{\Omega_h} (\nabla\delta\mathbf{M})^T \mathbf{j}_{\nabla\mathbf{M}}(\mathbf{M}^e) \nabla\mathbf{u} d\Omega \right| &\leq \sum_e \left( \int_{\Omega^e} |(\nabla\delta\mathbf{M})^T \mathbf{j}_{\nabla\mathbf{M}}(\mathbf{M}^e) \nabla\mathbf{u}| d\Omega \right) \\
&\leq C_y \sum_e \|\nabla\delta\mathbf{M}\|_{L^2(\Omega^e)} \|\nabla\mathbf{u}\|_{L^2(\Omega^e)},
\end{aligned} \tag{C.39}$$

$$\begin{aligned}
\left| \int_{\Omega_h} (\nabla\delta\mathbf{M})^T \mathbf{j}_{\mathbf{M}}(\mathbf{M}^e, \nabla\mathbf{M}^e) \mathbf{u} d\Omega \right| &\leq \sum_e \left( \int_{\Omega^e} |(\nabla\delta\mathbf{M})^T \mathbf{j}_{\mathbf{M}}(\mathbf{M}^e, \nabla\mathbf{M}^e) \mathbf{u}| d\Omega \right) \\
&\leq C_y \sum_e \|\nabla\delta\mathbf{M}\|_{L^2(\Omega^e)} \|\mathbf{u}\|_{L^2(\Omega^e)},
\end{aligned} \tag{C.40}$$

$$\begin{aligned}
\left| \int_{\partial_I\Omega_h \cup \partial_D\Omega_h} \llbracket \delta\mathbf{M}_n^T \rrbracket \left\langle \frac{\mathbf{j}_{\nabla\mathbf{M}}(\mathbf{M}^e) \mathcal{B}}{h_s} \right\rangle \llbracket \mathbf{u}_n \rrbracket dS \right| &= \left| \frac{1}{2} \sum_e \int_{\partial_I\Omega^e} \llbracket \delta\mathbf{M}_n^T \rrbracket \left\langle \frac{\mathbf{j}_{\nabla\mathbf{M}}(\mathbf{M}^e) \mathcal{B}}{h_s} \right\rangle \llbracket \mathbf{u}_n \rrbracket dS \right. \\
&+ \left. \sum_e \int_{\partial_D\Omega^e} \llbracket \delta\mathbf{M}_n^T \rrbracket \frac{\mathbf{j}_{\nabla\mathbf{M}}(\mathbf{M}^e) \mathcal{B}}{h_s} \llbracket \mathbf{u}_n \rrbracket dS \right| \leq \mathcal{B} C_y \sum_e \|\mathbf{h}_s^{-\frac{1}{2}} \llbracket \delta\mathbf{M}_n \rrbracket\|_{L^2(\partial\Omega^e)} \|\mathbf{h}_s^{-\frac{1}{2}} \llbracket \mathbf{u}_n \rrbracket\|_{L^2(\partial\Omega^e)},
\end{aligned} \tag{C.41}$$

$$\begin{aligned}
\left| \int_{\partial_I\Omega_h \cup \partial_D\Omega_h} \llbracket \mathbf{u}_n^T \rrbracket \langle \mathbf{j}_{\nabla\mathbf{M}}(\mathbf{M}^e) \nabla\delta\mathbf{M} \rangle dS \right| &= \left| \frac{1}{2} \sum_e \int_{\partial_I\Omega^e} \llbracket \mathbf{u}_n^T \rrbracket \langle \mathbf{j}_{\nabla\mathbf{M}}(\mathbf{M}^e) \nabla\delta\mathbf{M} \rangle dS \right. \\
&+ \left. \sum_e \int_{\partial_D\Omega^e} \llbracket \mathbf{u}_n^T \rrbracket \mathbf{j}_{\nabla\mathbf{M}}(\mathbf{M}^e) \nabla\delta\mathbf{M} dS \right| \leq C_y \sum_e \|\mathbf{h}_s^{\frac{1}{2}} \nabla\delta\mathbf{M}\|_{L^2(\partial\Omega^e)} \|\mathbf{h}_s^{-\frac{1}{2}} \llbracket \mathbf{u}_n \rrbracket\|_{L^2(\partial\Omega^e)},
\end{aligned} \tag{C.42}$$

$$\begin{aligned}
\left| \int_{\partial_I\Omega_h \cup \partial_D\Omega_h} \llbracket \delta\mathbf{M}_n^T \rrbracket \langle \mathbf{j}_{\nabla\mathbf{M}}(\mathbf{M}^e) \nabla\mathbf{u} \rangle dS \right| &= \left| \frac{1}{2} \sum_e \int_{\partial_I\Omega^e} \llbracket \delta\mathbf{M}_n^T \rrbracket \langle \mathbf{j}_{\nabla\mathbf{M}}(\mathbf{M}^e) \nabla\mathbf{u} \rangle dS \right. \\
&+ \left. \sum_e \int_{\partial_D\Omega^e} \llbracket \delta\mathbf{M}_n^T \rrbracket \mathbf{j}_{\nabla\mathbf{M}}(\mathbf{M}^e) \nabla\mathbf{u} dS \right| \leq C_y \sum_e \|\mathbf{h}_s^{\frac{1}{2}} \nabla\mathbf{u}\|_{L^2(\partial\Omega^e)} \|\mathbf{h}_s^{-\frac{1}{2}} \llbracket \delta\mathbf{M}_n \rrbracket\|_{L^2(\partial\Omega^e)},
\end{aligned} \tag{C.43}$$

and

$$\begin{aligned}
& \left| \int_{\partial_1 \Omega_h \cup \partial_D \Omega_h} \llbracket \delta \mathbf{M}_{\mathbf{n}}^T \rrbracket \langle \mathbf{j}_{\mathbf{M}}(\mathbf{M}^e, \nabla \mathbf{M}^e) \mathbf{u} \rangle dS \right| = \left| \frac{1}{2} \sum_e \int_{\partial_1 \Omega^e} \llbracket \delta \mathbf{M}_{\mathbf{n}}^T \rrbracket \langle \mathbf{j}_{\mathbf{M}}(\mathbf{M}^e, \nabla \mathbf{M}^e) \mathbf{u} \rangle dS \right. \\
& \left. + \sum_e \int_{\partial_D \Omega^e} \llbracket \delta \mathbf{M}_{\mathbf{n}}^T \rrbracket \mathbf{j}_{\mathbf{M}}(\mathbf{M}^e, \nabla \mathbf{M}^e) \mathbf{u} dS \right| \leq C_y \sum_e \left\| h_s^{\frac{1}{2}} \mathbf{u} \right\|_{L^2(\partial \Omega^e)} \left\| h_s^{-\frac{1}{2}} \llbracket \delta \mathbf{M}_{\mathbf{n}} \rrbracket \right\|_{L^2(\partial \Omega^e)}.
\end{aligned} \tag{C.44}$$

Therefore by combining the above results, we obtain:

$$\begin{aligned}
& | \mathcal{A}(\mathbf{M}^e; \mathbf{u}, \delta \mathbf{M}) + \mathcal{B}(\mathbf{M}^e; \mathbf{u}, \delta \mathbf{M}) | \\
& \leq C_y \sum_e \left\| \nabla \mathbf{u} \right\|_{L^2(\Omega^e)} \left\| \nabla \delta \mathbf{M} \right\|_{L^2(\Omega^e)} \\
& + C_y \sum_e \left\| \mathbf{u} \right\|_{L^2(\Omega^e)} \left\| \nabla \delta \mathbf{M} \right\|_{L^2(\Omega^e)} \\
& + \mathcal{B} C_y \sum_e \left\| h_s^{-\frac{1}{2}} \llbracket \mathbf{u}_{\mathbf{n}} \rrbracket \right\|_{L^2(\partial \Omega^e)} \left\| h_s^{-\frac{1}{2}} \llbracket \delta \mathbf{M}_{\mathbf{n}} \rrbracket \right\|_{L^2(\partial \Omega^e)} \\
& + C_y \sum_e \left\| h_s^{\frac{1}{2}} \nabla \mathbf{u} \right\|_{L^2(\partial \Omega^e)} \left\| h_s^{-\frac{1}{2}} \llbracket \delta \mathbf{M}_{\mathbf{n}} \rrbracket \right\|_{L^2(\partial \Omega^e)} \\
& + C_y \sum_e \left\| h_s^{-\frac{1}{2}} \llbracket \mathbf{u}_{\mathbf{n}} \rrbracket \right\|_{L^2(\partial \Omega^e)} \left\| h_s^{\frac{1}{2}} \nabla \delta \mathbf{M} \right\|_{L^2(\partial \Omega^e)} \\
& + C_y \sum_e \left\| h_s^{\frac{1}{2}} \mathbf{u} \right\|_{L^2(\partial \Omega^e)} \left\| h_s^{-\frac{1}{2}} \llbracket \delta \mathbf{M}_{\mathbf{n}} \rrbracket \right\|_{L^2(\partial \Omega^e)}.
\end{aligned} \tag{C.45}$$

Choosing  $C = \max(C_y, C_y \mathcal{B})$ , the previous equation is rewritten as:

$$\begin{aligned}
& | \mathcal{A}(\mathbf{M}^e; \mathbf{u}, \delta \mathbf{M}) + \mathcal{B}(\mathbf{M}^e; \mathbf{u}, \delta \mathbf{M}) | \leq C \sum_e \left\| \nabla \mathbf{u} \right\|_{L^2(\Omega^e)} \left\| \nabla \delta \mathbf{M} \right\|_{L^2(\Omega^e)} \\
& + C \sum_e \left\| \mathbf{u} \right\|_{L^2(\Omega^e)} \left\| \nabla \delta \mathbf{M} \right\|_{L^2(\Omega^e)} \\
& + C \sum_e \left\| h_s^{-\frac{1}{2}} \llbracket \mathbf{u}_{\mathbf{n}} \rrbracket \right\|_{L^2(\partial \Omega^e)} \left\| h_s^{-\frac{1}{2}} \llbracket \nabla \delta \mathbf{M}_{\mathbf{n}} \rrbracket \right\|_{L^2(\partial \Omega^e)} \\
& + C \sum_e \left\| h_s^{\frac{1}{2}} \nabla \mathbf{u} \right\|_{L^2(\partial \Omega^e)} \left\| h_s^{-\frac{1}{2}} \llbracket \delta \mathbf{M}_{\mathbf{n}} \rrbracket \right\|_{L^2(\partial \Omega^e)} \\
& + C \sum_e \left\| h_s^{-\frac{1}{2}} \llbracket \mathbf{u}_{\mathbf{n}} \rrbracket \right\|_{L^2(\partial \Omega^e)} \left\| h_s^{\frac{1}{2}} \nabla \delta \mathbf{M} \right\|_{L^2(\Omega^e)} \\
& + C \sum_e \left\| h_s^{\frac{1}{2}} \mathbf{u} \right\|_{L^2(\partial \Omega^e)} \left\| h_s^{-\frac{1}{2}} \llbracket \delta \mathbf{M}_{\mathbf{n}} \rrbracket \right\|_{L^2(\partial \Omega^e)}.
\end{aligned} \tag{C.46}$$

After some math, this becomes

$$\begin{aligned}
& | \mathcal{A}(\mathbf{M}^e; \mathbf{u}, \delta\mathbf{M}) + \mathcal{B}(\mathbf{M}^e; \mathbf{u}, \delta\mathbf{M}) | \\
& \leq C \sum_e \left[ \| \nabla \mathbf{u} \|_{L^2(\Omega^e)} + \| \mathbf{u} \|_{L^2(\Omega^e)} + h_s^{\frac{1}{2}} \| \mathbf{u} \|_{L^2(\partial\Omega^e)} \right. \\
& \quad \left. + h_s^{\frac{1}{2}} \| \nabla \mathbf{u} \|_{L^2(\partial\Omega^e)} + h_s^{-\frac{1}{2}} \| [\![\mathbf{u}_n]\!] \|_{L^2(\partial\Omega^e)} \right] \\
& \times \left[ \| \nabla \delta\mathbf{M} \|_{L^2(\Omega^e)} + \| \delta\mathbf{M} \|_{L^2(\Omega^e)} + h_s^{\frac{1}{2}} \| \delta\mathbf{M} \|_{L^2(\partial\Omega^e)} \right. \\
& \quad \left. + h_s^{\frac{1}{2}} \| \nabla \delta\mathbf{M} \|_{L^2(\partial\Omega^e)} + h_s^{-\frac{1}{2}} \| [\![\delta\mathbf{M}_n]\!] \|_{L^2(\partial\Omega^e)} \right]. \tag{C.47}
\end{aligned}$$

Using the Cauchy-Schwartz' inequality, Eq. (2.26), and the property  $2ab \leq a^2 + b^2$ , this last equation becomes

$$\begin{aligned}
& | \mathcal{A}(\mathbf{M}^e; \mathbf{u}, \delta\mathbf{M}) + \mathcal{B}(\mathbf{M}^e; \mathbf{u}, \delta\mathbf{M}) |^2 \\
& \leq C^2 \sum_e \left[ \| \nabla \mathbf{u} \|_{L^2(\Omega^e)} + \| \mathbf{u} \|_{L^2(\Omega^e)} + h_s^{\frac{1}{2}} \| \mathbf{u} \|_{L^2(\partial\Omega^e)} \right. \\
& \quad \left. + h_s^{\frac{1}{2}} \| \nabla \mathbf{u} \|_{L^2(\partial\Omega^e)} + h_s^{-\frac{1}{2}} \| [\![\mathbf{u}_n]\!] \|_{L^2(\partial\Omega^e)} \right]^2 \\
& \times \sum_{e'} \left[ \| \nabla \delta\mathbf{M} \|_{L^2(\Omega^{e'})} + \| \delta\mathbf{M} \|_{L^2(\Omega^{e'})} + h_s^{\frac{1}{2}} \| \delta\mathbf{M} \|_{L^2(\partial\Omega^{e'})} \right. \\
& \quad \left. + h_s^{\frac{1}{2}} \| \nabla \delta\mathbf{M} \|_{L^2(\partial\Omega^{e'})} + h_s^{-\frac{1}{2}} \| [\![\delta\mathbf{M}_n]\!] \|_{L^2(\partial\Omega^{e'})} \right]^2 \\
& \leq 4C^2 \sum_e \left[ \| \nabla \mathbf{u} \|_{L^2(\Omega^e)}^2 + \| \mathbf{u} \|_{L^2(\Omega^e)}^2 + h_s \| \mathbf{u} \|_{L^2(\partial\Omega^e)}^2 + \right. \\
& \quad \left. h_s \| \nabla \mathbf{u} \|_{L^2(\partial\Omega^e)}^2 + h_s^{-1} \| [\![\mathbf{u}_n]\!] \|_{L^2(\partial\Omega^e)}^2 \right] \times \\
& \sum_{e'} \left[ \| \nabla \delta\mathbf{M} \|_{L^2(\Omega^{e'})}^2 + \| \delta\mathbf{M} \|_{L^2(\Omega^{e'})}^2 + h_s \| \delta\mathbf{M} \|_{L^2(\partial\Omega^{e'})}^2 \right. \\
& \quad \left. + h_s \| \nabla \delta\mathbf{M} \|_{L^2(\partial\Omega^{e'})}^2 + h_s^{-1} \| [\![\delta\mathbf{M}_n]\!] \|_{L^2(\partial\Omega^{e'})}^2 \right]. \tag{C.48}
\end{aligned}$$

Considering 4 in C, and using the definition of the mesh dependent norm, Eq. (2.12), we get:

$$| \mathcal{A}(\mathbf{M}^e; \mathbf{u}, \delta\mathbf{M}) + \mathcal{B}(\mathbf{M}^e; \mathbf{u}, \delta\mathbf{M}) | \leq C \| \mathbf{u} \|_1 \| \delta\mathbf{M} \|_1 \quad \forall \mathbf{u}, \delta\mathbf{M} \in X. \tag{C.49}$$

Moreover, using Eq. (2.22), we obtain

$$| \mathcal{A}(\mathbf{M}^e; \mathbf{u}, \delta\mathbf{M}_h) + \mathcal{B}(\mathbf{M}^e; \mathbf{u}, \delta\mathbf{M}_h) | \leq C^k \| \mathbf{u} \|_1 \| \delta\mathbf{M}_h \| \quad \forall \mathbf{u} \in X, \delta\mathbf{M}_h \in X^k, \tag{C.50}$$

and again, using Eq. (2.22), we have

$$| \mathcal{A}(\mathbf{M}^e; \mathbf{u}_h, \delta\mathbf{M}_h) + \mathcal{B}(\mathbf{M}^e; \mathbf{u}_h, \delta\mathbf{M}_h) | \leq C^k \| \mathbf{u}_h \| \| \delta\mathbf{M}_h \| \quad \forall \mathbf{u}_h, \delta\mathbf{M}_h \in X^k. \tag{C.51}$$



## C.5 Uniqueness of the solution for Electro-Thermal coupling

Let us first show that for a given  $\boldsymbol{\xi} \in L^2(\Omega) \times L^2(\Omega)$ , there is a unique  $\boldsymbol{\phi}_h \in X^k$  such that

$$\mathcal{A}(\mathbf{M}^e; \delta \mathbf{M}_h, \boldsymbol{\phi}_h) + \mathcal{B}(\mathbf{M}^e; \delta \mathbf{M}_h, \boldsymbol{\phi}_h) = \sum_e \int_{\Omega_e} \boldsymbol{\varphi}^T \delta \mathbf{M}_h d\Omega \quad \forall \delta \mathbf{M}_h \in X^k. \quad (\text{C.52})$$

From Lemma 4.4.1, Eq. (4.108), with  $\delta \mathbf{M}_h = \boldsymbol{\phi}_h \in X^k$ ,  $\exists C_1^k, C_2^k$ , such that:

$$\mathcal{A}(\mathbf{M}^e; \boldsymbol{\phi}_h, \boldsymbol{\phi}_h) + \mathcal{B}(\mathbf{M}^e; \boldsymbol{\phi}_h, \boldsymbol{\phi}_h) \geq C_1^k \|\boldsymbol{\phi}_h\|^2 - C_2^k \|\boldsymbol{\phi}_h\|_{L^2(\Omega_h)}^2. \quad (\text{C.53})$$

Using  $\delta \mathbf{M}_h = \boldsymbol{\phi}_h$  in Eq. (C.52) thus yields

$$\begin{aligned} C_1^k \|\boldsymbol{\phi}_h\|^2 - C_2^k \|\boldsymbol{\phi}_h\|_{L^2(\Omega_h)}^2 &\leq \sum_e \int_{\Omega_e} \boldsymbol{\varphi}^T \boldsymbol{\phi}_h d\Omega \\ &\leq \|\boldsymbol{\varphi}\|_{L^2(\Omega_h)} \|\boldsymbol{\phi}_h\|_{L^2(\Omega_h)}, \end{aligned} \quad (\text{C.54})$$

or again

$$C_1^k \|\boldsymbol{\phi}_h\|^2 \leq \|\boldsymbol{\varphi}\|_{L^2(\Omega_h)} \|\boldsymbol{\phi}_h\|_{L^2(\Omega_h)} + C_2^k \|\boldsymbol{\phi}_h\|_{L^2(\Omega_h)}^2. \quad (\text{C.55})$$

Using the definition (2.11) of the energy norm, we have that  $\|\boldsymbol{\phi}_h\|_{L^2(\Omega_h)} \leq \|\boldsymbol{\phi}_h\|$ , and Eq. (C.56) becomes

$$C_1^k \|\boldsymbol{\phi}_h\|^2 \leq \|\boldsymbol{\varphi}\|_{L^2(\Omega_h)} \|\boldsymbol{\phi}_h\| + C_2^k \|\boldsymbol{\phi}_h\| \|\boldsymbol{\phi}_h\|_{L^2(\Omega_h)}. \quad (\text{C.56})$$

Hence, we have

$$\|\boldsymbol{\phi}_h\| \leq C_3^k \|\boldsymbol{\varphi}\|_{L^2(\Omega_h)} + C_4^k \|\boldsymbol{\phi}_h\|_{L^2(\Omega_h)}. \quad (\text{C.57})$$

In order to estimate  $\|\boldsymbol{\phi}_h\|_{L^2(\Omega_h)}$ , we use the auxiliary problem stated by Eq. (4.112), with  $\boldsymbol{\phi} = \boldsymbol{\phi}_h$ . Then it follows from [23, Theorem 8.3 and Lemma 9.17] that there exists a unique solution  $\boldsymbol{\psi} \in H^2(\Omega) \times H^2(\Omega)$  to the problem stated by Eq. (4.112), and the solution satisfies the elliptic property stated by Eq. (4.113). Multiplying Eq. (4.112) by  $\boldsymbol{\phi}_h$ , integrating on  $\Omega_h$ , and integrating by parts yield

$$\begin{aligned} &\sum_e \int_{\Omega_e} [\mathbf{j}_{\nabla \mathbf{M}}(\mathbf{M}^e) \nabla \boldsymbol{\psi} + \mathbf{j}_{\mathbf{M}}(\mathbf{M}^e, \nabla \mathbf{M}^e) \boldsymbol{\psi}]^T \nabla \boldsymbol{\phi}_h d\Omega \\ &- \sum_e \int_{\partial \Omega_e} [\mathbf{j}_{\nabla \mathbf{M}}(\mathbf{M}^e) \nabla \boldsymbol{\psi} + \mathbf{j}_{\mathbf{M}}(\mathbf{M}^e, \nabla \mathbf{M}^e) \boldsymbol{\psi}]^T \boldsymbol{\phi}_{h_n} dS = \int_{\Omega_h} \boldsymbol{\phi}_h^T \boldsymbol{\phi}_h d\Omega = \|\boldsymbol{\phi}_h\|_{L^2(\Omega_h)}^2. \end{aligned} \quad (\text{C.58})$$

As  $\boldsymbol{\psi} \in H^2(\Omega) \times H^2(\Omega)$  implies  $[\boldsymbol{\psi}] = [\nabla \boldsymbol{\psi}] = 0$  on  $\partial_I \Omega_h$  and  $[\boldsymbol{\psi}] = -\boldsymbol{\psi} = 0$  on  $\partial_D \Omega_h$ , we conclude that

$$\begin{cases} \int_{\Omega_h} [\mathbf{j}_{\nabla \mathbf{M}}(\mathbf{M}^e) \nabla \boldsymbol{\psi}]^T \nabla \boldsymbol{\phi}_h + \int_{\partial_I \Omega_h} [\mathbf{j}_{\nabla \mathbf{M}}(\mathbf{M}^e) \nabla \boldsymbol{\psi}]^T [\boldsymbol{\phi}_{h_n}] dS \\ \quad - \int_{\partial_D \Omega_h} [\mathbf{j}_{\nabla \mathbf{M}}(\mathbf{M}^e) \nabla \boldsymbol{\psi}]^T \boldsymbol{\phi}_{h_n} dS = \mathcal{A}(\mathbf{M}^e; \boldsymbol{\psi}, \boldsymbol{\phi}_h) \\ \int_{\Omega_h} [\mathbf{j}_{\mathbf{M}}(\mathbf{M}^e, \nabla \mathbf{M}^e) \boldsymbol{\psi}]^T \nabla \boldsymbol{\phi}_h d\Omega + \int_{\partial_I \Omega_h} [\mathbf{j}_{\mathbf{M}}(\mathbf{M}^e, \nabla \mathbf{M}^e) \boldsymbol{\psi}]^T [\boldsymbol{\phi}_{h_n}] dS \\ \quad - \int_{\partial_D \Omega_h} [\mathbf{j}_{\mathbf{M}}(\mathbf{M}^e, \nabla \mathbf{M}^e) \boldsymbol{\psi}]^T \boldsymbol{\phi}_{h_n} dS = \mathcal{B}(\mathbf{M}^e; \boldsymbol{\psi}, \boldsymbol{\phi}_h), \end{cases} \quad (\text{C.59})$$

leading to

$$\| \phi_h \|_{L^2(\Omega_h)}^2 = \mathcal{A}(\mathbf{M}^e; \psi, \phi_h) + \mathcal{B}(\mathbf{M}^e; \psi, \phi_h). \quad (\text{C.60})$$

Inserting  $I_h \psi$  the interpolant of  $\psi$  in  $X^k$ , this can be rewritten as

$$\begin{aligned} \| \phi_h \|_{L^2(\Omega_h)}^2 &= \mathcal{A}(\mathbf{M}^e; \psi - I_h \psi, \phi_h) + \mathcal{B}(\mathbf{M}^e; \psi - I_h \psi, \phi_h) \\ &\quad + \mathcal{A}(\mathbf{M}^e; I_h \psi, \phi_h) + \mathcal{B}(\mathbf{M}^e; I_h \psi, \phi_h). \end{aligned} \quad (\text{C.61})$$

From Eq. (C.52) for  $\varphi$ , in the particular case of  $\delta \mathbf{M}_h = I_h \psi$ , we have for one of the possible solutions  $\phi_h$

$$\begin{aligned} \mathcal{A}(\mathbf{M}^e; I_h \psi, \phi_h) + \mathcal{B}(\mathbf{M}^e; I_h \psi, \phi_h) &= \int_{\Omega_h} \varphi^T I_h \psi \\ &\leq \| \varphi \|_{L^2(\Omega_h)} \| I_h \psi \|_{L^2(\Omega_h)}. \end{aligned} \quad (\text{C.62})$$

Using Lemma 4.4.2, Eq. (4.110), and Lemma 2.4.6, Eq. (2.23), we get

$$\begin{aligned} | \mathcal{A}(\mathbf{M}^e; \psi - I_h \psi, \phi_h) + \mathcal{B}(\mathbf{M}^e; \psi - I_h \psi, \phi_h) | &\leq C^k \| \psi - I_h \psi \|_1 \| \phi_h \| \\ &\leq C^k h_s^{\mu-1} \| \psi \|_{H^s(\Omega_h)} \| \phi_h \|, \end{aligned} \quad (\text{C.63})$$

with  $\mu = \min \{s, k + 1\}$ .

Substituting Eq. (C.62) and Eq. (C.63), for  $s = 2$ , in Eq. (C.61), yields

$$\| \phi_h \|_{L^2(\Omega_h)}^2 \leq C^k h_s \| \psi \|_{H^2(\Omega_h)} \| \phi_h \| + \| \varphi \|_{L^2(\Omega_h)} \| I_h \psi \|_{L^2(\Omega_h)}, \quad (\text{C.64})$$

whereas, for  $h_s$  sufficient small, the term  $\| I_h \psi \|_{L^2(\Omega)}$  can be bounded using Lemma 2.4.6, Eq. (2.23), by

$$\begin{aligned} \| I_h \psi \|_{L^2(\Omega_h)} &\leq \| I_h \psi - \psi + \psi \|_{L^2(\Omega_h)} \\ &\leq \| I_h \psi - \psi \|_{L^2(\Omega_h)} + \| \psi \|_{L^2(\Omega_h)} \leq \| I_h \psi - \psi \|_1 + \| \psi \|_{H^2(\Omega_h)} \\ &\leq C^k h_s \| \psi \|_{H^2(\Omega_h)} + \| \psi \|_{H^2(\Omega_h)} \leq C^k \| \psi \|_{H^2(\Omega_h)}. \end{aligned} \quad (\text{C.65})$$

Equation (C.64) is thus rewritten for small  $h_s$

$$\| \phi_h \|_{L^2(\Omega_h)}^2 \leq C^k \| \psi \|_{H^2(\Omega_h)} \left( h_s \| \phi_h \| + \| \varphi \|_{L^2(\Omega_h)} \right). \quad (\text{C.66})$$

By using the regular ellipticity Eq. (4.113), we obtain

$$\| \phi_h \|_{L^2(\Omega_h)} \leq C^k h_s \| \phi_h \| + C^k \| \varphi \|_{L^2(\Omega_h)} \leq C^k \| \varphi \|_{L^2(\Omega_h)}, \quad (\text{C.67})$$

for small  $h_s$ . Hence we complete the proof of Lemma 4.4.3 by substituting Eq. (C.67) in Eq. (C.57)

$$\| \phi_h \| \leq C^k \| \varphi \|_{L^2(\Omega_h)}. \quad (\text{C.68})$$

The existence of the solution  $\phi_h$  to the problem stated by Eq. (C.52) follows from its uniqueness, which follows trivially from Eq. (C.68). Indeed for  $\varphi_1, \varphi_2 \in L^2(\Omega) \times L^2(\Omega)$ , we have

$$\| \phi_{h_1} - \phi_{h_2} \|_{L^2(\Omega_h)} \leq C^k \| \varphi_1 - \varphi_2 \|_{L^2(\Omega_h)}, \quad (\text{C.69})$$

and  $\phi_{h_1} = \phi_{h_2}$  if  $\varphi_1 = \varphi_2$ .

## C.6 The bound in the ball

We need to show that  $\mathbf{j}(\mathbf{x}; \mathbf{y}, \nabla \mathbf{y})$ ,  $\mathbf{j}_M(\mathbf{x}; \mathbf{y}, \nabla \mathbf{y})$ ,  $\mathbf{j}_{MM}(\mathbf{x}; \mathbf{y}, \nabla \mathbf{y})$ ,  $\mathbf{j}_{\nabla M}(\mathbf{x}; \mathbf{y})$ ,  $\mathbf{j}_{M\nabla M}(\mathbf{x}; \mathbf{y})$  are bounded for  $\mathbf{x} \in \bar{\Omega}$ ,  $\mathbf{y} \in O_\sigma(I_h \mathbf{M})$ .

To this end, we first show that  $\mathbf{y}$  and  $\nabla \mathbf{y}$  are bounded, by considering the ball  $O_\sigma(I_h \mathbf{M})$  with radius  $\sigma = h_s^{-\varepsilon} \|\mathbf{M}^e - I_h \mathbf{M}\|_1$ ,  $0 < \varepsilon < \frac{1}{4}$ . Therefore, we have

$$\|\mathbf{y} - \mathbf{M}^e\|_{W_\infty^1(\Omega)} \leq \|\mathbf{y} - I_h \mathbf{M}\|_{W_\infty^1(\Omega)} + \|I_h \mathbf{M} - \mathbf{M}^e\|_{W_\infty^1(\Omega)}. \quad (\text{C.70})$$

The first term of the right hand side of Eq. (C.70) can be bounded using the inverse inequality (2.19), yielding

$$\begin{aligned} \|\mathbf{y} - I_h \mathbf{M}\|_{W_\infty^1(\Omega)} &= \|\mathbf{y} - I_h \mathbf{M}\|_{L^\infty(\Omega)} + \|\nabla(\mathbf{y} - I_h \mathbf{M})\|_{L^\infty(\Omega)} \\ &\leq C_T^k h_s^{-1} \|\mathbf{y} - I_h \mathbf{M}\|_{L^2(\Omega)} + C_T^k h_s^{-1} \|\nabla(\mathbf{y} - I_h \mathbf{M})\|_{L^2(\Omega)} \\ &\leq C_T^k h_s^{-1} \|\mathbf{y} - I_h \mathbf{M}\|_{H^1(\Omega)} \leq C_T^k h_s^{-1} \|\mathbf{y} - I_h \mathbf{M}\|_1. \end{aligned} \quad (\text{C.71})$$

Using the interpolant inequality (2.14), the definition of the ball (4.119), and Eq. (4.121) for  $k \geq 2$  to bound the second term of the right hand side of Eq. (C.70), we have for  $h_s$  small enough

$$\begin{aligned} \|\mathbf{y} - \mathbf{M}^e\|_{W_\infty^1(\Omega)} &\leq C_T^k h_s^{-1} \|\mathbf{y} - I_h \mathbf{M}\|_1 + \|I_h \mathbf{M} - \mathbf{M}^e\|_{W_\infty^1(\Omega)} \\ &\leq C_T^k h_s^{-1-\varepsilon} \|\mathbf{M}^e - I_h \mathbf{M}\|_1 + C_D^k h_s^{\frac{1}{2}} \|\mathbf{M}^e\|_{H^{\frac{5}{2}}(\Omega_h)} \\ &\leq C_T^k C_M h_s^{\frac{1}{2}-\varepsilon} \|\mathbf{M}^e\|_{H^{\frac{5}{2}}(\Omega_h)} + C_D^k h_s^{\frac{1}{2}} \|\mathbf{M}^e\|_{H^{\frac{5}{2}}(\Omega_h)} \\ &\leq C_T^k C_M h_s^{\frac{1}{2}-\varepsilon} \|\mathbf{M}^e\|_{H^{\frac{5}{2}}(\Omega_h)} \quad \text{if } k \geq 2. \end{aligned} \quad (\text{C.72})$$

Hence, for small  $h_s$ ,  $\|\mathbf{y}\|_{W_\infty^1(\Omega)} \leq (1 + \sigma^*) \|\mathbf{M}^e\|_{W_\infty^1(\Omega)}$ , where  $0 < \sigma^* < 1$ , for  $k \geq 2$ . If  $\mathbf{M}^e \in H^{\frac{5}{2}}(\Omega) \times H^{\frac{5}{2}^+}(\Omega)$ , the value  $\mathbf{y}(\mathbf{x}) \in [(1 - \sigma^*)k_M, (1 + \sigma^*)K_M]$  is considered to derive the bounds, where  $0 < \sigma^* < 1$ ,  $k_M = \min \{\mathbf{M}^e(\mathbf{x}) : \mathbf{x} \in \bar{\Omega}\}$  and  $K_M = \max \{\mathbf{M}^e(\mathbf{x}) : \mathbf{x} \in \bar{\Omega}\}$ . Similarly, we consider the value of  $\frac{\partial \mathbf{y}}{\partial \mathbf{x}^i}(\mathbf{x}) \in [(1 - \sigma^*)k_{\nabla M}, (1 + \sigma^*)K_{\nabla M}]$ , such that  $k_{\nabla M} = \min \{\nabla \mathbf{M}^e(\mathbf{x}) : \mathbf{x} \in \bar{\Omega}\}$  and  $K_{\nabla M} = \max \{\nabla \mathbf{M}^e(\mathbf{x}) : \mathbf{x} \in \bar{\Omega}\}^2$ .

Since the nonlinear functions  $\mathbf{j}_M$ ,  $\mathbf{j}_{MM}$ ,  $\mathbf{j}_{\nabla M}$ ,  $\mathbf{j}_{M\nabla M}$  are continuous, they map the compact set  $[(1 - \sigma^*)k_M, (1 + \sigma^*)K_M] \times [(1 - \sigma^*)k_{\nabla M}, (1 + \sigma^*)K_{\nabla M}]$  into a compact set, hence the nonlinear term  $\mathbf{j}(\mathbf{x}; \mathbf{y}, \nabla \mathbf{y})$  and its derivatives  $\mathbf{j}_M(\mathbf{x}; \mathbf{y}, \nabla \mathbf{y})$ ,  $\mathbf{j}_{MM}(\mathbf{x}; \mathbf{y}, \nabla \mathbf{y})$ ,  $\mathbf{j}_{\nabla M}(\mathbf{x}; \mathbf{y})$ ,  $\mathbf{j}_{M\nabla M}(\mathbf{x}; \mathbf{y})$  are bounded in a ball around  $\mathbf{M}^e \in W_\infty^1(\Omega) \times W_\infty^1(\Omega)$ .

## C.7 Intermediate bounds derivation

The purpose of this section is to derive the bound of the nonlinear term  $\mathcal{N}$ .

First the term  $\|\boldsymbol{\zeta}\|_{L^2(\Omega^e)}$  is bounded by using its decomposition as  $\boldsymbol{\zeta} = \boldsymbol{\eta} + \boldsymbol{\xi}$ , where  $\boldsymbol{\eta} = \mathbf{M}^e - I_h \mathbf{M}$  and  $\boldsymbol{\xi} = I_h \mathbf{M} - \mathbf{y}$ , which gives

$$\sum_e \|\boldsymbol{\zeta}\|_{L^2(\Omega^e)}^2 \leq 2 \left( \sum_e \|\boldsymbol{\eta}\|_{L^2(\Omega^e)}^2 + \sum_e \|\boldsymbol{\xi}\|_{L^2(\Omega^e)}^2 \right). \quad (\text{C.73})$$

<sup>2</sup>By abuse of notations, in this context the min and max operator applied on vectors, mean we retain respectively the minimum and maximum value for each component.

Using the interpolation inequality (2.14) leads to

$$\sum_e \|\boldsymbol{\eta}\|_{L^2(\Omega^e)}^2 \leq C_{\mathcal{D}}^{k^2} h_s^{2\mu} \sum_e \|\mathbf{M}^e\|_{H^s(\Omega^e)}^2 = C_{\mathcal{D}}^{k^2} h_s^5 \sum_e \|\mathbf{M}^e\|_{H^{\frac{5}{2}}(\Omega^e)}^2 \quad \text{if } k \geq 2. \quad (\text{C.74})$$

An application of the norm definition, Eq. (2.12), and the definition of the ball, Eqs. (4.119, 4.120), give

$$\begin{aligned} \sum_e \|\boldsymbol{\xi}\|_{L^2(\Omega^e)}^2 &\leq C_{\mathcal{P}}^2 \|\boldsymbol{\xi}\|_1^2 \leq C_{\mathcal{P}}^2 \sigma^2 \\ &\leq C_{\mathcal{P}}^2 h_s^{2(\mu-1-\varepsilon)} \sum_e \|\mathbf{M}^e\|_{H^s(\Omega^e)}^2 = C_{\mathcal{P}}^2 h_s^{3-2\varepsilon} \sum_e \|\mathbf{M}^e\|_{H^{\frac{5}{2}}(\Omega^e)}^2 \quad \text{if } k \geq 2. \end{aligned} \quad (\text{C.75})$$

Combining Eq. (C.74, C.75), gives for  $h_s$  small enough

$$\begin{aligned} \sum_e \|\boldsymbol{\zeta}\|_{L^2(\Omega^e)}^2 &\leq C^{k^2} \sigma^2 \\ &\leq C^{k^2} h_s^{2(\mu-1-\varepsilon)} \sum_e \|\mathbf{M}^e\|_{H^s(\Omega^e)}^2 = C^{k^2} h_s^{3-2\varepsilon} \sum_e \|\mathbf{M}^e\|_{H^{\frac{5}{2}}(\Omega^e)}^2 \quad \text{if } k \geq 2. \end{aligned} \quad (\text{C.76})$$

Similarly, one can get

$$\sum_e \|\boldsymbol{\zeta}\|_{L^4(\Omega^e)}^4 \leq 4 \left( \sum_e \|\boldsymbol{\eta}\|_{L^4(\Omega^e)}^4 + \sum_e \|\boldsymbol{\xi}\|_{L^4(\Omega^e)}^4 \right). \quad (\text{C.77})$$

Using the interpolation inequality (2.14) leads to

$$\|\boldsymbol{\eta}\|_{L^4(\Omega^e)} \leq C_{\mathcal{D}}^k h_s^{\mu-\frac{1}{2}} \|\mathbf{M}^e\|_{H^s(\Omega^e)} = C_{\mathcal{D}}^k h_s^2 \|\mathbf{M}^e\|_{H^{\frac{5}{2}}(\Omega^e)} \quad \text{if } k \geq 2. \quad (\text{C.78})$$

Next,  $\|\boldsymbol{\xi}\|_{L^4(\Omega^e)}^4$  is bounded by applying, the inverse inequality (2.19), the definition of the norm (2.12), and the definition of the ball, Eqs. (4.119, 4.120), which yields

$$\begin{aligned} \sum_e \|\boldsymbol{\xi}\|_{L^4(\Omega^e)}^4 &\leq C_{\mathcal{I}}^{k^4} \left(\frac{1}{h_s}\right)^2 \sum_e \|\boldsymbol{\xi}\|_{L^2(\Omega^e)}^4 \\ &\leq C_{\mathcal{I}}^{k^4} \left(\frac{1}{h_s}\right)^2 \left( \sum_e \|\boldsymbol{\xi}\|_{L^2(\Omega^e)}^2 \right)^2 \leq C_{\mathcal{I}}^{k^4} h_s^{-2} \|\boldsymbol{\xi}\|_1^4 \leq C_{\mathcal{I}}^{k^4} h_s^{-2} \sigma^4 \\ &\leq C_{\mathcal{I}}^{k^4} h_s^{4(\mu-\frac{3}{2}-\varepsilon)} \|\mathbf{M}^e\|_{H^s(\Omega_h)}^4 = C_{\mathcal{I}}^{k^4} h_s^{4(1-\varepsilon)} \|\mathbf{M}^e\|_{H^{\frac{5}{2}}(\Omega_h)}^4 \quad \text{if } k \geq 2. \end{aligned} \quad (\text{C.79})$$

Combining Eqs. (C.78, C.79), gives for  $h_s$  small enough

$$\begin{aligned} \sum_e \|\boldsymbol{\zeta}\|_{L^4(\Omega^e)}^4 &\leq C^{k^4} h_s^{-2} \sigma^4 \\ &\leq C^{k^4} h_s^{4(\mu-\frac{3}{2}-\varepsilon)} \|\mathbf{M}^e\|_{H^s(\Omega_h)}^4 = C^{k^4} h_s^{4(1-\varepsilon)} \|\mathbf{M}^e\|_{H^{\frac{5}{2}}(\Omega_h)}^4 \quad \text{if } k \geq 2. \end{aligned} \quad (\text{C.80})$$

Proceeding by the same way,  $\sum_e \|\nabla \zeta\|_{L^2(\Omega^e)}^2$  can be estimated by applying the interpolation inequality (2.13), the definition of the norm (2.12), and the definition of the ball, Eqs. (4.119, 4.120), as

$$\begin{aligned}
\sum_e \|\nabla \zeta\|_{L^2(\Omega^e)}^2 &\leq 2 \left( \sum_e \|\nabla \boldsymbol{\eta}\|_{L^2(\Omega^e)}^2 + \sum_e \|\nabla \boldsymbol{\xi}\|_{L^2(\Omega^e)}^2 \right) \\
&\leq C_{\mathcal{D}}^{k^2} h_s^{2\mu-2} \sum_e \|\mathbf{M}^e\|_{H^s(\Omega^e)}^2 + 2 \|\boldsymbol{\xi}\|_1^2 \\
&\leq C_{\mathcal{D}}^{k^2} h_s^{2\mu-2} \sum_e \|\mathbf{M}^e\|_{H^s(\Omega^e)}^2 + 2\sigma^2 \\
&\leq C_{\mathcal{D}}^{k^2} h_s^{2\mu-2} \sum_e \|\mathbf{M}^e\|_{H^s(\Omega^e)}^2 + C_{\mathcal{I}}^{k^2} h_s^{2\mu-2-2\varepsilon} \sum_e \|\mathbf{M}^e\|_{H^s(\Omega^e)}^2 \\
&\leq C^{k^2} h_s^{2(\frac{3}{2}-\varepsilon)} \sum_e \|\mathbf{M}^e\|_{H^{\frac{5}{2}}(\Omega^e)}^2 \quad \text{if } k \geq 2.
\end{aligned} \tag{C.81}$$

Using the trace inequality (2.16) we have

$$\|\boldsymbol{\eta}\|_{L^4(\partial\Omega^e)}^4 \leq C_{\mathcal{T}} \left( h_s^{-1} \|\boldsymbol{\eta}\|_{L^4(\Omega^e)}^4 + \|\boldsymbol{\eta}\|_{L^6(\Omega^e)}^3 \|\nabla \boldsymbol{\eta}\|_{L^2(\Omega^e)} \right). \tag{C.82}$$

Calling the interpolation inequality (2.14) gives

$$\|\boldsymbol{\eta}\|_{W_4^0(\Omega^e)}^4 \leq C_{\mathcal{D}}^{k^4} h_s^{4(\mu-\frac{1}{2})} \|\mathbf{M}^e\|_{H^s(\Omega^e)}^4, \quad \text{and} \tag{C.83}$$

$$\|\boldsymbol{\eta}\|_{W_6^0(\Omega^e)}^3 \leq C_{\mathcal{D}}^{k^3} h_s^{3(\mu-\frac{2}{3})} \|\mathbf{M}^e\|_{H^s(\Omega^e)}^3. \tag{C.84}$$

Also, by the use of the interpolation inequality (2.13) one has

$$\|\nabla \boldsymbol{\eta}\|_{L^2(\Omega^e)} \leq \|\boldsymbol{\eta}\|_{H^1(\Omega^e)} \leq C_{\mathcal{D}}^k h_s^{\mu-1} \|\mathbf{M}^e\|_{H^s(\Omega^e)}. \tag{C.85}$$

Combining the last three equations results into

$$\|\boldsymbol{\eta}\|_{L^4(\partial\Omega^e)} \leq C_{\mathcal{T}}^{\frac{1}{4}} C_{\mathcal{D}}^k h_s^{\mu-\frac{3}{4}} \|\mathbf{M}^e\|_{H^{\frac{5}{2}}(\Omega^e)} \leq C_{\mathcal{T}}^{\frac{1}{4}} C_{\mathcal{D}}^k h_s^{\frac{7}{4}} \|\mathbf{M}^e\|_{H^{\frac{5}{2}}(\Omega^e)} \quad \text{if } k \geq 2. \tag{C.86}$$

Likewise, applying the trace inequality (2.16) and the interpolation inequality (2.14), leads to

$$\|\nabla \boldsymbol{\eta}\|_{L^4(\partial\Omega^e)}^4 \leq C_{\mathcal{T}} \left( h_s^{-1} \|\nabla \boldsymbol{\eta}\|_{L^4(\Omega^e)}^4 + \|\nabla \boldsymbol{\eta}\|_{L^6(\Omega^e)}^3 \|\nabla^2 \boldsymbol{\eta}\|_{L^2(\Omega^e)} \right), \tag{C.87}$$

with

$$\|\boldsymbol{\eta}\|_{W_4^1(\Omega^e)}^4 \leq C_{\mathcal{D}}^{k^4} h_s^{4(\mu-\frac{3}{2})} \|\mathbf{M}^e\|_{H^s(\Omega^e)}^4, \tag{C.88}$$

$$\|\boldsymbol{\eta}\|_{W_6^1(\Omega^e)}^3 \leq C_{\mathcal{D}}^{k^3} h_s^{3(\mu-\frac{5}{3})} \|\mathbf{M}^e\|_{H^s(\Omega^e)}^3, \tag{C.89}$$

$$\|\nabla^2 \boldsymbol{\eta}\|_{L^2(\Omega^e)} \leq \|\boldsymbol{\eta}\|_{W_2^2(\Omega^e)} \leq C_{\mathcal{D}}^k h_s^{\mu-2} \|\mathbf{M}^e\|_{H^s(\Omega^e)}. \tag{C.90}$$

Combining the last three equations gives

$$\| \nabla \boldsymbol{\eta} \|_{L^4(\partial\Omega^e)} \leq C_{\mathcal{T}}^{\frac{1}{4}} C_{\mathcal{D}}^k h_s^{\mu - \frac{7}{4}} \| \mathbf{M}^e \|_{H^s(\Omega^e)} = C_{\mathcal{T}}^{\frac{1}{4}} C_{\mathcal{D}}^k h_s^{\frac{3}{4}} \| \mathbf{M}^e \|_{H^{\frac{5}{2}}(\Omega^e)} \quad \text{if } k \geq 2. \quad (\text{C.91})$$

Next, the bound of  $\| \boldsymbol{\xi} \|_{L^4(\partial\Omega^e)}$  is estimated by applying the trace inequality (2.16) and the inverse inequality, Eqs. (2.19, 2.21), leading to

$$\| \boldsymbol{\xi} \|_{L^4(\partial\Omega^e)}^4 \leq C_{\mathcal{T}} \left( h_s^{-1} \| \boldsymbol{\xi} \|_{L^4(\Omega^e)}^4 + \| \boldsymbol{\xi} \|_{L^6(\Omega^e)}^3 \| \nabla \boldsymbol{\xi} \|_{L^2(\Omega^e)} \right), \quad (\text{C.92})$$

with

$$\| \boldsymbol{\xi} \|_{L^4(\Omega^e)}^4 \leq C_{\mathcal{I}}^k h_s^{-2} \| \boldsymbol{\xi} \|_{L^2(\Omega^e)}^4, \quad (\text{C.93})$$

$$\| \boldsymbol{\xi} \|_{L^6(\Omega^e)}^3 \leq C_{\mathcal{I}}^k h_s^{-2} \| \boldsymbol{\xi} \|_{L^2(\Omega^e)}^3, \quad (\text{C.94})$$

$$\| \nabla \boldsymbol{\xi} \|_{L^2(\Omega^e)} \leq C_{\mathcal{I}}^k h_s^{-1} \| \boldsymbol{\xi} \|_{L^2(\Omega^e)}. \quad (\text{C.95})$$

Combining the last three equations, then applying the definition of the norm (2.12) and the definition of the ball, Eqs. (4.119, 4.120), result into

$$\begin{aligned} \sum_e \| \boldsymbol{\xi} \|_{L^4(\partial\Omega^e)}^4 &\leq C_{\mathcal{T}} C_{\mathcal{I}}^k h_s^{-3} \sum_e \| \boldsymbol{\xi} \|_{L^2(\Omega^e)}^4 \leq C_{\mathcal{T}} C_{\mathcal{I}}^k C_{\mathcal{P}}^4 h_s^{-3} \| \boldsymbol{\xi} \|_1^4 \\ &\leq C_{\mathcal{T}} C_{\mathcal{I}}^k C_{\mathcal{P}}^4 h_s^{-3} \sigma^4 \\ &\leq C_{\mathcal{T}} C_{\mathcal{I}}^k C_{\mathcal{P}}^4 h_s^{4(\mu - \frac{7}{4} - \varepsilon)} \| \mathbf{M}^e \|_{H^s(\Omega_h)}^4 = C_{\mathcal{T}} C_{\mathcal{I}}^k C_{\mathcal{P}}^4 h_s^{4(\frac{3}{4} - \varepsilon)} \| \mathbf{M}^e \|_{H^{\frac{5}{2}}(\Omega_h)}^4 \quad \text{if } k \geq 2. \end{aligned} \quad (\text{C.96})$$

Then, using the inverse inequality (2.20), Lemma 2.4.3, Eq. (2.18), the definition of the norm (2.12), and the definition of the ball, Eqs. (4.119, 4.120), yields

$$\begin{aligned} \sum_e \| \nabla \boldsymbol{\xi} \|_{L^4(\partial\Omega^e)}^4 &\leq C_{\mathcal{I}}^k h_s^{-1} \sum_e \| \nabla \boldsymbol{\xi} \|_{L^2(\partial\Omega^e)}^4 \leq C_{\mathcal{I}}^k C_{\mathcal{K}}^k h_s^{-3} \sum_e \| \nabla \boldsymbol{\xi} \|_{L^2(\Omega^e)}^4 \\ &\leq C_{\mathcal{I}}^k C_{\mathcal{K}}^k h_s^{-3} \| \boldsymbol{\xi} \|_1^4 \leq C_{\mathcal{I}}^k C_{\mathcal{K}}^k h_s^{-3} \sigma^4 \\ &\leq C_{\mathcal{I}}^k C_{\mathcal{K}}^k h_s^{4(\mu - \frac{7}{4} - \varepsilon)} \| \mathbf{M}^e \|_{H^s(\Omega_h)}^4 = C_{\mathcal{I}}^k C_{\mathcal{K}}^k h_s^{4(\frac{3}{4} - \varepsilon)} \| \mathbf{M}^e \|_{H^{\frac{5}{2}}(\Omega_h)}^4 \quad \text{if } k \geq 2. \end{aligned} \quad (\text{C.97})$$

Moreover,  $\| \boldsymbol{\zeta} \|_{L^4(\partial\Omega^e)}$  can be bounded by the dominant term of its component as

$$\begin{aligned} \sum_e \| \boldsymbol{\zeta} \|_{L^4(\partial\Omega^e)}^4 &\leq C^k h_s^{-3} \sigma^4 \\ &\leq C^k h_s^{4(\mu - \frac{7}{4} - \varepsilon)} \| \mathbf{M}^e \|_{H^s(\Omega_h)}^4 = C^k h_s^{4(\frac{3}{4} - \varepsilon)} \| \mathbf{M}^e \|_{H^{\frac{5}{2}}(\Omega_h)}^4 \quad \text{if } k \geq 2. \end{aligned} \quad (\text{C.98})$$

By the same way, the bound of  $\| \nabla \boldsymbol{\zeta} \|_{L^4(\partial\Omega^e)}$  is the dominant term of its component (C.91, C.97), yielding

$$\begin{aligned} \sum_e \| \nabla \boldsymbol{\zeta} \|_{L^4(\partial\Omega^e)}^4 &\leq C^k h_s^{-3} \sigma^4 \\ &\leq C^k h_s^{4(\mu - \frac{7}{4} - \varepsilon)} \| \mathbf{M}^e \|_{H^s(\Omega_h)}^4 = C^k h_s^{4(\frac{3}{4} - \varepsilon)} \| \mathbf{M}^e \|_{H^{\frac{5}{2}}(\Omega_h)}^4 \quad \text{if } k \geq 2. \end{aligned} \quad (\text{C.99})$$

Now the bound of  $\| \llbracket \boldsymbol{\zeta} \rrbracket \|_{L^4(\partial\Omega^e)}^4$  can be evaluated from

$$\sum_e \| \llbracket \boldsymbol{\zeta} \rrbracket \|_{L^4(\partial\Omega^e)}^4 \leq 4 \left( \sum_e \| \llbracket \boldsymbol{\eta} \rrbracket \|_{L^4(\partial\Omega^e)}^4 + \sum_e \| \llbracket \boldsymbol{\xi} \rrbracket \|_{L^4(\partial\Omega^e)}^4 \right). \quad (\text{C.100})$$

Using Eq. (C.86), we have

$$\begin{aligned} \sum_e \| \llbracket \boldsymbol{\eta} \rrbracket \|_{L^4(\partial\Omega^e)}^4 &\leq 2 \sum_e \| \boldsymbol{\eta} \|_{L^4(\partial\Omega^e)}^4 \\ &\leq C_{\mathcal{T}} C_{\mathcal{D}}^{k^4} h_s^{4\mu-3} \sum_e \| \mathbf{M}^e \|_{H^s(\Omega^e)}^4 \\ &\leq C_{\mathcal{T}} C_{\mathcal{D}}^{k^4} h_s^7 \| \mathbf{M}_h \|_{H^s(\Omega_h)}^4 \text{ if } k \geq 2. \end{aligned} \quad (\text{C.101})$$

Then, applying the inverse inequality (2.20), the definition of the norm (2.12), and the definition of the ball, Eqs. (4.119, 4.120), yields

$$\begin{aligned} \sum_e \| \llbracket \boldsymbol{\xi} \rrbracket \|_{L^4(\partial\Omega^e)}^4 &\leq C_{\mathcal{I}}^{k^4} h_s^{-1} \sum_e \| \llbracket \boldsymbol{\xi} \rrbracket \|_{L^2(\partial\Omega^e)}^4 \leq C_{\mathcal{I}}^{k^4} h_s \sum_e \| h_s^{-\frac{1}{2}} \llbracket \boldsymbol{\xi} \rrbracket \|_{L^2(\partial\Omega^e)}^4 \\ &\leq C_{\mathcal{I}}^{k^4} C_{\mathcal{P}}^4 h_s \| \boldsymbol{\xi} \|_1^4 \leq C_{\mathcal{I}}^{k^4} C_{\mathcal{P}}^4 h_s \sigma^4 \\ &\leq C_{\mathcal{I}}^{k^4} C_{\mathcal{P}}^4 h_s^{4(\mu-\frac{3}{4}-\varepsilon)} \| \mathbf{M}^e \|_{H^s(\Omega_h)}^4 = C_{\mathcal{T}} C_{\mathcal{I}}^{k^4} C_{\mathcal{P}}^4 h_s^{4(\frac{7}{4}-\varepsilon)} \| \mathbf{M}^e \|_{H^{\frac{5}{2}}(\Omega_h)}^4 \text{ if } k \geq 2. \end{aligned} \quad (\text{C.102})$$

Combining Eqs. (C.101 and C.102), gives

$$\begin{aligned} \sum_e \| \llbracket \boldsymbol{\zeta} \rrbracket \|_{L^4(\partial\Omega^e)}^4 &\leq C^{k^4} h_s \sigma^4 \\ &\leq C^{k^4} h_s^{4(\mu-\frac{3}{4}-\varepsilon)} \| \mathbf{M}^e \|_{H^s(\Omega_h)}^4 = C^k h_s^{4(\frac{7}{4}-\varepsilon)} \| \mathbf{M}^e \|_{H^{\frac{5}{2}}(\Omega_h)}^4 \text{ if } k \geq 2. \end{aligned} \quad (\text{C.103})$$

Finally, by the use of the inverse inequality (2.19), we get Eq. (4.134), as

$$\| \delta \mathbf{M}_h \|_{L^4(\Omega^e)} \leq C_{\mathcal{I}}^k h_s^{-\frac{1}{2}} \| \delta \mathbf{M}_h \|_{L^2(\Omega^e)}, \quad (\text{C.104})$$

$$\| \nabla \delta \mathbf{M}_h \|_{L^4(\Omega^e)} \leq C_{\mathcal{I}}^k h_s^{-\frac{1}{2}} \| \nabla \delta \mathbf{M}_h \|_{L^2(\Omega^e)}, \quad (\text{C.105})$$

which implies

$$\begin{cases} | \delta \mathbf{M}_h |_{W_4^1(\Omega^e)} &\leq C_{\mathcal{I}}^k h_s^{-\frac{1}{2}} | \delta \mathbf{M}_h |_{H^1(\Omega^e)}, \\ \| \delta \mathbf{M}_h \|_{W_4^1(\Omega^e)} &\leq C_{\mathcal{I}}^k h_s^{-\frac{1}{2}} \| \delta \mathbf{M}_h \|_{H^1(\Omega^e)}. \end{cases} \quad (\text{C.106})$$

## C.8 The bound of the nonlinear term $\mathcal{N}(\mathbf{M}^e, \mathbf{y}; \delta\mathbf{M}_h)$

The first term of  $\mathcal{N}(\mathbf{M}^e, \mathbf{y}; \delta\mathbf{M}_h)$ , defined in Eq. (4.101), can be expanded using Eq. (4.91) as

$$\begin{aligned} \mathcal{I}_1 &= \int_{\Omega_h} (\nabla \delta\mathbf{M})_h^T \bar{\mathbf{R}}_j(\boldsymbol{\zeta}, \nabla \boldsymbol{\zeta}) d\Omega = \sum_e \int_{\Omega^e} (\nabla \delta\mathbf{M}_h)^T (\boldsymbol{\zeta}^T \bar{\mathbf{J}}_{\mathbf{M}\mathbf{M}}(\mathbf{y}, \nabla \mathbf{y}) \boldsymbol{\zeta}) d\Omega \\ &\quad + 2 \sum_e \int_{\Omega^e} (\nabla \delta\mathbf{M})_h^T (\boldsymbol{\zeta}^T \bar{\mathbf{J}}_{\mathbf{M}\nabla\mathbf{M}}(\mathbf{y}) \nabla \boldsymbol{\zeta}) d\Omega \quad (\text{C.107}) \\ &= \mathcal{I}_{11} + 2\mathcal{I}_{12}. \end{aligned}$$

The first term of the right hand side of Eq. (C.107) is bounded by using the generalized Hölder inequality (2.25), the generalized Cauchy-Schwartz' inequality (2.27), the definition of  $C_y$  in Eq. (4.93), and the bounds (4.122, 4.123, and 4.134) as

$$\begin{aligned} |\mathcal{I}_{11}| &= \left| \sum_e \int_{\Omega^e} (\nabla \delta\mathbf{M}_h)^T (\boldsymbol{\zeta}^T \bar{\mathbf{J}}_{\mathbf{M}\mathbf{M}}(\mathbf{y}, \nabla \mathbf{y}) \boldsymbol{\zeta}) d\Omega \right| \\ &\leq C_y \sum_e \|\boldsymbol{\zeta}\|_{L^4(\Omega^e)} \|\boldsymbol{\zeta}\|_{L^2(\Omega^e)} \|\nabla \delta\mathbf{M}_h\|_{L^4(\Omega^e)} \\ &\leq C_y \left( \sum_e \|\boldsymbol{\zeta}\|_{L^4(\Omega^e)}^4 \right)^{\frac{1}{4}} \left( \sum_e \|\boldsymbol{\zeta}\|_{L^2(\Omega^e)}^2 \right)^{\frac{1}{2}} \left( \sum_e \|\nabla \delta\mathbf{M}_h\|_{L^4(\Omega^e)}^4 \right)^{\frac{1}{4}} \quad (\text{C.108}) \\ &\leq C^k C_y h_s^{\mu-2-\varepsilon} \sigma \|\delta\mathbf{M}_h\|_{H^1(\Omega_h)} \|\mathbf{M}^e\|_{H^s(\Omega_h)}. \end{aligned}$$

