

## **Reference map approach to Eulerian thermomechanics using GENERIC**

Dirk Peschka<sup>1</sup>, Marita Thomas<sup>1,2</sup>, Andrea Zafferi<sup>2</sup>

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<sup>1</sup> Weierstrass Institute  
Mohrenstr. 39  
10117 Berlin  
Germany  
E-Mail: dirk.peschka@wias-berlin.de

<sup>2</sup> Freie Universität Berlin  
Arnimallee 9  
14195 Berlin  
E-Mail: thomas@fu-berlin.de  
zafferi@fu-berlin.de

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Edited by  
Weierstraß-Institut für Angewandte Analysis und Stochastik (WIAS)  
Leibniz-Institut im Forschungsverbund Berlin e. V.  
Mohrenstraße 39  
10117 Berlin  
Germany

Fax: +49 30 20372-303  
E-Mail: [preprint@wias-berlin.de](mailto:preprint@wias-berlin.de)  
World Wide Web: <http://www.wias-berlin.de/>

# Reference map approach to Eulerian thermomechanics using GENERIC

Dirk Peschka, Marita Thomas, Andrea Zafferi

*In memory of Wolfgang Dreyer, who we will always remember for  
his passion for thermodynamics and his love for a good argument.*

## Abstract

An Eulerian GENERIC model for thermo-viscoelastic materials with diffusive components is derived based on a transformation framework that maps a Lagrangian formulation to corresponding Eulerian coordinates. The key quantity describing the deformation in Eulerian coordinates is the inverse of the deformation, i.e. the *reference map*. The Eulerian model is formally constructed, and by reducing the GENERIC system to a damped Hamiltonian system, the isothermal limit is derived. A structure-preserving weak formulation is developed. As an example, the coupling of finite strain viscoelasticity and diffusion in a multiphase system governed by Lagrangian indicator functions is demonstrated.

## 1 Introduction

There is a plethora of thermomechanical models with diffusion that are relevant for numerous applications in the natural sciences. Among them, one can distinguish models for fluids or solids that may be either compressible or incompressible, cf. e.g. [46, 23, 32, 33, 45, 38]. These models can include diffusive or reactive components [11, 16, 12, 22] or even incorporate multiple phases, featuring phase transitions or phase separation [4, 3, 19, 1]. For solids, complex viscoelastic effects are relevant for hydrogels [35], in soft matter physics [20] as well as in geomechanics [42].

The wide applicability of these models, which all have a similar structure and thermodynamic basis, necessitates a unified thermomechanical framework that allows for large deformations. While thermo-viscoelastic models with large deformations are naturally formulated in the Lagrangian frame [46, 36, 41, 13, 6], this can be impractical for certain cases, e.g., when coupled with other effects that act in the current configuration, such as diffusion or fluid flow. In such situations an Eulerian formulation might be more suitable [56]. In a Lagrangian frame, compressible fluids and solids share a canonical skew-symmetric thermomechanical structure with irreversible dissipation but differ in their energy dependence on mechanical deformation, i.e., on the tensorial deformation gradient for hyperelastic solids and on the scalar volume for fluids. In contrast, in an Eulerian description, fluids and solids already differ in their choice of unknowns. Besides momentum as a state variable, fluid models typically track the volume via the Eulerian mass density, whereas solids evolve deformation via a tensor related to stress or strain [47, 55] transported by suitable Lie derivatives [36]. An alternative approach employs evolution equations for the vectorial *reference map* [30, 57], i.e., the inverse of the deformation, which is therefore sometimes also called in literature the *inverse map* [15, 54], *return map* [64], or *back-to-labels map* [14]. These approaches

can be especially useful when dealing with *Fluid-Structure Interaction* (FSI) problems [54, 57]. In [2], the authors implicitly also employ the reference map technique to evolve Eulerian displacements in a fluid–structure interaction problem involving capillary interfaces. This requires a careful and systematic consideration of the transformations between the Lagrangian reference configuration and the Eulerian deformed configuration in a thermodynamic framework.

In his book *Understanding Non-Equilibrium Thermodynamics*, Lebon presents a clear overview of the various schools that have evolved to study systems far from equilibrium [31]. There is no uniquely correct way to describe these processes, and different approaches have emerged based on distinct ideas of how to construct such theories. For example, classical irreversible thermodynamics is built on conservation laws and constitutive relations, while rational thermodynamics, pioneered by Truesdell [60], Coleman and Noll [46], follows a more systematic method to ensure consistency with the second law of thermodynamics. For fluids and mixtures, many well-developed theoretical extensions offer thermodynamically consistent formulations of complex systems, e.g. see *Thermo-Fluid Dynamics of Two-Phase Flow* by Ishii and Hibiki [28], *Thermodynamics of flowing systems: with internal microstructure* by Beris and Edwards [9], as well as the treatments by deGroot and Mazur in [18]. We also highlight the work *Continuum thermodynamics of chemically reacting fluid mixtures* by Dreyer and Bothe, who present a general model for diffusive and reactive mixtures and flows, along with an excellent overview of the different thermodynamic schools [12]. Similarly, for solids, dedicated texts such as *The mechanics and thermodynamics of continua* by Gurtin, Fried, and Anand provide rigorous frameworks that adhere to thermodynamic principles [25].

These approaches are complemented by more geometrical methods based on symplectic structures, Lie brackets, and gradient structures, such as the methods for metriplectic, port-Hamiltonian, or GENERIC systems [44, 43, 22, 37, 63, 38]. GENERIC, the acronym for *General Equations of Non-Equilibrium Reversible Irreversible Coupling*, is a thermodynamic formalism that was first introduced by Grmela and Öttinger [24, 50], based on the definition of thermodynamic potentials and geometric structures for conservative or reversible and for dissipative and irreversible processes, respectively. Grounded in thermodynamic functions like energy and entropy, the GENERIC formalism uses suitable geometric operators to generate the evolution of the state variables of the system. For over-damped systems, the structure of gradient flows can also ensure Onsager reciprocity by design [29, 48, 49, 20, 52]. Overall, these different approaches to thermomechanical systems are largely compatible and create a rich landscape of thermodynamic models — one that continues to spark lively debates about their respective advantages and disadvantages, with no final consensus among the thermodynamics community in sight.

In [66] we previously developed a mechanism to handle transformations between Lagrangian and Eulerian formulations of GENERIC systems and studied their implications on the thermodynamic formulation of systems of reactive multispecies fluids within the framework of GENERIC. In [59] it was shown that the GENERIC formalism extends to thermomechanical systems with state variables interacting between bulk and interfaces in terms of a weak formulation of GENERIC, which naturally encodes coupling conditions along the interfaces. Using such a weak formulation of GENERIC, in [53] we studied the transformation behaviour suited for a structure-preserving numerical discretization for a fluid-structure interaction problem using the reference map.

The main goal of this work is to provide an Eulerian GENERIC formulation for fluids and solids undergoing large deformations in terms of the reference map and show the feasibility of the weak form for structure-preserving numerical discretization. We establish two equivalent formulations in terms of Lagrangian and Eulerian quantities that are linked via a transformation map where we employ the *reference map*, i.e. the inverse of the deformation or flow map, as the variable to describe deformations.

In this spirit, section 2 introduces the Lagrangian and Eulerian kinematics and the GENERIC formalism augmented by a brief description of thermodynamics for solid materials. Subsequently, in section 3 we present a Lagrangian GENERIC system for thermo-viscoelastic materials and carry out a transformation to the Eulerian setting. We complement it by examples for the energy and entropy functionals and operators, and, by fast equilibration of temperature with a heat reservoir, reduce the GENERIC system to a damped Hamiltonian system. We conclude this work in section 4 with a weak formulation of the damped Hamiltonian system at the example

of a FSI problem, which is subsequently studied in numerical simulations. This example has two main purposes: Firstly, to show that the GENERIC structures previously introduced can be adapted to thermodynamically closed systems (in contrast to isolated systems treated by GENERIC) and, secondly, that the use of the reference map within this variational framework provides an alternative treatment to multiphase systems.

## 2 Kinematics and thermodynamics in the framework of GENERIC

We start by introducing the notations and definitions concerning the Lagrangian (reference) and the Eulerian (actual) configuration. In Section 2.2, we proceed with a brief discussion on thermodynamics of solid materials in connection with the previously defined quantities and ultimately we introduce the GENERIC framework.

### 2.1 Lagrangian and Eulerian kinematics

We consider a material that occupies in the Lagrangian or reference configuration the domain  $\bar{\Omega} \subset \mathbb{R}^d$  at time  $t = 0$ . At any time  $t \in [0, T]$  the Eulerian or actual domain  $\Omega(t)$  is connected to the initial data by the deformation or flow map  $\chi : [0, T] \times \bar{\Omega} \rightarrow \mathbb{R}^d$  such that  $\Omega(t) = \chi(t, \bar{\Omega})$ . Along with the flow map, deformations are measured through the deformation gradient  $\bar{F} : [0, T] \times \bar{\Omega} \rightarrow \mathbb{R}^{d \times d}$

$$\bar{F}(t, \bar{x}) := \bar{\nabla} \chi(t, \bar{x}).$$

Clearly, for the initial datum  $\chi(0, \bar{x}) = \bar{x}$  the deformation gradient is purely the identity matrix  $\bar{F}(0, \bar{x}) = \mathbb{I}_d$ . An important role in the energy functionals, see Remark 3.3, and in the thermodynamic formalism is played by its Jacobian  $\bar{V} := \det \bar{F}$ . Lastly, the description of a particle motion in Lagrangian coordinates is completed by its velocity field  $\bar{\nu}(t, \bar{x}) = \partial_t \chi(t, \bar{x})$ .

Assuming that the deformation  $\chi(t, \cdot)$  is invertible for every time  $t \in [0, T]$ , we introduce the *reference map*  $\alpha(t, \cdot) := \chi^{-1}(t, \cdot)$  that satisfies the identity relation

$$\alpha(t, \chi(t, \bar{x})) = \bar{x}, \quad \text{for any } (t, \bar{x}) \in [0, T] \times \bar{\Omega}. \quad (1)$$

From (1) one sees that the deformation gradient is the inverse gradient of the reference map, i.e.  $\bar{F}(t, x) = (\nabla \alpha(t, x))^{-1}$ . Throughout this paper we will denote quantities that are “naturally” defined in Lagrangian coordinates with a bar, while we will drop the bar for the Eulerian ones.

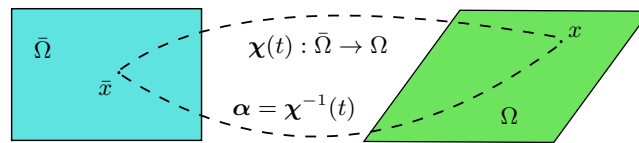


Figure 1: Schematic representation of the reference  $\bar{\Omega}$  and actual domain  $\Omega$  with the flow map  $\chi$  and the reference map  $\alpha$ .

### 2.2 Equilibrium thermomechanics

Since the GENERIC formalism relies on thermodynamic functionals and operators we first introduce some basic notions of equilibrium thermodynamics. It originated from the study of gases or fluids, see [62] and references therein for an historical review on the subject. One of the main observations of [66] is to identify the volume  $\bar{V}$  being an extensive thermodynamic variable with the determinant of the deformation gradient  $\bar{V} := \det \bar{F}$ .

To describe a fluid rheology only volumetric changes are relevant and thus only  $\bar{V}$  enters to the models. Instead, when modelling elastic solids, also deformations beyond pure volumetric changes have to be captured. Therefore, thermomechanical functionals and operators describing solid materials also have to include the dependency on other minors of the deformation gradient  $\bar{\mathbf{F}} = \bar{\nabla}\chi$  besides the determinant. By doing so, we will be able to treat general *hyperelastic* materials.

We follow the treatment of [61, 46, 25] and consider a state vector

$$\bar{\mathbf{q}}_{\bar{s}} := (\chi, \bar{\mathbf{c}}, \bar{s}) \quad (2)$$

formed by the vector of particle concentrations  $\bar{\mathbf{c}} = (\bar{c}_1, \dots, \bar{c}_N)$ , the deformation gradient  $\bar{\mathbf{F}} = \bar{\nabla}\chi$ , and the entropy density  $\bar{s}$ . Throughout this paper we will use a subscript  $z \in \{\bar{u}, \bar{s}, \bar{\theta}\}$  to stress the use of a specific thermodynamic variable in a given state vector, function or functional, as in (2) or (3). We then define the internal energy density of the system through an equation of state in natural variables

$$\bar{\mathcal{U}}_{\bar{s}}[\bar{\mathbf{q}}_{\bar{s}}] := \bar{\mathcal{U}}_{\bar{s}}(\bar{\mathbf{F}}, \bar{\mathbf{c}}, \bar{s}). \quad (3)$$

From the first and second law of thermodynamics we obtain the following fundamental relation between the state variables and their conjugate

$$D\bar{\mathcal{U}}_{\bar{s}} = \bar{\theta}_{\bar{s}} D\bar{s} + \bar{\Sigma}_{\bar{s}}^{\text{el}} : D\bar{\mathbf{F}} + \sum_{i=1}^N (\bar{\mu}_{\bar{s}})_i D\bar{c}_i. \quad (4)$$

Similar fundamental relations for solids can be found in [17, 7] and with a different strategy, introducing the concept of thermodynamic tension, in [8]. From (4), we recover the standard definitions of temperature  $\bar{\theta}_{\bar{s}}$ , chemical potential  $\bar{\mu}_{\bar{s}}$  and the elastic stress tensor  $\bar{\Sigma}_{\bar{s}}^{\text{el}}$ :

$$\bar{\theta}_{\bar{s}} := \frac{\partial \bar{\mathcal{U}}_{\bar{s}}}{\partial \bar{s}}, \quad \bar{\Sigma}_{\bar{s}}^{\text{el}} := \frac{\partial \bar{\mathcal{U}}_{\bar{s}}}{\partial \bar{\mathbf{F}}}, \quad \bar{\mu}_{\bar{s}} := \frac{\partial \bar{\mathcal{U}}_{\bar{s}}}{\partial \bar{\mathbf{c}}}. \quad (5)$$

This definition of elastic stress and its relation to  $\bar{\mathcal{U}}_{\bar{s}}$  is usually used in literature as the characterizing condition of hyperelastic materials, see [13, Ch.4]. Most of the theory of continuum mechanics of elastic bodies was developed independently from thermodynamics, which led to the assumption of constant temperature. For this and other practical reasons, often the Helmholtz free energy is used (or the Massieu potential, if more emphasis on dissipative processes is desired) to design constitutive laws for elastic materials. Let us briefly recall its definition. We define the Helmholtz free energy for the state vector  $\bar{\mathbf{q}}_{\bar{\theta}} = (\bar{\mathbf{F}}, \bar{\mathbf{c}}, \bar{\theta})$  in the following way:

$$\bar{\mathcal{F}}_{\bar{\theta}}(\bar{\mathbf{q}}_{\bar{\theta}}) = \int_{\Omega} \bar{\mathcal{F}}_{\bar{\theta}}[\bar{\mathbf{q}}_{\bar{\theta}}] d\bar{x} := \int_{\Omega} (\bar{\mathcal{U}}_{\bar{\theta}}[\bar{\mathbf{q}}_{\bar{\theta}}] - \bar{\theta} \bar{\mathcal{S}}_{\bar{\theta}}[\bar{\mathbf{q}}_{\bar{\theta}}]) d\bar{x}, \quad (6)$$

which is the Legendre transform of the internal energy  $\bar{\mathcal{U}}_{\bar{s}}$  wrt. the entropy  $\bar{s}$ . By means of the standard relations (5) we have:

$$\frac{\partial \bar{\mathcal{F}}_{\bar{\theta}}}{\partial \bar{\theta}} = -\bar{\mathcal{S}}_{\bar{\theta}}, \quad \frac{\partial^2 \bar{\mathcal{F}}_{\bar{\theta}}}{\partial \bar{\theta}^2} = -\frac{\bar{C}_{\bar{V}}}{\bar{\theta}}, \quad \frac{\partial \bar{\mathcal{F}}_{\bar{\theta}}}{\partial \bar{\mathbf{F}}} = \bar{\Sigma}^{\text{el}},$$

where  $\bar{C}_{\bar{V}}$  is the heat capacity at constant volume.

