

## **GENERIC framework for reactive fluid flows**

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submitted: May 7, 2021

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No. 2841  
Berlin 2021



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2020 *Mathematics Subject Classification.* 37K58, 76M30, 35Q35, 80A32, 80M30.

*Key words and phrases.* Reactive compressible flow, thermomechanical modeling, GENERIC, Navier-Stokes fluid, Lagrangian-Eulerian coordinates.

M. Thomas and A. Zafferi acknowledge the funding by the DFG-Collaborative Research Centre 1114 *Scaling cascades in complex systems* project # 235221301 *Dynamics of rock dehydration on multiple scales*. D. Peschka gratefully acknowledges the financial support by DFG-Priority Programme 2171 *Dynamic Wetting of Flexible, Adaptive, and Switchable Substrates* via project # 422792530. Additionally, M. Thomas acknowledges the partial funding by the project AA2-9 *Variational Methods for Viscoelastic Flows and Gelation* within the Berlin Mathematics Research Center MATH<sup>+</sup>. The authors also thank the Einstein Foundation for funding the Thematic Einstein Semester *Energy-based mathematical methods for reactive multiphase flows* within MATH<sup>+</sup> that has led to many fruitful discussions on the topic of variational modeling, in particular with M. Liero, A. Mielke, V. Mehrmann, B. Wagner, L. Heltai, and M.H. Farshbaf Shaker.

Edited by  
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## Abstract

We describe reactive fluid flows in terms of the formalism *General Equation for Non-Equilibrium Reversible-Irreversible Coupling* also known as GENERIC. Together with the formalism, we present the thermodynamical and mechanical foundations for the treatment of fluid flows using continuous fields and present a clear relation and transformation between a Lagrangian and an Eulerian formulation of the corresponding systems of partial differential equations. We bring the abstract framework to life by providing many physically relevant examples for reactive compressive fluid flows.

## 1 Introduction

Fluid flows lead to many complex phenomena on a wide variety of length and time scales [5, 11, 14]. Sometimes, a purely mechanical description of these phenomena in terms of force and mass balances, and rheology may be sufficient. However, in many modern applications, additional mechanisms such as reactions, diffusion, and thermal effects, are of particular importance, and need to be taken into account together with the fluid flow. In corresponding mathematical descriptions, a clear separation of reversible and irreversible effects is important in order to satisfy the principles of thermodynamics and mechanics, i.e., the laws of thermodynamics and the conservation laws of continuum mechanics.

Besides the Navier-Stokes equations the Euler equations are probably the best known description of fluid flow. The latter are the equations of motion for an ideal fluid without any dissipative effects, so that its dynamics is reversible and the total energy of the system is conserved, while its entropy remains constant. The Euler equations form a Hamiltonian system [65, 20], which can be formulated in a geometric description via a Poisson bracket and a Hamiltonian energy functional. The Hamiltonian description for the flow of an ideal fluid in Eulerian coordinates is obtained from the canonical form of the Poisson bracket in Lagrangian coordinates using the mapping between both coordinate representations [64, 52].

Many other thermodynamic processes are entirely dissipative in the sense that they can be modeled using an overdamped evolution, i.e., there is a balance of friction and driving forces. These evolution laws, also known as Onsager systems [68, 16] or gradient flows [1, 59], ensure thermodynamic consistency in terms of entropy increase and the validity of Onsager's reciprocity relations [58]. Historically, in fluid mechanics, these structures emerged from the concept of dissipation introduced by Helmholtz [73], Rayleigh [67] and Korteweg [35]. Rigorous derivations of Onsager systems from microscopic statistical models [47] can, for example, be performed using large deviation principles for particle systems involving diffusion and reaction.

In addition to purely geometric descriptions of reversible Hamiltonian or dissipative Onsager processes, there exists a plethora of schools of nonequilibrium thermodynamics [37, 55] that offer different, but mostly compatible, views on the coupling of reversible and dissipative processes. Without claiming to be exhaustive, we mention here classical irreversible thermodynamics [58, 63, 15], rational

thermodynamics [10, 69], extended irreversible thermodynamics [31], rational extended thermodynamics [54], GENERIC [27, 28, 44, 61] or port-Hamiltonian systems [71, 53]. Additionally, for fluid dynamics standard continuum mechanics approaches [29, 36, 4] are complemented by an extensive literature on variational approaches for complex fluids [6, 30, 24, 23].

Here we follow the GENERIC approach [27, 28, 44, 61] in order to provide a variational structure for the models under consideration. GENERIC, the acronym for General Equations of Non-Equilibrium Reversible Irreversible Coupling, characterizes the evolution of a thermodynamical system in terms of a state space  $\bar{\mathcal{Q}}$ , thermodynamical potentials such as total energy  $\bar{\mathcal{E}}$  and entropy  $\bar{\mathcal{S}}$  functionals, and geometric structures  $\bar{\mathbb{J}}$  and  $\bar{\mathbb{K}}$  which encode the reversible (Hamiltonian) or irreversible (Onsager) nature of a process. The evolution of a state vector  $\bar{\mathbf{q}} : [0, T] \rightarrow \bar{\mathcal{Q}}$  describing the mechanical and thermodynamical properties of the system is then given by

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

Compatibility with the laws of thermodynamics is encoded in the properties of  $\bar{\mathbb{J}}$  and  $\bar{\mathbb{K}}$ , and in combination with the noninteraction conditions (NIC)  $\bar{\mathbb{K}}(\bar{\mathbf{q}}) D\bar{\mathcal{E}}(\bar{\mathbf{q}}) \equiv 0$  and  $\bar{\mathbb{J}}(\bar{\mathbf{q}}) D\bar{\mathcal{S}}(\bar{\mathbf{q}}) \equiv 0$ , which ensure conservation of the total energy and increase of the entropy for thermodynamically closed systems.

The aim of this work is to give a mathematically detailed and practically accessible presentation of the GENERIC formulation for reactive compressible flows in Lagrangian and Eulerian coordinates, and to investigate transformations  $T : \bar{\mathcal{Q}} \rightarrow \mathcal{Q}$  of GENERIC formulations between different sets of variables and coordinate systems by means of invertible and noninvertible transformations, i.e., change of variables, change of coordinates, reductions, and extensions. A central theme of this work is the approach using integral functionals  $\bar{\mathcal{A}} : \bar{\mathcal{Q}} \rightarrow \mathbb{R}$  defined using densities  $\bar{A}$  such that  $\bar{\mathcal{A}}(\bar{\mathbf{q}}) = \int_{\bar{\Omega}} \bar{A}(\bar{\mathbf{q}}(\bar{x})) d\bar{x}$ . Here and in what follows  $\bar{\mathcal{Q}}$  is a real Banach space with dual space  $\bar{\mathcal{Q}}^*$ , and dual pairing  $\langle \cdot, \cdot \rangle_{\bar{\mathcal{Q}}} : \bar{\mathcal{Q}}^* \times \bar{\mathcal{Q}} \rightarrow \mathbb{R}$ . In order to write, e.g., the GENERIC evolution equations (G), it is assumed that the functional derivative

$$\langle D\bar{\mathcal{A}}(\bar{\mathbf{q}}), \bar{\mathbf{v}}_{\bar{\mathbf{q}}} \rangle_{\bar{\mathcal{Q}}} := \lim_{0 < h \rightarrow 0} \frac{1}{h} \int_{\bar{\Omega}} (\bar{A}(\bar{\mathbf{q}} + h\bar{\mathbf{v}}_{\bar{\mathbf{q}}}) - \bar{A}(\bar{\mathbf{q}})) d\bar{x}$$

with  $D\bar{\mathcal{A}}(\bar{\mathbf{q}}) \in \bar{\mathcal{Q}}^*$  exists for  $\bar{\mathbf{q}} \in \bar{\mathcal{Q}}$  and all variations  $\bar{\mathbf{v}}_{\bar{\mathbf{q}}} \in \bar{\mathcal{Q}}$ . Similarly, for a general map  $T : \bar{\mathcal{Q}} \rightarrow \mathcal{Q}$  between Banach spaces  $\bar{\mathcal{Q}}$  and  $\mathcal{Q}$ , the Gâteaux derivative is the linear map  $DT(\bar{\mathbf{q}}) : \bar{\mathcal{Q}} \rightarrow \mathcal{Q}$  defined by

$$DT(\bar{\mathbf{q}})\bar{\mathbf{v}}_{\bar{\mathbf{q}}} := \lim_{0 < h \rightarrow 0} \frac{1}{h} (T(\bar{\mathbf{q}} + h\bar{\mathbf{v}}_{\bar{\mathbf{q}}}) - T(\bar{\mathbf{q}})) \quad (\text{GD})$$

for all  $\bar{\mathbf{v}}_{\bar{\mathbf{q}}} \in \bar{\mathcal{Q}}$  with  $\|\bar{\mathbf{v}}_{\bar{\mathbf{q}}}\|_{\bar{\mathcal{Q}}} = 1$ . Hence, functional derivatives usually coincide with Gâteaux derivatives. The linear map  $DT(\bar{\mathbf{q}})$  is called *Fréchet derivative* if the limit passage in (GD) is uniform for all  $\bar{\mathbf{v}}_{\bar{\mathbf{q}}} \in \bar{\mathcal{Q}}$  with  $\|\bar{\mathbf{v}}_{\bar{\mathbf{q}}}\|_{\bar{\mathcal{Q}}} = 1$ . Let us stress that the results of this work are obtained under the *general smoothness prerequisite* that all functions, functionals, and operators involved are sufficiently smooth such that all the appearing derivatives do exist in a classical sense.

In this spirit, in Sec. 2 we first give a brief introduction to the thermomechanics of single-phase multicomponent systems in Lagrangian coordinates and to the kinematics of densities based on flow maps and their transformation to Eulerian coordinates. Details and the notation for thermodynamics will be briefly introduced in Sec. 2.1 and the kinematics of fields and transformations will be detailed in Sec. 2.2. Next, in Sec. 3 we will introduce basic ingredients for reversible Hamiltonian dynamics in Sec. 3.1 and for irreversible Onsager dynamics in Sec. 3.2. These are the building blocks of the coupled GENERIC formulation in Sec. 3.3. Invertible and noninvertible mappings of variational formulations, in particular the reduction formalism, will then be discussed in Sec. 3.4. For this, the validity

of so-called *closure conditions* will be crucial for a transformed structure to possess the properties of a GENERIC structure again. All formal constructions are supplemented with finite-dimensional examples. Starting in Sec. 4, these concepts are applied to fluid dynamics. First, in Sec. 4.1 the Hamiltonian description of ideal fluids is provided and in Sec. 4.2 extended to the Navier-Stokes equations. In Sec. 4.3 we study the limit case of a quasi-stationary flow. Next, in Sec. 5 we introduce additional irreversible processes that should be coupled to the fluid flow. The Onsager structure for reaction kinetics with detailed balance is discussed in Sec. 5.1, heat conduction is presented in Sec. 5.2, multi-component diffusion processes are shown in Sec. 5.3, and cross-coupling effects shortly discussed in Sec. 5.4. In the final Sec. 6 we couple all the structures for viscous fluid flows and the additional irreversible processes to construct the GENERIC system for reactive compressible viscous flows. Therefore, in Sec. 6.1 the GENERIC structure and the equations are presented in Lagrangian and Eulerian form for internal energy, entropy, and temperature as variables. Then, in Sec. 6.2 we provide evolution equations in terms of pressure and temperature variables for the Darcy flow.

## 2 Fundamentals of thermomechanics

In this section, we collect the main tools necessary to understand the GENERIC framework for reactive fluid flows: First, in Sec. 2.1 we review some generally known facts about equilibrium thermodynamics to introduce our notation and remind the reader of some key concepts. Subsequently, in Sec. 2.2 we combine the thermodynamical description with a Lagrangian formulation of continuum mechanics, focusing on the role of the kinematic relationships of deformations and densities as the basis for an operator approach to thermomechanics.

### 2.1 Equilibrium thermodynamics

In the following, we collect certain facts from equilibrium thermodynamics. This collection by no means replaces a proper lecture or textbook on thermodynamics [3, 56, 21]. It strictly focuses on aspects and relations that will be invoked in Sec. 2.2–6.

Continuum thermodynamics provides a description of many-particle systems, when individual particle trajectories become meaningless. Under certain homogeneity assumptions, one can define *state variables* for averaged macroscopic observables representing the thermodynamic state of a system. These variables can either measure a quality or quantity of the system and we distinguish the following two types of variables:

- a) **Extensive state variables** (quantity) behave additively when systems are brought into contact. Examples are the volume  $\bar{V} \in \mathbb{R}$ , the internal energy  $\bar{U} \in \mathbb{R}$ , the entropy  $\bar{S} \in \mathbb{R}$ , particle numbers  $\bar{C} \in \mathbb{R}^N$ , or momentum  $\bar{P} \in \mathbb{R}^d$ . In general we use capital roman letters to denote an extensive quantity, with the mass  $\bar{m}$  as the only exception from this convention. A general vector composed of extensive state variables is denoted by  $\bar{X}$ .
- b) **Intensive state variables** (quality) remain constant when systems are brought into contact. Examples for such properties are the pressure  $\bar{\pi} \in \mathbb{R}$ , the temperature  $\bar{\theta} \in \mathbb{R}$ , the chemical potential  $\bar{\mu} \in \mathbb{R}^N$ , or the velocity  $\bar{v} \in \mathbb{R}^d$ . In general we use small greek letters to denote intensive state variables. A general vector composed of intensive state variables is denoted by  $\bar{\eta}$ .