For the second term of the right hand side of Eq. (C.107), the generalized Hölder inequality (2.25), the generalized Cauchy-Schwartz' inequality (2.27), and the bounds (4.123, 4.124, and 4.134), imply that

$$\begin{aligned} |\mathcal{I}_{12}| &= \left| \sum_e \int_{\Omega^e} (\nabla \delta\mathbf{M}_h)^T (\boldsymbol{\zeta}^T \bar{\mathbf{J}}_{\mathbf{M}\nabla\mathbf{M}}(\mathbf{y}) \nabla \boldsymbol{\zeta}) d\Omega \right| \\ &\leq C_y \sum_e \|\boldsymbol{\zeta}\|_{L^4(\Omega^e)} \|\nabla \boldsymbol{\zeta}\|_{L^2(\Omega^e)} \|\nabla \delta\mathbf{M}_h\|_{L^4(\Omega^e)} \\ &\leq C_y \left( \sum_e \|\boldsymbol{\zeta}\|_{L^4(\Omega^e)}^4 \right)^{\frac{1}{4}} \left( \sum_e \|\nabla \boldsymbol{\zeta}\|_{L^2(\Omega^e)}^2 \right)^{\frac{1}{2}} \left( \sum_e \|\nabla \delta\mathbf{M}_h\|_{L^4(\Omega^e)}^4 \right)^{\frac{1}{4}} \quad (\text{C.109}) \\ &\leq C^k C_y h_s^{\mu-2-\varepsilon} \sigma \|\delta\mathbf{M}_h\|_{H^1(\Omega_h)} \|\mathbf{M}^e\|_{H^s(\Omega_h)}. \end{aligned}$$

Combining the above result leads to

$$\begin{aligned} |\mathcal{I}_1| &\leq C^k C_y h_s^{\mu-2-\varepsilon} \sigma \|\delta\mathbf{M}_h\|_{H^1(\Omega_h)} \|\mathbf{M}^e\|_{H^s(\Omega_h)} \\ &\leq C^k C_y C_M h_s^{\frac{1}{2}-\varepsilon} \sigma \|\delta\mathbf{M}_h\|_{H^1(\Omega_h)} \quad \text{if } k \geq 2. \end{aligned} \quad (\text{C.110})$$



The second term of  $\mathcal{N}(\mathbf{M}^e, \mathbf{y}; \delta \mathbf{M}_h)$ , defined in Eq. (4.101), becomes by using Eq. (4.91),

$$\begin{aligned}
\mathcal{I}_2 &= \int_{\partial_1 \Omega_h \cup \partial_D \Omega_h} \llbracket \delta \mathbf{M}_{h_n}^T \rrbracket \langle \bar{\mathbf{R}}_j(\boldsymbol{\zeta}, \nabla \boldsymbol{\zeta}) \rangle \, dS \\
&= \underbrace{\frac{1}{2} \sum_e \int_{\partial_1 \Omega^e} \llbracket \delta \mathbf{M}_{h_n}^T \rrbracket \langle \boldsymbol{\zeta}^{T\bar{}} \mathbf{j}_{\mathbf{M}\mathbf{M}}(\mathbf{y}, \nabla \mathbf{y}) \boldsymbol{\zeta} \rangle \, dS + \sum_e \int_{\partial_D \Omega^e} \llbracket \delta \mathbf{M}_{h_n}^T \rrbracket \langle \boldsymbol{\zeta}^{T\bar{}} \mathbf{j}_{\mathbf{M}\mathbf{M}}(\mathbf{y}, \nabla \mathbf{y}) \boldsymbol{\zeta} \rangle \, dS}_{\mathcal{I}_{21}} \\
&\quad + \underbrace{\sum_e \int_{\partial_1 \Omega^e} \llbracket \delta \mathbf{M}_{h_n}^T \rrbracket \langle \boldsymbol{\zeta}^{T\bar{}} \mathbf{j}_{\mathbf{M}\nabla \mathbf{M}}(\mathbf{y}) \nabla \boldsymbol{\zeta} \rangle \, dS + 2 \sum_e \int_{\partial_D \Omega^e} \llbracket \delta \mathbf{M}_{h_n}^T \rrbracket \langle \boldsymbol{\zeta}^{T\bar{}} \mathbf{j}_{\mathbf{M}\nabla \mathbf{M}}(\mathbf{y}) \nabla \boldsymbol{\zeta} \rangle \, dS}_{\mathcal{I}_{22}}.
\end{aligned} \tag{C.111}$$

The first term of the right hand side of Eq. (C.111) is estimated by using the generalized Hölder inequality (2.25), the generalized Cauchy-Schwartz' inequality (2.27), the definition of  $C_y$  in Eq. (4.93), and the bound (4.131)

$$\begin{aligned}
|\mathcal{I}_{21}| &\leq \sum_e \left| \int_{\partial \Omega^e} \llbracket \delta \mathbf{M}_{h_n}^T \rrbracket (\boldsymbol{\zeta}^{T\bar{}} \mathbf{j}_{\mathbf{M}\mathbf{M}}(\mathbf{y}, \nabla \mathbf{y}) \boldsymbol{\zeta}) \, dS \right| \\
&\leq C_y \sum_e \left[ h_s^{\frac{1}{2}} \|\boldsymbol{\zeta}\|_{L^4(\partial \Omega^e)}^2 \left( h_s^{-\frac{1}{2}} \|\llbracket \delta \mathbf{M}_{h_n}^T \rrbracket\|_{L^2(\partial \Omega^e)} \right) \right] \\
&\leq C_y h_s^{\frac{1}{2}} \left( \sum_e \|\boldsymbol{\zeta}\|_{L^4(\partial \Omega^e)}^4 \right)^{\frac{1}{2}} \left( \sum_e h_s^{-1} \|\llbracket \delta \mathbf{M}_{h_n}^T \rrbracket\|_{L^2(\partial \Omega^e)}^2 \right)^{\frac{1}{2}} \\
&\leq C_y h_s^{\frac{1}{2}} C^k h_s^{-\frac{3}{2}} \sigma^2 \left( \sum_e h_s^{-1} \|\llbracket \delta \mathbf{M}_{h_n} \rrbracket\|_{L^2(\partial \Omega^e)}^2 \right)^{\frac{1}{2}} \\
&\leq C^k C_y \|\mathbf{M}^e\|_{H^s(\Omega_h)} h_s^{\mu-2-\varepsilon} \sigma \left( \sum_e h_s^{-1} \|\llbracket \delta \mathbf{M}_{h_n} \rrbracket\|_{L^2(\partial \Omega^e)}^2 \right)^{\frac{1}{2}}.
\end{aligned} \tag{C.112}$$

The second term of the right hand side of Eq. (C.111) is bounded by applying the generalized Hölder inequality (2.25), the generalized Cauchy-Schwartz' inequality (2.27), the definition

of  $C_y$  in Eq. (4.93), and the bounds (4.131, 4.133), yielding

$$\begin{aligned}
|\mathcal{I}_{22}| &\leq 2 \sum_e \left| \int_{\partial\Omega^e} \llbracket \delta \mathbf{M}_{\mathbf{h}_n}^T \rrbracket (\boldsymbol{\zeta}^T \bar{\mathbf{j}}_{\mathbf{M}\nabla\mathbf{M}}(\mathbf{y}) \nabla \boldsymbol{\zeta}) \, dS \right| \\
&\leq 2C_y \sum_e \left[ h_s^{\frac{1}{2}} \|\nabla \boldsymbol{\zeta}\|_{L^4(\partial\Omega^e)} \|\boldsymbol{\zeta}\|_{L^4(\partial\Omega^e)} \left( h_s^{-\frac{1}{2}} \|\llbracket \delta \mathbf{M}_{\mathbf{h}_n}^T \rrbracket\|_{L^2(\partial\Omega^e)} \right) \right] \\
&\leq 2C_y h_s^{\frac{1}{2}} \left( \sum_e \|\boldsymbol{\zeta}\|_{L^4(\partial\Omega^e)}^4 \right)^{\frac{1}{4}} \left( \sum_e \|\nabla \boldsymbol{\zeta}\|_{L^4(\partial\Omega^e)}^4 \right)^{\frac{1}{4}} \left( \sum_e h_s^{-1} \|\llbracket \delta \mathbf{M}_{\mathbf{h}_n}^T \rrbracket\|_{L^2(\partial\Omega^e)}^2 \right)^{\frac{1}{2}} \\
&\leq C_y h_s^{\frac{1}{2}} C^k h_s^{-\frac{3}{2}} \sigma^2 \left( \sum_e h_s^{-1} \|\llbracket \delta \mathbf{M}_{\mathbf{h}_n} \rrbracket\|_{L^2(\partial\Omega^e)}^2 \right)^{\frac{1}{2}} \\
&\leq C^k C_y \|\mathbf{M}^e\|_{H^s(\Omega_h)} h_s^{\mu-2-\varepsilon} \sigma \left( \sum_e h_s^{-1} \|\llbracket \delta \mathbf{M}_{\mathbf{h}_n} \rrbracket\|_{L^2(\partial\Omega^e)}^2 \right)^{\frac{1}{2}}.
\end{aligned} \tag{C.113}$$

We now substitute Eqs. (C.112, C.113) in Eq. (C.111), to obtain the final bound of the second term of  $\mathcal{N}(\mathbf{M}^e, \mathbf{y}; \delta \mathbf{M}_h)$  as

$$\begin{aligned}
|\mathcal{I}_2| &\leq C^k C_y \|\mathbf{M}^e\|_{H^s(\Omega_h)} h_s^{\mu-2-\varepsilon} \sigma \left( h_s^{-1} \sum_e \|\llbracket \delta \mathbf{M}_{\mathbf{h}_n}^T \rrbracket\|_{L^2(\partial\Omega^e)}^2 \right)^{\frac{1}{2}} \\
&\leq C^k C_M h_s^{\frac{1}{2}-\varepsilon} \sigma \left( \sum_e h_s^{-1} \|\llbracket \delta \mathbf{M}_{\mathbf{h}_n} \rrbracket\|_{L^2(\partial\Omega^e)}^2 \right)^{\frac{1}{2}} \text{ if } k \geq 2.
\end{aligned} \tag{C.114}$$

Furthermore, for the third term of  $\mathcal{N}(\mathbf{M}^e, \mathbf{y}; \delta \mathbf{M}_h)$  as decomposed in Eq. (4.101), using Taylor series (4.89-4.91), the generalized Hölder inequality (2.25), the generalized Cauchy-Schwartz' inequality (2.27), the definition of  $C_y$  in Eq. (4.93), and the bounds (4.131, 4.132),

leads to

$$\begin{aligned}
|\mathcal{I}_3| &= \left| \frac{1}{2} \sum_e \int_{\partial_1 \Omega^e} \left[ \mathbf{M}_n^{eT} - \mathbf{y}_n^T \right] \langle (\mathbf{j}_{\nabla \mathbf{M}}(\mathbf{M}^e) - \mathbf{j}_{\nabla \mathbf{M}}(\mathbf{y})) \nabla \delta \mathbf{M}_h \rangle dS \right| \\
&\leq \sum_e \left| \int_{\partial_1 \Omega^e} \left[ \zeta_n^T \right] (\zeta^T \bar{\mathbf{j}}_{\nabla \mathbf{M}}(\mathbf{y}) \nabla \delta \mathbf{M}_h) dS \right| \\
&\leq C_y \sum_e \left[ h_s^{-\frac{1}{2}} \|\llbracket \zeta \rrbracket\|_{L^4(\partial \Omega^e)} \|\zeta\|_{L^4(\partial \Omega^e)} \left( h_s \|\nabla \delta \mathbf{M}_h\|_{L^2(\partial \Omega^e)}^2 \right)^{\frac{1}{2}} \right] \\
&\leq C_y h_s^{-\frac{1}{2}} \left( \sum_e \|\llbracket \zeta \rrbracket\|_{L^4(\partial \Omega^e)}^4 \right)^{\frac{1}{4}} \left( \sum_e \|\zeta\|_{L^4(\partial \Omega^e)}^4 \right)^{\frac{1}{4}} \left( \sum_e h_s \|\nabla \delta \mathbf{M}_h\|_{L^2(\partial \Omega^e)}^2 \right)^{\frac{1}{2}} \\
&\leq C_y h_s^{-\frac{1}{2}} C^k h_s^{-\frac{3}{4}} \sigma h_s^{\frac{1}{4}} \left( \sum_e h_s \|\delta \mathbf{M}_h\|_{H^1(\partial \Omega^e)}^2 \right)^{\frac{1}{2}} \\
&\leq C_y C^k \|\mathbf{M}^e\|_{H^s(\Omega_h)} h_s^{\mu-2-\varepsilon} \sigma \left( \sum_e h_s \|\delta \mathbf{M}_h\|_{H^1(\partial \Omega^e)}^2 \right)^{\frac{1}{2}} \\
&\leq C^k C_y C_M h_s^{\frac{1}{2}-\varepsilon} \sigma \left( \sum_e h_s \|\delta \mathbf{M}_h\|_{H^1(\partial \Omega^e)}^2 \right)^{\frac{1}{2}} \quad \text{if } k \geq 2.
\end{aligned} \tag{C.115}$$

Likewise, the fourth term of  $\mathcal{N}(\mathbf{M}^e, \mathbf{y}; \delta \mathbf{M}_h)$  defined in Eq. (4.101) is bounded using Taylor series (4.89-4.91), the generalized Hölder inequality (2.25), the generalized Cauchy-Schwartz' inequality (2.27), the definition of  $C_y$  in Eq. (4.93), and the bounds (4.131, 4.132) leading to

$$\begin{aligned}
|\mathcal{I}_4| &\leq \left| \frac{1}{2} \sum_e \int_{\partial_1 \Omega^e} \left[ \mathbf{M}_n^{eT} - \mathbf{y}_n^T \right] \left\langle \frac{\mathcal{B}}{h_s} (\mathbf{j}_{\nabla \mathbf{M}}(\mathbf{M}^e) - \mathbf{j}_{\nabla \mathbf{M}}(\mathbf{y})) \right\rangle \llbracket \delta \mathbf{M}_{h_n} \rrbracket dS \right| \\
&\leq \sum_e \left| \int_{\partial_1 \Omega^e} \left[ \zeta_n^T \right] \left( \frac{\mathcal{B}}{h_s} \zeta^T \bar{\mathbf{j}}_{\nabla \mathbf{M}}(\mathbf{y}) \right) \llbracket \delta \mathbf{M}_{h_n} \rrbracket dS \right| \\
&\leq C_y \sum_e \left[ h_s^{-\frac{1}{2}} \|\llbracket \zeta \rrbracket\|_{L^4(\partial \Omega^e)} \|\zeta\|_{L^4(\partial \Omega^e)} \left( h_s^{-1} \|\llbracket \delta \mathbf{M}_{h_n} \rrbracket\|_{L^2(\partial \Omega^e)}^2 \right)^{\frac{1}{2}} \right] \\
&\leq C_y h_s^{-\frac{1}{2}} \left( \sum_e \|\llbracket \zeta \rrbracket\|_{L^4(\partial \Omega^e)}^4 \right)^{\frac{1}{4}} \left( \sum_e \|\zeta\|_{L^4(\partial \Omega^e)}^4 \right)^{\frac{1}{4}} \left( \sum_e h_s^{-1} \|\llbracket \delta \mathbf{M}_{h_n} \rrbracket\|_{L^2(\partial \Omega^e)}^2 \right)^{\frac{1}{2}} \\
&\leq C_y h_s^{-\frac{1}{2}} C^k h_s^{\frac{1}{4}} \sigma h_s^{-\frac{3}{4}} \left( \sum_e h_s^{-1} \|\llbracket \delta \mathbf{M}_{h_n} \rrbracket\|_{L^2(\partial \Omega^e)}^2 \right)^{\frac{1}{2}} \\
&\leq C^k C_y \|\mathbf{M}^e\|_{H^s(\Omega_h)} h_s^{\mu-2-\varepsilon} \sigma \left( \sum_e h_s^{-1} \|\llbracket \delta \mathbf{M}_{h_n} \rrbracket\|_{L^2(\partial \Omega^e)}^2 \right)^{\frac{1}{2}} \\
&\leq C^k C_y C_M h_s^{\frac{1}{2}-\varepsilon} \sigma \left( \sum_e h_s^{-1} \|\llbracket \delta \mathbf{M}_{h_n} \rrbracket\|_{L^2(\partial \Omega^e)}^2 \right)^{\frac{1}{2}} \quad \text{if } k \geq 2.
\end{aligned} \tag{C.116}$$

Combining all the terms of  $\mathcal{N}(\mathbf{M}^e, \mathbf{y}; \delta \mathbf{M}_h)$ , Eqs. (C.110, C.114, C.115, C.116), yields

$$|\mathcal{N}(\mathbf{M}^e, \mathbf{y}; \delta \mathbf{M}_h)| \leq C^k C_y \|\mathbf{M}^e\|_{H^s(\Omega_h)} h_s^{\mu-2-\varepsilon} \sigma \left[ \|\delta \mathbf{M}_h\|_{H^1(\Omega_h)} + \left( \sum_e h_s \|\delta \mathbf{M}_h\|_{H^1(\partial\Omega^e)}^2 \right)^{\frac{1}{2}} + \left( \sum_e h_s^{-1} \|\llbracket \delta \mathbf{M}_h \rrbracket\|_{L^2(\partial\Omega^e)}^2 \right)^{\frac{1}{2}} \right]. \quad (\text{C.117})$$

## C.9 The bound of $\mathcal{N}$ used for $L^2$ -norm convergence rate derivation

The purpose of this section is to derive the bound of the nonlinear term  $\mathcal{N}$ , which is needed for the error estimation in the  $L^2$ -norm.

### C.9.1 Intermediate bounds for the $L^2$ -norm

The bounds of some terms, which will be used in the following analysis, are first established in this Appendix.

First the term  $\|\boldsymbol{\zeta}\|_{L^2(\Omega^e)}$  is bounded by using its decomposition  $\boldsymbol{\zeta} = \boldsymbol{\eta} + \boldsymbol{\xi}$ , where  $\boldsymbol{\eta} = \mathbf{M}^e - \mathbf{I}_h \mathbf{M}$  and  $\boldsymbol{\xi} = \mathbf{I}_h \mathbf{M} - \mathbf{M}_h$ , which gives

$$\sum_e \|\boldsymbol{\zeta}\|_{L^2(\Omega^e)}^2 \leq 2 \left( \sum_e \|\boldsymbol{\eta}\|_{L^2(\Omega^e)}^2 + \sum_e \|\boldsymbol{\xi}\|_{L^2(\Omega^e)}^2 \right). \quad (\text{C.118})$$

Using the interpolation inequality (2.14), leads to

$$\sum_e \|\boldsymbol{\eta}\|_{L^2(\Omega^e)}^2 \leq C_D^{k^2} h_s^{2\mu} \sum_e \|\mathbf{M}^e\|_{H^s(\Omega^e)}^2. \quad (\text{C.119})$$

An application of the definition of the norm (2.12), Eq. (4.155), and Lemma 2.4.6, Eq. (2.23), gives

$$\begin{aligned} \sum_e \|\boldsymbol{\xi}\|_{L^2(\Omega^e)}^2 &\leq C_P^2 \|\boldsymbol{\xi}\|_1^2 \leq C_P^2 C^{k'^2} \|\mathbf{I}_h \mathbf{M} - \mathbf{M}^e\|_1^2 \\ &\leq C_P^2 C^{k''^2} h_s^{2\mu-2} \sum_e \|\mathbf{M}^e\|_{H^s(\Omega^e)}^2. \end{aligned} \quad (\text{C.120})$$

Combining Eqs. (C.119, C.120) leads to

$$\begin{aligned} \sum_e \|\boldsymbol{\zeta}\|_{L^2(\Omega^e)}^2 &\leq 2 \left( C_D^{k^2} + C_P^2 C^{k''^2} \right) h_s^{2\mu-2} \sum_e \|\mathbf{M}^e\|_{H^s(\Omega^e)}^2 \\ &\leq C^{k^2} h_s^{2\mu-2} \sum_e \|\mathbf{M}^e\|_{H^s(\Omega^e)}^2. \end{aligned} \quad (\text{C.121})$$

Similarly, one can get

$$\sum_e \|\zeta\|_{L^4(\Omega^e)}^4 \leq 4 \left( \sum_e \|\boldsymbol{\eta}\|_{L^4(\Omega^e)}^4 + \sum_e \|\boldsymbol{\xi}\|_{L^4(\Omega^e)}^4 \right). \quad (\text{C.122})$$

Using the interpolation inequality (2.14) leads to

$$\|\boldsymbol{\eta}\|_{L^4(\Omega^e)} \leq C_{\mathcal{D}}^k h_s^{\mu-\frac{1}{2}} \|\mathbf{M}^e\|_{H^s(\Omega^e)}. \quad (\text{C.123})$$

Next,  $\|\boldsymbol{\xi}\|_{L^4(\Omega^e)}^4$  is bounded by applying the inverse inequality (2.19), the definition of the norm (2.12), and the a priori error estimate (4.155-4.156), which yields

$$\begin{aligned} \sum_e \|\boldsymbol{\xi}\|_{L^4(\Omega^e)}^4 &\leq C_{\mathcal{I}}^{k^4} \left( \frac{1}{h_s} \right)^2 \sum_e \|\boldsymbol{\xi}\|_{L^2(\Omega^e)}^4 \leq C_{\mathcal{I}}^{k^4} \left( \frac{1}{h_s} \right)^2 \|\boldsymbol{\xi}\|_1^4 \\ &\leq C_{\mathcal{I}}^{k^4} (C^{k'})^4 h_s^{4\mu-6} \|\mathbf{M}^e\|_{H^s(\Omega_h)}^4. \end{aligned} \quad (\text{C.124})$$

Combining Eq. (C.123, C.124), gives for  $h_s$  small enough

$$\sum_e \|\zeta\|_{L^4(\Omega^e)}^4 \leq 4 \left( C_{\mathcal{D}}^{k^4} + C_{\mathcal{I}}^{k^4} (C^{k'})^4 \right) h_s^{4\mu-6} \|\mathbf{M}^e\|_{H^s(\Omega_h)}^4 \leq (C^{k''})^4 h_s^{4\mu-6} \|\mathbf{M}^e\|_{H^s(\Omega_h)}^4. \quad (\text{C.125})$$

By the same way  $\sum_e \|\nabla\zeta\|_{L^2(\Omega^e)}^2$  can be estimated by applying the interpolation inequality, Eq. (2.14), the definition of the norm (2.12), the a priori error estimate (4.155-4.156), as

$$\begin{aligned} \sum_e \|\nabla\zeta\|_{L^2(\Omega^e)}^2 &\leq 2 \left( \sum_e \|\nabla\boldsymbol{\eta}\|_{L^2(\Omega^e)}^2 + \sum_e \|\nabla\boldsymbol{\xi}\|_{L^2(\Omega^e)}^2 \right) \\ &\leq 2 \left( C_{\mathcal{D}}^{k^2} h_s^{2\mu-2} \sum_e \|\mathbf{M}_h\|_{H^s(\Omega^e)}^2 + (C^{k'})^2 \|\mathbf{I}_h\mathbf{M} - \mathbf{M}^e\|_1^2 \right) \\ &\leq 2 \left( C_{\mathcal{D}}^{k^2} h_s^{2\mu-2} \sum_e \|\mathbf{M}^e\|_{H^{\frac{5}{2}}(\Omega^e)}^2 + (C^{k'})^2 h_s^{2\mu-2} \sum_e \|\mathbf{M}^e\|_{H^s(\Omega^e)}^2 \right) \\ &\leq (C^{k''})^2 h_s^{2\mu-2} \sum_e \|\mathbf{M}^e\|_{H^s(\Omega^e)}^2. \end{aligned} \quad (\text{C.126})$$

Then, using the trace inequality (2.16) yields

$$\|\boldsymbol{\eta}\|_{L^4(\partial\Omega^e)}^4 \leq C_{\mathcal{T}} \left( h_s^{-1} \|\boldsymbol{\eta}\|_{L^4(\Omega^e)}^4 + \|\boldsymbol{\eta}\|_{L^6(\Omega^e)}^3 \|\nabla\boldsymbol{\eta}\|_{L^2(\Omega^e)} \right). \quad (\text{C.127})$$

Calling the interpolation inequality (2.14) gives

$$\|\boldsymbol{\eta}\|_{W_4^0(\Omega^e)}^4 \leq C_{\mathcal{D}}^{k^4} h_s^{4(\mu-\frac{1}{2})} \|\mathbf{M}^e\|_{H^s(\Omega^e)}^4, \quad \text{and} \quad (\text{C.128})$$

$$\|\boldsymbol{\eta}\|_{W_6^0(\Omega^e)}^3 \leq C_{\mathcal{D}}^{k^3} h_s^{3(\mu-\frac{2}{3})} \|\mathbf{M}^e\|_{H^s(\Omega^e)}^3. \quad (\text{C.129})$$

Also by the use of the interpolation inequality (2.13), one has

$$\| \nabla \boldsymbol{\eta} \|_{L^2(\Omega^e)} \leq \| \boldsymbol{\eta} \|_{H^1(\Omega^e)} \leq C_{\mathcal{D}}^k h_s^{\mu-1} \| \mathbf{M}^e \|_{H^s(\Omega^e)}. \quad (\text{C.130})$$

Combining the last three equations results into

$$\| \boldsymbol{\eta} \|_{L^4(\partial\Omega^e)} \leq C_{\mathcal{T}}^{\frac{1}{4}} C_{\mathcal{D}}^k h_s^{\mu-\frac{3}{4}} \| \mathbf{M}^e \|_{H^s(\Omega^e)}. \quad (\text{C.131})$$

Likewise, the bound of  $\| \nabla \boldsymbol{\eta} \|_{L^4(\partial\Omega^e)}^4$  is obtained by applying the trace inequality (2.16) and the interpolation inequality (2.14), leading to

$$\| \nabla \boldsymbol{\eta} \|_{L^4(\partial\Omega^e)}^4 \leq C_{\mathcal{T}} \left( h_s^{-1} \| \nabla \boldsymbol{\eta} \|_{L^4(\Omega^e)}^4 + \| \nabla \boldsymbol{\eta} \|_{L^6(\Omega^e)}^3 \| \nabla^2 \boldsymbol{\eta} \|_{L^2(\Omega^e)} \right), \quad (\text{C.132})$$

with

$$\| \boldsymbol{\eta} \|_{W_{4}^1(\Omega^e)}^4 \leq C_{\mathcal{D}}^{k^4} h_s^{4(\mu-\frac{3}{2})} \| \mathbf{M}^e \|_{H^s(\Omega^e)}^4, \quad (\text{C.133})$$

$$\| \boldsymbol{\eta} \|_{W_{6}^1(\Omega^e)}^3 \leq C_{\mathcal{D}}^{k^3} h_s^{3(\mu-\frac{5}{3})} \| \mathbf{M}^e \|_{H^s(\Omega^e)}^3, \quad (\text{C.134})$$

$$\| \nabla^2 \boldsymbol{\eta} \|_{L^2(\Omega^e)} \leq \| \boldsymbol{\eta} \|_{W_{2}^2(\Omega^e)} \leq C_{\mathcal{D}}^k h_s^{\mu-2} \| \mathbf{M}^e \|_{H^s(\Omega^e)}. \quad (\text{C.135})$$

Combining the last three equations gives

$$\| \nabla \boldsymbol{\eta} \|_{L^4(\partial\Omega^e)} \leq C_{\mathcal{T}}^{\frac{1}{4}} C_{\mathcal{D}}^k h_s^{\mu-\frac{7}{4}} \| \mathbf{M}^e \|_{H^s(\Omega^e)}. \quad (\text{C.136})$$

Next, the bound of  $\| \boldsymbol{\xi} \|_{L^4(\partial\Omega^e)}$  is estimated by applying the trace inequality (2.16) and the inverse inequalities (2.19, 2.21), leading to

$$\| \boldsymbol{\xi} \|_{L^4(\partial\Omega^e)}^4 \leq C_{\mathcal{T}} \left( h_s^{-1} \| \boldsymbol{\xi} \|_{L^4(\Omega^e)}^4 + \| \boldsymbol{\xi} \|_{L^6(\Omega^e)}^3 \| \nabla \boldsymbol{\xi} \|_{L^2(\Omega^e)} \right), \quad (\text{C.137})$$

with

$$\| \boldsymbol{\xi} \|_{L^4(\Omega^e)}^4 \leq C_{\mathcal{I}}^{k^4} h_s^{-2} \| \boldsymbol{\xi} \|_{L^2(\Omega^e)}^4, \quad (\text{C.138})$$

$$\| \boldsymbol{\xi} \|_{L^6(\Omega^e)}^3 \leq C_{\mathcal{I}}^{k^3} h_s^{-2} \| \boldsymbol{\xi} \|_{L^2(\Omega^e)}^3, \quad (\text{C.139})$$

$$\| \nabla \boldsymbol{\xi} \|_{L^2(\Omega^e)} \leq C_{\mathcal{I}}^k h_s^{-1} \| \boldsymbol{\xi} \|_{L^2(\Omega^e)}. \quad (\text{C.140})$$

Combining the last three equations, then applying the definition of the norm (2.12), the a priori error estimate (4.155-4.156), result into

$$\begin{aligned} \sum_e \| \boldsymbol{\xi} \|_{L^4(\partial\Omega^e)}^4 &\leq C_{\mathcal{T}} C_{\mathcal{I}}^{k^4} h_s^{-3} \sum_e \| \boldsymbol{\xi} \|_{L^2(\Omega^e)}^4 \leq C_{\mathcal{T}} C_{\mathcal{I}}^{k^4} C_{\mathcal{P}}^4 h_s^{-3} \| \boldsymbol{\xi} \|_1^4 \\ &\leq C_{\mathcal{T}} C_{\mathcal{I}}^{k^4} C_{\mathcal{P}}^4 (C^{k'})^4 h_s^{-3} \| \mathbf{I}_h \mathbf{M} - \mathbf{M}^e \|_1^4 \\ &\leq C_{\mathcal{T}} C_{\mathcal{I}}^{k^4} C_{\mathcal{P}}^4 (C^{k'})^4 h_s^{4\mu-7} \| \mathbf{M}^e \|_{H^s(\Omega_h)}^4 \\ &\leq C^{k''^4} h_s^{4\mu-7} \| \mathbf{M}^e \|_{H^s(\Omega_h)}^4. \end{aligned} \quad (\text{C.141})$$

Then, using the inverse inequality (2.20), Lemma 2.4.3, Eq. (2.18), the definition of the norm, Eq. (2.12), and the a priori error estimate (4.155-4.156), yields

$$\begin{aligned} \sum_e \|\nabla \boldsymbol{\xi}\|_{L^4(\partial\Omega^e)}^4 &\leq C_{\mathcal{I}}^{k^4} h_s^{-1} \sum_e \|\nabla \boldsymbol{\xi}\|_{L^2(\partial\Omega^e)}^4 \leq C_{\mathcal{I}}^{k^4} C_{\mathcal{K}}^{k^4} h_s^{-3} \sum_e \|\nabla \boldsymbol{\xi}\|_{L^2(\Omega^e)}^4 \\ &\leq C_{\mathcal{I}}^{k^4} C_{\mathcal{K}}^{k^4} h_s^{-3} \|\boldsymbol{\xi}\|_1^4 \leq (C^{k'})^4 C_{\mathcal{I}}^{k^4} C_{\mathcal{K}}^{k^4} h_s^{-3} \|\mathbf{I}_h \mathbf{M} - \mathbf{M}^e\|_1^4 \\ &\leq (C^{k'})^4 C_{\mathcal{I}}^{k^4} C_{\mathcal{K}}^{k^4} h_s^{4\mu-7} \|\mathbf{M}^e\|_{H^s(\Omega_h)}^4. \end{aligned} \quad (\text{C.142})$$

Using these last result,  $\|\boldsymbol{\zeta}\|_{L^4(\partial\Omega^e)}$  can be bounded by the dominant of its component as

$$\begin{aligned} \sum_e \|\boldsymbol{\zeta}\|_{L^4(\partial\Omega^e)}^4 &\leq 4(C_{\mathcal{T}} C_{\mathcal{D}}^{k^4} h_s^{4\mu-3} + C_{\mathcal{T}} C_{\mathcal{I}}^{k^4} C_{\mathcal{P}}^4 (C^{k'})^4 h_s^{4\mu-7}) \|\mathbf{M}^e\|_{H^s(\Omega_h)}^4 \\ &\leq (C^{k''})^4 h_s^{4\mu-7} \|\mathbf{M}^e\|_{H^s(\Omega_h)}^4, \end{aligned} \quad (\text{C.143})$$

and similarly for the bound of  $\|\nabla \boldsymbol{\zeta}\|_{L^4(\partial\Omega^e)}$  by

$$\begin{aligned} \sum_e \|\nabla \boldsymbol{\zeta}\|_{L^4(\partial\Omega^e)}^4 &\leq 4(C_{\mathcal{T}} C_{\mathcal{D}}^{k^4} + (C^{k'})^4 C_{\mathcal{I}}^{k^4} C_{\mathcal{K}}^{k^4}) h_s^{4\mu-7} \|\mathbf{M}^e\|_{H^s(\Omega_h)}^4 \\ &\leq (C^{k''})^4 h_s^{4\mu-7} \|\mathbf{M}^e\|_{H^s(\Omega_h)}^4. \end{aligned} \quad (\text{C.144})$$

Now the bound of  $\|\llbracket \boldsymbol{\zeta} \rrbracket\|_{L^4(\partial\Omega^e)}$  can be computed as

$$\sum_e \|\llbracket \boldsymbol{\zeta} \rrbracket\|_{L^4(\partial\Omega^e)}^4 \leq 4 \left( \sum_e \|\llbracket \boldsymbol{\eta} \rrbracket\|_{L^4(\partial\Omega^e)}^4 + \sum_e \|\llbracket \boldsymbol{\xi} \rrbracket\|_{L^4(\partial\Omega^e)}^4 \right). \quad (\text{C.145})$$

Using Eq. (C.131), we have

$$\sum_e \|\llbracket \boldsymbol{\eta} \rrbracket\|_{L^4(\partial\Omega^e)}^4 \leq 2 \sum_e \|\boldsymbol{\eta}\|_{L^4(\partial\Omega^e)}^4 \leq C_{\mathcal{T}} C_{\mathcal{D}}^{k^4} h_s^{4\mu-3} \|\mathbf{M}^e\|_{H^s(\Omega^e)}^4. \quad (\text{C.146})$$

Then, applying the inverse inequality (2.20), the definition of the norm (2.12), and the a priori error estimate (4.155-4.156), yields

$$\begin{aligned} \sum_e \|\llbracket \boldsymbol{\xi} \rrbracket\|_{L^4(\partial\Omega^e)}^4 &\leq C_{\mathcal{I}}^{k^4} h_s^{-1} \sum_e \|\llbracket \boldsymbol{\xi} \rrbracket\|_{L^2(\partial\Omega^e)}^4 \leq C_{\mathcal{I}}^{k^4} h_s \sum_e \|h_s^{-\frac{1}{2}} \llbracket \boldsymbol{\xi} \rrbracket\|_{L^2(\partial\Omega^e)}^4 \\ &\leq C_{\mathcal{I}}^{k^4} h_s \|\boldsymbol{\xi}\|_1^4 \leq C_{\mathcal{I}}^{k^4} h_s \|\mathbf{I}_h \mathbf{M} - \mathbf{M}^e\|_1^4 \\ &\leq C_{\mathcal{I}}^{k^4} (C^{k'})^4 h_s^{4\mu-3} \|\mathbf{M}^e\|_{H^s(\Omega_h)}^4. \end{aligned} \quad (\text{C.147})$$

Combining Eqs. (C.146) and (C.147), gives

$$\sum_e \|\llbracket \boldsymbol{\zeta} \rrbracket\|_{L^4(\partial\Omega^e)}^4 \leq (C^{k''})^4 h_s^{4\mu-3} \|\mathbf{M}^e\|_{H^s(\Omega_h)}^4. \quad (\text{C.148})$$

Finally, by the use of the inverse inequality (2.19), we directly deduce

$$\|\mathbf{I}_h \boldsymbol{\psi}\|_{L^4(\Omega^e)} \leq C_{\mathcal{I}}^k h_s^{-\frac{1}{2}} \|\mathbf{I}_h \boldsymbol{\psi}\|_{L^2(\Omega^e)}, \quad (\text{C.149})$$

$$\| \nabla \mathbf{I}_h \boldsymbol{\psi} \|_{L^4(\Omega^e)} \leq C_{\mathcal{I}}^k h_s^{-\frac{1}{2}} \| \nabla \mathbf{I}_h \boldsymbol{\psi} \|_{L^2(\Omega^e)}, \quad (\text{C.150})$$

which implies

$$\begin{cases} | \mathbf{I}_h \boldsymbol{\psi} |_{W_4^1(\Omega^e)} & \leq C_{\mathcal{I}}^k h_s^{-\frac{1}{2}} | \mathbf{I}_h \boldsymbol{\psi} |_{H^1(\Omega^e)}, \\ \| \mathbf{I}_h \boldsymbol{\psi} \|_{W_4^1(\Omega^e)} & \leq C_{\mathcal{I}}^k h_s^{-\frac{1}{2}} \| \mathbf{I}_h \boldsymbol{\psi} \|_{H^1(\Omega^e)}. \end{cases} \quad (\text{C.151})$$

### C.9.2 Bound of $\mathcal{N}(\mathbf{M}^e, \mathbf{M}_h; \mathbf{I}_h \boldsymbol{\psi})$

The first term of  $\mathcal{N}(\mathbf{M}^e, \mathbf{M}_h; \mathbf{I}_h \boldsymbol{\psi})$ , developed in Eq. (4.101), can now be expanded using Eq. (4.91) as

$$\begin{aligned} \mathcal{I}_1 &= \int_{\Omega_h} \nabla \mathbf{I}_h \boldsymbol{\psi}^T \bar{\mathbf{R}}_j(\boldsymbol{\zeta}, \nabla \boldsymbol{\zeta}) d\Omega = \sum_e \int_{\Omega^e} \nabla \mathbf{I}_h \boldsymbol{\psi}^T (\boldsymbol{\zeta}^T \bar{\mathbf{J}}_{\mathbf{M}\mathbf{M}}(\mathbf{M}_h, \nabla \mathbf{M}_h) \boldsymbol{\zeta}) d\Omega \\ &\quad + 2 \sum_e \int_{\Omega^e} \nabla \mathbf{I}_h \boldsymbol{\psi}^T (\boldsymbol{\zeta}^T \bar{\mathbf{J}}_{\mathbf{M}\nabla \mathbf{M}}(\mathbf{M}_h) \nabla \boldsymbol{\zeta}) d\Omega \quad (\text{C.152}) \\ &= \mathcal{I}_{11} + \mathcal{I}_{12}, \end{aligned}$$

with  $\boldsymbol{\zeta} = \mathbf{M}^e - \mathbf{M}_h$ .

The first term of the right hand side of Eq. (C.152) is bounded using the generalized Hölder's inequality (2.25), the generalized Cauchy Schwartz' inequality (2.27), the definition of  $C_y$  in Eq. (4.93), and Eqs. (C.121, C.125, C.151)

$$\begin{aligned} | \mathcal{I}_{11} | &= \left| \sum_e \int_{\Omega^e} \nabla \mathbf{I}_h \boldsymbol{\psi}^T (\boldsymbol{\zeta}^T \bar{\mathbf{J}}_{\mathbf{M}\mathbf{M}}(\mathbf{M}_h, \nabla \mathbf{M}_h) \boldsymbol{\zeta}) d\Omega \right| \\ &\leq C_y \sum_e \| \boldsymbol{\zeta} \|_{L^4(\Omega^e)} \| \boldsymbol{\zeta} \|_{L^2(\Omega^e)} \| \nabla \mathbf{I}_h \boldsymbol{\psi} \|_{L^4(\Omega^e)} \\ &\leq C_y \left( \sum_e \| \boldsymbol{\zeta} \|_{L^4(\Omega^e)}^4 \right)^{\frac{1}{4}} \left( \sum_e \| \boldsymbol{\zeta} \|_{L^2(\Omega^e)}^2 \right)^{\frac{1}{2}} \left( \sum_e \| \nabla \mathbf{I}_h \boldsymbol{\psi} \|_{L^4(\Omega^e)}^4 \right)^{\frac{1}{4}} \quad (\text{C.153}) \\ &\leq C^{k''} C_y \| \mathbf{M}^e \|_{H^s(\Omega_h)}^2 h_s^{2\mu-3} | \mathbf{I}_h \boldsymbol{\psi} |_{H^1(\Omega_h)}. \end{aligned}$$

For the second term of the right hand side of Eq. (C.152), the generalized Hölder's inequality (2.25), the generalized Cauchy Schwartz' inequality (2.27), and Eqs. (C.125, C.126, C.150), imply that

$$\begin{aligned} | \mathcal{I}_{12} | &= \left| \sum_e \int_{\Omega^e} \nabla \mathbf{I}_h \boldsymbol{\psi}^T (\boldsymbol{\zeta}^T \bar{\mathbf{J}}_{\mathbf{M}\nabla \mathbf{M}}(\mathbf{M}_h) \nabla \boldsymbol{\zeta}) d\Omega \right| \\ &\leq C_y \sum_e \| \boldsymbol{\zeta} \|_{L^4(\Omega^e)} \| \nabla \boldsymbol{\zeta} \|_{L^2(\Omega^e)} \| \nabla \mathbf{I}_h \boldsymbol{\psi} \|_{L^4(\Omega^e)} \\ &\leq C_y \left( \sum_e \| \boldsymbol{\zeta} \|_{L^4(\Omega^e)}^4 \right)^{\frac{1}{4}} \left( \sum_e \| \nabla \boldsymbol{\zeta} \|_{L^2(\Omega^e)}^2 \right)^{\frac{1}{2}} \left( \sum_e \| \nabla \mathbf{I}_h \boldsymbol{\psi} \|_{L^4(\Omega_h)}^4 \right)^{\frac{1}{4}} \quad (\text{C.154}) \\ &\leq C^{k''} C_y \| \mathbf{M}^e \|_{H^s(\Omega_h)}^2 h_s^{2\mu-3} | \mathbf{I}_h \boldsymbol{\psi} |_{H^1(\Omega_h)}. \end{aligned}$$



Combining the above results, we have that

$$|\mathcal{I}_1| \leq C^{k''} C_y \|\mathbf{M}^e\|_{\mathbf{H}^s(\Omega_h)}^2 h_s^{2\mu-3} \|\mathbf{I}_h \boldsymbol{\psi}\|_{\mathbf{H}^1(\Omega_h)}. \quad (\text{C.155})$$

The second term of Eq. (4.101) can be expanded by the use of Eq. (4.91) as:

$$\begin{aligned} \mathcal{I}_2 &= \int_{\partial_1 \Omega_h \cup \partial_D \Omega_h} \llbracket \mathbf{I}_h \boldsymbol{\psi}_n^T \rrbracket \langle \bar{\mathbf{R}}_j(\boldsymbol{\zeta}, \nabla \boldsymbol{\zeta}) \rangle \, dS = \\ &\underbrace{\frac{1}{2} \sum_e \int_{\partial_1 \Omega^e} \llbracket \mathbf{I}_h \boldsymbol{\psi}_n^T \rrbracket \langle \boldsymbol{\zeta}^T \bar{\mathbf{j}}_{\mathbf{M}\mathbf{M}}(\mathbf{M}_h, \nabla \mathbf{M}_h) \boldsymbol{\zeta} \rangle \, dS + \sum_e \int_{\partial_D \Omega^e} \llbracket \mathbf{I}_h \boldsymbol{\psi}_n^T \rrbracket \langle \boldsymbol{\zeta}^T \bar{\mathbf{j}}_{\mathbf{M}\mathbf{M}}(\mathbf{M}_h, \nabla \mathbf{M}_h) \boldsymbol{\zeta} \rangle \, dS}_{\mathcal{I}_{21}} \\ &+ \underbrace{\sum_e \int_{\partial_1 \Omega^e} \llbracket \mathbf{I}_h \boldsymbol{\psi}_n^T \rrbracket \langle \boldsymbol{\zeta}^T \bar{\mathbf{j}}_{\mathbf{M}\nabla \mathbf{M}}(\mathbf{M}_h) \nabla \boldsymbol{\zeta} \rangle \, dS + 2 \sum_e \int_{\partial_D \Omega^e} \llbracket \mathbf{I}_h \boldsymbol{\psi}_n^T \rrbracket \langle \boldsymbol{\zeta}^T \bar{\mathbf{j}}_{\mathbf{M}\nabla \mathbf{M}}(\mathbf{M}_h) \nabla \boldsymbol{\zeta} \rangle \, dS}_{\mathcal{I}_{22}}. \end{aligned} \quad (\text{C.156})$$

The first term of the right hand side of Eq. (C.156) is estimated by using the Hölder's inequality (2.25), the generalized Cauchy Schwartz' inequality (2.27), the definition of  $C_y$  in Eq. (4.93), and Eq. (C.143), leading to

$$\begin{aligned} |\mathcal{I}_{21}| &\leq \sum_e \left| \int_{\partial \Omega^e} \llbracket \mathbf{I}_h \boldsymbol{\psi}_n^T \rrbracket (\boldsymbol{\zeta}^T \bar{\mathbf{j}}_{\mathbf{M}\mathbf{M}}(\mathbf{M}_h, \nabla \mathbf{M}_h) \boldsymbol{\zeta}) \, dS \right| \\ &\leq C_y \sum_e \left[ h_s^{\frac{1}{2}} \|\boldsymbol{\zeta}\|_{L^4(\partial \Omega^e)} \left( h_s^{-\frac{1}{2}} \|\llbracket \mathbf{I}_h \boldsymbol{\psi}_n^T \rrbracket\|_{L^2(\partial \Omega^e)} \right) \right] \\ &\leq C^{k''} C_y \|\mathbf{M}^e\|_{\mathbf{H}^s(\Omega_h)}^2 h_s^{\frac{1}{2}} h_s^{2\mu-\frac{7}{2}} \left( \sum_e h_s^{-1} \|\llbracket \mathbf{I}_h \boldsymbol{\psi}_n \rrbracket\|_{L^2(\partial \Omega^e)}^2 \right)^{\frac{1}{2}} \\ &\leq C^{k''} C_y \|\mathbf{M}^e\|_{\mathbf{H}^s(\Omega_h)}^2 h_s^{2\mu-3} \left( \sum_e h_s^{-1} \|\llbracket \mathbf{I}_h \boldsymbol{\psi}_n \rrbracket\|_{L^2(\partial \Omega^e)}^2 \right)^{\frac{1}{2}}. \end{aligned} \quad (\text{C.157})$$

Now, applying the Hölder's inequality (2.25), the generalized Cauchy Schwartz' inequality (2.27), Eq. (4.93), and Eqs. (C.143, C.144), the second term of the right hand side of Eq. (C.156) is bounded by

$$\begin{aligned} |\mathcal{I}_{22}| &\leq \sum_e \left| 2 \int_{\partial \Omega^e} \llbracket \mathbf{I}_h \boldsymbol{\psi}_n^T \rrbracket (\boldsymbol{\zeta}^T \bar{\mathbf{j}}_{\mathbf{M}\nabla \mathbf{M}}(\mathbf{M}_h) \nabla \boldsymbol{\zeta}) \, dS \right| \\ &\leq 2C_y \sum_e \left[ h_s^{\frac{1}{2}} \|\boldsymbol{\zeta}\|_{L^4(\partial \Omega^e)} \|\nabla \boldsymbol{\zeta}\|_{L^4(\partial \Omega^e)} \left( h_s^{-\frac{1}{2}} \|\llbracket \mathbf{I}_h \boldsymbol{\psi}_n^T \rrbracket\|_{L^2(\partial \Omega^e)} \right) \right] \\ &\leq C^{k''} C_y \|\mathbf{M}^e\|_{\mathbf{H}^s(\Omega_h)}^2 h_s^{\frac{1}{2}} h_s^{2\mu-\frac{7}{2}} \left( \sum_e h_s^{-1} \|\llbracket \mathbf{I}_h \boldsymbol{\psi}_n \rrbracket\|_{L^2(\partial \Omega^e)}^2 \right)^{\frac{1}{2}} \\ &\leq C^{k''} C_y \|\mathbf{M}^e\|_{\mathbf{H}^s(\Omega_h)}^2 h_s^{2\mu-3} \left( \sum_e h_s^{-1} \|\llbracket \mathbf{I}_h \boldsymbol{\psi}_n \rrbracket\|_{L^2(\partial \Omega^e)}^2 \right)^{\frac{1}{2}}. \end{aligned} \quad (\text{C.158})$$

By combining Eqs. (C.157) and Eq. (C.158), we have

$$|\mathcal{I}_2| \leq C^{k''} C_y \|\mathbf{M}^e\|_{\mathbf{H}^s(\Omega_h)}^2 h_s^{2\mu-3} \left( \sum_e h_s^{-1} \|\llbracket \mathbf{I}_h \boldsymbol{\psi}_n \rrbracket\|_{L^2(\partial\Omega^e)}^2 \right)^{\frac{1}{2}}. \quad (\text{C.159})$$

Furthermore, for the third term of  $\mathcal{N}(\mathbf{M}^e, \mathbf{M}_h; \mathbf{I}_h \boldsymbol{\psi})$ , Eq. (4.101), employing Taylor series, Eqs. (4.89-4.91), the generalized Hölder's inequality (2.25), the generalized Cauchy Schwartz (2.27), the definition of  $C_y$  in Eq. (4.93), and Eqs. (C.143, C.148), leads to

$$\begin{aligned} |\mathcal{I}_3| &= \left| \frac{1}{2} \sum_e \int_{\partial\Omega^e} \llbracket \mathbf{M}_n^{eT} - \mathbf{M}_{n_h}^T \rrbracket \langle (\mathbf{j}_{\nabla \mathbf{M}}(\mathbf{M}_h) - \mathbf{j}_{\nabla \mathbf{M}}(\mathbf{M}_h)) \nabla \mathbf{I}_h \boldsymbol{\psi} \rangle dS \right| \\ &\leq \sum_e \int_{\partial\Omega^e} | \llbracket \boldsymbol{\zeta}_n^T \rrbracket | | (\boldsymbol{\zeta}^T \bar{\mathbf{j}}_{\nabla \mathbf{M}}(\mathbf{M}_h) \nabla \mathbf{I}_h \boldsymbol{\psi}) | dS \\ &\leq C_y \sum_e h_s^{-\frac{1}{2}} \| \llbracket \boldsymbol{\zeta} \rrbracket \|_{L^4(\partial\Omega^e)} \| \boldsymbol{\zeta} \|_{L^4(\partial\Omega^e)} \left( h_s^{\frac{1}{2}} \| \nabla \mathbf{I}_h \boldsymbol{\psi} \|_{L^2(\partial\Omega^e)} \right) \\ &\leq C_y h_s^{-\frac{1}{2}} \left( \sum_e \| \llbracket \boldsymbol{\zeta} \rrbracket \|_{L^4(\partial\Omega^e)}^4 \right)^{\frac{1}{4}} \left( \sum_e \| \boldsymbol{\zeta} \|_{L^4(\partial\Omega^e)}^4 \right)^{\frac{1}{4}} \left( \sum_e h_s \| \nabla \mathbf{I}_h \boldsymbol{\psi} \|_{L^2(\partial\Omega^e)}^2 \right)^{\frac{1}{2}} \\ &\leq C^{k''} C_y \|\mathbf{M}^e\|_{\mathbf{H}^s(\Omega_h)}^2 h_s^{2\mu-3} \left( \sum_e h_s \| \mathbf{I}_h \boldsymbol{\psi} \|_{H^1(\partial\Omega^e)}^2 \right)^{\frac{1}{2}}. \end{aligned} \quad (\text{C.160})$$

Likewise, the fourth term of  $\mathcal{N}(\mathbf{M}^e, \mathbf{M}_h; \mathbf{I}_h \boldsymbol{\psi})$ , Eq. (4.101) is bounded using Taylor series, Eqs. (4.89-4.91), the generalized Hölder's inequality, the generalized Cauchy Schwartz' inequality (2.27), the definition of  $C_y$  in Eq. (4.93) and Eqs. (C.143, C.148) as

$$\begin{aligned} |\mathcal{I}_4| &= \left| \frac{1}{2} \sum_e \int_{\partial\Omega^e} \llbracket \mathbf{M}_n^{eT} - \mathbf{M}_{n_h}^T \rrbracket \left\langle \frac{\mathcal{B}}{h_s} (\mathbf{j}_{\nabla \mathbf{M}}(\mathbf{M}_h) - \mathbf{j}_{\nabla \mathbf{M}}(\mathbf{M}_h)) \right\rangle \llbracket \mathbf{I}_h \boldsymbol{\psi}_n \rrbracket dS \right| \\ &\leq \sum_e \int_{\partial\Omega^e} | \llbracket \boldsymbol{\zeta}_n^T \rrbracket | | \frac{\mathcal{B}}{h_s} \boldsymbol{\zeta}^T \bar{\mathbf{j}}_{\nabla \mathbf{M}}(\mathbf{M}_h) | | \llbracket \mathbf{I}_h \boldsymbol{\psi}_n \rrbracket | dS \\ &\leq C_y \sum_e h_s^{-\frac{1}{2}} \| \llbracket \boldsymbol{\zeta} \rrbracket \|_{L^4(\partial\Omega^e)} \| \boldsymbol{\zeta} \|_{L^4(\partial\Omega^e)} \left( h_s^{-\frac{1}{2}} \| \llbracket \mathbf{I}_h \boldsymbol{\psi}_n \rrbracket \|_{L(\partial\Omega^e)} \right) \\ &\leq C_y h_s^{-\frac{1}{2}} \left( \sum_e \| \llbracket \boldsymbol{\zeta} \rrbracket \|_{L^4(\partial\Omega^e)}^4 \right)^{\frac{1}{4}} \left( \sum_e \| \boldsymbol{\zeta} \|_{L^4(\partial\Omega^e)}^4 \right)^{\frac{1}{4}} \left( \sum_e h_s^{-1} \| \llbracket \mathbf{I}_h \boldsymbol{\psi}_n \rrbracket \|_{L^2(\partial\Omega^e)}^2 \right)^{\frac{1}{2}} \\ &\leq C^{k''} C_y \|\mathbf{M}^e\|_{\mathbf{H}^s(\Omega_h)}^2 h_s^{2\mu-3} \left( \sum_e h_s^{-1} \| \llbracket \mathbf{I}_h \boldsymbol{\psi}_n \rrbracket \|_{L^2(\partial\Omega^e)}^2 \right)^{\frac{1}{2}}. \end{aligned} \quad (\text{C.161})$$

By combining all the terms of  $\mathcal{N}(\mathbf{M}^e, \mathbf{M}_h; \mathbf{I}_h \boldsymbol{\psi})$ , Eqs. (C.155, C.159, C.160, C.161), we

have

$$\begin{aligned}
|\mathcal{N}(\mathbf{M}^e, \mathbf{M}_h; \mathbf{I}_h \boldsymbol{\psi})| &\leq C^{k''} C_y \|\mathbf{M}^e\|_{\mathbb{H}^s(\Omega_h)}^2 h_s^{2\mu-3} \left( |\mathbf{I}_h \boldsymbol{\psi}|_{H^1(\Omega_h)} + \left( \sum_e h_s |\mathbf{I}_h \boldsymbol{\psi}|_{H^1(\partial\Omega^e)}^2 \right)^{\frac{1}{2}} \right. \\
&\quad \left. + \left( \sum_e h_s^{-1} \|\llbracket \mathbf{I}_h \boldsymbol{\psi}_n \rrbracket\|_{L^2(\partial\Omega^e)}^2 \right)^{\frac{1}{2}} \right). \tag{C.162}
\end{aligned}$$

Moreover, using the definition of the energy norm Eq. (2.12), there exists a positive constant independent of  $h_s$ , such that

$$|\mathcal{N}(\mathbf{M}^e, \mathbf{M}_h; \mathbf{I}_h \boldsymbol{\psi})| \leq C^{k''} C_y \|\mathbf{M}^e\|_{\mathbb{H}^s(\Omega_h)}^2 h_s^{2\mu-3} \|\mathbf{I}_h \boldsymbol{\psi}\|_1, \tag{C.163}$$

or again using Eq. (2.22)

$$|\mathcal{N}(\mathbf{M}^e, \mathbf{M}_h; \mathbf{I}_h \boldsymbol{\psi})| \leq C^{k''} C_y \|\mathbf{M}^e\|_{\mathbb{H}^s(\Omega_h)}^2 h_s^{2\mu-3} \|\mathbf{I}_h \boldsymbol{\psi}\|. \tag{C.164}$$



# Appendix D

## Annexes related to chapter 5

### D.1 Stiffness matrix for Electro-Thermo-Mechanical coupling

The stiffness matrix, has been decomposed into nine sub-matrices with respect to the discretization of the five independent fields variables (3 for displacement  $\mathbf{u}$ , one for  $f_V$  and one for  $f_T$ ).

#### D.1.1 Expression of the force derivations

First  $\mathbf{K}_{\mathbf{uu}}$  is the derivative of the displacement contributions with respect to  $\mathbf{u}$ , is obtained from Eq. (5.65)

$$\begin{aligned} \frac{\partial \mathbf{F}_{\mathbf{u}|\mathbf{I}}^{\mathbf{a}}}{\partial \mathbf{u}^{\mathbf{b}}} &= \sum_e \int_{\Omega_0^e} \frac{\partial \mathbf{P}}{\partial \mathbf{u}^{\mathbf{b}}} \cdot \nabla_0 N_{\mathbf{u}}^{\mathbf{a}} d\Omega_0 \\ &= \sum_e \int_{\Omega_0^e} \nabla_0 N_{\mathbf{u}}^{\mathbf{a}} \cdot^2 \mathbf{C} \cdot^4 \nabla_0 N_{\mathbf{u}}^{\mathbf{b}} d\Omega_0, \end{aligned} \quad (\text{D.1})$$

where  $\mathbf{C} = \frac{\partial \mathbf{P}}{\partial \mathbf{F}}$ , and  $\cdot^2$  and  $\cdot^4$  mean to apply the contraction on the second and fourth component of  $\mathbf{C}$ .

Similarly, for the interface contribution<sup>1</sup>, from Eq. (5.67, 5.68 and 5.69) one can get

$$\frac{\partial \mathbf{F}_{\mathbf{u}|\mathbf{I}}^{\mathbf{a}\pm}}{\partial \mathbf{u}^{\mathbf{b}\pm}} = \frac{1}{2} \sum_s \int_{(\partial_1 \Omega_0)^s} (\pm N_{\mathbf{u}}^{\mathbf{a}\pm}) \mathbf{N}^- \cdot^2 \mathbf{C}^{\pm} \cdot^4 \nabla_0 N_{\mathbf{u}}^{\mathbf{b}\pm} dS_0, \quad (\text{D.2})$$

$$\frac{\partial \mathbf{F}_{\mathbf{u}|\mathbf{I}}^{\mathbf{a}\pm}}{\partial \mathbf{u}^{\mathbf{b}\pm}} = \frac{1}{2} \sum_s \int_{(\partial_1 \Omega_0)^s} (\pm N_{\mathbf{u}}^{\mathbf{b}\pm}) \mathbf{N}^- \cdot^2 \mathbf{H}^{\pm} \cdot^4 \nabla_0 N_{\mathbf{u}}^{\mathbf{a}\pm} dS_0, \quad (\text{D.3})$$

$$\frac{\partial \mathbf{F}_{\mathbf{u}|\mathbf{I}}^{\mathbf{a}\pm}}{\partial \mathbf{u}^{\mathbf{b}\pm}} = \sum_s \int_{(\partial_1 \Omega_0)^s} (\pm N_{\mathbf{u}}^{\mathbf{b}\pm}) \mathbf{N}^- \cdot^2 \left\langle \frac{\mathcal{H}\mathcal{B}}{h_s} \right\rangle \cdot^4 \mathbf{N}^- (\pm N_{\mathbf{u}}^{\mathbf{a}\pm}) dS_0. \quad (\text{D.4})$$

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<sup>1</sup>The contributions on  $\partial_D \Omega_h$  can be directly deduced by removing the factor (1/2) accordingly to the definition of the average flux on the Dirichlet boundary.