While the free energy can and should, in principle, depend arbitrarily on  $\bar{\mathbf{q}}_{\bar{\theta}}$ , we propose a simplified energy model that emphasizes the nonlinear elasticity of the system and adopts idealized assumptions for the dependence on temperature and concentration. This approach follows the strategy of ideal gas relationships for the concentration, assumes a constant (Eulerian) heat capacity, and ensures the distinction between classical extensive and intensive variables in the context of nonlinear elasticity. Accordingly, we propose the following form

$$\bar{\mathcal{F}}_{\bar{\theta}}[\bar{\mathbf{q}}_{\bar{\theta}}] := [\bar{\mathcal{F}}_{\text{mech}}(\bar{x}, \bar{\mathbf{F}}_{\text{iso}}) + \bar{\mathcal{F}}_{\text{int}}(\bar{x}, \bar{c}/\det(\bar{\mathbf{F}}), \bar{\theta}/\det(\bar{\mathbf{F}}), \bar{\theta})] \det(\bar{\mathbf{F}}), \quad (7a)$$

where  $\bar{\varrho}$  can be interpreted as the mass density. Its relation to the vector of concentrations  $\bar{c}$  will be specified later, cf. (16). In (7), the isochoric part of the deformation gradient  $\bar{\mathbf{F}}$  is defined as  $\bar{\mathbf{F}}_{\text{iso}} = \bar{\mathbf{F}}/(\det \bar{\mathbf{F}})^{1/d}$  for spatial dimension  $d$  so that  $\det(\bar{\mathbf{F}}_{\text{iso}}) \equiv 1$ . Here, elastic contributions (shear forces) are encoded in  $\mathcal{F}_{\text{mech}}$ , and the remaining thermal, chemical, and volumetric contributions come from the internal energy  $\mathcal{F}_{\text{int}}$ . We further distinguish in  $\mathcal{F}_{\text{int}}$  contributions due to elasticity and due to the diffusive species by

$$\mathcal{F}_{\text{int}}(\bar{x}, \bar{c}/\det \bar{\mathbf{F}}, \bar{\varrho}/\det \bar{\mathbf{F}}, \bar{\theta}) := \mathcal{F}_{\text{int}}^{\text{solid}}(\bar{x}, \bar{\varrho}/\det \bar{\mathbf{F}}, \bar{\theta}) + \mathcal{F}_{\text{int}}^{\text{diff}}(\bar{x}, \bar{c}/\det \bar{\mathbf{F}}, \bar{\theta}). \quad (7b)$$

A somewhat idealized choice is

$$\mathcal{F}_{\text{int}}^{\text{solid}}(\bar{x}, \frac{\bar{\varrho}}{\det \bar{\mathbf{F}}}, \bar{\theta}) := C_{\text{solid}} \bar{\theta} \left[ \ln \left( \frac{\bar{\theta}}{\bar{\theta}_{\text{ref}}} \right) - 1 \right] + \frac{K \bar{\varrho}^2}{2} \left( \frac{\det \bar{\mathbf{F}}}{\bar{\varrho}} - \frac{1}{\bar{\varrho}} \right)^2, \quad (7c)$$

$$\mathcal{F}_{\text{int}}^{\text{diff}}(\bar{x}, \frac{\bar{c}}{\det \bar{\mathbf{F}}}, \bar{\theta}) := \frac{\bar{c}}{\det \bar{\mathbf{F}}} k_B \bar{\theta} \left[ \ln \left( \frac{\bar{c}}{\det \bar{\mathbf{F}}} \lambda_{\bar{\theta}}^3 \right) - 1 \right], \quad (7d)$$

with the (thermal) de Broglie wavelength  $\lambda_{\bar{\theta}} \sim \bar{\theta}^{-1/2}$ , and further constants  $C_{\text{solid}}, K, k_B > 0$ . Using the above definitions, this gives rise to the simplified additive heat capacity

$$\bar{C}_{\bar{V}} = C_{\text{solid}} \det(\bar{\mathbf{F}}) + \frac{3}{2} k_B \bar{c}.$$

This implies that  $\bar{C}_{\bar{V}}$  is an extensive quantity, i.e., it scales 1-homogeneously with the other extensive quantities  $\bar{V} = \det \bar{\mathbf{F}}$  and  $\bar{c}$ . For dilute concentration the heat capacity is usually dominated by  $C_{\text{solid}} \det(\bar{\mathbf{F}})$ , which leads to a constant Eulerian heat capacity  $C_V = C_{\text{solid}}$ . The above construction relates the Eulerian free energy to its Lagrangian version (7) by

$$\mathcal{F}_{\theta}[\mathbf{q}_{\theta}] = \tilde{\mathcal{F}}_{\theta}[\bar{\mathbf{q}}_{\theta}(\mathbf{q}_{\theta})]/\det(\mathbf{F}), \quad \text{where } \mathbf{q}_{\theta} := (\alpha, \mathbf{c}, \theta),$$

is the Eulerian state vector, where we define  $\bar{\mathbf{q}}_{\theta}(\mathbf{q}_{\theta}) := (\alpha, \mathbf{c}V, \theta)$ . The origin of the relation to the Lagrangian state vector  $\bar{\mathbf{q}}_{\theta}$  via a transformation will be explained in section 3.2. With  $\varrho = \bar{\varrho} \circ \alpha/V$  we then have

$$\mathcal{F}_{\theta}(\mathbf{q}_{\theta}) = \int_{\Omega} \mathcal{F}_{\theta}[\mathbf{q}_{\theta}] dx, \quad \mathcal{F}_{\theta}[\mathbf{q}_{\theta}] = \mathcal{F}_{\text{mech}}(\alpha, \mathbf{F}_{\text{iso}}) + \mathcal{F}_{\text{int}}(\alpha, \mathbf{c}, \varrho, \theta). \quad (8)$$

## 2.3 Short introduction to GENERIC

The GENERIC (*General Equation for Non-Equilibrium Reversible-Irreversible Coupling*) formalism was firstly introduced by Grmela and Öttinger in [24, 50]. This variational approach aims to describe thermodynamically isolated systems by means of a state space  $\bar{\mathcal{Q}}$ , usually a Banach space with dual  $\bar{\mathcal{Q}}^*$  and we will denote with  $\langle \cdot, \cdot \rangle$  the canonical dual pairing between  $\bar{\mathcal{Q}}^*$  and  $\bar{\mathcal{Q}}$ . The framework is based on two thermodynamic potentials, the total energy  $\bar{\mathcal{E}} : \bar{\mathcal{Q}} \rightarrow \mathbb{R}$  and the total entropy  $\bar{\mathcal{S}} : \bar{\mathcal{Q}} \rightarrow \mathbb{R}$  of the system, and two geometric structures  $\bar{\mathbb{J}}$  and  $\bar{\mathbb{K}}$ . The geometric structures give rise to two bilinear forms of different nature that characterize the reversible, or Hamiltonian, dynamics and the irreversible, or dissipative, dynamics of the system. The Poisson structure  $\bar{\mathbb{J}}(\bar{\mathbf{q}}) : \bar{\mathcal{Q}}^* \rightarrow \bar{\mathcal{Q}}$  is antisymmetric, i.e.  $\bar{\mathbb{J}}(\bar{\mathbf{q}}) = -\bar{\mathbb{J}}^*(\bar{\mathbf{q}})$  for all  $\bar{\mathbf{q}} \in \bar{\mathcal{Q}}$ , and satisfies Jacobi's identity, whereas the Onsager operator  $\bar{\mathbb{K}}(\bar{\mathbf{q}}) : \bar{\mathcal{Q}}^* \rightarrow \bar{\mathcal{Q}}$  is symmetric, i.e.  $\bar{\mathbb{K}}(\bar{\mathbf{q}}) = \bar{\mathbb{K}}^*(\bar{\mathbf{q}})$  for all  $\bar{\mathbf{q}} \in \bar{\mathcal{Q}}$ , and positively semidefinite, i.e.  $\langle \bar{\xi}, \bar{\mathbb{K}}(\bar{\mathbf{q}}) \bar{\xi} \rangle \geq 0$  for all  $\bar{\xi} \in \bar{\mathcal{Q}}^*$ . The triplet  $(\bar{\mathcal{Q}}, \bar{\mathcal{E}}, \bar{\mathbb{J}})$  forms a Hamiltonian system for reversible processes, whereas the triplet  $(\bar{\mathcal{Q}}, \bar{\mathcal{S}}, \bar{\mathbb{K}})$  forms an Onsager system for irreversible dissipative processes. A GENERIC quintuple  $(\bar{\mathcal{Q}}, \bar{\mathcal{E}}, \bar{\mathcal{S}}, \bar{\mathbb{J}}, \bar{\mathbb{K}})$  couples the two via the so-called *Non-Interaction Conditions* (NIC), that can be stated as follows

$$\bar{\mathbb{J}}(\bar{\mathbf{q}}) D \bar{\mathcal{S}}(\bar{\mathbf{q}}) = 0 = \bar{\mathbb{K}}(\bar{\mathbf{q}}) D \bar{\mathcal{E}}(\bar{\mathbf{q}}) \quad (9a)$$

together with the mass conservation conditions

$$\bar{\mathbb{J}}(\bar{q})D\bar{\mathcal{M}}(\bar{q}) = 0 = \bar{\mathbb{K}}(\bar{q})D\bar{\mathcal{M}}(\bar{q}), \quad (9b)$$

for the total mass of the system  $\bar{\mathcal{M}} : \bar{\mathcal{Q}} \rightarrow \mathbb{R}$ . Altogether, (9a) and (9b) are called degeneracy conditions.

Above in (9) the letter D denotes the Fréchet derivative of the functionals, which is, for a functional  $\bar{\mathcal{A}} : \bar{\mathcal{Q}} \rightarrow \mathbb{R}$  defined by

$$\langle D\bar{\mathcal{A}}(\bar{q}), \bar{\xi} \rangle := \lim_{0 < h \rightarrow 0} \frac{1}{h} (\bar{\mathcal{A}}(\bar{q} + h\bar{\xi}) - \bar{\mathcal{A}}(\bar{q})), \quad (10)$$

where  $D\bar{\mathcal{A}}(\bar{q}) \in \bar{\mathcal{Q}}^*$ . We similarly introduce the Fréchet derivative  $DT(\bar{q})$  for general maps  $T : \bar{\mathcal{Q}} \rightarrow \bar{\mathcal{Q}}$ . Throughout this paper we work with integral functionals  $\bar{\mathcal{A}} : \bar{\mathcal{Q}} \rightarrow \mathbb{R}$  that act on the state  $\bar{q} \in \bar{\mathcal{Q}}$ . The state is a map  $\bar{q} : [0, T] \times \Omega \rightarrow \mathbb{R}^k$ ,  $k \in \mathbb{N}$ . With a density  $\bar{\mathcal{A}} : \Omega \times \mathbb{R}^k \times \mathbb{R}^{k \times d} \rightarrow \mathbb{R}$ , the integral functional  $\bar{\mathcal{A}}$  is given by

$$\bar{\mathcal{A}}(\bar{q}) := \int_{\Omega} \bar{\mathcal{A}}[\bar{q}] d\bar{x}.$$

where we used the abbreviation  $\bar{\mathcal{A}}[\bar{q}] := \bar{\mathcal{A}}(\bar{x}, \bar{q}, \nabla \bar{q})$  to simplify notation. Based on this representation, we will use for both the functional derivative (10) and for the derivative of the density the symbol D, so that for all  $\bar{q}, \bar{\xi} \in \bar{\mathcal{Q}}$

$$\begin{aligned} \langle D\bar{\mathcal{A}}(\bar{q}), \bar{\xi} \rangle &= \int_{\Omega} D\bar{\mathcal{A}}[\bar{q}] \cdot \bar{\xi} d\bar{x}, \quad \text{where} \\ D\bar{\mathcal{A}}[\bar{q}] \cdot \bar{\xi} &= (\partial_{\bar{q}} \bar{\mathcal{A}}(\bar{x}, \bar{q}, \nabla \bar{q}) - \nabla \cdot \partial_{\nabla \bar{q}} \bar{\mathcal{A}}(\bar{x}, \bar{q}, \nabla \bar{q})) \cdot \bar{\xi}. \end{aligned} \quad (11)$$

Based on above definitions for a GENERIC system  $(\bar{\mathcal{Q}}, \bar{\mathcal{E}}, \bar{\mathcal{S}}, \bar{\mathbb{J}}, \bar{\mathbb{K}})$  the evolution of a state vector  $\bar{q} : [0, T] \rightarrow \bar{\mathcal{Q}}$  is governed by the following equation

$$\partial_t \bar{q} = \bar{\mathbb{J}}(\bar{q})D\bar{\mathcal{E}}(\bar{q}) + \bar{\mathbb{K}}(\bar{q})D\bar{\mathcal{S}}(\bar{q}). \quad (12)$$

Conditions (9) together with the properties of the operators  $\bar{\mathbb{J}}$  and  $\bar{\mathbb{K}}$  ensure the compatibility of the system with the laws of thermodynamics. In fact, by assuming that the chain rule holds true, for every solution to (12) one has the following inequality for the time derivative of the entropy

$$\begin{aligned} \frac{d}{dt} \bar{\mathcal{S}}(\bar{q}(t)) &= \langle D\bar{\mathcal{S}}(\bar{q}), \partial_t \bar{q} \rangle = \langle D\bar{\mathcal{S}}(\bar{q}), \bar{\mathbb{J}}(\bar{q})D\bar{\mathcal{E}}(\bar{q}) + \bar{\mathbb{K}}(\bar{q})D\bar{\mathcal{S}}(\bar{q}) \rangle \\ &= \langle D\bar{\mathcal{E}}(\bar{q}), -\bar{\mathbb{J}}(\bar{q})D\bar{\mathcal{S}}(\bar{q}) \rangle + \langle D\bar{\mathcal{S}}(\bar{q}), \bar{\mathbb{K}}(\bar{q})D\bar{\mathcal{S}}(\bar{q}) \rangle \\ &= \langle D\bar{\mathcal{S}}(\bar{q}), \bar{\mathbb{K}}(\bar{q})D\bar{\mathcal{S}}(\bar{q}) \rangle \geq 0. \end{aligned}$$

Analogously, one can prove that the total energy of the system is conserved for a solution of (12), i.e.,

$$\frac{d}{dt} \bar{\mathcal{E}}(\bar{q}(t)) = 0.$$

### 3 Nonequilibrium thermomechanical model with diffusion

In this section we present a GENERIC model for thermo-viscoelastic materials. Firstly, we provide a Lagrangian formulation  $(\bar{\mathcal{Q}}, \bar{\mathcal{E}}, \bar{\mathcal{S}}, \bar{\mathbb{J}}, \bar{\mathbb{K}})$ . Then we define Eulerian variables and perform a transformation of the functionals and related geometric structures resulting in a corresponding Eulerian GENERIC system  $(\bar{\mathcal{Q}}, \bar{\mathcal{E}}, \bar{\mathcal{S}}, \bar{\mathbb{J}}, \bar{\mathbb{K}})$ .