In general, intensive  $\bar{\eta}$  and extensive  $\bar{X}$  state vectors are not independent but related by an *equation*

of state like

$$\bar{A} = \bar{A}(\bar{\boldsymbol{\eta}}, \bar{\mathbf{X}}) \quad \text{or} \quad \bar{\alpha} = \bar{\alpha}(\bar{\boldsymbol{\eta}}, \bar{\mathbf{X}}),$$

for some components  $\alpha = \bar{\eta}_i$  or  $\bar{A} = \bar{X}_j$ . For convenience, we use the same symbols to denote the state and the corresponding equation of state. With this notation, extensive and intensive states are characterized by the following homogeneity properties.

**Definition 2.1** Consider a thermodynamic system with extensive variables  $\bar{\mathbf{X}}$  and intensive variables  $\bar{\boldsymbol{\eta}}$ . Then:

i) an extensive equation of state  $\bar{A}$  satisfies

$$\bar{A}(\bar{\boldsymbol{\eta}}, \bar{\mathbf{X}}) = \lambda^{-1} \bar{A}(\bar{\boldsymbol{\eta}}, \lambda \bar{\mathbf{X}}) \quad (1a)$$

for all  $\lambda \in (0, \infty)$  and  $\bar{A}(\bar{\boldsymbol{\eta}}, \mathbf{0}) = 0$ , i.e.,  $\bar{A}$  is 1-homogeneous with respect to extensive variables.

ii) an intensive equation of state  $\bar{\alpha}$  satisfies

$$\bar{\alpha}(\bar{\boldsymbol{\eta}}, \bar{\mathbf{X}}) = \bar{\alpha}(\bar{\boldsymbol{\eta}}, \lambda \bar{\mathbf{X}}) \quad (1b)$$

for all  $\lambda \in (0, \infty)$ , i.e.,  $\bar{\alpha}$  is 0-homogeneous with respect to the extensive variables.

**Remark 2.2** The microscopic origins of the homogeneity properties (1) are rarely discussed in detail[3]. However, Def. 2.1 and its foundation is crucial for the following construction as it allows us to pick an extensive variable from  $\bar{\mathbf{X}}$ , usually the volume  $\bar{V}$ , and define a reduced vector of extensive and intensive variables  $\mathbf{X} = \bar{\mathbf{X}}/\bar{V}$ , resulting in the reduced equations of state

$$A(\boldsymbol{\eta}, \mathbf{X}) := \bar{V}^{-1} \bar{A}(\bar{\boldsymbol{\eta}}, \bar{\mathbf{X}}), \quad (2a)$$

$$\alpha(\boldsymbol{\eta}, \mathbf{X}) := \bar{\alpha}(\bar{\boldsymbol{\eta}}, \bar{\mathbf{X}}), \quad (2b)$$

and with  $\boldsymbol{\eta} = \bar{\boldsymbol{\eta}}$ . Note that the selected variable  $\bar{V}$  is no more contained in the reduced state vector  $\mathbf{X}$ . \*

A thermodynamic state vector  $\bar{\mathbf{q}} = (\bar{\boldsymbol{\eta}}, \bar{\mathbf{X}}) \in \bar{\mathcal{Q}}$  is assumed to be composed of a (possibly empty) vector of intensive state variables  $\bar{\boldsymbol{\eta}}$  and a vector of (at least one) extensive state variables  $\bar{\mathbf{X}}$ , which are independent and chosen such that, together with the equations of state, the thermodynamic state of the system is fully characterized. Equivalently the system can be described in terms of the reduced variables  $\mathbf{q} = (\boldsymbol{\eta}, \mathbf{X}) \in \mathcal{Q}$  and the reduced equations of state. In Sec. 2.2 we will see that the description in  $\bar{\mathcal{Q}}$  corresponds to the thermodynamic description in Lagrangian coordinates, whereas the Eulerian description will be formulated in  $\mathcal{Q}$ .

For the characterization of thermodynamic equilibria, the entropy  $\bar{S}$  and internal energy  $\bar{U}$  play a special role. For thermodynamically isolated systems, their critical points determine the thermodynamic equilibrium. For non-isolated systems, thermodynamic equilibria are characterized by corresponding Legendre transformations of  $\bar{S}$  and  $\bar{U}$ . In the following we give one possible characterization of a thermodynamic system based on a description using the extensive internal energy  $\bar{U}$  as a generating equation of state. We assume that the state variable  $\bar{\mathbf{q}}$  is given by the extensive state variables

$$\bar{\mathbf{q}} := (\bar{C}, \bar{V}, \bar{S}),$$

which are the *natural variables* for the internal energy, i.e.,  $\bar{U} = \bar{U}(\bar{\mathbf{C}}, \bar{V}, \bar{S})$  with

$$\begin{aligned} \bar{\mathbf{C}} & \quad \text{the vector of particle concentrations } [\text{m}^{-d}], \\ \bar{V} & \quad \text{the volume density } [1], \\ \bar{S} & \quad \text{the entropy density } [\text{JK}^{-1}\text{m}^{-d}], \end{aligned}$$

and  $d \in \mathbb{N}$  the space dimension. In order to tie in with continuum mechanics, the units of all extensive thermodynamic variables are divided by the  $d$ -dimensional volume, so that extensive variables indeed are densities.

We now introduce the internal energy (internal energy per  $d$ -dimensional unit volume) of the thermodynamical system in equilibrium as an equation of state depending on  $\bar{\mathbf{q}} := (\bar{\mathbf{C}}, \bar{V}, \bar{S}) \in \bar{\mathcal{Q}}$ , i.e.,

$$\bar{U}(\bar{\mathbf{q}}) \quad \text{the internal energy density } [\text{Jm}^{-d}], \quad (3)$$

and  $\bar{U} : \bar{\mathcal{Q}} \rightarrow \mathbb{R}$  is an equation of state for the extensive internal energy. As a consequence of the first and second law of thermodynamics we have the fundamental relation

$$d\bar{U} = \bar{\theta}d\bar{S} - \bar{\pi}d\bar{V} + \sum_{i=1}^N \bar{\mu}_i d\bar{\mathbf{C}}_i, \quad (4)$$

that pairs the total differential of each extensive variable with an intensive variable and gives rise to an internal energy differential. The pairs of extensive and intensive variables are also called *conjugate variables*. By (4), the intensive thermodynamic state variables temperature  $\bar{\theta}$ , pressure  $\bar{\pi}$ , and chemical potential  $\bar{\mu}$  are defined as the following partial derivatives of  $\bar{U}$

$$\bar{\theta} := \frac{\partial \bar{U}}{\partial \bar{S}} \quad \text{temperature } [\text{K}], \quad (5a)$$

$$\bar{\pi} := -\frac{\partial \bar{U}}{\partial \bar{V}} \quad \text{pressure } [\text{Nm}^{d-1}], \quad (5b)$$

$$\bar{\mu} := \frac{\partial \bar{U}}{\partial \bar{\mathbf{C}}} \quad \text{chemical potential } [\text{J}]. \quad (5c)$$

By the positive 1-homogeneity (1a) of the internal energy density it is  $\bar{U}(\lambda\bar{\mathbf{C}}, \lambda\bar{V}, \lambda\bar{S}) = \lambda\bar{U}(\bar{\mathbf{C}}, \bar{V}, \bar{S})$  which upon differentiation with respect to  $\lambda$  yields

$$\bar{U}(\bar{\mathbf{C}}, \bar{V}, \bar{S}) = \bar{\theta}\bar{S} - \bar{\pi}\bar{V} + \bar{\mu} \cdot \bar{\mathbf{C}}. \quad (6)$$

Calculating the total differential from (6) and comparing with (4) reveals the *Gibbs-Duhem* relation

$$0 = \bar{S}d\bar{\theta} - \bar{V}d\bar{\pi} + \bar{\mathbf{C}} \cdot d\bar{\mu}.$$

This expresses that intensive variables  $(\bar{\mu}, \bar{\pi}, \bar{\theta})$  are not independent. Hence, when characterizing the thermodynamical system in equilibrium through a set of independent variables, at least one of them must be extensive [3, Sec. 5.6.5].

By inverting (6) with respect to  $\bar{S}$  one finds the entropy as an equation of state

$$\bar{S}(\bar{\mathbf{q}}_{\bar{U}}) = \bar{S}(\bar{\mathbf{C}}, \bar{V}, \bar{U}). \quad (7a)$$

in terms of its natural variables  $\bar{\mathbf{q}}_{\bar{U}} := (\bar{\mathbf{C}}, \bar{V}, \bar{U})$ . By the rule for differentiating the inverse, the chain rule, and the definitions (5) it follows that

$$\frac{1}{\bar{\theta}} = \frac{\partial \bar{S}}{\partial \bar{U}}, \quad \frac{\bar{\pi}}{\bar{\theta}} = \frac{\partial \bar{S}}{\partial \bar{V}}, \quad \frac{\bar{\mu}}{\bar{\theta}} = -\frac{\partial \bar{S}}{\partial \bar{\mathbf{C}}}. \quad (7b)$$

thermodynamic potential	symbol	definition	fundamental relation	natural variables
internal energy density	$\bar{U}$	$\bar{U} = \bar{\theta}\bar{S} - \bar{\pi}\bar{V} + \bar{\mu} \cdot \bar{C}$	$d\bar{U} = \bar{\theta}d\bar{S} - \bar{\pi}d\bar{V} + \bar{\mu} \cdot d\bar{C}$	$\bar{C}, \bar{V}, \bar{S}$
enthalpy density	$\bar{H}$	$\bar{H} = \bar{U} + \bar{\pi}\bar{V}$	$d\bar{H} = \bar{\theta}d\bar{S} + \bar{V}d\bar{\pi} + \bar{\mu} \cdot d\bar{C}$	$\bar{C}, \bar{\pi}, \bar{S}$
Helmholtz free energy density	$\bar{F}$	$\bar{F} = \bar{U} - \bar{\theta}\bar{S}$	$d\bar{F} = -\bar{S}d\bar{\theta} - \bar{\pi}d\bar{V} + \bar{\mu} \cdot d\bar{C}$	$\bar{C}, \bar{V}, \bar{\theta}$
Gibbs free energy density	$\bar{G}$	$\bar{G} = \bar{U} + \bar{\pi}\bar{V} - \bar{\theta}\bar{S}$	$d\bar{G} = -\bar{S}d\bar{\theta} + \bar{V}d\bar{\pi} + \bar{\mu} \cdot d\bar{C}$	$\bar{C}, \bar{\pi}, \bar{\theta}$
Landau free energy density	$\bar{\Phi}_G$	$\bar{\Phi}_G = \bar{U} - \bar{\theta}\bar{S} - \bar{\mu} \cdot \bar{C}$	$d\bar{\Phi}_G = -\bar{S}d\bar{\theta} - \bar{\pi}d\bar{V} - \bar{C} \cdot d\bar{\mu}$	$\bar{\mu}, \bar{V}, \bar{\theta}$
entropy density	$\bar{S}$	$\bar{S} = \frac{\bar{U}}{\bar{\theta}} + \frac{\bar{\pi}}{\bar{\theta}}\bar{V} - \frac{\bar{\mu}}{\bar{\theta}} \cdot \bar{C}$	$d\bar{S} = \frac{1}{\bar{\theta}}d\bar{U} + \frac{\bar{\pi}}{\bar{\theta}}d\bar{V} - \frac{\bar{\mu}}{\bar{\theta}} \cdot d\bar{C}$	$\bar{C}, \bar{V}, \bar{U}$
Helmholtz free entropy density	$\bar{J}$	$\bar{J} = \bar{S} - \bar{\theta}^{-1}\bar{U} = \frac{-1}{\bar{\theta}}\bar{F}$	$d\bar{J} = -\bar{U}d\frac{1}{\bar{\theta}} + \frac{\bar{\pi}}{\bar{\theta}}d\bar{V} - \frac{\bar{\mu}}{\bar{\theta}} \cdot d\bar{C}$	$\bar{C}, \bar{V}, \frac{1}{\bar{\theta}}$
Gibbs free entropy density	$\bar{Y}$	$\bar{Y} = \bar{S} - \frac{1}{\bar{\theta}}(\bar{U} + \bar{\pi}\bar{V}) = \frac{-1}{\bar{\theta}}\bar{G}$	$d\bar{Y} = -\bar{U}d\frac{1}{\bar{\theta}} - \bar{V}d\frac{\bar{\pi}}{\bar{\theta}} - \frac{\bar{\mu}}{\bar{\theta}} \cdot d\bar{C}$	$\bar{C}, \frac{\bar{\pi}}{\bar{\theta}}, \frac{1}{\bar{\theta}}$

Table 1: List of common thermodynamic potentials (free energy [Jm<sup>-d</sup>] and free entropy [JK<sup>-1</sup>m<sup>-d</sup>] densities)

The most common Legendre transforms of the internal energy  $\bar{U}$  are the enthalpy  $\bar{H}$ , the Helmholtz free energy  $\bar{F}$ , the Gibbs free energy  $\bar{G}$ , and the Landau free energy (also Grand potential)  $\bar{\Phi}_G$ . Starting from the state equation (7a) for the entropy, Legendre transform results in thermodynamic potentials which are *free entropies* or *Massieu-Planck potentials* [42, 62]. All the mentioned thermodynamic potentials are extensive quantities and more details are gathered in Tab. 1.