Then stiffness matrix  $\mathbb{K}_{\mathbf{u}f_V}$  corresponding to the forces for the mechanical part with respect to  $f_V$  and reads

$$\frac{\partial \mathbf{F}_{\mathbf{u}int}^a}{\partial f_V^b} = \sum_e \int_{\Omega_0^e} \nabla_0 N_{\mathbf{u}}^a \cdot \frac{\partial \mathbf{P}}{\partial f_V} N_{f_V}^b d\Omega_0, \quad (D.5)$$

$$\frac{\partial \mathbf{F}_{\mathbf{u}I1}^{a\pm}}{\partial f_V^{b\pm}} = \frac{1}{2} \sum_s \int_{(\partial_I \Omega_0)^s} (\pm N_{\mathbf{u}}^{a\pm}) \frac{\partial \mathbf{P}^{\pm}}{\partial f_V^{\pm}} \cdot \mathbf{N}^- N_{f_V}^{b\pm} dS_0. \quad (D.6)$$

The stiffness matrix corresponding to the forces for the mechanical part with respect to  $f_T$  is  $\mathbb{K}_{\mathbf{u}f_T}$ <sup>2</sup> and reads

$$\frac{\partial \mathbf{F}_{\mathbf{u}int}^a}{\partial f_T^b} = \sum_e \int_{\Omega_0^e} \nabla_0 N_{\mathbf{u}}^a \cdot \frac{\partial \mathbf{P}}{\partial f_T} N_{f_T}^b d\Omega_0, \quad (D.7)$$

$$\frac{\partial \mathbf{F}_{\mathbf{u}I1}^{a\pm}}{\partial f_T^{b\pm}} = \frac{1}{2} \sum_s \int_{(\partial_I \Omega_0)^s} (\pm N_{\mathbf{u}}^{a\pm}) \frac{\partial \mathbf{P}^{\pm}}{\partial f_T^{\pm}} \cdot \mathbf{N}^- N_{f_T}^{b\pm} dS_0. \quad (D.8)$$

Secondly, the derivative of the electrical contributions with respect to the displacement  $\mathbf{u}$  is  $\mathbb{K}_{f_V \mathbf{u}}$  and derives from Eqs. (5.70, 5.71)

$$\begin{aligned} \frac{\partial F_{f_V ext}^a}{\partial \mathbf{u}^b} &= - \sum_s \int_{(\partial_D \Omega_0)^s} \bar{f}_V \mathbf{N} \cdot \left( \frac{\partial \mathbf{L}_1(\mathbf{F}_h, \bar{f}_T)}{\partial \mathbf{F}^b} \cdot \nabla_0 N_{\mathbf{u}}^b \right) \cdot \nabla_0 N_{f_V}^a dS_0 \\ &- \sum_s \int_{(\partial_D \Omega_0)^s} \bar{f}_T \mathbf{N} \cdot \left( \frac{\partial \mathbf{L}_2(\mathbf{F}_h, \bar{f}_V, \bar{f}_T)}{\partial \mathbf{F}^b} \cdot \nabla_0 N_{\mathbf{u}}^b \right) \cdot \nabla_0 N_{f_V}^{a\pm} dS_0 \\ &+ \sum_s \int_{(\partial_D \Omega_0)^s} \bar{f}_V \mathbf{N} \cdot \left( \frac{\partial \mathbf{L}_1(\mathbf{F}_h, \bar{f}_T)}{\partial \mathbf{F}^b} \cdot \nabla_0 N_{\mathbf{u}}^b \frac{\mathcal{B}}{h_s} \right) \cdot \mathbf{N} N_{f_V}^a dS_0 \\ &+ \sum_s \int_{(\partial_D \Omega_0)^s} \bar{f}_T \mathbf{N} \cdot \left( \frac{\partial \mathbf{L}_2(\mathbf{F}_h, \bar{f}_V, \bar{f}_T)}{\partial \mathbf{F}^b} \cdot \nabla_0 N_{\mathbf{u}}^b \frac{\mathcal{B}}{h_s} \right) \cdot \mathbf{N} N_{f_V}^a dS_0, \end{aligned} \quad (D.9)$$

$$\frac{\partial F_{f_V int}^a}{\partial \mathbf{u}^b} = \sum_e \int_{\Omega_0^e} \nabla_0 N_{f_V}^a \cdot \frac{\partial \mathbf{J}_e}{\partial \mathbf{F}} \cdot \nabla_0 N_{\mathbf{u}}^b d\Omega_0, \quad (D.10)$$

and then using Eqs. (5.73, 5.74, and 5.75), we have

$$\frac{\partial F_{f_V I1}^{a\pm}}{\partial \mathbf{u}^{b\pm}} = \frac{1}{2} \sum_s \int_{(\partial_I \Omega_0)^s} (\pm N_{f_V}^{a\pm}) \frac{\partial \mathbf{J}_e^{\pm}}{\partial \mathbf{F}^{\pm}} \cdot \nabla_0 N_{\mathbf{u}}^{b\pm} \cdot \mathbf{N}^- dS_0, \quad (D.11)$$

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<sup>2</sup>There is one more additional term in  $\frac{\partial \mathbf{F}_{\mathbf{u}I1}^{a\pm}}{\partial f_T^{b\pm}}$  on the Dirichlet boundary, which is  $\sum_s \int_{(\partial_D \Omega_0)^s} (N_{\mathbf{u}}^a) \left( 2 \frac{\boldsymbol{\alpha}^{th} : \boldsymbol{\mathcal{H}}}{f_T^2} N_{f_T}^b \right) \cdot \mathbf{N}^- dS_0$ .

$$\begin{aligned} \frac{\partial F_{f_{V12}}^{a\pm}}{\partial \mathbf{u}^{b\pm}} &= \frac{1}{2} \sum_s \int_{(\partial_1 \Omega_0)^s} \llbracket f_{V_h} \rrbracket (\nabla_0 N_{f_V}^{a\pm} \cdot \frac{\partial \mathbf{L}_1^\pm}{\partial \mathbf{F}^\pm} \cdot \nabla_0 N_{\mathbf{u}}^{b\pm}) \cdot \mathbf{N}^- dS_0 \\ &+ \frac{1}{2} \sum_s \int_{(\partial_1 \Omega_0)^s} \llbracket f_{T_h} \rrbracket (\nabla_0 N_{f_V}^{a\pm} \cdot \frac{\partial \mathbf{L}_2^\pm}{\partial \mathbf{F}^\pm} \cdot \nabla_0 N_{\mathbf{u}}^{b\pm}) \cdot \mathbf{N}^- dS_0, \end{aligned} \quad (D.12)$$

$$\begin{aligned} \frac{\partial F_{f_{V13}}^{a\pm}}{\partial \mathbf{u}^{b\pm}} &= \frac{1}{2} \sum_s \int_{(\partial_1 \Omega_0)^s} \llbracket f_{V_h} \rrbracket \mathbf{N}^- \cdot \left( \frac{\partial \mathbf{L}_1^\pm}{\partial \mathbf{F}^\pm} \frac{\mathcal{B}}{h_s} \cdot \nabla_0 N_{\mathbf{u}}^{b\pm} \right) \cdot \mathbf{N}^- (\pm N_{f_V}^{a\pm}) dS_0 \\ &+ \frac{1}{2} \sum_s \int_{(\partial_1 \Omega_0)^s} (\pm N_{f_V}^{a\pm}) \mathbf{N}^- \cdot \left( \frac{\partial \mathbf{L}_2^\pm}{\partial \mathbf{F}^\pm} \frac{\mathcal{B}}{h_s} \cdot \nabla_0 N_{\mathbf{u}}^{b\pm} \right) \cdot \mathbf{N}^- \llbracket f_{T_h} \rrbracket dS_0. \end{aligned} \quad (D.13)$$

Moreover, the derivative of the electrical contributions with respect to  $f_V$  is  $\mathbb{K}_{f_V f_V}$ , and from Eq. (5.71), we have for the volume term

$$\frac{\partial F_{f_{Vint}}^a}{\partial f_V^b} = \sum_e \int_{\Omega_0^e} \frac{\partial \mathbf{J}_e}{\partial f_V} \cdot \nabla_0 N_{f_V}^a N_{f_V}^b d\Omega_0 + \sum_e \int_{\Omega_0^e} \nabla_0 N_{f_V}^a \cdot \frac{\partial \mathbf{J}_e}{\partial \nabla_0 f_V} \cdot \nabla_0 N_{f_V}^b d\Omega_0, \quad (D.14)$$

and for the interface terms, by calling Eqs. (5.73, 5.74, and 5.75), we have

$$\begin{aligned} \frac{\partial F_{f_{V11}}^{a\pm}}{\partial f_V^{b\pm}} &= \frac{1}{2} \sum_s \int_{(\partial_1 \Omega_0)^s} (\pm N_{f_V}^{a\pm}) \frac{\partial \mathbf{J}_e^\pm}{\partial f_V^\pm} \cdot \mathbf{N}^- N_{f_V}^{b\pm} dS_0 \\ &+ \frac{1}{2} \sum_s \int_{(\partial_1 \Omega_0)^s} (\pm N_{f_V}^{a\pm}) \mathbf{N}^- \cdot \frac{\partial \mathbf{J}_e^\pm}{\partial \nabla_0 f_V^\pm} \cdot \nabla_0 N_{f_V}^{b\pm} dS_0, \end{aligned} \quad (D.15)$$

$$\begin{aligned} \frac{\partial F_{f_{V12}}^{a\pm}}{\partial f_V^{b\pm}} &= \frac{1}{2} \sum_s \int_{(\partial_1 \Omega_0)^s} (\pm N_{f_V}^{b\pm}) \left( \mathbf{L}_1^\pm \cdot \nabla_0 N_{f_V}^{a\pm} \right) \cdot \mathbf{N}^- dS_0 \\ &+ \frac{1}{2} \sum_s \int_{(\partial_1 \Omega_0)^s} \llbracket f_{T_h} \rrbracket \left( \frac{\partial \mathbf{L}_2^\pm}{\partial f_V^\pm} \cdot \nabla_0 N_{f_V}^{a\pm} N_{f_V}^{b\pm} \right) \cdot \mathbf{N}^- dS_0, \end{aligned} \quad (D.16)$$

$$\begin{aligned} \frac{\partial F_{f_{V13}}^{a\pm}}{\partial f_V^{b\pm}} &= \sum_s \int_{(\partial_1 \Omega_0)^s} (\pm N_{f_V}^{a\pm}) \mathbf{N}^- \cdot \left\langle \frac{\mathbf{L}_1 \mathcal{B}}{h_s} \right\rangle \cdot \mathbf{N}^- (\pm N_{f_V}^{b\pm}) dS_0 \\ &+ \sum_s \int_{(\partial_1 \Omega_0)^s} (\pm N_{f_V}^{a\pm}) \mathbf{N}^- \cdot \left\langle \frac{\partial \mathbf{L}_2}{\partial f_V} \frac{\mathcal{B}}{h_s} \right\rangle \cdot \mathbf{N}^- N_{f_V}^{b\pm} \llbracket f_{T_h} \rrbracket dS_0. \end{aligned} \quad (D.17)$$

Similarly, the derivatives of the forces for the electrical contribution with respect to  $f_T$  give  $\mathbb{K}_{f_V f_T}$  and read

$$\frac{\partial F_{f_{Vint}}^a}{\partial f_T^b} = \sum_e \int_{\Omega_0^e} \frac{\partial \mathbf{J}_e}{\partial f_T} \cdot \nabla_0 N_{f_V}^a N_{f_T}^b d\Omega_0 + \sum_e \int_{\Omega_0^e} \nabla_0 N_{f_V}^a \cdot \frac{\partial \mathbf{J}_e}{\partial \nabla_0 f_T} \cdot \nabla_0 N_{f_T}^b d\Omega_0, \quad (D.18)$$

then for the interface terms by recalling Eqs. (5.73, 5.74, and 5.75), one can get

$$\begin{aligned} \frac{\partial F_{f_{T11}}^{a\pm}}{\partial f_T^{b\pm}} &= \frac{1}{2} \sum_s \int_{(\partial_1 \Omega_0)^s} (\pm N_{f_V}^{a\pm}) \frac{\partial \mathbf{J}_e^\pm}{\partial f_T} \cdot \mathbf{N}^- N_{f_T}^{b\pm} dS_0 \\ &+ \frac{1}{2} \sum_s \int_{(\partial_1 \Omega_0)^s} (\pm N_{f_V}^{a\pm}) \mathbf{N}^- \cdot \frac{\partial \mathbf{J}_e^\pm}{\partial \nabla_0 f_T} \cdot \nabla_0 N_{f_T}^{b\pm} dS_0, \end{aligned} \quad (D.19)$$

$$\begin{aligned}
\frac{\partial \mathbf{F}_{f_{V12}}^{a\pm}}{\partial \mathbf{f}_T^{\pm}} &= \frac{1}{2} \sum_s \int_{(\partial_T \Omega_0)^s} \llbracket f_{V_h} \rrbracket \left( \frac{\partial \mathbf{L}_1^\pm}{\partial \mathbf{f}_T^\pm} \cdot \nabla_0 \mathbf{N}_{f_V}^{a\pm} \mathbf{N}_{f_T}^{b\pm} \right) \cdot \mathbf{N}^- dS_0 \\
&+ \frac{1}{2} \sum_s \int_{(\partial_T \Omega_0)^s} \llbracket f_{T_h} \rrbracket \left( \frac{\partial \mathbf{L}_2^\pm}{\partial \mathbf{f}_T^\pm} \cdot \nabla_0 \mathbf{N}_{f_V}^{a\pm} \mathbf{N}_{f_T}^{b\pm} \right) \cdot \mathbf{N}^- dS_0 \\
&+ \frac{1}{2} \sum_s \int_{(\partial_T \Omega_0)^s} (\pm \mathbf{N}_{f_T}^{b\pm}) (\mathbf{L}_2^\pm \cdot \nabla_0 \mathbf{N}_{f_V}^{a\pm}) \cdot \mathbf{N}^- dS_0,
\end{aligned} \tag{D.20}$$

$$\begin{aligned}
\frac{\partial \mathbf{F}_{f_{V13}}^{a\pm}}{\partial \mathbf{f}_T^{\pm}} &= \frac{1}{2} \sum_s \int_{(\partial_T \Omega_0)^s} \llbracket f_{V_h} \rrbracket \mathbf{N}^- \cdot \frac{\partial \mathbf{L}_1^\pm}{\partial \mathbf{f}_T^\pm} \frac{\mathcal{B}}{h_s} \cdot \mathbf{N}^- \mathbf{N}_{f_T}^{b\pm} (\pm \mathbf{N}_{f_V}^{a\pm}) dS_0 \\
&+ \sum_s \int_{(\partial_T \Omega_0)^s} (\pm \mathbf{N}_{f_V}^{a\pm}) \mathbf{N}^- \cdot \left\langle \frac{\mathbf{L}_2 \mathcal{B}}{h_s} \right\rangle \cdot \mathbf{N}^- (\pm \mathbf{N}_{f_T}^{b\pm}) dS_0 \\
&+ \frac{1}{2} \sum_s \int_{(\partial_T \Omega_0)^s} (\pm \mathbf{N}_{f_V}^{a\pm}) \mathbf{N}^- \cdot \frac{\partial \mathbf{L}_2^\pm}{\partial \mathbf{f}_T^\pm} \frac{\mathcal{B}}{h_s} \cdot \mathbf{N}^- \mathbf{N}_{f_T}^{b\pm} \llbracket f_{T_h} \rrbracket dS_0.
\end{aligned} \tag{D.21}$$

The derivative of the thermal contributions with respect to the displacement  $\mathbf{u}$  is  $\mathbf{K}_{f_T \mathbf{u}}$ , and is obtained from Eq. (5.76, 5.77)

$$\begin{aligned}
\frac{\partial \mathbf{F}_{f_{T \text{ext}}}^a}{\partial \mathbf{u}^b} &= - \sum_s \int_{(\partial_D \Omega_0)^s} \bar{f}_T \mathbf{N} \cdot \left( \frac{\partial \mathbf{J}_{y1}(\mathbf{F}_h, \bar{f}_V, \bar{f}_T)}{\partial \mathbf{F}^b} \cdot \nabla_0 \mathbf{N}_{\mathbf{u}}^b \right) \cdot \nabla_0 \mathbf{N}_{f_T}^a dS_0 \\
&- \sum_s \int_{(\partial_D \Omega_0)^s} \bar{f}_V \mathbf{N} \cdot \left( \frac{\partial \mathbf{L}_2(\mathbf{F}_h, \bar{f}_V, \bar{f}_T)}{\partial \mathbf{F}^b} \cdot \nabla_0 \mathbf{N}_{\mathbf{u}}^b \right) \cdot \nabla_0 \mathbf{N}_{f_T}^a dS_0 \\
&+ \sum_s \int_{(\partial_D \Omega_0)^s} \bar{f}_T \mathbf{N} \cdot \left( \frac{\partial \mathbf{J}_{y1}(\mathbf{F}_h, \bar{f}_V, \bar{f}_T)}{\partial \mathbf{F}^b} \cdot \nabla_0 \mathbf{N}_{\mathbf{u}}^b \right) \frac{\mathcal{B}}{h_s} \cdot \mathbf{N} \mathbf{N}_{f_T}^a dS_0 \\
&+ \sum_s \int_{(\partial_D \Omega_0)^s} \bar{f}_V \mathbf{N} \cdot \left( \frac{\partial \mathbf{L}_2(\mathbf{F}_h, \bar{f}_V, \bar{f}_T)}{\partial \mathbf{F}^b} \cdot \nabla_0 \mathbf{N}_{\mathbf{u}}^b \right) \frac{\mathcal{B}}{h_s} \cdot \mathbf{N} \mathbf{N}_{f_T}^a dS_0,
\end{aligned} \tag{D.22}$$

$$\frac{\partial \mathbf{F}_{f_{T \text{int}}}^a}{\partial \mathbf{u}^b} = \sum_e \int_{\Omega_0^e} \nabla_0 \mathbf{N}_{f_T}^a \cdot \frac{\partial \mathbf{J}_y}{\partial \mathbf{F}} \cdot \nabla_0 \mathbf{N}_{\mathbf{u}}^b d\Omega_0 + \sum_e \int_{\Omega_0^e} \frac{\partial \bar{F}}{\partial \mathbf{F}} \cdot \nabla_0 \mathbf{N}_{\mathbf{u}}^b \mathbf{N}_{f_T}^a d\Omega_0, \tag{D.23}$$

and from Eqs. (5.79, 5.80, and 5.81)

$$\frac{\partial \mathbf{F}_{f_{T11}}^a}{\partial \mathbf{u}^{b\pm}} = \frac{1}{2} \sum_s \int_{(\partial_T \Omega_0)^s} (\pm \mathbf{N}_{f_T}^{a\pm}) \mathbf{N}^- \cdot \frac{\partial \mathbf{J}_y^\pm}{\partial \mathbf{F}^\pm} \cdot \nabla_0 \mathbf{N}_{\mathbf{u}}^{b\pm} dS_0, \tag{D.24}$$

$$\begin{aligned}
\frac{\partial \mathbf{F}_{f_{T12}}^{a\pm}}{\partial \mathbf{u}^{b\pm}} &= \frac{1}{2} \sum_s \int_{(\partial_T \Omega_0)^s} \llbracket f_{T_h} \rrbracket \left( \nabla_0 \mathbf{N}_{f_T}^{a\pm} \cdot \frac{\mathbf{J}_{y1}^\pm}{\partial \mathbf{F}^\pm} \cdot \nabla_0 \mathbf{N}_{\mathbf{u}}^{b\pm} \right) \cdot \mathbf{N}^- dS_0 \\
&+ \frac{1}{2} \sum_s \int_{(\partial_T \Omega_0)^s} \llbracket f_{V_h} \rrbracket \left( \nabla_0 \mathbf{N}_{f_T}^{a\pm} \cdot \frac{\partial \mathbf{L}_2^\pm}{\partial \mathbf{F}^\pm} \cdot \nabla_0 \mathbf{N}_{\mathbf{u}}^{b\pm} \right) \cdot \mathbf{N}^- dS_0,
\end{aligned} \tag{D.25}$$

$$\begin{aligned}
\frac{\partial \mathbf{F}_{f_{T13}}^{a\pm}}{\partial \mathbf{u}^{b\pm}} &= + \frac{1}{2} \sum_s \int_{(\partial_T \Omega_0)^s} (\pm \mathbf{N}_{f_T}^{a\pm}) \mathbf{N}^- \cdot \left( \frac{\partial \mathbf{J}_{y1}^\pm}{\partial \mathbf{F}^\pm} \frac{\mathcal{B}}{h_s} \cdot \nabla_0 \mathbf{N}_{\mathbf{u}}^{b\pm} \right) \cdot \mathbf{N}^- \llbracket f_{T_h} \rrbracket dS_0 \\
&+ \frac{1}{2} \sum_s \int_{(\partial_T \Omega_0)^s} \llbracket f_{V_h} \rrbracket \mathbf{N}^- \cdot \left( \frac{\partial \mathbf{L}_2^\pm}{\partial \mathbf{F}^\pm} \frac{\mathcal{B}}{h_s} \cdot \nabla_0 \mathbf{N}_{\mathbf{u}}^{b\pm} \right) \cdot \mathbf{N}^- (\pm \mathbf{N}_{f_T}^{a\pm}) dS_0.
\end{aligned} \tag{D.26}$$



The derivatives of the thermal contributions with respect to  $f_T$  is  $\mathbf{K}_{f_T f_T}$  read, for the volume term Eq. (5.77)

$$\begin{aligned} \frac{\partial F_{f_{Tint}}^a}{\partial f_T^b} &= \sum_e \int_{\Omega_0^e} \frac{\partial \mathbf{J}_y}{\partial f_T} \cdot \nabla_0 N_{f_T}^a N_{f_T}^b d\Omega_0 + \sum_e \int_{\Omega_0^e} \nabla_0 N_{f_T}^a \cdot \frac{\partial \mathbf{J}_y}{\partial \nabla_0 f_T} \cdot \nabla_0 N_{f_T}^b d\Omega_0 \\ &- \sum_e \int_{\Omega_0^e} \rho_0 \frac{\partial_t y}{\partial f_T} N_{f_T}^b N_{f_T}^a d\Omega_0 + \sum_e \int_{\Omega_0^e} \frac{\partial \bar{F}}{\partial f_T} N_{f_T}^b N_{f_T}^a d\Omega_0, \end{aligned} \quad (D.27)$$

and the derivatives of the interface forces are computed by calling Eqs. (5.79, 5.80, and 5.81)

$$\begin{aligned} \frac{\partial F_{f_{T11}}^{a\pm}}{\partial f_T^{b\pm}} &= \frac{1}{2} \sum_s \int_{(\partial_1 \Omega_0)^s} (\pm N_{f_T}^{a\pm}) \frac{\partial \mathbf{J}_y^\pm}{\partial f_T^\pm} \cdot \mathbf{N}^- N_{f_T}^{b\pm} dS_0 \\ &+ \frac{\gamma}{2} \sum_s \int_{(\partial_1 \Omega_0)^s} (\pm N_{f_T}^{a\pm}) \left( \frac{\partial \mathbf{J}_y^\pm}{\partial \nabla_0 f_T^\pm} \cdot \nabla_0 N_{f_T}^{b\pm} \right) \cdot \mathbf{N}^- dS_0, \end{aligned} \quad (D.28)$$

$$\begin{aligned} \frac{\partial F_{f_{T12}}^{a\pm}}{\partial f_T^{b\pm}} &= \frac{1}{2} \sum_s \int_{(\partial_1 \Omega_0)^s} (\pm N_{f_T}^{b\pm}) \left( \mathbf{J}_{y1}^\pm \cdot \nabla_0 N_{f_T}^{a\pm} \right) \cdot \mathbf{N}^- dS_0 \\ &+ \frac{1}{2} \sum_s \int_{(\partial_1 \Omega_0)^s} \llbracket f_{T_h} \rrbracket \left( \frac{\mathbf{J}_{y1}^\pm}{\partial f_T^\pm} \cdot \nabla_0 N_{f_T}^{a\pm} N_{f_T}^{b\pm} \right) \cdot \mathbf{N}^- dS_0 \\ &+ \frac{1}{2} \sum_s \int_{(\partial_1 \Omega_0)^s} \llbracket f_{V_h} \rrbracket \left( \frac{\partial \mathbf{L}_2^\pm}{\partial f_T^\pm} \cdot \nabla_0 N_{f_T}^{a\pm} N_{f_T}^{b\pm} \right) \cdot \mathbf{N}^- dS_0, \end{aligned} \quad (D.29)$$

and

$$\begin{aligned} \frac{\partial F_{f_{T13}}^{a\pm}}{\partial f_T^{b\pm}} &= \sum_s \int_{(\partial_1 \Omega_0)^s} (\pm N_{f_T}^{a\pm}) \mathbf{N}^- \cdot \left\langle \frac{\mathbf{J}_{y1} \mathcal{B}}{h_s} \right\rangle \cdot \mathbf{N}^- (\pm N_{f_T}^{b\pm}) dS_0 \\ &+ \frac{1}{2} \sum_s \int_{(\partial_1 \Omega_0)^s} (\pm N_{f_T}^{a\pm}) \mathbf{N}^- \cdot \frac{\partial \mathbf{J}_{y1}^\pm}{\partial f_T^\pm} \frac{\mathcal{B}}{h_s} \cdot \mathbf{N}^- N_{f_T}^{b\pm} \llbracket f_{T_h} \rrbracket dS_0 \\ &+ \frac{1}{2} \sum_s \int_{(\partial_1 \Omega_0)^s} \llbracket f_{V_h} \rrbracket \mathbf{N}^- \cdot \frac{\partial \mathbf{L}_2^\pm}{\partial f_T^\pm} \frac{\mathcal{B}}{h_s} \cdot \mathbf{N}^- N_{f_T}^{b\pm} (\pm N_{f_T}^{a\pm}) dS_0. \end{aligned} \quad (D.30)$$

The last part is the derivative of the thermal forces contribution with respect to  $f_V$  is  $\mathbf{K}_{f_T f_V}$

$$\begin{aligned} \frac{\partial F_{f_{Tint}}^a}{\partial f_V^b} &= \sum_e \int_{\Omega_0^e} \frac{\partial \mathbf{J}_y}{\partial f_V} \cdot \nabla_0 N_{f_T}^a N_{f_V}^b d\Omega_0 + \sum_e \int_{\Omega_0^e} \nabla_0 N_{f_T}^a \cdot \frac{\partial \mathbf{J}_y}{\partial \nabla_0 f_V} \cdot \nabla_0 N_{f_V}^b d\Omega_0 \\ &- \sum_e \int_{\Omega_0^e} \rho_0 \frac{\partial_t y}{\partial f_V} N_{f_V}^b N_{f_T}^a d\Omega_0, \end{aligned} \quad (D.31)$$

and the derivatives of the interface forces are computed by recalling Eqs. (5.79, 5.80 and 5.81)

$$\begin{aligned} \frac{\partial F_{f_{T11}}^{a\pm}}{\partial f_V^{b\pm}} &= \frac{1}{2} \sum_s \int_{(\partial_1 \Omega_0)^s} (\pm N_{f_T}^{a\pm}) \frac{\partial \mathbf{J}_y^\pm}{\partial f_V^\pm} \cdot \mathbf{N}^- N_{f_V}^{b\pm} dS_0 \\ &+ \frac{1}{2} \sum_s \int_{(\partial_1 \Omega_0)^s} (\pm N_{f_T}^{a\pm}) \mathbf{N}^- \cdot \frac{\partial \mathbf{J}_y^\pm}{\partial \nabla_0 f_V^\pm} \cdot \nabla_0 N_{f_V}^{b\pm} dS_0, \end{aligned} \quad (D.32)$$

$$\begin{aligned}
\frac{\partial \mathbf{F}_{f_{T12}}^{a\pm}}{\partial f_V^{b\pm}} &= \frac{1}{2} \sum_s \int_{(\partial_1 \Omega_0)^s} \llbracket f_{T_h} \rrbracket \left( \frac{\partial \mathbf{J}_{y1}^\pm}{\partial f_V^\pm} \cdot \nabla_0 N_{f_T}^{a\pm} N_{f_V}^{b\pm} \right) \cdot \mathbf{N}^- dS_0 \\
&+ \frac{1}{2} \sum_s \int_{(\partial_1 \Omega_0)^s} (\pm N_{f_V}^{b\pm}) (\mathbf{L}_2^\pm \cdot \nabla_0 N_{f_T}^{a\pm}) \cdot \mathbf{N}^- dS_0 \\
&+ \frac{1}{2} \sum_s \int_{(\partial_1 \Omega_0)^s} \llbracket f_{V_h} \rrbracket \left( \frac{\partial \mathbf{L}_2^\pm}{\partial f_V^\pm} \cdot \nabla_0 N_{f_T}^{a\pm} N_{f_V}^{b\pm} \right) \cdot \mathbf{N}^- dS_0,
\end{aligned} \tag{D.33}$$

$$\begin{aligned}
\frac{\partial \mathbf{F}_{f_{T13}}^{a\pm}}{\partial f_V^{b\pm}} &= \frac{1}{2} \sum_s \int_{(\partial_1 \Omega_0)^s} \llbracket f_{T_h} \rrbracket \mathbf{N}^- \cdot \frac{\partial \mathbf{J}_{y1}^\pm}{\partial f_V^\pm} \frac{\mathcal{B}}{h_s} \cdot \mathbf{N}^- N_{f_V}^{b\pm} (\pm N_{f_T}^a) dS_0 \\
&+ \sum_s \int_{(\partial_1 \Omega_0)^s} (\pm N_{f_V}^{b\pm}) \mathbf{N}^- \cdot \left\langle \frac{\mathbf{L}_2 \mathcal{B}}{h_s} \right\rangle \cdot \mathbf{N}^- (\pm N_{f_T}^{a\pm}) dS_0 \\
&+ \frac{1}{2} \sum_s \int_{(\partial_1 \Omega_0)^s} \llbracket f_{V_h} \rrbracket \mathbf{N}^- \cdot \frac{\partial \mathbf{L}_2^\pm}{\partial f_V^\pm} \frac{\mathcal{B}}{h_s} \cdot \mathbf{N}^- N_{f_V}^{b\pm} (\pm N_{f_T}^{a\pm}) dS_0.
\end{aligned} \tag{D.34}$$

### D.1.2 Expression of the constitutive law derivations

The derivative of first Piola-Kirchhoff with respect to the deformation gradient  $\frac{\partial \mathbf{P}}{\partial \mathbf{F}}$  and to the temperature  $\frac{\partial \mathbf{P}}{\partial T}$  are given in Appendix E.1 and E.2, then  $\frac{\partial \mathbf{P}}{\partial f_T}$  is computed as follows

$$\frac{\partial \mathbf{P}}{\partial f_T} = \frac{\partial \mathbf{P}}{\partial T} \frac{\partial T}{\partial f_T} + \frac{\partial \mathbf{P}}{\partial V} \frac{\partial V}{\partial f_T}. \tag{D.35}$$

where  $\frac{\partial T}{\partial f_T} = \frac{-1}{f_T^2}$  and  $\frac{\partial V}{\partial f_T} = \frac{f_V}{f_T^2}$ . In our case  $\frac{\partial \mathbf{P}}{\partial V} = 0$  as the Electro-Mechanical coupling is not considered.

The other derivatives related to the electrical and thermal contributions are give here. First the derivative of the electrical current flow with respect to  $f_V$  is obtained using (5.20)

$$\frac{\partial \mathbf{J}_e}{\partial f_V} = \frac{\partial \mathbf{L}_1}{\partial f_V} \cdot \nabla_0 f_T + \frac{\partial \mathbf{L}_2}{\partial f_V} \cdot \nabla_0 f_V, \tag{D.36}$$

where the derivative of  $\frac{\partial \mathbf{L}_1}{\partial f_V}$  and  $\frac{\partial \mathbf{L}_2}{\partial f_V}$  are obtained using Eq. (5.17)

$$\frac{\partial \mathbf{L}_1}{\partial f_V} = 0, \tag{D.37}$$

$$\frac{\partial \mathbf{L}_2}{\partial f_V} = -\frac{1}{f_T^2} \mathbf{L}(\mathbf{F}). \tag{D.38}$$

The derivative of the electrical current flow with respect to  $f_T$  is computed from (5.20)

$$\frac{\partial \mathbf{J}_e}{\partial f_T} = \frac{\partial \mathbf{L}_1}{\partial f_T} \cdot \nabla_0 f_T + \frac{\partial \mathbf{L}_2}{\partial f_T} \cdot \nabla_0 f_V, \tag{D.39}$$

where  $\frac{\partial \mathbf{L}_1}{\partial f_T}$  and  $\frac{\partial \mathbf{L}_2}{\partial f_T}$  are computed by recalling Eq. (5.17)

$$\frac{\partial \mathbf{L}_1}{\partial f_T} = -\frac{1}{f_T^2} \mathbf{L}(\mathbf{F}), \quad (\text{D.40})$$

$$\frac{\partial \mathbf{L}_2}{\partial f_T} = 2 \frac{f_V}{f_T^3} \mathbf{L}(\mathbf{F}) - 2\alpha \frac{1}{f_T^3} \mathbf{L}(\mathbf{F}). \quad (\text{D.41})$$

The derivative with respect to the gradient of  $f_V$  and  $f_T$  are

$$\frac{\partial \mathbf{J}_e}{\partial \nabla_0 f_V} = \mathbf{L}_1(\mathbf{F}), \quad \frac{\partial \mathbf{J}_e}{\partial \nabla_0 f_T} = \mathbf{L}_2(\mathbf{F}). \quad (\text{D.42})$$

The derivative of energy flux with respect to  $f_T$  is obtained from:

$$\frac{\partial \mathbf{J}_y}{\partial f_T} = \frac{\partial \mathbf{J}_{y_1}}{\partial f_T} \cdot \nabla_0 f_T + \frac{\partial \mathbf{L}_2}{\partial f_T} \cdot \nabla_0 f_V, \quad (\text{D.43})$$

where  $\frac{\partial \mathbf{J}_{y_1}}{\partial f_T}$  is computed from Eq. (5.17) as

$$\frac{\partial \mathbf{J}_{y_1}}{\partial f_T} = -\frac{2}{f_T^3} \mathbf{K}(\mathbf{F}) + 6\alpha \frac{f_V}{f_T^4} \mathbf{L}(\mathbf{F}) - \alpha^2 \frac{3}{f_T^4} \mathbf{L}(\mathbf{F}) - \frac{3f_V^2}{f_T^4} \mathbf{L}(\mathbf{F}), \quad (\text{D.44})$$

Moreover

$$\frac{\partial \mathbf{J}_y}{\partial f_V} = \frac{\partial \mathbf{J}_{y_1}}{\partial f_V} \cdot \nabla_0 f_T + \frac{\partial \mathbf{L}_2}{\partial f_V} \cdot \nabla_0 f_V, \quad (\text{D.45})$$

where using Eq. (5.17), we have

$$\frac{\partial \mathbf{J}_{y_1}}{\partial f_V} = -2\alpha \frac{1}{f_T^3} \mathbf{L}(\mathbf{F}) + \frac{2f_V}{f_T^3} \mathbf{L}(\mathbf{F}). \quad (\text{D.46})$$

The derivative of energy flux with respect to the gradient of  $f_T$  and  $f_V$  are

$$\frac{\partial \mathbf{J}_y}{\partial \nabla_0 f_T} = \mathbf{J}_{y_1}, \quad \frac{\partial \mathbf{J}_y}{\partial \nabla_0 f_V} = \mathbf{L}_2. \quad (\text{D.47})$$

The derivative of the electric current flow with respect to the deformation gradient is obtained from Eq. (5.20)

$$\frac{\partial \mathbf{J}_e}{\partial \mathbf{F}} = \frac{\partial \mathbf{L}_1}{\partial \mathbf{F}} \cdot \nabla_0 f_V + \frac{\partial \mathbf{L}_2}{\partial \mathbf{F}} \cdot \nabla_0 f_T, \quad (\text{D.48})$$

where

$$\frac{\partial \mathbf{L}_1}{\partial \mathbf{F}} = \frac{1}{f_T} \frac{\partial \mathbf{L}(\mathbf{F})}{\partial \mathbf{F}}, \quad (\text{D.49})$$

and

$$\frac{\partial \mathbf{L}_2}{\partial \mathbf{F}} = \left( -\frac{f_V}{f_T^2} + \alpha \frac{1}{f_T^2} \right) \frac{\partial \mathbf{L}(\mathbf{F})}{\partial \mathbf{F}}. \quad (\text{D.50})$$

According to the definition of  $\mathbf{L}(\mathbf{F})$  in Eq. (5.5), its derivative with respect to the deformation gradient is

$$\frac{\partial \mathbf{L}_{KL}}{\partial \mathbf{F}_{Nm}} = -\mathbf{F}_{Km}^{-1} \mathbf{L}_{NL} - \mathbf{L}_{KN} \mathbf{F}_{Lm}^{-1} + \mathbf{L}_{KL} \mathbf{F}_{Nm}^{-1}. \quad (\text{D.51})$$

Similarly, we have

$$\frac{\partial \mathbf{J}_y}{\partial \mathbf{F}} = \frac{\partial \mathbf{J}_{y_1}}{\partial \mathbf{F}} \cdot \nabla_0 f_T + \frac{\partial \mathbf{L}_2}{\partial \mathbf{F}} \cdot \nabla_0 f_V, \quad (\text{D.52})$$

where

$$\frac{\partial \mathbf{J}_{y_1}}{\partial \mathbf{F}} = \frac{1}{f_T^2} \frac{\partial \mathbf{K}(\mathbf{F})}{\partial \mathbf{F}} + \left( -2\alpha \frac{f_V}{f_T^3} + \alpha^2 \frac{1}{f_T^3} + \frac{f_V^2}{f_T^3} \right) \frac{\partial \mathbf{L}}{\partial \mathbf{F}}, \quad (\text{D.53})$$

where  $\frac{\partial \mathbf{L}}{\partial \mathbf{F}}$  is already computed in Eq. (D.51), while  $\frac{\partial \mathbf{K}}{\partial \mathbf{F}}$  can be computed using Eq. (5.12) as

$$\frac{\partial \mathbf{K}_{KL}}{\partial \mathbf{F}_{Nm}} = -\mathbf{F}_{Km}^{-1} \mathbf{K}_{NL} - \mathbf{K}_{KN} \mathbf{F}_{Lm}^{-1} + \mathbf{K}_{KL} \mathbf{F}_{Nm}^{-1}. \quad (\text{D.54})$$

## D.2 Lower bound for Electro-Thermo-Mechanical coupling

In order to prove Lemma 5.4.1, let us first use Eq. (5.115) and Eq. (5.116), yielding

$$\begin{aligned} & \mathcal{A}(\mathbf{G}^e; \delta \mathbf{G}_h, \delta \mathbf{G}_h) + \mathcal{B}(\mathbf{G}^e; \delta \mathbf{G}_h, \delta \mathbf{G}_h) \\ &= \int_{\Omega_h} (\nabla \delta \mathbf{G}_h)^T \mathbf{w}_{\nabla \mathbf{G}}(\mathbf{G}^e) \nabla \delta \mathbf{G}_h d\Omega + \int_{\partial_1 \Omega_h \cup \partial_D \Omega_h} \llbracket \delta \mathbf{G}_{hn}^T \rrbracket \langle \mathbf{w}_{\nabla \mathbf{G}}(\mathbf{G}^e) \nabla \delta \mathbf{G}_h \rangle dS \\ &+ \int_{\partial_1 \Omega_h \cup \partial_D \Omega_h} \llbracket \delta \mathbf{G}_{hn}^T \rrbracket \langle \mathbf{w}_{\nabla \mathbf{G}}(\mathbf{G}^e) \nabla \delta \mathbf{G}_h \rangle dS \\ &+ \int_{\partial_1 \Omega_h \cup \partial_D \Omega_h} \llbracket \delta \mathbf{G}_{hn}^T \rrbracket \left\langle \frac{\mathcal{B}}{h_s} \mathbf{w}_{\nabla \mathbf{G}}(\mathbf{G}^e) \right\rangle \llbracket \delta \mathbf{G}_{hn} \rrbracket dS \\ &+ \int_{\Omega_h} (\nabla \delta \mathbf{G}_h)^T \mathbf{w}_{\mathbf{G}}(\mathbf{G}^e, \nabla \mathbf{G}^e) \delta \mathbf{G}_h d\Omega + \int_{\partial_1 \Omega_h \cup \partial_D \Omega_h} \llbracket \delta \mathbf{G}_{hn}^T \rrbracket \langle \mathbf{w}_{\mathbf{G}}(\mathbf{G}^e, \nabla \mathbf{G}^e) \delta \mathbf{G}_h \rangle dS \\ &+ \int_{\Omega_h} \delta \mathbf{G}_h^T \mathbf{d}_{\nabla \mathbf{G}}(\mathbf{G}^e) \nabla \delta \mathbf{G}_h d\Omega + \int_{\Omega_h} \delta \mathbf{G}_h^T \mathbf{d}_{\mathbf{G}}(\mathbf{G}^e, \nabla \mathbf{G}^e) \delta \mathbf{G}_h d\Omega \\ &+ \int_{\partial_1 \Omega_h \cup \partial_D \Omega_h} \llbracket \delta \mathbf{G}_{hn}^T \mathbf{d}_{\nabla \mathbf{G}}^T(\mathbf{G}^e) \rrbracket \langle \delta \mathbf{G}_h \rangle dS \quad \forall \delta \mathbf{G}_h \in X^k. \end{aligned} \quad (\text{D.55})$$

This equation can be rewritten as

$$\begin{aligned}
\mathcal{A}(\mathbf{G}^e; \delta \mathbf{G}_h, \delta \mathbf{G}_h) + \mathcal{B}(\mathbf{G}^e; \delta \mathbf{G}_h, \delta \mathbf{G}_h) &= \int_{\Omega_h} (\nabla \delta \mathbf{G}_h)^T \mathbf{w}_{\nabla \mathbf{G}}(\mathbf{G}^e) \nabla \delta \mathbf{G}_h d\Omega \\
&+ \int_{\Omega_h} (\nabla \delta \mathbf{G}_h)^T \mathbf{w}_{\mathbf{G}}(\mathbf{G}^e, \nabla \mathbf{G}^e) \delta \mathbf{G}_h d\Omega \\
&+ \int_{\Omega_h} (\nabla \delta \mathbf{G}_h)^T (\mathbf{d}_{\nabla \mathbf{G}}^T(\mathbf{G}^e) \delta \mathbf{G}_h) d\Omega \\
&+ \int_{\Omega_h} \delta \mathbf{G}_h^T \mathbf{d}_{\mathbf{G}}(\mathbf{G}^e, \nabla \mathbf{G}^e) \delta \mathbf{G}_h d\Omega \\
&+ 2 \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \llbracket \delta \mathbf{G}_{h_n}^T \rrbracket \langle \mathbf{w}_{\nabla \mathbf{G}}(\mathbf{G}^e) \nabla \delta \mathbf{G}_h \rangle dS \\
&+ \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \llbracket \delta \mathbf{G}_{h_n}^T \rrbracket \langle \mathbf{w}_{\mathbf{G}}(\mathbf{G}^e, \nabla \mathbf{G}^e) \delta \mathbf{G}_h \rangle dS \\
&+ \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \llbracket \delta \mathbf{G}_{h_n}^T \rrbracket \left\langle \frac{\mathcal{B}}{h_s} \mathbf{w}_{\nabla \mathbf{G}}(\mathbf{G}^e) \right\rangle \llbracket \delta \mathbf{G}_{h_n} \rrbracket dS \\
&+ \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \llbracket \delta \mathbf{G}_{h_n}^T \mathbf{d}_{\nabla \mathbf{G}}^T(\mathbf{G}^e) \rrbracket \langle \delta \mathbf{G}_h \rangle dS.
\end{aligned} \tag{D.56}$$

By Eqs. (5.102) and (5.118), Eq. (D.56) gives

$$\begin{aligned}
\mathcal{A}(\mathbf{G}^e; \delta \mathbf{G}_h, \delta \mathbf{G}_h) + \mathcal{B}(\mathbf{G}^e; \delta \mathbf{G}_h, \delta \mathbf{G}_h) &\geq \\
\sum_e C_\alpha \|\nabla \delta \mathbf{G}_h\|_{L^2(\Omega^e)}^2 + \sum_e C_\alpha \|\delta \mathbf{G}_h\|_{L^2(\Omega^e)}^2 \\
- 2C_y \sum_e \|\nabla \delta \mathbf{G}_h\|_{L^2(\Omega^e)} \|\delta \mathbf{G}_h\|_{L^2(\Omega^e)} \\
- 2 \sum_s C_y \left| \int_{(\partial_{DI}\Omega)^s} \llbracket \delta \mathbf{G}_{h_n} \rrbracket \langle \nabla \delta \mathbf{G}_h \rangle dS \right| \\
- 2 \sum_s C_y \left| \int_{(\partial_{DI}\Omega)^s} \llbracket \delta \mathbf{G}_{h_n} \rrbracket \langle \delta \mathbf{G}_h \rangle dS \right| + \sum_s C_\alpha \frac{\mathcal{B}}{h_s} \|\llbracket \delta \mathbf{G}_{h_n} \rrbracket\|_{L^2((\partial_{DI}\Omega)^s)}^2,
\end{aligned} \tag{D.57}$$

where  $\int_{\partial_I \Omega_h} + \int_{\partial_D \Omega_h} = \sum_s \int_{(\partial_{DI}\Omega)^s}$ .

The fourth and fifth terms of the right hand side in Eq. (D.57) can be estimated using

Cauchy-Schwartz' inequality, Eq. (2.26),

$$\begin{aligned}
& 2C_y \sum_s \left| \int_{(\partial_{DI}\Omega)^s} \llbracket \delta \mathbf{G}_{h_n} \rrbracket \langle \nabla \delta \mathbf{G}_h \rangle \, dS \right| + 2C_y \sum_s \left| \int_{(\partial_{DI}\Omega)^s} \llbracket \delta \mathbf{G}_{h_n} \rrbracket \langle \delta \mathbf{G}_h \rangle \, dS \right| \\
& \leq 2C_y \left( \sum_s \frac{1}{h_s} \|\llbracket \delta \mathbf{G}_{h_n} \rrbracket\|_{L^2((\partial_{DI}\Omega)^s)}^2 \right)^{\frac{1}{2}} \left( \sum_s h_s \|\langle \nabla \delta \mathbf{G}_h \rangle\|_{L^2((\partial_{DI}\Omega)^s)}^2 \right)^{\frac{1}{2}} \\
& + 2C_y \left( \sum_s \frac{1}{h_s} \|\llbracket \delta \mathbf{G}_{h_n} \rrbracket\|_{L^2((\partial_{DI}\Omega)^s)}^2 \right)^{\frac{1}{2}} \left( \sum_s h_s \|\langle \delta \mathbf{G}_h \rangle\|_{L^2((\partial_{DI}\Omega)^s)}^2 \right)^{\frac{1}{2}} \\
& \leq 2C_y \left( \sum_s \frac{1}{h_s} \|\llbracket \delta \mathbf{G}_{h_n} \rrbracket\|_{L^2((\partial_{DI}\Omega)^s)}^2 \right)^{\frac{1}{2}} \left[ \left( \sum_s h_s \|\langle \nabla \delta \mathbf{G}_h \rangle\|_{L^2((\partial_{DI}\Omega)^s)}^2 \right)^{\frac{1}{2}} \right. \\
& \left. + \left( \sum_s h_s \|\langle \delta \mathbf{G}_h \rangle\|_{L^2((\partial_{DI}\Omega)^s)}^2 \right)^{\frac{1}{2}} \right], \tag{D.58}
\end{aligned}$$

where the term  $h_s \|\langle \nabla \delta \mathbf{G}_h \rangle\|_{L^2((\partial_{DI}\Omega)^s)}^2$  can be bounded using the trace inequality on the finite element space (2.18), with

$$\begin{aligned}
\sum_s h_s \|\langle \nabla \delta \mathbf{G}_h \rangle\|_{L^2((\partial_{DI}\Omega)^s)}^2 &= \frac{1}{2} \sum_e h_s \|\langle \nabla \delta \mathbf{G}_h \rangle\|_{L^2(\partial_1 \Omega^e)}^2 + \sum_e h_s \|\nabla \delta \mathbf{G}_h\|_{L^2(\partial_D \Omega^e)}^2 \\
&\leq \sum_e h_s \|\nabla \delta \mathbf{G}_h\|_{L^2(\partial \Omega^e)}^2 \leq C_{\mathcal{K}}^2 \sum_e \|\nabla \delta \mathbf{G}_h\|_{L^2(\Omega^e)}^2. \tag{D.59}
\end{aligned}$$

Then using the trace inequality, Eq. (2.16), and inverse inequality, Eq. (2.21), we observe that

$$\begin{aligned}
\sum_s h_s \|\langle \delta \mathbf{G}_h \rangle\|_{L^2((\partial_{DI}\Omega)^s)}^2 &= \frac{1}{2} \sum_e h_s \|\langle \delta \mathbf{G}_h \rangle\|_{L^2(\partial_1 \Omega^e)}^2 + \sum_e h_s \|\delta \mathbf{G}_h\|_{L^2(\partial_D \Omega^e)}^2 \\
&\leq \sum_e h_s \|\delta \mathbf{G}_h\|_{L^2(\partial \Omega^e)}^2 \\
&\leq C_{\mathcal{T}} \sum_e \left( \|\delta \mathbf{G}_h\|_{L^2(\Omega^e)}^2 + h_s \|\delta \mathbf{G}_h\|_{L^2(\Omega^e)} \|\nabla \delta \mathbf{G}_h\|_{L^2(\Omega^e)} \right) \\
&\leq \sum_e C_{\mathcal{T}} (C_{\mathcal{I}}^k + 1) \|\delta \mathbf{G}_h\|_{L^2(\Omega^e)}^2. \tag{D.60}
\end{aligned}$$

Therefore Eq. (D.58) is rewritten as

$$\begin{aligned}
& 2C_y \sum_s \left| \int_{(\partial_{DI}\Omega)^s} \llbracket \delta \mathbf{G}_{h_n} \rrbracket \langle \nabla \delta \mathbf{G}_h \rangle \, dS \right| + 2C_y \sum_s \left| \int_{(\partial_{DI}\Omega)^s} \llbracket \delta \mathbf{G}_{h_n} \rrbracket \langle \delta \mathbf{G}_h \rangle \, dS \right| \\
& \leq C_y \left( \sum_s \frac{1}{h_s} \|\llbracket \delta \mathbf{G}_{h_n} \rrbracket\|_{L^2((\partial_{DI}\Omega)^s)}^2 \right)^{\frac{1}{2}} \left( \sum_e \max(4C_{\mathcal{T}}(C_{\mathcal{I}}^k + 1), 4C_{\mathcal{K}}^2) \|\delta \mathbf{G}_h\|_{H^1(\Omega^e)}^2 \right)^{\frac{1}{2}}. \tag{D.61}
\end{aligned}$$

Finally, by the use of the  $\xi$ -inequality  $-\xi > 0 : |ab| \leq \frac{\xi}{4}a^2 + \frac{1}{\xi}b^2$  with  $\xi = \frac{C_\alpha}{C_y \max(4C_{\mathcal{T}}(C_{\mathcal{I}}^k+1), 4C_{\mathcal{K}}^k)}$ , we arrive at

$$\begin{aligned} & 2C_y \sum_s \left| \int_{(\partial_{\text{DI}}\Omega)^s} \llbracket \delta \mathbf{G}_{\text{hn}} \rrbracket \langle \nabla \delta \mathbf{G}_h \rangle \, \text{dS} \right| + 2C_y \sum_s \left| \int_{(\partial_{\text{DI}}\Omega)^s} \llbracket \delta \mathbf{G}_{\text{hn}} \rrbracket \langle \delta \mathbf{G}_h \rangle \, \text{dS} \right| \\ & \leq \frac{C_\alpha}{4} \sum_e \|\delta \mathbf{G}_h\|_{\text{H}^1(\Omega^e)}^2 + \frac{C_y^2}{C_\alpha} \max(4C_{\mathcal{T}}(C_{\mathcal{I}}^k+1), 4C_{\mathcal{K}}^k) \sum_s \frac{1}{h_s} \|\llbracket \delta \mathbf{G}_{\text{hn}} \rrbracket\|_{\text{L}^2((\partial_{\text{DI}}\Omega)^s)}^2. \end{aligned} \quad (\text{D.62})$$

For the third term of the right hand side of Eq. (D.57), choosing  $\xi = \frac{2C_\alpha}{C_y}$  and applying the  $\xi$ -inequality, we find

$$\begin{aligned} \sum_e 2C_y \|\nabla \delta \mathbf{G}_h\|_{\text{L}^2(\Omega^e)} \|\delta \mathbf{G}_h\|_{\text{L}^2(\Omega^e)} & \leq \frac{2C_y}{\xi} \sum_e \|\delta \mathbf{G}_h\|_{\text{L}^2(\Omega^e)}^2 + \frac{2C_y \xi}{4} \sum_e \|\nabla \delta \mathbf{G}_h\|_{\text{L}^2(\Omega^e)}^2 \\ & \leq \frac{C_y^2}{C_\alpha} \sum_e \|\delta \mathbf{G}_h\|_{\text{L}^2(\Omega^e)}^2 + \frac{C_\alpha}{4} \sum_e \|\nabla \delta \mathbf{G}_h\|_{\text{L}^2(\Omega^e)}^2. \end{aligned} \quad (\text{D.63})$$

If we substitute Eqs. (D.62) and (D.63) in Eq. (D.57), we thus obtain the following result:

$$\begin{aligned} & \mathcal{A}(\mathbf{G}^e; \delta \mathbf{G}_h, \delta \mathbf{G}_h) + \mathcal{B}(\mathbf{G}^e; \delta \mathbf{G}_h, \delta \mathbf{G}_h) \\ & \geq \frac{C_\alpha}{2} \sum_e \|\nabla \delta \mathbf{G}_h\|_{\text{L}^2(\Omega^e)}^2 + C_\alpha \sum_e \|\delta \mathbf{G}_h\|_{\text{L}^2(\Omega^e)}^2 \\ & \quad - \left( \frac{C_y^2}{C_\alpha} + \frac{C_\alpha}{4} \right) \sum_e \|\delta \mathbf{G}_h\|_{\text{L}^2(\Omega^e)}^2 \\ & \quad + \left[ \mathcal{B}C_\alpha - \frac{C_y^2}{C_\alpha} \max(4C_{\mathcal{T}}(C_{\mathcal{I}}^k+1), 4C_{\mathcal{K}}^k) \right] h_s^{-1} \sum_e \|\llbracket \delta \mathbf{G}_{\text{hn}} \rrbracket\|_{\text{L}^2(\partial\Omega^e)}^2. \end{aligned} \quad (\text{D.64})$$

Therefore

$$\begin{aligned} & \mathcal{A}(\mathbf{G}^e; \delta \mathbf{G}_h, \delta \mathbf{G}_h) + \mathcal{B}(\mathbf{G}^e; \delta \mathbf{G}_h, \delta \mathbf{G}_h) \geq \frac{C_\alpha}{2} \sum_e \|\nabla \delta \mathbf{G}_h\|_{\text{L}^2(\Omega^e)}^2 - \left( \frac{C_y^2}{C_\alpha} + \frac{5C_\alpha}{4} \right) \sum_e \|\delta \mathbf{G}_h\|_{\text{L}^2(\Omega^e)}^2 \\ & \quad + \left[ \mathcal{B}C_\alpha - \frac{C_y^2}{C_\alpha} \max(4C_{\mathcal{T}}(C_{\mathcal{I}}^k+1), 4C_{\mathcal{K}}^k) \right] h_s^{-1} \sum_e \|\llbracket \delta \mathbf{G}_{\text{hn}} \rrbracket\|_{\text{L}^2(\partial\Omega^e)}^2. \end{aligned} \quad (\text{D.65})$$

This last relation can be rewritten as

$$\begin{aligned} & \mathcal{A}(\mathbf{G}^e; \delta \mathbf{G}_h, \delta \mathbf{G}_h) + \mathcal{B}(\mathbf{G}^e; \delta \mathbf{G}_h, \delta \mathbf{G}_h) \geq C_1^k \left[ \sum_e \|\nabla \delta \mathbf{G}_h\|_{\text{L}^2(\Omega^e)}^2 + h_s^{-1} \sum_e \|\llbracket \delta \mathbf{G}_{\text{hn}} \rrbracket\|_{\text{L}^2(\partial\Omega^e)}^2 \right] \\ & \quad - C_2^k \|\delta \mathbf{G}_h\|_{\text{L}^2(\Omega_h)}^2 \quad \forall \delta \mathbf{G}_h \in \mathbf{X}^k. \end{aligned} \quad (\text{D.66})$$

where  $C_1^k = \min\left(\frac{C_\alpha}{2}, \mathcal{B}C_\alpha - \frac{C_y^2}{C_\alpha} \max(4C_{\mathcal{T}}(C_{\mathcal{I}}^k + 1), 4C_{\mathcal{K}}^{k^2})\right)$ , which is positive when  $\mathcal{B} > \frac{C_y^2}{C_\alpha} \max(4C_{\mathcal{T}}(C_{\mathcal{I}}^k + 1), 4C_{\mathcal{K}}^{k^2})$ , and  $C_2^k = \frac{C_y^2}{C_\alpha} + \frac{5C_\alpha}{4} > 0$ .

Therefore, comparing with the definition of the mesh dependent norm, Eq. (2.10), we have

$$\mathcal{A}(\mathbf{G}^e; \delta\mathbf{G}_h, \delta\mathbf{G}_h) + \mathcal{B}(\mathbf{G}^e; \delta\mathbf{G}_h, \delta\mathbf{G}_h) \geq C_1^k \|\delta\mathbf{G}_h\|_*^2 - C_2^k \|\delta\mathbf{G}_h\|_{L^2(\Omega_h)}^2 \quad \forall \delta\mathbf{G}_h \in X^k. \quad (\text{D.67})$$

Moreover, starting from Eq. (D.64) and choosing  $C_2^k = \frac{C_y^2}{C_\alpha} + \frac{3C_\alpha}{4}$ , we rewrite the expression in terms of the norm (2.11) as

$$\mathcal{A}(\mathbf{G}^e; \delta\mathbf{G}_h, \delta\mathbf{G}_h) + \mathcal{B}(\mathbf{G}^e; \delta\mathbf{G}_h, \delta\mathbf{G}_h) \geq C_1^k \|\delta\mathbf{G}_h\|^2 - C_2^k \|\delta\mathbf{G}_h\|_{L^2(\Omega_h)}^2 \quad \forall \delta\mathbf{G}_h \in X^k. \quad (\text{D.68})$$

Hence, this shows that the stability of the method is conditioned by the constant  $\mathcal{B}$ , which should be large enough.