One of the main goals of this article is to construct two equivalent formulations of the physical system, one in terms of the Lagrangian or reference configuration and the other in terms of the Eulerian or actual configuration



$$\begin{array}{ccc}
\partial_t \bar{\mathbf{q}} = \bar{\mathbb{J}}(\bar{\mathbf{q}}) D\bar{\mathcal{E}}(\bar{\mathbf{q}}) + \bar{\mathbb{K}}(\bar{\mathbf{q}}) D\bar{\mathcal{S}}(\bar{\mathbf{q}}) & \xrightarrow{\text{solution}} & \bar{\mathbf{q}}(t) \in \bar{\mathcal{Q}} \\
\downarrow \mathbb{L} & & \downarrow T_{LE} \\
\partial_t \mathbf{q} = \mathbb{J}(\mathbf{q}) D\mathcal{E}(\mathbf{q}) + \mathbb{K}(\mathbf{q}) D\mathcal{S}(\mathbf{q}) & \xrightarrow{\text{solution}} & \mathbf{q}(t) \in \mathcal{Q}
\end{array}$$

Figure 2: Diagram showing the mapping relations between two GENERIC systems  $(\bar{\mathcal{Q}}, \bar{\mathcal{E}}, \bar{\mathcal{S}}, \bar{\mathbb{J}}, \bar{\mathbb{K}})$  and  $(\mathcal{Q}, \mathcal{E}, \mathcal{S}, \mathbb{J}, \mathbb{K})$  and between their respective solutions  $\bar{\mathbf{q}}, \mathbf{q}$ .

within the GENERIC framework. Here we collect notions and results about transformations and changes of coordinates for GENERIC systems that we will use later without any further proof. A detailed discussion and its relation to thermodynamics can be found in [66]. The family of relevant transformations consists of Fréchet differentiable maps between two state spaces

$$T_{LE} : \bar{\mathcal{Q}} \rightarrow \mathcal{Q} \quad \text{with Fréchet derivative } \mathbb{L}(\bar{\mathbf{q}}) := DT_{LE}(\bar{\mathbf{q}}). \quad (13)$$

Given two GENERIC systems  $(\bar{\mathcal{Q}}, \bar{\mathcal{E}}, \bar{\mathcal{S}}, \bar{\mathbb{J}}, \bar{\mathbb{K}}), (\mathcal{Q}, \mathcal{E}, \mathcal{S}, \mathbb{J}, \mathbb{K})$ , we say that the *closure conditions* are satisfied if

$$\mathcal{E}(T_{LE}(\bar{\mathbf{q}})) = \bar{\mathcal{E}}(\bar{\mathbf{q}}), \quad \mathcal{S}(T_{LE}(\bar{\mathbf{q}})) = \bar{\mathcal{S}}(\bar{\mathbf{q}}), \quad \mathcal{M}(T_{LE}(\bar{\mathbf{q}})) = \bar{\mathcal{M}}(\bar{\mathbf{q}}) \quad (14a)$$

$$\mathbb{J}(T_{LE}(\bar{\mathbf{q}})) = \mathbb{L}(\bar{\mathbf{q}}) \bar{\mathbb{J}}(\bar{\mathbf{q}}) \mathbb{L}^*(\bar{\mathbf{q}}), \quad (14b)$$

$$\mathbb{K}(T_{LE}(\bar{\mathbf{q}})) = \mathbb{L}(\bar{\mathbf{q}}) \bar{\mathbb{K}}(\bar{\mathbf{q}}) \mathbb{L}^*(\bar{\mathbf{q}}), \quad (14c)$$

with  $\mathbb{L}^*(\bar{\mathbf{q}})$  the adjoint operator of  $\mathbb{L}(\bar{\mathbf{q}})$ . This transformation mechanism is shown in the following diagram 2, which illustrates the existence of a transformed structure  $(\mathcal{Q}, \mathcal{E}, \mathcal{S}, \mathbb{J}, \mathbb{K})$  whose solutions agree with the mapped solutions  $\mathbf{q}(t) = T_{LE}(\bar{\mathbf{q}}(t))$ .

### 3.1 Lagrangian GENERIC system

**States.** We consider a time-evolving thermo-viscoelastic solid material in the reference configuration, described by the vector of state variables

$$\bar{\mathbf{q}} := \begin{pmatrix} \chi : \bar{\Omega} \rightarrow \mathbb{R}^d \\ \bar{\mathbf{m}} : \bar{\Omega} \rightarrow \mathbb{R}^d \\ \bar{\mathbf{c}} : \bar{\Omega} \rightarrow \mathbb{R}^N \\ \bar{\theta} : \bar{\Omega} \rightarrow \mathbb{R} \end{pmatrix} \in \bar{\mathcal{Q}}, \quad (15)$$

with the deformation  $\chi$  from Sec. 2.1, the linear momentum  $\bar{\mathbf{m}}$ , the vector of concentrations  $\bar{\mathbf{c}}$  of  $N$  species and the temperature  $\bar{\theta}$ . We assume the existence of a constant  $N$ -tuple of molar masses  $\mathbf{M} \in \mathbb{R}^N$ , such that the mass density  $\bar{\rho} : \bar{\Omega} \rightarrow \mathbb{R}$  can be expressed as a function of  $\bar{\mathbf{c}}$  via

$$\bar{\rho}(t, \bar{x}) = \bar{\rho}_0(\bar{x}) + \bar{\mathbf{c}}(t, \bar{x}) \cdot \mathbf{M}. \quad (16)$$

Condition (9b) imposes a strict restriction on the evolution of the function  $\bar{\mathbf{c}}$  and its relation with  $\mathbf{M}$ . In fact, the operators  $\bar{\mathbb{J}}$  and  $\bar{\mathbb{K}}$  have to be constructed in such a way that (9b) is satisfied, which in our barycentric setting enforces the condition  $\bar{\mathbf{c}}(t, \bar{x}) \cdot \mathbf{M} = 0$  for any  $(t, \bar{x}) \in [0, T] \times \bar{\Omega}$ .

The linear momentum relates to the velocity field by

$$\bar{\mathbf{m}}(t, \bar{x}) := \bar{\rho}(t, \bar{x}) \bar{\mathbf{v}}(t, \bar{x}) \quad \text{for every } (t, \bar{x}) \in [0, T] \times \bar{\Omega}.$$

The choice of the temperature as the “thermodynamic” variable is clearly not exclusive but it is made here in order to compare our result with the literature and to be closer to thermodynamic potentials that are used in this

scenario, see eq. (7) and Remark 3.2, Remark 3.3. In the Lagrangian and Eulerian formulation of this system we will not perform a change of the thermodynamic variable to  $\bar{u}$  or  $\bar{s}$  and thus we drop the  $\bar{\theta}$ -subscript from the state variable from now on.

**Driving functionals.** We consider the total energy functional  $\bar{\mathcal{E}} : \bar{\mathcal{Q}} \rightarrow \mathbb{R}$  as the sum of the kinetic energy  $\bar{\mathcal{K}} : \bar{\mathcal{Q}} \rightarrow \mathbb{R}$  and the internal energy  $\bar{\mathcal{U}} : \bar{\mathcal{Q}} \rightarrow \mathbb{R}$ , i.e.,

$$\bar{\mathcal{E}}(\bar{q}) := \bar{\mathcal{K}}(\bar{q}) + \bar{\mathcal{U}}(\bar{q}) \quad \text{with} \quad (17a)$$

$$\bar{\mathcal{K}}(\bar{q}) := \int_{\bar{\Omega}} \bar{\mathcal{K}}[\bar{q}] \, d\bar{x} = \int_{\bar{\Omega}} \frac{|\bar{\mathbf{m}}|^2}{2\bar{\varrho}(t, \bar{x})} \, d\bar{x} \quad \text{kinetic energy,} \quad (17b)$$

$$\bar{\mathcal{U}}(\bar{q}) := \int_{\bar{\Omega}} \bar{\mathcal{U}}[\bar{q}] \, d\bar{x} = \int_{\bar{\Omega}} \bar{\mathcal{U}}(\bar{x}, \bar{\mathbf{F}}, \bar{\mathbf{c}}, \bar{\theta}) \, d\bar{x} \quad \text{internal energy.} \quad (17c)$$

We emphasize here the  $\bar{\theta}$ -dependence of the internal energy density  $\bar{\mathcal{U}}$ , in view of the computation of the driving force  $D\bar{\mathcal{E}}$  and the verification of the non-interaction conditions (9a). Moreover, we highlight the dependence of  $\bar{\mathcal{U}}$  on the deformation gradient  $\bar{\mathbf{F}}$ , since this is a feature of solid materials, as discussed previously. Similarly to the total energy, we consider an entropy functional of the following form:

$$\bar{\mathcal{S}}(\bar{q}) := \int_{\bar{\Omega}} \bar{\mathcal{S}}[\bar{q}] \, d\bar{x} = \int_{\bar{\Omega}} \bar{\mathcal{S}}(\bar{x}, \bar{\mathbf{F}}, \bar{\mathbf{c}}, \bar{\theta}) \, d\bar{x}. \quad (18)$$

We now compute the Fréchet derivatives for the densities of the functionals in (17)

$$D\bar{\mathcal{E}}(\bar{q}) = \begin{pmatrix} D_{\mathbf{x}}\bar{\mathcal{U}}[\bar{q}] \\ D_{\bar{\mathbf{m}}}\bar{\mathcal{K}}[\bar{q}] \\ D_{\bar{\mathbf{c}}}(\bar{\mathcal{K}}[\bar{q}] + \bar{\mathcal{U}}[\bar{q}]) \\ D_{\bar{\theta}}\bar{\mathcal{U}}[\bar{q}] \end{pmatrix} = \begin{pmatrix} -\bar{\nabla} \cdot (\partial_{\bar{\mathbf{F}}}\bar{\mathcal{U}}) \\ \bar{\mathbf{v}} \\ -\frac{|\bar{\mathbf{v}}|^2}{2} + \partial_{\bar{\mathbf{c}}}\bar{\mathcal{U}} \\ \bar{C}_{\bar{V}} \end{pmatrix}, \quad (19a)$$

where  $\bar{C}_{\bar{V}}$  is the heat capacity. For the total entropy in (18) we get

$$D\bar{\mathcal{S}}(\bar{q}) = \begin{pmatrix} D_{\mathbf{x}}\bar{\mathcal{S}}[\bar{q}] \\ D_{\bar{\mathbf{m}}}\bar{\mathcal{S}}[\bar{q}] \\ D_{\bar{\mathbf{c}}}\bar{\mathcal{S}}[\bar{q}] \\ D_{\bar{\theta}}\bar{\mathcal{S}}[\bar{q}] \end{pmatrix} = \begin{pmatrix} -\bar{\nabla} \cdot (\partial_{\bar{\mathbf{F}}}\bar{\mathcal{S}}) \\ 0 \\ \partial_{\bar{\mathbf{c}}}\bar{\mathcal{S}} \\ \frac{\bar{C}_{\bar{V}}}{\bar{\theta}} \end{pmatrix}. \quad (19b)$$

**Geometric structures.** For reversible dynamics, we consider the Poisson operator

$$\bar{\mathbb{J}}(\bar{q}) := \begin{pmatrix} 0 & \mathbb{I}_d & 0 & 0 \\ -\mathbb{I}_d & 0 & 0 & \bar{\mathbb{J}}^{\bar{\mathbf{m}}\bar{\theta}} \\ 0 & 0 & 0 & 0 \\ 0 & \bar{\mathbb{J}}^{\bar{\theta}\bar{\mathbf{m}}} & 0 & 0 \end{pmatrix}, \quad \text{with} \quad (20)$$

$$\bar{\mathbb{J}}^{\bar{\mathbf{m}}\bar{\theta}}(\bar{q})[\bar{\eta}_{\bar{\theta}}] := -\bar{\nabla} \cdot (\bar{\eta}_{\bar{\theta}}\bar{\theta}\bar{C}_{\bar{V}}^{-1}\partial_{\bar{\mathbf{F}}}\bar{\mathcal{S}}), \quad \bar{\mathbb{J}}^{\bar{\theta}\bar{\mathbf{m}}}(\bar{q})[\bar{\eta}_{\bar{\mathbf{m}}}] := -\bar{\theta}\bar{C}_{\bar{V}}^{-1}\bar{\nabla}\bar{\eta}_{\bar{\mathbf{m}}} : \partial_{\bar{\mathbf{F}}}\bar{\mathcal{S}},$$

and where  $\bar{\eta} = (\bar{\eta}_{\mathbf{x}}, \bar{\eta}_{\bar{\mathbf{m}}}, \bar{\eta}_{\bar{\mathbf{c}}}, \bar{\eta}_{\bar{\theta}})$  is used here as a placeholder for the functional derivatives. This operator conforms with the non-canonical reversible operator for fluids and it can be derived from the canonical Poisson operator, e.g. see [44], by means of the transformation and closure conditions (14b), when mapping the entropy  $\bar{s}$  to the temperature  $\bar{\theta}$ . A detailed transformation is carried out in [66]. We can readily verify that  $\bar{\mathbb{J}}$  is linear and skew-symmetric, and that it satisfies the non-interaction conditions (9a), i.e.  $\bar{\mathbb{J}}(\bar{q})D\bar{\mathcal{S}}(\bar{q}) = 0$ , where one needs to use the thermodynamic relation  $\partial_{\bar{\theta}}\bar{\mathcal{S}} = \bar{C}_{\bar{V}}/\bar{\theta}$ .

The irreversible dynamics is characterized in our considered problem by three processes: heat conduction, diffusion of species, and viscous dissipation in the solid. In order to write a suitable operator we exploit the

additive property of the Onsager systems. As introduced for reaction diffusion systems [39], we split the Onsager operator  $\mathbb{K}$  into contributions and write  $\mathbb{K}(\bar{\mathbf{q}}) = \mathbb{K}^{\text{heat}}(\bar{\mathbf{q}}) + \mathbb{K}^{\text{diff}}(\bar{\mathbf{q}}) + \mathbb{K}^{\text{vi}}(\bar{\mathbf{q}})$ . Heat conduction is modelled

$$\mathbb{K}^{\text{heat}}(\bar{\mathbf{q}}) := \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \mathbb{K}_{\theta\theta}^{\text{heat}}(\bar{\mathbf{q}}) \end{pmatrix}, \quad \text{where} \quad (21a)$$

$$\mathbb{K}_{\theta\theta}^{\text{heat}}(\bar{\mathbf{q}})[\bar{\eta}_\theta] := -\frac{1}{\bar{C}_V(\bar{\mathbf{q}})} \bar{\nabla} \cdot \left[ \text{Cof}(\bar{\mathbf{F}}) \bar{\theta}^2 \bar{k}_{\text{heat}}(\bar{\mathbf{q}}) \bar{\mathbf{F}}^{-\top} \bar{\nabla} \left( \frac{\bar{\eta}_\theta}{\bar{C}_V} \right) \right], \quad (21b)$$

with  $\bar{k} = \bar{k}_{\text{heat}}(\bar{\mathbf{q}}) > 0$  and the cofactor matrix  $\text{Cof}(\bar{\mathbf{F}}) = \det(\bar{\mathbf{F}}) \bar{\mathbf{F}}^{-\top}$ . The dependence on  $\bar{\mathbf{F}}$  will become clearer later, when mapping to Eulerian coordinates, since it will be used to relate Lagrangian gradient  $\bar{\nabla}$  to Eulerian  $\nabla$ . Symmetry and positive semi-definiteness are readily verified and by setting  $\bar{\eta}_\theta = D_\theta \bar{\mathcal{E}} \equiv \partial_\theta \bar{\mathcal{U}} = \bar{C}_V$ , one sees immediately that the NIC  $\mathbb{K}^{\text{heat}} D \bar{\mathcal{E}} \equiv \mathbf{0}$  is satisfied.

The contribution due to diffusion of species, although different in nature, shares a structure similar to (21). We set

$$\mathbb{K}^{\text{diff}}(\bar{\mathbf{q}}) := \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & \mathbb{K}_{\mathbf{c}\mathbf{c}}^{\text{diff}}(\bar{\mathbf{q}}) & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad (22a)$$

$$\mathbb{K}_{\mathbf{c}\mathbf{c}}^{\text{diff}}(\bar{\mathbf{q}}) := -\bar{\nabla} \cdot [\bar{\mathbb{M}}(\bar{\mathbf{q}}) \bar{\nabla}(\bar{\eta}_{\mathbf{c}}) \bar{\mathbf{F}}^{-1} \text{Cof}(\bar{\mathbf{F}})]. \quad (22b)$$

Here  $\bar{\mathbb{M}}(\bar{\mathbf{q}}) \in \mathbb{R}^{N \times N}$  is the mobility matrix. In order to ensure mass conservation and (9a) we ask the  $N$ -tuple of molar masses  $\bar{\mathbf{M}}$  to lie in the kernel of  $\bar{\mathbb{M}}(\bar{\mathbf{q}})$ . The construction of diffusion coefficients satisfying this requirement is explored in [66].