Assuming that the thermodynamic potentials from Tab. 1 are twice continuously differentiable, the calculation of the mixed second-order derivatives taking into account Schwartz's theorem provides the so-called *Maxwell relations*. This allows us to get a hold of changes in entropy by changes of directly measurable quantities and restricts the response functions, e.g., heat capacities, expansion coefficients. In order to explore further aspects of these thermodynamic response functions, we use the reduced internal energy and entropy introduced in Remark 2.2

$$\begin{aligned}\bar{V}U(\mathbf{C}, S) &:= \bar{U}(\bar{C}, \bar{V}, \bar{S}), \\ \bar{V}S(\mathbf{C}, U) &:= \bar{S}(\bar{C}, \bar{V}, \bar{U}),\end{aligned}\tag{8}$$

with volume-specific extensive concentration  $\mathbf{C} = \bar{C}/\bar{V}$ , entropy  $S = \bar{S}/\bar{V}$ , and internal energy  $U = \bar{U}/\bar{V}$ , and compute the second derivatives

$$\begin{aligned}\frac{\partial^2 \bar{U}}{\partial \bar{\mathbf{q}}^2} &= \begin{pmatrix} \frac{\partial^2 \bar{U}}{\partial \bar{\mathbf{C}}^2} & \frac{\partial^2 \bar{U}}{\partial \bar{\mathbf{C}} \partial \bar{V}} & \frac{\partial^2 \bar{U}}{\partial \bar{\mathbf{C}} \partial \bar{S}} \\ \frac{\partial^2 \bar{U}}{\partial \bar{\mathbf{C}} \partial \bar{V}} & \frac{\partial^2 \bar{U}}{\partial \bar{V}^2} & \frac{\partial^2 \bar{U}}{\partial \bar{S} \partial \bar{V}} \\ \frac{\partial^2 \bar{U}}{\partial \bar{\mathbf{C}} \partial \bar{S}} & \frac{\partial^2 \bar{U}}{\partial \bar{S} \partial \bar{V}} & \frac{\partial^2 \bar{U}}{\partial \bar{S}^2} \end{pmatrix} \\ &= \frac{1}{\bar{V}} \begin{pmatrix} \alpha & -S\gamma - \alpha\mathbf{C} & \gamma \\ -S\gamma^\top - \mathbf{C}^\top\alpha & \mathbf{C} \cdot \alpha\mathbf{C} + S^2\beta + 2S\mathbf{C} \cdot \gamma & -\mathbf{C} \cdot \gamma - S\beta \\ \gamma^\top & -\mathbf{C} \cdot \gamma - S\beta & \beta \end{pmatrix},\end{aligned}\tag{9a}$$

where the parameters  $\alpha \in \mathbb{R}_{\text{sym}}^{N \times N}$ ,  $\beta \in \mathbb{R}$ ,  $\gamma \in \mathbb{R}^N$  depend on  $\bar{\mathbf{q}} = (\bar{C}, \bar{V}, \bar{S})$ . Similarly, by interchanging entropy and internal energy in (9a), we can introduce the capacities for the entropy defined by

$$\begin{aligned}\alpha &:= \frac{\partial^2 U}{\partial \mathbf{C}^2}, & \beta &:= \frac{\partial^2 U}{\partial S^2}, & \gamma &:= \frac{\partial^2 U}{\partial \mathbf{C} \partial S}, \\ \alpha_S &:= \frac{\partial^2 S}{\partial \mathbf{C}^2}, & \beta_S &:= \frac{\partial^2 S}{\partial U^2}, & \gamma_S &:= \frac{\partial^2 S}{\partial \mathbf{C} \partial U},\end{aligned}\tag{9b}$$

to relate the second derivatives  $\partial^2 \bar{S} / \partial \bar{\mathbf{q}}^2$  encoded in  $\alpha_S, \beta_S, \gamma_S$  to the second derivatives  $\partial^2 \bar{U} / \partial \bar{\mathbf{q}}^2$



from (9a) encoded in  $\alpha, \beta, \gamma$ . By taking derivatives of the identity  $U(\mathbf{C}, S(\mathbf{C}, u)) = u$  this gives

$$\begin{aligned}\alpha_S &= -\frac{1}{\bar{\theta}}\alpha + (\gamma \otimes \frac{\boldsymbol{\mu}}{\bar{\theta}^2} + \frac{\boldsymbol{\mu}}{\bar{\theta}^2} \otimes \gamma) - \frac{1}{\bar{\theta}^3}(\boldsymbol{\mu} \otimes \boldsymbol{\mu})\beta, \\ \beta_S &= -\frac{1}{\bar{\theta}^3}\beta, \\ \gamma_S &= -\frac{1}{\bar{\theta}^2}\gamma + \frac{\boldsymbol{\mu}}{\bar{\theta}^3}\beta,\end{aligned}\tag{9c}$$

and will be useful for change of variables later.

These second derivatives of the internal energy can be related to the standard response functions, i.e., heat capacity at constant volume  $\bar{C}_{\bar{V}}$ , adiabatic compressibility  $\bar{\kappa}_{\bar{S}}$ , and latent heat at constant volume  $\bar{\Lambda}_{\bar{V}}$ , defined as

$$\bar{C}_{\bar{V}} := \left( \frac{\partial \bar{U}}{\partial \bar{\theta}} \right)_{\bar{V}}, \quad \bar{\kappa}_{\bar{S}} := -\frac{1}{\bar{V}} \left( \frac{\partial \bar{V}}{\partial \bar{\pi}} \right)_{\bar{S}}, \quad \bar{\Lambda}_{\bar{V}} := \bar{\theta} \left( \frac{\partial \bar{S}}{\partial \bar{V}} \right)_{\bar{\theta}}.$$

Using the definitions and general thermodynamic relations, we immediately find the relations of the second derivatives to  $\bar{C}_{\bar{V}}$  and  $\bar{\kappa}_{\bar{S}}$  and  $\bar{\Lambda}_{\bar{V}}$  as

$$\frac{\partial^2 \bar{U}}{\partial \bar{S}^2} = \frac{\bar{\theta}}{\bar{C}_{\bar{V}}}, \quad \frac{\partial^2 \bar{U}}{\partial \bar{V}^2} = \frac{1}{\bar{V} \bar{\kappa}_{\bar{S}}}, \quad \frac{\partial^2 \bar{U}}{\partial \bar{V} \partial \bar{S}} = \frac{-\bar{\Lambda}_{\bar{V}}}{\bar{C}_{\bar{V}}}.\tag{10}$$

which now entirely define all second derivatives of  $\bar{U}$  or of  $\bar{S}$  for a single component system  $N = 1$ .

Later we will use the following thermodynamic description of the ideal gas in some examples.

**Example 2.3 (Ideal gas)** The ideal gas is a thermodynamic system of gas particles in the absence of particle interactions. It has the well-known equation of state  $\bar{\pi} \bar{V} = k_{\text{B}} \bar{\theta} \bar{C}$ , where  $k_{\text{B}} = 1.3805 \cdot 10^{-23} \text{ J K}^{-1}$  is the Boltzmann constant. The thermodynamic state is entirely determined by the entropy  $\bar{S} = \bar{S}(\bar{C}, \bar{V}, \bar{U})$ , which for a three-dimensional monoatomic ideal gas is given by the Sackur-Tetrode equation

$$\bar{S}(\bar{C}, \bar{V}, \bar{U}) := \bar{C} k_{\text{B}} \left[ \log \left( \frac{\bar{V}}{\bar{C}} \left( \frac{4\pi M \bar{U}}{3h^2 \bar{C}} \right)^{\frac{3}{2}} \right) + \frac{5}{2} \right].\tag{11}$$

Upon differentiation with respect to its natural variables we get

$$\frac{1}{\bar{\theta}} = \frac{\partial \bar{S}}{\partial \bar{U}} = \frac{3}{2} \frac{\bar{C} k_{\text{B}}}{\bar{U}},\tag{12a}$$

$$\frac{\bar{\pi}}{\bar{\theta}} = \frac{\partial \bar{S}}{\partial \bar{V}} = \frac{k_{\text{B}} \bar{C}}{\bar{V}},\tag{12b}$$

$$-\frac{\bar{\mu}}{\bar{\theta}} = \frac{\partial \bar{S}}{\partial \bar{C}} = k_{\text{B}} \log \left( \frac{\bar{V}}{\bar{C}} \left( \frac{4\pi M \bar{U}}{3h^2 \bar{C}} \right)^{\frac{3}{2}} \right).\tag{12c}$$

This can be rewritten in the more common form

$$\bar{U} = \frac{3}{2} k_{\text{B}} \bar{C} \bar{\theta}, \quad \bar{\pi} \bar{V} = k_{\text{B}} \bar{C} \bar{\theta}.\tag{13}$$

Note that the normalization  $\frac{4\pi M}{3h^2}$  in  $\bar{S}$  using the gas particle mass  $M$  and the Planck's constant  $h$  is based on quantum-statistical arguments and fixes the additive ambiguity of the entropy [57]. Rewriting this into an expression for the internal energy we obtain

$$\bar{U}(\bar{C}, \bar{V}, \bar{S}) = \frac{3h^2 \bar{C}}{4\pi M} \left( \frac{\bar{C}}{\bar{V}} \right)^{\frac{2}{3}} \exp \left( \frac{2}{3} \frac{\bar{S}}{k_{\text{B}} \bar{C}} - \frac{5}{3} \right).\tag{14}$$

These potentials are the basis for transformations to other variables. The thermodynamics of the ideal gas still allows some further level of variation. Gas particles in three spatial dimensions are

characterized by the number of degrees of freedom per molecule  $f \in \mathbb{N}$ . For a monoatomic ideal gas  $f = 3$ , for diatomic molecules  $f = 5$ , and for full three-dimensional molecules  $f = 6$ . We can also express the heat capacity ratio using  $f$  as

$$\frac{\bar{C}_\pi}{\bar{C}_V} =: \frac{f+2}{f}.$$

With  $f$  the entropy in natural variables becomes

$$\bar{S}(\bar{C}, \bar{V}, \bar{U}) := \bar{C} k_B \left[ \log \left( \frac{\bar{V}}{\bar{C}} \left( \frac{\alpha \bar{U}}{\bar{C}} \right)^{\frac{f}{2}} \right) + \frac{f+2}{2} \right],$$

where  $\alpha$  is a dimensional normalization constant depending on quantum-statistical arguments that give rise to a specific effective density of states for the thermodynamical system. For a monoatomic gas in  $d$  dimensions we have  $\alpha = \frac{4\pi M}{3h^2}$  and  $f = d$ . This gives the slightly more general equation of state

$$\bar{U} = \frac{f}{2} k_B \bar{C} \bar{\theta}, \quad \bar{\pi} \bar{V} = k_B \bar{C} \bar{\theta}, \quad \bar{\mu} = \frac{f+2}{2} k_B \bar{\theta}.$$

Based on these expression for the thermodynamic potential of a single-component ideal gas, the extension to a multicomponent monoatomic ideal gas reads

$$\bar{F}(\bar{C}, \bar{V}, \bar{\theta}) := \sum_{i=1}^N \bar{C}_i k_B \bar{\theta} \left[ \log \left( \frac{\bar{C}_i}{\bar{V}} \lambda_{i,\bar{\theta}}^3 \right) - 1 \right], \quad (15)$$

where the thermal de Broglie wavelength depends on the particle type through the mass as

$$\lambda_{i,\bar{\theta}} := \sqrt{\frac{h^2}{2\pi M_i k_B \bar{\theta}}} = C_{\text{therm}} \bar{\theta}^{-1/2}, \quad (16)$$

producing the same equation of state as in (13) but with the total number of particles  $\bar{C} = \sum_{i=1}^N \bar{C}_i$ .  
\*

## 2.2 Kinematics of flow maps and densities

In this section, we introduce the basic kinematic ingredients from continuum mechanics needed to incorporate equilibrium thermodynamics into a variational framework for compressible reactive fluid flows. The key idea is the consistent use of *flow map*  $\chi(t)$  and momentum  $\bar{P}(t)$  as elements of an abstract state space  $\bar{Q}$ . Based on the definitions in Sec. 2.1, we additionally connect the concept of the motion of material by flow maps with the concept of extensive and intensive thermodynamic state variables as elements of the state space  $\bar{Q}$ . This description will allow us to systematically relate quantities in the Lagrangian and the Eulerian frame.

Therefore, we consider the motion of a material occupying at time  $t \in [0, T]$ , an open, bounded set  $\Omega(t) \subset \mathbb{R}^d$ . At the initial time  $t = 0$ , this domain is denoted by  $\bar{\Omega} := \Omega(0)$ . We call  $\bar{\Omega}$  the *reference* or *Lagrangian* domain and  $\Omega(t)$  the *current* or *Eulerian* domain for any  $t \in (0, T]$ . As a special case, the Eulerian domain can be fixed  $\Omega(t) \equiv \Omega$  but in general it is time-dependent. At any time, the letter  $x$  denotes coordinates in the current domain  $x \in \Omega(t)$ , whereas the letter  $\bar{x}$  represents coordinates in the reference domain  $\bar{x} \in \bar{\Omega}$ , cf. Fig. 1.

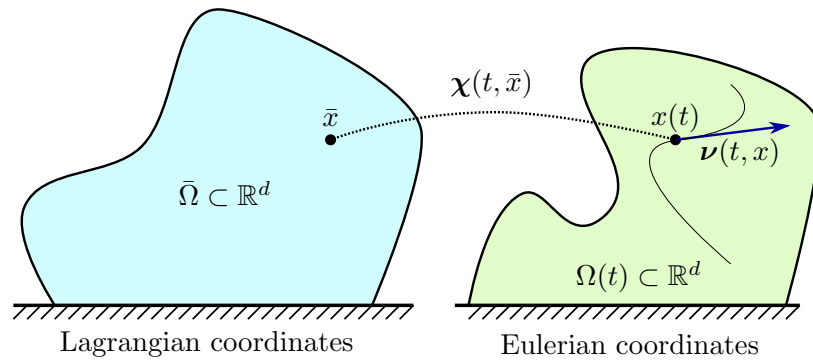


Figure 1: Flow map facilitates transport in space.