### D.3 Upper bound for Electro-Thermo-Mechanical coupling

The upper bound of the bi-linear form is determined, by recalling Eq. (5.115) and Eq. (5.116), for  $\mathbf{m}, \delta\mathbf{G} \in X$

$$\begin{aligned} \mathcal{A}(\mathbf{G}^e; \mathbf{m}, \delta\mathbf{G}) + \mathcal{B}(\mathbf{G}^e; \mathbf{m}, \delta\mathbf{G}) &= \int_{\Omega_h} (\nabla\delta\mathbf{G})^T \mathbf{w}_{\nabla\mathbf{G}}(\mathbf{G}^e) \nabla\mathbf{m} d\Omega \\ &+ \int_{\partial_1\Omega_h \cup \partial_D\Omega_h} \llbracket \delta\mathbf{G}_n^T \rrbracket \langle \mathbf{w}_{\nabla\mathbf{G}}(\mathbf{G}^e) \nabla\mathbf{m} \rangle dS + \int_{\partial_1\Omega_h \cup \partial_D\Omega_h} \llbracket \mathbf{m}_n^T \rrbracket \langle \mathbf{w}_{\nabla\mathbf{G}}(\mathbf{G}^e) \nabla\delta\mathbf{G} \rangle dS \\ &+ \int_{\partial_1\Omega_h \cup \partial_D\Omega_h} \llbracket \delta\mathbf{G}_n^T \rrbracket \left\langle \frac{\mathcal{B}}{h_s} \mathbf{w}_{\nabla\mathbf{G}}(\mathbf{G}^e) \right\rangle \llbracket \mathbf{m}_n \rrbracket dS + \int_{\Omega_h} (\nabla\delta\mathbf{G})^T \mathbf{w}_{\mathbf{G}}(\mathbf{G}^e, \nabla\mathbf{G}^e) \mathbf{m} d\Omega \quad (\text{D.69}) \\ &+ \int_{\partial_1\Omega_h \cup \partial_D\Omega_h} \llbracket \delta\mathbf{G}_n^T \rrbracket \langle \mathbf{w}_{\mathbf{G}}(\mathbf{G}^e, \nabla\mathbf{G}^e) \mathbf{m} \rangle dS + \int_{\Omega_h} \delta\mathbf{G}^T (\mathbf{d}_{\mathbf{G}}(\mathbf{G}^e, \nabla\mathbf{G}^e) \mathbf{m}) d\Omega \\ &+ \int_{\Omega_h} \delta\mathbf{G}^T (\mathbf{d}_{\nabla\mathbf{G}}(\mathbf{G}^e) \nabla\mathbf{m}) d\Omega + \int_{\partial_1\Omega_h \cup \partial_D\Omega_h} \llbracket \mathbf{m}_n^T \mathbf{d}_{\nabla\mathbf{G}}^T(\mathbf{G}^e) \rrbracket \langle \delta\mathbf{G} \rangle dS. \end{aligned}$$

Every term in the right hand side of Eq. (D.69) is bounded using the Hölder's inequality, Eq. (2.24), and the bound (5.118). This successively results in

$$\begin{aligned} \left| \int_{\Omega_h} (\nabla\delta\mathbf{G})^T \mathbf{w}_{\nabla\mathbf{G}}(\mathbf{G}^e) \nabla\mathbf{m} d\Omega \right| &\leq \sum_e \left( \int_{\Omega^e} |(\nabla\delta\mathbf{G})^T \mathbf{w}_{\nabla\mathbf{G}}(\mathbf{G}^e) \nabla\mathbf{m}| d\Omega \right) \\ &\leq C_y \sum_e \|\nabla\delta\mathbf{G}\|_{L^2(\Omega^e)} \|\nabla\mathbf{m}\|_{L^2(\Omega^e)}, \end{aligned} \quad (\text{D.70})$$

$$\begin{aligned} \left| \int_{\Omega_h} (\nabla\delta\mathbf{G})^T \mathbf{w}_{\mathbf{G}}(\mathbf{G}^e, \nabla\mathbf{G}^e) \mathbf{m} d\Omega \right| &\leq \sum_e \left( \int_{\Omega^e} |(\nabla\delta\mathbf{G})^T \mathbf{w}_{\mathbf{G}}(\mathbf{G}^e, \nabla\mathbf{G}^e) \mathbf{m}| d\Omega \right) \\ &\leq C_y \sum_e \|\nabla\delta\mathbf{G}\|_{L^2(\Omega^e)} \|\mathbf{m}\|_{L^2(\Omega^e)}, \end{aligned} \quad (\text{D.71})$$



$$\left| \int_{\Omega_h} \delta \mathbf{G}^T \mathbf{d}_{\mathbf{G}}(\mathbf{G}^e) \mathbf{m} d\Omega \right| \leq C_y \sum_e \|\delta \mathbf{G}\|_{L^2(\Omega^e)} \|\mathbf{m}\|_{L^2(\Omega^e)}, \quad (\text{D.72})$$

$$\left| \int_{\Omega_h} \delta \mathbf{G}^T \mathbf{d}_{\nabla \mathbf{G}}(\mathbf{G}^e) \nabla \mathbf{m} d\Omega \right| \leq C_y \sum_e \|\delta \mathbf{G}\|_{L^2(\Omega^e)} \|\nabla \mathbf{m}\|_{L^2(\Omega^e)}, \quad (\text{D.73})$$

$$\begin{aligned} & \left| \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \llbracket \delta \mathbf{G}_n^T \rrbracket \left\langle \frac{\mathbf{w}_{\nabla \mathbf{G}}(\mathbf{G}^e) \mathcal{B}}{h_s} \right\rangle \llbracket \mathbf{m}_n \rrbracket dS \right| \\ &= \left| \sum_e \int_{\partial_D \Omega^e} \llbracket \delta \mathbf{G}_n^T \rrbracket \frac{\mathbf{w}_{\nabla \mathbf{G}}(\mathbf{G}^e) \mathcal{B}}{h_s} \llbracket \mathbf{m}_n \rrbracket dS \right. \\ & \quad \left. + \frac{1}{2} \sum_e \int_{\partial_I \Omega^e} \llbracket \delta \mathbf{G}_n^T \rrbracket \left\langle \frac{\mathbf{w}_{\nabla \mathbf{G}}(\mathbf{G}^e) \mathcal{B}}{h_s} \right\rangle \llbracket \mathbf{m}_n \rrbracket dS \right| \\ & \leq \mathcal{B} \sum_e C_y \|\mathbf{h}_s^{-\frac{1}{2}} \llbracket \delta \mathbf{G}_n \rrbracket\|_{L^2(\partial \Omega^e)} \|\mathbf{h}_s^{-\frac{1}{2}} \llbracket \mathbf{m}_n \rrbracket\|_{L^2(\partial \Omega^e)}, \end{aligned} \quad (\text{D.74})$$

$$\begin{aligned} & \left| \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \llbracket \mathbf{m}_n^T \rrbracket \langle \mathbf{w}_{\nabla \mathbf{G}}(\mathbf{G}^e) \nabla \delta \mathbf{G} \rangle dS \right| = \left| \frac{1}{2} \sum_e \int_{\partial_I \Omega^e} \llbracket \mathbf{m}_n^T \rrbracket \langle \mathbf{w}_{\nabla \mathbf{G}}(\mathbf{G}^e) \nabla \delta \mathbf{G} \rangle dS \right. \\ & \quad \left. + \sum_e \int_{\partial_D \Omega^e} \llbracket \mathbf{m}_n^T \rrbracket \mathbf{w}_{\nabla \mathbf{G}}(\mathbf{G}^e) \nabla \delta \mathbf{G} dS \right| \leq C_y \sum_e \|\mathbf{h}_s^{\frac{1}{2}} \nabla \delta \mathbf{G}\|_{L^2(\partial \Omega^e)} \|\mathbf{h}_s^{-\frac{1}{2}} \llbracket \mathbf{m}_n \rrbracket\|_{L^2(\partial \Omega^e)}, \end{aligned} \quad (\text{D.75})$$

$$\begin{aligned} & \left| \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \llbracket \delta \mathbf{G}_n^T \rrbracket \langle \mathbf{w}_{\nabla \mathbf{G}}(\mathbf{G}^e) \nabla \mathbf{m} \rangle dS \right| = \left| \frac{1}{2} \sum_e \int_{\partial_I \Omega^e} \llbracket \delta \mathbf{G}_n^T \rrbracket \langle \mathbf{w}_{\nabla \mathbf{G}}(\mathbf{G}^e) \nabla \mathbf{m} \rangle dS \right. \\ & \quad \left. + \sum_e \int_{\partial_D \Omega^e} \llbracket \delta \mathbf{G}_n^T \rrbracket \mathbf{w}_{\nabla \mathbf{G}}(\mathbf{G}^e) \nabla \mathbf{m} dS \right| \leq C_y \sum_e \|\mathbf{h}_s^{\frac{1}{2}} \nabla \mathbf{m}\|_{L^2(\partial \Omega^e)} \|\mathbf{h}_s^{-\frac{1}{2}} \llbracket \delta \mathbf{G}_n \rrbracket\|_{L^2(\partial \Omega^e)}, \end{aligned} \quad (\text{D.76})$$

$$\begin{aligned} & \left| \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \llbracket \delta \mathbf{G}_n^T \rrbracket \langle \mathbf{w}_{\mathbf{G}}(\mathbf{G}^e, \nabla \mathbf{G}^e) \mathbf{m} \rangle dS \right| = \left| \frac{1}{2} \sum_e \int_{\partial_I \Omega^e} \llbracket \delta \mathbf{G}_n^T \rrbracket \langle \mathbf{w}_{\mathbf{G}}(\mathbf{G}^e, \nabla \mathbf{G}^e) \mathbf{m} \rangle dS \right. \\ & \quad \left. + \sum_e \int_{\partial_D \Omega^e} \llbracket \delta \mathbf{G}_n^T \rrbracket \mathbf{w}_{\mathbf{G}}(\mathbf{G}^e, \nabla \mathbf{G}^e) \mathbf{m} dS \right| \leq C_y \sum_e \|\mathbf{h}_s^{\frac{1}{2}} \mathbf{m}\|_{L^2(\partial \Omega^e)} \|\mathbf{h}_s^{-\frac{1}{2}} \llbracket \delta \mathbf{G}_n \rrbracket\|_{L^2(\partial \Omega^e)}, \end{aligned} \quad (\text{D.77})$$

and

$$\begin{aligned} & \left| \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \llbracket \mathbf{m}_n^T \mathbf{d}_{\nabla \mathbf{G}}^T(\mathbf{G}^e) \rrbracket \langle \delta \mathbf{G} \rangle dS \right| = \left| \frac{1}{2} \sum_e \int_{\partial_I \Omega^e} \llbracket \mathbf{m}_n^T \mathbf{d}_{\nabla \mathbf{G}}^T(\mathbf{G}^e) \rrbracket \langle \delta \mathbf{G} \rangle dS \right. \\ & \quad \left. + \sum_e \int_{\partial_D \Omega^e} \llbracket \mathbf{m}_n^T \mathbf{d}_{\nabla \mathbf{G}}^T(\mathbf{G}^e) \rrbracket \langle \delta \mathbf{G} \rangle dS \right| \leq C_y \sum_e \|\mathbf{h}_s^{\frac{1}{2}} \delta \mathbf{G}\|_{L^2(\partial \Omega^e)} \|\mathbf{h}_s^{-\frac{1}{2}} \llbracket \mathbf{m}_n \rrbracket\|_{L^2(\partial \Omega^e)}. \end{aligned} \quad (\text{D.78})$$

Thereby, in combining the above results, we thus obtain:

$$\begin{aligned}
| \mathcal{A}(\mathbf{G}^e; \mathbf{m}, \delta \mathbf{G}) + \mathcal{B}(\mathbf{G}^e; \mathbf{m}, \delta \mathbf{G}) | &\leq C_y \sum_e \|\nabla \mathbf{m}\|_{L^2(\Omega^e)} \|\nabla \delta \mathbf{G}\|_{L^2(\Omega^e)} \\
&+ C_y \sum_e \|\nabla \mathbf{m}\|_{L^2(\Omega^e)} \|\delta \mathbf{G}\|_{L^2(\Omega^e)} \\
&+ C_y \sum_e \|\mathbf{m}\|_{L^2(\Omega^e)} \|\nabla \delta \mathbf{G}\|_{L^2(\Omega^e)} \\
&+ C_y \sum_e \|\mathbf{m}\|_{L^2(\Omega^e)} \|\delta \mathbf{G}\|_{L^2(\Omega^e)} \\
&+ \mathcal{B}C_y \sum_e \|\mathbf{h}_s^{-\frac{1}{2}} \llbracket \mathbf{m}_n \rrbracket\|_{L^2(\partial\Omega^e)} \|\mathbf{h}_s^{-\frac{1}{2}} \llbracket \delta \mathbf{G}_n \rrbracket\|_{L^2(\partial\Omega^e)} \\
&+ C_y \sum_e \|\mathbf{h}_s^{\frac{1}{2}} \nabla \mathbf{m}\|_{L^2(\partial\Omega^e)} \|\mathbf{h}_s^{-\frac{1}{2}} \llbracket \delta \mathbf{G}_n \rrbracket\|_{L^2(\partial\Omega^e)} \\
&+ C_y \sum_e \|\mathbf{h}_s^{-\frac{1}{2}} \llbracket \mathbf{m}_n \rrbracket\|_{L^2(\partial\Omega^e)} \|\mathbf{h}_s^{\frac{1}{2}} \nabla \delta \mathbf{G}\|_{L^2(\partial\Omega^e)} \\
&+ C_y \sum_e \|\mathbf{h}_s^{\frac{1}{2}} \mathbf{m}\|_{L^2(\partial\Omega^e)} \|\mathbf{h}_s^{-\frac{1}{2}} \llbracket \delta \mathbf{G}_n \rrbracket\|_{L^2(\partial\Omega^e)} \\
&+ C_y \sum_e \|\mathbf{h}_s^{\frac{1}{2}} \delta \mathbf{G}\|_{L^2(\partial\Omega^e)} \|\mathbf{h}_s^{-\frac{1}{2}} \llbracket \mathbf{m}_n \rrbracket\|_{L^2(\partial\Omega^e)} .
\end{aligned} \tag{D.79}$$

Choosing  $C = \max(C_y, C_y \mathcal{B})$ , the previous equation is rewritten as:

$$\begin{aligned}
| \mathcal{A}(\mathbf{G}^e; \mathbf{m}, \delta \mathbf{G}) + \mathcal{B}(\mathbf{G}^e; \mathbf{m}, \delta \mathbf{G}) | &\leq C \sum_e \|\nabla \mathbf{m}\|_{L^2(\Omega^e)} \|\nabla \delta \mathbf{G}\|_{L^2(\Omega^e)} \\
&+ C \sum_e \|\nabla \mathbf{m}\|_{L^2(\Omega^e)} \|\delta \mathbf{G}\|_{L^2(\Omega^e)} \\
&+ C \sum_e \|\mathbf{m}\|_{L^2(\Omega^e)} \|\nabla \delta \mathbf{G}\|_{L^2(\Omega^e)} \\
&+ C \sum_e \|\mathbf{m}\|_{L^2(\Omega^e)} \|\delta \mathbf{G}\|_{L^2(\Omega^e)} \\
&+ C \sum_e \|\mathbf{h}_s^{-\frac{1}{2}} \llbracket \mathbf{m}_n \rrbracket\|_{L^2(\partial\Omega^e)} \|\mathbf{h}_s^{-\frac{1}{2}} \llbracket \nabla \delta \mathbf{G}_n \rrbracket\|_{L^2(\partial\Omega^e)} \tag{D.80} \\
&+ C \sum_e \|\mathbf{h}_s^{\frac{1}{2}} \nabla \mathbf{m}\|_{L^2(\partial\Omega^e)} \|\mathbf{h}_s^{-\frac{1}{2}} \llbracket \delta \mathbf{G}_n \rrbracket\|_{L^2(\partial\Omega^e)} \\
&+ C \sum_e \|\mathbf{h}_s^{-\frac{1}{2}} \llbracket \mathbf{m}_n \rrbracket\|_{L^2(\partial\Omega^e)} \|\mathbf{h}_s^{\frac{1}{2}} \nabla \delta \mathbf{G}\|_{L^2(\partial\Omega^e)} \\
&+ C \sum_e \|\mathbf{h}_s^{\frac{1}{2}} \mathbf{m}\|_{L^2(\partial\Omega^e)} \|\mathbf{h}_s^{-\frac{1}{2}} \llbracket \delta \mathbf{G}_n \rrbracket\|_{L^2(\partial\Omega^e)} \\
&+ C \sum_e \|\mathbf{h}_s^{\frac{1}{2}} \delta \mathbf{G}\|_{L^2(\partial\Omega^e)} \|\mathbf{h}_s^{-\frac{1}{2}} \llbracket \mathbf{m}_n \rrbracket\|_{L^2(\partial\Omega^e)} .
\end{aligned}$$

After some maths, this becomes

$$\begin{aligned}
| \mathcal{A}(\mathbf{G}^e; \mathbf{m}, \delta \mathbf{G}) + \mathcal{B}(\mathbf{G}^e; \mathbf{m}, \delta \mathbf{G}) | &\leq C \sum_e \left[ \left\| \nabla \mathbf{m} \right\|_{L^2(\Omega^e)} + \left\| \mathbf{m} \right\|_{L^2(\Omega^e)} + h_s^{\frac{1}{2}} \left\| \mathbf{m} \right\|_{L^2(\partial \Omega^e)} \right. \\
&\quad \left. + h_s^{\frac{1}{2}} \left\| \nabla \mathbf{m} \right\|_{L^2(\partial \Omega^e)} + h_s^{-\frac{1}{2}} \left\| \llbracket \mathbf{m}_n \rrbracket \right\|_{L^2(\partial \Omega^e)} \right] \\
&\quad \times \left[ \left\| \nabla \delta \mathbf{G} \right\|_{L^2(\Omega^e)} + \left\| \delta \mathbf{G} \right\|_{L^2(\Omega^e)} + h_s^{\frac{1}{2}} \left\| \delta \mathbf{G} \right\|_{L^2(\partial \Omega^e)} \right. \\
&\quad \left. + h_s^{\frac{1}{2}} \left\| \nabla \delta \mathbf{G} \right\|_{L^2(\partial \Omega^e)} + h_s^{-\frac{1}{2}} \left\| \llbracket \delta \mathbf{G}_n \rrbracket \right\|_{L^2(\partial \Omega^e)} \right]. \tag{D.81}
\end{aligned}$$

Using the Cauchy-Schwartz' inequality, Eq. (2.26), and the property  $2ab \leq a^2 + b^2$ , this last equation becomes

$$\begin{aligned}
&| \mathcal{A}(\mathbf{G}^e; \mathbf{m}, \delta \mathbf{G}) + \mathcal{B}(\mathbf{G}^e; \mathbf{m}, \delta \mathbf{G}) |^2 \\
&\leq C^2 \sum_e \left[ \left\| \nabla \mathbf{m} \right\|_{L^2(\Omega^e)} + \left\| \mathbf{m} \right\|_{L^2(\Omega^e)} + h_s^{\frac{1}{2}} \left\| \mathbf{m} \right\|_{L^2(\partial \Omega^e)} \right. \\
&\quad \left. + h_s^{\frac{1}{2}} \left\| \nabla \mathbf{m} \right\|_{L^2(\partial \Omega^e)} + h_s^{-\frac{1}{2}} \left\| \llbracket \mathbf{m}_n \rrbracket \right\|_{L^2(\partial \Omega^e)} \right]^2 \\
&\quad \times \sum_{e'} \left[ \left\| \nabla \delta \mathbf{G} \right\|_{L^2(\Omega^{e'})} + \left\| \delta \mathbf{G} \right\|_{L^2(\Omega^{e'})} + h_s^{\frac{1}{2}} \left\| \delta \mathbf{G} \right\|_{L^2(\partial \Omega^{e'})} \right. \\
&\quad \left. + h_s^{\frac{1}{2}} \left\| \nabla \delta \mathbf{G} \right\|_{L^2(\partial \Omega^{e'})} + h_s^{-\frac{1}{2}} \left\| \llbracket \delta \mathbf{G}_n \rrbracket \right\|_{L^2(\partial \Omega^{e'})} \right]^2 \tag{D.82} \\
&\leq 4C^2 \sum_e \left[ \left\| \nabla \mathbf{m} \right\|_{L^2(\Omega^e)}^2 + \left\| \mathbf{m} \right\|_{L^2(\Omega^e)}^2 + h_s \left\| \mathbf{m} \right\|_{L^2(\partial \Omega^e)}^2 + \right. \\
&\quad \left. h_s \left\| \nabla \mathbf{m} \right\|_{L^2(\partial \Omega^e)}^2 + h_s^{-1} \left\| \llbracket \mathbf{m}_n \rrbracket \right\|_{L^2(\partial \Omega^e)}^2 \right] \times \\
&\quad \sum_{e'} \left[ \left\| \nabla \delta \mathbf{G} \right\|_{L^2(\Omega^{e'})}^2 + \left\| \delta \mathbf{G} \right\|_{L^2(\Omega^{e'})}^2 + h_s \left\| \delta \mathbf{G} \right\|_{L^2(\partial \Omega^{e'})}^2 \right. \\
&\quad \left. + h_s \left\| \nabla \delta \mathbf{G} \right\|_{L^2(\partial \Omega^{e'})}^2 + h_s^{-1} \left\| \llbracket \delta \mathbf{G}_n \rrbracket \right\|_{L^2(\partial \Omega^{e'})}^2 \right].
\end{aligned}$$

Considering 4 in C, and using the definition of the mesh dependent norm, Eq. (2.12), we get:

$$| \mathcal{A}(\mathbf{G}^e; \mathbf{m}, \delta \mathbf{G}) + \mathcal{B}(\mathbf{G}^e; \mathbf{m}, \delta \mathbf{G}) | \leq C \left\| \mathbf{m} \right\|_1 \left\| \delta \mathbf{G} \right\|_1 \quad \forall \mathbf{m}, \delta \mathbf{G} \in X. \tag{D.83}$$

Moreover, using Eq. (2.22), we obtain

$$| \mathcal{A}(\mathbf{G}^e; \mathbf{m}, \delta \mathbf{G}_h) + \mathcal{B}(\mathbf{G}^e; \mathbf{m}, \delta \mathbf{G}_h) | \leq C^k \left\| \mathbf{m} \right\|_1 \left\| \delta \mathbf{G}_h \right\| \quad \forall \mathbf{m} \in X, \delta \mathbf{G}_h \in X^k, \tag{D.84}$$

and again, using Eq. (2.22), we have

$$| \mathcal{A}(\mathbf{G}^e; \mathbf{m}_h, \delta \mathbf{G}_h) + \mathcal{B}(\mathbf{G}^e; \mathbf{m}_h, \delta \mathbf{G}_h) | \leq C^k \left\| \mathbf{m}_h \right\| \left\| \delta \mathbf{G}_h \right\| \quad \forall \mathbf{m}_h, \delta \mathbf{G}_h \in X^k. \tag{D.85}$$

## D.4 Uniqueness of the solution for Electro-Thermo-Mechanical coupling

Let us first show that for a given  $\boldsymbol{\varphi} \in [L^2(\Omega)]^d \times L^2(\Omega) \times L^2(\Omega)$ , there is a unique  $\boldsymbol{\phi}_h \in X^k$  such that

$$\mathcal{A}(\mathbf{G}^e; \delta \mathbf{G}_h, \boldsymbol{\phi}_h) + \mathcal{B}(\mathbf{G}^e; \delta \mathbf{G}_h, \boldsymbol{\phi}_h) = \sum_e \int_{\Omega_e} \boldsymbol{\varphi}^T \delta \mathbf{G}_h d\Omega \quad \forall \delta \mathbf{G}_h \in X^k. \quad (\text{D.86})$$

Lemma 5.4.1, Eq. (5.122), with  $\delta \mathbf{G}_h = \boldsymbol{\phi}_h \in X^k$ , implies that  $\exists C_1^k, C_2^k$  such that

$$\mathcal{A}(\mathbf{G}^e; \boldsymbol{\phi}_h, \boldsymbol{\phi}_h) + \mathcal{B}(\mathbf{G}^e; \boldsymbol{\phi}_h, \boldsymbol{\phi}_h) \geq C_1^k \|\boldsymbol{\phi}_h\|^2 - C_2^k \|\boldsymbol{\phi}_h\|_{L^2(\Omega_h)}^2. \quad (\text{D.87})$$

Choosing  $\delta \mathbf{G}_h = \boldsymbol{\phi}_h$  in Eq. (D.86) thus yields

$$C_1^k \|\boldsymbol{\phi}_h\|^2 - C_2^k \|\boldsymbol{\phi}_h\|_{L^2(\Omega_h)}^2 \leq \sum_e \int_{\Omega} \boldsymbol{\varphi}^T \boldsymbol{\phi}_h d\Omega \leq \|\boldsymbol{\varphi}\|_{L^2(\Omega_h)} \|\boldsymbol{\phi}_h\|_{L^2(\Omega_h)}, \quad (\text{D.88})$$

or again

$$C_1^k \|\boldsymbol{\phi}_h\|^2 \leq \|\boldsymbol{\varphi}\|_{L^2(\Omega_h)} \|\boldsymbol{\phi}_h\|_{L^2(\Omega_h)} + C_2^k \|\boldsymbol{\phi}_h\|_{L^2(\Omega_h)}^2. \quad (\text{D.89})$$

By the use of the the energy norm definition (2.11), we thus deduce  $\|\boldsymbol{\phi}_h\|_{L^2(\Omega_h)} \leq \|\boldsymbol{\phi}_h\|$ , and Eq. (D.90) becomes

$$C_1^k \|\boldsymbol{\phi}_h\|^2 \leq \|\boldsymbol{\varphi}\|_{L^2(\Omega_h)} \|\boldsymbol{\phi}_h\| + C_2^k \|\boldsymbol{\phi}_h\| \|\boldsymbol{\phi}_h\|_{L^2(\Omega_h)}. \quad (\text{D.90})$$

Hence, we have

$$\|\boldsymbol{\phi}_h\| \leq C_3^k \|\boldsymbol{\varphi}\|_{L^2(\Omega_h)} + C_4^k \|\boldsymbol{\phi}_h\|_{L^2(\Omega_h)}. \quad (\text{D.91})$$

The term  $\|\boldsymbol{\phi}_h\|_{L^2(\Omega_h)}$  can be estimated as follows using the auxiliary problem stated by Eq. (5.126), with  $\boldsymbol{\phi} = \boldsymbol{\phi}_h$ . Then it follows from [23, Theorem 8.3 and Lemma 9.17] that there exists a unique solution  $\boldsymbol{\psi} \in [H^2(\Omega)]^d \times H^2(\Omega) \times H^2(\Omega)$  to the problem stated by Eq. (5.126), and the solution satisfies the elliptic property stated by Eq. (5.127). Multiplying Eq. (5.126) by  $\boldsymbol{\phi}_h$ , then integrating on  $\Omega_h$ , and integrating by parts, lead to

$$\begin{aligned} & \sum_e \int_{\Omega_e} [\mathbf{w}_{\nabla \mathbf{G}}(\mathbf{G}^e) \nabla \boldsymbol{\psi} + \mathbf{w}_{\mathbf{G}}(\mathbf{G}^e, \nabla \mathbf{G}^e) \boldsymbol{\psi}]^T \nabla \boldsymbol{\phi}_h d\Omega \\ & - \sum_e \int_{\partial \Omega_e} [\mathbf{w}_{\nabla \mathbf{G}}(\mathbf{G}^e) \nabla \boldsymbol{\psi} + \mathbf{w}_{\mathbf{G}}(\mathbf{G}^e, \nabla \mathbf{G}^e) \boldsymbol{\psi}]^T \boldsymbol{\phi}_{h_n} dS \\ & + \sum_e \int_{\Omega_e} [\mathbf{d}_{\nabla \mathbf{G}}(\mathbf{G}^e) \nabla \boldsymbol{\psi}]^T \boldsymbol{\phi}_h d\Omega + \sum_e \int_{\Omega_e} [\mathbf{d}_{\mathbf{G}}(\mathbf{G}^e) \boldsymbol{\psi}]^T \boldsymbol{\phi}_h d\Omega = \|\boldsymbol{\phi}_h\|_{L^2(\Omega_h)}^2. \end{aligned} \quad (\text{D.92})$$

As  $\boldsymbol{\psi} \in [H^2(\Omega)]^d \times H^2(\Omega) \times H^2(\Omega)$  implies  $[\boldsymbol{\psi}] = [[\nabla \boldsymbol{\psi}]] = 0$  on  $\partial_I \Omega_h$  and  $[\boldsymbol{\psi}] = -\boldsymbol{\psi} = 0$  on  $\partial_D \Omega_h$ , we conclude by comparing to Eqs. (5.115, 5.116) that

$$\left\{ \begin{array}{l} \int_{\Omega_h} [\mathbf{w}_{\nabla \mathbf{G}}(\mathbf{G}^e) \nabla \boldsymbol{\psi}]^T \nabla \boldsymbol{\phi}_h + \int_{\partial_I \Omega_h} [\mathbf{w}_{\nabla \mathbf{G}}(\mathbf{G}^e) \nabla \boldsymbol{\psi}]^T [[\boldsymbol{\phi}_{h_n}]] dS \\ - \int_{\partial_D \Omega_h} [\mathbf{w}_{\nabla \mathbf{G}}(\mathbf{G}^e) \nabla \boldsymbol{\psi}]^T \boldsymbol{\phi}_{h_n} dS = \mathcal{A}(\mathbf{G}^e; \boldsymbol{\psi}, \boldsymbol{\phi}_h) \\ \int_{\Omega_h} [\mathbf{w}_{\mathbf{G}}(\mathbf{G}^e, \nabla \mathbf{G}^e) \boldsymbol{\psi}]^T \nabla \boldsymbol{\phi}_h d\Omega + \int_{\partial_I \Omega_h} [\mathbf{w}_{\mathbf{G}}(\mathbf{G}^e, \nabla \mathbf{G}^e) \boldsymbol{\psi}]^T [[\boldsymbol{\phi}_{h_n}]] dS \\ - \int_{\partial_D \Omega_h} [\mathbf{w}_{\mathbf{G}}(\mathbf{G}^e, \nabla \mathbf{G}^e) \boldsymbol{\psi}]^T \boldsymbol{\phi}_{h_n} dS + \int_{\Omega_h} \boldsymbol{\phi}_h^T \mathbf{d}_{\nabla \mathbf{G}}(\mathbf{G}^e) \nabla \boldsymbol{\psi} d\Omega \\ + \int_{\Omega_h} \boldsymbol{\phi}_h^T \mathbf{d}_{\mathbf{G}}(\mathbf{G}^e) \boldsymbol{\psi} d\Omega = \mathcal{B}(\mathbf{G}^e; \boldsymbol{\psi}, \boldsymbol{\phi}_h), \end{array} \right. \quad (\text{D.93})$$

leading to

$$\| \phi_h \|_{L^2(\Omega_h)}^2 = \mathcal{A}(\mathbf{G}^e; \psi, \phi_h) + \mathcal{B}(\mathbf{G}^e; \psi, \phi_h). \quad (\text{D.94})$$

Inserting  $I_h \psi$  the interpolant of  $\psi$  in  $X^k$ , this can be rewritten as

$$\begin{aligned} \| \phi_h \|_{L^2(\Omega_h)}^2 &= \mathcal{A}(\mathbf{G}^e; \psi - I_h \psi, \phi_h) + \mathcal{B}(\mathbf{G}^e; \psi - I_h \psi, \phi_h) \\ &\quad + \mathcal{A}(\mathbf{G}^e; I_h \psi, \phi_h) + \mathcal{B}(\mathbf{G}^e; I_h \psi, \phi_h). \end{aligned} \quad (\text{D.95})$$

From Eq. (D.86), in the particular case of  $\delta \mathbf{G}_h = I_h \psi$ , assuming there are several solutions to Eq. (D.86), we have for one solution  $\phi_h$

$$\begin{aligned} \mathcal{A}(\mathbf{G}^e; I_h \psi, \phi_h) + \mathcal{B}(\mathbf{G}^e; I_h \psi, \phi_h) &= \int_{\Omega_h} \varphi I_h \psi d\Omega \\ &\leq \| \varphi \|_{L^2(\Omega_h)} \| I_h \psi \|_{L^2(\Omega_h)}. \end{aligned} \quad (\text{D.96})$$

Now an application of Lemma 5.4.2, Eq. (5.124), with Lemma 2.4.6, Eq. (2.23), yields

$$\begin{aligned} | \mathcal{A}(\mathbf{G}^e; \psi - I_h \psi, \phi_h) + \mathcal{B}(\mathbf{G}^e; \psi - I_h \psi, \phi_h) | &\leq C^k \| \psi - I_h \psi \|_1 \| \phi_h \| \\ &\leq C^k h_s^{\mu-1} \| \psi \|_{H^s(\Omega_h)} \| \phi_h \|, \end{aligned} \quad (\text{D.97})$$

with  $\mu = \min \{s, k + 1\}$ .

Substituting Eq. (D.96) and Eq. (D.97), for  $s = 2$ , in Eq. (D.95), yields

$$\| \phi_h \|_{L^2(\Omega_h)}^2 \leq C^k h_s \| \psi \|_{H^2(\Omega_h)} \| \phi_h \| + \| \varphi \|_{L^2(\Omega_h)} \| I_h \psi \|_{L^2(\Omega_h)}, \quad (\text{D.98})$$

whereas, for  $h_s$  sufficient small, the term  $\| I_h \psi \|_{L^2(\Omega)}$  can be bounded using Lemma 2.4.6, Eq. (2.23), by

$$\begin{aligned} \| I_h \psi \|_{L^2(\Omega_h)} &\leq \| I_h \psi - \psi + \psi \|_{L^2(\Omega_h)} \\ &\leq \| I_h \psi - \psi \|_{L^2(\Omega_h)} + \| \psi \|_{L^2(\Omega_h)} \leq \| I_h \psi - \psi \|_1 + \| \psi \|_{H^2(\Omega_h)} \\ &\leq C^k h_s \| \psi \|_{H^2(\Omega_h)} + \| \psi \|_{H^2(\Omega_h)} \leq C^k \| \psi \|_{H^2(\Omega_h)}. \end{aligned} \quad (\text{D.99})$$

Eq. (D.98) is thus rewritten for small  $h_s$

$$\| \phi_h \|_{L^2(\Omega_h)}^2 \leq C^k \| \psi \|_{H^2(\Omega_h)} \left( h_s \| \phi_h \| + \| \varphi \|_{L^2(\Omega_h)} \right). \quad (\text{D.100})$$

By using the regular ellipticity Eq. (5.127), we obtain

$$\| \phi_h \|_{L^2(\Omega_h)} \leq C^k h_s \| \phi_h \| + C^k \| \varphi \|_{L^2(\Omega_h)} \leq C^k \| \varphi \|_{L^2(\Omega_h)}, \quad (\text{D.101})$$

for small  $h_s$ . Hence we complete the proof of Lemma 5.4.3 by substituting Eq. (D.101) in Eq. (D.91)

$$\| \phi_h \| \leq C^k \| \varphi \|_{L^2(\Omega_h)}. \quad (\text{D.102})$$

Indeed, the existence of the solution  $\phi_h$  to the problem stated by Eq. (D.86) follows from the uniqueness, which follows trivially from Eq. (D.102). Indeed for  $\varphi_1, \varphi_2 \in [L^2(\Omega)]^3 \times L^2(\Omega) \times L^2(\Omega)$ , we have

$$\| \phi_{h_1} - \phi_{h_2} \|_{L^2(\Omega_h)} \leq C^k \| \varphi_1 - \varphi_2 \|_{L^2(\Omega_h)}, \quad (\text{D.103})$$

and  $\phi_{h_1} = \phi_{h_2}$  if  $\varphi_1 = \varphi_2$ .

## D.5 The bound of the nonlinear term $\mathcal{N}(\mathbf{G}^e, \mathbf{y}; \delta\mathbf{G}_h)$

### D.5.1 Bounds of different contributions

The bound of  $\mathcal{N}(\mathbf{G}^e, \mathbf{y}; \delta\mathbf{G}_h)$  follows from the argumentation reported in [25] and the bound of the nonlinear term  $\mathcal{N}(\mathbf{G}^e, \mathbf{y}; \delta\mathbf{G}_h)$  is nominated by the term with the largest bound.

Indeed the bound of the first forth terms of Eq. (5.114) follow from the argumentation reported in Chapter 4 after replacing  $\mathbf{M}^e, \delta\mathbf{M}_h, \mathbf{j}$  by  $\mathbf{G}^e, \delta\mathbf{G}_h, \mathbf{w}$  respectively. Henceforth, only the final results are given for the first forth terms as

$$\begin{aligned} |\mathcal{I}_1| &= \left| \int_{\Omega_h} (\nabla \delta\mathbf{G}_h)^\top \langle \bar{\mathbf{R}}_w(\zeta, \nabla \zeta) \rangle d\Omega \right| \\ &\leq C^k C_y h_s^{\mu-2-\varepsilon} \sigma \|\delta\mathbf{G}_h\|_{H^1(\Omega_h)} \|\mathbf{G}^e\|_{H^s(\Omega_h)}, \end{aligned} \quad (\text{D.104})$$

$$\begin{aligned} |\mathcal{I}_2| &= \left| \int_{\partial_I \Omega_h \cup \partial_D \Omega_h} \llbracket \delta\mathbf{G}_{h_n}^\top \rrbracket \langle \bar{\mathbf{R}}_w(\zeta, \nabla \zeta) \rangle dS \right| \\ &\leq C^k C_y \|\mathbf{G}^e\|_{H^s(\Omega_h)} h_s^{\mu-2-\varepsilon} \sigma \left( \sum_e h_s^{-1} \|\llbracket \delta\mathbf{G}_{h_n} \rrbracket\|_{L^2(\partial\Omega^e)}^2 \right)^{\frac{1}{2}}, \end{aligned} \quad (\text{D.105})$$

$$\begin{aligned} |\mathcal{I}_3| &= \left| \int_{\partial_I \Omega_h} \llbracket \mathbf{G}_n^{eT} - \mathbf{y}_n^T \rrbracket \langle (\mathbf{w}_{\nabla \mathbf{G}}(\mathbf{G}^e) - \mathbf{w}_{\nabla \mathbf{G}}(\mathbf{y})) \nabla \delta\mathbf{G}_h \rangle dS \right| \\ &\leq C_y C^k \|\mathbf{G}^e\|_{H^s(\Omega_h)} h_s^{\mu-2-\varepsilon} \sigma \left( \sum_e h_s \|\delta\mathbf{G}_h\|_{H^1(\partial\Omega^e)}^2 \right)^{\frac{1}{2}}, \end{aligned} \quad (\text{D.106})$$

$$\begin{aligned} |\mathcal{I}_4| &= \left| \int_{\partial_I \Omega_h} \llbracket \mathbf{G}_n^{eT} - \mathbf{y}_n^T \rrbracket \left\langle \frac{\mathcal{B}}{h_s} (\mathbf{w}_{\nabla \mathbf{G}}(\mathbf{G}^e) - \mathbf{w}_{\nabla \mathbf{G}}(\mathbf{y})) \right\rangle \llbracket \delta\mathbf{G}_{h_n} \rrbracket dS \right| \\ &\leq C^k C_y \|\mathbf{G}^e\|_{H^s(\Omega_h)} h_s^{\mu-2-\varepsilon} \sigma \left( \sum_e h_s^{-1} \|\llbracket \delta\mathbf{G}_{h_n} \rrbracket\|_{L^2(\partial\Omega^e)}^2 \right)^{\frac{1}{2}}. \end{aligned} \quad (\text{D.107})$$

It should be noted that all the intermediate bounds  $\left( \sum_e \|\zeta\|_{L^4(\Omega^e)}^4 \right)^{\frac{1}{4}}$ ,  $\left( \sum_e \|\nabla \zeta\|_{L^2(\Omega^e)}^2 \right)^{\frac{1}{2}}$ ,  $\left( \sum_e \|\nabla \zeta\|_{L^2(\Omega^e)}^2 \right)^{\frac{1}{2}}$ ,  $\left( \sum_e \|\zeta\|_{L^4(\partial\Omega^e)}^4 \right)^{\frac{1}{4}}$ ,  $\left( \sum_e \|\llbracket \zeta \rrbracket\|_{L^4(\partial\Omega^e)}^4 \right)^{\frac{1}{4}}$ ,  $\left( \sum_e \|\nabla \zeta\|_{L^4(\partial\Omega^e)}^4 \right)^{\frac{1}{4}}$ ,  $\|\delta\mathbf{G}_h\|_{W_4^1(\Omega^e)}$ , and  $\|\delta\mathbf{G}_h\|_{W_4^1(\Omega^e)}$  can be derived by the same spirit as in Lemma 4.4.4, after replacing  $\mathbf{M}^e, I_h \mathbf{M}$  and  $\delta\mathbf{M}_h$  by  $\mathbf{G}^e, I_h \mathbf{G}$  and  $\delta\mathbf{G}_h$  respectively. We will use the bounds (4.122-4.134) of Chapter 4 directly.

Then the bound of the fifth term is derived as follows, using Eq. (D.124)

$$\begin{aligned}
|\mathcal{I}_5| &= \left| \int_{\partial_t \Omega_h \cup \partial_D \Omega_h} [(\mathbf{G}^e - \mathbf{G}_h)^T \bar{\mathbf{o}}_{\mathbf{G}}^T(\mathbf{G}_h)(\mathbf{G}^e - \mathbf{G}_h)] \langle \delta \mathbf{G}_{h_n} \rangle dS \right| \\
&\leq 2C_y \sum_e \left| \int_{\partial_t \Omega^e \cup \partial_D \Omega^e} [(\mathbf{G}^e - \mathbf{G}_h)^T] \mathbf{I}(\mathbf{G}^e - \mathbf{G}_h) \delta \mathbf{G}_{h_n} dS \right| \\
&\quad + \frac{1}{8} C_y \sum_e \left| \int_{\partial_t \Omega^e} [(\mathbf{G}^e - \mathbf{G}_h)^T] \mathbf{I} [(\mathbf{G}^e - \mathbf{G}_h)] [\delta \mathbf{G}_{h_n}] dS \right| \\
&\leq |\mathcal{I}_{51}| + |\mathcal{I}_{52}|.
\end{aligned} \tag{D.108}$$

Therefore, with  $\boldsymbol{\zeta} = \mathbf{G}^e - \mathbf{G}_h$ , one has

$$\begin{aligned}
|\mathcal{I}_{51}| &\leq 2C_y \sum_e \left| \int_{\partial \Omega^e} [\boldsymbol{\zeta}^T] \mathbf{I}(\boldsymbol{\zeta} \delta \mathbf{G}_{h_n}) dS \right| \\
&\leq 2C_y \sum_e \left[ h_s^{-\frac{1}{2}} \|\llbracket \boldsymbol{\zeta} \rrbracket\|_{L^4(\partial \Omega^e)} \|\boldsymbol{\zeta}\|_{L^4(\partial \Omega^e)} \left( h_s \|\delta \mathbf{G}_h\|_{L^2(\partial \Omega^e)}^2 \right)^{\frac{1}{2}} \right] \\
&\leq 2C_y h_s^{-\frac{1}{2}} \left( \sum_e \|\llbracket \boldsymbol{\zeta} \rrbracket\|_{L^4(\partial \Omega^e)}^4 \right)^{\frac{1}{4}} \left( \sum_e \|\boldsymbol{\zeta}\|_{L^4(\partial \Omega^e)}^4 \right)^{\frac{1}{4}} \left( \sum_e h_s \|\delta \mathbf{G}_h\|_{L^2(\partial \Omega^e)}^2 \right)^{\frac{1}{2}} \\
&\leq 2C_y h_s^{-\frac{1}{2}} C^k h_s^{-\frac{3}{4}} \sigma h_s^{\frac{1}{4}} \sigma \left( \sum_e h_s \|\delta \mathbf{G}_h\|_{L^2(\partial \Omega^e)}^2 \right)^{\frac{1}{2}} \\
&\leq 2C_y C^k \|\mathbf{G}^e\|_{H^s(\Omega_h)} h_s^{\mu-2-\varepsilon} \sigma \left( \sum_e h_s \|\delta \mathbf{G}_h\|_{L^2(\partial \Omega^e)}^2 \right)^{\frac{1}{2}},
\end{aligned} \tag{D.109}$$

where we have used the generalized Hölder's inequality (2.25), the generalized Cauchy-Schwartz' inequality (2.27), the definition of  $C_y$  in Eq. (5.118), and the bounds (4.131,

4.132). Similarly we have the following bound for  $\mathcal{I}_{52}$

$$\begin{aligned}
|\mathcal{I}_{52}| &\leq C_y \frac{1}{8} \sum_e \left| \int_{\partial\Omega^e} [(\mathbf{G}^e - \mathbf{G}_h)^T] \mathbf{I} [\mathbf{G}^e - \mathbf{G}_h] [\delta\mathbf{G}_{h_n}] dS \right| \\
&\leq \frac{1}{8} C_y \sum_e \left| \int_{\partial\Omega^e} [\boldsymbol{\zeta}^T] \mathbf{I} [\boldsymbol{\zeta}] [\delta\mathbf{G}_{h_n}] dS \right| \\
&\leq \frac{1}{8} C_y \sum_e \left[ h_s^{\frac{1}{2}} \|\boldsymbol{\zeta}\|_{L^4(\partial\Omega^e)} \|\boldsymbol{\zeta}\|_{L^4(\partial\Omega^e)} \left( h_s^{-1} \|\delta\mathbf{G}_h\|_{L^2(\partial\Omega^e)}^2 \right)^{\frac{1}{2}} \right] \\
&\leq \frac{1}{8} C_y h_s^{\frac{1}{2}} \left( \sum_e \|\boldsymbol{\zeta}\|_{L^4(\partial\Omega^e)}^4 \right)^{\frac{1}{4}} \left( \sum_e \|\boldsymbol{\zeta}\|_{L^4(\partial\Omega^e)}^4 \right)^{\frac{1}{4}} \left( \sum_e h_s^{-1} \|\delta\mathbf{G}_h\|_{L^2(\partial\Omega^e)}^2 \right)^{\frac{1}{2}} \\
&\leq \frac{1}{8} C_y h_s^{\frac{1}{2}} C^k h_s^{\frac{1}{4}} \sigma h_s^{\frac{1}{4}} \sigma \left( \sum_e h_s^{-1} \|\delta\mathbf{G}_h\|_{L^2(\partial\Omega^e)}^2 \right)^{\frac{1}{2}} \\
&\leq \frac{1}{8} C_y C^k \|\mathbf{G}^e\|_{H^s(\Omega_h)} h_s^{\mu-\varepsilon} \sigma \left( \sum_e h_s^{-1} \|\delta\mathbf{G}_h\|_{L^2(\partial\Omega^e)}^2 \right)^{\frac{1}{2}}.
\end{aligned} \tag{D.110}$$

By combining Eqs. (D.109, and D.110), we have

$$\begin{aligned}
|\mathcal{I}_5| &\leq 2C_y C^k \|\mathbf{G}^e\|_{H^s(\Omega_h)} h_s^{\mu-2-\varepsilon} \sigma \left( \sum_e h_s \|\delta\mathbf{G}_h\|_{L^2(\partial\Omega^e)}^2 \right)^{\frac{1}{2}} \\
&\quad + \frac{1}{8} C_y C^k \|\mathbf{G}^e\|_{H^s(\Omega_h)} h_s^{\mu-\varepsilon} \sigma \left( \sum_e h_s^{-1} \|\delta\mathbf{G}_h\|_{L^2(\partial\Omega^e)}^2 \right)^{\frac{1}{2}}
\end{aligned} \tag{D.111}$$

Finally to bound the last term of the right hand side of Eq. (5.109), we rewrite it using Eq. (5.109) as

$$\begin{aligned}
\mathcal{I}_6 &= \int_{\Omega_h} \delta\mathbf{G}_h^T \bar{\mathbf{R}}_d(\boldsymbol{\zeta}, \nabla\boldsymbol{\zeta}) d\Omega = \sum_e \int_{\Omega^e} \delta\mathbf{G}_h^T (\boldsymbol{\zeta}^T \bar{\mathbf{d}}_{\mathbf{G}\mathbf{G}}(\mathbf{y}, \nabla\mathbf{y}) \boldsymbol{\zeta}) d\Omega \\
&\quad + 2 \sum_e \int_{\Omega^e} \delta\mathbf{G}_h^T (\boldsymbol{\zeta}^T \bar{\mathbf{d}}_{\mathbf{G}\nabla\mathbf{G}}(\mathbf{y}) \nabla\boldsymbol{\zeta}) d\Omega \\
&= \mathcal{I}_{61} + 2\mathcal{I}_{62}.
\end{aligned} \tag{D.112}$$

The first part is bounded by

$$\begin{aligned}
|\mathcal{I}_{61}| &\leq \left| \sum_e \int_{\Omega^e} \delta\mathbf{G}_h^T (\boldsymbol{\zeta}^T \bar{\mathbf{d}}_{\mathbf{G}\mathbf{G}}(\mathbf{y}, \nabla\mathbf{y}) \boldsymbol{\zeta}) d\Omega \right| \leq C_y \sum_e \|\boldsymbol{\zeta}\|_{L^4(\Omega^e)} \|\boldsymbol{\zeta}\|_{L^4(\Omega^e)} \|\delta\mathbf{G}_h\|_{L^2(\Omega^e)} \\
&\leq C_y \left( \sum_e \|\boldsymbol{\zeta}\|_{L^4(\Omega^e)}^4 \right)^{\frac{1}{4}} \left( \sum_e \|\boldsymbol{\zeta}\|_{L^4(\Omega^e)}^4 \right)^{\frac{1}{4}} \left( \sum_e \|\delta\mathbf{G}_h\|_{L^2(\Omega^e)}^2 \right)^{\frac{1}{2}} \\
&\leq C^k C_y h_s^{\mu-2-\varepsilon} \sigma \|\delta\mathbf{G}_h\|_{L^2(\Omega_h)} \|\mathbf{G}^e\|_{H^s(\Omega_h)}.
\end{aligned} \tag{D.113}$$



This bound is estimated by recalling the generalized Hölder inequality (2.25), the generalized Cauchy-Schwartz' inequality (2.27), the definition of  $C_y$  in Eq. (5.118), and the bound (4.123).

The second part can be estimated in the same way using the generalized Hölder's inequality (2.25), the generalized Cauchy-Schwartz' inequality (2.27), the definition of  $C_y$  in Eq. (5.118), the bounds (4.123, 4.124), and the inverse inequality of Lemma 2.4.4

$$\begin{aligned}
|\mathcal{I}_{62}| &\leq \left| \sum_e \int_{\Omega^e} \delta \mathbf{G}_h^T (\boldsymbol{\zeta}^T \bar{\mathbf{d}}_{\mathbf{G}\nabla\mathbf{G}}(\mathbf{y}) \nabla \boldsymbol{\zeta}) \, d\Omega \right| \leq C_y \sum_e \|\boldsymbol{\zeta}\|_{L^4(\Omega^e)} \|\nabla \boldsymbol{\zeta}\|_{L^2(\Omega^e)} \|\delta \mathbf{G}_h\|_{L^4(\Omega^e)} \\
&\leq C_y \left( \sum_e \|\boldsymbol{\zeta}\|_{L^4(\Omega^e)}^4 \right)^{\frac{1}{4}} \left( \sum_e \|\nabla \boldsymbol{\zeta}\|_{L^2(\Omega^e)}^2 \right)^{\frac{1}{2}} \left( \sum_e \|\delta \mathbf{G}_h\|_{L^4(\Omega^e)}^4 \right)^{\frac{1}{4}} \\
&\leq C^k C_y h_s^{\mu-2-\varepsilon} \sigma \|\delta \mathbf{G}_h\|_{L^2(\Omega_h)} \|\mathbf{G}^e\|_{H^s(\Omega_h)}.
\end{aligned} \tag{D.114}$$

Substituting Eqs. (D.113, D.114) in Eq. (D.112), we get

$$|\mathcal{I}_6| \leq C^k C_y h_s^{\mu-2-\varepsilon} \sigma \|\delta \mathbf{G}_h\|_{L^2(\Omega_h)} \|\mathbf{G}^e\|_{H^s(\Omega_h)}. \tag{D.115}$$

Combining Eqs. (D.104, D.105, D.106, D.107, D.108, and D.115), yields the bound of  $\mathcal{N}(\mathbf{G}^e, \mathbf{y}; \delta \mathbf{G}_h)$

$$\begin{aligned}
|\mathcal{N}(\mathbf{G}^e, \mathbf{y}; \delta \mathbf{G}_h)| &\leq C^k C_y \|\mathbf{G}^e\|_{H^s(\Omega_h)} h_s^{\mu-2-\varepsilon} \sigma \left[ \|\delta \mathbf{G}_h\|_{H^1(\Omega_h)} \right. \\
&\quad \left. + \left( \sum_e h_s \|\delta \mathbf{G}_h\|_{H^1(\partial\Omega^e)}^2 \right)^{\frac{1}{2}} \left( + \sum_e h_s^{-1} \|\llbracket \delta \mathbf{G}_{h_n} \rrbracket\|_{L^2(\partial\Omega^e)}^2 \right)^{\frac{1}{2}} \right].
\end{aligned} \tag{D.116}$$

### D.5.2 Declaration related to the fifth term of $\mathcal{N}(\mathbf{G}^e, \mathbf{y}; \delta \mathbf{G}_h)$

Using the identities  $\llbracket ab \rrbracket = \llbracket a \rrbracket \langle b \rangle + \langle a \rangle \llbracket b \rrbracket$  and  $\langle a \rangle \langle b \rangle = \langle ab \rangle - \frac{1}{4} \llbracket a \rrbracket \llbracket b \rrbracket$  on  $\partial_t \Omega_h$ , the term  $\llbracket (\mathbf{G}^e - \mathbf{G}_h)^T \bar{\mathbf{o}}_{\mathbf{G}}^T(\mathbf{G}_h) (\mathbf{G}^e - \mathbf{G}_h) \rrbracket \langle \delta \mathbf{G}_{h_n} \rangle$  can be rewritten with an abuse of notations on the product operator as

$$\begin{aligned}
\llbracket (\mathbf{G}^e - \mathbf{G}_h)^T \bar{\mathbf{o}}_{\mathbf{G}}^T(\mathbf{G}_h) (\mathbf{G}^e - \mathbf{G}_h) \rrbracket \langle \delta \mathbf{G}_{h_n} \rangle &= \langle (\mathbf{G}^e - \mathbf{G}_h)^T \bar{\mathbf{o}}_{\mathbf{G}}^T(\mathbf{G}_h) \rangle \llbracket \mathbf{G}^e - \mathbf{G}_h \rrbracket \langle \delta \mathbf{G}_{h_n} \rangle \\
&\quad + \llbracket (\mathbf{G}^e - \mathbf{G}_h)^T \bar{\mathbf{o}}_{\mathbf{G}}^T(\mathbf{G}_h) \rrbracket \langle \mathbf{G}^e - \mathbf{G}_h \rangle \langle \delta \mathbf{G}_{h_n} \rangle \\
&= \langle (\mathbf{G}^e - \mathbf{G}_h)^T \bar{\mathbf{o}}_{\mathbf{G}}^T(\mathbf{G}_h) \delta \mathbf{G}_{h_n} \rangle \llbracket \mathbf{G}^e - \mathbf{G}_h \rrbracket \\
&\quad - \frac{1}{4} \llbracket (\mathbf{G}^e - \mathbf{G}_h)^T \bar{\mathbf{o}}_{\mathbf{G}}^T(\mathbf{G}_h) \rrbracket \llbracket \mathbf{G}^e - \mathbf{G}_h \rrbracket \llbracket \delta \mathbf{G}_{h_n} \rrbracket \\
&\quad + \llbracket (\mathbf{G}^e - \mathbf{G}_h)^T \bar{\mathbf{o}}_{\mathbf{G}}^T(\mathbf{G}_h) \rrbracket \langle \mathbf{G}^e - \mathbf{G}_h \rangle \langle \delta \mathbf{G}_{h_n} \rangle.
\end{aligned} \tag{D.117}$$

Now, we need to solve explicitly the term  $\llbracket (\mathbf{G}^e - \mathbf{G}_h)^T \bar{\mathbf{o}}_{\mathbf{G}}^T(\mathbf{G}_h) \rrbracket$ , where  $\bar{\mathbf{o}}_{\mathbf{G}}^T(\mathbf{G}_h)$  is equal by analogy to Eq. (4.92) to

$$\bar{\mathbf{o}}_{\mathbf{G}}(\mathbf{G}_h) = \int_0^1 (1-t) \mathbf{o}_{\mathbf{G}}(\mathbf{V}^t) dt, \tag{D.118}$$

with  $\mathbf{V}^t = \mathbf{G}^e + t(\mathbf{G}_h - \mathbf{G}^e)$ . As  $\mathbf{o}_G$  only involves terms in  $\frac{2}{f_T^3}$ , we compute  $\bar{\alpha}$  the nonzero component.

$$\bar{\alpha} = 3K\alpha_{th} \int_0^1 (1-t) \left( \frac{2}{[f_T^e + t(f_T - f_T^e)]^3} \right) dt. \quad (D.119)$$

For simplicity, let us define  $\lambda$  as

$$\lambda = \int_0^1 (1-t) \frac{2}{[f_T^e + t(f_T - f_T^e)]^3} dt. \quad (D.120)$$

Setting  $a = 1 - t$ ,  $da = -dt$ ,  $db = \frac{2dt}{[f_T^e + t(f_T - f_T^e)]^3}$ , and  $b = \frac{-1}{(f_T - f_T^e)[f_T^e + t(f_T - f_T^e)]^2}$ , such that  $\lambda$  can be rewritten as

$$\begin{aligned} \lambda &= \left[ \frac{t-1}{(f_T - f_T^e)[f_T^e + t(f_T - f_T^e)]^2} \right]_0^1 - \int_0^1 \frac{dt}{(f_T - f_T^e)[f_T^e + t(f_T - f_T^e)]^2} \\ &= \frac{1}{(f_T - f_T^e)f_T^e} - \left[ \frac{-1}{(f_T - f_T^e)^2[f_T^e + t(f_T - f_T^e)]} \right]_0^1 \\ &= \frac{1}{(f_T - f_T^e)f_T^e} + \frac{1}{(f_T - f_T^e)^2 f_T} - \frac{1}{(f_T - f_T^e)^2 f_T^e} \\ &= \frac{1}{(f_T - f_T^e)f_T^e} + \frac{1}{(f_T - f_T^e)^2} \left( \frac{f_T^e - f_T}{f_T f_T^e} \right) = \frac{1}{(f_T - f_T^e)f_T^e} - \frac{1}{(f_T - f_T^e)} \frac{1}{f_T f_T^e} \\ &= \frac{-1}{(f_T - f_T^e)} \left( \frac{f_T^e - f_T}{f_T f_T^e} \right) = \frac{1}{f_T f_T^e}. \end{aligned} \quad (D.121)$$

It can be noticed that to evaluate  $\llbracket (\mathbf{G}^e - \mathbf{G}_h)^T \mathbf{o}_G^T (\mathbf{G}_h) \rrbracket$ , we need  $\lambda(f_T^e - f_T)$  which reads

$$\lambda(f_T^e - f_T) = \frac{1}{f_T f_T^e} (f_T^e - f_T) = \frac{1}{f_T^e} \left( \frac{1}{f_T} - \frac{1}{f_T^e} \right), \quad (D.122)$$

and the jump of the last result is

$$\llbracket \lambda(f_T^e - f_T) \rrbracket = \begin{cases} \frac{1}{f_T^e} \left( \frac{1}{f_T^+} - \frac{1}{f_T^-} - \frac{1}{f_T} + \frac{1}{f_T^e} \right) = -\frac{1}{f_T^e} \left( \frac{f_T^- - f_T^+}{f_T^+ f_T^-} \right) = -\frac{1}{f_T^e f_T^+ f_T^-} \llbracket f_T - f_T^e \rrbracket \text{ on } \partial_I \Omega_h \\ \frac{1}{f_T f_T^e} (f_T - f_T^e) = -\frac{1}{f_T f_T^e} \llbracket f_T - f_T^e \rrbracket \text{ on } \partial_D \Omega_h. \end{cases} \quad (D.123)$$

Hence considering this equation in the matrix form, and then substituting it in Eq. (D.117), lead to

$$\begin{aligned}
& \left| \sum_e \int_{\partial_t \Omega^e \cup \partial_D \Omega^e} [(\mathbf{G}^e - \mathbf{G}_h)^T \bar{\mathbf{o}}_{\mathbf{G}}^T(\mathbf{G}_h) (\mathbf{G}^e - \mathbf{G}_h)] \langle \delta \mathbf{G}_{h_n} \rangle dS \right| \\
& \leq \frac{1}{2} \left| \sum_e \int_{\partial_t \Omega^e} \langle (\mathbf{G}^e - \mathbf{G}_h)^T \bar{\mathbf{o}}_{\mathbf{G}}^T(\mathbf{G}_h) \delta \mathbf{G}_{h_n} \rangle [(\mathbf{G}^e - \mathbf{G}_h)] dS \right| \\
& + \frac{1}{8} \left| \sum_e \int_{\partial_t \Omega^e} [(\mathbf{G}^e - \mathbf{G}_h)^T \bar{\mathbf{o}}_{\mathbf{G}}^T(\mathbf{G}_h)] [(\mathbf{G}^e - \mathbf{G}_h)] [\delta \mathbf{G}_{h_n}] dS \right| \\
& + \frac{1}{2} \left| \sum_e \int_{\partial_t \Omega^e} [(\mathbf{G}^e - \mathbf{G}_h)^T \bar{\mathbf{o}}_{\mathbf{G}}^T(\mathbf{G}_h)] \langle \mathbf{G}^e - \mathbf{G}_h \rangle \langle \delta \mathbf{G}_{h_n} \rangle dS \right| \\
& + \left| \sum_e \int_{\partial_D \Omega^e} [(\mathbf{G}^e - \mathbf{G}_h)] \bar{\mathbf{o}}_{\mathbf{G}}^T(\mathbf{G}_h) (\mathbf{G}^e - \mathbf{G}_h) \delta \mathbf{G}_{h_n} dS \right| \tag{D.124} \\
& \leq \sum_e \left| \int_{\partial_t \Omega^e} (\mathbf{G}^e - \mathbf{G}_h)^T \mathbf{I} [(\mathbf{G}^e - \mathbf{G}_h)] \delta \mathbf{G}_{h_n} dS \right| \\
& + \frac{1}{8} \sum_e \left| \int_{\partial_t \Omega^e} [(\mathbf{G}^e - \mathbf{G}_h)^T] \mathbf{I} [(\mathbf{G}^e - \mathbf{G}_h)] [\delta \mathbf{G}_{h_n}] dS \right| \\
& + \sum_e \left| \int_{\partial_t \Omega^e} [(\mathbf{G}^e - \mathbf{G}_h)^T] \mathbf{I} (\mathbf{G}^e - \mathbf{G}_h) \delta \mathbf{G}_{h_n} dS \right| \\
& + \sum_e \left| \int_{\partial_D \Omega^e} [(\mathbf{G}^e - \mathbf{G}_h)^T] \mathbf{I} (\mathbf{G}^e - \mathbf{G}_h) \delta \mathbf{G}_{h_n} dS \right|
\end{aligned}$$

where  $\mathbf{I}$  is a matrix of unit norm and has the same size of  $\bar{\mathbf{o}}_{\mathbf{G}}^T$ .