The viscous dissipation operator together with the driving force  $D \bar{\mathcal{F}}$  generates the viscous stress  $\bar{\Sigma}^{\text{vi}}$ . However, finding a physically acceptable viscous stress can be an insidious task, as pointed out in [5]. We tackle this problem similarly to the heat conduction and construct the viscous Onsager operator by "pulling back" the Eulerian Onsager operator for a Stokes fluid, which is defined e.g. in [51, Ch.4.6]. We recall the notation for the symmetric gradient  $\bar{\nabla}_s \bar{\mathbf{a}} := \frac{1}{2}(\bar{\nabla} \bar{\mathbf{a}} \bar{\mathbf{F}}^{-1} + \bar{\mathbf{F}}^{-\top} \bar{\nabla} \bar{\mathbf{a}}^\top)$  and introduce a positive semi-definite fourth-order tensor  $\bar{\Lambda}(\bar{\mathbf{q}})$ . We then represent the viscous Onsager operator  $\mathbb{K}^{\text{vi}}$  in the following block-matrix structure:

$$\mathbb{K}^{\text{vi}}(\bar{\mathbf{q}}) := \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \mathbb{K}_{\bar{\mathbf{m}}\bar{\mathbf{m}}}^{\text{vi}}(\bar{\mathbf{q}}) & 0 & \mathbb{K}_{\bar{\mathbf{m}}\bar{\theta}}^{\text{vi}}(\bar{\mathbf{q}}) \\ 0 & 0 & 0 & 0 \\ 0 & \mathbb{K}_{\bar{\theta}\bar{\mathbf{m}}}^{\text{vi}}(\bar{\mathbf{q}}) & 0 & \mathbb{K}_{\bar{\theta}\bar{\theta}}^{\text{vi}}(\bar{\mathbf{q}}) \end{pmatrix}, \quad (23a)$$

$$\mathbb{K}_{\bar{\mathbf{m}}\bar{\mathbf{m}}}^{\text{vi}}(\bar{\mathbf{q}})[\bar{\eta}_{\bar{\mathbf{m}}}] := -\bar{\nabla} \cdot [\bar{\theta} \bar{\Lambda}(\bar{\mathbf{q}}) : \bar{\nabla}_s \bar{\eta}_{\bar{\mathbf{m}}} \text{Cof}(\bar{\mathbf{F}})], \quad (23b)$$

$$\mathbb{K}_{\bar{\mathbf{m}}\bar{\theta}}^{\text{vi}}(\bar{\mathbf{q}})[\bar{\eta}_{\bar{\theta}}] := \bar{\nabla} \cdot \left[ \bar{\theta} \bar{\Lambda}(\bar{\mathbf{q}}) : \bar{\nabla}_s \bar{\nu} \text{Cof}(\bar{\mathbf{F}}) \frac{\bar{\eta}_{\bar{\theta}}}{\bar{C}_V} \right], \quad (23c)$$

$$\mathbb{K}_{\bar{\theta}\bar{\mathbf{m}}}^{\text{vi}}(\bar{\mathbf{q}})[\bar{\eta}_{\bar{\mathbf{m}}}] := -\frac{1}{\bar{C}_V} \bar{\nabla}_s \bar{\nu} : \bar{\theta} \bar{\Lambda}(\bar{\mathbf{q}}) : \bar{\nabla}_s \bar{\eta}_{\bar{\mathbf{m}}} \bar{V}, \quad (23d)$$

$$\mathbb{K}_{\bar{\theta}\bar{\theta}}^{\text{vi}}(\bar{\mathbf{q}})[\bar{\eta}_{\bar{\theta}}] := \frac{\bar{\eta}_{\bar{\theta}}}{\bar{C}_V} \bar{\nabla}_s \bar{\nu} : \bar{\theta} \bar{\Lambda}(\bar{\mathbf{q}}) : \bar{\nabla}_s \bar{\nu} \bar{V}. \quad (23e)$$

The operator so defined satisfies the symmetry condition, i.e.,  $\mathbb{K} \equiv \mathbb{K}^*$  and the positive semi-definiteness, i.e.,  $\langle \bar{\eta}, \mathbb{K}^{\text{vi}} \bar{\eta} \rangle \geq 0$  for all  $\bar{\eta} \in \bar{\mathcal{Q}}^*$ . As before, by taking  $\bar{\eta}_{\bar{\mathbf{m}}} = D_{\bar{\mathbf{m}}} \bar{\mathcal{E}} \equiv \bar{\nu}$  and  $\bar{\eta}_{\bar{\theta}} = D_{\bar{\theta}} \bar{\mathcal{E}} \equiv \bar{C}_V$  we check that the non-interaction condition  $\mathbb{K}^{\text{vi}} D \bar{\mathcal{E}} \equiv \mathbf{0}$  is satisfied. In order to obtain the Stokes viscosity, we choose  $\bar{\Lambda}$  as

$$\bar{\Lambda}(\bar{\mathbf{q}}) := 2\bar{\lambda} \mathbb{I}_d^4 + \bar{\xi} (\mathbb{I}_d^2 \otimes \mathbb{I}_d^2), \quad (23f)$$

where  $\bar{\lambda} > 0$  and  $\bar{\xi} + \frac{2\bar{\lambda}}{d} > 0$  are the shear and bulk viscosity, respectively, and might be state-dependent. The fourth- and second-order identity tensors are denoted by  $\mathbb{I}_d^4$  and  $\mathbb{I}_d^2$ . With this choice of  $\bar{\Lambda}$ , the viscous Onsager

operator for fluids is retrieved. The product of a fourth order tensor  $A$  with a second order tensor  $B$  gives the second-order tensor with components in the following sense  $(A : B)_{ij} = A_{ijkl}B_{kl}$ .

By collecting the above definitions we have a GENERIC quintuple  $(\bar{\mathcal{Q}}, \bar{\mathcal{E}}, \bar{\mathcal{S}}, \bar{\mathbb{J}}, \bar{\mathbb{K}})$  and by applying the operators (20)-(23) to the driving forces (19), the evolution law  $\partial_t \bar{q} = \bar{\mathbb{J}}(\bar{q})D\bar{\mathcal{E}}(\bar{q}) + \bar{\mathbb{K}}(\bar{q})D\bar{\mathcal{S}}(\bar{q})$  results in the PDE-system

$$\partial_t \chi = \frac{\bar{m}}{\bar{\rho}}, \quad (24a)$$

$$\partial_t \bar{m} = \bar{\nabla} \cdot (\bar{\Sigma}^{\text{el}} + \bar{\Sigma}^{\text{vi}}) - \bar{W}, \quad (24b)$$

$$\partial_t \bar{c} = -\bar{\nabla} \cdot [\text{Cof}(\bar{F})\bar{\mathbb{M}}\bar{F}^{-\top} \bar{\nabla}(\partial_{\bar{c}}\bar{\mathcal{S}})] \quad (24c)$$

$$\bar{C}_{\bar{V}} \partial_t \bar{\theta} = \bar{\theta} \bar{\nabla} \bar{\nu} : \partial_{\bar{F}} \bar{\mathcal{S}} + \bar{\nabla}_s \bar{\nu} : \bar{\Sigma}^{\text{vi}} \bar{F}^{\top} + \bar{\nabla} \cdot (\text{Cof}(\bar{F})\bar{k}\bar{F}^{-\top} \bar{\nabla} \bar{\theta}), \quad (24d)$$

where  $\bar{\Sigma}^{\text{vi}} := \bar{\Lambda} \bar{\nabla}_s \bar{\nu} \text{Cof}(\bar{F})$  is the viscous stress and  $\bar{\Sigma}^{\text{el}} := \partial_{\bar{F}}(\bar{\mathcal{U}} - \bar{\theta} \bar{\mathcal{S}})$ . By including the second gradient of the deformation  $\chi$ , i.e.,  $\bar{\nabla} \bar{F}$  in the entropy and energy we would extend our model to the description of the so-called *2nd-grade non-simple materials* and by taking the overdamped limit we recover the equations and the structures presented in [41].

**Remark 3.1** (Frame indifference of stresses). *One of the requirements for having a physically consistent model is for the elastic and viscous stresses to be invariant under rigid motions. For the elastic stress tensor  $\bar{\Sigma}^{\text{el}}$ , this is ensured if, for example, the internal energy  $\bar{\mathcal{U}}$  and the entropy  $\bar{\mathcal{S}}$  depend on  $\bar{F}$  only through the right Cauchy-Green tensor  $\bar{F}^{\top} \bar{F}$ , see [13, Theorem 4.2-1] for more details. For the viscous stress tensor being frame indifferent is equivalent to satisfy the following condition for some  $\tilde{\Sigma} : \mathbb{R}^{d \times d} \times \mathbb{R}^{d \times d} \rightarrow \mathbb{R}^{d \times d}$ , cf. [40]:*

$$\bar{\Sigma}^{\text{vi}}(\bar{F}, \partial_t \bar{F}) = \bar{F} \tilde{\Sigma}(\bar{F}^{\top} \bar{F}, \bar{F}^{\top} \partial_t \bar{F} + \partial_t \bar{F}^{\top} \bar{F}).$$

*For dissipation structures as in (23f) one can see that this condition is satisfied for  $\tilde{\Sigma}(\bar{F}, \partial_t \bar{F}) := \bar{\Lambda}(\bar{q})(\bar{F}^{\top} \bar{F})^{-1} \frac{1}{2}(\bar{F}^{\top} \partial_t \bar{F} + \partial_t \bar{F}^{\top} \bar{F})(\bar{F}^{\top} \bar{F})^{-1} \sqrt{\det(\bar{F}^{\top} \bar{F})}$  where we recall that  $\bar{\nabla} \bar{\nu} = \partial_t \bar{F}$ .* \*

**Remark 3.2** (Hyperelastic material). *In this setting, the dependence of  $\bar{\mathcal{U}}$  on  $\bar{F}$  is the main distinguishing trait in modelling elastic responses of the solid material. Following [13, Ch. 4], the so-called Ogden's materials are described by a Helmholtz free energy, whose mechanical contribution is:*

$$\bar{\mathcal{F}}(\bar{F}) := \sum_{i=1}^M \alpha_i \text{tr}(\bar{F}^{\top} \bar{F})^{\gamma_i/2} + \sum_{j=1}^N \beta_j \text{tr}(\text{Cof}(\bar{F}^{\top} \bar{F}))(\bar{F}^{\top})^{\delta_j/2} + \kappa(\det \bar{F}),$$

*where  $\alpha_i > 0, \beta_j > 0, \gamma_i \geq 1, \delta_j \geq 1$ , and  $\kappa : (0, +\infty) \rightarrow \mathbb{R}$  is a convex function satisfying  $\kappa(y) \rightarrow +\infty$  as  $y \rightarrow 0^+$  and subjected to suitable growth as  $y \rightarrow +\infty$ . Other types of hyperelastic materials are the compressible Mooney-Rivlin materials, whose energy can be expressed as follows*

$$\bar{\mathcal{F}}(\bar{F}) := \alpha \text{tr}|\bar{F}|^2 + \beta |\text{Cof}(\bar{F})|^2 + \kappa(\det \bar{F}),$$

*where  $\kappa(y) = cy^2 - d \log(y), c \geq 0, d \geq 0$ . If  $\beta = 0$ , then one recovers an equation for a compressible neo-Hookean material. With the function  $\kappa(\cdot)$  related to volumetric variations and  $c = 0, d = 0$  one recovers the incompressible limit.*

**Remark 3.3** (Pure volumetric deformation). *Murnaghan's equation of state is widely used in geosciences, see e.g. [26], to model the behaviour of a solid under high pressures and it relates the pressure  $\bar{\pi}$  to the volume  $\bar{V}$ , the temperature  $\bar{\theta}$  and the bulk modulus  $\kappa_{\bar{\theta}}$  through the following equation of state*

$$\bar{\pi}(\bar{V}, \bar{\theta}) = \frac{\kappa_{\bar{\theta}}(\bar{\theta})}{\kappa'_{\bar{\theta}}} \left[ \left( \frac{\bar{V}_{\text{ref}}(\bar{\theta})}{\bar{V}} \right)^{\partial_{\bar{\pi}} \kappa_{\bar{\theta}}} - 1 \right] \quad (25)$$

with  $\bar{V}_{\text{ref}}(\bar{\theta})$  being a reference value of the volume obtained from

$$\bar{V}_{\text{ref}}(\bar{\theta}) = \bar{V}(\bar{\pi}_{\text{ref}}, \bar{\theta}_{\text{ref}}) \left[ 1 + a(\bar{\theta} - \bar{\theta}_{\text{ref}}) - 20a(\sqrt{\bar{\theta}} - \sqrt{\bar{\theta}_{\text{ref}}}) \right],$$

where  $\bar{\pi} = 1\text{bar}$ ,  $\bar{\theta}_{\text{ref}} = 298\text{K}$  and  $a > 0$ . We recall that the bulk modulus is defined through the following standard thermodynamic relation

$$\kappa_{\bar{\theta}} := -\bar{V} \left( \frac{\partial \bar{\pi}}{\partial \bar{V}} \right)_{\bar{\theta}}.$$

If we assume  $\partial_{\bar{\pi}} \kappa_{\bar{\theta}}$  to be constant (usually one has  $\partial_{\bar{\pi}} \kappa_{\bar{\theta}} \approx 4$ ) then the equation of state (25) is induced by a free energy density of the following type

$$\bar{\mathcal{F}}(\bar{V}, \bar{\theta}) = \frac{\kappa_{\bar{\theta}}(\bar{\theta})}{\partial_{\bar{\pi}} \kappa_{\bar{\theta}}} \bar{V} \left[ \frac{1}{\partial_{\bar{\pi}} \kappa_{\bar{\theta}} - 1} \left( \frac{\bar{V}_{\text{ref}}}{\bar{V}} \right)^{\partial_{\bar{\pi}} \kappa_{\bar{\theta}}} + 1 \right] - \frac{\kappa_{\bar{\theta}}(\bar{\theta}) \bar{V}_{\text{ref}}(\bar{\theta})}{\partial_{\bar{\pi}} \kappa_{\bar{\theta}} - 1}. \quad (26)$$

This fact can be easily checked by computing the pressure, which is given as the derivative of the free energy density  $\bar{\mathcal{F}} = \bar{\mathcal{F}}(\bar{V}, \bar{\theta})$

$$\bar{\pi} = -\frac{\partial \bar{\mathcal{F}}}{\partial \bar{V}}.$$

Let us remark that this energy density involves the deformation gradient only through purely volumetric contributions via  $\bar{V} = \det \bar{\mathbf{F}}$ .