In the same spirit, we indicate state variables or state functions  $\bar{A}$ ,  $\bar{\alpha}$  defined on the Lagrangian domain  $\bar{\Omega}$  with a bar and their Eulerian counterparts  $A$ ,  $\alpha$  defined on the current domain  $\Omega(t)$  without a bar. This applies in particular to all thermodynamic state variables previously defined in Sec. 2.1, which for a non-equilibrium system depend both on time  $t \in [0, T]$  and on Lagrangian coordinates  $\bar{x} \in \bar{\Omega}$  or Eulerian coordinates  $x \in \Omega$ . Accordingly,  $\bar{\mathcal{Q}}$  denotes the Lagrangian state space and  $\mathcal{Q}$  the Eulerian counterpart of these state variables (functions). Moreover, we synonymously use  $\bar{A}(t)$  to denote state variables  $\bar{A}(t, \bar{x})$  and equations of state  $\bar{A}(\bar{q}(t, \bar{x}))$ . When discussing equations of state for the same variable  $\bar{A}$  or  $\bar{\alpha}$  in dependence of different sets of variables, e.g.,  $\bar{q}_{\bar{S}}$  and  $\bar{q}_{\bar{U}}$ , then for brevity we use  $\bar{A}_{\diamond}$  or  $\bar{\alpha}_{\diamond}$  with state space  $\bar{\mathcal{Q}}_{\diamond}$  and  $\diamond \in \{\bar{S}, \bar{U}\}$ . When no confusion is possible, we omit this index. This will be the case if the natural variables of a thermodynamic potential are used.

Extensive quantities are denoted by capital roman letters and in general, the corresponding integrated quantity is always denoted with the same letter in calligraphic font, e.g., see (19). This notation is applied in particular to the total energy  $\mathcal{E}$ , internal energy  $\mathcal{U}$ , and the entropy  $\mathcal{S}$  of a thermomechanical system. Moreover, when ambiguities are ruled out, we shall sometimes omit the dependence of a variable on time and space and write  $\bar{A} = \bar{A}(t, \bar{x})$  or  $\bar{q} = \bar{q}(t, \bar{x})$  and similarly in Eulerian coordinates. Throughout this work we equivalently use the dot and  $\partial_t$  to indicate partial derivatives with respect to time of state variables and functions, e.g.,  $\dot{\bar{A}} = \partial_t \bar{A} = \partial_t \bar{A}(t, \bar{x})$ , e.g., see (18h).

**Definition 2.4 (Deformation, flow map, velocity)** A map  $\chi : \bar{\Omega} \rightarrow \mathbb{R}^d$  with properties i)-iii) is called a deformation:

- i)  $\chi : \bar{\Omega} \rightarrow \mathbb{R}^d$  is invertible with  $\chi^{-1}$  the inverse map,
- ii) the map  $\chi$  is continuously differentiable for all  $\bar{x} \in \bar{\Omega}$ ,
- iii) the map  $\chi$  preserves orientation  $\det \bar{\nabla} \chi > 0$ .

We denote  $\bar{\mathcal{Q}}_{\chi} := \{\chi : \bar{\Omega} \rightarrow \mathbb{R}^d \text{ with properties i)-iii)}\}$  the set of deformations.

A map  $\chi : [0, T] \times \bar{\Omega} \rightarrow \mathbb{R}^d$  is called a flow map, if it satisfies the following properties:

- iv)  $\chi(t) \in \bar{\mathcal{Q}}_{\chi}$  for all  $t \in [0, T]$ ,
- v)  $\chi(0, \bar{x}) = \bar{x}$  for all  $\bar{x} \in \bar{\Omega}$  at initial time  $t = 0$ .

For any  $\bar{\omega} \subset \bar{\Omega}$  we set

$$\chi(t, \bar{\omega}) := \{x \in \mathbb{R}^d, \exists \bar{x} \in \bar{\omega} \text{ s.t. } x = \chi(t, \bar{x})\},$$

hence in particular  $\Omega(t) := \chi(t, \bar{\Omega})$ .

For a flow map  $\chi(t)$  and time  $t \in [0, T]$ , the corresponding Lagrangian velocity  $\bar{\nu}(t) : \bar{\Omega} \rightarrow \mathbb{R}^d$  is given by

$$\bar{\nu}(t, \bar{x}) = \partial_t \chi(t, \bar{x}), \quad (17a)$$

and the associated Eulerian velocity  $\nu(t) : \Omega(t) \rightarrow \mathbb{R}^d$  is defined as  $\bar{\nu} = \nu \circ \chi$ , i.e.,

$$\nu(t, x) = (\partial_t \chi)(t, \chi^{-1}(t, x)). \quad (17b)$$

In turn, for given Eulerian velocity  $\nu$ , the flow map can be reconstructed by solving the ODE-Cauchy problem

$$\partial_t \chi(t, \bar{x}) = \nu(t, \chi(t, \bar{x})) \quad \text{and} \quad \chi(0, \bar{x}) = \bar{x}, \quad (17c)$$

which is called the kinematic condition.

Next we establish connections between the properties of flow maps and the thermodynamic volume density  $\bar{V}$ .

**Lemma 2.5 (Jacobi matrix  $\bar{F}$  and volume  $\bar{V}$ )** Let  $\chi : [0, T] \times \bar{\Omega} \rightarrow \mathbb{R}^d$  be a flow map satisfying properties iv)-v) of Def. 2.4. Let  $\bar{F}(t) : \bar{\Omega} \rightarrow \mathbb{R}^{d \times d}$  denote its Jacobian, i.e., for all  $t \in [0, T]$

$$\bar{F}(t) := \bar{\nabla} \chi(t), \quad (18a)$$

and  $\bar{V}(t) : \bar{\Omega} \rightarrow \mathbb{R}$  the associated volume density, i.e.,

$$\bar{V}(t) = T_{\bar{V}}(\chi(t)) := \det \bar{F}(t), \quad (18b)$$

where  $T_{\bar{V}} : \bar{\mathcal{Q}}_{\chi} \rightarrow (0, \infty)$  maps a flow map to its volume density.

Then, for all  $t \in [0, T]$  the volume density  $\bar{V}(t)$  is strictly positive, the Jacobian  $\bar{F}(t)$  is invertible, and the total volume of the domain  $\Omega(t)$  is

$$\int_{\Omega(t)} 1 dx = \int_{\bar{\Omega}} \bar{V}(t, \bar{x}) d\bar{x}. \quad (18c)$$

Furthermore, the Fréchet derivative of the map  $T_{\bar{V}}$  is given by [9][p. 10f]

$$\mathbb{D}T_{\bar{V}}(\chi)\square = \partial_{\bar{F}} \det(\bar{F}) : \bar{\nabla}\square = \text{Cof}(\bar{F}) : \bar{\nabla}\square, \quad (18d)$$

$$\text{with } \text{Cof}(\mathbf{A}) := (\det \mathbf{A})\mathbf{A}^{-\top}, \quad (18e)$$

the cofactor matrix for any invertible  $\mathbf{A} \in \mathbb{R}^{d \times d}$ . Above, the  $\square$  indicates the placement of functions in the definition of linear operators acting on these functions (to the right) and the Frobenius scalar product and norm are

$$\mathbf{A} : \mathbf{B} := \sum_{i,j=1}^d A_{ij} B_{ij}, \quad |\mathbf{A}|^2 = \mathbf{A} : \mathbf{A}, \quad (18f)$$

for all  $\mathbf{A}, \mathbf{B} \in \mathbb{R}^{d \times d}$ . For  $\bar{\nabla} \chi$  continuously differentiable there holds the Piola identity [9][p. 39]

$$\bar{\nabla} \cdot \text{Cof}(\bar{\nabla} \chi) = 0 \quad \text{in } \bar{\Omega}. \quad (18g)$$

Moreover, with  $\dot{\bar{F}} = \partial_t \bar{F} = \bar{\nabla} \dot{\chi}$ , the volume density evolves as [19][L. 5.3]

$$\dot{\bar{V}} = \partial_t \bar{V} = \mathbb{D}T_{\bar{V}}(\chi)\dot{\chi} = \text{Cof}(\bar{F}) : \dot{\bar{F}}. \quad (18h)$$

Note that the flow map  $\chi$  has the unit of a length and  $\bar{F}, \bar{V}$  are dimensionless quantities measuring the deformation of the reference volume.

Next, we discuss how the thermodynamic quantities from Section 2.1 are mapped from  $\bar{\Omega}$  to the current domain  $\Omega(t)$  and study their associated transport relations. Extensive state variable  $\bar{A} : [0, T] \times \bar{\Omega} \rightarrow \mathbb{R}$  as introduced on p. 3 in a) satisfy the identity

$$\mathcal{A}(t) = \int_{\bar{\omega}} \bar{A}(t) d\bar{x} = \int_{\chi(t, \bar{\omega})} A(t) dx, \quad (19)$$

for any  $\bar{\omega} \subset \bar{\Omega}$  and the value of  $\mathcal{A}(t)$  is independent of the choice of coordinates. As introduced in Remark 2.2,  $\bar{A}$  is the extensive quantity in Lagrangian coordinates and  $A$  is the reduced variable in Eulerian coordinates. In addition, the calligraphic letter  $\mathcal{A}$  denotes the integrated quantity. Similarly, using the definition in b), p. 3, the value of intensive quantities is independent of the coordinate frame. Taking into account the transformation rules for integrals thus results in the following transformation relations for extensive and intensive variables.

**Definition 2.6 (Transformation of coordinates)** *Let  $t \in [0, T]$  be fixed, and at time  $t$  let  $\chi : \bar{\Omega} \rightarrow \Omega(t)$  be a deformation with properties i)-iii) of Def. 2.4, and  $\bar{V} = T_{\bar{V}}(\chi)$  the associated volume density. Let  $\bar{A} : \bar{\Omega} \rightarrow \mathbb{R}$  be an extensive thermodynamic state variable and  $\bar{\alpha} : \bar{\Omega} \rightarrow \mathbb{R}$  be an intensive thermodynamic state variable in Lagrangian coordinates. Then, the corresponding extensive state variable  $A : \Omega \rightarrow \mathbb{R}$  and the corresponding intensive state variable  $\alpha : \Omega \rightarrow \mathbb{R}$  in Eulerian coordinates are defined by*

$$A \circ \chi := \frac{\bar{A}}{\bar{V}}, \quad (20a)$$

$$\alpha \circ \chi := \bar{\alpha}, \quad (20b)$$

*i.e.,  $A(\chi(\bar{x})) = \bar{V}(\bar{x})^{-1} \bar{A}(\bar{x})$  and  $\alpha(\chi(\bar{x})) = \bar{\alpha}(\bar{x})$ . Relations (20) define a nonlinear transformation*

$$T_{LE} : \bar{\mathcal{Q}} \rightarrow \mathcal{Q},$$

*between the Lagrangian state space  $\bar{\mathcal{Q}}$  and the Eulerian state space  $\mathcal{Q}$ . For fluids, the latter contains all the transformed state variables from  $\bar{\mathcal{Q}}$ , except for  $\chi$  and  $\bar{V}$ .*

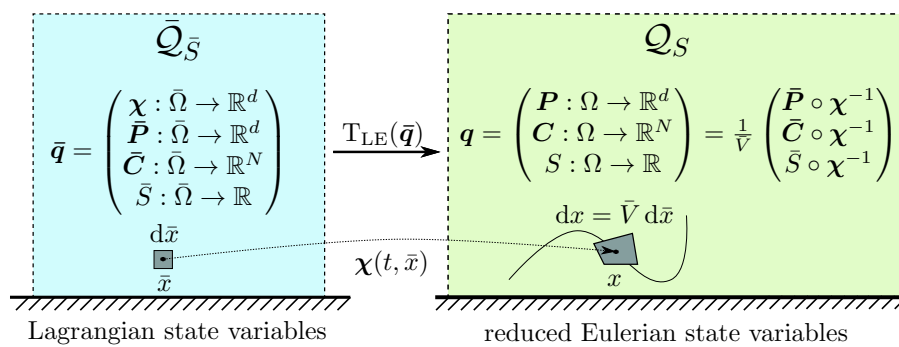


Figure 2: Illustration of the mapping from Lagrangian to Eulerian state space, where the flow map  $\chi$  and the momentum  $\bar{P}$  characterize the mechanical state and, e.g., entropy and concentration are the thermodynamic state variables.

In Fig. 2 the workings of the map  $T_{LE}$  is illustrated. Note that we also consider vector-valued extensive and intensive quantities, where then (20) applies to each component. For concise notation, we collect here our notation for vector- and tensor-valued functions, and the transformation rules for their gradients.