## Appendix E

# Annexes related to chapter 6

### E.1 Tangent of the carbon fiber

The first Piola-Kirchhoff is evaluated from the second Piola-Kirchhoff as

$$\mathbf{P}_{xJ} = \mathbf{F}_{xI} \mathbf{S}_{IJ} = \mathbf{F}_{xI} (\mathbf{S}_{IJ}^{\text{is}} + \mathbf{S}_{IJ}^{\text{tr}}). \quad (\text{E.1})$$

The derivative of  $\mathbf{P}$  with respect to the deformation gradient is computed components by components

$$\frac{\partial \mathbf{S}_{IJ}^{\text{is}}}{\partial \mathbf{C}_{KL}} = \frac{\lambda}{2} \mathbf{C}_{IJ}^{-1} \mathbf{C}_{KL}^{-1} - \frac{1}{2} (\lambda \ln J - \mathbf{G}^{\text{TT}} - 3\lambda \alpha_{\text{th}} (T - T_0)) (\mathbf{C}_{IK}^{-1} \mathbf{C}_{JL}^{-1} + \mathbf{C}_{IL}^{-1} \mathbf{C}_{JK}^{-1}), \quad (\text{E.2})$$

$$\begin{aligned} \frac{\partial \mathbf{S}_{IJ}^{\text{tr}}}{\partial \mathbf{C}_{KL}} &= 2\beta^{\text{tr}} (\mathbf{C}_{IJ}^{-1} \mathbf{A}_K \mathbf{A}_L + \mathbf{C}_{KL}^{-1} \mathbf{A}_I \mathbf{A}_J) + 4\gamma^{\text{tr}} \mathbf{A}_I \mathbf{A}_J \mathbf{A}_K \mathbf{A}_L \\ &\quad - \mathbf{I}_{JK} \alpha^{\text{tr}} \mathbf{A}_I \mathbf{A}_L - \mathbf{I}_{IK} \alpha^{\text{tr}} \mathbf{A}_J \mathbf{A}_L - \beta^{\text{tr}} (\mathbf{I}_4 - 1) (\mathbf{C}_{IK}^{-1} \mathbf{C}_{JL}^{-1} + \mathbf{C}_{IL}^{-1} \mathbf{C}_{JK}^{-1}). \end{aligned} \quad (\text{E.3})$$

which result in

$$\frac{\partial \mathbf{P}_{xJ}}{\partial \mathbf{F}_{kL}} = \mathbf{I}_{xk} (\mathbf{S}_{JL}^{\text{is}} + \mathbf{S}_{JL}^{\text{tr}}) + \mathbf{F}_{xI} \left( \frac{\partial \mathbf{S}_{IJ}^{\text{is}}}{\partial \mathbf{C}_{DN}} + \frac{\partial \mathbf{S}_{IJ}^{\text{tr}}}{\partial \mathbf{C}_{DN}} \right) (\mathbf{I}_{DL} \mathbf{F}_{kN} + \mathbf{I}_{NL} \mathbf{F}_{kD}). \quad (\text{E.4})$$

The derivative of  $\mathbf{P}$  with respect to temperature reads

$$\frac{\partial \mathbf{P}_{xJ}}{\partial T} = \mathbf{F}_{xI} \left( \frac{\partial \mathbf{S}_{IJ}^{\text{is}}}{\partial T} + \frac{\partial \mathbf{S}_{IJ}^{\text{tr}}}{\partial T} \right), \quad (\text{E.5})$$

with

$$\frac{\partial \mathbf{S}_{IJ}^{\text{is}}}{\partial T} = -3\lambda \alpha_{\text{th}} \mathbf{C}_{IJ}^{-1}, \quad (\text{E.6})$$

and

$$\frac{\partial \mathbf{S}_{IJ}^{\text{tr}}}{\partial T} = -12\beta^{\text{tr}} \alpha_{\text{th}} \mathbf{A}_I \mathbf{A}_J. \quad (\text{E.7})$$

## E.2 Predictor-corrector and stiffness computation for SMP

### E.2.1 Predictor-corrector for the first mechanism ( $\alpha = 1$ )

In this step we will solve the system of equations that has to be developed.

#### E.2.1.1 Flow rule

The plastic part of the deformation gradient in the incremental form can be derived from the continuous form Eq. (6.56) as

$$\mathbf{F}_{(n+1)}^{p(1)} = \exp(\Delta \mathbf{D}^{p(1)}) \mathbf{F}_{(n)}^{p(1)}, \quad (\text{E.8})$$

where

$$\Delta \mathbf{D}^{p(1)} = \Delta \epsilon^{p(1)} \left( \frac{\mathbf{M}_0^{e(1)}}{2\bar{\tau}(1)} \right), \quad (\text{E.9})$$

and the elastic part of the deformation becomes

$$\mathbf{F}_{(n+1)}^{e(1)} = \mathbf{F}_{(n+1)} \mathbf{F}_{(n)}^{p(1)-1} \exp[(\Delta \epsilon^{p(1)}) \frac{\mathbf{M}_0^{e(1)}}{2\bar{\tau}(1)}]^{-1}, \quad (\text{E.10})$$

where  $\mathbf{M}_0^{e(1)}$  is the deviatoric part of Mandel stress. Let us define the normal  $\mathbf{N}^{(1)}$  as

$$\mathbf{N}^{(1)} = \frac{\mathbf{M}_0^{e(1)}}{\sqrt{2}|\mathbf{M}_0^{e(1)}|}. \quad (\text{E.11})$$

Then  $\mathbf{F}^{e(1)}$ , Eq. (E.10), can be rewritten under the form

$$\mathbf{F}_{n+1}^{e(1)} = \mathbf{F}_{(n+1)} \mathbf{F}_{(n)}^{p(1)-1} \left[ \exp(\Delta \epsilon^{p(1)} \mathbf{N}^{(1)}) \right]^{-1}, \quad (\text{E.12})$$

and we have

$$\mathbf{C}_{(n+1)}^{e(1)} = \left[ \exp(\Delta \epsilon^{p(1)} \mathbf{N}^{(1)}) \right]^{-T} \mathbf{C}_{(\text{pr})}^{e(1)} \left[ \exp(\Delta \epsilon^{p(1)} \mathbf{N}^{(1)}) \right]^{-1}, \quad (\text{E.13})$$

where  $\mathbf{C}_{(\text{pr})}^{e(1)} = \mathbf{F}_{(n)}^{p(1)-T} \mathbf{F}_{(n+1)}^T \mathbf{F}_{(n+1)} \mathbf{F}_{(n)}^{p(1)-1}$ . In order to compute  $\mathbf{M}^{e(1)}$  from Eq. (6.50), we need first to compute the elastic strain

$$\mathbf{E}^{e(1)} = \ln \sqrt{\mathbf{C}_{(n+1)}^{e(1)}}, \quad (\text{E.14})$$

which becomes using Eq. (E.10)

$$\mathbf{E}_{(n+1)}^{e(1)} = \frac{1}{2} \ln \left\{ \left[ \exp(\Delta \epsilon^{p(1)} \mathbf{N}^{(1)}) \right]^{-T} \mathbf{C}_{(\text{pr})}^{e(1)} \left[ \exp(\Delta \epsilon^{p(1)} \mathbf{N}^{(1)}) \right]^{-1} \right\}, \quad (\text{E.15})$$

The deviatoric part can thus be evaluated as

$$\mathbf{E}_0^{e(1)} = \frac{1}{2} \left( \ln(\mathbf{C}_{(\text{pr})}^{e(1)}) \right)_0 - \Delta \epsilon^{p(1)} \mathbf{N}^{(1)}, \quad (\text{E.16})$$

and the volume part as

$$\text{tr} \mathbf{E}^{e(1)} = \frac{1}{2} \text{tr} \left( \ln(\mathbf{C}_{(\text{pr})}^{e(1)}) \right), \quad (\text{E.17})$$

where we have dropped the subscript  $(n+1)$  for conciseness.

### E.2.1.2 Mandel stress

Using Eqs. (E.16) and (E.17), then Mandel stress Eq. (6.50) can be expressed as

$$\mathbf{M}^{e(1)} = G \left( \ln(\mathbf{C}_{(pr)}^{e(1)}) \right)_0 - 2G\Delta\epsilon^{p(1)}\mathbf{N}^{(1)} + \frac{1}{2}K \operatorname{tr} \left( \ln(\mathbf{C}_{(pr)}^{e(1)}) \right) \mathbf{I} - 3K\alpha_{th}(T - T_0)\mathbf{I}. \quad (\text{E.18})$$

From this equation one can deduce

$$\operatorname{tr}\mathbf{M}^{e(1)} = \frac{3}{2}K \operatorname{tr} \left( \ln(\mathbf{C}_{(pr)}^{e(1)}) \right) - 9K\alpha_{th}(T - T_0), \quad (\text{E.19})$$

$$\mathbf{M}_0^{e(1)} = G \left( \ln(\mathbf{C}_{(pr)}^{e(1)}) \right)_0 - 2G\Delta\epsilon^{p(1)}\mathbf{N}^{(1)}. \quad (\text{E.20})$$

Thus, from Eq. (E.11) and Eq. (E.20), one can conclude that:

$$\mathbf{N}^{(1)} = \frac{\left( \ln(\mathbf{C}_{(pr)}^{e(1)}) \right)_0}{\sqrt{2} \left| \left( \ln(\mathbf{C}_{(pr)}^{e(1)}) \right)_0 \right|}. \quad (\text{E.21})$$

Note that  $\mathbf{N}^{(1)}$  is constant during the plastic corrections because of Eq. (E.21).

### E.2.1.3 Shear stress

Let us compute  $\mathbf{M}_0^{e(1)} : \mathbf{N}^{(1)}$  from Eq. (6.25), we get

$$\mathbf{M}_0^{e(1)} : \mathbf{N}^{(1)} = \frac{\mathbf{M}_0^{e(1)} : \mathbf{M}_0^{e(1)}}{\sqrt{2}|\mathbf{M}_0^{e(1)}|} = \frac{|\mathbf{M}_0^{e(1)}|}{\sqrt{2}} = \bar{\tau}^{(1)}. \quad (\text{E.22})$$

Moreover, starting from Eq. (E.20)

$$\begin{aligned} \mathbf{M}_0^{e(1)} : \mathbf{N}^{(1)} &= G\sqrt{2} \left| \left( \ln(\mathbf{C}_{(pr)}^{e(1)}) \right)_0 \right| \mathbf{N}^{(1)} : \mathbf{N}^{(1)} - 2G\Delta\epsilon^{p(1)} \mathbf{N}^{(1)} : \mathbf{N}^{(1)} \\ &= \frac{G}{\sqrt{2}} \left| \left( \ln(\mathbf{C}_{(pr)}^{e(1)}) \right)_0 \right| - G\Delta\epsilon^{p(1)}, \end{aligned} \quad (\text{E.23})$$

and combining Eq. (E.22) and Eq. (E.23) gives the equivalent shear stress

$$\bar{\tau}^{(1)} = \frac{G}{\sqrt{2}} \left| \left( \ln(\mathbf{C}_{(pr)}^{e(1)}) \right)_0 \right| - G\Delta\epsilon^{p(1)}. \quad (\text{E.24})$$

Then the governing equation for the net shear stress of the thermally activated flow one has successively the final expression of Eq. (E.35) as

$$\tau^{e(1)} = \frac{G}{\sqrt{2}} \left| \left( \ln(\mathbf{C}_{(pr)}^{e(1)}) \right)_0 \right| - G\Delta\epsilon^{p(1)} - (S_a + S_b + \alpha_p \bar{p}), \quad (\text{E.25})$$

where  $\bar{p} = -\frac{1}{3}\operatorname{tr}\mathbf{M}^{e(1)}$ , is obtained using Eq. (E.19), as

$$\bar{p} = -\frac{1}{3}\operatorname{tr}\mathbf{M}^{e(1)} = -\left[ \frac{1}{2}K \operatorname{tr} \left( \ln(\mathbf{C}_{(pr)}^{e(1)}) \right) - 3K\alpha_{th}(T - T_0) \right]. \quad (\text{E.26})$$

Using the previous equation and Eq. (6.52) we may rewrite the evolution equation for  $\tau^{e(1)}$  (E.25) as

$$\begin{aligned} \dot{\tau}_1^{e(1)} &= \frac{G}{\sqrt{2}} \left| \left( \ln(\mathbf{C}_{(pr)}^{e(1)}) \right)_0 \right| - G\Delta\epsilon^{p(1)} + \frac{1}{2}\alpha_p K \operatorname{tr} \left( \ln(\mathbf{C}_{(pr)}^{e(1)}) \right) \\ &\quad - 3\alpha_p K\alpha_{th}(T - T_0) - S_a - S_b. \end{aligned} \quad (\text{E.27})$$

### E.2.1.4 Internal variables

The time incremental form for internal variable for  $S_a$ , can be derived from Eq. (6.65)

$$S_{a(n+1)} = S_{a(n)} + h_a (S_{a(n+\beta)}^* - S_{a(n+\beta)}) \Delta \epsilon^{P(1)}, \quad (\text{E.28})$$

where  $\beta$  is a constant value between  $[0, 1]$  with

$$S_{a(n+\beta)} = \beta S_{a(n+1)} + (1 - \beta) S_{a(n)}, \quad (\text{E.29})$$

$$S_{a(n+\beta)}^* = \beta S_{a(n+1)}^* + (1 - \beta) S_{a(n)}^*. \quad (\text{E.30})$$

This last term is computed using Eq. (6.66)

$$\varphi_{(n+1)} = \varphi_{(n)} + g (\varphi_{(n+\beta)}^* - \varphi_{(n+\beta)}) \Delta \epsilon^{P(1)}. \quad (\text{E.31})$$

as

$$S_a^* = b(\varphi^* - \varphi), \quad (\text{E.32})$$

with

$$\varphi^*(\dot{\epsilon}^{P(1)}, T) = \begin{cases} z \left(1 - \frac{T}{T_g}\right)^r + h_g \left(\frac{\dot{\epsilon}^{P(1)}}{\epsilon_r}\right)^s & \text{if } (T \leq T_g) \text{ and } (\dot{\epsilon}^{P(1)} > 0), \\ zh_g \left(\frac{\dot{\epsilon}^{P(1)}}{\epsilon_r}\right)^s & \text{if } (T > T_g) \text{ and } (\dot{\epsilon}^{P(1)} > 0). \end{cases} \quad (\text{E.33})$$

In this previous equation,  $(z, r, s, h_g)$  are constant properties, in particular  $h_g$  is introduced to get small value of  $\varphi^*$  instead of 0 for  $T > T_g$ , and this in turn avoids the big slope of  $\Delta \epsilon^{P(1)}$  between above and below glass transition temperature.

The incremental form of the plastic shear strain rate, Eq. (6.58) is rewritten

$$\Delta \epsilon^{P(1)} = \begin{cases} 0 & \text{if } \tau^{e(1)} \leq 0, \\ \Delta h \epsilon_0^{(1)} \exp\left(-\frac{1}{\xi}\right) \exp\left(-\frac{Q}{K_B T}\right) \left[\sinh\left(\frac{\tau^{e(1)} * V}{2 K_B T}\right)\right]^{1/m} & \text{if } \tau^{e(1)} > 0, \end{cases} \quad (\text{E.34})$$

where

$$\tau^{e(1)} = \bar{\tau}^{(1)} - (S_{a(n+1)} + S_{b(n+1)} + \alpha_p \bar{p}), \quad (\text{E.35})$$

$\tau^{e(1)}$  denotes a net shear stress for the thermally activated flow, and  $\alpha_p \geq 0$  is a parameter introduced to account for the pressure sensitivity,  $\bar{p}$  is the normal pressure which has negative value of hydrostatic stress, and  $\bar{\tau}^{(1)}$  is the equivalent shear stress.

The evaluation of the internal variables follows from Eqs. (E.28-E.34), where by combining Eqs. (E.29, E.30) in (E.28), we have

$$S_{a(n+1)} = \frac{S_{a(n)} + h_a \beta S_{a(n+1)}^* \Delta \epsilon^{P(1)} + h_a (1 - \beta) (S_{a(n)}^* - S_{a(n)}) \Delta \epsilon^{P(1)}}{1 + \beta h_a \Delta \epsilon^{P(1)}}. \quad (\text{E.36})$$

In the same way, from Eq. (E.31) we get

$$\varphi_{(n+1)} = \frac{\varphi_{(n)} + g \beta \varphi_{(n+1)}^* \Delta \epsilon^{P(1)} + g (1 - \beta) (\varphi_{(n)}^* - \varphi_{(n)}) \Delta \epsilon^{P(1)}}{1 + \beta g \Delta \epsilon^{P(1)}}. \quad (\text{E.37})$$



The missing terms read

$$S_{a(n+1)}^* = b(\varphi_{(n+1)}^* - \varphi_{(n+1)}), \quad (\text{E.38})$$

with

$$\varphi_{(n+1)}^* = \begin{cases} z\left(1 - \frac{T}{T_g}\right)^r + h_g \left(\frac{\Delta\epsilon^{P(1)}}{\Delta t\epsilon_r}\right)^s & \text{if } (T \leq T_g) \text{ and } (\dot{\epsilon}^{P(1)} > 0), \\ z(h_g)^r \left(\frac{\Delta\epsilon^{P(1)}}{\Delta t\epsilon_r}\right)^s & \text{if } (T > T_g) \text{ and } (\dot{\epsilon}^{P(1)} > 0), \end{cases} \quad (\text{E.39})$$

and hence Eq. (E.37) becomes for  $T \leq T_g$

$$\varphi_{(n+1)} = \frac{\varphi_{(n)} + g\beta z \left(1 - \frac{T}{T_g}\right)^r + h_g \left(\frac{\Delta\epsilon^{P(1)}}{\Delta t\epsilon_r}\right)^s \Delta\epsilon^{P(1)} + g(1 - \beta)(\varphi_{(n)}^* - \varphi_{(n)})\Delta\epsilon^{P(1)}}{1 + \beta g\Delta\epsilon^{P(1)}}, \quad (\text{E.40})$$

Eq. (E.38) becomes for  $T \leq T_g$

$$S_{(n+1)}^* = \frac{b \left( z \left(1 - \frac{T}{T_g}\right)^r + h_g \left(\frac{\Delta\epsilon^{P(1)}}{\Delta t\epsilon_r}\right)^s - \varphi_{(n)} - g(1 - \beta)(\varphi_{(n)}^* - \varphi_{(n)})\Delta\epsilon^{P(1)} \right)}{1 + \beta g\Delta\epsilon^{P(1)}}, \quad (\text{E.41})$$

and Eq. (E.36) becomes for  $T \leq T_g$

$$S_{a(n+1)} = \frac{S_{a(n)} + h_a(1 - \beta)(S_{a(n)}^* - S_{a(n)})\Delta\epsilon^{P(1)}}{1 + \beta h_a\Delta\epsilon^{P(1)}} + \frac{h_a\beta b \left( z \left(1 - \frac{T}{T_g}\right)^r + h_g \left(\frac{\Delta\epsilon^{P(1)}}{\Delta t\epsilon_r}\right)^s - \varphi_{(n)} - g(1 - \beta)(\varphi_{(n)}^* - \varphi_{(n)})\Delta\epsilon^{P(1)} \right) \Delta\epsilon^{P(1)}}{(1 + \beta h_a\Delta\epsilon^{P(1)})(1 + \beta g\Delta\epsilon^{P(1)})}. \quad (\text{E.42})$$

Similarly, for  $T > T_g$ , we have

$$S_{a(n+1)} = \frac{S_{a(n)} + h_a(1 - \beta)(S_{a(n)}^* - S_{a(n)})\Delta\epsilon^{P(1)}}{1 + \beta h_a\Delta\epsilon^{P(1)}} + \frac{h_a\beta b \left( z(h_g) \left(\frac{\Delta\epsilon^{P(1)}}{\Delta t\epsilon_r}\right)^s - \varphi_{(n)} - g(1 - \beta)(\varphi_{(n)}^* - \varphi_{(n)})\Delta\epsilon^{P(1)} \right) \Delta\epsilon^{P(1)}}{(1 + \beta h_a\Delta\epsilon^{P(1)})(1 + \beta g\Delta\epsilon^{P(1)})}. \quad (\text{E.43})$$

Finally Eq. (6.69) becomes

$$S_b = S_{b0} + H_b(\bar{\lambda} - 1)^a, \quad \bar{\lambda} = \sqrt{\text{tr}\mathbf{C}^{(1)}/3}, \quad (\text{E.44})$$

with  $H_b(T)$  defined in Eq. (6.70).

Finally the glass transition temperature  $T_g$ , Eq. (6.44) is computed as

$$T_g = \begin{cases} T_r & \text{if } \dot{\epsilon} \leq \epsilon_r, \\ T_r + n\log\left(\frac{\dot{\epsilon}}{\epsilon_r}\right) & \text{if } \dot{\epsilon} > \epsilon_r, \end{cases} \quad (\text{E.45})$$

where  $\dot{\epsilon}$  is computed using Eq. (6.40), which in turn is computed using Eq.(6.42), thus one has

$$\mathbf{D}_{\text{ix(sym)}} = \frac{1}{2\Delta t} \ln \left( \mathbf{F}_{(n+1)\text{iA}} \mathbf{F}_{(n)\text{Ax}}^{-1} + \mathbf{F}_{(n)\text{Ai}}^{-1} \mathbf{F}_{(n+1)\text{xA}} \right). \quad (\text{E.46})$$

### E.2.1.5 Non-linear system of equations

Thereafter the residual equation for the first micromechanisms can be defined from Eq. (6.59)

$$\Omega^{(1)} = \tau^{e(1)} - \left( \bar{\tau}^{(1)} - (S_a + S_b + \alpha_p \bar{p}^{(1)}) \right). \quad (\text{E.47})$$

From Eq. (E.34) let us define  $L(T)$  to simplify the equation

$$L(T) = \begin{cases} \dot{\epsilon}_0^{(1)} \Delta t \exp\left(-\frac{1}{\xi_{\text{gl}}}\right) \exp\left(-\frac{Q(T)}{K_B T}\right) & \text{if } T \leq T_g, \\ \dot{\epsilon}_0^{(1)} \Delta t \exp\left(-\frac{1}{(\xi_{\text{gl}} + d(T - T_g))}\right) \exp\left(-\frac{Q(T)}{K_B T}\right) & \text{if } T > T_g, \end{cases} \quad (\text{E.48})$$

where  $Q(T)$  is defined in Eq. (6.61), and  $W(T)$  as

$$W(T) = \frac{V}{2K_B T}, \quad (\text{E.49})$$

which allow rewriting (E.34) as

$$\Delta \epsilon^{p(1)} = \begin{cases} L(T) [\sinh(\tau^{e(1)} W(T))]^{1/m} & \text{if } \tau^{e(1)} > 0, \\ 0 & \text{if } \tau^{e(1)} \leq 0. \end{cases} \quad (\text{E.50})$$

This equation can be rewritten

$$\tau^{e(1)} = \frac{1}{W(T)} \operatorname{arcsinh} \left( \frac{\Delta \epsilon^{p(1)}}{L(T)} \right)^m. \quad (\text{E.51})$$

So the residual defined by Eq. (E.47) becomes, using Eq. (E.27)

$$\begin{aligned} \Omega^{(1)} &= \frac{1}{W(T)} \operatorname{arcsinh} \left( \frac{\Delta \epsilon^{p(1)}}{L(T)} \right)^m - \frac{G(T)}{\sqrt{2}} \left| \ln(\mathbf{C}_{(\text{pr})}^{e(1)}) \right|_0 + G(T) \Delta \epsilon^{p(1)} \\ &\quad - \frac{1}{2} \alpha_p K(T) \operatorname{tr} \left( \ln(\mathbf{C}_{(\text{pr})}^{e(1)}) \right) + 3 \alpha_p K(T) \alpha_{\text{th}} (T - T_0) + S_{a(n+1)}(T) + S_b(T). \end{aligned} \quad (\text{E.52})$$

For both cases ( $T \leq T_g$ ) the associated Newton-Raphson (NR) scheme reads

$$\Omega^{(1)} + \frac{\partial \Omega^{(1)}}{\partial \Delta \epsilon^{p(1)}} \Big|_{\bar{\mathbf{C}}_{\text{pr}}^{e(1)}} \Delta \Delta \epsilon^{p(1)} = 0. \quad (\text{E.53})$$

This system is iteratively solved using the Jacobian, which is defined as  $J_1^{(1)} = \frac{\partial \Omega^{(1)}}{\partial \Delta \epsilon^{p(1)}} \Big|_{\bar{\mathbf{C}}_{\text{pr}}^{e(1)}}$ , leading to

$$\Delta \Delta \epsilon^{p(1)} = -J_1^{(1)-1} \Omega^{(1)}, \quad (\text{E.54})$$

with the updated step

$$\Delta\epsilon^{p(1)} \leftarrow \Delta\epsilon^{p(1)} + \Delta\Delta\epsilon^{p(1)}. \quad (\text{E.55})$$

The iterations continue until convergence until a specified tolerance is achieved.

Let us now compute the derivative of the components of  $\Omega^{(1)}$ , and let us start by computing  $\frac{\partial\tau^{e(1)}}{\partial\Delta\epsilon^{p(1)}}$  by calling Eq. (E.51)

$$\begin{aligned} \frac{\partial\tau^{e(1)}}{\partial\Delta\epsilon^{p(1)}} &= \frac{\partial}{\partial\Delta\epsilon^{p(1)}} \left( \frac{1}{W(T)} \operatorname{arcsinh}\left(\frac{\Delta\epsilon^{p(1)}}{L(T)}\right)^m \right) \\ &= \frac{m}{W(T)L(T)} \frac{1}{\sqrt{\left(\frac{\Delta\epsilon^{p(1)}}{L(T)}\right)^{2m} + 1}} \left(\frac{\Delta\epsilon^{p(1)}}{L(T)}\right)^{m-1}. \end{aligned} \quad (\text{E.56})$$

By doing some calculations we can get the derivative of  $S_a$ , Eq. (E.43), with respect to  $\Delta\epsilon^{p(1)}$  for  $T \leq T_g$ ,

$$\begin{aligned} \frac{\partial S_{a(n+1)}}{\partial\Delta\epsilon^{p(1)}} &= \frac{h_a(1-\beta)(S_{a(n)}^* - S_{a(n)})(1 + \beta h_a \Delta\epsilon_1^{p(1)}) - \beta h_a(S_{a(n)} + h_a(1-\beta)(S_{a(n)}^* - S_{a(n)})\Delta\epsilon^{p(1)}}{(1 + \beta h_a \Delta\epsilon^{p(1)})^2} \\ &+ \frac{\frac{sh_a\beta b}{\Delta t\epsilon_r} z \left( \left(1 - \frac{T}{T_g}\right)^r + h_g \right) \left(\frac{\Delta\epsilon^{p(1)}}{\Delta t\epsilon_r}\right)^{s-1} \Delta\epsilon^{p(1)}}{(1 + \beta h_a \Delta\epsilon^{p(1)})(1 + \beta g \Delta\epsilon^{p(1)})} + \frac{h_a\beta b z \left( \left(1 - \frac{T}{T_g}\right)^r + h_g \right) \left(\frac{\Delta\epsilon^{p(1)}}{\Delta t\epsilon_r}\right)^s}{(1 + \beta h_a \Delta\epsilon^{p(1)})(1 + \beta g \Delta\epsilon^{p(1)})} \\ &- \frac{h_a\beta b \left( g(1-\beta)(\varphi_{(n)}^* - \varphi_{(n)})\Delta\epsilon^{p(1)} \right)}{(1 + \beta h_a \Delta\epsilon^{p(1)})(1 + \beta g \Delta\epsilon^{p(1)})} - \frac{h_a\beta b \left( \varphi_{(n)} + g(1-\beta)(\varphi_{(n)}^* - \varphi_{(n)})\Delta\epsilon^{p(1)} \right)}{(1 + \beta h_a \Delta\epsilon^{p(1)})(1 + \beta g \Delta\epsilon^{p(1)})} \\ &+ \frac{(\beta^2 h_a(1 + \beta g \Delta\epsilon^{p(1)}) + \beta^2 g(1 + \beta h_a \Delta\epsilon^{p(1)}))(h_a b(\varphi_{(n)}) \Delta\epsilon^{p(1)})}{(1 + \beta h_a \Delta\epsilon^{p(1)})^2(1 + \beta g \Delta\epsilon^{p(1)})^2} \\ &+ \frac{(\beta^2 h_a(1 + \beta g \Delta\epsilon^{p(1)}) + \beta^2 g(1 + \beta h_a \Delta\epsilon^{p(1)}))(h_a b g(1-\beta)(\varphi_{(n)}^* - \varphi_{(n)})\Delta\epsilon^{p(1)}) \Delta\epsilon^{p(1)}}{(1 + \beta h_a \Delta\epsilon^{p(1)})^2(1 + \beta g \Delta\epsilon^{p(1)})^2} \\ &- \frac{(\beta^2 h_a(1 + \beta g \Delta\epsilon^{p(1)}) + \beta^2 g(1 + \beta h_a \Delta\epsilon^{p(1)})) \left( h_a b(z \left( \left(1 - \frac{T}{T_g}\right)^r + h_g \right) \left(\frac{\Delta\epsilon_1^{p(1)}}{\Delta t\epsilon_r}\right)^s \right) \Delta\epsilon^{p(1)}}{(1 + \beta h_a \Delta\epsilon^{p(1)})^2(1 + \beta g \Delta\epsilon^{p(1)})^2}, \end{aligned} \quad (\text{E.57})$$

and for the second case  $T > T_g$ , from Eq. (E.43)

$$\begin{aligned}
\frac{\partial S_{a(n+1)}}{\partial \Delta \epsilon^{P(1)}} &= \frac{h_a(1-\beta)(S_{a(n)}^* - S_{a(n)})}{(1+\beta h_a \Delta \epsilon^{P(1)})} - \frac{\beta h_a (S_{a(n)} + h_a(1-\beta)(S_{a(n)}^* - S_{a(n)}) \Delta \epsilon^{P(1)})}{(1+\beta h_a \Delta \epsilon^{P(1)})^2} \\
&+ \frac{\frac{sh_a \beta b}{\Delta t \epsilon_r} z h_g \left(\frac{\Delta \epsilon^{P(1)}}{\Delta t \epsilon_r}\right)^{s-1} \Delta \epsilon^{P(1)}}{(1+\beta h_a \Delta \epsilon^{P(1)})(1+\beta g \Delta \epsilon^{P(1)})} + \frac{h_a \beta b z h_g \left(\frac{\Delta \epsilon_1^{P(1)}}{\Delta t \epsilon_r}\right)^s}{(1+\beta h_a \Delta \epsilon^{P(1)})(1+\beta g \Delta \epsilon^{P(1)})} \\
&\frac{h_a \beta b \left(\varphi_{(n)} + g(1-\beta)(\varphi_{(n)}^* - \varphi_{(n)}) \Delta \epsilon^{P(1)}\right)}{(1+\beta h_a \Delta \epsilon^{P(1)})(1+\beta g \Delta \epsilon^{P(1)})} \\
&\frac{h_a \beta b \left(g(1-\beta)(\varphi_{(n)}^* - \varphi_{(n)})\right) \Delta \epsilon^{P(1)}}{(1+\beta h_a \Delta \epsilon^{P(1)})(1+\beta g \Delta \epsilon^{P(1)})} \\
&+ \frac{(\beta^2 h_a(1+\beta g \Delta \epsilon^{P(1)}) + \beta^2 g(1+\beta h_a \Delta \epsilon^{P(1)})) h_a b(\varphi_{(n)}) \Delta \epsilon^{P(1)}}{(1+\beta h_a \Delta \epsilon^{P(1)})^2(1+\beta g \Delta \epsilon^{P(1)})^2} \\
&+ \frac{(\beta^2 h_a(1+\beta g \Delta \epsilon^{P(1)}) + \beta^2 g(1+\beta h_a \Delta \epsilon^{P(1)})) h_a b(g(1-\beta)(\varphi_{(n)}^* - \varphi_{(n)}) \Delta \epsilon^{P(1)}) \Delta \epsilon^{P(1)}}{(1+\beta h_a \Delta \epsilon^{P(1)})^2(1+\beta g \Delta \epsilon^{P(1)})^2} \\
&\frac{(\beta^2 h_a(1+\beta g \Delta \epsilon^{P(1)}) + \beta^2 g(1+\beta h_a \Delta \epsilon^{P(1)}))(h_a b z h_g \left(\frac{\Delta \epsilon_1^{P(1)}}{\Delta t \epsilon_r}\right)^s) \Delta \epsilon^{P(1)}}{(1+\beta h_a \Delta \epsilon^{P(1)})^2(1+\beta g \Delta \epsilon^{P(1)})^2}.
\end{aligned} \tag{E.58}$$

By combining Eqs. (E.56 and E.57 or E.58) we obtain the Jacobian and the system is iteratively solved for  $T \leq T_g$  using

$$j^{(1)} = \frac{\partial \Omega^{(1)}}{\partial \Delta \epsilon^{P(1)}} \Big|_{\mathbf{C}_{pr}^{e(1)}} = \frac{m}{W(T)L(T)} \frac{1}{\sqrt{\left(\frac{\Delta \epsilon^{P(1)}}{L(T)}\right)^{2m} + 1}} \left(\frac{\Delta \epsilon^{P(1)}}{L(T)}\right)^{m-1} + G + \frac{\partial S_{a(n+1)}}{\partial \Delta \epsilon^{P(1)}}. \tag{E.59}$$

### E.2.1.6 Converged solution

The first Piola-Kirchhoff stress tensor, is given by  $\mathbf{P} = 2\mathbf{F} \frac{\partial \psi^{e(1)}}{\partial \mathbf{C}}$  can be derived from Eq. (6.46)

$$\begin{aligned}
\mathbf{P}_{iA}^{(1)} &= 2\mathbf{F}_{iN} \frac{\partial \psi^{e(1)}}{\partial \mathbf{C}_{NA}} = 2\mathbf{F}_{iN}^{(1)} \frac{\partial \psi^{e(1)}}{\partial \mathbf{E}_{KL}^{e(1)}} \frac{\partial \mathbf{E}_{KL}^{e(1)}}{\partial \mathbf{C}_{MS}^{e(1)}} \frac{\partial \mathbf{C}_{MS}^{e(1)}}{\partial \mathbf{C}_{NA}} \\
&= \mathbf{F}_{iN} \mathbf{F}_{NM}^{p(1)-1} \mathcal{L}_{KLMS}^e \frac{\partial \psi^{e(1)}}{\partial \mathbf{E}_{KL}^{e(1)}} \mathbf{F}_{AS}^{p(1)-1} \\
&= \mathbf{F}_{iM}^{e(1)} \mathcal{L}_{KLMS}^e \frac{\partial \psi^{e(1)}}{\partial \mathbf{E}_{KL}^{e(1)}} \mathbf{F}_{SA}^{p(1)-T} \\
&= \mathbf{F}_{iM}^{e(1)} \mathcal{L}_{KLMS}^e \mathbf{M}_{KL}^{e(1)} \mathbf{F}_{SA}^{p(1)-T}.
\end{aligned} \tag{E.60}$$

Note that  $\mathbf{M}^{e(1)}$  is computed from Eq. (E.18),  $\mathcal{L}^e$  is an approximated matrix for the derivative of  $\ln\sqrt{\mathbf{C}^{e(1)}}$  with respect to  $\mathbf{C}^{e(1)}$ , such that  $\mathcal{L}^e = 2\frac{\partial\ln\sqrt{\mathbf{C}^{e(1)}}}{\partial\mathbf{C}^{e(1)}} = \frac{\partial\ln\mathbf{C}^{e(1)}}{\partial\mathbf{C}^{e(1)}}$ .

The previous equation allows us to evaluate the first Piola-Kirchhoff stress in terms of the elastic and plastic parts of the deformation gradient. Then using these results, the derivative of the Piola-Kirchhoff stress tensor with respect to the deformation can be evaluated as

$$\begin{aligned}\frac{\partial\mathbf{P}_{iA}^{(1)}}{\partial\mathbf{F}_{jC}} &= \frac{\partial(\mathbf{F}_{iM}^{e(1)}\mathcal{L}_{KLMs}^e\mathbf{M}_{KL}^{e(1)}\mathbf{F}_{SA}^{p(1)-T})}{\partial\mathbf{F}_{jC}} \\ &= \frac{\partial\mathbf{F}_{iM}^{e(1)}}{\partial\mathbf{F}_{jC}}\mathcal{L}_{KLMs}^e\mathbf{M}_{KL}^{e(1)}\mathbf{F}_{SA}^{p(1)-T} + \mathbf{F}_{iM}^{e(1)}\mathcal{L}_{KLMs}^e\frac{\partial\mathbf{M}_{KL}^{e(1)}}{\partial\mathbf{F}_{jC}}\mathbf{F}_{SA}^{p(1)-T} \\ &\quad + \mathbf{F}_{iM}^{e(1)}\frac{\partial\mathcal{L}_{KLMs}^e}{\partial\mathbf{F}_{jC}}\mathbf{M}_{KL}^{e(1)}\mathbf{F}_{SA}^{p(1)-T} + \mathbf{F}_{iM}^{e(1)}\mathcal{L}_{KLMs}^e\mathbf{M}_{KL}^{e(1)}\frac{\partial\mathbf{F}_{SA}^{p(1)-T}}{\partial\mathbf{F}_{jC}}.\end{aligned}\quad (\text{E.61})$$

The derivative of the inverse of the plastic deformation gradient is given by

$$\frac{\partial\mathbf{F}_{XY}^{p(1)-1}}{\partial\mathbf{F}_{jC}} = -\mathbf{F}_{XE}^{p(1)-1}\frac{\partial\mathbf{F}_{EZ}^{p(1)}}{\partial\mathbf{F}_{jC}}\mathbf{F}_{ZY}^{p(1)-1}.\quad (\text{E.62})$$

The derivative of the elastic deformation gradient with respect to the deformation gradient reads

$$\frac{\partial\mathbf{F}_{iM}^{e(1)}}{\partial\mathbf{F}_{jC}} = \frac{\partial(\mathbf{F}_{iG}\mathbf{F}_{GM}^{p(1)-1})}{\partial\mathbf{F}_{jC}} = \left(\delta_{ij}\mathbf{F}_{CM}^{p(1)-1} - \mathbf{F}_{iG}\mathbf{F}_{GX}^{p(1)-1}\frac{\partial\mathbf{F}_{XY}^{p(1)}}{\partial\mathbf{F}_{jC}}\mathbf{F}_{yM}^{p(1)-1}\right).\quad (\text{E.63})$$

The derivative of  $\mathcal{L}^e$  follows from

$$\begin{aligned}\frac{\partial\mathcal{L}_{KLMs}^e}{\partial\mathbf{F}_{jC}} &= \frac{\partial\mathcal{L}_{KLMs}^e}{\partial\mathbf{C}_{QV}^{e(1)}}\frac{\partial\mathbf{C}_{QV}^{e(1)}}{\partial\mathbf{F}_{EU}^{e(1)}}\frac{\partial\mathbf{F}_{EU}^{e(1)}}{\partial\mathbf{F}_{jC}} \\ &= \frac{\partial\mathcal{L}_{KLMs}^e}{\partial\mathbf{C}_{QV}^{e(1)}}\left(\delta_{QU}\mathbf{F}_{EV}^{e(1)} + \mathbf{F}_{EQ}^{e(1)}\delta_{VU}\right)\frac{\partial\mathbf{F}_{EU}^{e(1)}}{\partial\mathbf{F}_{jC}}.\end{aligned}\quad (\text{E.64})$$

To evaluate these three terms, the derivative of the plastic deformation gradient is obtained from its definition Eq. (6.95), leading to

$$\begin{aligned}\frac{\partial\mathbf{F}_{(n+1)EZ}^{p(1)}}{\partial\mathbf{F}_{jC}} &= \frac{\partial\exp(\Delta\mathbf{D}_{EZ}^{(1)})}{\partial\Delta\mathbf{D}_{OP}^{(1)}}\frac{\partial\Delta\mathbf{D}_{OP}^{(1)}}{\partial\mathbf{F}_{jC}}\mathbf{F}_{(n)IZ}^{p(1)} \\ &= \mathcal{Z}_{EIOP}\left[\mathbf{N}_{OP}^{(1)}\frac{\partial\Delta\epsilon^{p(1)}}{\partial\mathbf{F}_{jC}} + \Delta\epsilon^{p(1)}\frac{\partial\mathbf{N}_{OP}^{(1)}}{\partial\mathbf{F}_{jC}}\right]\mathbf{F}_{(n)IZ}^{p(1)},\end{aligned}\quad (\text{E.65})$$

where  $\mathcal{Z}$  is an approximated matrix for the derivative of exponential of  $\mathbf{C}^{e(1)}$  with respect to  $\mathbf{C}^{e(1)}$ , such that  $\mathcal{Z} = \frac{\partial\exp\mathbf{C}^{e(1)}}{\partial\mathbf{C}^{e(1)}}$ . The derivative of the missing terms can be computed by deriving the residual  $\Omega^{(1)}$ , Eq. (E.47), with respect to right Cauchy tensor  $\mathbf{C}^{e(1)}$ , yielding

$$\frac{\partial\Omega^{(1)}}{\partial\mathbf{F}_{jC}}\Big|_{\Delta\epsilon^{p(1)}} + \frac{\partial\Omega^{(1)}}{\partial\Delta\epsilon^{p(1)}}\frac{\partial\Delta\epsilon^{p(1)}}{\partial\mathbf{F}_{jC}} = 0,\quad (\text{E.66})$$

$$\implies \frac{\partial \Delta \epsilon^{\text{P}(1)}}{\partial \mathbf{F}_{\text{jC}}} = -j^{(1)-1} \frac{\partial \Omega^{(1)}}{\partial \mathbf{F}_{\text{jC}}} \Big|_{\Delta \epsilon^{\text{P}(1)}}. \quad (\text{E.67})$$

The derivative of the residual with respect to the deformation gradient tensor is obtained from

$$\frac{\partial \Omega^{(1)}}{\partial \mathbf{F}_{\text{jC}}} \Big|_{\Delta \epsilon^{\text{P}(1)}} = \left( \mathbf{F}_{(\text{pr})\text{WH}}^{\text{P}(1)-1} \frac{\partial \Omega^{(1)}}{\partial \mathbf{C}_{(\text{pr})\text{HT}}^{\text{e}(1)}} \mathbf{F}_{(\text{pr})\text{TV}}^{\text{P}(1)-\text{T}} + \frac{\partial \Omega^{(1)}}{\partial \mathbf{C}_{\text{WV}}} \right) (\mathbf{F}_{\text{jV}} \boldsymbol{\delta}_{\text{WC}} + \mathbf{F}_{\text{jW}} \boldsymbol{\delta}_{\text{VC}}). \quad (\text{E.68})$$

Let us compute the derivative of the components of  $\Omega^{(1)}$  given by Eq. (E.52). First one has

$$\frac{\partial \text{tr} \left( \ln(\mathbf{C}_{(\text{pr})}^{\text{e}(1)}) \right)}{\partial \mathbf{C}_{(\text{pr})\text{HT}}^{\text{e}(1)}} = \frac{\partial \text{tr} \left( \ln(\mathbf{C}_{(\text{pr})}^{\text{e}(1)}) \right)}{\partial \left( \ln(\mathbf{C}_{(\text{pr})\text{XO}}^{\text{e}(1)}) \right)} \frac{\partial \left( \ln(\mathbf{C}_{(\text{pr})\text{XO}}^{\text{e}(1)}) \right)}{\partial \mathbf{C}_{(\text{pr})\text{HT}}^{\text{e}(1)}} = \boldsymbol{\delta}_{\text{XO}} \mathcal{L}_{(\text{pr})\text{XOHT}}^{\text{e}}, \quad (\text{E.69})$$

and then, one has

$$\frac{\partial \left( \ln(\mathbf{C}_{(\text{pr})\text{KL}}^{\text{e}(1)}) \right)_0}{\partial \mathbf{C}_{(\text{pr})\text{HT}}^{\text{e}(1)}} = \frac{\partial \left( \left( \ln(\mathbf{C}_{(\text{pr})\text{KL}}^{\text{e}(1)}) - \frac{1}{3} \text{tr} \ln(\mathbf{C}_{(\text{pr})}^{\text{e}(1)}) \delta_{\text{KL}} \right) \right)}{\partial \mathbf{C}_{(\text{pr})\text{HT}}^{\text{e}(1)}} = \mathcal{L}_{(\text{pr})\text{KLHT}}^{\text{e}} - \frac{1}{3} \boldsymbol{\delta}_{\text{YZ}} \mathcal{L}_{(\text{pr})\text{YZHT}}^{\text{e}} \delta_{\text{KL}}, \quad (\text{E.70})$$

where  $\mathcal{L}_{(\text{pr})}^{\text{e}} = \frac{\partial \ln \mathbf{C}_{(\text{pr})}^{\text{e}(1)}}{\partial \mathbf{C}_{(\text{pr})}^{\text{e}(1)}}$ . Now let us compute the derivative of  $\mathbf{N}^{(1)}$  by recalling Eq. (E.21).

First one has

$$\begin{aligned} \frac{\partial \left( \ln(\mathbf{C}_{\text{pr}}^{\text{e}(1)}) \right)_0}{\partial \mathbf{C}_{(\text{pr})\text{HT}}^{\text{e}}} &= \frac{\partial \sqrt{\left( \ln(\mathbf{C}_{(\text{pr})\text{OM}}^{\text{e}(1)}) \right)_0 \left( \ln(\mathbf{C}_{(\text{pr})\text{OM}}^{\text{e}(1)}) \right)_0}}{\partial \left( \mathbf{C}_{(\text{pr})\text{HT}}^{\text{e}} \right)} \\ &= \sqrt{2} \mathbf{N}_{\text{OM}}^{(1)} \mathcal{L}_{\text{OMHT}}^{\text{e}} - \frac{\sqrt{2}}{3} \mathbf{N}_{\text{OM}}^{(1)} \boldsymbol{\delta}_{\text{YZ}} \mathcal{L}_{\text{YZHT}}^{\text{e}} \boldsymbol{\delta}_{\text{OM}} \\ &= \sqrt{2} \mathbf{N}_{\text{OM}}^{(1)} \mathcal{L}_{\text{OMHT}}^{\text{e}}. \end{aligned} \quad (\text{E.71})$$

The derivative of glass transition temperature with respect to the deformation gradient is obtained from Eq. (6.44), with

$$\frac{\partial T_{\text{g}}}{\partial \mathbf{F}_{\text{jC}}} = \begin{cases} 0 & \text{if } \dot{\epsilon} \leq \epsilon_{\text{r}} \\ \frac{n}{\dot{\epsilon}} \frac{\partial \dot{\epsilon}}{\partial \mathbf{F}_{\text{jC}}} & \text{if } \dot{\epsilon} > \epsilon_{\text{r}} \end{cases} \quad (\text{E.72})$$

Using Eq. (6.40), one has

$$\begin{aligned} \frac{\partial \dot{\epsilon}}{\partial \mathbf{F}_{\text{jC}}} &= \frac{\sqrt{2} |\mathbf{D}_{0(\text{sym})}|}{\partial \mathbf{F}_{\text{jC}}} \\ &= \sqrt{2} \mathbf{D}_{\text{ix}(0\text{sym})} |\mathbf{D}_{0(\text{sym})}|^{-1} \left( \frac{\partial \mathbf{D}_{\text{ix}(\text{sym})}}{\partial \mathbf{F}_{\text{jC}}} - \frac{1}{3} \boldsymbol{\delta}_{\text{yz}} \frac{\partial \mathbf{D}_{\text{yz}(\text{sym})}}{\partial \mathbf{F}_{\text{jC}}} \boldsymbol{\delta}_{\text{ix}} \right), \end{aligned} \quad (\text{E.73})$$

where using Eq. (E.46), thus one has

$$\begin{aligned} \frac{\partial \mathbf{D}_{\text{ix(sym)}}}{\partial \mathbf{F}_{(n+1)\text{jC}}} &= \frac{1}{2\Delta t} \frac{\partial \ln \left( \mathbf{F}_{(n+1)\text{iA}} \mathbf{F}_{(n)\text{Ax}}^{-1} + \mathbf{F}_{(n)\text{Ai}}^{-1} \mathbf{F}_{(n+1)\text{xA}} \right)}{\partial \left( \mathbf{F}_{(n+1)\text{zB}} \mathbf{F}_{(n)\text{By}}^{-1} + \mathbf{F}_{(n)\text{Bz}}^{-1} \mathbf{F}_{(n+1)\text{yB}} \right)} \frac{\partial \left( \mathbf{F}_{(n+1)\text{zB}} \mathbf{F}_{(n)\text{By}}^{-1} + \mathbf{F}_{(n)\text{Bz}}^{-1} \mathbf{F}_{(n+1)\text{yB}} \right)}{\partial \mathbf{F}_{(n+1)\text{jC}}} \\ &= \frac{1}{2\Delta t} \mathcal{L}_{\text{ixzy}} \left( \delta_{\text{zj}} \mathbf{F}_{(n)\text{Cy}}^{-1} + \delta_{\text{yj}} \mathbf{F}_{(n)\text{Cz}}^{-1} \right), \end{aligned} \quad (\text{E.74})$$

where  $\mathcal{L}$  is the approximated matrix for the derivative of  $\ln \left( \mathbf{F}_{(n+1)} \mathbf{F}_{(n)}^{-1} + \mathbf{F}_{(n)}^{-1} \mathbf{F}_{(n+1)} \right)$  with respect to  $\left( \mathbf{F}_{(n+1)} \mathbf{F}_{(n)}^{-1} + \mathbf{F}_{(n)}^{-1} \mathbf{F}_{(n+1)} \right)$ .

The derivative of Poisson ratio with respect to the deformation gradient can be computed by

$$\frac{\partial \nu(\mathbf{T})}{\partial \mathbf{F}_{\text{jC}}} = \frac{\partial \nu(\mathbf{T})}{\partial T_{\text{g}}} \frac{\partial T_{\text{g}}}{\partial \mathbf{F}_{\text{jC}}} \quad (\text{E.75})$$

where the derivative of Poisson ratio with respect to glass transition temperature using Eq. (6.55) is

$$\frac{\partial \nu(\mathbf{T})}{\partial T_{\text{g}}} = \frac{1}{2\Delta} (\nu_{\text{gl}} - \nu_{\text{r}}) (1 - \tanh^2 \left( \frac{1}{\Delta} (T - T_{\text{g}}) \right)). \quad (\text{E.76})$$

Similarly, using Eq. (6.52), the derivative of the shear modulus  $G$  reads

$$\frac{\partial G}{\partial \mathbf{F}_{\text{jC}}} = \frac{\partial G}{\partial T_{\text{g}}} \frac{\partial T_{\text{g}}}{\partial \mathbf{F}_{\text{jC}}}, \quad (\text{E.77})$$

with

$$\frac{\partial G(\mathbf{T})}{\partial T_{\text{g}}} = \begin{cases} \frac{1}{2\Delta} (G_{\text{gl}} - G_{\text{r}}) (1 - \tanh^2 \left( \frac{1}{\Delta} (T - T_{\text{g}}) \right)) + M_{\text{gl}} & \text{if } T \leq T_{\text{g}} \\ \frac{1}{2\Delta} (G_{\text{gl}} - G_{\text{r}}) (1 - \tanh^2 \left( \frac{1}{\Delta} (T - T_{\text{g}}) \right)) + M_{\text{r}} & \text{if } T > T_{\text{g}}. \end{cases} \quad (\text{E.78})$$

By the same way, one can get the derivative of the bulk modulus Eq. (6.55), with respect to the deformation gradient as follows

$$\frac{\partial K}{\partial \mathbf{F}_{\text{jC}}} = \frac{\partial K}{\partial T_{\text{g}}} \frac{\partial T_{\text{g}}}{\partial \mathbf{F}_{\text{jC}}}, \quad (\text{E.79})$$

$$\frac{\partial K(\mathbf{T})}{\partial T_{\text{g}}} = \frac{\partial G(\mathbf{T})}{\partial T_{\text{g}}} \frac{2(1 + \nu)}{3(1 - 2\nu)} + G(\mathbf{T}) \left( \frac{2 \frac{\partial \nu}{\partial T_{\text{g}}} (1 - 2\nu) + 4 \frac{\partial \nu}{\partial T_{\text{g}}} (1 + \nu)}{3(1 - 2\nu)^2} \right). \quad (\text{E.80})$$

By the same way, using Eq. (6.70), gives

$$\frac{\partial H_{\text{b}}(\mathbf{T})}{\partial \mathbf{F}_{\text{jC}}} = \begin{cases} \left[ \frac{1}{2\Delta} (H_{\text{gl}} - H_{\text{r}}) (1 - \tanh^2 \left( \frac{1}{\Delta} (T - T_{\text{g}}) \right)) + L_{\text{gl}} \right] \frac{\partial T_{\text{g}}}{\partial \mathbf{F}_{\text{jC}}} & \text{if } T \leq T_{\text{g}}, \\ \left[ \frac{1}{2\Delta} (H_{\text{gl}} - H_{\text{r}}) (1 - \tanh^2 \left( \frac{1}{\Delta} (T - T_{\text{g}}) \right)) + L_{\text{r}} \right] \frac{\partial T_{\text{g}}}{\partial \mathbf{F}_{\text{jC}}} & \text{if } T > T_{\text{g}}. \end{cases} \quad (\text{E.81})$$

By calling Eqs. (E.42, E.43), one has

$$\frac{\partial S_{a(n+1)}}{\partial T_g} = \begin{cases} \frac{r h_a / \beta b z T}{T_g^2} \left(1 - \frac{T}{T_g}\right)^{r-1} \left(\frac{\Delta \epsilon^{p(1)}}{\Delta t \epsilon_r}\right)^s \Delta \epsilon^{p(1)} & \text{if } T \leq T_g, \\ 0 & \text{if } T > T_g. \end{cases} \quad (\text{E.82})$$

Now let us compute the derivative of  $\alpha_{\text{th}}$  with respect to the glass transition temperature by using Eq. (6.53):

$$\frac{\partial \alpha_{\text{th}}(T - T_0)}{\partial \mathbf{F}_{jC}} = \frac{\partial \alpha_{\text{th}}(T - T_0)}{\partial T_g} \frac{\partial T_g}{\partial \mathbf{F}_{jC}}, \quad (\text{E.83})$$

where

$$\frac{\partial \alpha_{\text{th}}(T - T_0)}{\partial T_g} = \begin{cases} 0 & \text{if } T \leq T_g \text{ and } T_0 \leq T_g, \\ -\alpha_{gl} + \alpha_r & \text{if } T \leq T_g \text{ and } T_0 > T_g, \\ -\alpha_r + \alpha_{gl} & \text{if } T > T_g \text{ and } T_0 \leq T_g, \\ 0 & \text{if } T > T_g \text{ and } T_0 > T_g. \end{cases} \quad (\text{E.84})$$

Moreover, we need to compute  $\frac{\partial L(T)}{\partial \mathbf{F}_{jC}}$  by recalling Eq. (E.48)

$$\frac{\partial L(T)}{\partial \mathbf{F}_{jC}} = -\frac{\epsilon_0^{(1)} \Delta t}{TK_B} \exp\left(-\frac{1}{\xi_{gl}}\right) \exp\left(-\frac{Q}{K_B T}\right) \frac{\partial Q}{\partial \mathbf{F}_{jC}} \quad \text{if } T \leq T_g, \quad (\text{E.85})$$

and

$$\begin{aligned} \frac{\partial L(T)}{\partial \mathbf{F}_{jC}} &= -\frac{\epsilon_0^{(1)} \Delta t}{TK_B} \exp\left(-\frac{1}{(\xi_{gl} + d(T - T_g))}\right) \exp\left(-\frac{Q}{K_B T}\right) \frac{\partial Q}{\partial \mathbf{F}_{jC}} \\ &\quad -\epsilon_0^{(1)} \Delta t \exp\left(-\frac{1}{(\xi_{gl} + d(T - T_g))}\right) \exp\left(-\frac{Q}{K_B T}\right) \frac{d}{(\xi_{gl} + d(T - T_g))^2} \frac{\partial T_g}{\partial \mathbf{F}_{jC}} \quad \text{if } T > T_g, \end{aligned} \quad (\text{E.86})$$

where  $\frac{\partial Q(T)}{\partial \mathbf{F}}$  is computed, after recalling Eq. (6.61)

$$\frac{\partial Q(T)}{\partial \mathbf{F}_{jC}} = \left[ \frac{1}{2\Delta} (Q_{gl} - Q_r) \left(1 - \tanh^2\left(\frac{1}{\Delta}(T - T_g)\right)\right) \right] \frac{\partial T_g}{\partial \mathbf{F}_{jC}}. \quad (\text{E.87})$$



Eventually, by gathering Eqs. (E.75-E.87), Eq. (E.68) becomes

$$\begin{aligned}
\frac{\partial \Omega^{(1)}}{\partial \mathbf{F}_{jC}} \Big|_{\Delta \epsilon^{p(1)}} &= -\frac{2mK_B T}{V} \frac{1}{\sqrt{\left(\frac{\Delta \epsilon^{p(1)}}{L(T)}\right)^{2m} + 1}} (\Delta \epsilon^{p(1)})^m (L(T))^{-m-1} \frac{\partial L(T)}{\partial \mathbf{F}_{jC}} \\
&\quad - \frac{1}{\sqrt{2}} \frac{\partial G(T)}{\partial \mathbf{F}_{jC}} \Big|_{\left(\ln(\mathbf{C}_{pr}^{e(1)})\right)_0} + \frac{\partial G(T)}{\partial \mathbf{F}_{jC}} \Delta \epsilon^{p(1)} - \frac{1}{2} \alpha_p \frac{\partial K(T)}{\partial \mathbf{F}_{jC}} \text{tr} \left( \ln(\mathbf{C}_{pr}^{e(1)}) \right) \\
&\quad + 3 \alpha_p \frac{\partial K(T)}{\partial \mathbf{F}_{jC}} \alpha_{th}(T - T_0) + 3 \alpha_p K(T) \frac{\partial \alpha_{th}(T - T_0)}{\partial \mathbf{F}_{jC}} + \frac{\partial S_{a(n+1)}}{\partial \mathbf{F}_{jC}} \\
&\quad + \left[ -G(T) \mathbf{N}_{OM}^{(1)} \mathcal{L}_{OMHX}^e - \frac{1}{2} \alpha_p K(T) \delta_{YZ} \mathcal{L}_{(pr)YZHX}^e \right] \\
&\quad \mathbf{F}_{(pr)WH}^{p(1)-1} \mathbf{F}_{(pr)VX}^{p(1)-1} (\mathbf{F}_{jV} \delta_{WC} + \mathbf{F}_{jW} \delta_{VC}) + \frac{\partial H_b(T)}{\partial \mathbf{F}_{jC}} \left( \sqrt{\frac{\text{tr} \mathbf{C}}{3}} - 1 \right)^a \\
&\quad + \frac{a}{2} H_b(T) \left( \sqrt{\frac{\text{tr} \mathbf{C}}{3}} - 1 \right)^{a-1} \frac{1}{\sqrt{3 \text{tr} \mathbf{C}}} \delta_{WV} (\mathbf{F}_{jV} \delta_{WC} + \mathbf{F}_{jW} \delta_{VC}).
\end{aligned} \tag{E.88}$$

Therefore, Eq. (E.67) becomes

$$\frac{\partial \Delta \epsilon^{p(1)}}{\partial \mathbf{F}_{jC}} = -\frac{1}{J} \frac{\partial \Omega^{(1)}}{\partial \mathbf{F}_{jC}} \Big|_{\Delta \epsilon^{p(1)}}. \tag{E.89}$$

By the same way of the first term of Eq. (E.68), the derivative of  $\mathbf{N}^{(1)}$  Eq. (E.21) reads

$$\begin{aligned}
\frac{\partial \mathbf{N}_{OP}^{(1)}}{\partial \mathbf{C}_{WV}^{(1)}} &= \frac{\partial \mathbf{N}_{OP}^{(1)}}{\partial \mathbf{C}_{(pr)HX}^{e(1)}} \mathbf{F}_{(pr)WH}^{p(1)-1} \mathbf{F}_{(pr)VX}^{p(1)-1} \\
&= \frac{1}{\sqrt{2}} \left( \mathcal{L}_{(pr)OPHX}^e - \frac{1}{3} \delta_{YZ} \mathcal{L}_{(pr)YZHX}^e \delta_{OP} \right) \Big|_{\left(\ln(\mathbf{C}_{pr}^{e(1)})\right)_0}^{-1} \mathbf{F}_{(pr)WH}^{p(1)-1} \mathbf{F}_{(pr)VX}^{p(1)-1} \\
&\quad - \mathbf{N}_{QM}^{(1)} \Big|_{\left(\ln(\mathbf{C}_{pr}^{e(1)})\right)_0}^{-2} \left( \ln(\mathbf{C}_{(pr)OP}^{e(1)}) \right)_0 \mathcal{L}_{QMHX}^e \mathbf{F}_{(pr)WH}^{p(1)-1} \mathbf{F}_{(pr)VX}^{p(1)-1}.
\end{aligned} \tag{E.90}$$

which gives

$$\frac{\partial \mathbf{N}_{OP}^{(1)}}{\partial \mathbf{F}_{jC}} = \frac{\partial \mathbf{N}_{OP}^{(1)}}{\partial \mathbf{C}_{WV}^{(1)}} (\mathbf{F}_{jV} \delta_{WC} + \mathbf{F}_{jW} \delta_{VC}). \tag{E.91}$$

Combining Eqs. (E.89) and (E.91) in Eq. (E.65) leads to the final expression of the derivative of the equivalent plastic deformation.