### 3.2 Eulerian GENERIC system $(\mathcal{Q}, \mathcal{E}, \mathcal{S}, \mathbb{J}, \mathbb{K})$

In this subsection we consider the GENERIC system  $(\bar{\mathcal{Q}}, \bar{\mathcal{E}}, \bar{\mathcal{S}}, \bar{\mathbb{J}}, \bar{\mathbb{K}})$  previously defined in Section 3.1 and perform a change of variables from Lagrangian to Eulerian coordinates using the map  $\mathbb{T}_{\text{LE}}$  introduced in (13). We will use the reference map  $\alpha$  defined in (1) as one of the state variables. We recall that  $\alpha(t, \cdot)$  is the inverse of the deformation  $\chi(t)$  at time  $t$ , i.e.,  $\alpha(t, \chi(t, \bar{x})) = \bar{x}$  for every  $(t, \bar{x}) \in [0, \mathbb{T}] \times \bar{\Omega}$ . Eulerian fields will be denoted without a bar. For intensive variables the Eulerian fields result by simply composing the Lagrangian field with  $\alpha$ , as for  $\mathbf{F} = \bar{\mathbf{F}} \circ \alpha$ ,  $V = \bar{V} \circ \alpha$ ,  $\nu = \bar{\nu} \circ \alpha$ . For extensive variables the transformation additionally involves a division by  $\bar{V}$ , as can be seen in particular in equations (27b) and (27c). The new Eulerian state vector  $\mathbf{q}$  is defined through the map  $\mathbb{T}_{\text{LE}} : \bar{\mathcal{Q}} \rightarrow \mathcal{Q}$

$$\mathbf{q} = \begin{pmatrix} \alpha : \Omega \rightarrow \mathbb{R}^d \\ \mathbf{m} : \Omega \rightarrow \mathbb{R}^d \\ \mathbf{c} : \Omega \rightarrow \mathbb{R}^N \\ \theta : \Omega \rightarrow \mathbb{R} \end{pmatrix} = \mathbb{T}_{\text{LE}}(\bar{\mathbf{q}}) \in \mathcal{Q}, \text{ where} \quad (27a)$$

$$\mathbf{m} = \frac{\bar{\mathbf{m}}}{\bar{V}} \circ \alpha, \quad (27b)$$

$$\mathbf{c} = \frac{\bar{\mathbf{c}}}{\bar{V}} \circ \alpha, \quad (27c)$$

$$\theta = \bar{\theta} \circ \alpha. \quad (27d)$$

Here, based on the results of [66], momentum and concentrations are mapped as extensive variables, while the temperature as an intensive variable is transformed by simply applying the reference map. Since we are not going to perform any further change of variables, we omit the subscript that would mark the dependence on the temperature  $\theta$ , as previously introduced in (2) and below. One can verify that the driving functionals (17) and

(18) indeed satisfy the closure conditions (14a) under the mapping (27):

$$\mathcal{E}(\mathbf{q}) := \mathcal{K}(\mathbf{q}) + \mathcal{U}(\mathbf{q}) \quad \text{with} \quad (28a)$$

$$\mathcal{K}(\mathbf{q}) := \int_{\Omega} \frac{|\mathbf{m}|^2}{2\varrho} dx, \text{ where } \varrho = \frac{\bar{\varrho} \circ \boldsymbol{\alpha}}{V} + \mathbf{c} \cdot \mathbf{M}, \quad \text{kinetic energy,} \quad (28b)$$

$$\mathcal{U}(\mathbf{q}) := \int_{\Omega} \mathcal{U}(\boldsymbol{\alpha}, \mathbf{F}, \mathbf{c}, \theta) dx \quad \text{internal energy,} \quad (28c)$$

$$\mathcal{S}(\mathbf{q}) := \int_{\Omega} \mathcal{S}(\boldsymbol{\alpha}, \mathbf{F}, \mathbf{c}, \theta) dx \quad \text{entropy,} \quad (28d)$$

where  $\bar{\mathcal{U}}(\boldsymbol{\alpha}, \mathbf{F}, \mathbf{c}V, \theta) = \mathcal{U}(\boldsymbol{\alpha}, \mathbf{F}, \mathbf{c}, \theta)V$  and  $\bar{\mathcal{S}}(\boldsymbol{\alpha}, \mathbf{F}, \mathbf{c}V, \theta) = \mathcal{S}(\boldsymbol{\alpha}, \mathbf{F}, \mathbf{c}, \theta)V$ , cf. with the free energy (8). For the densities of the internal energy  $\mathcal{U}$  and entropy  $\mathcal{S}$  we have highlighted the  $\boldsymbol{\alpha}$ -dependency and distinguished it from  $\mathbf{F}$ . This distinction will simplify the computation of their functional derivative and will clarify that only the derivatives of these functionals wrt.  $\mathbf{F}$  contribute in the final PDE system. Furthermore, observe that the third component of  $\mathcal{U}$  and  $\mathcal{S}$  is  $\bar{\mathbf{c}} = \mathbf{c}V$  from (27c). The driving forces are given by the Fréchet derivatives of (28):

$$\mathrm{D}\mathcal{E}[\mathbf{q}] = \left( \mathrm{D}_{\boldsymbol{\alpha}} \left( \frac{|\mathbf{m}|}{2\varrho^2} + \frac{\bar{\mathcal{U}}}{V} \right), \boldsymbol{\nu}, -\frac{|\mathbf{m}|^2}{2\varrho^2} \mathbf{M} + \partial_{\bar{\mathbf{c}}} \bar{\mathcal{U}}, \frac{\partial_{\theta} \bar{\mathcal{U}}}{V} \right)^{\top}, \quad \text{where } \bar{\mathbf{c}} = \mathbf{c}V \quad (29a)$$

$$\mathrm{D}\mathcal{S}[\mathbf{q}] = \left( \mathrm{D}_{\boldsymbol{\alpha}} \mathcal{S}, 0, \partial_{\bar{\mathbf{c}}} \bar{\mathcal{S}}, \frac{C_V}{\theta} \right)^{\top}. \quad (29b)$$

Following (13) and below, the Lagrangian rates  $\partial_t \bar{\mathbf{q}}$  are mapped through the derivative of the Lagrangian-Eulerian transformation:

$$\mathrm{DT}_{\mathrm{LE}}(\bar{\mathbf{q}}) : \bar{\mathcal{Q}} \rightarrow \mathcal{Q}, \quad \mathrm{DT}_{\mathrm{LE}}(\bar{\mathbf{q}}) = \begin{pmatrix} -\nabla \boldsymbol{\alpha} & 0 & 0 & 0 \\ -\nabla \cdot (\bar{\mathbf{m}} \otimes \square) & \frac{\square}{\bar{V}} & 0 & 0 \\ -\nabla \cdot (\bar{\mathbf{c}} \otimes \square) & 0 & \frac{\square}{\bar{V}} & 0 \\ -\square \cdot \nabla \bar{\theta} & 0 & 0 & 1 \end{pmatrix}. \quad (30a)$$

This mapping induces the following relations between Lagrangian  $\partial_t \bar{\mathbf{q}}$  and Eulerian velocities  $\partial_t \mathbf{q}$ :

$$\begin{pmatrix} \partial_t \boldsymbol{\alpha} \\ \partial_t \bar{\mathbf{m}} \\ \partial_t \bar{\mathbf{c}} \\ \partial_t \bar{\theta} \end{pmatrix} = \mathrm{DT}_{\mathrm{LE}}(\bar{\mathbf{q}}) \begin{pmatrix} \partial_t \boldsymbol{\chi} \\ \partial_t \bar{\mathbf{m}} \\ \partial_t \bar{\mathbf{c}} \\ \partial_t \bar{\theta} \end{pmatrix} = \begin{pmatrix} -(\nabla \boldsymbol{\alpha}) \partial_t \boldsymbol{\chi} \\ -\bar{V}^{-1} \partial_t \bar{\mathbf{m}} - \nabla \cdot (\bar{V}^{-1} \bar{\mathbf{m}} \otimes \partial_t \boldsymbol{\chi}) \\ -\bar{V}^{-1} \partial_t \bar{\mathbf{c}} - \nabla \cdot (\bar{V}^{-1} \bar{\mathbf{c}} \otimes \partial_t \boldsymbol{\chi}) \\ \partial_t \bar{\theta} - \partial_t \boldsymbol{\chi} \cdot \nabla \bar{\theta} \end{pmatrix}, \quad (30b)$$

where the Eulerian gradient is acting on Lagrangian variables at the point  $\bar{x} = \boldsymbol{\alpha}(x)$ . The adjoint operator  $\mathrm{DT}_{\mathrm{LE}}^* : \mathcal{Q}^* \rightarrow \bar{\mathcal{Q}}^*$  maps driving forces and can be obtained by integration by parts of the expression  $\langle \boldsymbol{\eta}, \mathrm{DT}_{\mathrm{LE}} \bar{\mathbf{v}} \rangle_{\mathcal{Q}} = \langle \mathrm{DT}_{\mathrm{LE}}^* \boldsymbol{\eta}, \bar{\mathbf{v}} \rangle_{\bar{\mathcal{Q}}}$  valid for any sufficiently smooth  $\boldsymbol{\eta} \in \mathcal{Q}^*$  and any  $\bar{\mathbf{v}} \in \bar{\mathcal{Q}}$ , see (11) for the dual pairing. Using  $\mathrm{DT}_{\mathrm{LE}}$  from (30a) this leads to

$$\mathrm{DT}_{\mathrm{LE}}^*(\bar{\mathbf{q}}) = \begin{pmatrix} -\bar{V} \nabla \boldsymbol{\alpha}^{\top} & (\bar{\nabla} \square)^{\top} \bar{\mathbf{F}}^{-1} \bar{\mathbf{m}} & (\bar{\nabla} \square)^{\top} \bar{\mathbf{F}}^{-1} \bar{\mathbf{c}} & -\square \bar{V} \bar{\mathbf{F}}^{-\top} \bar{\nabla} \bar{\theta} \\ 0 & \square & 0 & 0 \\ 0 & 0 & \square & 0 \\ 0 & 0 & 0 & \bar{V} \square \end{pmatrix}. \quad (30c)$$

The transformed geometric structures  $\mathbb{J}(\mathbf{q}), \mathbb{K}(\mathbf{q}) : \mathcal{Q}^* \rightarrow \mathcal{Q}$  are directly computed using the transformation operators  $\mathrm{DT}_{\mathrm{LE}}, \mathrm{DT}_{\mathrm{LE}}^*$  as follows

$$\begin{aligned} \mathbb{J}(\mathbf{q}) &= \mathrm{DT}_{\mathrm{LE}}(\bar{\mathbf{q}}) \bar{\mathbb{J}}(\bar{\mathbf{q}}) \mathrm{DT}_{\mathrm{LE}}^*(\bar{\mathbf{q}}) \\ &= \begin{pmatrix} 0 & -\nabla \boldsymbol{\alpha} & 0 & 0 \\ \nabla \boldsymbol{\alpha}^{\top} & -(\nabla \square)^{\top} \bar{\mathbf{m}} - \nabla \cdot (\bar{\mathbf{m}} \otimes \square) & -(\nabla \square)^{\top} \bar{\mathbf{c}} & \nabla \theta + \frac{1}{\bar{V}} \bar{\mathbb{J}}^{\bar{\mathbf{m}} \bar{\theta}}[\square V] \\ 0 & -\nabla \cdot (\bar{\mathbf{c}} \otimes \square) & 0 & 0 \\ 0 & -\square \cdot \nabla \theta + \bar{\mathbb{J}}^{\bar{\theta} \bar{\mathbf{m}}} & 0 & 0 \end{pmatrix}, \end{aligned} \quad (31)$$

where the momentum-temperature related entries are obtained from (20) in terms of

$$\frac{1}{V} \mathbb{J}^{\bar{m}\bar{\theta}}[\eta_\theta V] = -\nabla \cdot \left( \frac{\theta}{C_V} \eta_\theta \partial_{\mathbf{F}} \mathcal{S} \mathbf{F}^\top \right), \quad \mathbb{J}^{\bar{\theta}\bar{m}}[\eta_m] = -\frac{\theta}{C_V} \nabla \eta_m : \frac{\partial_{\mathbf{F}} \mathcal{S}_\theta \mathbf{F}^{-\top}}{V}$$

by exploiting Piola's identity  $\bar{\nabla} \cdot (\bar{V} \bar{\mathbf{F}}^{-\top}) = \mathbf{0}$  as well as the transformation rule  $(\bar{\nabla} \cdot \bar{\mathbf{A}}) \bar{\mathbf{F}}^{-\top} = \nabla \cdot (\bar{\mathbf{A}} \circ \alpha)$  for any  $\bar{\mathbf{A}} \in \mathbb{R}^{d \times d}$ .

Similarly, we obtain or the Onsager operator

$$\mathbb{K}(\mathbf{q}) = \text{DT}_{\text{LE}}(\bar{\mathbf{q}}) \bar{\mathbb{K}}(\bar{\mathbf{q}}) \text{DT}_{\text{LE}}^*(\bar{\mathbf{q}}) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \mathbb{K}_{mm}(\mathbf{q}) & 0 & \mathbb{K}_{m\theta}(\mathbf{q}) \\ 0 & 0 & \mathbb{K}_{cc}(\mathbf{q}) & 0 \\ 0 & \mathbb{K}_{\theta m}(\mathbf{q}) & 0 & \mathbb{K}_{\theta\theta}(\mathbf{q}) \end{pmatrix}, \quad (32a)$$

where the entries have been transformed to

$$\mathbb{K}_{mm}(\mathbf{q}) \eta_m = -\nabla \cdot [\theta \mathbf{\Lambda}(\mathbf{q}) \nabla_s \eta_m], \quad (32b)$$

$$\mathbb{K}_{m\theta}(\mathbf{q}) \eta_\theta = \nabla \cdot \left[ \theta \mathbf{\Lambda}(\mathbf{q}) \frac{\eta_\theta}{C_V} \nabla_s \nu \right], \quad (32c)$$

$$\mathbb{K}_{cc}(\mathbf{q}) \eta_c = -\nabla \cdot (\mathbb{M}(\mathbf{q}) \eta_c), \quad (32d)$$

$$\mathbb{K}_{\theta m}(\mathbf{q}) \eta_m = -\frac{\theta}{C_V} \nabla_s \nu : \mathbf{\Lambda}(\mathbf{q}) : \frac{\eta_\theta}{C_V} \nabla_s \eta_m, \quad (32e)$$

$$\mathbb{K}_{\theta\theta}(\mathbf{q}) \eta_\theta = \frac{\theta}{C_V} \nabla_s \nu : \mathbf{\Lambda}(\mathbf{q}) : \nabla_s \nu - \frac{1}{C_V} \nabla \cdot \left( k_{\text{heat}}(\mathbf{q}) \theta^2 \nabla \frac{\eta_\theta}{C_V} \right). \quad (32f)$$

It can be readily checked that the NIC are satisfied and thus the transformation has led to a GENERIC quintuple  $(\mathcal{Q}, \mathcal{E}, \mathcal{S}, \mathbb{J}, \mathbb{K})$  in the Eulerian frame. We obtain the evolution by replacing  $\eta$  in (32) with  $\eta = \text{D}\mathcal{S}[\mathbf{q}]$  from (29b) and correspondingly let  $\text{D}\mathcal{E}[\mathbf{q}]$  from (29a) act on the Poisson structure (31). This leads to PDE system

$$\partial_t \alpha + (\nabla \alpha) \nu = \mathbf{0}, \quad (33a)$$

$$\partial_t \mathbf{m} + \nabla \cdot (\mathbf{m} \otimes \nu) = \nabla \cdot (\sigma^{\text{el}} + \sigma^{\text{vi}}), \quad (33b)$$

$$\partial_t \mathbf{c} + \nabla \cdot (\mathbf{c} \otimes \nu) = -\nabla \cdot (\mathbb{M} \partial_{\bar{\mathbf{c}}} \bar{\mathcal{S}}), \quad (33c)$$

$$C_V (\partial_t \theta + \nu \cdot \nabla \theta) = -\theta \nabla \nu : \partial_{\mathbf{F}} \mathcal{S} \frac{\mathbf{F}^{-\top}}{V} + \nabla_s \nu : \sigma^{\text{vi}} + \nabla \cdot (k_{\text{heat}} \nabla \theta), \quad (33d)$$

$$\text{with } \sigma^{\text{el}} = \partial_{\mathbf{F}} (\mathcal{U} - \theta \bar{\mathcal{S}}) \mathbf{F}^\top V^{-1} \text{ and } \sigma^{\text{vi}} = \mathbf{\Lambda} : \nabla_s \nu. \quad (33e)$$

where the viscous contribution to the Cauchy stress is generated by  $\sigma^{\text{vi}} = \mathbb{K}_{m\theta}(\mathbf{q}) \eta_\theta$  with  $\eta_\theta = C_V / \theta$ . In order to obtain (33b) some non-trivial computations are involved, which we explain in the following. For this, we look more detailed at the terms that arise by the computation of the second component  $(\mathbb{J}(\mathbf{q}) \text{D}\mathcal{E}[\mathbf{q}])_2$  with  $\text{D}\mathcal{E}[\mathbf{q}]$  from (29a) and the Poisson operator  $\mathbb{J}(\mathbf{q})$  from (31). In particular, it is

$$\begin{aligned} & (\mathbb{J}(\mathbf{q}) \text{D}\mathcal{E}[\mathbf{q}])_2 \\ &= \left( \nabla \alpha^\top \partial_\alpha \left( \frac{|\mathbf{m}|^2}{2\varrho} \right) - \left( \nabla \frac{\mathbf{m}}{\varrho} \right)^\top \mathbf{m} - \nabla \cdot \left( \mathbf{m} \otimes \frac{\mathbf{m}}{\varrho} \right) + \left( \nabla \frac{|\mathbf{m}|^2}{2\varrho^2} \mathbf{M} \right)^\top \mathbf{c} \right) \\ &+ \left( \mathbf{F}^{-\top} \text{D}_\alpha \frac{\mathcal{U}}{V} - \nabla (\partial_{\bar{\mathbf{c}}} \mathcal{U})^\top \mathbf{c} + \frac{\partial_\theta \mathcal{U}}{V} \nabla \theta - \nabla \cdot \left( \frac{\theta \partial_\theta \mathcal{U}}{C_V} \frac{\partial_{\mathbf{F}} \mathcal{S}}{V} \mathbf{F}^\top \right) \right), \end{aligned} \quad (34)$$

where we have used that  $\nu = \mathbf{m} / \varrho$  as well as  $\nabla \alpha = \mathbf{F}^{-1}$ . We will verify now that the first term on the right-hand side of (34) gives the transport term  $\nabla \cdot (\mathbf{m} \otimes \nu)$  in the momentum balance (33b) and that the second term on the right-hand side of (34) results in the elastic part  $\sigma^{\text{el}}$  of the Cauchy stress given in (33e).