**Definition 2.7** Let  $\Omega \subset \mathbb{R}^d$  with the usual scalar product of Euclidean space. The tensor product of two vector fields  $\mathbf{a} : \Omega \rightarrow \mathbb{R}^M$  and  $\mathbf{b} : \Omega \rightarrow \mathbb{R}^N$  results in the second-order tensor field  $(\mathbf{a} \otimes \mathbf{b}) : \Omega \rightarrow \mathbb{R}^{M \times N}$  with

$$(\mathbf{a} \otimes \mathbf{b})_{ij}(x) := \mathbf{a}_i(x)\mathbf{b}_j(x). \quad (21a)$$

Consider a differentiable, scalar function  $f : \Omega \rightarrow \mathbb{R}$  in Eulerian coordinates. Its Eulerian gradient is the usual  $d$ -dimensional vector field  $\nabla f : \Omega \rightarrow \mathbb{R}^d$  defined

$$\nabla f(x) := (\partial_{x_i} f(x))_{i=1}^d \in \mathbb{R}^d. \quad (21b)$$

For differentiable, vector-valued or multicomponent functions  $\mathbf{c} : \Omega \rightarrow \mathbb{R}^N$  the gradient  $\nabla \mathbf{c} : \Omega \rightarrow \mathbb{R}^{N \times d}$  is

$$\nabla \mathbf{c}(x) := ((\partial_{x_j} c_i(x))_{i=1}^N)_{j=1}^d \in \mathbb{R}^{N \times d}. \quad (21c)$$

Consequently, for any second-order tensor  $\boldsymbol{\sigma} : \Omega \rightarrow \mathbb{R}^{N \times d}$  and vector field  $\mathbf{v} : \Omega \rightarrow \mathbb{R}^d$  their Eulerian divergence is

$$\nabla \cdot \boldsymbol{\sigma}(x) := \left( \sum_{j=1}^d \partial_{x_j} \boldsymbol{\sigma}_{ij}(x) \right)_{i=1}^N \in \mathbb{R}^N, \quad (21d)$$

$$\nabla \cdot \mathbf{v}(x) := \sum_{j=1}^d \partial_{x_j} v_j(x) = \nabla \mathbf{v}(x) : \mathbb{I}_d \in \mathbb{R}, \quad (21e)$$

with  $\mathbb{I}_d \in \mathbb{R}^{d \times d}$  the identity matrix. The Lagrangian gradients  $\bar{\nabla} \bar{f}$ ,  $\bar{\nabla} \bar{\mathbf{v}}$  of differentiable, scalar- and vector-valued functions  $\bar{f} : \bar{\Omega} \rightarrow \mathbb{R}$ ,  $\bar{\mathbf{v}} : \bar{\Omega} \rightarrow \mathbb{R}^N$ , and the Lagrangian divergence  $\bar{\nabla} \cdot \bar{\boldsymbol{\sigma}}$  are defined analogously. Suppose that above functions are related by a coordinate transformation using a smooth deformation  $\chi : \bar{\Omega} \rightarrow \Omega$  as in Def. 2.4, i.e.,  $f(\chi(\bar{x})) := \bar{f}(\bar{x})$  and  $\mathbf{v}(\chi(\bar{x})) := \bar{\mathbf{v}}(\bar{x})$  for all  $\bar{x} \in \bar{\Omega}$ . Then, their gradients are related as follows

$$\nabla f(x) = \bar{\mathbf{F}}^{-\top}(\bar{x}) \bar{\nabla} \bar{f}(\bar{x}), \quad (21f)$$

$$\nabla \mathbf{v}(x) = \bar{\nabla} \bar{\mathbf{v}}(\bar{x}) \bar{\mathbf{F}}^{-1}(\bar{x}), \quad (21g)$$

with  $\bar{\mathbf{F}} = \bar{\nabla} \chi$  and  $x = \chi(\bar{x})$ . Using that  $\mathbf{A} : (\mathbf{BC}) = \mathbf{AC}^\top : \mathbf{B}$  with (21g) one finds for the Eulerian divergence the Lagrangian representation

$$\nabla \cdot \mathbf{v} = \mathbb{I}_d : (\bar{\nabla} \bar{\mathbf{v}}) \bar{\mathbf{F}}^{-1} = (\det \bar{\mathbf{F}})^{-1} \text{Cof } \bar{\mathbf{F}} : \bar{\nabla} \bar{\mathbf{v}}. \quad (21h)$$

While the transformation in Def.s 2.6 & 2.7 does not depend on time itself, in general we map time-dependent state variables, i.e.,  $\mathbf{q}(t) = \mathbb{T}_{\text{LE}}(\bar{\mathbf{q}}(t))$ .

Based on the transformation behavior defined in (20) the evolution laws for  $A$  and  $\alpha$  can be derived. Differentiating (20b) with respect to time directly gives

$$(\dot{\alpha} + \boldsymbol{\nu} \cdot \nabla \alpha)_{t,x=\chi(t,\bar{x})} = \dot{\bar{\alpha}}(t, \bar{x}). \quad (22a)$$

Similarly, differentiating (20a) with respect to time and using (18h) gives

$$(\dot{A} + \boldsymbol{\nu} \cdot \nabla A)_{t,x=\chi(t,\bar{x})} = \frac{\dot{A}}{\bar{V}} - \frac{\bar{A} \dot{\bar{V}}}{\bar{V}^2} = \frac{\dot{A}}{\bar{V}} - \frac{\bar{A}}{\bar{V}} \bar{\mathbf{F}}^{-\top} : \bar{\nabla} \dot{\chi}.$$

Then the identity  $\bar{A} \bar{V}^{-1} \bar{\mathbf{F}}^{-\top} : \bar{\nabla} \dot{\chi} = (A \nabla \cdot \boldsymbol{\nu})_{t,x=\chi(t,\bar{x})}$  and rearranging terms finally yields

$$\left( \dot{A} + \nabla \cdot (A \boldsymbol{\nu}) \right)_{t,x=\chi(t,\bar{x})} = \frac{\dot{A}(t, \bar{x})}{\bar{V}(t, \bar{x})}. \quad (22b)$$

In the special cases where  $\bar{\alpha}$  and  $\bar{A}$  do not depend on time, then (22a) becomes the transport equation and (22b) becomes the continuity equation. Using the nonlinear coordinate transformation  $T_{LE}$ , from the evolution laws (22a) and (22b) one directly recovers the following formal relations between the partial time derivatives of the quantities in Lagrangian and Eulerian coordinates:

**Lemma 2.8** *Let  $\chi : [0, T] \times \bar{\Omega} \rightarrow \mathbb{R}^d$  be a flow map satisfying properties iv)-v) of Def. 2.4. Let  $\bar{w} \in \{\bar{\alpha}, \bar{A}\}$  be an intensive or extensive state variable in Lagrangian coordinates, and  $T_{LE} : \bar{Q}_\chi \times \bar{Q}_{\bar{w}} \rightarrow Q_w$  the coordinate transformation  $T_{LE}(\chi; \bar{w}) = w$  given by relations (20). Then,*

$$\dot{w} = D_{\bar{w}} T_{LE}(\chi; \bar{w}) \dot{\bar{w}} + D_\chi T_{LE}(\chi; \bar{w}) \dot{\chi} \quad (23)$$

*takes the form (22a) for intensive variables and (22b) for extensive variables.*

Here,  $D_{\bar{w}} T_{LE}(\chi; \bar{w})$  denotes the Fréchet derivative of  $T_{LE}$  with respect to  $w$ , and  $D_\chi T_{LE}(\chi; \bar{w})$  with similar meaning. Thus, in general (23) provides an affine relation between the Eulerian partial time derivative  $\dot{w}$  and its Lagrangian counterpart  $\dot{\bar{w}}$ . Accordingly, in case that also  $\chi$  is part of the state vector, the Fréchet derivative  $DT_{LE}$  even gives a linear relation, as will be seen in Lemma 3.13. This property will be crucial throughout Sec. 3–6 for the Lagrangian-Eulerian reduction of GENERIC systems.

As a direct consequence of (22b) one finds the following definition of locally conserved quantities.

**Lemma 2.9 (Locally conserved quantities)** *An extensive thermodynamic quantity  $A$  satisfies the continuity equation (22b), if and only if it is constant in Lagrangian coordinates  $\bar{A}(t, \bar{x}) = \bar{A}(0, \bar{x})$ . Such a quantity will be called locally conserved.*

For single-phase flows, the mass density is a *locally conserved* quantity. Thus, the Eulerian mass density satisfies the continuity equation

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{v}) = 0. \quad (24a)$$

The corresponding Lagrangian mass density is defined by

$$\bar{\rho}(\bar{x}) = \sum_{i=1}^N M_i \bar{C}_i(t, \bar{x}) \equiv \mathbf{M} \cdot \bar{\mathbf{C}}, \quad (24b)$$

where  $\bar{\mathbf{C}} \in \mathbb{R}^N$  is the vector of particle densities and  $\mathbf{M} = (M_i)_{i=1 \dots N} \in \mathbb{R}^N$  is the constant mass per particle. Note that  $\bar{\rho}$  being independent of time sets an essential and nontrivial constraint on the values of  $\bar{C}_i$  and their evolution. The mass density  $\bar{\rho}$  is an extensive quantity resulting in the total mass

$$\mathcal{M} = \int_{\bar{\Omega}} \bar{\rho} d\bar{x}. \quad (24c)$$

We also point out that for reversible (isentropic) Hamiltonian dynamics the entropy  $\bar{S}$  is locally conserved and in the absence of diffusion and reactions the particle concentrations  $\bar{\mathbf{C}}$  are locally conserved.

### 3 Thermomechanical modelling via GENERIC

We present a variational framework that allows us to connect the thermodynamics of Sec. 2.1 with the kinematic description of continuum mechanics of Sec. 2.2 and to treat isolated systems outside equilibrium. This is related to the formulation of evolution laws using conservation laws that should be satisfied by a thermomechanical system. From a thermodynamical point of view this concerns the first and the second law of thermodynamics, i.e., the conservation of total energy for the reversible dynamics and the increase of entropy for the dissipative dynamics. Additionally, we need to ensure the conservation of mass and from the mechanical point of view also the conservation of linear momentum has to be taken into account. The GENERIC approach is closely related to the notion of *metriplectic systems* [51].

It is the aim of this section to introduce the building blocks of the GENERIC framework and its general properties: The triple  $(\bar{Q}, \bar{\mathcal{E}}, \bar{\mathbb{J}})$  for reversible dynamics in Sec. 3.1 and the triple  $(\bar{Q}, \bar{\mathcal{S}}, \bar{\mathbb{K}})$  for dissipative dynamics in Sec. 3.2, which are coupled in a GENERIC system as a quintuple  $(\bar{Q}, \bar{\mathcal{E}}, \bar{\mathcal{S}}, \bar{\mathbb{J}}, \bar{\mathbb{K}})$  under the constraint of a so-called *non-interaction condition* or *degeneracy condition* [27, 28, 44, 17] in Sec. 3.3. Transformations of these structures between different Lagrangian and Eulerian coordinates and between different sets of variables will be considered in Sec. 3.4.

#### 3.1 Hamiltonian systems $(\bar{Q}, \bar{\mathcal{E}}, \bar{\mathbb{J}})$ for reversible dynamics

The evolution of conservative systems is governed by reversible processes. The driving potential for reversible dynamics is the total energy functional of the system  $\bar{\mathcal{E}} : \bar{Q} \rightarrow \mathbb{R}$ , defined on a suitable state space  $\bar{Q}$ . In our applications  $\bar{Q}$  usually is a Banach space with dual space  $\bar{Q}^*$  and the dual pairing  $\langle \cdot, \cdot \rangle_{\bar{Q}} : \bar{Q}^* \times \bar{Q} \rightarrow \mathbb{R}$ . We denote the set of infinitely-often Fréchet-differentiable functionals mapping from the state space  $\bar{Q}$  to  $\mathbb{R}$  by

$$\bar{\mathcal{X}} := \{\bar{\Phi} : \bar{Q} \rightarrow \mathbb{R}, \bar{\Phi} \text{ is smooth}\}. \quad (25)$$

This includes but is not restricted to linear functionals. In particular it is assumed that  $\bar{\mathcal{E}} \in \bar{\mathcal{X}}$ . The geometric structure associated with reversible dynamics is generated by a Poisson bracket

$$\{\cdot, \cdot\} : \bar{\mathcal{X}} \times \bar{\mathcal{X}} \rightarrow \bar{\mathcal{X}}, \quad (26a)$$

which is a skewsymmetric bilinear form, i.e.,

$$\{\bar{\mathcal{F}}, \bar{\mathcal{G}}\} = -\{\bar{\mathcal{G}}, \bar{\mathcal{F}}\}, \quad (26b)$$

that satisfies Jacobi's identity, i.e.,

$$\{\bar{\mathcal{F}}, \{\bar{\mathcal{G}}, \bar{\mathcal{H}}\}\} + \{\bar{\mathcal{H}}, \{\bar{\mathcal{F}}, \bar{\mathcal{G}}\}\} + \{\bar{\mathcal{G}}, \{\bar{\mathcal{H}}, \bar{\mathcal{F}}\}\} = 0, \quad (26c)$$

and the Leibniz rule, i.e.,

$$\{\bar{\mathcal{F}}\bar{\mathcal{G}}, \bar{\mathcal{H}}\} = \bar{\mathcal{F}}\{\bar{\mathcal{G}}, \bar{\mathcal{H}}\} + \{\bar{\mathcal{F}}, \bar{\mathcal{H}}\}\bar{\mathcal{G}}, \quad (26d)$$

for all  $\bar{\mathcal{F}}, \bar{\mathcal{G}}, \bar{\mathcal{H}} \in \bar{\mathcal{X}}$ . With the dual pairing  $\langle \cdot, \cdot \rangle_{\bar{Q}}$  and with a given linear operator  $\bar{\mathbb{J}}(\bar{q}) : \bar{Q}^* \rightarrow \bar{Q}$ , one can introduce a bracket as follows

$$\{\bar{\mathcal{F}}, \bar{\mathcal{G}}\}(\bar{q}) := \langle D_{\bar{q}}\bar{\mathcal{F}}(\bar{q}), \bar{\mathbb{J}}(\bar{q})D_{\bar{q}}\bar{\mathcal{G}}(\bar{q}) \rangle_{\bar{Q}}, \quad (27a)$$



for all  $\bar{\mathcal{F}}, \bar{\mathcal{G}} \in \bar{\mathcal{X}}$  and  $\bar{\mathbf{q}} \in \bar{\mathcal{Q}}$ . Then, the skewsymmetry of the Poisson bracket (26b) translates into the skewsymmetry of  $\bar{\mathbb{J}}(\bar{\mathbf{q}}) : \bar{\mathcal{Q}}^* \rightarrow \bar{\mathcal{Q}}$ , i.e.,

$$\bar{\mathbb{J}}(\bar{\mathbf{q}}) = -\bar{\mathbb{J}}^*(\bar{\mathbf{q}}) \quad \text{for all } \bar{\mathbf{q}} \in \bar{\mathcal{Q}}. \quad (27b)$$

Here, the operator  $\bar{\mathbb{J}}^* : \bar{\mathcal{Q}}^* \rightarrow \bar{\mathcal{Q}}^{**}$  denotes the adjoint of the linear operator  $\bar{\mathbb{J}}$  and  $\bar{\mathcal{Q}}^{**}$  is the bidual of  $\bar{\mathcal{Q}}$ . The Leibniz rule (26d) for the bracket (27a) follows from the product rule for the Fréchet derivative. Instead, Jacobi's identity (26c) for state-dependent  $\bar{\mathbb{J}}(\bar{\mathbf{q}})$  states an additional, nontrivial constraint [27, 28] that generalizes the commutation law for partial derivatives [12] and that needs to be verified for the bracket (27a), see also Remark 3.2.