Furthermore, the derivative of Mandel stress can be computed using Eq. (E.18)

$$\begin{aligned}
\frac{\partial \mathbf{M}_{\text{KL}}^{e(1)}}{\partial \mathbf{F}_{\text{jC}}} &= \frac{\partial \mathbf{M}_{\text{KL}}^{e(1)}}{\partial \mathbf{F}_{\text{jC}}} + \frac{\partial \mathbf{M}_{\text{KL}}^{e(1)}}{\partial \mathbf{C}_{\text{WV}}} \frac{\partial \mathbf{C}_{\text{WV}}}{\partial \mathbf{F}_{\text{jC}}} = \frac{\partial \mathbf{M}_{\text{KL}}^{e(1)}}{\partial \mathbf{F}_{\text{jC}}} + \frac{\partial \mathbf{M}_{\text{KL}}^{(1)}}{\partial \mathbf{C}_{\text{WV}}} (\mathbf{F}_{\text{jV}} \boldsymbol{\delta}_{\text{WC}} + \mathbf{F}_{\text{jW}} \boldsymbol{\delta}_{\text{VC}}) \\
&+ \frac{\partial \text{G}}{\partial \mathbf{F}_{\text{jC}}} \left( \ln(\mathbf{C}_{(\text{pr})\text{KL}}^{e(1)}) \right)_0 - 2 \frac{\partial \text{G}}{\partial \mathbf{F}_{\text{jC}}} \Delta \epsilon^{\text{P}(1)} \mathbf{N}_{\text{KL}}^{(1)} \\
&- 3 \frac{\partial \text{K}}{\partial \mathbf{F}_{\text{jC}}} \alpha_{\text{th}}(\text{T} - \text{T}_0) \boldsymbol{\delta}_{\text{KL}} - 3 \text{K} \frac{\partial \alpha_{\text{th}}(\text{T} - \text{T}_0)}{\partial \mathbf{F}_{\text{jC}}} \boldsymbol{\delta}_{\text{KL}} + \frac{1}{2} \frac{\partial \text{K}}{\partial \mathbf{F}_{\text{jC}}} \text{tr} \left( \ln(\mathbf{C}_{(\text{pr})}^{e(1)}) \right) \boldsymbol{\delta}_{\text{KL}} \\
&+ \left[ \text{G} (\mathcal{L}_{\text{KLHX}}^e - \frac{1}{3} \boldsymbol{\delta}_{\text{YZ}} \mathcal{L}_{\text{YZHX}}^e \boldsymbol{\delta}_{\text{KL}}) \mathbf{F}_{(\text{pr})\text{WH}}^{\text{P}(1)-1} \mathbf{F}_{(\text{pr})\text{VX}}^{\text{P}(1)-1} + \frac{1}{2} \text{K} \boldsymbol{\delta}_{\text{SU}} \mathcal{L}_{\text{SUHX}}^e \boldsymbol{\delta}_{\text{KL}} \mathbf{F}_{(\text{pr})\text{WH}}^{\text{P}(1)-1} \mathbf{F}_{(\text{pr})\text{VX}}^{\text{P}(1)-1} \right] \\
&(\mathbf{F}_{\text{jV}}^{(1)} \boldsymbol{\delta}_{\text{WC}} + \mathbf{F}_{\text{jW}}^{(1)} \boldsymbol{\delta}_{\text{VC}}) - 2 \text{G} \frac{\partial \Delta \epsilon^{\text{P}(1)}}{\partial \mathbf{F}_{\text{jC}}} \mathbf{N}_{\text{KL}}^{(1)} - 2 \text{G} \Delta \epsilon^{\text{P}(1)} \frac{\partial \mathbf{N}_{\text{KL}}^{(1)}}{\partial \mathbf{F}_{\text{jC}}}.
\end{aligned} \tag{E.92}$$

By combining Eqs. (E.62, E.63, E.64, E.65, E.89, E.91 and E.92) in Eq. (E.61) one gets the final expression of the derivative of the Piola-Kirchhoff stress tensor with respect to the deformation gradient.

In the following, the derivative of Piola-Kirchhoff stress tensor with respect of the temperature for the first mechanisms  $\frac{\partial \mathbf{P}}{\partial \text{T}}$  is developed

$$\begin{aligned}
\frac{\partial \mathbf{P}_{\text{iA}}^{(1)}}{\partial \text{T}} &= \frac{\partial (\mathbf{F}_{\text{iN}} \mathbf{F}_{\text{NM}}^{\text{P}(1)-1} \mathcal{L}_{\text{KLMS}}^e \mathbf{M}_{\text{KL}}^{e(1)} \mathbf{F}_{\text{SA}}^{\text{P}(1)-\text{T}})}{\partial \text{T}} \\
&= \mathbf{F}_{\text{iN}} \frac{\partial \mathbf{F}_{\text{NM}}^{\text{P}(1)-1}}{\partial \text{T}} \mathcal{L}_{\text{KLMS}}^e \mathbf{M}_{\text{KL}}^{e(1)} \mathbf{F}_{\text{SA}}^{\text{P}(1)-\text{T}} + \mathbf{F}_{\text{iN}} \mathbf{F}_{\text{NM}}^{\text{P}(1)-1} \mathcal{L}_{\text{KLMS}}^e \frac{\partial \mathbf{M}_{\text{KL}}^{e(1)}}{\partial \text{T}} \mathbf{F}_{\text{SA}}^{\text{P}(1)-\text{T}} \\
&+ \mathbf{F}_{\text{iN}} \mathbf{F}_{\text{NM}}^{\text{P}(1)-1} \frac{\partial \mathcal{L}_{\text{KLMS}}^e}{\partial \text{T}} \mathbf{M}_{\text{KL}}^{e(1)} \mathbf{F}_{\text{SA}}^{\text{P}(1)-\text{T}} + \mathbf{F}_{\text{iN}} \mathbf{F}_{\text{NM}}^{\text{P}(1)-1} \mathcal{L}_{\text{KLMS}}^e \mathbf{M}_{\text{KL}}^{e(1)} \frac{\partial \mathbf{F}_{\text{SA}}^{\text{P}(1)-\text{T}}}{\partial \text{T}}.
\end{aligned} \tag{E.93}$$

The term related to the fourth term of Eq. (E.93) can be derived as

$$\begin{aligned}
\frac{\partial \mathcal{L}_{\text{KLMS}}^e}{\partial \text{T}} &= \frac{\partial \mathcal{L}_{\text{KLMS}}^e}{\partial \mathbf{C}_{\text{QV}}^{e(1)}} \frac{\partial \mathbf{C}_{\text{QV}}^{e(1)}}{\partial \mathbf{F}_{\text{EU}}^{e(1)}} \frac{\partial \mathbf{F}_{\text{EU}}^{e(1)}}{\partial \text{T}} \\
&= \frac{\partial \mathcal{L}_{\text{KLMS}}^e}{\partial \mathbf{C}_{\text{QV}}^{e(1)}} \left( \boldsymbol{\delta}_{\text{QU}} \mathbf{F}_{\text{EV}}^{e(1)} + \mathbf{F}_{\text{EQ}}^{e(1)} \boldsymbol{\delta}_{\text{VU}} \right) \mathbf{F}_{\text{EW}} \frac{\partial \mathbf{F}_{\text{WU}}^{\text{P}(1)-1}}{\partial \text{T}},
\end{aligned} \tag{E.94}$$

where  $\frac{\partial \mathcal{L}^e}{\partial \mathbf{C}^{e(1)}}$  is obtained from the logarithmic approximation. The derivative of the plastic deformation gradient with respect to temperature reads

$$\begin{aligned}
\frac{\partial \mathbf{F}_{(\text{n}+1)\text{EZ}}^{\text{P}(1)}}{\partial \text{T}} &= \frac{\partial \exp(\Delta \epsilon^{\text{P}(1)} \mathbf{N}^{(1)})_{\text{EI}}}{\partial \text{T}} \mathbf{F}_{(\text{n})\text{IZ}}^{\text{P}} \\
&= \frac{\partial \exp(\Delta \epsilon^{\text{P}(1)} \mathbf{N}^{(1)})_{\text{EI}}}{\partial (\Delta \epsilon^{\text{P}(1)} \mathbf{N}^{(1)})_{\text{OP}}} \frac{\partial (\Delta \epsilon^{\text{P}(1)} \mathbf{N}^{(1)})_{\text{OP}}}{\partial \text{T}} \mathbf{F}_{(\text{n})\text{IZ}}^{\text{P}(1)} \\
&= \boldsymbol{\mathcal{Z}}_{\text{EIOP}} \mathbf{N}_{\text{OP}}^{(1)} \frac{\partial \Delta \epsilon^{\text{P}(1)}}{\partial \text{T}} \mathbf{F}_{(\text{n})\text{IZ}}^{\text{P}(1)},
\end{aligned} \tag{E.95}$$

which immediately gives the derivative of the inverse of the plastic deformation:

$$\frac{\partial \mathbf{F}_{XY}^{\mathbf{P}(1)-1}}{\partial \mathbf{T}} = -\mathbf{F}_{XE}^{\mathbf{P}(1)-1} \frac{\partial \mathbf{F}_{EZ}^{\mathbf{P}(1)}}{\partial \mathbf{T}} \mathbf{F}_{ZY}^{\mathbf{P}(1)-1}. \quad (\text{E.96})$$

In order to get  $\frac{\partial \Delta \epsilon^{\mathbf{P}(1)}}{\partial \mathbf{T}}$ , the derivative of the residual  $\Omega^{(1)}$ , Eq.(E.52), with respect to the temperature should be computed

$$\frac{\partial \Omega^{(1)}}{\partial \mathbf{T}} \Big|_{\Delta \epsilon^{\mathbf{P}(1)}} + \frac{\partial \Omega^{(1)}}{\partial \Delta \epsilon^{\mathbf{P}(1)}} \frac{\partial \Delta \epsilon^{\mathbf{P}(1)}}{\partial \mathbf{T}} = 0 \quad (\text{E.97})$$

$$\implies \frac{\partial \Delta \epsilon^{\mathbf{P}(1)}}{\partial \mathbf{T}} = -(\mathcal{J}_1^{-1}) \frac{\partial \Omega^{(1)}}{\partial \mathbf{T}} \Big|_{\Delta \epsilon^{\mathbf{P}(1)}}. \quad (\text{E.98})$$

We need to calculate the derivative of the residual  $\Omega^{(1)}$  with respect to the temperature  $\mathbf{T}$ . From Eq. (6.61) one has

$$\frac{\partial Q(\mathbf{T})}{\partial \mathbf{T}} = -\frac{1}{2\Delta} (Q_{gl} - Q_r) (1 - \tanh^2(\frac{1}{\Delta}(\mathbf{T} - \mathbf{T}_g))). \quad (\text{E.99})$$

From Eq. (6.54), one also has

$$\frac{\partial \nu(\mathbf{T})}{\partial \mathbf{T}} = -\frac{1}{2\Delta} (\nu_{gl} - \nu_r) (1 - \tanh^2(\frac{1}{\Delta}(\mathbf{T} - \mathbf{T}_g))), \quad (\text{E.100})$$

and from Eqs. (6.52), one has

$$\frac{\partial G(\mathbf{T})}{\partial \mathbf{T}} = \begin{cases} -\frac{1}{2\Delta} (G_{gl} - G_r) (1 - \tanh^2(\frac{1}{\Delta}(\mathbf{T} - \mathbf{T}_g))) - M_{gl} & \text{if } \mathbf{T} \leq \mathbf{T}_g, \\ -\frac{1}{2\Delta} (G_{gl} - G_r) (1 - \tanh^2(\frac{1}{\Delta}(\mathbf{T} - \mathbf{T}_g))) - M_r & \text{if } \mathbf{T} > \mathbf{T}_g. \end{cases} \quad (\text{E.101})$$

The derivative of the bulk modulus, Eq. (6.55), reads

$$\frac{\partial K(\mathbf{T})}{\partial \mathbf{T}} = \frac{\partial G(\mathbf{T})}{\partial \mathbf{T}} \frac{2(1+\nu)}{3(1-2\nu)} + G(\mathbf{T}) \left( \frac{2 \frac{\partial \nu}{\partial \mathbf{T}} (1-2\nu) + 4 \frac{\partial \nu}{\partial \mathbf{T}} (1+\nu)}{3(1-2\nu)^2} \right), \quad (\text{E.102})$$

and the derivative of the thermal strain Eq. (6.53), reads

$$\frac{\partial \alpha_{th}(\mathbf{T} - \mathbf{T}_0)}{\partial \mathbf{T}} = \begin{cases} \alpha_{gl} & \text{if } \mathbf{T} \leq \mathbf{T}_g \text{ and } \mathbf{T}_0 \leq \mathbf{T}_g, \\ \alpha_r & \text{if } \mathbf{T} \leq \mathbf{T}_g \text{ and } \mathbf{T}_0 > \mathbf{T}_g. \end{cases} \quad (\text{E.103})$$

The derivative of The derivative of Eq. (E.48), reads

$$\frac{\partial L(\mathbf{T})}{\partial \mathbf{T}} = \epsilon_0^{(1)} \Delta t \exp\left(-\frac{1}{\xi_{gl}}\right) \exp\left(-\frac{Q}{K_B T}\right) \left( \frac{-\frac{\partial Q(\mathbf{T})}{\partial \mathbf{T}} K_B T + Q K_B}{K_B^2 T^2} \right) \quad \text{if } \mathbf{T} \leq \mathbf{T}_g, \quad (\text{E.104})$$

The derivative of Eq. (E.48) reads

$$\begin{aligned} \frac{\partial L(\mathbf{T})}{\partial \mathbf{T}} &= \epsilon_0^{(1)} \Delta t \exp\left(-\frac{1}{(\xi_{gl} + d(\mathbf{T} - \mathbf{T}_g))}\right) \exp\left(-\frac{Q(\mathbf{T})}{K_B T}\right) \frac{d}{(\xi_{gl} + d(\mathbf{T} - \mathbf{T}_g))^2} \\ &+ \epsilon_0^{(1)} \Delta t \exp\left(-\frac{1}{(\xi_{gl} + d(\mathbf{T} - \mathbf{T}_g))}\right) \exp\left(-\frac{Q(\mathbf{T})}{K_B T}\right) \left( \frac{-\frac{\partial Q(\mathbf{T})}{\partial \mathbf{T}} K_B T + Q K_B}{K_B^2 T^2} \right) \quad \text{if } \mathbf{T} > \mathbf{T}_g. \end{aligned} \quad (\text{E.105})$$

Also, the derivative of Eq. (6.70) is expressed as

$$\frac{\partial H_b(T)}{\partial T} = \begin{cases} -\frac{1}{2\Delta}(H_{gl} - H_r)(1 - \tanh^2(\frac{1}{\Delta}(T - T_g))) - L_{gl} & \text{if } T \leq T_g \\ -\frac{1}{2\Delta}(H_{gl} - H_r)(1 - \tanh^2(\frac{1}{\Delta}(T - T_g))) - L_r & \text{if } T > T_g. \end{cases} \quad (\text{E.106})$$

Eventually from Eqs. (E.42, E.43), we have

$$\frac{\partial S_{a(n+1)}}{\partial T} = \begin{cases} -\frac{r h_a \beta b}{T_g} z(1 - \frac{T}{T_g})^{r-1} \left( \frac{\Delta \epsilon^{p(1)}}{\Delta t \epsilon_r} \right)^s \Delta \epsilon^{p(1)} & \text{if } T \leq T_g, \\ 0 & \text{if } T > T_g. \end{cases} \quad (\text{E.107})$$

After substituting Eqs. (E.99- E.107), in Eq. (E.52), one has

$$\begin{aligned} \frac{\partial \Omega^{(1)}}{\partial T} &= \frac{2K_B}{V} \operatorname{arcsinh} \left( \frac{\Delta \epsilon_1^{p(1)}}{L(T)} \right)^m - \frac{2mK_B T}{V} \frac{1}{\sqrt{\left( \frac{\Delta \epsilon^{p(1)}}{L(T)} \right)^{2m} + 1}} (\Delta \epsilon^{p(1)})^m (L(T))^{-m-1} \frac{\partial L(T)}{\partial T} \\ &\quad - \frac{1}{\sqrt{2}} \frac{\partial G(T)}{\partial T} \left| \left( \ln(\mathbf{C}_{pr}^{e(1)}) \right)_0 \right| + \frac{\partial G(T)}{\partial T} \Delta \epsilon_1^{p(1)} - \frac{1}{2} \alpha_p \frac{\partial K(T)}{\partial T} \operatorname{tr} \left( \ln(\mathbf{C}_{pr}^{e(1)}) \right) \\ &\quad + 3 \alpha_p K(T) \left( \frac{\partial \alpha_{th}(T - T_0)}{\partial T} \right) + 3 \alpha_p \frac{\partial K(T)}{\partial T} \alpha_{th}(T - T_0) \\ &\quad + \frac{\partial H_b(T)}{\partial T} (\sqrt{\operatorname{tr} \mathbf{C}/3} - 1)^a + \frac{\partial S_{a(n+1)}}{\partial T}. \end{aligned} \quad (\text{E.108})$$

Therefore, the derivative of the plastic shear strain rate with respect to the temperature can be evaluated from Eq. (E.98). Finally by substituting Eq. (E.98) in Eq. (E.95) yields the derivative of plastic deformation gradient.

Eventually, by using Eqs. (E.89, E.101, E.102, and E.103) we can evaluate the missing term of Eq. (E.93) as

$$\begin{aligned} \frac{\partial \mathbf{M}_{KL}^{e(1)}}{\partial T} &= \frac{\partial G(T)}{\partial T} \left( \ln(\mathbf{C}_{(pr)KL}^{e(1)}) \right)_0 - 2 \frac{\partial G(T)}{\partial T} \Delta \epsilon^{p(1)} \mathbf{N}_{KL}^{(1)} - 2G(T) \frac{\partial \Delta \epsilon^{p(1)}}{\partial T} \mathbf{N}_{KL}^{(1)} \\ &\quad - 3 \frac{\partial K(T)}{\partial T} \alpha_{th}(T - T_0) \boldsymbol{\delta}_{KL} - 3K(T) \frac{\partial \alpha_{th}(T - T_0)}{\partial T} \boldsymbol{\delta}_{KL} + \frac{1}{2} \frac{\partial K(T)}{\partial T} \operatorname{tr} \left( \ln(\mathbf{C}_{(pr)}^{e(1)}) \right) \boldsymbol{\delta}_{KL} \end{aligned} \quad (\text{E.109})$$

Combining Eqs. (E.95, E.96 and E.109) in Eq. (E.93) yields the final expression of the derivative of the first Piola-Kirchhoff stress tensor with respect to the temperature.

## E.2.2 Predictor-corrector for second mechanism ( $\alpha = 2$ )

As explained in Section 6.3.4.3, the second mechanism is purely deviatoric.

### E.2.2.1 Flow rule

Let us define the normal direction as

$$\mathbf{N}^{(2)} = \frac{\mathbf{M}^{e(2)}}{\sqrt{2} |\mathbf{M}^{e(2)}|}. \quad (\text{E.110})$$

Then one can write the elastic deformation gradient Eq. (6.13) from the incremental form of the plastic flow Eq. (6.28) as

$$\bar{\mathbf{F}}^{e(2)} = \bar{\mathbf{F}}^{(2)} \mathbf{F}_{(n)}^{p(2)-1} \left[ \exp(\dot{\epsilon}_0^{(2)} \Delta t \left( \frac{\bar{\tau}^{(2)}}{S^{(2)}(T)} \right)^{\frac{1}{m}} \mathbf{N}^{(2)}) \right]^{-1}. \quad (\text{E.111})$$

Therefore, the elastic right Cauchy tensor reads

$$\bar{\mathbf{C}}^{e(2)} = \left[ \exp(\Delta \epsilon^{p(2)} \mathbf{N}^{(2)}) \right]^{-T} \bar{\mathbf{C}}_{(\text{pr})}^{e(2)} \left[ \exp(\Delta \epsilon^{p(2)} \mathbf{N}^{(2)}) \right]^{-1}, \quad (\text{E.112})$$

with  $\bar{\mathbf{C}}_{(\text{pr})}^{e(2)} = \mathbf{F}_{(n)}^{p(2)-T} \mathbf{F}_{(n+1)}^T \mathbf{F}_{(n+1)} \mathbf{F}_{(n)}^{p(2)-1}$

### E.2.2.2 Mandel stress

Using Eq. (6.76), one has

$$\mathbf{S}^{e(2)} = J^{-\frac{2}{3}} \mu^{(2)} \left( 1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)} - 3}{I_m^{(2)}} \right)^{-1} \left\{ \mathbf{I} - \frac{1}{3} (\text{tr} \bar{\mathbf{C}}^{e(2)}) \right. \\ \left. \left[ \exp(\dot{\epsilon}_0^{(2)} \Delta t \left( \frac{\bar{\tau}^{(2)}}{S^{(2)}(T)} \right)^{\frac{1}{m}} \mathbf{N}^{(2)}) \right] \bar{\mathbf{C}}_{(\text{pr})}^{e(2)-1} \left[ \exp(\dot{\epsilon}_0^{(2)} \Delta t \left( \frac{\bar{\tau}^{(2)}}{S^{(2)}(T)} \right)^{\frac{1}{m}} \mathbf{N}^{(2)}) \right]^T \right\}. \quad (\text{E.113})$$

Thereby, using Eq. (6.79), yields

$$\mathbf{M}^{e(2)} = \mu^{(2)} \left( 1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)} - 3}{I_m^{(2)}} \right)^{-1} \left\{ -\frac{1}{3} (\text{tr} \bar{\mathbf{C}}^{e(2)}) \mathbf{I} + \left[ \exp(\dot{\epsilon}_0^{(2)} \Delta t \left( \frac{\bar{\tau}^{(2)}}{S^{(2)}(T)} \right)^{\frac{1}{m}} \mathbf{N}^{(2)}) \right]^{-T} \right. \\ \left. \bar{\mathbf{C}}_{(\text{pr})}^{e(2)} \left[ \exp(\dot{\epsilon}_0^{(2)} \Delta t \left( \frac{\bar{\tau}^{(2)}}{S^{(2)}(T)} \right)^{\frac{1}{m}} \mathbf{N}^{(2)}) \right]^{-1} \right\}. \quad (\text{E.114})$$

### E.2.2.3 Shear strain

Combining Eq. (6.25) with Eq. (E.114), yields

$$\bar{\tau}^{(2)} = \frac{1}{\sqrt{2}} |\mu^{(2)} \left( 1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)} - 3}{I_m^{(2)}} \right)^{-1} \left\{ -\frac{1}{3} (\text{tr} \bar{\mathbf{C}}^{e(2)}) + \left[ \exp(\dot{\epsilon}_0^{(2)} \Delta t \left( \frac{\bar{\tau}^{(2)}}{S^{(2)}(T)} \right)^{\frac{1}{m}} \mathbf{N}^{(2)}) \right]^{-T} \right. \\ \left. \bar{\mathbf{C}}_{(\text{pr})}^{e(2)} \left[ \exp(\dot{\epsilon}_0^{(2)} \Delta t \left( \frac{\bar{\tau}^{(2)}}{S^{(2)}(T)} \right)^{\frac{1}{m}} \mathbf{N}^{(2)}) \right]^{-1} \right\}|. \quad (\text{E.115})$$

### E.2.2.4 Non-linear system of equations

The Mandel stress is the solution of the system for the mechanism 2, which is stated as

$$\mathbf{M}^{e(2)} = \mathbf{C}^{e(2)} \mathbf{S}^{e(2)} = f(\Delta \epsilon^p(2), \mathbf{N}^{(2)})|_{\bar{\mathbf{C}}_{(\text{pr})}^{e(2)}, \mathbf{J}} = f(\bar{\tau}^{(2)}, \mathbf{N}^{(2)})|_{\bar{\mathbf{C}}_{(\text{pr})}^{e(2)}, \mathbf{J}} = f(\mathbf{M}^{e(2)})|_{\bar{\mathbf{C}}_{(\text{pr})}^{e(2)}, \mathbf{J}}. \quad (\text{E.116})$$

Notice that  $(\bar{\mathbf{C}}_{\text{pr}}^{e(2)})$  and  $(\mathbf{J})$  are constant during the resolution of the system. Using the results here above, Eq. (E.116) is written in the implicit residual form

$$\begin{aligned} \boldsymbol{\Omega}^{(2)} = & \mathbf{M}^{e(2)} - \mu^{(2)} \left(1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)} - 3}{I_m^{(2)}}\right)^{-1} \left\{ -\frac{1}{3} (\text{tr} \bar{\mathbf{C}}^{e(2)}) \mathbf{I} \right. \\ & + \left[ \exp(\dot{\epsilon}_0^{(2)} \Delta t \left(\frac{|\mathbf{M}^{e(2)}|}{\sqrt{2} S^{(2)}(\text{T})}\right)^{\frac{1}{m}} \frac{\mathbf{M}^{e(2)}}{\sqrt{2} |\mathbf{M}^{e(2)}|} \right]^{-\text{T}} \bar{\mathbf{C}}_{(\text{pr})}^{e(2)} \left[ \exp(\dot{\epsilon}_0^{(2)} \Delta t \left(\frac{|\mathbf{M}^{e(2)}|}{\sqrt{2} S^{(2)}(\text{T})}\right)^{\frac{1}{m}} \right. \\ & \left. \left. \frac{\mathbf{M}^{e(2)}}{\sqrt{2} |\mathbf{M}^{e(2)}|} \right) \right]^{-1} \right\} = 0. \end{aligned} \quad (\text{E.117})$$

The associated Newton-Raphson scheme reads

$$\boldsymbol{\Omega}^{(2)} + \frac{\partial \boldsymbol{\Omega}^{(2)}}{\partial \mathbf{M}^{e(2)}}|_{\bar{\mathbf{C}}_{(\text{pr})}^{e(2)}, \mathbf{J}} \Delta \mathbf{M}^{e(2)} = 0. \quad (\text{E.118})$$

Let us define Jaccobian matrix as  $\mathbf{j}_2 = \frac{\partial \boldsymbol{\Omega}^{(2)}}{\partial \mathbf{M}^{e(2)}}|_{\bar{\mathbf{C}}_{(\text{pr})}^{e(2)}, \mathbf{J}}$ , which leads to

$$\Delta \mathbf{M}^{e(2)} = -\mathbf{j}_2^{-1} \boldsymbol{\Omega}^{(2)}. \quad (\text{E.119})$$

The solution is then updated by

$$\mathbf{M}^{e(2)} \leftarrow \mathbf{M}^{e(2)} + \Delta \mathbf{M}^{e(2)}, \quad (\text{E.120})$$

and the iterations continue until convergence to a specified tolerance is achieved.

One has now to compute the Jacobian using Eq. (E.117), leading to

$$\begin{aligned} \frac{\partial \boldsymbol{\Omega}_{\text{US}}^{(2)}}{\partial \mathbf{M}_{\text{CD}}^{e(2)}} = & \frac{\partial}{\partial \mathbf{M}_{\text{CD}}^{e(2)}} \left( \mathbf{M}_{\text{US}}^{e(2)} - \mu^{(2)} \left(1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)} - 3}{I_m^{(2)}}\right)^{-1} \left\{ -\frac{1}{3} \text{tr} \bar{\mathbf{C}}^{e(2)} \boldsymbol{\delta}_{\text{US}} \right. \right. \\ & + \left[ \exp(\dot{\epsilon}_0^{(2)} \Delta t \left(\frac{|\mathbf{M}^{e(2)}|}{\sqrt{2} S^{(2)}(\text{T})}\right)^{\frac{1}{m}} \frac{\mathbf{M}^{e(2)}}{\sqrt{2} |\mathbf{M}^{e(2)}|} \right]_{\text{UR}}^{-\text{T}} \\ & \left. \left. \bar{\mathbf{C}}_{(\text{pr})\text{RQ}}^{e(2)} \left[ \exp(\dot{\epsilon}_0^{(2)} \Delta t \left(\frac{|\mathbf{M}^{e(2)}|}{\sqrt{2} S^{(2)}(\text{T})}\right)^{\frac{1}{m}} \frac{\mathbf{M}^{e(2)}}{\sqrt{2} |\mathbf{M}^{e(2)}|} \right]_{\text{QS}}^{-1} \right\} \right). \end{aligned} \quad (\text{E.121})$$

Let us successively compute the derivatives of the components of  $\boldsymbol{\Omega}^{(2)}$ . First one has

$$\frac{\partial \text{tr} \bar{\mathbf{C}}^{e(2)}}{\partial \mathbf{M}_{\text{CD}}^{e(2)}} = \frac{\partial \text{tr} \bar{\mathbf{C}}^{e(2)}}{\partial \bar{\mathbf{C}}_{\text{YZ}}^{e(2)}} \frac{\partial \bar{\mathbf{C}}_{\text{YZ}}^{e(2)}}{\partial \mathbf{M}_{\text{CD}}^{e(2)}} = \boldsymbol{\delta}_{\text{YZ}} \frac{\partial \bar{\mathbf{C}}_{\text{YZ}}^{e(2)}}{\partial \mathbf{M}_{\text{CD}}^{e(2)}}, \quad (\text{E.122})$$

with Eq. (E.112)

$$\frac{\partial \bar{\mathbf{C}}_{YZ}^{e(2)}}{\partial \mathbf{M}_{CD}^{e(2)}} = \frac{\partial}{\partial \mathbf{M}_{CD}^{e(2)}} \left\{ \left[ \exp(\dot{\epsilon}_0^{(2)} \Delta t) \left( \frac{|\mathbf{M}^{e(2)}|}{\sqrt{2S^{(2)}(T)}} \right)^{\frac{1}{m}} \frac{\mathbf{M}^{e(2)}}{\sqrt{2}|\mathbf{M}^{e(2)}|} \right]_{YI}^{-T} \bar{\mathbf{C}}_{PIJ}^{e(2)} \right. \\ \left. \left[ \exp(\dot{\epsilon}_0^{(2)} \Delta t) \left( \frac{|\mathbf{M}^{e(2)}|}{\sqrt{2S^{(2)}(T)}} \right)^{\frac{1}{m}} \frac{\mathbf{M}^{e(2)}}{\sqrt{2}|\mathbf{M}^{e(2)}|} \right]_{JZ}^{-1} \right\}. \quad (\text{E.123})$$

Let us define  $y = \frac{\epsilon_0^{(2)} \Delta t S^{(2)}(T)^{-\frac{1}{m}}}{\sqrt{2}^{\frac{m+1}{m}}}$ , then one gets

$$\frac{\partial \left[ \exp(y|\mathbf{M}^{e(2)}|^{\frac{1-m}{m}} \mathbf{M}^{e(2)}) \right]_{YI}^{-T}}{\partial \mathbf{M}_{CD}^{e(2)}} = \frac{\partial \left[ \exp(y|\mathbf{M}^{e(2)}|^{\frac{1-m}{m}} \mathbf{M}^{e(2)}) \right]_{YI}^{-T}}{\partial \left[ \exp(y|\mathbf{M}^{e(2)}|^{\frac{1-m}{m}} \mathbf{M}^{e(2)}) \right]_{AB}} \frac{\partial \left[ \exp(y|\mathbf{M}^{e(2)}|^{\frac{1-m}{m}} \mathbf{M}^{e(2)}) \right]_{AB}}{\partial (y|\mathbf{M}^{e(2)}|^{\frac{1-m}{m}} \mathbf{M}_{KL}^{e(2)})} \\ \frac{\partial (y|\mathbf{M}^{e(2)}|^{\frac{1-m}{m}} \mathbf{M}_{KL}^{e(2)})}{\partial \mathbf{M}_{CD}^{e(2)}}. \quad (\text{E.124})$$

To evaluate this derivation, we use

$$\frac{\partial \left[ \exp(y|\mathbf{M}^{e(2)}|^{\frac{1-m}{m}} \mathbf{M}^{e(2)}) \right]_{YI}^{-T}}{\partial \left[ \exp(y|\mathbf{M}^{e(2)}|^{\frac{1-m}{m}} \mathbf{M}^{e(2)}) \right]_{AB}} = - \left[ \exp(y|\mathbf{M}^{e(2)}|^{\frac{1-m}{m}} \mathbf{M}^{e(2)}) \right]_{YB}^{-T} \left[ \exp(y|\mathbf{M}^{e(2)}|^{\frac{1-m}{m}} \mathbf{M}^{e(2)}) \right]_{AI}^{-T}, \quad (\text{E.125})$$

$$\frac{\partial \left[ \exp(y|\mathbf{M}^{e(2)}|^{\frac{1-m}{m}} \mathbf{M}^{e(2)}) \right]_{AB}}{\partial (y|\mathbf{M}^{e(2)}|^{\frac{1-m}{m}} \mathbf{M}_{KL}^{e(2)})} = \mathcal{Z}_{ABKL}, \quad (\text{E.126})$$

$$\frac{\partial |\mathbf{M}^{e(2)}|}{\partial \mathbf{M}^{e(2)}} = \frac{\partial \sqrt{\mathbf{M}^{e(2)} : \mathbf{M}^{e(2)}}}{\partial \mathbf{M}^{e(2)}} = \frac{\mathbf{M}^{e(2)} : \mathcal{I}}{|\mathbf{M}^{e(2)}|}, \quad (\text{E.127})$$

and

$$\frac{\partial (y|\mathbf{M}^{e(2)}|^{\frac{1-m}{m}} \mathbf{M}_{KL}^{e(2)})}{\partial \mathbf{M}_{CD}^{e(2)}} = y \left( \frac{\partial (|\mathbf{M}^{e(2)}|^{\frac{1-m}{m}})}{\partial \mathbf{M}_{CD}^{e(2)}} \mathbf{M}_{KL}^{e(2)} + |\mathbf{M}^{e(2)}|^{\frac{1-m}{m}} \frac{\partial (\mathbf{M}_{KL}^{e(2)})}{\partial \mathbf{M}_{CD}^{e(2)}} \right) \\ = y \left( \frac{1-m}{m} |\mathbf{M}^{e(2)}|^{\frac{1-3m}{m}} \mathbf{M}_{CD}^{e(2)} \mathbf{M}_{KL}^{e(2)} + |\mathbf{M}^{e(2)}|^{\frac{1-m}{m}} \mathcal{I}_{KLCD} \right), \quad (\text{E.128})$$

where  $\mathcal{I}_{KLCD} = \frac{1}{2}(\delta_{KD}\delta_{LC} + \delta_{KL}\delta_{CD})$ . Then by inserting Eqs. (E.125- E.128) in Eq. (E.124) we have

$$\frac{\partial \left[ \exp(y|\mathbf{M}^{e(2)}|^{\frac{1-m}{m}} \mathbf{M}^{e(2)}) \right]_{YI}^{-T}}{\partial \mathbf{M}_{CD}^{e(2)}} = - \left[ \exp(y|\mathbf{M}^{e(2)}|^{\frac{1-m}{m}} \mathbf{M}^{e(2)}) \right]_{YB}^{-T} \left[ \exp(y|\mathbf{M}^{e(2)}|^{\frac{1-m}{m}} \mathbf{M}^{e(2)}) \right]_{AI}^{-T} \\ \mathcal{Z}_{ABKL} y \left( \frac{1-m}{m} |\mathbf{M}^{e(2)}|^{\frac{1-3m}{m}} \mathbf{M}_{CD}^{e(2)} \mathbf{M}_{KL}^{e(2)} + |\mathbf{M}^{e(2)}|^{\frac{1-m}{m}} \mathcal{I}_{KLCD} \right). \quad (\text{E.129})$$

By the same way as to derive Eq. (E.124), we can compute the following derivative

$$\frac{\partial \left[ \exp(y|\mathbf{M}^{e(2)}| \frac{1-m}{m} \mathbf{M}^{e(2)}) \right]_{\text{JZ}}^{-1}}{\partial \mathbf{M}_{\text{CD}}^{e(2)}} = \frac{\partial \left[ \exp(y|\mathbf{M}^{e(2)}| \frac{1-m}{m} \mathbf{M}^{e(2)}) \right]_{\text{JZ}}^{-1}}{\partial \left[ \exp(y|\mathbf{M}^{e(2)}| \frac{1-m}{m} \mathbf{M}^{e(2)}) \right]_{\text{AB}}} \frac{\partial \left[ \exp(y|\mathbf{M}^{e(2)}| \frac{1-m}{m} \mathbf{M}^{e(2)}) \right]_{\text{AB}}^{-1}}{\partial (y|\mathbf{M}^{e(2)}| \frac{1-m}{m} \mathbf{M}_{\text{KL}}^{e(2)})} \frac{\partial (y|\mathbf{M}^{e(2)}| \frac{1-m}{m} \mathbf{M}_{\text{KL}}^{e(2)})}{\partial \mathbf{M}_{\text{CD}}^{e(2)}}. \quad (\text{E.130})$$

By combining the above result, we have

$$\begin{aligned} \frac{\partial \bar{\mathbf{C}}_{\text{YZ}}^{e(2)}}{\partial \mathbf{M}_{\text{CD}}^{e(2)}} &= -y \left[ \exp(y|\mathbf{M}^{e(2)}| \frac{1-m}{m} \mathbf{M}^{e(2)}) \right]_{\text{YB}}^{-\text{T}} \left[ \exp(y|\mathbf{M}^{e(2)}| \frac{1-m}{m} \mathbf{M}^{e(2)}) \right]_{\text{AI}}^{-\text{T}} \mathbf{Z}_{\text{ABKL}} \\ &\quad \left( \frac{1-m}{m} |\mathbf{M}^{e(2)}| \frac{1-3m}{m} \mathbf{M}_{\text{CD}}^{e(2)} \mathbf{M}_{\text{KL}}^{e(2)} + |\mathbf{M}^{e(2)}| \frac{1-m}{m} \mathcal{I}_{\text{KLCD}} \right) \bar{\mathbf{C}}_{(\text{pr})\text{IJ}}^{e(2)} \left[ \exp(y|\mathbf{M}^{e(2)}| \frac{1-m}{m} \mathbf{M}^{e(2)}) \right]_{\text{JZ}}^{-1} \\ &\quad - y \left[ \exp(y|\mathbf{M}^{e(2)}| \frac{1-m}{m} \mathbf{M}^{e(2)}) \right]_{\text{YI}}^{-\text{T}} \bar{\mathbf{C}}_{(\text{pr})\text{IJ}}^{e(2)} \left[ \exp(y|\mathbf{M}^{e(2)}| \frac{1-m}{m} \mathbf{M}^{e(2)}) \right]_{\text{JA}}^{-1} \\ &\quad \left[ \exp(y|\mathbf{M}^{e(2)}| \frac{1-m}{m} \mathbf{M}^{e(2)}) \right]_{\text{BZ}}^{-1} \mathbf{Z}_{\text{ABKL}} \\ &\quad \left( \frac{1-m}{m} |\mathbf{M}^{e(2)}| \frac{1-3m}{m} \mathbf{M}_{\text{CD}}^{e(2)} \mathbf{M}_{\text{KL}}^{e(2)} + |\mathbf{M}^{e(2)}| \frac{1-m}{m} \mathcal{I}_{\text{KLCD}} \right). \end{aligned} \quad (\text{E.131})$$

Combining Eqs. (E.123, E.131) leads to the final expression of Eq. (E.121), and the system Eq. (E.119) is iteratively solved using the Jaccobian matrix

$$\begin{aligned} \mathbf{jz} &= \frac{\partial \Omega_{\text{US}}^{(2)}}{\partial \mathbf{M}_{\text{CD}}^{e(2)}} = \mathcal{I}_{\text{USCD}} - \frac{\mu^{(2)}}{I_{\text{m}}^{(2)}} \left( 1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)} - 3}{I_{\text{m}}^{(2)}} \right)^{-2} \frac{\partial \text{tr} \bar{\mathbf{C}}^{e(2)}}{\partial \mathbf{M}_{\text{CD}}^{e(2)}} \left\{ -\frac{1}{3} \text{tr} \bar{\mathbf{C}}^{e(2)} \delta_{\text{US}} \right. \\ &\quad \left. + \left[ \exp(y|\mathbf{M}^{e(2)}| \frac{1-m}{m} \mathbf{M}^{e(2)}) \right]_{\text{UR}}^{-\text{T}} \bar{\mathbf{C}}_{(\text{pr})\text{RQ}}^{e(2)} \left[ \exp(y|\mathbf{M}^{e(2)}| \frac{1-m}{m} \mathbf{M}^{e(2)}) \right]_{\text{QS}}^{-1} \right\} \\ &\quad - \mu^{(2)} \left( 1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)} - 3}{I_{\text{m}}^{(2)}} \right)^{-1} \left[ -\frac{1}{3} \frac{\partial \text{tr} \bar{\mathbf{C}}^{e(2)}}{\partial \mathbf{M}_{\text{CD}}^{e(2)}} \delta_{\text{US}} - y \left[ \exp(y|\mathbf{M}^{e(2)}| \frac{1-m}{m} \mathbf{M}^{e(2)}) \right]_{\text{UB}}^{-\text{T}} \right. \\ &\quad \left[ \exp(y|\mathbf{M}^{e(2)}| \frac{1-m}{m} \mathbf{M}^{e(2)}) \right]_{\text{AR}}^{-\text{T}} \mathbf{Z}_{\text{ABKL}} \left( \frac{1-m}{m} |\mathbf{M}^{e(2)}| \frac{1-3m}{m} \mathbf{M}_{\text{CD}}^{e(2)} \mathbf{M}_{\text{KL}}^{e(2)} + |\mathbf{M}^{e(2)}| \frac{1-m}{m} \mathcal{I}_{\text{KLCD}} \right) \\ &\quad \bar{\mathbf{C}}_{(\text{pr})\text{RQ}}^{e(2)} \left[ \exp(y|\mathbf{M}^{e(2)}| \frac{1-m}{m} \mathbf{M}^{e(2)}) \right]_{\text{QS}}^{-1} - y \left[ \exp(y|\mathbf{M}^{e(2)}| \frac{1-m}{m} \mathbf{M}^{e(2)}) \right]_{\text{UR}}^{-\text{T}} \bar{\mathbf{C}}_{(\text{pr})\text{RQ}}^{e(2)} \\ &\quad \left[ \exp(y|\mathbf{M}^{e(2)}| \frac{1-m}{m} \mathbf{M}^{e(2)}) \right]_{\text{QA}}^{-1} \left[ \exp(y|\mathbf{M}^{e(2)}| \frac{1-m}{m} \mathbf{M}^{e(2)}) \right]_{\text{BS}}^{-1} \mathbf{Z}_{\text{ABKL}} \\ &\quad \left. \left( \frac{1-m}{m} |\mathbf{M}^{e(2)}| \frac{1-3m}{m} \mathbf{M}_{\text{CD}}^{e(2)} \mathbf{M}_{\text{KL}}^{e(2)} + |\mathbf{M}^{e(2)}| \frac{1-m}{m} \mathcal{I}_{\text{KLCD}} \right) \right]. \end{aligned} \quad (\text{E.132})$$



### E.2.2.5 Converged solution

Let us now compute the tangent for the second mechanism. From the first Piola-Kirchhoff stress defined in Eq. (6.23), one can get its derivative with respect of the deformation gradient as

$$\begin{aligned}
\frac{\partial \mathbf{P}_{iA}^{(2)}}{\partial \mathbf{F}_{jC}} &= \frac{\partial (\mathbf{F}_{iW} \mathbf{F}_{WD}^{p(2)-1} \mathbf{S}_{DB}^{e(2)} \mathbf{F}_{BA}^{p(2)-T})}{\partial \mathbf{F}_{jC}} \\
&= \delta_{ij} \delta_{WC} \mathbf{F}_{WD}^{p(2)-1} \mathbf{S}_{DB}^{e(2)} \mathbf{F}_{BA}^{p(2)-T} + \mathbf{F}_{iW} \frac{\partial \mathbf{F}_{WD}^{p(2)-1}}{\partial \mathbf{F}_{jC}} \mathbf{S}_{DB}^{e(2)} \mathbf{F}_{BA}^{p(2)-T} \\
&+ \mathbf{F}_{iW} \mathbf{F}_{WD}^{p(2)-1} \mathbf{S}_{DB}^{e(2)} \frac{\partial \mathbf{F}_{BA}^{p(2)-T}}{\partial \mathbf{F}_{jC}} + \mathbf{F}_{iW} \mathbf{F}_{WD}^{p(2)-1} \frac{\partial \mathbf{S}_{DB}^{e(2)}}{\partial \bar{\mathbf{F}}_{qM}^{e(2)}} \frac{\partial \bar{\mathbf{F}}_{qM}^{e(2)}}{\partial \mathbf{F}_{jC}} \mathbf{F}_{BA}^{p(2)-T} \\
&+ \mathbf{F}_{iW} \mathbf{F}_{WD}^{p(2)-1} \frac{\partial \mathbf{S}_{DB}^{e(2)}}{\partial \bar{\mathbf{F}}_{qM}^{e(2)}} \frac{\partial \bar{\mathbf{F}}_{qM}^{e(2)}}{\partial J} \frac{\partial J}{\partial \mathbf{F}_{jC}} \mathbf{F}_{BA}^{p(2)-T} + \mathbf{F}_{iW} \mathbf{F}_{WD}^{p(2)-1} \frac{\partial \mathbf{S}_{DB}^{(2)}}{\partial J} \frac{\partial J}{\partial \mathbf{F}_{jC}} \mathbf{F}_{BA}^{p(2)-T} \\
&+ \mathbf{F}_{iW} \mathbf{F}_{WD}^{p(2)-1} \frac{\partial \mathbf{S}_{DB}^{(2)}}{\partial \mu^{(2)}(T)} \frac{\partial \mu^{(2)}(T)}{\partial T_g} \frac{\partial T_g}{\partial \mathbf{F}_{jC}} \mathbf{F}_{BA}^{p(2)-T} \\
&+ \mathbf{F}_{iW} \mathbf{F}_{WD}^{p(2)-1} \frac{\partial \mathbf{S}_{DB}^{(2)}}{\partial S^{(2)}(T)} \frac{\partial S^{(2)}(T)}{\partial T_g} \frac{\partial T_g}{\partial \mathbf{F}_{jC}} \mathbf{F}_{BA}^{p(2)-T},
\end{aligned} \tag{E.133}$$

where the derivative of plastic deformation gradient can be computed by using Eq. (6.81, 6.82)

$$\begin{aligned}
\frac{\partial \mathbf{F}_{(n+1)EZ}^{p(2)}}{\partial \mathbf{F}_{jC}} &= \frac{\partial \exp(\Delta \mathbf{D}^{p(2)})_{EZ}}{\partial \mathbf{F}_{jC}} \mathbf{F}_{(n)IZ}^{p(2)} \\
&= \frac{\partial \exp(\Delta \epsilon^{p(2)} \mathbf{N}^{(2)})_{EI}}{\partial \mathbf{F}_{jC}} \mathbf{F}_{(n)IZ}^{p(2)} \\
&= \frac{\partial \exp(\Delta \epsilon^{p(2)} \mathbf{N}^{(2)})_{EI}}{\partial (\Delta \epsilon^{p(2)} \mathbf{N}^{(2)})_{OP}} \frac{\partial (\Delta \epsilon^{p(2)} \mathbf{N}^{(2)})_{OP}}{\partial \mathbf{F}_{jC}} \mathbf{F}_{(n)IZ}^{p(2)} \\
&= \mathcal{Z}_{EIOP} \left[ \mathbf{N}_{OP}^{(2)} \frac{\partial \Delta \epsilon^{p(2)}}{\partial \mathbf{F}_{jC}} + \Delta \epsilon^{p(2)} \frac{\partial \mathbf{N}_{OP}^{(2)}}{\partial \mathbf{F}_{jC}} \right] \mathbf{F}_{(n)IZ}^{p(2)}.
\end{aligned} \tag{E.134}$$

The derivatives of the inverse of the plastic deformation gradient  $\mathbf{F}^{p(2)-1}$  and of the elastic deformation mapping  $\mathbf{F}^{e(2)}$  are obtained similarly to mechanism 1, Eq. (E.62) and Eq. (E.63) respectively. Therefore, the deviatoric part derivative reads

$$\frac{\partial \bar{\mathbf{F}}_{qM}^{e(2)}}{\partial \mathbf{F}_{jC}} = J^{-\frac{1}{3}} \frac{\partial \mathbf{F}_{qM}^{e(2)}}{\partial \mathbf{F}_{jC}} = J^{-\frac{1}{3}} \left( \delta_{qJ} \mathbf{F}_{CM}^{p(2)-1} - \mathbf{F}_{qG} \mathbf{F}_{GX}^{p(2)-1} \frac{\partial \mathbf{F}_{XY}^{p(2)}}{\partial \mathbf{F}_{jC}} \mathbf{F}_{YM}^{p(2)-1} \right). \tag{E.135}$$

Further, the derivative of the fourth term in Eq. (E.133) is computed as follows

$$\begin{aligned} \frac{\partial \mathbf{S}_{\text{DB}}^{e(2)}}{\partial \bar{\mathbf{F}}_{\text{qM}}^{e(2)}} \frac{\partial \bar{\mathbf{F}}_{\text{qM}}^{e(2)}}{\partial \mathbf{F}_{\text{jC}}} &= \left[ J^{-\frac{2}{3}} \mu^{(2)} \frac{\partial (1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)} - 3}{I_{\text{m}}^{(2)}})^{-1}}{\partial \bar{\mathbf{F}}_{\text{qM}}^{e(2)}} [\delta_{\text{DB}} - \frac{1}{3} (\text{tr} \bar{\mathbf{C}}^{e(2)}) \bar{\mathbf{C}}_{\text{DB}}^{e(2)-1}] \right. \\ &\quad \left. + J^{-\frac{2}{3}} \mu^{(2)} (1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)} - 3}{I_{\text{m}}^{(2)}})^{-1} (-1/3) \frac{\partial (\text{tr} \bar{\mathbf{C}}^{e(2)} \bar{\mathbf{C}}_{\text{DB}}^{e(2)-1})}{\partial \bar{\mathbf{F}}_{\text{qM}}^{e(2)}} \right] \\ &\quad J^{-\frac{1}{3}} \left( \delta_{\text{qj}} \mathbf{F}_{\text{CM}}^{\text{p}(2)-1} + \mathbf{F}_{\text{qG}}^{(2)} \frac{\partial \mathbf{F}_{\text{GM}}^{\text{p}(2)-1}}{\partial \mathbf{F}_{\text{jC}}} \right). \end{aligned} \quad (\text{E.136})$$

Let us first compute

$$\frac{\partial (1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)} - 3}{I_{\text{m}}^{(3)}})^{-1}}{\partial \bar{\mathbf{F}}_{\text{qM}}^{e(3)}} = -(1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)} - 3}{I_{\text{m}}^{(3)}})^{-2} \frac{\partial \text{tr} \bar{\mathbf{C}}^{e(2)}}{\partial \bar{\mathbf{F}}_{\text{qM}}^{e(2)}} \left( \frac{-1}{I_{\text{m}}} \right). \quad (\text{E.137})$$

Using

$$\frac{\partial \text{tr} \bar{\mathbf{C}}^{e(2)}}{\partial \bar{\mathbf{F}}_{\text{qM}}^{e(2)}} = \frac{\partial \text{tr} \bar{\mathbf{C}}^{e(2)}}{\partial \bar{\mathbf{C}}_{\text{DF}}^{e(2)}} \frac{\partial \bar{\mathbf{C}}_{\text{DF}}^{e(2)}}{\partial \bar{\mathbf{F}}_{\text{qM}}^{e(2)}} = \delta_{\text{DF}} \left( \frac{\partial (\bar{\mathbf{F}}_{\text{kD}}^{e(2)} \bar{\mathbf{F}}_{\text{kF}}^{e(2)})}{\partial \bar{\mathbf{F}}_{\text{qM}}^{e(2)}} \right) = 2 \bar{\mathbf{F}}_{\text{qM}}^{e(2)}, \quad (\text{E.138})$$

and inserting Eq. (E.138) in Eq. (E.137), yields

$$\frac{\partial (1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)} - 3}{I_{\text{m}}^{(2)}})^{-1}}{\partial \bar{\mathbf{F}}_{\text{qM}}^{e(2)}} = \frac{2}{I_{\text{m}}} (1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)} - 3}{I_{\text{m}}^{(2)}})^{-2} \bar{\mathbf{F}}_{\text{qM}}^{e(2)}. \quad (\text{E.139})$$

Then we can compute:

$$\frac{\partial (\text{tr} \bar{\mathbf{C}}^{e(2)} \bar{\mathbf{C}}_{\text{DB}}^{e(2)-1})}{\partial \bar{\mathbf{F}}_{\text{qM}}^{e(2)}} = \frac{\partial \text{tr} \bar{\mathbf{C}}^{e(2)}}{\partial \bar{\mathbf{F}}_{\text{qM}}^{e(2)}} \bar{\mathbf{C}}_{\text{DB}}^{e(2)-1} + \text{tr} \bar{\mathbf{C}}^{e(2)} \frac{\partial \bar{\mathbf{C}}_{\text{DB}}^{e(2)-1}}{\partial \bar{\mathbf{F}}_{\text{qM}}^{e(2)}}, \quad (\text{E.140})$$

with

$$\begin{aligned} \frac{\partial \bar{\mathbf{C}}_{\text{DB}}^{e(2)-1}}{\partial \bar{\mathbf{F}}_{\text{qM}}^{e(2)}} &= \frac{\partial \bar{\mathbf{F}}_{\text{Dk}}^{e(2)-1} \bar{\mathbf{F}}_{\text{Bk}}^{e(2)-1}}{\partial \bar{\mathbf{F}}_{\text{qM}}^{e(2)}} = \frac{\partial \bar{\mathbf{F}}_{\text{Dk}}^{e(2)-1}}{\partial \bar{\mathbf{F}}_{\text{qM}}^{e(2)}} \bar{\mathbf{F}}_{\text{Bk}}^{e(2)-1} + \bar{\mathbf{F}}_{\text{Dk}}^{e(2)-1} \frac{\partial \bar{\mathbf{F}}_{\text{Bk}}^{e(2)-1}}{\partial \bar{\mathbf{F}}_{\text{qM}}^{e(2)}} \\ &= -\bar{\mathbf{F}}_{\text{Dq}}^{e(2)-1} \bar{\mathbf{F}}_{\text{Mk}}^{e(2)-1} \bar{\mathbf{F}}_{\text{Bk}}^{e(2)-1} - \bar{\mathbf{F}}_{\text{Dk}}^{e(2)-1} \bar{\mathbf{F}}_{\text{Bq}}^{e(2)-1} \bar{\mathbf{F}}_{\text{Mk}}^{e(2)-1}, \end{aligned} \quad (\text{E.141})$$

as  $\frac{\partial \bar{\mathbf{F}}_{\text{Dk}}^{-1}}{\partial \bar{\mathbf{F}}_{\text{qM}}} = -\bar{\mathbf{F}}_{\text{Dq}}^{-1} \bar{\mathbf{F}}_{\text{Mk}}^{-1}$ . Then using Eqs. (E.141, E.138), the relation (E.140) becomes

$$\begin{aligned} \frac{\partial (\text{tr} \bar{\mathbf{C}}^{e(2)} \bar{\mathbf{C}}_{\text{DB}}^{e(2)-1})}{\partial \bar{\mathbf{F}}_{\text{qM}}^{e(2)}} &= 2 \bar{\mathbf{F}}_{\text{qM}}^{e(2)} \bar{\mathbf{C}}_{\text{DB}}^{e(2)-1} - \text{tr} \bar{\mathbf{C}}^{e(2)} \left( \bar{\mathbf{F}}_{\text{Dq}}^{e(2)-1} \bar{\mathbf{F}}_{\text{Mk}}^{e(2)-1} \bar{\mathbf{F}}_{\text{Bk}}^{e(2)-1} + \bar{\mathbf{F}}_{\text{Dk}}^{e(2)-1} \bar{\mathbf{F}}_{\text{Bq}}^{e(2)-1} \bar{\mathbf{F}}_{\text{Mk}}^{e(2)-1} \right) \\ &= 2 \bar{\mathbf{F}}_{\text{qM}}^{e(2)} \bar{\mathbf{C}}_{\text{DB}}^{e(2)-1} - \text{tr} \bar{\mathbf{C}}^{e(2)} \left( \bar{\mathbf{F}}_{\text{Dq}}^{e(2)-1} \bar{\mathbf{C}}_{\text{MB}}^{e(2)-1} + \bar{\mathbf{C}}_{\text{DM}}^{e(2)-1} \bar{\mathbf{F}}_{\text{Bq}}^{e(2)-1} \right). \end{aligned} \quad (\text{E.142})$$