Indeed, from the first term on the right-hand side of (34) we calculate the transport term  $\nabla \cdot (\mathbf{m} \otimes \boldsymbol{\nu})$  as follows:

$$\begin{aligned} & \nabla \alpha^\top \partial_\alpha \left( \frac{|\mathbf{m}|^2}{2\varrho} \right) - \left( \nabla \frac{\mathbf{m}}{\varrho} \right)^\top \mathbf{m} - \nabla \cdot \left( \mathbf{m} \otimes \frac{\mathbf{m}}{\varrho} \right) + \left( \nabla \frac{|\mathbf{m}|^2}{2\varrho^2} M \right)^\top \mathbf{c} \\ &= -\frac{\mathbf{F}^\top}{V} \frac{|\mathbf{m}|^2}{2\varrho^2} \partial_\alpha \bar{\varrho}_0 + \nabla \left( \frac{\mathbf{m}}{\varrho} \right)^\top \frac{\mathbf{m}}{\varrho} \frac{\bar{\varrho}_0}{V} + \frac{\mathbf{F}^\top}{V} \frac{|\mathbf{m}|^2}{2\varrho^2} \partial_\alpha \bar{\varrho}_0 \\ & \quad - \left( \nabla \frac{\mathbf{m}}{\varrho} \right)^\top \mathbf{m} - \nabla \cdot \left( \mathbf{m} \otimes \frac{\mathbf{m}}{\varrho} \right) + \left( \nabla \frac{\mathbf{m}}{\varrho} \right)^\top \frac{\mathbf{m}}{\varrho} (M \cdot \mathbf{c}) = -\nabla \cdot (\mathbf{m} \otimes \boldsymbol{\nu}), \end{aligned}$$

which then moves with minus to the left-hand side of (33b). In the calculation above we have used Piola's identity in Eulerian coordinates  $\nabla \cdot (\mathbf{F}^\top V^{-1}) = \mathbf{0}$ , the definition of  $\varrho$  and the relation  $\boldsymbol{\nu} = \mathbf{m}\varrho^{-1}$ .

To see that the elastic part  $\boldsymbol{\sigma}^{\text{el}}$  of the Cauchy stress in (33b) arises from the second term on the right-hand side of (34) we calculate

$$\begin{aligned} & \mathbf{F}^{-\top} D_\alpha \frac{\bar{\mathcal{U}}}{V} - \nabla (\partial_{\bar{\mathbf{c}}} \bar{\mathcal{U}})^\top \mathbf{c} + \frac{\partial_\theta \bar{\mathcal{U}}}{V} \nabla \theta - \nabla \cdot \left( \frac{\theta \partial_\theta \bar{\mathcal{U}}}{\bar{C}_V} \frac{\partial_{\mathbf{F}} \bar{\mathcal{S}}}{V} \mathbf{F}^\top \right) \\ & \quad - \sum_k \mathbf{c}_k \nabla \partial_{\bar{\mathbf{c}}_k} \bar{\mathcal{U}} + \frac{\partial_\theta \bar{\mathcal{U}}}{V} \nabla \theta - \nabla \cdot \left( \theta \frac{\partial_{\mathbf{F}} \bar{\mathcal{S}}}{V} \mathbf{F}^\top \right) \\ &= \mathbf{F}^{-\top} \frac{\partial_\alpha \bar{\mathcal{U}}}{V} + \nabla \cdot \left( \frac{\partial_{\mathbf{F}} \bar{\mathcal{U}}}{V} \mathbf{F}^\top \right) + \sum_{i,j} \frac{\partial_{\mathbf{F}_{ij}} \bar{\mathcal{U}}}{V} \nabla \mathbf{F}_{ij} + \sum_k \frac{\nabla (\partial_{\bar{\mathbf{c}}_k} \bar{\mathcal{U}} \mathbf{c}_k V)}{V} - \frac{\nabla \bar{\mathcal{U}}}{V} \\ & \quad - \sum_k \mathbf{c}_k \nabla \partial_{\bar{\mathbf{c}}_k} \bar{\mathcal{U}} + \frac{\partial_\theta \bar{\mathcal{U}}}{V} \nabla \theta - \nabla \cdot \left( \theta \frac{\partial_{\mathbf{F}} \bar{\mathcal{S}}}{V} \mathbf{F}^\top \right) \\ &= \nabla \cdot \left( \partial_{\mathbf{F}} (\bar{\mathcal{U}} - \theta \bar{\mathcal{S}}) \mathbf{F}^\top V^{-1} \right) = \nabla \cdot \boldsymbol{\sigma}^{\text{el}}. \end{aligned}$$

Above, we explicitly computed  $D_\alpha \bar{\mathcal{U}}$  and exploited  $\partial_\theta \bar{\mathcal{U}} = \bar{C}_V$ . We have also repeatedly used the Piola's identity in Eulerian coordinates  $\nabla \cdot (\mathbf{F}^\top V^{-1}) = \mathbf{0}$ , and collect all terms that are generated by  $V^{-1} \nabla \bar{\mathcal{U}}$ .

### 3.3 Damped Hamiltonian limit

The GENERIC formalism was introduced to describe isolated systems, i.e., systems with no exchange of mass or energy with the surroundings. Yet, the geometric structures and thermodynamic potentials presented here can be adapted to the case of closed system, i.e., systems that exchange heat/energy but no mass with the surroundings. Following the work of Mielke [38] we show that a damped Hamiltonian system arises by coupling the GENERIC system with a heat bath and in particular that the corresponding evolution equation has a similar structure as the GENERIC evolution equation (12).

To do so, we consider a GENERIC quintuple  $(\mathcal{Q}, \mathcal{E}, \mathcal{S}, \mathbb{J}, \mathbb{K})$  and we split the state vector in order to highlight the thermodynamic variable in last position  $\mathbf{q}_z = (\mathbf{w}, z)$ , where  $z \in \{e, s, \theta\}$  is a placeholder for the total energy  $e$ , the total entropy  $s$  or the temperature  $\theta$  while  $\mathbf{w}$  collects all remaining variables; cf. (27) where  $\mathbf{w} = (\boldsymbol{\alpha}, \mathbf{m}, \mathbf{c})$  and  $z = \theta$ . We highlight that for  $z = e$ , resp.  $z = s$ , the total energy, resp. entropy, of the system is simply  $\mathcal{E}_e(\mathbf{q}_e) := \int_\Omega e \, dx$ , resp.  $\mathcal{S}_s(\mathbf{q}_s) := \int_\Omega s \, dx$ , which produces the driving force

$$D\mathcal{E}_e(\mathbf{q}_e) = (0, 1)^\top, \quad \text{resp. } D\mathcal{S}_s(\mathbf{q}_s) = (0, 1)^\top.$$

This choice of thermodynamic variables simplifies the implementation of the non-interaction conditions (9a),  $\mathbb{J}_s(\mathbf{q}_s) D\mathcal{S}_s(\mathbf{q}_s) \equiv 0$ ,  $\mathbb{K}_e(\mathbf{q}_e) D\mathcal{E}_e(\mathbf{q}_e) \equiv 0$ . This can be ensured by the two geometric operators  $\mathbb{J}_s = \begin{pmatrix} \mathbb{J}_{\mathbf{w}\mathbf{w}} & \mathbb{J}_{\mathbf{w}s} \\ \mathbb{J}_{s\mathbf{w}} & 0 \end{pmatrix}$  and  $\mathbb{K}_e = \begin{pmatrix} \mathbb{K}_{\mathbf{w}\mathbf{w}} & \mathbb{K}_{\mathbf{w}e} \\ \mathbb{K}_{e\mathbf{w}} & \mathbb{K}_{ee} \end{pmatrix}$ , where the off-diagonal entries are a combination of first and second order differential operators and the entry  $\mathbb{K}_{ee}$  relates to heat conduction processes, cf. (32f). We refer to [66] for more examples.



For  $z \in \{e, s\}$ , we now consider the two transformations

$$T_z : \mathcal{Q}_z \rightarrow \mathcal{Q}_\theta, \quad \mathbf{q}_z = (\mathbf{w}, z) \mapsto \mathbf{q} = \mathbf{q}_\theta = (\mathbf{w}, \theta),$$

that map the total energy and total entropy to the temperature. Similarly to (30a) and (30c), their Fréchet derivatives  $DT_z(\mathbf{q}) = \mathbb{L}_z(\mathbf{q})$  and adjoints  $\mathbb{L}_z^*(\mathbf{q})$  are given by

$$\mathbb{L}_z(\mathbf{q}) = DT_z(\mathbf{q}) := \begin{pmatrix} \mathbb{L}_w & 0 \\ D_w z(\mathbf{q}) & \partial_\theta z(\mathbf{q}) \end{pmatrix}^{-1} = \begin{pmatrix} \mathbb{L}_w & 0 \\ -D_w z(\mathbf{q})/\partial_\theta z(\mathbf{q}) & 1/\partial_\theta z(\mathbf{q}) \end{pmatrix}, \quad (35)$$

$$\mathbb{L}_z^*(\mathbf{q}) = DT_z^*(\mathbf{q}) := \begin{pmatrix} \mathbb{L}_w & -D_w^* z(\mathbf{q})/\partial_\theta z(\mathbf{q}) \\ 0 & 1/\partial_\theta z(\mathbf{q}) \end{pmatrix}. \quad (36)$$

Here, in contrast to (30a) and (30c), we have represented these operators in terms of the variables of the image  $\mathbf{q} = \mathbf{q}_\theta$ . Given a GENERIC system written in terms of  $\mathbf{q} = \mathbf{q}_\theta$ , we consider the closure conditions (14) applied to the GENERIC evolution equation

$$\partial_t \mathbf{q} = \mathbb{L}_s(\mathbf{q}) \mathbb{J}_s(\mathbf{q}) \mathbb{L}_s^*(\mathbf{q}) D\mathcal{E}(\mathbf{q}) + \mathbb{L}_e(\mathbf{q}) \mathbb{K}_e(\mathbf{q}) \mathbb{L}_e^*(\mathbf{q}) D\mathcal{S}(\mathbf{q}), \quad (37)$$

By applying the adjoint  $DT_z^*$  to the driving forces, one can see that, for the remaining variables  $\mathbf{w}$  the Helmholtz free energy and the Massieu potential are the thermodynamic driving potentials:

$$DT_s^*(\mathbf{q}) D\mathcal{E}[\mathbf{q}] = \begin{pmatrix} D_w \mathcal{E}[\mathbf{q}] - \frac{\partial_\theta \mathcal{E}}{\partial_\theta \mathcal{S}} D_w \mathcal{S}[\mathbf{q}] \\ \frac{\partial_\theta \mathcal{E}}{\partial_\theta \mathcal{S}}[\mathbf{q}] \end{pmatrix}, \quad (38a)$$

$$DT_e^*(\mathbf{q}) D\mathcal{S}[\mathbf{q}] = \begin{pmatrix} D_w \mathcal{S}[\mathbf{q}] - \frac{\partial_\theta \mathcal{S}}{\partial_\theta \mathcal{E}} D_w \mathcal{E}[\mathbf{q}] \\ \frac{\partial_\theta \mathcal{S}}{\partial_\theta \mathcal{E}}[\mathbf{q}] \end{pmatrix}. \quad (38b)$$

In fact, we recall that the *Gibbs relation* implies  $\partial_\theta \mathcal{E}/\partial_\theta \mathcal{S} = \theta$  and that the Helmholtz free energy is obtained from a Legendre transformation of the total energy resulting in the densities  $\mathcal{F} = \mathcal{E} - \theta \mathcal{S}$ . Hence, the first entry of (38a) can be interpreted as the derivative of the Helmholtz free energy density  $\mathcal{F}$  with respect to  $\mathbf{w}$ , while equation (38b) presents the derivative of the so-called Massieu potential  $\mathcal{M} = -\theta^{-1} \mathcal{F} = \mathcal{S} - \theta^{-1} \mathcal{E}$ . Overall, equation (37) can be rewritten as:

$$\begin{pmatrix} \partial_t \mathbf{w} \\ \partial_t \theta \end{pmatrix} = \begin{pmatrix} -\frac{D_w \mathcal{S}}{\partial_\theta \mathcal{S}} \mathbb{J}_{ww} + \frac{\mathbb{J}_{Sw}}{\partial_\theta \mathcal{S}} & -\frac{D_w \mathcal{S}}{\partial_\theta \mathcal{S}} \mathbb{J}_{wS} \\ \frac{\mathbb{K}_{ww}}{\partial_\theta \mathcal{E}} + \frac{\mathbb{K}_{ew}}{\partial_\theta \mathcal{E}} & -\frac{D_w \mathcal{E}}{\partial_\theta \mathcal{E}} \mathbb{K}_{we} + \frac{\mathbb{K}_{ee}}{\partial_\theta \mathcal{E}} \end{pmatrix} \begin{pmatrix} D_w \mathcal{F} \\ \theta \end{pmatrix} + \begin{pmatrix} \frac{\mathbb{K}_{ww}}{\partial_\theta \mathcal{E}} + \frac{\mathbb{K}_{ew}}{\partial_\theta \mathcal{E}} & -\frac{D_w \mathcal{E}}{\partial_\theta \mathcal{E}} \mathbb{K}_{we} + \frac{\mathbb{K}_{ee}}{\partial_\theta \mathcal{E}} \end{pmatrix} \begin{pmatrix} -D_w \mathcal{F}/\theta \\ 1/\theta \end{pmatrix}. \quad (39)$$

Observe that the operators so derived do not satisfy the properties required for a Poisson structure  $\mathbb{J}$  or an Onsager operator  $\mathbb{K}$ . We further assume that the system is in thermal equilibrium, i.e.  $\theta \equiv \theta^* \in (0, \infty)$ . This procedure can be done in different ways: by adding a further dissipative contribution to the operators, see [38], by coupling the system with an external heat bath resulting in independent evolution on the boundary, see [59], or by considering a two-phase system with one phase being a thermal source, see [65]. By solely focusing on the evolution of  $\mathbf{w}$ , we obtain the following

$$\partial_t \mathbf{w} = \left( \mathbb{J}_{ww}(\mathbf{w}, \theta^*) - \frac{1}{\theta^*} \mathbb{K}_{ww}(\mathbf{w}, \theta^*) \right) D_w \mathcal{F}(\mathbf{w}, \theta^*), \quad (40)$$

where  $\theta^*$  plays the role of an external parameter. Observe that in this case  $\mathbb{J}_{ww}$  is again skew-symmetric and satisfies the Jacobi's identity and  $\mathbb{K}_{ww}$  is symmetric and positively semidefinite, which would allow us to identify once more  $\mathbb{J}_{ww}$  with the conservative and  $\mathbb{K}_{ww}$  with the dissipative dynamics. The symmetry and skew-symmetry properties are still valid since  $\mathbb{K}_{ww}$  and  $\mathbb{J}_{ww}$  are principal minors of  $\mathbb{K}$  and  $\mathbb{J}$ . The Jacobi's identity is satisfied in view of [42, Prop. A.1] and the positive semidefiniteness thanks to Sylvester's criterion, see e.g. [27, Thm. 7.2.5].