In view of the above properties of a Poisson bracket, we call the operator  $\bar{\mathbb{J}}$  with properties (27) a Poisson structure or Poisson operator [41, 27, 28, 44]. We remark that  $\bar{\mathbb{J}}$  is also called a cosymplectic structure or cosymplectic operator [41, 52]. Since this is the geometric structure underlying Hamiltonian mechanics together with the energy functional  $\bar{\mathcal{E}} : \bar{\mathcal{Q}} \rightarrow \mathbb{R}$  (Hamiltonian) defined on an appropriate state space  $\bar{\mathcal{Q}}$ , we call the triple  $(\bar{\mathcal{Q}}, \bar{\mathcal{E}}, \bar{\mathbb{J}})$  a Hamiltonian system. Based on  $(\bar{\mathcal{Q}}, \bar{\mathcal{E}}, \bar{\mathbb{J}})$ , for  $\bar{\mathbf{q}} : [0, T] \rightarrow \bar{\mathcal{Q}}$  and  $t \in [0, T]$ , the equations of motion are given by

$$\partial_t \bar{\mathbf{q}}(t) = \bar{\mathbb{J}}(\bar{\mathbf{q}}(t)) D\bar{\mathcal{E}}(\bar{\mathbf{q}}(t)) \quad \text{in } \bar{\mathcal{Q}}. \quad (28)$$

Assume now that  $\bar{\mathcal{Q}}$  is a reflexive Banach space so that  $\bar{\mathcal{Q}}^{**} \equiv \bar{\mathcal{Q}}$ . Then, by the skewsymmetry of  $\bar{\mathbb{J}}(\bar{\mathbf{q}})$  we have

$$\langle \bar{\xi}_1, \bar{\mathbb{J}}(\bar{\mathbf{q}}) \bar{\xi}_2 \rangle_{\bar{\mathcal{Q}}} = \langle \bar{\xi}_2, \bar{\mathbb{J}}^*(\bar{\mathbf{q}}) \bar{\xi}_1 \rangle_{\bar{\mathcal{Q}}} = \langle \bar{\xi}_2, -\bar{\mathbb{J}}(\bar{\mathbf{q}}) \bar{\xi}_1 \rangle_{\bar{\mathcal{Q}}} \quad (29)$$

for all  $\bar{\xi}_1, \bar{\xi}_2 \in \bar{\mathcal{Q}}^*$ , and therefore  $\langle \bar{\xi}, \bar{\mathbb{J}}(\bar{\mathbf{q}}) \bar{\xi} \rangle_{\bar{\mathcal{Q}}} = 0$  for any  $\bar{\xi} \in \bar{\mathcal{Q}}^*$ . Hence, by the chain rule and as a direct consequence of skewsymmetry, it follows for a Hamiltonian system  $(\bar{\mathcal{Q}}, \bar{\mathcal{E}}, \bar{\mathbb{J}})$  that the total energy is conserved along a solution  $\bar{\mathbf{q}} : [0, T] \rightarrow \bar{\mathcal{Q}}$  of (28), i.e.,

$$\frac{d}{dt} \bar{\mathcal{E}}(\bar{\mathbf{q}}(t)) = \langle D\bar{\mathcal{E}}(\bar{\mathbf{q}}(t)), \partial_t \bar{\mathbf{q}}(t) \rangle_{\bar{\mathcal{Q}}} = \langle D\bar{\mathcal{E}}(\bar{\mathbf{q}}(t)), \bar{\mathbb{J}}(\bar{\mathbf{q}}(t)) D\bar{\mathcal{E}}(\bar{\mathbf{q}}(t)) \rangle_{\bar{\mathcal{Q}}} = 0. \quad (30)$$

**Remark 3.1** By (27a), the mapping property (26a) of the Poisson bracket and Jacobi's identity (26c) impose certain requirements on the state-dependent Poisson operator  $\bar{\mathbb{J}}(\cdot)$ . In order to have the expressions in (26c) well-defined, it has to be ensured that each of the three terms above to the right is an element of  $\bar{\mathcal{Q}}^*$ , so that for all for all  $\bar{\mathcal{F}}, \bar{\mathcal{G}} \in \bar{\mathcal{X}}$ ,  $\bar{\mathbf{q}} \in \bar{\mathcal{Q}}$  it is

$$D_{\bar{\mathbf{q}}} \langle D_{\bar{\mathbf{q}}} \bar{\mathcal{F}}(\bar{\mathbf{q}}), \bar{\mathbb{J}}(\bar{\mathbf{q}}) D_{\bar{\mathbf{q}}} \bar{\mathcal{G}}(\bar{\mathbf{q}}) \rangle_{\bar{\mathcal{Q}}} \in \bar{\mathcal{Q}}^*. \quad (31a)$$

Moreover, mapping property (26a) further requires that

$$\bar{\mathbb{J}}(\cdot) \bar{\xi} : \bar{\mathcal{Q}} \rightarrow \bar{\mathcal{Q}} \text{ is a smooth map for all } \bar{\xi} \in \bar{\mathcal{Q}}^*. \quad (31b)$$

In conclusion, we have the following statement:

*Assume that (31) holds true. Then the bracket generated by  $\bar{\mathbb{J}}$  via (27a) is a smooth map, i.e.,*  $\{\circ, \circ\}_{\bar{\mathcal{Q}}} := \langle D_{\bar{\mathbf{q}}} \circ, \bar{\mathbb{J}} D_{\bar{\mathbf{q}}} \circ \rangle_{\bar{\mathcal{Q}}} : \bar{\mathcal{X}} \times \bar{\mathcal{X}} \rightarrow \bar{\mathcal{X}}$ , *and the terms in (26c) are well-defined.* (32)

\*

**Remark 3.2** In finite dimensions the Jacobi identity can be simplified [52] to

$$\sum_l \bar{\mathbb{J}}_{il} \partial_{\bar{q}_l} \bar{\mathbb{J}}_{jk} + \bar{\mathbb{J}}_{jl} \partial_{\bar{q}_l} \bar{\mathbb{J}}_{ki} + \bar{\mathbb{J}}_{kl} \partial_{\bar{q}_l} \bar{\mathbb{J}}_{ij} = 0, \quad (33)$$

which is easier to check than Jacobi's identity (26c). While this is satisfied for Poisson structures that do not depend on the state, e.g., canonical structures, this can be non-trivial to check when the Poisson structure depends on the state variable. \*

**Example 3.3 (Newton's laws)** Consider the finite-dimensional state vector  $\bar{\mathbf{q}} = (\bar{\mathbf{x}}, \bar{\mathbf{p}}) \in \bar{\mathcal{Q}} = \mathbb{R}^{2d}$  with the position vector  $\bar{\mathbf{x}} \in \mathbb{R}^d$  and the linear momentum  $\bar{\mathbf{p}} \in \mathbb{R}^d$ . Since  $\bar{\mathcal{Q}}$  is finite-dimensional, we have  $\bar{\mathcal{Q}}^* \equiv \bar{\mathcal{Q}}$  and the dual pairing can be identified with the scalar product. Furthermore, we introduce the *canonical form* of the Poisson structure

$$\bar{\mathbb{J}}(\bar{\mathbf{q}}) = \bar{\mathbb{J}}_{\text{can}} := \begin{pmatrix} 0 & +\mathbb{I}_d \\ -\mathbb{I}_d & 0 \end{pmatrix}, \quad (34a)$$

with  $\mathbb{I}_d \in \mathbb{R}^{d \times d}$  the  $(d \times d)$ -identity matrix. The Poisson structure  $\bar{\mathbb{J}}_{\text{can}} : \mathbb{R}^{2d} \rightarrow \mathbb{R}^{2d}$  is linear and skewsymmetric, i.e.,  $\bar{\mathbb{J}}_{\text{can}}^* = -\bar{\mathbb{J}}_{\text{can}}$ , and defines the Poisson bracket

$$\begin{aligned} \{\bar{\mathcal{F}}, \bar{\mathcal{G}}\} &= D\bar{\mathcal{F}} \cdot \bar{\mathbb{J}}_{\text{can}} D\bar{\mathcal{G}} \\ &= \sum_{i,j=1}^{2d} \partial_{\bar{q}_i} \bar{\mathcal{F}} \bar{\mathbb{J}}_{\text{can}_{ij}} \partial_{\bar{q}_j} \bar{\mathcal{G}} = \sum_{i=1}^d \left( \frac{\partial \bar{\mathcal{G}}}{\partial \bar{p}_i} \frac{\partial \bar{\mathcal{F}}}{\partial \bar{x}_i} - \frac{\partial \bar{\mathcal{F}}}{\partial \bar{p}_i} \frac{\partial \bar{\mathcal{G}}}{\partial \bar{x}_i} \right) \end{aligned}$$

for all smooth functions  $\bar{\mathcal{F}}, \bar{\mathcal{G}} : \bar{\mathcal{Q}} \rightarrow \mathbb{R}$ . Using (33) Jacobi's identity is directly confirmed. We introduce the Hamiltonian  $\bar{\mathcal{E}} : \bar{\mathcal{Q}} \rightarrow \mathbb{R}$  as follows

$$\bar{\mathcal{E}}(\bar{\mathbf{q}}) = \frac{|\bar{\mathbf{p}}|^2}{2M} + \bar{U}_{\text{pot}}(\bar{\mathbf{x}}), \quad (34b)$$

with  $M > 0$  the (particle) mass and  $\bar{U}_{\text{pot}} : \mathbb{R}^d \rightarrow \mathbb{R}$  the potential energy. With the driving force

$$D_{\bar{\mathbf{q}}} \bar{\mathcal{E}}(\bar{\mathbf{q}}) = \begin{pmatrix} \bar{\nabla} \bar{U}_{\text{pot}}(\bar{\mathbf{x}}) \\ \frac{\bar{\mathbf{p}}}{M} \end{pmatrix}$$

the Newton's equations for  $\bar{\mathbf{q}} : [0, T] \rightarrow \bar{\mathcal{Q}}$  generated by the Hamiltonian system  $(\bar{\mathcal{Q}}, \bar{\mathcal{E}}, \bar{\mathbb{J}})$  are

$$\begin{aligned} \partial_t \bar{\mathbf{x}} &= +\frac{\bar{\mathbf{p}}}{M}, \\ \partial_t \bar{\mathbf{p}} &= -\bar{\nabla} \bar{U}_{\text{pot}}(\bar{\mathbf{x}}). \end{aligned}$$

with the conservative force being the gradient of the potential energy  $\bar{U}_{\text{pot}}$ , i.e.,  $(\bar{\nabla} \bar{U}_{\text{pot}})_i = \partial_{\bar{x}_i} \bar{U}_{\text{pot}}$ ,  $i = 1, \dots, d$ . \*

### 3.2 Gradient systems $(\bar{\mathcal{Q}}, \bar{\mathcal{S}}, \bar{\mathbb{K}})$ for irreversible dynamics

Gradient systems describe the dynamics of irreversible, dissipative effects. Like Hamiltonian systems for conservative dynamics, also gradient systems are characterized by a triple  $(\bar{\mathcal{Q}}, \bar{\mathcal{S}}, \bar{\mathbb{K}})$  given by a state space  $\bar{\mathcal{Q}}$ , a driving functional  $\bar{\mathcal{S}} : \bar{\mathcal{Q}} \rightarrow \mathbb{R}$ , and a geometric structure  $\bar{\mathbb{K}} : \bar{\mathcal{Q}}^* \rightarrow \bar{\mathcal{Q}}$ . Based on  $(\bar{\mathcal{Q}}, \bar{\mathcal{S}}, \bar{\mathbb{K}})$  the evolution equation for the state vector  $\bar{\mathbf{q}} : [0, T] \rightarrow \bar{\mathcal{Q}}$  reads

$$\partial_t \bar{\mathbf{q}}(t) = \bar{\mathbb{K}}(\bar{\mathbf{q}}(t)) D_{\bar{\mathbf{q}}} \bar{\mathcal{S}}(\bar{\mathbf{q}}(t)) \quad \text{in } \bar{\mathcal{Q}}. \quad (36)$$