As a result, Eq. (E.136) can easily be obtained

$$\begin{aligned} \frac{\partial \mathbf{S}_{\text{DB}}^{e(2)}}{\partial \bar{\mathbf{F}}_{\text{qM}}^{e(2)}} \frac{\partial \bar{\mathbf{F}}_{\text{qM}}^{e(2)}}{\partial \mathbf{F}_{\text{jC}}} &= \mathbf{J}^{-1} \mu^{(2)} \frac{2}{\mathbf{I}_{\text{m}}^{(2)}} \left(1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)} - 3}{\mathbf{I}_{\text{m}}^{(2)}}\right)^{-2} \bar{\mathbf{F}}_{\text{qM}}^{e(2)} \left[ \boldsymbol{\delta}_{\text{DB}} - \frac{1}{3} (\text{tr} \bar{\mathbf{C}}^{e(2)}) \bar{\mathbf{C}}_{\text{DB}}^{e(2)-1} \right] \frac{\partial \mathbf{F}_{\text{qM}}^{e(2)}}{\partial \mathbf{F}_{\text{jC}}} \\ &\quad - \frac{1}{3} \mathbf{J}^{-1} \mu^{(2)} \left(1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)} - 3}{\mathbf{I}_{\text{m}}^{(2)}}\right)^{-1} [2 \bar{\mathbf{F}}_{\text{qM}}^{e(2)} \bar{\mathbf{C}}_{\text{DB}}^{e(2)-1} - \text{tr} \bar{\mathbf{C}}^{e(2)} (\bar{\mathbf{F}}_{\text{Dq}}^{e(2)-1} \bar{\mathbf{F}}_{\text{Mk}}^{e(2)-1} \bar{\mathbf{F}}_{\text{Bk}}^{e(2)-1} \\ &\quad + \bar{\mathbf{F}}_{\text{Dk}}^{e(2)-1} \bar{\mathbf{F}}_{\text{Bq}}^{e(2)-1} \bar{\mathbf{F}}_{\text{Mk}}^{e(2)-1})] \frac{\partial \mathbf{F}_{\text{qM}}^{e(2)}}{\partial \mathbf{F}_{\text{jC}}}. \end{aligned} \quad (\text{E.143})$$

Since

$$\frac{\partial \mathbf{J}}{\partial \mathbf{F}_{\text{jC}}} = \frac{\partial (\det \mathbf{F})}{\partial \mathbf{F}_{\text{jC}}} = \mathbf{J} \mathbf{F}_{\text{jC}}^{-\text{T}}, \quad (\text{E.144})$$

and since

$$\frac{\partial \bar{\mathbf{F}}_{\text{qM}}^{e(2)}}{\partial \mathbf{J}} = \frac{\partial (\mathbf{J}^{-\frac{1}{3}} \mathbf{F}_{\text{qM}}^{e(2)})}{\partial \mathbf{J}} = \frac{-1}{3} \mathbf{J}^{-\frac{4}{3}} \mathbf{F}_{\text{qM}}^{e(2)} = \frac{-1}{3} \mathbf{J}^{-1} \bar{\mathbf{F}}_{\text{qM}}^{e(2)}, \quad (\text{E.145})$$

The fifth term in Eq. (E.133) is computed as follows, using Eqs. (E.143, E.144, and E.145)

$$\begin{aligned} \frac{\partial \mathbf{S}_{\text{DB}}^{e(2)}}{\partial \bar{\mathbf{F}}_{\text{qM}}^{e(2)}} \frac{\partial \bar{\mathbf{F}}_{\text{qM}}^{e(2)}}{\partial \mathbf{J}} \frac{\partial \mathbf{J}}{\partial \mathbf{F}_{\text{jC}}} &= -\mathbf{J}^{-\frac{2}{3}} \mu^{(2)} \frac{2}{3 \mathbf{I}_{\text{m}}^{(2)}} \left(1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)} - 3}{\mathbf{I}_{\text{m}}^{(2)}}\right)^{-2} \bar{\mathbf{F}}_{\text{qM}}^{e(2)} \left[ \boldsymbol{\delta}_{\text{DB}} - \frac{1}{3} (\text{tr} \bar{\mathbf{C}}^{e(2)}) \bar{\mathbf{C}}_{\text{DB}}^{e(2)-1} \right] \bar{\mathbf{F}}_{\text{qM}}^{e(2)} \mathbf{F}_{\text{jC}}^{-\text{T}} \\ &\quad + \frac{1}{9} \mathbf{J}^{-\frac{2}{3}} \mu^{(2)} \left(1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)} - 3}{\mathbf{I}_{\text{m}}^{(2)}}\right)^{-1} [2 \bar{\mathbf{F}}_{\text{qM}}^{e(2)} \bar{\mathbf{C}}_{\text{DB}}^{e(2)-1} - \text{tr} \bar{\mathbf{C}}^{e(2)} (\bar{\mathbf{F}}_{\text{Dq}}^{e(2)-1} \bar{\mathbf{F}}_{\text{Mk}}^{e(2)-1} \bar{\mathbf{F}}_{\text{Bk}}^{e(2)-1} \\ &\quad + \bar{\mathbf{F}}_{\text{Dk}}^{e(2)-1} \bar{\mathbf{F}}_{\text{Bq}}^{e(2)-1} \bar{\mathbf{F}}_{\text{Mk}}^{e(2)-1})] \bar{\mathbf{F}}_{\text{qM}}^{e(2)} \mathbf{F}_{\text{jC}}^{-\text{T}}. \end{aligned} \quad (\text{E.146})$$

Then for sixth term in Eq. (E.133) is evaluated from Eq. (E.113) and read

$$\frac{\partial \mathbf{S}_{\text{DB}}^{(2)}}{\partial \mathbf{J}} \frac{\partial \mathbf{J}}{\partial \mathbf{F}_{\text{jC}}} = -\frac{2}{3} \mathbf{S}_{\text{AB}}^{(2)} \mathbf{F}_{\text{jC}}^{-\text{T}}. \quad (\text{E.147})$$

The derivative of the glass transition temperature with respect to deformation, i.e. the seventh term, is already performed in Eq. (E.72). Therefore from the definition of the first Piola-Kirchhoff stress for the second mechanisms, Eq. (6.76), we have

$$\begin{aligned} \frac{\partial \mathbf{S}_{\text{DB}}^{e(2)}}{\partial \mu^{(2)}(\text{T})} \frac{\partial \mu^{(2)}(\text{T})}{\partial \mathbf{F}_{\text{jC}}} &= \frac{\partial}{\partial \mu^{(2)}(\text{T})} \left\{ \mathbf{J}^{-\frac{2}{3}} \mu^{(2)}(\text{T}) \left(1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)} - 3}{\mathbf{I}_{\text{m}}^{(2)}}\right)^{-1} \right. \\ &\quad \left. \left[ \boldsymbol{\delta}_{\text{DB}} - \frac{1}{3} (\text{tr} \bar{\mathbf{C}}^{e(2)}) \bar{\mathbf{C}}_{\text{DB}}^{e(2)-1} \right] \right\} \frac{\partial \mu^{(2)}(\text{T})}{\partial \mathbf{F}_{\text{jC}}}, \end{aligned} \quad (\text{E.148})$$

where

$$\frac{\partial \mu^{(2)}(\text{T})}{\partial \mathbf{F}_{\text{jC}}} = \frac{\partial \mu^{(2)}(\text{T})}{\partial \text{T}_{\text{g}}} \frac{\partial \text{T}_{\text{g}}}{\partial \mathbf{F}_{\text{jC}}}. \quad (\text{E.149})$$

Using Eq. (6.75)

$$\frac{\partial \mu^{(2)}(\mathbf{T})}{\partial \mathbf{T}_g} = N \mu_g^{(2)} \exp(-N(\mathbf{T} - \mathbf{T}_g)) = N \mu^{(2)}(\mathbf{T}), \quad (\text{E.150})$$

which leads to

$$\frac{\partial \mathbf{S}_{\text{DB}}^{e(2)}}{\partial \mu^{(2)}(\mathbf{T})} \frac{\partial \mu^{(2)}(\mathbf{T})}{\partial \mathbf{T}_g} \frac{\partial \mathbf{T}_g}{\partial \mathbf{F}_{\text{jC}}} = N \mathbf{S}_{\text{DB}}^{e(2)} \frac{\partial \mathbf{T}_g}{\partial \mathbf{F}_{\text{jC}}}. \quad (\text{E.151})$$

By the same way, the eighth term follows from

$$\begin{aligned} \frac{\partial \mathbf{S}_{\text{DB}}^{e(2)}}{\partial S^{(2)}(\mathbf{T})} \frac{\partial S^{(2)}(\mathbf{T})}{\partial \mathbf{F}_{\text{jC}}} &= J^{-\frac{2}{3}} \left[ \mu^{(2)} \frac{\partial (1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)} - 3}{I_m^{(2)}})^{-1}}{\partial S^{(2)}(\mathbf{T})} [\boldsymbol{\delta}_{\text{DB}} - \frac{1}{3} (\text{tr} \bar{\mathbf{C}}^{e(2)}) \bar{\mathbf{C}}_{\text{DB}}^{e(2)-1}] \right. \\ &\quad \left. + J^{-\frac{2}{3}} \mu^{(2)} (1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)} - 3}{I_m^{(2)}})^{-1} (-1/3) \frac{\partial (\text{tr} \bar{\mathbf{C}}^{e(2)} \bar{\mathbf{C}}_{\text{DB}}^{e(2)-1})}{\partial S^{(2)}(\mathbf{T})} \right] \frac{\partial S^{(2)}(\mathbf{T})}{\partial \mathbf{F}_{\text{jC}}}. \end{aligned} \quad (\text{E.152})$$

We have

$$\begin{aligned} \frac{\partial (\text{tr} \bar{\mathbf{C}}^{e(2)} \bar{\mathbf{C}}_{\text{DB}}^{e(2)-1})}{\partial S^{(2)}(\mathbf{T})} &= \frac{\partial \text{tr} \bar{\mathbf{C}}^{e(2)}}{\partial S^{(2)}(\mathbf{T})} \bar{\mathbf{C}}_{\text{DB}}^{e(2)-1} + \text{tr} \bar{\mathbf{C}}^{e(2)} \frac{\partial \bar{\mathbf{C}}_{\text{DB}}^{e(2)-1}}{\partial S^{(2)}(\mathbf{T})} \\ &= \frac{\partial \text{tr} \bar{\mathbf{C}}^{e(2)}}{\partial S^{(2)}(\mathbf{T})} \bar{\mathbf{C}}_{\text{DB}}^{e(2)-1} - \text{tr} \bar{\mathbf{C}}^{e(2)} \bar{\mathbf{C}}_{\text{DF}}^{(2)-1} \bar{\mathbf{C}}_{\text{GB}}^{(2)-1} \frac{\partial \bar{\mathbf{C}}_{\text{FG}}^{e(2)}}{\partial S^{(2)}(\mathbf{T})}, \end{aligned} \quad (\text{E.153})$$

also from Eq. (6.85), we have

$$\frac{\partial S^{(2)}(\mathbf{T})}{\partial \mathbf{T}_g} \frac{\partial \mathbf{T}_g}{\partial \mathbf{F}_{\text{jC}}} = \frac{1}{2\Delta_2} (S_{\text{gl}}^{(2)} - S_{\text{r}}^{(2)}) (1 - \tanh^2(\frac{1}{\Delta_2}(\mathbf{T} - \mathbf{T}_g))) \frac{\partial \mathbf{T}_g}{\partial \mathbf{F}_{\text{jC}}}, \quad (\text{E.154})$$

and the eighth term becomes

$$\begin{aligned} \frac{\partial \mathbf{S}_{\text{DB}}^{e(2)}}{\partial S^{(2)}(\mathbf{T})} \frac{\partial S^{(2)}(\mathbf{T})}{\partial \mathbf{T}_g} \frac{\partial \mathbf{T}_g}{\partial \mathbf{F}_{\text{jC}}} &= \left( \frac{1}{I_m} J^{-\frac{2}{3}} \mu^{(2)} (1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)} - 3}{I_m^{(2)}})^{-2} \frac{\partial \text{tr} \bar{\mathbf{C}}^{e(2)}}{\partial S^{(2)}(\mathbf{T})} [\boldsymbol{\delta}_{\text{DB}} - \frac{1}{3} (\text{tr} \bar{\mathbf{C}}^{e(2)}) \bar{\mathbf{C}}_{\text{DB}}^{e(2)-1}] \right. \\ &\quad \left. - \frac{1}{3} J^{-\frac{2}{3}} \mu^{(2)} (1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)} - 3}{I_m^{(2)}})^{-1} \left[ \frac{\partial \text{tr} \bar{\mathbf{C}}^{e(2)}}{\partial \mathbf{F}_{\text{jC}}} \bar{\mathbf{C}}_{\text{DB}}^{e(2)-1} - \text{tr} \bar{\mathbf{C}}^{e(2)} \bar{\mathbf{C}}_{\text{DF}}^{e(2)-1} \bar{\mathbf{C}}_{\text{GB}}^{(2)-1} \frac{\partial \bar{\mathbf{C}}_{\text{FG}}^{e(2)}}{\partial S^{(2)}(\mathbf{T})} \right] \right) \\ &\quad \frac{\partial S^{(2)}(\mathbf{T})}{\partial \mathbf{T}_g} \frac{\partial \mathbf{T}_g}{\partial \mathbf{F}_{\text{jC}}}. \end{aligned} \quad (\text{E.155})$$

Combining Eqs. (E.143, E.143, E.146, E.147, and E.155) leads to the final expression of Eq. (E.133). However, the following terms are missing:  $\frac{\partial \Delta_{\epsilon^{\text{P}(2)}}}{\partial \mathbf{F}_{\text{jX}}}$ ,  $\frac{\partial \mathbf{F}_{\text{EZ}(n+1)}^{\text{P}(2)}}{\partial \mathbf{F}_{\text{jC}}}$ . In order to get the missing derivatives, let us compute the derivative of the residual Eq. (E.118)

$$\frac{\partial \boldsymbol{\Omega}_{\text{US}}^{(2)}}{\partial \mathbf{F}_{\text{jC}}} + \frac{\partial \boldsymbol{\Omega}_{\text{US}}^{(2)}}{\partial \mathbf{M}_{\text{CD}}^{e(2)}} \frac{\partial \mathbf{M}_{\text{CD}}^{e(2)}}{\partial \mathbf{F}_{\text{jC}}} = 0. \quad (\text{E.156})$$

Thereby

$$\implies \frac{\partial \mathbf{M}_{CD}^{e(2)}}{\partial \mathbf{F}_{jC}^{(2)}} = -\mathbf{J}_{CDUS}^{-1} \frac{\partial \Omega_{US}^{(2)}}{\partial \mathbf{F}_{jC}^{(2)}} \Big|_{\mathbf{M}^{e(2)}}. \quad (\text{E.157})$$

Let us now compute  $\frac{\partial \Omega_{US}^{(2)}}{\partial \mathbf{F}_{jC}^{(2)}}$  from Eq. (E.117)

$$\begin{aligned} \frac{\partial \Omega_{US}^{(2)}}{\partial \mathbf{F}_{jX}} &= \frac{\partial}{\partial \mathbf{F}_{jX}} (\mathbf{M}_{US}^{e(2)} - \mu^{(2)} (1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)}}{\mathbf{I}_m^{(2)}} - 3)^{-1}) \left\{ -\frac{1}{3} \text{tr} \bar{\mathbf{C}}^{e(2)} \boldsymbol{\delta}_{US} \right. \\ &+ \left[ \exp(\dot{\epsilon}_0^{(2)} \Delta t (\frac{|\mathbf{M}^{e(2)}|}{\sqrt{2S^{(2)}(T)}})^{\frac{1}{m}} \frac{\mathbf{M}^{e(2)}}{\sqrt{2}|\mathbf{M}^{e(2)}|}) \right]_{UR}^{-T} \\ &\left. \bar{\mathbf{C}}_{(pr)RQ}^{e(2)} \left[ \exp(\dot{\epsilon}_0^{(2)} \Delta t (\frac{|\mathbf{M}^{e(2)}|}{\sqrt{2S^{(2)}(T)}})^{\frac{1}{m}} \frac{\mathbf{M}^{e(2)}}{\sqrt{2}|\mathbf{M}^{e(2)}|}) \right]_{QS}^{-1} \right\} = 0. \end{aligned} \quad (\text{E.158})$$

The derivative of the terms dependent on  $\bar{\mathbf{C}}_{(pr)}^{e(2)}$  are obtained through the derivative with respect to Cauchy strain tensor as

$$\frac{\partial}{\partial \bar{\mathbf{C}}_{AB}} = \frac{\partial}{\partial \bar{\mathbf{C}}_{(pr)HT}^{e(2)}} : \mathbf{F}_{(pr)AH}^{p(2)-1} \mathbf{F}_{(pr)BT}^{p(2)-1}, \quad (\text{E.159})$$

and reads

$$\Omega_{\mathbf{M}^{e(2)}, \bar{\mathbf{C}}}^{(2)} = \mathbf{F}_{(pr)}^{p(2)-1} \cdot \Omega_{\mathbf{M}^{e(2)}, \bar{\mathbf{C}}_{(pr)}^e}^{(2)} \cdot \mathbf{F}_{(pr)}^{p(2)-T}. \quad (\text{E.160})$$

The derivative of  $\bar{\mathbf{C}}$  with respect to  $\mathbf{F}$  is

$$\frac{\partial \bar{\mathbf{C}}}{\partial \mathbf{F}_{jX}} = J^{-\frac{2}{3}} \mathcal{I}_{ABWV} (\mathbf{F}_{jV} \boldsymbol{\delta}_{WX} + \mathbf{F}_{jW} \boldsymbol{\delta}_{VX}), \quad (\text{E.161})$$

where we have used in the previous equation the following result

$$\frac{\partial \bar{\mathbf{C}}_{AB}^{(2)}}{\partial \mathbf{C}_{WV}^{(2)}} = J^{-\frac{2}{3}} \frac{\partial \mathbf{C}_{AB}^{(2)}}{\partial \mathbf{C}_{WV}^{(2)}} = J^{-\frac{2}{3}} \mathcal{I}_{ABWV}. \quad (\text{E.162})$$

Let us define  $\mathbf{G} = (\dot{\epsilon}_0^{(2)} \Delta t (\frac{|\mathbf{M}^{e(2)}|}{\sqrt{2S^{(2)}(T)}})^{\frac{1}{m}} \frac{\mathbf{M}^{e(2)}}{\sqrt{2}|\mathbf{M}^{e(2)}|})$ . Therefore, combining Eqs. (E.158,

E.160) yields

$$\begin{aligned}
\frac{\partial \Omega_{\text{US}}^{(2)}}{\partial \mathbf{F}_{\text{jX}}} &= \mathbf{F}_{\text{AHpr}}^{\text{p}(2)-1} \left[ -\mu^{(2)} \frac{\partial (1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)} - 3}{I_{\text{m}}^{(2)}})^{-1}}{\partial \bar{\mathbf{C}}_{(\text{pr})\text{HT}}^{e(2)}} \left\{ -\frac{1}{3} \text{tr} \bar{\mathbf{C}}^{e(2)} \boldsymbol{\delta}_{\text{US}} + [\exp(\mathbf{G})]_{\text{UR}}^{-\text{T}} \bar{\mathbf{C}}_{(\text{pr})\text{RQ}}^{e(2)} [\exp(\mathbf{G})]_{\text{QS}}^{-1} \right\} \right. \\
&\quad \left. - \mu^{(2)} \left( 1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)} - 3}{I_{\text{m}}^{(2)}} \right)^{-1} \left\{ \frac{\partial (-\frac{1}{3} \text{tr} \bar{\mathbf{C}}^{e(2)}) \boldsymbol{\delta}_{\text{US}}}{\partial \bar{\mathbf{C}}_{(\text{pr})\text{HT}}^{e(2)}} + [\exp(\mathbf{G})]_{\text{UR}}^{-\text{T}} \frac{\partial \bar{\mathbf{C}}_{(\text{pr})\text{RQ}}^{e(2)}}{\partial \bar{\mathbf{C}}_{(\text{pr})\text{HT}}^{e(2)}} [\exp(\mathbf{G})]_{\text{QS}}^{-1} \right\} \right] \\
&\quad \mathbf{F}_{\text{BTpr}}^{\text{p}(2)-1} \mathbf{J}^{-\frac{2}{3}} \mathcal{I}_{\text{ABWV}} (\mathbf{F}_{\text{jV}} \boldsymbol{\delta}_{\text{WX}} + \mathbf{F}_{\text{jW}} \boldsymbol{\delta}_{\text{VX}}) \\
&\quad - \mu^{(2)} \frac{\partial (1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)} - 3}{I_{\text{m}}^{(2)}})^{-1}}{\partial \mathbf{F}_{\text{jX}}} \left\{ -\frac{1}{3} \text{tr} \bar{\mathbf{C}}^{e(2)} \boldsymbol{\delta}_{\text{US}} + [\exp(\mathbf{G})]_{\text{UR}}^{-\text{T}} \bar{\mathbf{C}}_{(\text{pr})\text{RQ}}^{e(2)} [\exp(\mathbf{G})]_{\text{QS}}^{-1} \right\} \\
&\quad - \mu^{(2)} \left( 1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)} - 3}{I_{\text{m}}^{(2)}} \right)^{-1} \left\{ \frac{\partial (-\frac{1}{3} \text{tr} \bar{\mathbf{C}}^{e(2)})}{\partial S^{(2)}(\text{T})} \frac{\partial S^{(2)}(\text{T})}{\partial \mathbf{F}_{\text{jX}}} \boldsymbol{\delta}_{\text{US}} \right\} \\
&\quad - \mu^{(2)} \left( 1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)} - 3}{I_{\text{m}}^{(2)}} \right)^{-1} \left\{ \frac{[\partial \exp(\mathbf{G})]_{\text{UR}}^{-\text{T}}}{\partial S^{(2)}(\text{T})} \frac{\partial S^{(2)}(\text{T})}{\partial \mathbf{F}_{\text{jX}}} \bar{\mathbf{C}}_{(\text{pr})\text{RQ}}^{e(2)} [\exp(\mathbf{G})]_{\text{QS}}^{-1} \right. \\
&\quad \left. + [\exp(\mathbf{G})]_{\text{UR}}^{-\text{T}} \bar{\mathbf{C}}_{(\text{pr})\text{RQ}}^{e(2)} \frac{[\partial \exp(\mathbf{G})]_{\text{QS}}^{-1}}{\partial S^{(2)}(\text{T})} \frac{\partial S^{(2)}(\text{T})}{\partial \mathbf{F}_{\text{jX}}} \right\} \\
&\quad - \frac{\partial \mu^{(2)}(\text{T})}{\partial \text{T}_{\text{g}}} \frac{\partial \text{T}_{\text{g}}}{\partial \mathbf{F}_{\text{jX}}} \left( 1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)} - 3}{I_{\text{m}}^{(2)}} \right)^{-1} \left\{ -\frac{1}{3} \text{tr} \bar{\mathbf{C}}^{e(2)} \boldsymbol{\delta}_{\text{US}} + [\exp(\mathbf{G})]_{\text{UR}}^{-\text{T}} \bar{\mathbf{C}}_{(\text{pr})\text{RQ}}^{e(2)} [\exp(\mathbf{G})]_{\text{QS}}^{-1} \right\}.
\end{aligned} \tag{E.163}$$

Let us calculate the required derivatives for the previous equation components. We have

$$\begin{aligned}
\frac{\partial \text{tr} \bar{\mathbf{C}}^{e(2)}}{\partial \bar{\mathbf{C}}_{(\text{pr})\text{HT}}^{e(2)}} &= \frac{\partial \text{tr} \bar{\mathbf{C}}^{e(2)}}{\partial \bar{\mathbf{C}}_{\text{FM}}^{e(2)}} \frac{\partial \bar{\mathbf{C}}_{\text{FM}}^{e(2)}}{\partial \bar{\mathbf{C}}_{(\text{pr})\text{HT}}^{e(2)}} \\
&= [\exp(\mathbf{G})]_{\text{MK}}^{-\text{T}} \mathcal{I}_{\text{KLHT}} [\exp(\mathbf{G})]_{\text{LM}}^{-1},
\end{aligned} \tag{E.164}$$

$$\begin{aligned}
\frac{\partial (1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)} - 3}{I_{\text{m}}^{(2)}})^{-1}}{\partial \bar{\mathbf{C}}_{(\text{pr})\text{HT}}^{e(2)}} &= \frac{1}{I_{\text{m}}} \left( 1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)} - 3}{I_{\text{m}}^{(2)}} \right)^{-2} \frac{\partial \text{tr} \bar{\mathbf{C}}^{e(2)}}{\partial \bar{\mathbf{C}}_{(\text{pr})\text{HT}}^{e(2)}} \\
&= \frac{1}{I_{\text{m}}} \left( 1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)} - 3}{I_{\text{m}}^{(2)}} \right)^{-2} [\exp(\mathbf{G})]_{\text{MK}}^{-\text{T}} \mathcal{I}_{\text{KLHT}} [\exp(\mathbf{G})]_{\text{LM}}^{-1}.
\end{aligned} \tag{E.165}$$

Let us define  $\mathbf{W} = (\dot{\epsilon}_0^{(2)} \Delta t (\frac{|\mathbf{M}^{e(2)}|}{\sqrt{2}})^{\frac{1}{\text{m}}} \frac{\mathbf{M}^{e(2)}}{\sqrt{2} |\mathbf{M}^{e(2)}|})$ , which leads to

$$\frac{\partial \bar{\mathbf{C}}^{e(2)}}{\partial S^{(2)}(\text{T})} \frac{\partial S^{(2)}(\text{T})}{\partial \mathbf{F}_{\text{jC}}} = \frac{\partial}{\partial \mathbf{F}_{\text{jC}}} \left\{ \left[ \exp(\mathbf{W} (S^{(2)}(\text{T}))^{\frac{-1}{\text{m}}}) \right]_{\text{YI}}^{-\text{T}} \bar{\mathbf{C}}_{(\text{pr})\text{IJ}}^{e(2)} \left[ \exp(\mathbf{W} (S^{(2)}(\text{T}))^{\frac{-1}{\text{m}}}) \right]_{\text{JZ}}^{-1} \right\}. \tag{E.166}$$

and thus

$$\frac{\partial \left[ \exp(\mathbf{WS}^{(2)}(\mathbf{T})^{\frac{-1}{m}}) \right]_{\text{UR}}^{-\text{T}}}{\partial \mathbf{S}^{(2)}(\mathbf{T})} \frac{\partial \mathbf{S}^{(2)}(\mathbf{T})}{\partial \mathbf{F}_{\text{jC}}} = \frac{\partial \left[ \exp(\mathbf{WS}^{(2)}(\mathbf{T})^{\frac{-1}{m}}) \right]_{\text{UR}}^{-\text{T}}}{\partial \left[ \exp(\mathbf{WS}^{(2)}(\mathbf{T})^{\frac{-1}{m}}) \right]_{\text{AB}}} \frac{\partial \left[ \exp(\mathbf{WS}^{(2)}(\mathbf{T})^{\frac{-1}{m}}) \right]_{\text{AB}}}{\partial (\mathbf{WS}^{(2)}(\mathbf{T})^{\frac{-1}{m}})_{\text{KL}}} \frac{\partial (\mathbf{WS}^{(2)}(\mathbf{T})^{\frac{-1}{m}})_{\text{KL}}}{\partial \mathbf{S}^{(2)}(\mathbf{T})} \frac{\partial \mathbf{S}^{(2)}(\mathbf{T})}{\partial \mathbf{F}_{\text{jC}}}, \quad (\text{E.167})$$

with

$$\frac{\partial \left[ \exp(\mathbf{WS}^{(2)}(\mathbf{T})^{\frac{-1}{m}}) \right]_{\text{UR}}^{-\text{T}}}{\partial \left[ \exp(\mathbf{WS}^{(2)}(\mathbf{T})^{\frac{-1}{m}}) \right]_{\text{AB}}} = - \left[ \exp(\mathbf{WS}^{(2)}(\mathbf{T})^{\frac{-1}{m}}) \right]_{\text{UB}}^{-\text{T}} \left[ \exp(\mathbf{WS}(\mathbf{T})^{\frac{-1}{m}}) \right]_{\text{AR}}^{-\text{T}}, \quad (\text{E.168})$$

$$\frac{\partial \left[ \exp(\mathbf{W}(\mathbf{S}^{(2)}(\mathbf{T})^{\frac{-1}{m}})) \right]_{\text{AB}}}{\partial (\mathbf{WS}(\mathbf{T})^{\frac{-1}{m}})_{\text{KL}}} = \mathbf{Z}_{\text{ABKL}}. \quad (\text{E.169})$$

$$\frac{\partial (\mathbf{WS}^{(2)}(\mathbf{T})^{\frac{-1}{m}})_{\text{KL}}}{\partial \mathbf{S}^{(2)}(\mathbf{T})} \frac{\partial \mathbf{S}^{(2)}(\mathbf{T})}{\partial \mathbf{F}_{\text{jC}}} = - \frac{\mathbf{W}}{m} (\mathbf{S}(\mathbf{T})^{(2)})^{\frac{-1-m}{m}} \frac{\partial \mathbf{S}^{(2)}(\mathbf{T})}{\partial \mathbf{F}_{\text{jC}}}. \quad (\text{E.170})$$

Substituting Eqs. (E.167- E.170) in Eq. (E.166), leads to

$$\frac{\partial \left[ \exp(\mathbf{WS}^{(2)}(\mathbf{T})^{\frac{-1}{m}}) \right]_{\text{UR}}^{-\text{T}}}{\partial \mathbf{S}^{(2)}(\mathbf{T})} \frac{\partial \mathbf{S}^{(2)}(\mathbf{T})}{\partial \mathbf{F}_{\text{jC}}} = \left[ \exp(\mathbf{WS}^{(2)}(\mathbf{T})^{\frac{-1}{m}}) \right]_{\text{UB}}^{-\text{T}} \left[ \exp(\mathbf{WS}^{(2)}(\mathbf{T})^{\frac{-1}{m}}) \right]_{\text{AR}}^{-\text{T}} \mathbf{Z}_{\text{ABKL}} \frac{\mathbf{W}}{m} (\mathbf{S}(\mathbf{T})^{(2)})^{\frac{-1-m}{m}} \frac{\partial \mathbf{S}^{(2)}(\mathbf{T})}{\partial \mathbf{F}_{\text{jC}}}. \quad (\text{E.171})$$

By the same way, we have

$$\frac{\partial \left[ \exp(\mathbf{WS}(\mathbf{T})^{\frac{-1}{m}}) \right]_{\text{QS}}^{-1}}{\partial \mathbf{S}^{(2)}(\mathbf{T})} \frac{\partial \mathbf{S}^{(2)}(\mathbf{T})}{\partial \mathbf{F}_{\text{jC}}} = \left[ \exp(\mathbf{WS}^{(2)}(\mathbf{T})^{\frac{-1}{m}}) \right]_{\text{QB}}^{-1} \left[ \exp(\mathbf{WS}^{(2)}(\mathbf{T})^{\frac{-1}{m}}) \right]_{\text{AS}}^{-1} \mathbf{Z}_{\text{ABKL}} \frac{\mathbf{W}}{m} (\mathbf{S}^{(2)}(\mathbf{T}))^{\frac{-1-m}{m}} \frac{\partial \mathbf{S}^{(2)}(\mathbf{T})}{\partial \mathbf{F}_{\text{jC}}}. \quad (\text{E.172})$$

Therefore, combining the previous equations gives the derivative Eq. (E.166) as

$$\begin{aligned}
\frac{\partial \bar{\mathbf{C}}_{YZ}^{e(2)}}{\partial \mathbf{S}^{(2)}(\mathbf{T})} \frac{\partial \mathbf{S}^{(2)}(\mathbf{T})}{\partial \mathbf{F}_{jC}} &= \frac{\mathbf{W}_{KL}}{m} \left[ \exp(\mathbf{W}(\mathbf{S}^{(2)}(\mathbf{T}))^{\frac{-1}{m}}) \right]_{YB}^{-T} \left[ \exp(\mathbf{W}(\mathbf{S}^{(2)}(\mathbf{T}))^{\frac{-1}{m}}) \right]_{AI}^{-T} \\
&\quad \mathbf{Z}_{ABKL} \mathbf{S}^{(2)}(\mathbf{T})^{\frac{-1-m}{m}} \frac{\partial \mathbf{S}^{(2)}(\mathbf{T})}{\partial \mathbf{F}_{jC}} \bar{\mathbf{C}}_{(pr)IJ}^{e(2)} \left[ \exp(\mathbf{W}(\mathbf{S}^{(2)}(\mathbf{T}))^{\frac{-1}{m}}) \right]_{ZJ}^{-1} \\
&\quad + \frac{\mathbf{W}_{KL}}{m} \left[ \exp(\mathbf{W}(\mathbf{S}^{(2)}(\mathbf{T}))^{\frac{-1}{m}}) \right]_{YI}^{-T} \bar{\mathbf{C}}_{(pr)IJ}^{e(2)} \left[ \exp(\mathbf{W}(\mathbf{S}^{(2)}(\mathbf{T}))^{\frac{-1}{m}}) \right]_{JA}^{-1} \\
&\quad \left[ \exp(\mathbf{W}(\mathbf{S}^{(2)}(\mathbf{T}))^{\frac{-1}{m}}) \right]_{BZ}^{-1} \mathbf{Z}_{ABKL} \mathbf{S}^{(2)}(\mathbf{T})^{\frac{-1-m}{m}} \frac{\partial \mathbf{S}^{(2)}(\mathbf{T})}{\partial \mathbf{F}_{jC}}.
\end{aligned} \tag{E.173}$$

The combination of Eqs. (E.165 and E.173) enables the first derivative of the residual in term of deformation gradient to be obtained as

$$\begin{aligned}
\frac{\partial \Omega_{US}^{(2)}}{\partial \mathbf{F}_{jX}} &= \mathbf{F}_{AHpr}^{p(2)-1} \left[ -\mu^{(2)} \frac{1}{I_m} \left( 1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)}}{I_m^{(2)}} - 3 \right)^{-2} [\exp(\mathbf{G})]_{MK}^{-T} \right. \\
&\quad \left. \mathbf{I}_{KLHT} [\exp(\mathbf{G})]_{LM}^{-1} \left\{ -\frac{1}{3} \text{tr} \bar{\mathbf{C}}^{e(2)} \delta_{US} + [\exp(\mathbf{G})]_{UR}^{-T} \bar{\mathbf{C}}_{(pr)RQ}^{e(2)} [\exp(\mathbf{G})]_{QS}^{-1} \right\} \right. \\
&\quad \left. - \mu^{(2)} \left( 1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)}}{I_m^{(2)}} - 3 \right)^{-1} \left\{ -\frac{1}{3} [\exp(\mathbf{G})]_{MK}^{-T} \mathbf{I}_{KLHT} [\exp(\mathbf{G})]_{LM}^{-1} \delta_{US} \right. \right. \\
&\quad \left. \left. + [\exp(\mathbf{G})]_{UR}^{-T} \mathbf{I}_{RQHT} [\exp(\mathbf{G})]_{QS}^{-1} \right\} \right] \mathbf{F}_{BT(pr)}^{p(2)-1} \mathbf{J}^{-\frac{2}{3}} \mathbf{I}_{ABWV} (\mathbf{F}_{jV} \delta_{WX} + \mathbf{F}_{jW} \delta_{VX}) \\
&\quad - \mu^{(2)} \frac{1}{I_m} \left( 1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)}}{I_m^{(2)}} - 3 \right)^{-2} \frac{\partial (\text{tr} \bar{\mathbf{C}}^{e(2)})}{\partial \mathbf{S}^{(2)}(\mathbf{T})} \frac{\partial \mathbf{S}^{(2)}(\mathbf{T})}{\partial \mathbf{F}_{jC}} \\
&\quad \left\{ -\frac{1}{3} \text{tr} \bar{\mathbf{C}}^{e(2)} \delta_{US} + [\exp(\mathbf{G})]_{UR}^{-T} \bar{\mathbf{C}}_{(pr)RQ}^{e(2)} [\exp(\mathbf{G})]_{QS}^{-1} \right\} \\
&\quad - \mu^{(2)} \left( 1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)}}{I_m^{(2)}} - 3 \right)^{-1} \left\{ -\frac{1}{3} \frac{\partial (\text{tr} \bar{\mathbf{C}}^{e(2)})}{\partial \mathbf{S}^{(2)}(\mathbf{T})} \delta_{US} \frac{\partial \mathbf{S}^{(2)}(\mathbf{T})}{\partial \mathbf{F}_{jC}} \right\} \\
&\quad - \mu^{(2)} \left( 1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)}}{I_m^{(2)}} - 3 \right)^{-1} \left\{ \left[ \exp(\mathbf{W}(\mathbf{S}(\mathbf{T}))^{\frac{-1}{m}}) \right]_{UB}^{-T} \left[ \exp(\mathbf{W}(\mathbf{S}(\mathbf{T}))^{\frac{-1}{m}}) \right]_{AR}^{-T} \mathbf{Z}_{ABKL} \right. \\
&\quad \left. \frac{\mathbf{W}_{KL}}{m} (\mathbf{S}^{(2)}(\mathbf{T}))^{\frac{-1-m}{m}} \frac{\partial \mathbf{S}^{(2)}(\mathbf{T})}{\partial \mathbf{F}_{jX}} \bar{\mathbf{C}}_{(pr)RQ}^{e(2)} [\exp(\mathbf{G})]_{QS}^{-1} \right. \\
&\quad \left. + [\exp(\mathbf{G})]_{UR}^{-T} \bar{\mathbf{C}}_{(pr)RQ}^{e(2)} \left[ \exp(\mathbf{W}(\mathbf{S}^2(\mathbf{T}))^{\frac{-1}{m}}) \right]_{QA}^{-1} \left[ \exp(\mathbf{W}(\mathbf{S}^2(\mathbf{T}))^{\frac{-1}{m}}) \right]_{BS}^{-1} \mathbf{Z}_{ABKL} \right. \\
&\quad \left. \frac{\mathbf{W}_{KL}}{m} (\mathbf{S}^{(2)}(\mathbf{T}))^{\frac{-1-m}{m}} \frac{\partial \mathbf{S}^{(2)}(\mathbf{T})}{\partial \mathbf{F}_{jC}} \right\} - N \mu^{(2)}(\mathbf{T}) \frac{\partial T_g}{\partial \mathbf{F}_{jX}} \left( 1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)}}{I_m^{(2)}} - 3 \right)^{-1} \\
&\quad \left\{ -\frac{1}{3} \text{tr} \bar{\mathbf{C}}^{e(2)} \delta_{US} + [\exp(\mathbf{G})]_{UR}^{-T} \bar{\mathbf{C}}_{(pr)RQ}^{e(2)} [\exp(\mathbf{G})]_{QS}^{-1} \right\}.
\end{aligned} \tag{E.174}$$

Thereafter, by using the equation (E.157), one can evaluate the derivative of  $\mathbf{M}^{e(2)}$  with respect to the deformation gradient.



Next, the derivative of the plastic deformation increment can be computed from Eq. (6.84) as

$$\begin{aligned} \frac{\partial \Delta \epsilon^{p(2)}}{\partial \mathbf{F}_{jX}} &= \frac{\partial}{\partial \mathbf{F}_{jX}} \left( \dot{\epsilon}_0^{(2)} \Delta t \left( \frac{|\mathbf{M}^{e(2)}|}{\sqrt{2}S^{(2)}(T)} \right)^{\frac{1}{m}} \right) \\ &= \frac{\dot{\epsilon}_0^{(2)} \Delta t}{(\sqrt{2}S^{(2)}(T))^{\frac{1}{m}}} \frac{\partial |\mathbf{M}^{e(2)}|^{\frac{1}{m}}}{\partial \mathbf{F}_{jX}} \\ &\quad - \frac{\dot{\epsilon}_0^{(2)} \Delta t}{m} \left( \frac{|\mathbf{M}^{e(2)}|}{\sqrt{2}} \right)^{\frac{1}{m}} \left( S^{(2)}(T) \right)^{\frac{-1-m}{m}} \frac{\partial S^{(2)}(T)}{\partial \mathbf{F}_{jC}}, \end{aligned} \quad (\text{E.175})$$

where we need to compute the following derivatives

$$\begin{aligned} \frac{\partial |\mathbf{M}^{e(2)}|^{\frac{1}{m}}}{\partial \mathbf{F}_{jX}} &= \frac{1}{m} |\mathbf{M}^{e(2)}|^{\frac{1-m}{m}} \frac{\partial \sqrt{\mathbf{M}_{CD}^{e(2)} : \mathbf{M}_{CD}^{e(2)}}}{\partial \mathbf{F}_{jX}} \\ &= \frac{1}{m} |\mathbf{M}^{e(2)}|^{\frac{1-2m}{m}} \left( \frac{\partial \mathbf{M}_{CD}^{e(2)}}{\partial \mathbf{F}_{jX}} \mathbf{M}_{CD}^{e(2)} \right), \end{aligned} \quad (\text{E.176})$$

and  $\frac{\partial S^{(2)}(T)}{\partial \mathbf{F}_{jC}}$  is given by Eq. (E.154). Similarly, we can get the derivative of the normal with respect to the deformation as

$$\begin{aligned} \frac{\partial \mathbf{N}_{OP}^{(2)}}{\partial \mathbf{F}_{jX}} &= \frac{\partial}{\partial \mathbf{F}_{jX}} \left( \frac{\mathbf{M}_{OP}^{e(2)}}{\sqrt{2}|\mathbf{M}^{e(2)}|} \right) \\ &= \frac{1}{\sqrt{2}} \left[ \frac{\partial \mathbf{M}_{OP}^{e(2)}}{\partial \mathbf{F}_{jX}} |\mathbf{M}^{e(2)}|^{-1} - |\mathbf{M}^{e(2)}|^{-3} \mathbf{M}_{OP}^{e(2)} \frac{\partial \mathbf{M}_{CD}^{e(2)}}{\partial \mathbf{F}_{jX}} \mathbf{M}_{CD}^{e(2)} \right]. \end{aligned} \quad (\text{E.177})$$

The derivative of the plastic deformation mapping is obtained from its definition Eq. (6.95). By combining Eqs. (E.177 and E.175) in Eq. (E.134) yields the derivative of plastic deformation with respect to the deformation gradient

$$\begin{aligned} \frac{\partial \mathbf{F}_{EZ(n+1)}^{p(2)}}{\partial \mathbf{F}_{jC}} &= \frac{\partial \mathbf{D}_{EZ}^{p(2)}}{\partial \mathbf{F}_{jC}} \mathbf{F}_{IZ(n)}^{p(2)} \\ &= \mathcal{Z}_{IEOP} \left[ \mathbf{N}_{OP} \frac{\partial \Delta \epsilon^{p(2)}}{\partial \mathbf{F}_{jC}} + \Delta \epsilon^{p(2)} \frac{\partial \mathbf{N}_{OP}}{\partial \mathbf{F}_{jC}} \right] \mathbf{F}_{IZ(n)}^{p(2)} \\ &= \mathcal{Z}_{IEOP} \left[ \frac{\mathbf{M}_{OP}^{e(2)}}{\sqrt{2}|\mathbf{M}^{e(2)}|} \frac{\partial \Delta \epsilon^{p(2)}}{\partial \mathbf{F}_{jC}} + \Delta \epsilon^{p(2)} \frac{\partial \mathbf{N}_{OP}}{\partial \mathbf{F}_{jC}} \right] \mathbf{F}_{IZ(n)}^{p(2)}, \end{aligned} \quad (\text{E.178})$$

where  $\mathcal{Z} = \frac{\partial \exp \mathbf{C}}{\partial \mathbf{C}}$ .

By substituting Eqs. (E.143, E.143, E.146, E.147, E.173 and E.178) in Eq. (E.133), leads to the derivative of the first Piola-Kirchhof with respect to the deformation gradient

as follows

$$\begin{aligned}
\frac{\partial \mathbf{P}_{iA}^{(2)}}{\partial \mathbf{F}_{jC}} &= \boldsymbol{\delta}_{ij} \mathbf{F}_{CD}^{p(2)-1} \mathbf{S}_{DB}^{e(2)} \mathbf{F}_{BA}^{p(2)-T} + \mathbf{F}_{iW} \frac{\partial \mathbf{F}_{WD}^{p(2)-1}}{\partial \mathbf{F}_{jC}} \mathbf{S}_{DB}^{e(2)} \mathbf{F}_{BA}^{p(2)-T} + \mathbf{F}_{iW} \mathbf{F}_{WD}^{p(2)-1} \mathbf{S}_{DB}^{e(2)} \frac{\partial \mathbf{F}_{BA}^{p(2)-T}}{\partial \mathbf{F}_{jC}} \\
&+ \mathbf{F}_{iW} \mathbf{F}_{WD}^{p(2)-1} \left\{ J^{-1} \mu^{(2)} \frac{2}{I_m^{(2)}} \left(1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)}}{I_m^{(2)}} - 3\right)^{-2} \bar{\mathbf{F}}_{qM}^{e(2)} \left[ \boldsymbol{\delta}_{DB} - \frac{1}{3} (\text{tr} \bar{\mathbf{C}}^{e(2)}) \bar{\mathbf{C}}_{DB}^{e(2)-1} \right] \right. \\
&\frac{\partial \bar{\mathbf{F}}_{qM}^{e(2)}}{\partial \mathbf{F}_{jC}} - \frac{1}{3} J^{-1} \mu^{(2)} \left(1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)}}{I_m^{(2)}} - 3\right)^{-1} \\
&\left. \left[ 2 \bar{\mathbf{F}}_{qM}^{e(2)} \bar{\mathbf{C}}_{DB}^{e(2)-1} - \text{tr} \bar{\mathbf{C}}^{e(2)} (\bar{\mathbf{F}}_{Dq}^{e(2)-1} \bar{\mathbf{F}}_{Mk}^{e(2)-1} \bar{\mathbf{F}}_{Bk}^{e(2)-1} + \bar{\mathbf{F}}_{Dk}^{e(2)-1} \bar{\mathbf{F}}_{Bq}^{e(2)-1} \bar{\mathbf{F}}_{Mk}^{e(2)-1}) \right] \frac{\partial \bar{\mathbf{F}}_{qM}^{e(2)}}{\partial \mathbf{F}_{jC}} \right\} \mathbf{F}_{BA}^{p(2)-T} \\
&+ \mathbf{F}_{iW} \mathbf{F}_{WD}^{p(2)-1} \left\{ \frac{-2}{3 I_m^{(2)}} J^{-\frac{2}{3}} \mu^{(2)} \left(1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)}}{I_m^{(2)}} - 3\right)^{-2} \bar{\mathbf{F}}_{qM}^{e(2)} \left[ \boldsymbol{\delta}_{DB} - \frac{1}{3} (\text{tr} \bar{\mathbf{C}}^{e(2)}) \bar{\mathbf{C}}_{DB}^{e(2)-1} \right] \bar{\mathbf{F}}_{qM}^{e(2)} \mathbf{F}_{jC}^{-T} \right. \\
&+ \frac{1}{9} J^{-\frac{2}{3}} \mu^{(2)} \left(1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)}}{I_m^{(2)}} - 3\right)^{-1} \left[ 2 \bar{\mathbf{F}}_{qM}^{e(2)} \bar{\mathbf{C}}_{DB}^{e(2)-1} - \text{tr} \bar{\mathbf{C}}^{e(2)} (\bar{\mathbf{F}}_{Dq}^{e(2)-1} \bar{\mathbf{F}}_{Mk}^{e(2)-1} \bar{\mathbf{F}}_{Bk}^{e(2)-1} \right. \\
&+ \left. \left. \bar{\mathbf{F}}_{Dk}^{e(2)-1} \bar{\mathbf{F}}_{Bq}^{e(2)-1} \bar{\mathbf{F}}_{Mk}^{e(2)-1}) \right] \bar{\mathbf{F}}_{qM}^{e(2)} \mathbf{F}_{jC}^{-T} \right\} \mathbf{F}_{BA}^{p(2)-T} \\
&- \mathbf{F}_{iW} \mathbf{F}_{WD}^{p(2)-1} \left\{ \frac{2}{3} J^{-\frac{2}{3}} \mu^{(2)} \left(1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)}}{I_m^{(2)}} - 3\right)^{-1} \left[ \boldsymbol{\delta}_{DB} - \frac{1}{3} (\text{tr} \bar{\mathbf{C}}^{e(2)}) \bar{\mathbf{C}}_{DB}^{e(2)-1} \right] \mathbf{F}_{jC}^{-T} \right\} \mathbf{F}_{BA}^{p(2)-T} \\
&+ \mathbf{F}_{iW} \mathbf{F}_{WD}^{p(2)-1} \left\{ N \frac{\partial T_g}{\partial \mathbf{F}_{jC}} \mathbf{S}_{DB}^{e(2)} + \frac{1}{I_m} J^{-\frac{2}{3}} \mu^{(2)} \left(1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)}}{I_m^{(2)}} - 3\right)^{-2} \frac{\partial \text{tr} \bar{\mathbf{C}}^{e(2)}}{\partial S^{(2)}(T)} \left[ \boldsymbol{\delta}_{DB} - \frac{1}{3} (\text{tr} \bar{\mathbf{C}}^{e(2)}) \bar{\mathbf{C}}_{DB}^{e(2)-1} \right] \right. \\
&\left. \frac{-1}{3} J^{-\frac{2}{3}} \mu^{(2)} \left(1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)}}{I_m^{(2)}} - 3\right)^{-1} \left[ \frac{\partial \text{tr} \bar{\mathbf{C}}^{e(2)}}{\partial S^{(2)}(T)} \bar{\mathbf{C}}_{DB}^{e(2)-1} - \text{tr} \bar{\mathbf{C}}^{e(2)} \bar{\mathbf{C}}_{DF}^{e(2)-1} \bar{\mathbf{C}}_{GB}^{(2)-1} \frac{\partial \bar{\mathbf{C}}_{FG}^{e(2)}}{\partial S^{(2)}(T)} \right] \frac{\partial S^{(2)}(T)}{\partial \mathbf{F}_{jC}} \right\} \mathbf{F}_{BA}^{p(2)-T}.
\end{aligned} \tag{E.179}$$

### E.2.2.6 Derivation of first Piola-Kirchhoff strain with respect to temperature

The remaining part of the tangent is the derivative of the first Piola-Kirchhoff stress in terms of the temperature  $\frac{\partial \mathbf{P}^{(2)}}{\partial T}$ , which can be deduced by computing the derivative of the residual Eq. (E.118) with respect to the temperature :

$$\begin{aligned}
\frac{\partial \mathbf{P}_{iA}^{(2)}}{\partial T} &= \frac{\partial (\mathbf{F}_{iW} \mathbf{F}_{WD}^{p(2)-1} \mathbf{S}_{DB}^{e(2)} \mathbf{F}_{BA}^{p(2)-T})}{\partial T} \\
&= \mathbf{F}_{iW} \frac{\partial \mathbf{F}_{WD}^{p(2)-1}}{\partial T} \mathbf{S}_{DB}^{e(2)} \mathbf{F}_{BA}^{p(2)-T} + \mathbf{F}_{iW} \mathbf{F}_{WD}^{p(2)-1} \frac{\partial \mathbf{S}_{DB}^{e(2)}}{\partial T} \mathbf{F}_{BA}^{p(2)-T} \\
&\quad + \mathbf{F}_{iW} \mathbf{F}_{WD}^{p(2)-1} \mathbf{S}_{DB}^{e(2)} \frac{\partial \mathbf{F}_{BA}^{p(2)-T}}{\partial T}.
\end{aligned} \tag{E.180}$$

The derivative of plastic deformation gradient with respect to the temperature is obtained

by

$$\begin{aligned} \frac{\partial \mathbf{F}_{\text{EZ}(n+1)}^{\text{P}(2)}}{\partial T} &= \frac{\partial \exp(\Delta \epsilon^{\text{P}(2)} \mathbf{N}^{(2)})_{\text{EI}}}{\partial T} \mathbf{F}_{\text{IZ}(n)}^{\text{P}(2)} \\ &= \mathbf{Z}_{\text{EIOP}} \left[ \frac{\mathbf{M}_{\text{OP}}^{\text{e}(2)}}{\sqrt{2} |\mathbf{M}^{\text{e}(2)}|} \frac{\partial \Delta \epsilon^{\text{P}(2)}}{\partial T} + \Delta \epsilon^{\text{P}(2)} \frac{\partial \mathbf{N}_{\text{OP}}}{\partial T} \right] \mathbf{F}_{\text{IZ}(n)}^{\text{P}(2)}, \end{aligned} \quad (\text{E.181})$$

which immediately gives the derivative of the inverse of plastic deformation gradient

$$\frac{\partial \mathbf{F}_{\text{XY}}^{\text{P}(2)-1}}{\partial T} = -\mathbf{F}_{\text{XE}}^{\text{P}(2)-1} \frac{\partial \mathbf{F}_{\text{EZ}}^{\text{P}(2)}}{\partial T} \mathbf{F}_{\text{ZY}}^{\text{P}(2)-1}. \quad (\text{E.182})$$

In order to get the derivative of the plastic deformation gradient in terms of the temperature, we need to compute it from the residual defined in Eq. (E.117) as

$$\frac{\partial \Omega_{\text{US}}^{(2)}}{\partial T} \Big|_{\mathbf{M}^{\text{e}(2)}} + \frac{\partial \Omega_{\text{US}}^{(2)}}{\partial \mathbf{M}_{\text{CD}}^{\text{e}(2)}} \frac{\partial \mathbf{M}_{\text{CD}}^{\text{e}(2)}}{\partial T} = 0, \quad (\text{E.183})$$

which yields

$$\Rightarrow \frac{\partial \mathbf{M}_{\text{CD}}^{\text{e}(2)}}{\partial T} = -(\mathbf{J}_2^{-1})_{\text{CDUS}} \frac{\partial \Omega_{\text{US}}^{(2)}}{\partial T} \Big|_{\mathbf{M}^{\text{e}(2)}}. \quad (\text{E.184})$$

We need to calculate the derivative of the residual  $\Omega^{(2)}$  with respect to the temperature  $T$

$$\begin{aligned} \frac{\partial \Omega_{\text{US}}^{(2)}}{\partial T} &= \frac{\partial}{\partial T} (\mathbf{M}_{\text{US}}^{\text{e}(2)} - \mu^{(2)} (1 - \frac{\text{tr} \bar{\mathbf{C}}^{\text{e}(2)}}{I_{\text{m}}^{(2)}} - 3)^{-1}) \left\{ -\frac{1}{3} \text{tr} \bar{\mathbf{C}}^{\text{e}(2)} \boldsymbol{\delta}_{\text{US}} \right. \\ &+ \left[ \exp(\dot{\epsilon}_0^{(2)} \Delta t \left( \frac{|\mathbf{M}^{\text{e}(2)}|}{\sqrt{2} S^{(2)}(T)} \right)^{\frac{1}{\text{m}}} \frac{\mathbf{M}^{\text{e}(2)}}{\sqrt{2} |\mathbf{M}^{\text{e}(2)}|} \right]_{\text{UR}}^{-\text{T}} \\ &\left. \bar{\mathbf{C}}_{(\text{pr})\text{RQ}}^{\text{e}(2)} \left[ \exp(\dot{\epsilon}_0^{(2)} \Delta t \left( \frac{|\mathbf{M}^{\text{e}(2)}|}{\sqrt{2} S^{(2)}(T)} \right)^{\frac{1}{\text{m}}} \frac{\mathbf{M}^{\text{e}(2)}}{\sqrt{2} |\mathbf{M}^{\text{e}(2)}|} \right]_{\text{QS}}^{-1} \right\}. \end{aligned} \quad (\text{E.185})$$

Let us define  $\mathbf{W} = \frac{\epsilon_0^{(2)} \Delta t |\mathbf{M}^{e(2)}|_{\frac{1}{m}} \mathbf{N}}{\sqrt{2}^{\frac{1}{m}}}$ , then we get

$$\begin{aligned}
\frac{\partial \boldsymbol{\Omega}_{\text{US}}^{(2)}}{\partial \mathbf{T}} &= -\frac{\partial \mu^{(2)}}{\partial \mathbf{T}} \left(1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)}}{\mathbf{I}_m^{(2)}} - 3\right)^{-1} \left\{ -\frac{1}{3} \text{tr} \bar{\mathbf{C}}^{e(2)} \boldsymbol{\delta}_{\text{US}} \right. \\
&+ \left[ \exp(\mathbf{W} (\mathbf{S}^{(2)}(\mathbf{T}))^{\frac{-1}{m}}) \right]_{\text{UR}}^{-\text{T}} \bar{\mathbf{C}}_{(\text{pr})\text{RQ}}^{e(2)} \left[ \exp(\mathbf{W} (\mathbf{S}^{(2)}(\mathbf{T}))^{\frac{-1}{m}}) \right]_{\text{QS}}^{-1} \Big\} \\
&- \mu^{(2)} \frac{\partial \left(1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)}}{\mathbf{I}_m^{(2)}} - 3\right)^{-1}}{\partial \mathbf{T}} \left\{ -\frac{1}{3} \text{tr} \bar{\mathbf{C}}^{e(2)} \boldsymbol{\delta}_{\text{US}} \right. \\
&+ \left[ \exp(\mathbf{W} (\mathbf{S}^{(2)}(\mathbf{T}))^{\frac{-1}{m}}) \right]_{\text{UR}}^{-\text{T}} \bar{\mathbf{C}}_{(\text{pr})\text{RQ}}^{e(2)} \left[ \exp(\mathbf{W} (\mathbf{S}^{(2)}(\mathbf{T}))^{\frac{-1}{m}}) \right]_{\text{QS}}^{-1} \Big\} \\
&- \mu^{(2)} \left(1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)}}{\mathbf{I}_m^{(2)}} - 3\right)^{-1} \left\{ -\frac{1}{3} \frac{\partial \text{tr} \bar{\mathbf{C}}^{e(2)}}{\partial \mathbf{T}} \boldsymbol{\delta}_{\text{US}} \right. \\
&+ \frac{\partial \left[ \exp(\mathbf{W} (\mathbf{S}^{(2)}(\mathbf{T}))^{\frac{-1}{m}}) \right]_{\text{UR}}^{-\text{T}} \bar{\mathbf{C}}_{(\text{pr})\text{RQ}}^{e(2)} \left[ \exp(\mathbf{W} (\mathbf{S}^{(2)}(\mathbf{T}))^{\frac{-1}{m}}) \right]_{\text{QS}}^{-1}}{\partial \mathbf{T}} \\
&+ \left. \left[ \exp(\mathbf{W} (\mathbf{S}^{(2)}(\mathbf{T}))^{\frac{-1}{m}}) \right]_{\text{UR}}^{-\text{T}} \bar{\mathbf{C}}_{(\text{pr})\text{RQ}}^{e(2)} \frac{\partial \left[ \exp(\mathbf{W} (\mathbf{S}^{(2)}(\mathbf{T}))^{\frac{-1}{m}}) \right]_{\text{QS}}^{-1}}{\partial \mathbf{T}} \right\}. \tag{E.186}
\end{aligned}$$

Let us compute the derivative of the components. First let us recall equation (6.75), yielding

$$\frac{\partial \mu^{(2)}}{\partial \mathbf{T}} = -N \mu_g^{(2)} \exp(-N(\mathbf{T} - \mathbf{T}_g)) = -N \mu^{(2)}. \tag{E.187}$$

Also from Eq. (6.85), we have

$$\frac{\partial \mathbf{S}^{(2)}(\mathbf{T})}{\partial \mathbf{T}} = -\frac{1}{2\Delta_2} (\mathbf{S}_{\text{gl}}^{(2)} - \mathbf{S}_{\text{r}}^{(2)}) (1 - \tanh^2(\frac{1}{\Delta_2}(\mathbf{T} - \mathbf{T}_g))). \tag{E.188}$$