## 4 Eulerian diffusion and finite strain in a multiphase system

We dedicate this section to introduce a weak formulation of (40) based on the definition of suitable bilinear forms derived from the operators  $\mathbb{J}$  and  $\mathbb{K}$  previously discussed. Additionally, we provide a numerical example inspired by the theory of fluid-structure interaction (FSI) problems to highlight the benefits of this variational framework. In the spirit of [10] or [21], for example, this construction has the goal to construct a class of structure-preserving schemes.

**Weak form of damped Hamiltonian systems.** Based on previous work [53, 58], we can reformulate a damped Hamiltonian evolution, i.e. (40), for the state variable  $\mathbf{q} : [0, T] \rightarrow \mathcal{Q}$  and the free energy  $\mathcal{F}$

$$\partial_t \mathbf{q} = (\mathbb{J}(\mathbf{q}) - \mathbb{K}(\mathbf{q})) \mathbb{D}\mathcal{F}(\mathbf{q}), \quad (41)$$

as a saddle-point problem. Therefore, we introduce variables  $\boldsymbol{\eta} = (\eta_\alpha, \eta_m, \eta_c) \in \mathcal{V}$  and an operator  $\mathbb{B} : \mathcal{Q} \rightarrow \mathcal{V}^*$  such that for every  $\mathbf{q} \in \mathcal{Q}$  we find  $\boldsymbol{\eta} \in \mathcal{V}$  such that  $\mathbb{B}^* \boldsymbol{\eta} = \mathbb{D}\mathcal{F}(\mathbf{q}) \in \mathcal{Q}^*$ . Multiplying (41) with  $\mathbb{B}$  from the left and inserting  $\boldsymbol{\eta}$  then results in the operator equation in saddle-point form

$$\mathbb{A}(\mathbf{q}) \boldsymbol{\eta} - \mathbb{B} \partial_t \mathbf{q} = 0, \quad (42a)$$

$$\mathbb{B}^* \boldsymbol{\eta} = \mathbb{D}\mathcal{F}(\mathbf{q}), \quad (42b)$$

which holds in  $\mathcal{V}^* \times \mathcal{Q}^*$  and where  $\mathbb{A}(\mathbf{q}) = \mathbb{B}[\mathbb{J}(\mathbf{q}) - \mathbb{K}(\mathbf{q})] \mathbb{B}^* : \mathcal{V} \rightarrow \mathcal{V}^*$ . This operator equation is equivalent to  $\partial_t \mathbf{q}$  and  $\boldsymbol{\eta}$  being a stationary points of the functional

$$\mathcal{R}(\cdot, \cdot; \mathbf{q}) : \mathcal{V}^* \times \mathcal{Q}^* \rightarrow \mathbb{R}, \quad \mathcal{R}(\mathbf{v}, \boldsymbol{\xi}; \mathbf{q}) = -\frac{1}{2} \langle \mathbb{A}(\mathbf{q}) \boldsymbol{\eta}, \boldsymbol{\eta} \rangle_{\mathcal{V}} + \langle \mathbb{B} \mathbf{v}, \boldsymbol{\eta} \rangle_{\mathcal{V}} + \langle \mathbb{D}\mathcal{F}(\mathbf{q}), \mathbf{v} \rangle_{\mathcal{Q}}$$

with respect to  $\mathbf{v}, \boldsymbol{\xi}$  for given  $\mathbf{q}$ . In [53] we show how the operators need to be chosen for an Eulerian approach to nonlinear elasticity that is generated from a corresponding Lagrangian model. Furthermore, in [66] a similar construction is presented for compressible flows with diffusion and reactions. Similar structures have been analysed in the context of poroelasticity [21].

**Free energy and bilinear forms.** As an example we consider here the dynamics  $\mathbf{q} : [0, T] \rightarrow \mathcal{Q}$  of a compressible isothermal multiphase system with state variables

$$\mathbf{q} = \begin{pmatrix} \boldsymbol{\alpha} : \Omega \rightarrow \mathbb{R}^d \\ \mathbf{m} : \Omega \rightarrow \mathbb{R}^d \\ \mathbf{c} : \Omega \rightarrow \mathbb{R}^N \end{pmatrix} \in \mathcal{Q}; \quad (43)$$

lateron, in the numerical example we set  $d = 2$  and  $N = 1$ . We showcase an Eulerian formulation of nonlinear elasticity in a multiphase setting coupled to diffusion. The multiphase character is introduced by a Lagrangian indicator function

$$\bar{\iota}_0(\bar{x}) = \begin{cases} 1 & \text{if } x \in \Omega_s, \\ 0 & \text{if } x \in \Omega_l, \end{cases} \quad (44)$$

where  $\bar{\Omega} = \bar{\Omega}_s \cup \bar{\Omega}_l$  is built from the mutually disjoint solid and liquid phase. Similarly, we use  $\bar{\iota}_\varepsilon : \bar{\Omega} \rightarrow [0, 1]$  a smooth approximation of  $\bar{\iota}_0$  as  $\varepsilon \rightarrow 0$ , see Figure 3. Note that if  $\bar{\iota}_\varepsilon$  can be expressed explicitly, then  $\iota_\varepsilon$  can also be written explicitly as its composition with  $\boldsymbol{\alpha}$ . Consequently, derivatives of  $\iota_\varepsilon$  with respect to  $x, t$  and also  $\boldsymbol{\alpha}$  can be computed explicitly. The Eulerian indicator function  $\iota_\varepsilon := \bar{\iota}_\varepsilon \circ \boldsymbol{\alpha}$  satisfies a continuity equation  $\partial_t \iota_\varepsilon + \boldsymbol{\nu} \cdot \nabla \iota_\varepsilon = 0$ . One major advantage of the reference map is that we can explicitly express the time and space dependence of material parameters  $p_s, p_l \in \mathbb{R}$  of the solid or liquid phase via the smoothed indicator function by

$$p_\varepsilon(t, x) = p_s \bar{\iota}_\varepsilon(\boldsymbol{\alpha}(t, x)) + p_l (1 - \bar{\iota}_\varepsilon(\boldsymbol{\alpha}(t, x))), \quad (45)$$

which can also be simply expressed as  $p_\varepsilon = p_s \iota_\varepsilon + p_l (1 - \iota_\varepsilon)$ . More generally, any spatial heterogeneity in the Lagrangian frame can be explicitly represented by composition with the reference map  $\boldsymbol{\alpha}$ . For this example, we

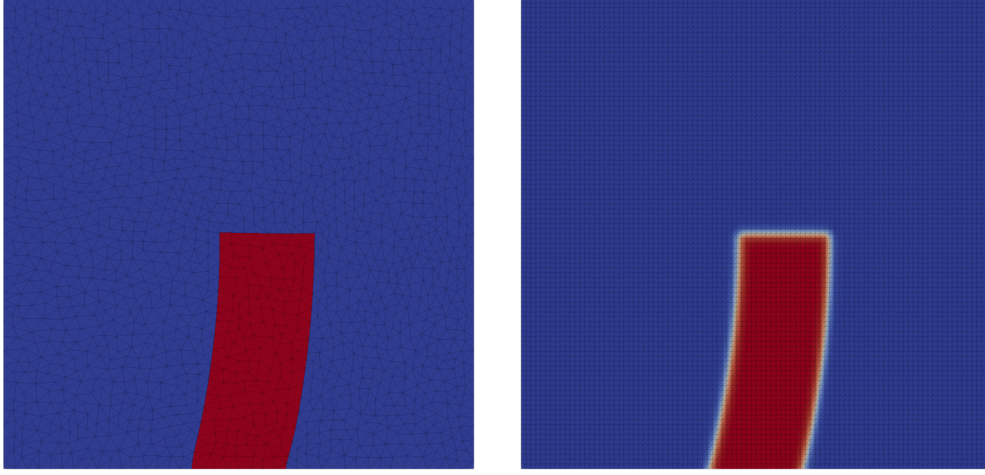


Figure 3: (left) transformed sharp indicator  $\iota_0 = \bar{\iota}_0 \circ \alpha$  on deformed mesh with initial displacement  $\bar{\mathbf{u}}(t = 0, \bar{x}, \bar{y}) = \bar{x}\bar{y}(1 - \bar{x})(1 - \bar{y})$  and corresponding diffuse indicator  $\iota_\varepsilon$  for  $\varepsilon = 10^{-2}$  on a domain  $\Omega = \bar{\Omega} = [0, 1]^2$  with solid  $\bar{\Omega}_s = [0.4, 0.6] \times [0, 0.5]$  (red) and liquid  $\bar{\Omega}_l = \bar{\Omega} \setminus \Omega_s$  (blue).

use the subscript  $\varepsilon$  to indicate the interpolation of two material parameters  $(p_s, p_l)$  via the smoothed indicator and the return map for general tuples of real-valued parameters.

This allows us to write the Eulerian energy of the isothermal system as

$$\mathcal{F}(\mathbf{q}) = \int_{\Omega} \frac{|\mathbf{m}|^2}{2\rho_\varepsilon} + \mathcal{F}_\varepsilon[\mathbf{q}] \, dx, \quad \mathcal{F}_\varepsilon[\mathbf{q}] = \mathcal{F}_\varepsilon^{\text{mech}}(\mathbf{F}_{\text{iso}}) + \mathcal{F}_\varepsilon^{\text{int}}(\mathbf{c}), \quad (46a)$$

and, following (45), we define the mass density as

$$\rho_\varepsilon(t, x) = V(t, x)^{-1} (\bar{\rho}_s \bar{\iota}_\varepsilon(\alpha(t, x)) + \bar{\rho}_l (1 - \bar{\iota}_\varepsilon(\alpha(t, x)))) \quad (46b)$$

with referential mass densities  $\bar{\rho}_s, \bar{\rho}_l \in (0, \infty)$ . Similarly, we use an elastic energy

$$\mathcal{F}_\varepsilon^{\text{mech}}(\mathbf{F}_{\text{iso}}) = \frac{1}{V} \left[ \frac{G_\varepsilon}{2} \text{tr}(\mathbb{C}_{\text{iso}} - \mathbb{I}) + \frac{K_\varepsilon}{2} (V - 1)^2 \right], \quad (46c)$$

$$\mathcal{F}_\varepsilon^{\text{int}}(\mathbf{c}) = k_\varepsilon \mathbf{c} \left( \log \left( \frac{\mathbf{c}}{\mathbf{c}_{\text{ref}, \varepsilon}} \right) - 1 \right), \quad (46d)$$

with the deformation gradient  $\mathbf{F} = \nabla \alpha^{-1}$ , its Jacobian  $V = \det \mathbf{F}$  and the isochoric part  $\mathbf{F}_{\text{iso}} = V^{-1/d} \mathbf{F}$ . Furthermore,  $\mathbb{C}_{\text{iso}} = \mathbf{F}_{\text{iso}}^T \mathbf{F}_{\text{iso}}$  denotes the isochoric part of the right Cauchy-Green tensor  $G_\varepsilon = G_s \iota_\varepsilon + G_l (1 - \iota_\varepsilon)$  captures the energy due to distortion of the solid or liquid phase,  $K_\varepsilon = K_s \iota_\varepsilon + K_l (1 - \iota_\varepsilon)$  encodes compressibility and  $k_\varepsilon = k_s \iota_\varepsilon + k_l (1 - \iota_\varepsilon)$  encodes the contribution of  $\mathbf{c}$  to the heat capacity. Note, when calculating  $D\mathcal{F}$ , then the derivatives of functions such as  $\rho_\varepsilon$  with respect to  $\alpha$  need to be taken fully into account to produce a consistent force balance. This form of a saddle-point structure is suitable for numerical treatment, as by testing (42) directly translates into the weak form

$$\mathbf{a}(\boldsymbol{\eta}, \boldsymbol{\xi}; \mathbf{q}) - \mathbf{b}(\boldsymbol{\xi}, \partial_t \mathbf{q}) = 0, \quad (47a)$$

$$\mathbf{b}(\boldsymbol{\eta}, \mathbf{v}) = \langle D\mathcal{F}(\mathbf{q}), \mathbf{v} \rangle, \quad (47b)$$

where  $\mathbf{a}(\boldsymbol{\eta}, \boldsymbol{\xi}; \mathbf{q}) := \mathbf{j}(\boldsymbol{\eta}, \boldsymbol{\xi}; \mathbf{q}) - \mathbf{k}(\boldsymbol{\eta}, \boldsymbol{\xi}; \mathbf{q})$  with the skew-symmetric bilinear form  $\mathbf{j}(\boldsymbol{\eta}, \boldsymbol{\xi}; \mathbf{q}) = \langle \mathbb{B}\mathbb{J}(\mathbf{q}) \mathbb{B}^* \boldsymbol{\eta}, \boldsymbol{\xi} \rangle$  and  $\mathbf{k}(\boldsymbol{\eta}, \boldsymbol{\xi}; \mathbf{q}) := \langle \mathbb{B}\mathbb{K}(\mathbf{q}) \mathbb{B}^* \boldsymbol{\eta}, \boldsymbol{\xi} \rangle$  is a symmetric positive bilinear form. We have  $\mathbf{v} = (v_\alpha, v_m, v_c) \in \mathcal{Q}$ ,

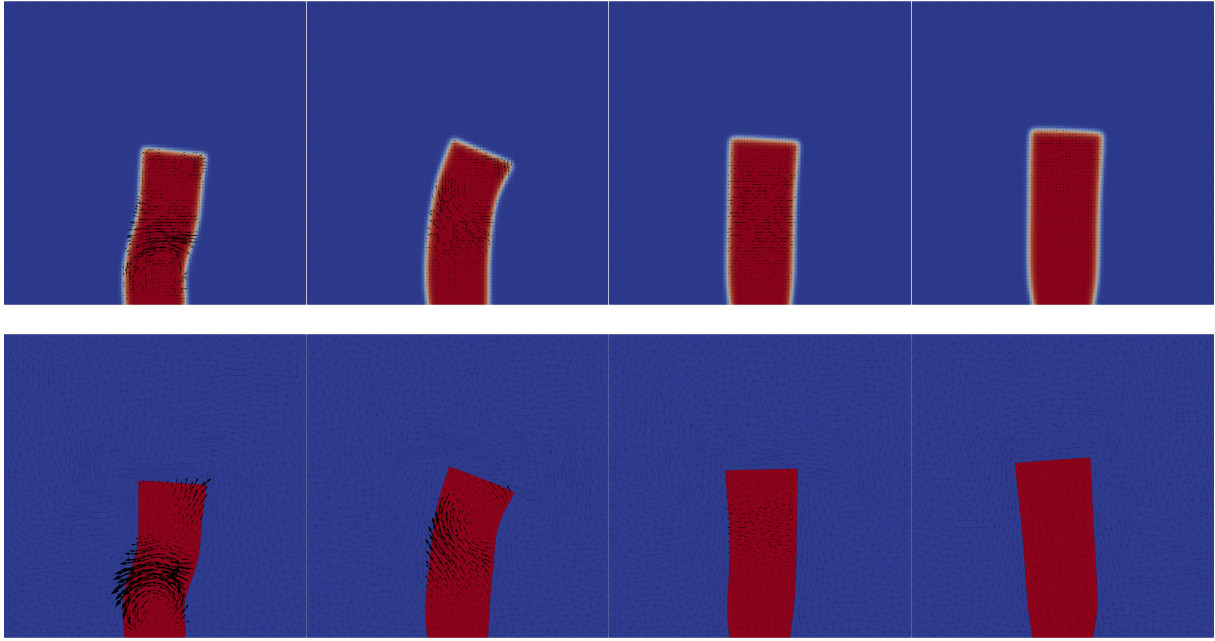


Figure 4: **(top row)** Eulerian solution of Equation (49) with parameters from Table 1 showing the indicator function  $\iota_\varepsilon$  (shading blue  $\iota_\varepsilon = 0$  and red  $\iota_\varepsilon = 1$ ) and momentum (black arrows) for different times increasing from left to right and **(bottom row)** Lagrangian solution with sharp indicator  $\iota_0$  on deformed mesh (shading) and momentum (black arrows) at the same times as in top row.

$\partial_t \mathbf{q} = (\partial_t \boldsymbol{\alpha}, \partial_t \mathbf{m}, \partial_t \mathbf{c}) \in \mathcal{Q}$  and  $\boldsymbol{\eta} = (\eta_\alpha, \eta_m, \eta_c) \in \mathcal{V}$  and  $\boldsymbol{\xi} = (\xi_\alpha, \xi_m, \xi_c) \in \mathcal{V}$ , where

$$j(\boldsymbol{\eta}, \boldsymbol{\xi}; \mathbf{q}) = \int_{\Omega} [\nabla \boldsymbol{\alpha}^T \xi_\alpha - \nabla \xi_m^T \mathbf{m}] \cdot \eta_m - [\nabla \boldsymbol{\alpha}^T \eta_\alpha - \nabla \eta_m^T \mathbf{m}] \cdot \xi_m + c [\nabla \xi_c \cdot \eta_m - \nabla \eta_c \cdot \xi_m] dx \quad (48a)$$

$$k(\boldsymbol{\eta}, \boldsymbol{\xi}; \mathbf{q}) = \int_{\Omega} \mu_\varepsilon \nabla_s \eta_m \cdot \nabla_s \xi_m + D_\varepsilon(\mathbf{c}) \nabla \eta_c \cdot \nabla \xi_c dx \quad (48b)$$

$$b(\boldsymbol{\eta}, \mathbf{v}) = \int_{\Omega} \eta_\alpha \cdot v_\alpha + \eta_m \cdot v_m + \eta_c \cdot v_c dx \quad (48c)$$

We note that the bilinear forms so introduced are consistent with the previous definition of reversible (31) and irreversible (32) operators after transformation to the isothermal system (40).

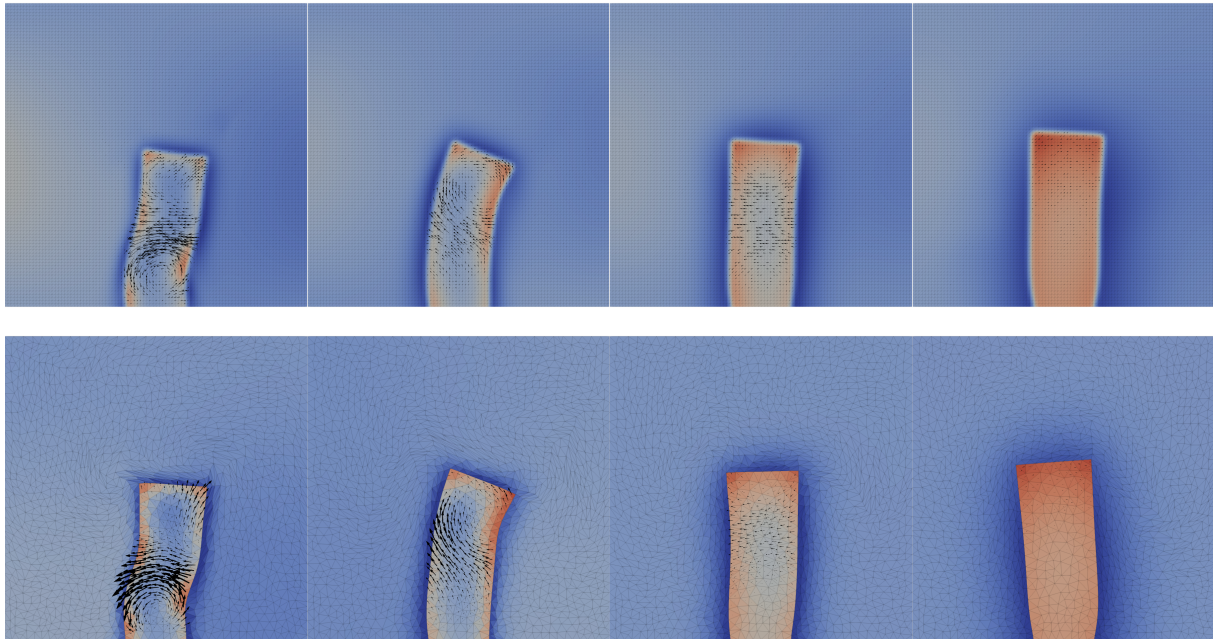


Figure 5: (**top row**) Eulerian solution of Equation (49) with parameters from Table 1 showing the concentration  $c$  (increasing from blue to red) and momentum (black arrows) for different times increasing from left to right and (**bottom row**) Lagrangian solution with concentration on deformed mesh (shading) and momentum (black arrows) at the same times.

**Numerical example.** This structure-preserving weak form is discretized in space using finite elements and in time with a semi-implicit scheme, where  $D\mathcal{F}$  is computed fully-implicit, whereas the dependence of  $\mathbf{a}$  on  $\boldsymbol{\eta}$  is treated implicitly and the dependence on the state  $\mathbf{q}$  is treated explicitly. Therefore, for given  $\mathbf{q}^{n-1}, \boldsymbol{\eta}^{n-1}$  we seek  $\mathbf{q}^n, \boldsymbol{\eta}^n$  such that

$$\mathbf{a}(\boldsymbol{\eta}^n, \boldsymbol{\xi}; \mathbf{q}^{n-1}) - \mathbf{b}(\boldsymbol{\xi}^n, \frac{1}{\tau}(\mathbf{q}^n - \mathbf{q}^{n-1})) = 0 \quad (49a)$$

$$\mathbf{b}(\boldsymbol{\eta}^n, \mathbf{v}) = \langle D\mathcal{F}(\mathbf{q}^n), \mathbf{v} \rangle, \quad (49b)$$

for all  $\mathbf{v}, \boldsymbol{\xi}$ . For this Eulerian formulation scalar and vectorial  $P_1$  finite elements are used throughout.

Parameter	$G_i$	$K_i$	$\mu_i$	$\bar{\varrho}_i$	$k_i$	$c_{\text{ref},i}$	$D_i$
fluid ( $i = f$ )	$10^{-4}$	1	$10^{-4}$	$10^{-2}$	1	1	$10^{-2}$
solid ( $i = s$ )	$10^1$	1	$10^{-4}$	$10^0$	1	2	$10^{-2}$

Table 1: Simulation parameters for fluid and solid phases for  $\bar{\Omega} = \Omega = [0, 1]^2$ ,  $\bar{\Omega}_s = [0.4, 0.6] \times [0, 0.5]$  and phase-indicator  $\bar{\iota}_\varepsilon$  with  $\varepsilon = 0.01$ .

Numerical solutions for this Eulerian formulation (49) based on the material parameters in Table 1 are compared with their Lagrangian counterparts in Figure 4 and Figure 5. We omit the Lagrangian formulation of the problem and refer instead to [53] for details. In the example shown in Figure 4 and the corresponding energies in Figure 6 one can observe an oscillatory motion of the system due to inertia. The aspect ratio of mass densities  $\bar{\varrho}_s : \bar{\varrho}_l = 100 : 1$  causes the momentum to be concentrated in the solid phase, i.e. the black arrows are mainly visible in the solid phase. Slight differences between Lagrangian and Eulerian solutions are due to the finite  $\varepsilon$  and rather large time steps. The oscillation ceases quite quickly due to the large viscosity in solid and liquid phase. Furthermore, Figure 6 clearly shows that during the evolution the (total) energy decreases whereas the solid phase expands significantly by almost 40%. To understand the expansion, one can assume a homogeneous state. In the solid phase, one can then use the stationary state variables as  $V(x) = V_s \in (0, \infty)$  and



$c(x) = c_s$ , while in the liquid phase, the state variables are  $V(x) = V_l \in (0, \infty)$  and  $c(x) = c_l$ . Importantly, the evolution conserves total concentration  $C$  and total volume  $V$ , which are expressed as

$$C = c_s V_s |\bar{\Omega}_s| + c_l V_l |\bar{\Omega}_l|, \quad V = V_s |\bar{\Omega}_s| + V_l |\bar{\Omega}_l| = 1. \quad (50)$$

This conservation property allows  $c_l$  and  $V_l$  to be expressed in terms of  $c_s$  and  $V_s$ . Consequently, the free energy of the homogeneous system can be written as a function of the two real parameters  $c_s$  and  $V_s$ . As shown in Figure 7, the free energy exhibits a minimum at  $c_s \approx c_{\text{ref},s} = 2$  and  $V_s \approx 2$  and explains the solids expansion.

The example above demonstrates that a thermodynamically consistent, unified formulation can be constructed for a multiphase system that allows for large deformations. The usage of the reference map  $\alpha$  allows to state the weak formulation of the nonlinear PDE in spatial (Eulerian) coordinates while retaining information about the reference configuration, which can be useful when Lagrangian material properties need to be accessed, e.g. via material indicator functions. However, for fluid flows with large distortion, it might be non-trivial to ensure the invertibility of  $\alpha$ , resp.  $\chi$ , and a more classical discretization of compressible flows in terms of density  $\varrho$  and momentum  $\mathbf{m}$  as the state variables might be more suitable.

By using Equation (47) together with the bilinear forms (48), a natural structure-preserving discretization is obtained that ensures thermodynamic consistency, although one needs to be careful in a multiphase setting to compute all derivatives with respect to the indicator functions  $\iota_\varepsilon = \bar{\iota}_\varepsilon \circ \alpha$  consistently. This can be an intricate process, which is best handled by discretization frameworks that support automatic differentiation of expressions and functionals, e.g. FEniCS [34]. Once such a formulation is available, multiphase and multiphysics problems, e.g. the coupling of multiphase flows and diffusion, can be discretized in space with relative ease via finite element methods.

The proposed structure introduces additional terms, which make the equations appear more complicated at first glance, and the usual structure of the momentum balance becomes only apparent after certain terms cancel. While this might imply additional complexity, it remains an open question whether these additional terms, which stem from structure preservation, could be beneficial for numerical stability.

## 5 Conclusions and summary

We presented a GENERIC quintuple  $(\mathcal{Q}, \mathcal{E}, \mathcal{S}, \mathbb{J}, \mathbb{K})$  for materials at large strain with diffusion processes in Eulerian coordinates, where the *reference* map  $\alpha(1)$  is used as the main variable governing the deformation. We also introduced the corresponding Lagrangian GENERIC system  $(\mathcal{Q}, \mathcal{E}, \mathcal{S}, \mathbb{J}, \mathbb{K})$  and showed its connection

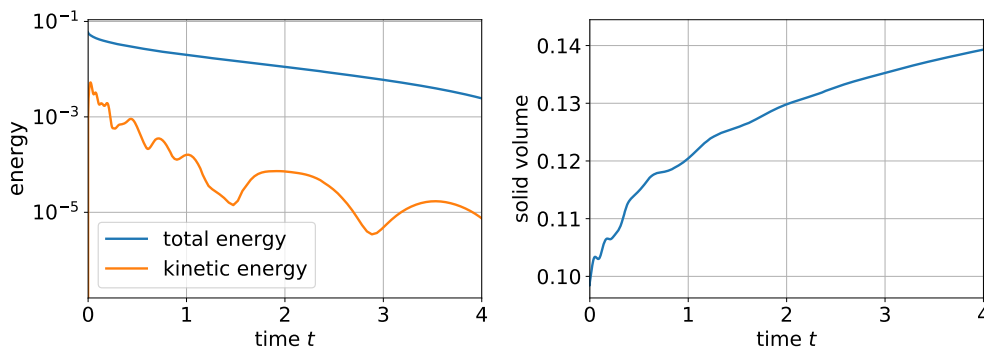


Figure 6: (left panel) Total energy  $\mathcal{F}(\mathbf{q}(t))$  (shifted by a constant) and kinetic energy  $\mathcal{K}(\mathbf{q}(t))$  and (right panel) solid volume  $\int_{\Omega} \iota_\varepsilon(t, x) dx$  as functions of time  $0 \leq t \leq 4$ . The solid domains  $\bar{\Omega}_s = \Omega_s(t=0) = [0.4, 0.6] \times [0, 0.5]$  initial volume is 0.1, which is well approximated by  $\iota_\varepsilon$ .

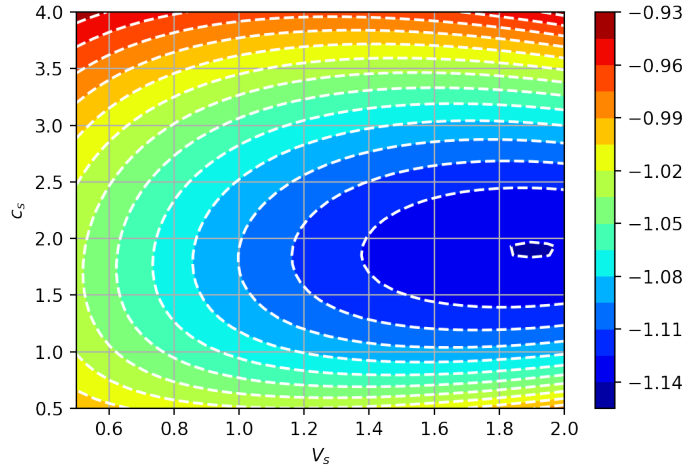


Figure 7: Contour plot of energy  $\mathcal{F}(\mathbf{q})$  as a function of an assumed homogeneous (constant in space) solid concentration  $c_s$  and volume  $V_s$  for parameters in Table 1. Also the liquid concentration  $c_l$  and volume  $V_l$  are assumed homogeneous and are determined from conservation laws.

to  $(\mathcal{Q}, \mathcal{E}, \mathcal{S}, \mathbb{J}, \mathbb{K})$  via a transformation mapping Lagrangian to Eulerian state variables  $T_{LE} : \bar{\mathcal{Q}} \rightarrow \mathcal{Q}$ . The thermodynamical functionals and geometric structures are then linked through a linearization of this map  $DT_{LE}(\bar{\mathbf{q}}) = \mathbb{L}(\bar{\mathbf{q}})$  and through the *closure conditions* (14). In order to systematically structure this approach we introduced kinematics and thermodynamics in the Eulerian and Lagrangian frame. Finally, we constructed a structure-preserving discretization based on a saddle-point structure relying on symmetry-preserving bilinear forms  $a = j - k$  with skew-symmetric  $j$  and symmetric positive  $k$ . We presented an example with fluid-structure interaction and diffusion based on indicator functions, which is similar to other contemporary methods for fluid-structure interaction that explicitly evolve level sets [57].

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