Let us start to compute the derivative of the components of  $\bar{\mathbf{C}}^{e(2)}$

$$\frac{\partial \bar{\mathbf{C}}^{e(2)}}{\partial \mathbf{T}} = \frac{\partial}{\partial \mathbf{T}} \left\{ \left[ \exp(\mathbf{W} (\mathbf{S}^{(2)}(\mathbf{T}))^{\frac{-1}{m}}) \right]_{\text{YI}}^{-\text{T}} \bar{\mathbf{C}}_{(\text{pr})\text{IJ}}^{e(2)} \left[ \exp(\mathbf{W} (\mathbf{S}^{(2)}(\mathbf{T}))^{\frac{-1}{m}}) \right]_{\text{JZ}}^{-1} \right\}. \tag{E.189}$$

$$\begin{aligned}
\frac{\partial \left[ \exp(\mathbf{W} (\mathbf{S}^{(2)}(\mathbf{T}))^{\frac{-1}{m}}) \right]_{\text{YI}}^{-\text{T}}}{\partial \mathbf{T}} &= \frac{\partial \left[ \exp(\mathbf{W} (\mathbf{S}^{(2)}(\mathbf{T}))^{\frac{-1}{m}}) \right]_{\text{YI}}^{-\text{T}}}{\partial \left[ \exp(\mathbf{W} (\mathbf{S}^{(2)}(\mathbf{T}))^{\frac{-1}{m}}) \right]_{\text{AB}}^{-1}} \frac{\partial \left[ \exp(\mathbf{W} (\mathbf{S}^{(2)}(\mathbf{T}))^{\frac{-1}{m}}) \right]_{\text{AB}}^{-1}}{\partial \left[ (\mathbf{W} (\mathbf{S}^{(2)}(\mathbf{T}))^{\frac{-1}{m}}) \right]_{\text{KL}}^{-1}} \\
&\quad \frac{\partial \left[ (\mathbf{W} (\mathbf{S}^{(2)}(\mathbf{T}))^{\frac{-1}{m}}) \right]_{\text{KL}}^{-1}}{\partial \mathbf{T}}, \tag{E.190}
\end{aligned}$$

where

$$\frac{\partial \left[ \exp(\mathbf{W} (S^{(2)}(T))^{\frac{-1}{m}}) \right]_{YI}^{-T}}{\partial \left[ \exp(\mathbf{W} (S^{(2)}(T))^{\frac{-1}{m}}) \right]_{AB}} = - \left[ \exp(\mathbf{W} (S^{(2)}(T))^{\frac{-1}{m}}) \right]_{YB}^{-T} \left[ \exp(\mathbf{W} (S^{(2)}(T))^{\frac{-1}{m}}) \right]_{AI}^{-T}, \quad (\text{E.191})$$

also

$$\frac{\partial \left[ \exp(\mathbf{W} (S^{(2)}(T))^{\frac{-1}{m}}) \right]_{AB}}{\partial \left[ (\mathbf{W} (S^{(2)}(T))^{\frac{-1}{m}}) \right]_{KL}} = \mathbf{Z}_{ABKL}, \quad (\text{E.192})$$

and

$$\begin{aligned} \frac{\partial \left[ (\mathbf{W} (S^{(2)}(T))^{\frac{-1}{m}}) \right]_{KL}}{\partial T} &= \frac{-\mathbf{W}_{KL} S^{(2)}(T)^{\frac{-1-m}{m}} \frac{\partial S^{(2)}(T)}{\partial T}}{m} \\ &= \frac{\mathbf{W}_{KL} S^{(2)}(T)^{\frac{-1-m}{m}} (S_g - S_r) \text{sech}^2 \left( \frac{1}{\Delta_2} (T - T_g) \right)}{2m\Delta_2}. \end{aligned} \quad (\text{E.193})$$

Combining Eqs. (E.125, E.192 and E.193) in Eq. (E.190) one gets

$$\begin{aligned} \frac{\partial \left[ \exp(\mathbf{W} (S^{(2)}(T))^{\frac{-1}{m}}) \right]_{YI}^{-T}}{\partial T} &= \frac{\mathbf{W}_{KL}}{m} \left[ \exp(\mathbf{W} (S^{(2)}(T))^{\frac{-1}{m}}) \right]_{YB}^{-T} \left[ \exp(\mathbf{W} (S^{(2)}(T))^{\frac{-1}{m}}) \right]_{AI}^{-T} \\ &\quad \mathbf{Z}_{ABKL} S^{(2)}(T)^{\frac{-1-m}{m}} \frac{\partial S^{(2)}(T)}{\partial T}. \end{aligned} \quad (\text{E.194})$$

By the same way of (E.190) we can compute

$$\begin{aligned} \frac{\partial \left[ \exp(\mathbf{W} (S^{(2)}(T))^{\frac{-1}{m}}) \right]_{JZ}^{-1}}{\partial T} &= \frac{\partial \left[ \exp(\mathbf{W} (S^{(2)}(T))^{\frac{-1}{m}}) \right]_{JZ}^{-1}}{\partial \left[ \exp(\mathbf{W} (S^{(2)}(T))^{\frac{-1}{m}}) \right]_{AB}} \frac{\partial \left[ \exp(\mathbf{W} (S^{(2)}(T))^{\frac{-1}{m}}) \right]_{AB}}{\partial \left[ \mathbf{W} (S^{(2)}(T))^{\frac{-1}{m}} \right]_{KL}} \\ &\quad \frac{\partial \left[ \mathbf{W} (S^{(2)}(T))^{\frac{-1}{m}} \right]_{KL}}{\partial T}. \end{aligned} \quad (\text{E.195})$$

So with reference to Eq. (E.189), one can get

$$\begin{aligned} \frac{\partial \bar{\mathbf{C}}_{YZ}^{e(2)}}{\partial T} &= \frac{\mathbf{W}_{KL}}{m} \left[ \exp(\mathbf{W} (S^{(2)}(T))^{\frac{-1}{m}}) \right]_{YB}^{-T} \left[ \exp(\mathbf{W} (S^{(2)}(T))^{\frac{-1}{m}}) \right]_{AI}^{-T} \\ &\quad \mathbf{Z}_{ABKL} S^{(2)}(T)^{\frac{-1-m}{m}} \frac{\partial S^{(2)}(T)}{\partial T} \bar{\mathbf{C}}_{(pr)IJ}^{e(2)} \left[ \exp(\mathbf{W} (S^{(2)}(T))^{\frac{-1}{m}}) \right]_{ZJ}^{-1} \\ &\quad + \frac{\mathbf{W}_{KL}}{m} \left[ \exp(\mathbf{W} (S^{(2)}(T))^{\frac{-1}{m}}) \right]_{YI}^{-T} \bar{\mathbf{C}}_{(pr)IJ}^{e(2)} \left[ \exp(\mathbf{W} (S^{(2)}(T))^{\frac{-1}{m}}) \right]_{JA}^{-1} \\ &\quad \left[ \exp(\mathbf{W} (S^{(2)}(T))^{\frac{-1}{m}}) \right]_{BZ}^{-1} \mathbf{Z}_{ABKL} S^{(2)}(T)^{\frac{-1-m}{m}} \frac{\partial S^{(2)}(T)}{\partial T}. \end{aligned} \quad (\text{E.196})$$

We thus have directly

$$\frac{\partial \text{tr} \bar{\mathbf{C}}^{e(2)}}{\partial T} = \frac{\partial \text{tr} \bar{\mathbf{C}}^{e(2)}}{\partial \mathbf{C}_{YZ}^{e(2)}} \frac{\partial \bar{\mathbf{C}}_{YZ}^{e(2)}}{\partial T} = \boldsymbol{\delta}_{YZ} \frac{\partial \bar{\mathbf{C}}_{YZ}^{e(2)}}{\partial T}, \text{ and} \quad (\text{E.197})$$

$$\frac{\partial (1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)} - 3}{I_m^{(2)}})^{-1}}{\partial T} = \frac{1}{I_m} (1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)} - 3}{I_m^{(2)}})^{-2} \frac{\partial \text{tr} \bar{\mathbf{C}}^{e(2)}}{\partial T}. \quad (\text{E.198})$$

Combining Eqs. (E.194, E.197 and E.198) leads to the final expression of derivative of the residual with respect to temperature Eq. (E.186) becomes

$$\begin{aligned} \frac{\partial \Omega_{US}^{(2)}}{\partial T} = & + N \mu_g^{(2)} \exp(-N(T - T_g)) (1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)} - 3}{I_m^{(2)}})^{-1} \left\{ -\frac{1}{3} \text{tr} \bar{\mathbf{C}}^{e(2)} \boldsymbol{\delta}_{US} \right. \\ & + \left[ \exp(\mathbf{W} (S^{(2)}(T))^{\frac{-1}{m}}) \right]_{UR}^{-T} \bar{\mathbf{C}}_{pr(RQ)}^{e(2)} \left[ \exp(\mathbf{W} (S^{(2)}(T))^{\frac{-1}{m}}) \right]_{QS}^{-1} \left. \right\} \\ & - \frac{\mu^{(2)}}{I_m} (1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)} - 3}{I_m^{(2)}})^{-2} \frac{\partial \text{tr} \bar{\mathbf{C}}^{e(2)}}{\partial T} \left\{ -\frac{1}{3} \text{tr} \bar{\mathbf{C}}^{e(2)} \boldsymbol{\delta}_{US} \right. \\ & + \left[ \exp(\mathbf{W} (S^{(2)}(T))^{\frac{-1}{m}}) \right]_{UR}^{-T} \bar{\mathbf{C}}_{(pr)RQ}^{e(2)} \left[ \exp(\mathbf{W} (S^{(2)}(T))^{\frac{-1}{m}}) \right]_{QS}^{-1} \left. \right\} \\ & - \mu^{(2)} (1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)} - 3}{I_m^{(2)}})^{-1} \left\{ -\frac{1}{3} \frac{\partial \text{tr} \bar{\mathbf{C}}^{e(2)}}{\partial T} \boldsymbol{\delta}_{US} \right. \quad (\text{E.199}) \\ & + \frac{\mathbf{W}_{KL}}{m} \left[ \exp(\mathbf{W} (S^{(2)}(T))^{\frac{-1}{m}}) \right]_{UB}^{-T} \left[ \exp(\mathbf{W} (S^{(2)}(T))^{\frac{-1}{m}}) \right]_{AR}^{-T} \\ & \boldsymbol{\mathcal{Z}}_{ABKL} S^{(2)}(T)^{\frac{-1-m}{m}} \frac{\partial S^{(2)}(T)}{\partial T} \bar{\mathbf{C}}_{(pr)RQ}^{e(2)} \left[ \exp(\mathbf{W} (S^{(2)}(T))^{\frac{-1}{m}}) \right]_{QS}^{-1} \\ & + \frac{\mathbf{W}_{KL}}{m} \left[ \exp(\mathbf{W} (S^{(2)}(T))^{\frac{-1}{m}}) \right]_{UR}^{-T} \bar{\mathbf{C}}_{(pr)RQ}^{e(2)} \left[ \exp(\mathbf{W} (S^{(2)}(T))^{\frac{-1}{m}}) \right]_{QA}^{-1} \\ & \left. \left[ \exp(\mathbf{W} (S^{(2)}(T))^{\frac{-1}{m}}) \right]_{BS}^{-1} \boldsymbol{\mathcal{Z}}_{ABKL} S^{(2)}(T)^{\frac{-1-m}{m}} \frac{\partial S^{(2)}(T)}{\partial T} \right\}. \end{aligned}$$

Hence, substituting Eq. (E.199) in Eq. (E.184) one has successively the final expression of  $\frac{\partial \mathbf{M}_{CD}^{e(2)}}{\partial T}$ .

The components for the derivative of the plastic deformation gradient can be computed as

$$\begin{aligned} \frac{\partial \Delta \epsilon^{p(2)}}{\partial T} &= \frac{\partial}{\partial T} \left( \dot{\epsilon}_0^{(2)} \Delta t \left( \frac{|\mathbf{M}^{e(2)}|}{\sqrt{2} S^{(2)}(T)} \right)^{\frac{1}{m}} \right) \\ &= \frac{\partial (S^{(2)}(T))^{\frac{-1}{m}}}{\partial T} \left( \dot{\epsilon}_0^{(2)} \Delta t \left( \frac{|\mathbf{M}^{e(2)}|}{\sqrt{2}} \right)^{\frac{1}{m}} \right) + \left( \dot{\epsilon}_0^{(2)} \Delta t \left( \frac{1}{\sqrt{2} S^{(2)}(T)} \right)^{\frac{1}{m}} \right) \frac{\partial (|\mathbf{M}^{e(2)}|)^{\frac{1}{m}}}{\partial T}, \quad (\text{E.200}) \end{aligned}$$

where

$$\begin{aligned}\frac{\partial |\mathbf{M}^{e(2)}|^{\frac{1}{m}}}{\partial T} &= \frac{1}{m} |\mathbf{M}^{e(2)}|^{\frac{1-m}{m}} \frac{\partial \sqrt{\mathbf{M}_{CD}^{e(2)} : \mathbf{M}_{CD}^{e(2)}}}{\partial T} \\ &= -\frac{1}{m} |\mathbf{M}^{e(2)}|^{\frac{1-2m}{m}} \mathbf{J}_{2CDUS}^{-1} \frac{\partial \Omega_{US}^{(2)}}{\partial T} \mathbf{M}_{CD}^{e(2)}.\end{aligned}\quad (\text{E.201})$$

Substituting Eq. (E.201) in Eq. (E.200), gives

$$\begin{aligned}\frac{\partial \Delta \epsilon^p(2)}{\partial T} &= -\frac{\dot{\epsilon}_0^{(2)} \Delta t}{m} \left( \frac{|\mathbf{M}^{e(2)}|}{\sqrt{2}} \right)^{\frac{1}{m}} S^{(2)}(T)^{\frac{-1-m}{m}} \frac{\partial S^{(2)}(T)}{\partial T} \\ &\quad + \frac{1}{m} \left( \frac{\dot{\epsilon}_0^{(2)} \Delta t}{(\sqrt{2} S^{(2)}(T))^{\frac{1}{m}}} \right) |\mathbf{M}^{e(2)}|^{\frac{1-2m}{m}} \frac{\partial \mathbf{M}_{CD}^{e(2)}}{\partial T} \mathbf{M}_{CD}^{e(2)}.\end{aligned}\quad (\text{E.202})$$

Moreover, one has

$$\begin{aligned}\frac{\partial \mathbf{N}_{OP}^{(2)}}{\partial T} &= \frac{\partial}{\partial T} \left( \frac{\mathbf{M}_{OP}^{e(2)}}{\sqrt{2} |\mathbf{M}^{e(2)}|} \right) = \frac{\partial}{\partial T} \left( \frac{\mathbf{M}_{OP}^{e(2)} |\mathbf{M}^{e(2)}|^{-1}}{\sqrt{2}} \right) \\ &= -\frac{1}{\sqrt{2}} \mathbf{J}_{2OPUS}^{-1} \frac{\partial \Omega_{US}^{(2)}}{\partial T} |\mathbf{M}^{e(2)}|^{-1} + \frac{1}{\sqrt{2}} |\mathbf{M}^{e(2)}|^{-3} \mathbf{M}_{OP}^{e(2)} \mathbf{J}_{2CDUS}^{-1} \frac{\partial \Omega_{US}^{(2)}}{\partial T} \mathbf{M}_{CD}^{e(2)},\end{aligned}\quad (\text{E.203})$$

and

$$\frac{\partial \bar{\tau}^{(2)}}{\partial T} = \frac{1}{\sqrt{2}} \frac{\partial |\mathbf{M}^{e(2)}|}{\partial T} = -\frac{\mathbf{M}_{CD}^{e(2)}}{|\mathbf{M}^{e(2)}|} \mathbf{J}_{2CDUS}^{-1} \frac{\partial \Omega_{US}^{(2)}}{\partial T}.\quad (\text{E.204})$$

Combining Eqs. (E.203 and E.202) in Eq. (E.181) yields the derivative of plastic deformation gradient with respect to the temperature

$$\begin{aligned}\frac{\partial \mathbf{F}_{EZ(n+1)}^{p(2)}}{\partial T} &= \mathbf{Z}_{EIOP} \left[ \frac{\mathbf{M}_{OP}^{e(2)}}{\sqrt{2} |\mathbf{M}^{e(2)}|} \frac{\partial \Delta \epsilon^p(2)}{\partial T} + \Delta \epsilon^p(2) \frac{\partial \mathbf{N}_{OP}}{\partial T} \right] \mathbf{F}_{IZ(n)}^{p(2)} \\ &= \mathbf{Z}_{EIOP} \left[ \frac{\mathbf{M}_{OP}^{e(2)}}{\sqrt{2} |\mathbf{M}^{e(2)}|} \left\{ \left( -\dot{\epsilon}_0^{(2)} \Delta t \left( \frac{|\mathbf{M}^{e(2)}|}{\sqrt{2}} \right)^{\frac{1}{m}} \right) \frac{1}{2m \Delta_2} S^{(2)}(T)^{\frac{-1-m}{m}} (S_{gl}^{(2)} - S_r^{(2)}) \right. \right. \\ &\quad \left. \left. \operatorname{sech}^2 \left( \frac{1}{\Delta_2} (T - T_g) \right) + \frac{1}{m} \left( \frac{\dot{\epsilon}_0^{(2)} \Delta t}{(\sqrt{2} S^{(2)}(T))^{\frac{1}{m}}} \right) |\mathbf{M}^{e(2)}|^{\frac{1-2m}{m}} \frac{\partial \mathbf{M}_{CD}^{e(2)}}{\partial T} \mathbf{M}_{CD}^{e(2)} \right\} \right. \\ &\quad \left. + \Delta \epsilon^p(2) \left\{ \frac{\partial \mathbf{M}_{CD}^{e(2)}}{\partial T} |\mathbf{M}^{e(2)}|^{-1} - |\mathbf{M}^{e(2)}|^{-3} \mathbf{M}_{OP}^{e(2)} \frac{\partial \mathbf{M}_{CD}^{e(2)}}{\partial T} \mathbf{M}_{CD}^{e(2)} \right\} \right] \mathbf{F}_{IZ(n)}^{p(2)}.\end{aligned}\quad (\text{E.205})$$

The second term of Eq. (E.180) is obtained as

$$\begin{aligned} \frac{\partial \mathbf{S}_{\text{DB}}^{e(2)}}{\partial T} = & \left\{ J^{-\frac{2}{3}} \left( \frac{\partial \mu^{(2)}}{\partial T} \right) \left( 1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)} - 3}{\mathbf{I}_m^{(2)}} \right)^{-1} \left[ \boldsymbol{\delta}_{\text{DB}} - \frac{1}{3} (\text{tr} \bar{\mathbf{C}}^{e(2)}) \bar{\mathbf{C}}_{\text{DB}}^{e(2)-1} \right] \right. \\ & + J^{-\frac{2}{3}} \left[ \mu^{(2)} \frac{\partial \left( 1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)} - 3}{\mathbf{I}_m^{(2)}} \right)^{-1}}{\partial T} \left[ \boldsymbol{\delta}_{\text{DB}} - \frac{1}{3} (\text{tr} \bar{\mathbf{C}}^{e(2)}) \bar{\mathbf{C}}_{\text{DB}}^{e(2)-1} \right] \right. \\ & \left. \left. + J^{-\frac{2}{3}} \mu^{(2)} \left( 1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)} - 3}{\mathbf{I}_m^{(2)}} \right)^{-1} \left( -\frac{1}{3} \right) \frac{\partial (\text{tr} \bar{\mathbf{C}}^{e(2)} \bar{\mathbf{C}}_{\text{DB}}^{e(2)-1})}{\partial T} \right] \right\}. \end{aligned} \quad (\text{E.206})$$

As we know

$$\begin{aligned} \frac{\partial (\text{tr} \bar{\mathbf{C}}^{e(2)} \bar{\mathbf{C}}_{\text{DB}}^{e(2)-1})}{\partial T} &= \frac{\partial \text{tr} \bar{\mathbf{C}}^{e(2)}}{\partial T} \bar{\mathbf{C}}_{\text{DB}}^{e(2)-1} + \text{tr} \bar{\mathbf{C}}^{e(2)} \frac{\partial \bar{\mathbf{C}}_{\text{DB}}^{e(2)-1}}{\partial T} \\ &= \frac{\partial \text{tr} \bar{\mathbf{C}}^{e(2)}}{\partial T} \bar{\mathbf{C}}_{\text{DB}}^{e(2)-1} + \text{tr} \bar{\mathbf{C}}^{e(2)} \frac{\partial \bar{\mathbf{C}}_{\text{DB}}^{e(2)-1}}{\partial \bar{\mathbf{C}}_{\text{FG}}^{e(2)}} \frac{\partial \bar{\mathbf{C}}_{\text{FG}}^{e(2)}}{\partial T} \\ &= \frac{\partial \text{tr} \bar{\mathbf{C}}^{e(2)}}{\partial T} \bar{\mathbf{C}}_{\text{DB}}^{e(2)-1} - \text{tr} \bar{\mathbf{C}}^{e(2)} \bar{\mathbf{C}}_{\text{DF}}^{(2)-1} \bar{\mathbf{C}}_{\text{GB}}^{(2)-1} \frac{\partial \bar{\mathbf{C}}_{\text{FG}}^{e(2)}}{\partial T}, \end{aligned} \quad (\text{E.207})$$

Eq. (E.206) becomes

$$\begin{aligned} \frac{\partial \mathbf{S}_{\text{DB}}^{e(2)}}{\partial T} = & \left\{ -N \mu_g^{(2)} J^{-\frac{2}{3}} \exp(-N(T - T_g)) \left( 1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)} - 3}{\mathbf{I}_m^{(2)}} \right)^{-1} \left[ \boldsymbol{\delta}_{\text{DB}} - \frac{1}{3} (\text{tr} \bar{\mathbf{C}}^{e(2)}) \bar{\mathbf{C}}_{\text{DB}}^{e(2)-1} \right] \right. \\ & + \frac{1}{\mathbf{I}_m} J^{-\frac{2}{3}} \mu^{(2)} \left( 1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)} - 3}{\mathbf{I}_m^{(2)}} \right)^{-2} \frac{\partial \text{tr} \bar{\mathbf{C}}^{e(2)}}{\partial T} \left[ \boldsymbol{\delta}_{\text{DB}} - \frac{1}{3} (\text{tr} \bar{\mathbf{C}}^{e(2)}) \bar{\mathbf{C}}_{\text{DB}}^{e(2)-1} \right] \\ & \left. - \frac{1}{3} J^{-\frac{2}{3}} \mu^{(2)} \left( 1 - \frac{\text{tr} \bar{\mathbf{C}}^{e(2)} - 3}{\mathbf{I}_m^{(2)}} \right)^{-1} \left[ \frac{\partial \text{tr} \bar{\mathbf{C}}^{e(2)}}{\partial T} \bar{\mathbf{C}}_{\text{DB}}^{e(2)-1} - \text{tr} \bar{\mathbf{C}}^{e(2)} \bar{\mathbf{C}}_{\text{DF}}^{e(2)-1} \bar{\mathbf{C}}_{\text{GB}}^{(2)-1} \frac{\partial \bar{\mathbf{C}}_{\text{FG}}^{e(2)}}{\partial T} \right] \right\}. \end{aligned} \quad (\text{E.208})$$

We should calculate the derivatives of  $\text{tr} \bar{\mathbf{C}}^{e(2)}$  and  $\bar{\mathbf{C}}^{e(2)}$  with respect to the temperature.

After defining for simplicity  $V = \frac{\epsilon_0^{(2)} \Delta t}{\sqrt{2} \frac{m+1}{m}}$ , we have

$$\begin{aligned} \frac{\partial \bar{\mathbf{C}}_{\text{DB}}^{e(2)}}{\partial T} = & \frac{\partial \left[ \exp \left( \frac{V |\mathbf{M}^{e(2)}|^{\frac{1-m}{m}} \mathbf{M}^{e(2)}}{S^{(2)}(T)^{\frac{1}{m}}} \right) \right]_{\text{DR}}^{-T} \bar{\mathbf{C}}_{(\text{pr})\text{RQ}}^{e(2)} \left[ \exp \left( \frac{V |\mathbf{M}^{e(2)}|^{\frac{1-m}{m}} \mathbf{M}^{e(2)}}{S^{(2)}(T)^{\frac{1}{m}}} \right) \right]_{\text{QB}}^{-1}}{\partial T} \\ & + \left[ \exp \left( \frac{V |\mathbf{M}^{e(2)}|^{\frac{1-m}{m}} \mathbf{M}^{e(2)}}{S^{(2)}(T)^{\frac{1}{m}}} \right) \right]_{\text{DR}}^{-T} \bar{\mathbf{C}}_{(\text{pr})\text{RQ}}^{e(2)} \frac{\partial \left[ \exp \left( \frac{V |\mathbf{M}^{e(2)}|^{\frac{1-m}{m}} \mathbf{M}^{e(2)}}{S^{(2)}(T)^{\frac{1}{m}}} \right) \right]_{\text{QB}}^{-1}}{\partial T}. \end{aligned} \quad (\text{E.209})$$



First we have, after using the definition of  $\mathbf{W} = \frac{\epsilon_0^{(2)} \Delta t |\mathbf{M}^{e(2)}|^{\frac{1}{m}} \mathbf{N}}{\sqrt{2}^{\frac{1}{m}}}$

$$\frac{\partial \left[ \exp \left( \mathbf{WS}^{(2)}(\mathbf{T})^{\frac{-1}{m}} \right) \right]_{\text{DR}}^{-\text{T}}}{\partial \mathbf{T}} = \frac{\partial \left[ \exp \left( \mathbf{DS}^{(2)}(\mathbf{T})^{\frac{-1}{m}} \right) \right]_{\text{DR}}^{-\text{T}}}{\partial \left[ \exp \left( \mathbf{WS}^{(2)}(\mathbf{T})^{\frac{-1}{m}} \right) \right]_{\text{NO}}} \frac{\partial \left[ \exp \left( \mathbf{WS}^{(2)}(\mathbf{T})^{\frac{-1}{m}} \right) \right]_{\text{NO}}}{\partial \left( \mathbf{WS}^{(2)}(\mathbf{T})^{\frac{-1}{m}} \right)} \quad (\text{E.210})$$

$$\frac{\partial \left( \mathbf{WS}^{(2)}(\mathbf{T})^{\frac{-1}{m}} \right)}{\partial \mathbf{T}},$$

with

$$\frac{\partial \left[ \exp \left( \mathbf{WS}^{(2)}(\mathbf{T})^{\frac{-1}{m}} \right) \right]_{\text{DR}}^{-\text{T}}}{\partial \left[ \exp \left( \mathbf{WS}^{(2)}(\mathbf{T})^{\frac{-1}{m}} \right) \right]_{\text{NO}}} = - \left[ \exp \left( \mathbf{WS}^{(2)}(\mathbf{T})^{\frac{-1}{m}} \right) \right]_{\text{DO}}^{-\text{T}} \left[ \exp \left( \mathbf{WS}^{(2)}(\mathbf{T})^{\frac{-1}{m}} \right) \right]_{\text{NR}}^{-\text{T}}, \quad (\text{E.211})$$

and

$$\frac{\partial \left[ \exp \left( \mathbf{WS}^{(2)}(\mathbf{T})^{\frac{-1}{m}} \right) \right]_{\text{NO}}}{\partial \left( \mathbf{WS}^{(2)}(\mathbf{T})^{\frac{-1}{m}} \right)_{\text{KL}}} = \mathbf{Z}_{\text{NOKL}}. \quad (\text{E.212})$$

Using Eq. (6.85) gives

$$\begin{aligned} \frac{\partial \left( \mathbf{WS}^{(2)}(\mathbf{T})^{\frac{-1}{m}} \right)}{\partial \mathbf{T}} &= \mathbf{V} \left( \frac{\partial |\mathbf{M}^{e(2)}|^{\frac{1-m}{m}}}{\partial \mathbf{T}} \mathbf{M}_{\text{KL}}^{e(2)} + |\mathbf{M}^{e(2)}|^{\frac{1-m}{m}} \frac{\partial (\mathbf{M}_{\text{KL}}^{e(2)})}{\partial \mathbf{T}} \right) (\mathbf{S}^{(2)}(\mathbf{T}))^{\frac{-1}{m}} \\ &+ \mathbf{V} |\mathbf{M}^{e(2)}|^{\frac{1-m}{m}} \mathbf{M}_{\text{KL}}^{e(2)} \frac{\partial \mathbf{S}^{(2)}(\mathbf{T})^{\frac{-1}{m}}}{\partial \mathbf{T}} \\ &= \mathbf{V} \left( \frac{1-m}{m} |\mathbf{M}^{e(2)}|^{\frac{1-3m}{m}} \frac{\partial (\mathbf{M}_{\text{RQ}}^{e(2)})}{\partial \mathbf{T}} \mathbf{M}_{\text{RQ}}^{e(2)} \mathbf{M}_{\text{KL}}^{e(2)} + |\mathbf{M}^{e(2)}|^{\frac{1-m}{m}} \frac{\partial (\mathbf{M}_{\text{KL}}^{e(2)})}{\partial \mathbf{T}} \right) (\mathbf{S}^{(2)}(\mathbf{T}))^{\frac{-1}{m}} \\ &- \mathbf{V} |\mathbf{M}^{e(2)}|^{\frac{1-m}{m}} \mathbf{M}_{\text{KL}}^{e(2)} \frac{1}{m} \mathbf{S}^{(2)}(\mathbf{T})^{\frac{-1-m}{m}} \frac{\partial \mathbf{S}^{(2)}(\mathbf{T})}{\partial \mathbf{T}}. \end{aligned} \quad (\text{E.213})$$

By combining Eqs. (E.211, E.212 and E.213) yields

$$\begin{aligned} \frac{\partial \left[ \exp \left( \mathbf{WS}^{(2)}(\mathbf{T})^{\frac{-1}{m}} \right) \right]_{\text{DR}}^{-\text{T}}}{\partial \mathbf{T}} &= - \left[ \exp \left( \mathbf{WS}^{(2)}(\mathbf{T})^{\frac{-1}{m}} \right) \right]_{\text{DO}}^{-\text{T}} \left[ \exp \left( \mathbf{WS}^{(2)}(\mathbf{T})^{\frac{-1}{m}} \right) \right]_{\text{NR}}^{-\text{T}} \\ &\mathbf{Z}_{\text{NOKL}} \mathbf{V} \left\{ \left( -\frac{1-m}{m} |\mathbf{M}^{e(2)}|^{\frac{1-3m}{m}} (\mathbf{J}^2)^{-1} \right)_{\text{RQUS}} \frac{\partial \Omega_{\text{US}}^{(2)}}{\partial \mathbf{T}} \mathbf{M}_{\text{RQ}}^{e(2)} \mathbf{M}_{\text{KL}}^{e(2)} \right. \\ &- \left. |\mathbf{M}^{e(2)}|^{\frac{1-m}{m}} (\mathbf{J}^2)^{-1} \right)_{\text{KLUS}} \frac{\partial \Omega_{\text{US}}^{(2)}}{\partial \mathbf{T}} \right\} (\mathbf{S}^{(2)}(\mathbf{T}))^{\frac{-1}{m}} \\ &+ |\mathbf{M}^{e(2)}|^{\frac{1-m}{m}} \mathbf{M}_{\text{KL}}^{e(2)} \frac{1}{2m\Delta_2} \mathbf{S}^{(2)}(\mathbf{T})^{\frac{-1-m}{m}} (\mathbf{S}_g^{(2)} - \mathbf{S}_r^{(2)}) \\ &\left. \text{sech}^2 \left( \frac{1}{\Delta_2} (\mathbf{T} - \mathbf{T}_g) \right) \right\}. \end{aligned} \quad (\text{E.214})$$

By the same way, we have

$$\frac{\partial \left[ \exp \left( \mathbf{WS}^{(2)}(\mathbb{T})^{\frac{-1}{m}} \right) \right]_{\text{QB}}^{-1}}{\partial \mathbb{T}} = \frac{\partial \left[ \exp \left( \mathbf{WS}^{(2)}(\mathbb{T})^{\frac{-1}{m}} \right) \right]_{\text{QB}}^{-1}}{\partial \left[ \exp \left( \mathbf{WS}^{(2)}(\mathbb{T})^{\frac{-1}{m}} \right) \right]_{\text{NO}}} \frac{\partial \left[ \exp \left( \mathbf{WS}^{(2)}(\mathbb{T})^{\frac{-1}{m}} \right) \right]_{\text{NO}}}{\partial \left( \mathbf{WS}^{(2)}(\mathbb{T})^{\frac{-1}{m}} \right)_{\text{KL}}} \cdot \quad (\text{E.215})$$

$$\frac{\partial \left( \mathbf{WS}^{(2)}(\mathbb{T})^{\frac{-1}{m}} \right)_{\text{KL}}}{\partial \mathbb{T}}.$$

Altogether, we have

$$\begin{aligned} \frac{\partial \bar{\mathbf{C}}_{\text{DB}}^{e(2)}}{\partial \mathbb{T}} &= - \left[ \exp \left( \mathbf{WS}(\mathbb{T})^{(2)\frac{-1}{m}} \right) \right]_{\text{DO}}^{-\text{T}} \left[ \exp \left( \mathbf{WS}(\mathbb{T})^{(2)\frac{-1}{m}} \right) \right]_{\text{NR}}^{-\text{T}} \\ &\mathcal{Z}_{\text{NOKLV}} \left\{ \left( -\frac{1-m}{m} |\mathbf{M}^{e(2)}|^{\frac{1-3m}{m}} \frac{\partial \mathbf{M}_{\text{XY}}^{e(2)}}{\partial \mathbb{T}} \mathbf{M}_{\text{XY}}^{e(2)} \mathbf{M}_{\text{KL}}^{e(2)} - |\mathbf{M}^{e(2)}|^{\frac{1-m}{m}} \frac{\partial \mathbf{M}_{\text{KL}}^{e(2)}}{\partial \mathbb{T}} \right) \mathbf{S}^{(2)}(\mathbb{T})^{\frac{-1}{m}} \right\} \\ &+ |\mathbf{M}^{e(2)}|^{\frac{1-m}{m}} \mathbf{M}_{\text{KL}}^{e(2)} \frac{1}{m} \mathbf{S}^{(2)}(\mathbb{T})^{\frac{-1-m}{m}} \frac{\partial \mathbf{S}^{(2)}(\mathbb{T})}{\partial \mathbb{T}} \left\} \bar{\mathbf{C}}_{(\text{pr})\text{RQ}}^{e(2)} \left[ \exp \left( \mathbf{WS}^{(2)}(\mathbb{T})^{\frac{-1}{m}} \right) \right]_{\text{QB}}^{-1} \\ &- \left[ \exp \left( \mathbf{WS}^{(2)}(\mathbb{T})^{\frac{-1}{m}} \right) \right]_{\text{DR}}^{-\text{T}} \bar{\mathbf{C}}_{(\text{pr})\text{RQ}}^{e(2)} \left[ \exp \left( \mathbf{WS}^{(2)}(\mathbb{T})^{\frac{-1}{m}} \right) \right]_{\text{QN}}^{-1} \left[ \exp \left( \mathbf{WS}^{(2)}(\mathbb{T})^{\frac{-1}{m}} \right) \right]_{\text{OB}}^{-1} \\ &\mathcal{Z}_{\text{NOKLV}} \left\{ \left( -\frac{1-m}{m} |\mathbf{M}^{e(2)}|^{\frac{1-3m}{m}} \frac{\partial \mathbf{M}_{\text{RQ}}^{e(2)}}{\partial \mathbb{T}} \mathbf{M}_{\text{RQ}}^{e(2)} \mathbf{M}_{\text{KL}}^{e(2)} - |\mathbf{M}^{e(2)}|^{\frac{1-m}{m}} \frac{\partial \mathbf{M}_{\text{KL}}^{e(2)}}{\partial \mathbb{T}} \right) \mathbf{S}^{(2)}(\mathbb{T})^{\frac{-1}{m}} \right\} \\ &+ |\mathbf{M}^{e(2)}|^{\frac{1-m}{m}} \mathbf{M}_{\text{KL}}^{e(2)} \frac{1}{m} \mathbf{S}^{(2)}(\mathbb{T})^{\frac{-1-m}{m}} \frac{\partial \mathbf{S}^{(2)}(\mathbb{T})}{\partial \mathbb{T}} \left\}. \end{aligned} \quad (\text{E.216})$$

Finally, we have

$$\frac{\partial \text{tr} \bar{\mathbf{C}}^{e(2)}}{\partial \mathbb{T}} = \frac{\partial \text{tr} \bar{\mathbf{C}}^{e(2)}}{\partial \bar{\mathbf{C}}_{\text{DB}}^{e(2)}} \frac{\partial \bar{\mathbf{C}}_{\text{DB}}^{e(2)}}{\partial \mathbb{T}} = \boldsymbol{\delta}_{\text{DB}} \frac{\partial \bar{\mathbf{C}}_{\text{DB}}^{e(2)}}{\partial \mathbb{T}}. \quad (\text{E.217})$$

As a result, we get  $\frac{\partial \mathbf{S}^{e(2)}}{\partial \mathbb{T}}$ , thereafter, by combining Eqs. (E.205, E.208, E.216 and E.217), which leads to the final expression of  $\frac{\partial \mathbf{P}^{(2)}}{\partial \mathbb{T}}$ , Eq. (E.180).

### E.2.3 Predictor-corrector for third mechanism ( $\alpha = 3$ )

As explained in Section 6.3.4.4 only a nonlinear spring is used, accordingly we have  $\mathbf{F}^{\text{p}(3)} = \mathbf{I}$ , then  $\mathbf{F}^{e(3)} = \mathbf{F}$  and we can directly use the relations Eq. (6.90) and Eq. (6.92)

### E.2.3.1 Piola-Kirchhoff stress

The first Piola-Kirchhoff stress tensor can be computed from Eq. (6.90) by

$$\begin{aligned} \mathbf{P}_{iB}^{(3)} &= \mathbf{F}_{iA} \mathbf{S}_{AB}^{(3)} \\ &= \mathbf{F}_{iA} J^{-\frac{2}{3}} \mu^{(3)} \left(1 - \frac{\text{tr}\bar{\mathbf{C}} - 3}{I_m^{(3)}}\right)^{-1} \left[\delta_{AB} - \frac{1}{3}(\text{tr}\bar{\mathbf{C}}^{(3)})\bar{\mathbf{C}}_{(AB)}^{-1}\right]. \end{aligned} \quad (\text{E.218})$$

### E.2.3.2 Converged solution

The derivative of the first Piola-Kirchhoff stress tensor can be evaluated as

$$\begin{aligned} \frac{\mathbf{P}_{iB}^{(3)}}{\partial \mathbf{F}_{jC}} &= \frac{\partial \mathbf{P}_{iB}^{(3)}}{\partial \mathbf{F}_{jC}} = \frac{\partial (\mathbf{F}_{iA} \mathbf{S}_{AB}^{(3)})}{\partial \mathbf{F}_{jC}} = \frac{\partial \mathbf{F}_{iA}}{\partial \mathbf{F}_{jC}} \mathbf{S}_{AB} + \mathbf{F}_{iA} \frac{\partial \mathbf{S}_{AB}^{(3)}}{\partial \mathbf{F}_{jC}} \\ &= \delta_{ij} \delta_{AC} \mathbf{S}_{AB}^{(3)} + \mathbf{F}_{iA} \left( \frac{\partial \mathbf{S}_{AB}^{(3)}}{\partial \bar{\mathbf{F}}_{qM}} \frac{\partial \bar{\mathbf{F}}_{qM}}{\partial \mathbf{F}_{jC}} + \frac{\partial \mathbf{S}_{AB}^{(3)}}{\partial J} \frac{\partial J}{\partial \mathbf{F}_{jC}} \right). \end{aligned} \quad (\text{E.219})$$

As we have

$$\frac{\partial \bar{\mathbf{F}}_{qM}}{\partial \mathbf{F}_{jC}} = J^{-\frac{1}{3}} \frac{\partial \mathbf{F}_{qM}}{\partial \mathbf{F}_{jC}} = J^{-\frac{1}{3}} \delta_{qj} \delta_{MC}, \quad (\text{E.220})$$

the derivative of the second term of Eq. (E.219) can be computed as

$$\begin{aligned} \frac{\partial \mathbf{S}_{AB}^{(3)}}{\partial \bar{\mathbf{F}}_{qM}} \frac{\partial \bar{\mathbf{F}}_{qM}}{\partial \mathbf{F}_{jC}} &= \frac{\partial}{\partial \mathbf{F}_{qM}} \left( J^{-\frac{2}{3}} \mu^{(3)} \left(1 - \frac{\text{tr}\bar{\mathbf{C}} - 3}{I_m^{(3)}}\right)^{-1} \left[\delta_{AB} - \frac{1}{3}(\text{tr}\bar{\mathbf{C}})\bar{\mathbf{C}}_{AB}^{-1}\right] \right) J^{-\frac{1}{3}} \delta_{qj} \delta_{MC} \\ &= \left( J^{-\frac{2}{3}} \mu^{(3)} \frac{\partial \left(1 - \frac{\text{tr}\bar{\mathbf{C}} - 3}{I_m^{(3)}}\right)^{-1}}{\partial \bar{\mathbf{F}}_{qM}} \left[\delta_{AB} - \frac{1}{3}(\text{tr}\bar{\mathbf{C}})\bar{\mathbf{C}}_{AB}^{-1}\right] \right. \\ &\quad \left. + J^{-\frac{2}{3}} \mu^{(3)} \left(1 - \frac{\text{tr}\bar{\mathbf{C}} - 3}{I_m^{(3)}}\right)^{-1} (-1/3) \frac{\partial (\text{tr}\bar{\mathbf{C}}\bar{\mathbf{C}}_{AB}^{-1})}{\partial \bar{\mathbf{F}}_{qM}} \right) J^{-\frac{1}{3}} \delta_{qj} \delta_{MC}. \end{aligned} \quad (\text{E.221})$$

Let us first compute

$$\frac{\partial \left(1 - \frac{\text{tr}\bar{\mathbf{C}} - 3}{I_m^{(3)}}\right)^{-1}}{\partial \bar{\mathbf{F}}_{qM}} = -\left(1 - \frac{\text{tr}\bar{\mathbf{C}} - 3}{I_m^{(3)}}\right)^{-2} \frac{\partial \text{tr}\bar{\mathbf{C}}}{\partial \bar{\mathbf{F}}_{qM}} \left(\frac{-1}{I_m^{(3)}}\right), \quad (\text{E.222})$$

with

$$\frac{\partial \text{tr}\bar{\mathbf{C}}}{\partial \bar{\mathbf{F}}_{qM}} = \frac{\partial \text{tr}\bar{\mathbf{C}}}{\partial \mathbf{C}_{Df}} \frac{\partial \mathbf{C}_{Df}}{\partial \bar{\mathbf{F}}_{qM}} = \delta_{Df} \left( \frac{\partial (\bar{\mathbf{F}}_{kD} \bar{\mathbf{F}}_{kf})}{\partial \bar{\mathbf{F}}_{qM}} \right) = 2\bar{\mathbf{F}}_{qM}. \quad (\text{E.223})$$

Then Eq. (E.222), becomes

$$\frac{\partial \left(1 - \frac{\text{tr}\bar{\mathbf{C}} - 3}{I_m^{(3)}}\right)^{-1}}{\partial \bar{\mathbf{F}}_{qM}} = \frac{2}{I_m^{(3)}} \left(1 - \frac{\text{tr}\bar{\mathbf{C}} - 3}{I_m^{(3)}}\right)^{-2} \bar{\mathbf{F}}_{qM}. \quad (\text{E.224})$$

Then we can compute

$$\frac{\partial(\text{tr}\bar{\mathbf{C}}\bar{\mathbf{C}}_{AB}^{-1})}{\partial\bar{\mathbf{F}}_{qM}} = \frac{\partial\text{tr}\bar{\mathbf{C}}}{\partial\bar{\mathbf{F}}_{qM}}\bar{\mathbf{C}}_{AB}^{-1} + \text{tr}\bar{\mathbf{C}}\frac{\partial\bar{\mathbf{C}}_{AB}^{-1}}{\partial\bar{\mathbf{F}}_{qM}}, \quad (\text{E.225})$$

with

$$\begin{aligned} \frac{\partial\bar{\mathbf{C}}_{AB}^{-1}}{\partial\bar{\mathbf{F}}_{qM}} &= \frac{\partial\bar{\mathbf{F}}_{Ak}^{-1}\bar{\mathbf{F}}_{Bk}^{-1}}{\partial\bar{\mathbf{F}}_{qM}} = \frac{\partial\bar{\mathbf{F}}_{Ak}^{-1}}{\partial\bar{\mathbf{F}}_{qM}}\bar{\mathbf{F}}_{Bk}^{-1} + \bar{\mathbf{F}}_{Ak}^{-1}\frac{\partial\bar{\mathbf{F}}_{Bk}^{-1}}{\partial\bar{\mathbf{F}}_{qM}} \\ &= -\bar{\mathbf{F}}_{Aq}^{-1}\bar{\mathbf{F}}_{Mk}^{-1}\bar{\mathbf{F}}_{Bk}^{-1} - \bar{\mathbf{F}}_{Ak}^{-1}\bar{\mathbf{F}}_{Bq}^{-1}\bar{\mathbf{F}}_{Mk}^{-1}, \end{aligned} \quad (\text{E.226})$$

as  $\frac{\partial\bar{\mathbf{F}}_{Ak}^{-1}}{\partial\bar{\mathbf{F}}_{qM}} = -\bar{\mathbf{F}}_{Aq}^{-1}\bar{\mathbf{F}}_{Mk}^{-1}$ .

Using Eq. (E.226) and Eq. (E.223), the relation (E.225) becomes

$$\frac{\partial(\text{tr}\bar{\mathbf{C}}\bar{\mathbf{C}}_{AB}^{-1})}{\partial\bar{\mathbf{F}}_{qM}} = 2\bar{\mathbf{F}}_{qM}\bar{\mathbf{C}}_{AB}^{-1} - \text{tr}\bar{\mathbf{C}}\left(\bar{\mathbf{F}}_{Aq}^{-1}\bar{\mathbf{C}}_{MB}^{-1} + \bar{\mathbf{C}}_{AM}^{-1}\bar{\mathbf{F}}_{Bq}^{-1}\right). \quad (\text{E.227})$$

Thus Eq. (E.221) is rewritten as

$$\begin{aligned} \frac{\partial\mathbf{S}_{AB}^{(3)}}{\partial\bar{\mathbf{F}}_{qM}}\frac{\partial\bar{\mathbf{F}}_{qM}}{\partial\bar{\mathbf{F}}_{jC}} &= \left\{ \frac{2}{I_m^{(3)}}J^{-1}\mu^{(3)}\left(1 - \frac{\text{tr}\bar{\mathbf{C}} - 3}{I_m^{(3)}}\right)^{-2}\bar{\mathbf{F}}_{jC}[\delta_{AB} - \frac{1}{3}(\text{tr}\bar{\mathbf{C}})\bar{\mathbf{C}}_{AB}^{-1}] \right. \\ &\quad - \frac{2}{3}J^{-1}\mu^{(3)}\left(1 - \frac{\text{tr}\bar{\mathbf{C}} - 3}{I_m^{(3)}}\right)^{-1}\bar{\mathbf{F}}_{jC}\bar{\mathbf{C}}_{AB}^{-1} \\ &\quad \left. + \frac{1}{3}J^{-1}\mu^{(3)}\left(1 - \frac{\text{tr}\bar{\mathbf{C}} - 3}{I_m^{(3)}}\right)^{-1}\text{tr}\bar{\mathbf{C}}\left(\bar{\mathbf{F}}_{Aj}^{-1}\bar{\mathbf{F}}_{Ck}^{-1}\bar{\mathbf{F}}_{Bk}^{-1} + \bar{\mathbf{F}}_{Ak}^{-1}\bar{\mathbf{F}}_{Bj}^{-1}\bar{\mathbf{F}}_{Ck}^{-1}\right) \right\}. \end{aligned} \quad (\text{E.228})$$

The third term of Eq. (E.219) can be computed by using

$$\frac{\partial J}{\partial\bar{\mathbf{F}}_{jC}} = \frac{\partial(\det\mathbf{F})}{\partial\bar{\mathbf{F}}_{jC}} = \mathbf{J}\bar{\mathbf{F}}_{jC}^{-T} = \mathbf{J}\bar{\mathbf{F}}_{Cj}^{-1}, \quad (\text{E.229})$$

as

$$\frac{\partial\mathbf{S}_{AB}^{(3)}}{\partial J}\frac{\partial J}{\partial\bar{\mathbf{F}}_{jC}} = -\frac{2}{3}\mathbf{S}_{AB}^{(3)}\bar{\mathbf{F}}_{jC}^{-T}. \quad (\text{E.230})$$

Combining Eqs. (E.228 and E.230) and replacing  $\mathbf{F}_{iA}$  by  $J^{\frac{1}{3}}\bar{\mathbf{F}}_{iA}$ , leads to the final expression of Eq. (E.219) as

$$\begin{aligned} \mathbf{Tangent}_{iBjC}^{(3)} &= \frac{\partial\mathbf{P}_{iB}}{\partial\bar{\mathbf{F}}_{jC}} = \delta_{ij}\delta_{AC}\mathbf{S}_{AB} \\ &\quad + \frac{2}{I_m^{(3)}}J^{-\frac{2}{3}}\mu^{(3)}\left(1 - \frac{\text{tr}\bar{\mathbf{C}} - 3}{I_m^{(3)}}\right)^{-2}[\bar{\mathbf{F}}_{iB}\bar{\mathbf{F}}_{jC} - \frac{1}{3}(\text{tr}\bar{\mathbf{C}})\bar{\mathbf{F}}_{Bi}^{-1}\bar{\mathbf{F}}_{jC}] \\ &\quad - \frac{2}{3}J^{-\frac{2}{3}}\mu^{(3)}\left(1 - \frac{\text{tr}\bar{\mathbf{C}} - 3}{I_m^{(3)}}\right)^{-1}\bar{\mathbf{F}}_{Bi}^{-1}\bar{\mathbf{F}}_{jC} \\ &\quad + \frac{1}{3}J^{-\frac{2}{3}}\mu^{(3)}\left(1 - \frac{\text{tr}\bar{\mathbf{C}} - 3}{I_m^{(3)}}\right)^{-1}\text{tr}\bar{\mathbf{C}}\left(\delta_{ij}\bar{\mathbf{C}}_{BC}^{-1} + \bar{\mathbf{F}}_{Ci}^{-1}\bar{\mathbf{F}}_{Bj}^{-1}\right) \\ &\quad - \frac{2}{3}\bar{\mathbf{F}}_{iA}\mathbf{S}_{AB}\bar{\mathbf{F}}_{Cj}^{-1}. \end{aligned} \quad (\text{E.231})$$

### E.2.3.3 Derivation with respect to temperature

Since the material parameters for this mechanisms are temperature independent, this leads to

$$\frac{\partial \mathbf{P}^{(3)}}{\partial T} = 0. \quad (\text{E.232})$$

### E.2.4 Evaluation of the heat source

The derivative of the right side of Eq. (6.36), which will be called  $w$ , with respect to the deformation and temperature can be computed as follows,

$$W = -\rho_0 c_v \dot{T} + Q_r + v \left( \bar{\tau}^{(1)} \Delta \epsilon^{p(1)} \frac{1}{\Delta t} + \bar{\tau}^{(2)} \Delta \epsilon^{p(2)} \frac{1}{\Delta t} \right), \quad (\text{E.233})$$

where  $\Delta t$  is the time step. Now let us define the following variable for simplicity

$$A^{(\alpha)} = (\bar{\tau}^{(\alpha)} \Delta \epsilon^{p(\alpha)}) \frac{1}{\Delta t}. \quad (\text{E.234})$$

First we derive with respect to the deformation gradient

$$\frac{\partial W}{\partial \mathbf{F}} = - \sum \rho_0 \frac{\partial c_v}{\partial \mathbf{F}} \dot{T} + \sum \frac{\partial A^{(\alpha)}}{\partial \mathbf{F}} v, \quad (\text{E.235})$$

and

$$\frac{\partial c_v}{\partial \mathbf{F}} = \frac{\partial c_v}{\partial T_g} \frac{\partial T_g}{\partial \mathbf{F}}. \quad (\text{E.236})$$

By calling Eq.(6.39), yields

$$\frac{\partial c_v}{\partial T_g} = \begin{cases} c_1 & \text{if } T \leq T_g \\ 0 & \text{if } T > T_g. \end{cases} \quad (\text{E.237})$$

Then using Eq. (E.234), one has

$$\frac{\partial A^{(\alpha)}}{\partial \mathbf{F}} = \left( \bar{\tau}^{(\alpha)} \frac{\partial \Delta \epsilon^{p(\alpha)}}{\partial \mathbf{F}} + \frac{\partial \bar{\tau}^{(\alpha)}}{\partial \mathbf{F}} \Delta \epsilon^{p(\alpha)} \right) \frac{1}{\Delta t}. \quad (\text{E.238})$$

For the first mechanisms, we have

$$\begin{aligned} \frac{\bar{\tau}^{(1)}}{\partial \mathbf{F}_{jX}} &= \frac{1}{\sqrt{2}} \frac{|\mathbf{M}_0^{e(1)}|}{\partial \mathbf{F}_{jC}} = \frac{1}{\sqrt{2}} \frac{\mathbf{M}_{0(CD)}^{e(1)}}{|\mathbf{M}_0^{e(1)}|} \frac{\partial \mathbf{M}_{0(CD)}^{e(1)}}{\partial \mathbf{F}_{jX}} \\ &= \frac{1}{\sqrt{2}} \frac{\mathbf{M}_{0(CD)}^{e(1)}}{|\mathbf{M}_0^{e(1)}|} \left( \frac{\partial \mathbf{M}_{CD}^{e(1)}}{\partial \mathbf{F}_{jX}} - \frac{1}{3} \delta_{AB} \frac{\partial \mathbf{M}_{AB}^{e(1)}}{\partial \mathbf{F}_{jX}} \delta_{CD} \right), \end{aligned} \quad (\text{E.239})$$

and  $\frac{\partial \Delta \epsilon^{p(1)}}{\partial \mathbf{F}}$  have been evaluated in Eq. (E.89). Upon substitution of  $\frac{\partial \Delta \epsilon^{p(1)}}{\partial \mathbf{F}}$  and  $\frac{\partial \bar{\tau}^{(1)}}{\partial \mathbf{F}}$  in Eq. (E.238) one has the derivative of the term related to plasticity with respect to deformation.

By the same way of mechanism 1, we compute the derivative of  $A^{(2)}$  with respect to the deformation.

$$\frac{\partial A^{(2)}}{\partial \mathbf{F}} = \left( \bar{\tau}^{(2)} \frac{\partial \Delta \epsilon^{P(2)}}{\partial \mathbf{F}} + \frac{\partial \bar{\tau}^{(2)}}{\partial \mathbf{F}} \Delta \epsilon^{P(2)} \right) \frac{1}{\Delta t}. \quad (\text{E.240})$$

The derivative of  $\frac{\partial \Delta \epsilon^{P(2)}}{\partial \mathbf{F}_{jX}}$  has been computed in Eq. (E.200). As we know  $\bar{\tau}^{(2)} = \frac{1}{\sqrt{2}} |\mathbf{M}^{e(2)}|$ , we have

$$\begin{aligned} \frac{\bar{\tau}^{(2)}}{\partial \mathbf{F}_{jX}} &= \frac{1}{\sqrt{2}} \frac{|\mathbf{M}^{e(2)}|}{\partial \mathbf{F}_{jC}} = \frac{1}{\sqrt{2}} \frac{\mathbf{M}_{CD}^{e(2)}}{|\mathbf{M}^{e(2)}|} \frac{\partial \mathbf{M}_{CD}^{e(2)}}{\partial \mathbf{F}_{jX}} \\ &= -\frac{1}{\sqrt{2}} \frac{\mathbf{M}_{CD}^{e(2)}}{|\mathbf{M}^{e(2)}|} \mathbf{J}^2_{CDUS}^{-1} \frac{\partial \Omega_{US}^{(2)}}{\partial \mathbf{F}_{jX}}, \end{aligned} \quad (\text{E.241})$$

where  $\frac{\partial \Omega_{US}^{(2)}}{\partial \mathbf{F}_{jX}}$  has been computed in Eq. (E.174). By substituting Eqs. (E.241) and (E.175) in the previous equation (E.240), one has its solution.

Secondly, the derivative of the thermal source is

$$\frac{\partial W}{\partial T} = -\sum \rho_0 \frac{\partial c_v}{\partial T} \dot{T} - \sum \rho_0 \frac{c_v}{\Delta t} + \sum \frac{\partial A^{(\alpha)}}{\partial T} v, \quad (\text{E.242})$$

where

$$\frac{\partial c_v}{\partial T} = \begin{cases} -c_1 & \text{if } T \leq T_g, \\ 0 & \text{if } T > T_g, \end{cases} \quad (\text{E.243})$$

and

$$\frac{\partial A^{(\alpha)}}{\partial T} = \left( \bar{\tau}^{(\alpha)} \frac{\partial \Delta \epsilon^{P(\alpha)}}{\partial T} + \Delta \epsilon^{P(\alpha)} \frac{\partial \bar{\tau}^{(\alpha)}}{\partial T} \right) \frac{1}{\Delta t}. \quad (\text{E.244})$$

For the first mechanism, we have

$$\frac{\partial A^{(1)}}{\partial T} = (\bar{\tau}^{(1)} \frac{\partial \Delta \epsilon^{P(1)}}{\partial T} + \frac{\partial \bar{\tau}^{(1)}}{\partial T} \Delta \epsilon^{P(1)}) \frac{1}{\Delta t}, \quad (\text{E.245})$$

where  $\frac{\partial \Delta \epsilon^{P(1)}}{\partial T}$  has been already computed in Eq. (E.200), then  $\frac{\partial \bar{\tau}^{(1)}}{\partial T}$  is computed by using Eq. (E.22)

$$\begin{aligned} \frac{\partial \bar{\tau}^{(1)}}{\partial T} &= \frac{1}{\sqrt{2}} \frac{|\mathbf{M}_0^{e(1)}|}{\partial T} = \frac{1}{\sqrt{2}} \frac{\mathbf{M}_{0(CD)}^{e(1)}}{|\mathbf{M}_0^{e(1)}|} \frac{\partial \mathbf{M}_{0(CD)}^{e(1)}}{\partial T} \\ &= \frac{1}{\sqrt{2}} \frac{\mathbf{M}_{0(CD)}^{e(1)}}{|\mathbf{M}_0^{e(1)}|} \left( \frac{\partial \mathbf{M}_{(CD)}^{e(1)}}{\partial T} - \frac{1}{3} \delta_{AB} \frac{\partial \mathbf{M}_{(AB)}^{e(1)}}{\partial T} \delta_{CD} \right). \end{aligned} \quad (\text{E.246})$$

By substituting Eq. (E.109) in Eq. (E.246), we can get the derivative of the term related to placticity with respect to temperature.

By the same way the derivative of  $A$  with respect to temperature for the second mechanism is computed as

$$\frac{\partial A^{(2)}}{\partial T} = (\bar{\tau}^{(2)} \frac{\partial \Delta \epsilon^{P(2)}}{\partial T} + \Delta \epsilon^{P(2)} \frac{\partial \bar{\tau}^{(2)}}{\partial T}) \frac{1}{\Delta t}, \quad (\text{E.247})$$

where  $\frac{\partial \Delta e^{(2)}}{\partial T}$  has been computed in Eq. (E.158), and

$$\begin{aligned} \frac{\partial \bar{\tau}^{(2)}}{\partial T} &= \frac{1}{\sqrt{2}} \frac{|\mathbf{M}^{e(2)}|}{\partial T} = \frac{\mathbf{M}_{CD}^{e(2)}}{|\mathbf{M}^{e(2)}|} \frac{\partial \mathbf{M}_{CD}^{e(2)}}{\partial T} \\ &= - \frac{\mathbf{M}_{CD}^{e(2)}}{|\mathbf{M}^{e(2)}|} \mathbf{J}_{CDUS}^{-1} \frac{\partial \boldsymbol{\Omega}_{US}^{(2)}}{\partial T}. \end{aligned} \quad (\text{E.248})$$

By substituting Eq. (E.203) and Eq. (E.248) in the previous equation (E.247), one can get its expression.