Again,  $\bar{Q}$  is a Banach space with dual space  $\bar{Q}^*$  and  $\langle \cdot, \cdot \rangle_{\bar{Q}}$  the dual pairing. The driving functional is either the entropy  $\bar{S}$  or a free energy functional, and the geometric structure is imposed by an operator  $\bar{\mathbb{K}}(\bar{q}) : \bar{Q}^* \rightarrow \bar{Q}$  with the following properties for all  $\bar{q} \in \bar{Q}$ :

$$\bullet \bar{\mathbb{K}}(\bar{q}) \text{ is symmetric, i.e. } \bar{\mathbb{K}}(\bar{q}) = \bar{\mathbb{K}}^*(\bar{q}), \quad (37a)$$

$$\bullet \bar{\mathbb{K}}(\bar{q}) \text{ is positively semidefinite, i.e. } \langle \bar{\xi}, \bar{\mathbb{K}}(\bar{q})\bar{\xi} \rangle_{\bar{Q}} \geq 0. \quad (37b)$$

The symmetry property (37a) of  $\bar{\mathbb{K}}$  is a generalization of Onsager's reciprocity principle [58], which provides reciprocal relations between rates and their thermodynamically conjugate forces in certain thermodynamical non-equilibrium systems. The positive semidefiniteness (37b) is a manifestation of the second law of thermodynamics. In other words, the positive semidefiniteness of  $\bar{\mathbb{K}}$  ensures the increase of entropy:

$$\frac{d}{dt} \bar{S}(\bar{q}(t)) = \langle D\bar{S}(\bar{q}(t)), \partial_t \bar{q}(t) \rangle_{\bar{Q}} = \langle D\bar{S}(\bar{q}(t)), \bar{\mathbb{K}}(\bar{q}(t)) D\bar{S}(\bar{q}(t)) \rangle_{\bar{Q}} \geq 0. \quad (38)$$

In the light of Onsager's reciprocity principle, we call the operator  $\bar{\mathbb{K}}$  that contributes the geometric structure to a gradient system  $(\bar{Q}, \bar{S}, \bar{\mathbb{K}})$  by properties (37) an *Onsager operator*. In the same way as  $\bar{\mathbb{J}}$  generates a Poisson bracket for reversible dynamics with the aid of the dual pairing, cf. (27a), the Onsager operator  $\bar{\mathbb{K}}$  generates a dissipative bracket [27, 28, 51, 6]  $[\cdot, \cdot] : \bar{\mathcal{X}} \times \bar{\mathcal{X}} \rightarrow \bar{\mathcal{X}}$  defined as

$$[\bar{\mathcal{F}}, \bar{\mathcal{G}}](\bar{q}) := \langle D_{\bar{q}} \bar{\mathcal{F}}(\bar{q}), \bar{\mathbb{K}}(\bar{q}) D_{\bar{q}} \bar{\mathcal{G}}(\bar{q}) \rangle_{\bar{Q}}, \quad (39)$$

for all  $\bar{\mathcal{F}}, \bar{\mathcal{G}} \in \bar{\mathcal{X}}$  and any  $\bar{q} \in \bar{Q}$ .

The irreversible dynamics also allows for an equivalent description [43] via the non-negative dual dissipation potential  $\bar{\Psi}^* : \bar{Q} \times \bar{Q}^* \rightarrow \mathbb{R}$

$$\bar{\Psi}^*(\bar{q}; \bar{\xi}) = \frac{1}{2} \langle \bar{\xi}, \bar{\mathbb{K}}(\bar{q}) \bar{\xi} \rangle_{\bar{Q}}, \quad (40)$$

which is quadratic in the thermodynamic driving force  $\bar{\xi} \in \bar{Q}^*$ . More generally,  $\bar{\Psi}^*(\bar{q}; \cdot)$  can be non-quadratic, but nonnegative, convex, with the property  $\bar{\Psi}^*(\bar{q}; 0) = 0$  for any  $\bar{q} \in \bar{Q}$ . Then, the triple  $(\bar{Q}, \bar{S}, \bar{\Psi}^*)$  is a *generalized* gradient system and its evolution equation reads

$$\partial_t \bar{q}(t) = D_{\bar{\xi}} \bar{\Psi}^*(\bar{q}(t); D\bar{S}(\bar{q}(t))) \quad \text{in } \bar{Q}. \quad (41)$$

The extension to nonquadratic dissipation potentials (41) is relevant, for example, for materials with a rate-independent hysteretic evolution of the internal variable [44] or for reactions with cosh-type dissipation potential motivated by large-deviation principles [46, 39]. We point out that evolution equations (36) and (41) are rate equations, where the Onsager operator  $\bar{\mathbb{K}}$ , or more generally, the non-linear operator  $D_{\bar{\xi}} \bar{\Psi}^*(\bar{q}; \cdot)$  maps the thermodynamic driving force  $D\bar{S}(\bar{q}) \in \bar{Q}^*$  to a rate  $\partial_t \bar{q} \in \bar{Q}$ .

By exploiting the convexity of the dual dissipation potential one obtains via Legendre transform its convex conjugate, the dissipation potential  $\bar{\Psi} : \bar{Q} \times \bar{Q} \rightarrow \mathbb{R}$ . Based on  $\bar{\Psi}(\bar{q}; \bar{v})$ , the evolution law (41) can be equivalently formulated as a force balance

$$D_{\bar{v}} \bar{\Psi}(\bar{q}; \partial_t \bar{q}(t)) = D\bar{S}(\bar{q}(t)) \quad \text{in } \bar{Q}^*. \quad (42a)$$

If  $\bar{\Psi}^*(\bar{q}; \cdot)$  is quadratic as in (40) and defined via an invertible operator  $\bar{\mathbb{K}}(\bar{q})$ , then the dissipation potential is  $\bar{\Psi}(\bar{q}; \bar{v}) = \frac{1}{2} \langle \bar{\mathbb{K}}(\bar{q})^{-1} \bar{v}, \bar{v} \rangle_{\bar{Q}}$  for all rates  $\bar{v} \in \bar{Q}$ . With the inverse operator  $\bar{\mathbb{K}}(\bar{q})^{-1} : \bar{Q} \rightarrow \bar{Q}^*$ , the force balance becomes

$$\bar{\mathbb{K}}(\bar{q})^{-1} \partial_t \bar{q}(t) = D\bar{S}(\bar{q}(t)) \quad \text{in } \bar{Q}^*. \quad (42b)$$

In comparison to force balance (42), the formulation of dissipative dynamics in terms of a rate equation (36), i.e., in terms of Onsager operators and dual dissipation potentials, has the advantage that different dissipative mechanisms related to one state variable can be included to the system simply by adding the corresponding dual dissipation potentials or equivalently by adding the Onsager operators. For example, for different dissipative effects  $i \in \{1, \dots, k\}$  related to the state vector  $\bar{q}$  described by dual dissipation potentials  $\bar{\Psi}_i^*$  and corresponding Onsager operators  $\bar{\mathbb{K}}_i = D_{\bar{\xi}} \bar{\Psi}_i^*(\bar{q}; \bar{\xi})$ , e.g.,  $i \in \{\text{heat, viscosity, reaction, diffusion, } \dots\}$ , the dual dissipation potential describing the total, coupled dissipative dynamics is obtained as the sum of the relevant dissipative processes  $i$ , i.e.,  $\bar{\Psi}_{\text{tot}}^*(\bar{q}; \bar{\xi}) = \sum_{i=1}^k \bar{\Psi}_i^*(\bar{q}; \bar{\xi})$  and accordingly  $\bar{\mathbb{K}}_{\text{tot}}(\bar{q}) := \sum_{i=1}^k \bar{\mathbb{K}}_i(\bar{q})$ . Instead, the corresponding formulation in terms of the total dissipation potential  $\bar{\Psi}_{\text{tot}}$  is less straight forward since the Legendre transform of the sum  $\bar{\Psi}_{\text{tot}}^*(\bar{q}; \bar{\xi}) = \sum_{i=1}^k \bar{\Psi}_i^*(\bar{q}; \bar{\xi})$  involves an inf-convolution. We exploit in Sections 5.4 and 6 the coupling of different dissipative effects by summing the different dual dissipation potentials, resp. their Onsager operators.

**Example 3.4 (Viscous damped evolution)** Consider the finite-dimensional state variable  $\bar{q} \equiv \bar{x} = (\bar{x}_1, \dots, \bar{x}_d)^\top \in \mathbb{R}^d = \bar{Q}$  given by the position vector and a potential energy as the sole contribution to the free energy, which is the driving functional for isothermal systems, i.e.,  $\bar{U}(\bar{q}) = \bar{U}_{\text{pot}}(\bar{x})$ . We introduce the state-dependent dual dissipation potential  $\bar{\Psi}^* : \bar{Q} \times \bar{Q}^* \rightarrow \mathbb{R}$  for viscous damping by

$$\bar{\Psi}_{\text{vd}}^*(\bar{x}; \bar{\xi}) := \frac{1}{2} \bar{\xi} \cdot \bar{K}_{\text{vd}}(\bar{x}) \bar{\xi}, \quad (43a)$$

with positively semidefinite, symmetric  $\bar{K}_{\text{vd}} : \bar{Q} \rightarrow \mathbb{R}^{d \times d}$ . This gives the Onsager operator for viscous damping

$$\bar{\mathbb{K}}_{\text{vd}}(\bar{x}) \bar{\xi} = D_{\bar{\xi}} \bar{\Psi}_{\text{vd}}^*(\bar{x}; \bar{\xi}) = \bar{K}_{\text{vd}}(\bar{x}) \bar{\xi}. \quad (43b)$$

The properties of  $\bar{K}_{\text{vd}}$  ensure that  $\bar{\mathbb{K}}_{\text{vd}}$  is a linear, symmetric, and positively semidefinite operator. The triple  $(\bar{Q}, \bar{\mathcal{F}}, \bar{\mathbb{K}}_{\text{vd}})$  leads to the system of evolution equations

$$\partial_t \bar{x} = -\bar{\mathbb{K}}_{\text{vd}}(\bar{x}) D_{\bar{x}} \bar{U}(\bar{x}) = -\bar{K}_{\text{vd}}(\bar{x}) \bar{\nabla} \bar{U}_{\text{pot}}(\bar{x}), \quad (43c)$$

where the Onsager operator  $\bar{\mathbb{K}}_{\text{vd}}$  transforms the force  $-D\bar{U} = -\bar{\nabla} \bar{U}_{\text{pot}}$  into a rate  $\partial_t \bar{x}$ . Suppose now that  $\bar{\mathbb{K}}_{\text{vd}}(\bar{x}) = \bar{K}_{\text{vd}}(\bar{x})$  is even positively definite for all  $\bar{x} \in \mathbb{R}^d$ . Then, the dissipation potential  $\bar{\Psi}_{\text{vd}} : \bar{Q} \times \bar{Q} \rightarrow \mathbb{R}$  can be defined as

$$\bar{\Psi}_{\text{vd}}(\bar{x}; \bar{v}) := \frac{1}{2} \bar{v} \cdot \bar{K}_{\text{vd}}^{-1}(\bar{x}) \bar{v} \quad (43d)$$

with rates  $\bar{v} = \partial_t \bar{x}$ , and the evolution can be equivalently rewritten as the force balance

$$0 = \partial_{\bar{v}} \bar{\Psi}_{\text{vd}}(\bar{x}; \partial_t \bar{x}) + D_{\bar{x}} \bar{U}(\bar{x}) = \bar{G}_{\text{vd}}(\bar{x}) \partial_t \bar{x} + \bar{\nabla} \bar{U}_{\text{pot}}(\bar{x}),$$

with  $\bar{G}_{\text{vd}} = \bar{K}_{\text{vd}}^{-1}$ . If either  $\bar{G}_{\text{vd}}(\bar{x})$  or  $\bar{K}_{\text{vd}}(\bar{x})$  has a kernel, this results in algebraic constraints where either the rate or the force in this subspace vanishes at  $\bar{x}$ . \*

### 3.3 GENERIC systems $(\bar{Q}, \bar{\mathcal{E}}, \bar{\mathcal{S}}, \bar{\mathbb{J}}, \bar{\mathbb{K}})$ for coupled dynamics

A GENERIC system provides a description of isolated systems using the quintuple  $(\bar{Q}, \bar{\mathcal{E}}, \bar{\mathcal{S}}, \bar{\mathbb{J}}, \bar{\mathbb{K}})$ , where the triple  $(\bar{Q}, \bar{\mathcal{E}}, \bar{\mathbb{J}})$  is a Hamiltonian system and  $(\bar{Q}, \bar{\mathcal{S}}, \bar{\mathbb{K}})$  is an Onsager system. In addition to the structural relations (27) and (37) for the Poisson and the Onsager operator, there are the following nontrivial coupling conditions required to hold

$$\bar{\mathbb{K}}D\bar{\mathcal{E}} \equiv 0 \quad \text{and} \quad \bar{\mathbb{J}}D\bar{\mathcal{S}} \equiv 0, \quad (44a)$$

$$\bar{\mathbb{K}}D\bar{\mathcal{M}} \equiv 0 \quad \text{and} \quad \bar{\mathbb{J}}D\bar{\mathcal{M}} \equiv 0, \quad (44b)$$

which we call *noninteraction conditions*. Then, the combined evolution equations have the form

$$\partial_t \bar{q} = \bar{\mathbb{J}}(\bar{q})D_{\bar{q}}\bar{\mathcal{E}}(\bar{q}) + \bar{\mathbb{K}}(\bar{q})D_{\bar{q}}\bar{\mathcal{S}}(\bar{q}), \quad (45)$$

which clearly shows the reversible and the irreversible part of the dynamics. The noninteraction conditions (44a) ensure that the driving force of reversible dynamics  $D\bar{\mathcal{E}}$  is in the kernel of the operator for irreversible dynamics and vice versa. Similar constraints for quantities that are conserved under reversible and irreversible processes are added to the formalism using (44b). Throughout this work we satisfy the conservation of total mass  $\bar{\mathcal{M}}$  by construction using the constraint (24). Note that the noninteraction conditions (44) express that the operators  $\bar{\mathbb{J}}$  and  $\bar{\mathbb{K}}$  have a nontrivial kernel. The noninteraction conditions have the following direct implications [27, 28, 44], see also Sec. A.2:

**Theorem 3.5 (Consequences of conditions (44))** *Let  $(\bar{Q}, \bar{\mathcal{E}}, \bar{\mathcal{S}}, \bar{\mathbb{J}}, \bar{\mathbb{K}})$  be a GENERIC system satisfying the noninteraction conditions (44) and  $\bar{q} : [0, T] \rightarrow \bar{Q}$  a solution of the GENERIC evolution equations (45). Then the system also has the following properties:*

i) *In accordance with the first law of thermodynamics, the total energy  $\bar{\mathcal{E}}$  is conserved:*

$$\frac{d}{dt}\bar{\mathcal{E}}(\bar{q}(t)) = 0. \quad (46a)$$

ii) *In accordance with the second law of thermodynamics, the entropy  $\bar{\mathcal{S}}$  is increasing:*

$$\frac{d}{dt}\bar{\mathcal{S}}(\bar{q}(t)) \geq 0. \quad (46b)$$

iii) *The total mass  $\bar{\mathcal{M}}$  is conserved:*

$$\frac{d}{dt}\bar{\mathcal{M}}(\bar{q}(t)) = 0. \quad (46c)$$

iv) *Stationary states are governed by the maximum entropy principle, i.e., states  $\bar{q}_*$  that maximize the entropy under the constraint*

$$\bar{\mathcal{E}}(\bar{q}_*) = \bar{\mathcal{E}}_0 \quad \text{and} \quad \bar{\mathcal{M}}(\bar{q}_*) = \bar{\mathcal{M}}_0, \quad (46d)$$

*for any attainable  $\bar{\mathcal{E}}_0, \bar{\mathcal{M}}_0 \in \mathbb{R}$ , are stationary.*

**Example 3.6 (GENERIC system)** We now couple Example 3.3 of a finite-dimensional Hamiltonian system with Example 3.4 of a finite-dimensional gradient system to construct a GENERIC system. Now, the state variable is given by the vector  $\bar{q} = (\bar{x}, \bar{p}, \bar{S}) \in \bar{Q} = \mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}$  with  $\bar{x}$  the position vector,  $\bar{p}$  the linear momentum, and  $\bar{S}$  the entropy.

The driving functionals are the total energy for reversible and the entropy for dissipative processes

$$\bar{\mathcal{E}}(\bar{\mathbf{q}}) = \bar{E}_{\text{kin}}(\bar{\mathbf{q}}) + \bar{U}(\bar{\mathbf{q}}) \quad \text{and} \quad \bar{\mathcal{S}}(\bar{\mathbf{q}}) = \bar{S},$$

where the internal energy  $\bar{U}$  contains thermal and mechanical contributions and  $\bar{E}_{\text{kin}} = \frac{|\bar{\mathbf{p}}|^2}{2M}$ . Using the equation of state for the ideal gas (14), we set

$$\bar{U}(\bar{\mathbf{q}}) = \bar{U}_{\text{pot}}(\bar{\mathbf{x}}) + \bar{U}_{\text{heat}}(\bar{S}) \quad \text{with} \quad \bar{U}_{\text{heat}}(\bar{S}) = C \exp\left(\frac{\bar{S}}{C_V}\right).$$

Accordingly, the driving forces are

$$D\bar{\mathcal{E}}(\bar{\mathbf{q}}) = \begin{pmatrix} \nabla \bar{U}_{\text{pot}}(\bar{\mathbf{x}}) \\ \frac{\bar{\mathbf{p}}}{M} \\ \bar{\theta} \end{pmatrix}, \quad D\bar{\mathcal{S}}(\bar{\mathbf{q}}) = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix},$$

with positive temperature  $\bar{\theta} = \partial_{\bar{S}} \bar{U}_{\text{heat}} = \bar{C}_V^{-1} \bar{U}_{\text{heat}} > 0$ . Embedding the canonical Poisson structure (34a) that generates Newtons laws into the Poisson operator by

$$\bar{\mathbb{J}}(\bar{\mathbf{q}}) = \begin{pmatrix} \bar{\mathbb{J}}_{\text{can}} & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & +\mathbb{I}_d & 0 \\ -\mathbb{I}_d & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad (47a)$$

ensures that the noninteraction condition  $\bar{\mathbb{J}}D\bar{\mathcal{S}} \equiv 0$  from (44a) is satisfied. The Poisson operator  $\bar{\mathbb{J}}$  from (47a) is skewsymmetric and satisfies Jacobi's identity. However,  $\bar{\mathbb{J}}$  is non-canonical and non-invertible due to the degeneracy in the last line and column. Moreover, similar to (43c) we reuse the Onsager operator

$$\bar{\mathbb{K}}_{\text{visc}}(\bar{\mathbf{q}}) = \bar{\theta} \begin{pmatrix} 0 & 0 & 0 \\ 0 & \bar{K}_{\text{visc}}(\bar{\mathbf{q}}) & -\bar{\theta}^{-1} \bar{K}_{\text{visc}}(\bar{\mathbf{q}}) \bar{\nu} \\ 0 & -\bar{\theta}^{-1} \bar{\nu}^\top \bar{K}_{\text{visc}}(\bar{\mathbf{q}}) & \bar{\theta}^{-2} \bar{\nu}^\top \bar{K}_{\text{visc}}(\bar{\mathbf{q}}) \bar{\nu} \end{pmatrix}, \quad (47b)$$

for the GENERIC structure, with the velocity  $\bar{\nu} = \bar{\mathbf{p}}/\bar{M}$  and symmetric, positively semidefinite matrix-valued  $\bar{K}_{\text{visc}} : \bar{\mathcal{Q}} \rightarrow \mathbb{R}^{d \times d}$ . The matrix  $\bar{\mathbb{K}}_{\text{visc}}(\bar{\mathbf{q}})$  is also symmetric and positively semidefinite for all  $\bar{\mathbf{q}} \in \bar{\mathcal{Q}}$ , since for every  $\bar{\xi} = (\bar{\xi}_{\bar{\mathbf{x}}}, \bar{\xi}_{\bar{\mathbf{p}}}, \bar{\xi}_{\bar{S}}) \in \bar{\mathcal{Q}}^*$  and with  $\bar{\mathbf{w}} := \bar{\xi}_{\bar{\mathbf{p}}} - \bar{\theta}^{-1} \bar{\nu} \bar{\xi}_{\bar{S}}$  the dual dissipation potential satisfies

$$\bar{\Psi}_{\text{visc}}^*(\bar{\mathbf{q}}; \bar{\xi}) = \frac{1}{2} \langle \bar{\xi}, \bar{\mathbb{K}}_{\text{visc}} \bar{\xi} \rangle = \bar{\theta} \bar{\mathbf{w}}^\top \bar{K}_{\text{visc}}(\bar{\mathbf{q}}) \bar{\mathbf{w}} \geq 0. \quad (47c)$$

The evolution equations (45) for the GENERIC system  $(\bar{\mathcal{Q}}, \bar{\mathcal{E}}, \bar{\mathcal{S}}, \bar{\mathbb{J}}, \bar{\mathbb{K}}_{\text{visc}})$  then read

$$\partial_t \bar{\mathbf{x}} = \bar{M}^{-1} \bar{\mathbf{p}} \equiv \bar{\nu}, \quad (48a)$$

$$\partial_t \bar{\mathbf{p}} = -\nabla \bar{U}_{\text{pot}}(\bar{\mathbf{x}}) - \bar{K}_{\text{visc}}(\bar{\mathbf{q}}) \bar{\nu}, \quad (48b)$$

$$\partial_t \bar{S} = \bar{\theta}^{-1} \bar{\nu}^\top \bar{K}_{\text{visc}}(\bar{\mathbf{q}}) \bar{\nu}, \quad (48c)$$

and an exemplarily solution in  $d = 1$  is shown in Fig. 3.

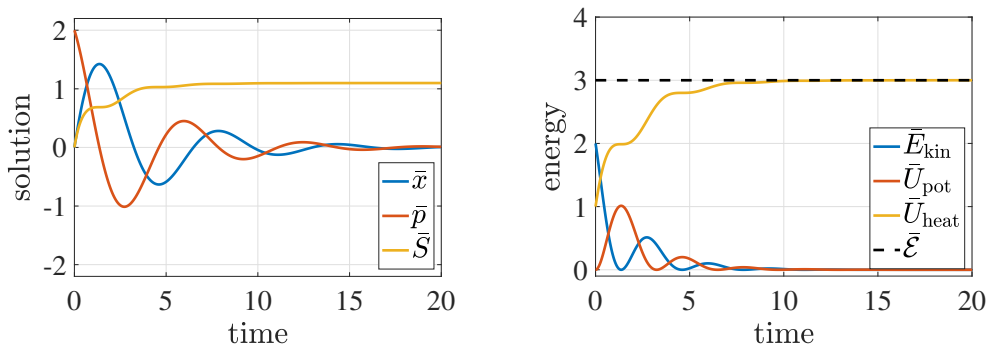


Figure 3: Example solution of GENERIC system in  $d = 1$  with  $\bar{M} = C = \bar{C}_{\bar{V}} = 1$ ,  $\bar{K}_{\text{visc}} = 2$ ,  $\bar{U}_{\text{pot}}(\bar{x}) = \frac{1}{2}\bar{x}^2$  and initial data  $\bar{x}(0) = 0$ ,  $\bar{p}(0) = 2$ ,  $\bar{S}(0) = 0$ . Left panel shows oscillating solution with increasing entropy, whereas right panel shows energy components for total conserved energy  $\bar{\mathcal{E}}$ .

Alternatively, (48a) can be differentiated with respect to time and combined with (48b) to obtain the usual second-order rate equation

$$\bar{M}\partial_t^2\bar{x} = -\bar{\nabla}\bar{U}_{\text{pot}}(\bar{x}) - \bar{K}_{\text{visc}}(\bar{q})\partial_t\bar{x}, \quad (48b^*)$$

as the momentum balance together with the entropy evolution (48c). Note that (48b), resp. (48b<sup>\*</sup>), is a force balance whereas the corresponding evolution law (43c) for the pure gradient system is a rate equation. We obtain the same dynamics when neglecting inertia  $\bar{M} = 0$  and setting  $\bar{K}_{\text{visc}}(\bar{q}) = \bar{K}_{\text{vd}}^{-1}(\bar{x})$ . This is due to the fact that momentum balance (48b) decouples from the evolution law (48c).

\*

### 3.4 Change of variables and coordinates in GENERIC

Next, we discuss transformations of the state variables  $\mathbb{T} : \hat{\mathcal{Q}} \rightarrow \tilde{\mathcal{Q}}$  involved in the GENERIC framework and how this affects the GENERIC evolution equation (45). In particular, we are answering the question, under what condition a transformed evolution is again generated by a GENERIC system so that this diagram commutes:

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

where  $\mathbb{L}(\hat{\mathbf{q}}) := \mathbb{D}_{\hat{\mathbf{q}}}\mathbb{T}(\hat{\mathbf{q}})$  is the Fréchet derivative of  $\mathbb{T}$  in  $\hat{\mathbf{q}}$ . We consider two classes of transformations: The first one, denoted by  $\mathbb{T}_{\text{LE}}$ , accounts for a change of coordinates from the Lagrangian to the Eulerian frame, and the second one, denoted by  $\mathbb{T}_{\text{v}}$ , carries out a change of thermodynamic state variables. The coordinate transform  $\mathbb{T}_{\text{LE}}$  from the Lagrangian to the Eulerian frame involves the flow map and for each thermodynamic variable it is realized through the mappings introduced in Definition 2.6. We first explain the general strategy common to both types of transformations  $\mathbb{T}_{\text{v}}$  and  $\mathbb{T}_{\text{LE}}$ , and discuss the individual details separately in Sec. 3.4.1 and 3.4.2.

Consider a transformation  $\mathbb{T} : \hat{\mathcal{Q}} \rightarrow \tilde{\mathcal{Q}}$  that is a continuously differentiable map from a Banach space  $\hat{\mathcal{Q}}$  to a Banach space  $\tilde{\mathcal{Q}}$ . Let  $\tilde{\mathbf{q}} = \mathbb{T}(\hat{\mathbf{q}}) \in \tilde{\mathcal{Q}}$  for an element  $\hat{\mathbf{q}} \in \hat{\mathcal{Q}}$ . We point out that  $\mathbb{T}$  need not

to be invertible, which is in particular the case for transformations of the type  $T_{LE}$ . Nevertheless, if  $T$  were invertible, transformed functionals  $\tilde{\mathcal{A}} : \tilde{\mathcal{Q}} \rightarrow \mathbb{R}$  can always be defined by

$$\tilde{\mathcal{A}}(\tilde{\mathbf{q}}) := \hat{\mathcal{A}}(T^{-1}(\tilde{\mathbf{q}})) \text{ for all } \tilde{\mathbf{q}} \in \tilde{\mathcal{Q}}. \quad (49)$$

However, in order to well-define the mapping of the GENERIC system also for non-invertible transformations, one needs to impose certain *closure conditions* [52].

**Definition 3.7 (Closure conditions)** Consider a GENERIC system  $(\hat{\mathcal{Q}}, \hat{\mathcal{E}}, \hat{\mathcal{S}}, \hat{\mathbb{J}}, \hat{\mathbb{K}})$  and let  $T : \hat{\mathcal{Q}} \rightarrow \tilde{\mathcal{Q}}$  be a smooth map between Banach spaces  $\hat{\mathcal{Q}}$  and  $\tilde{\mathcal{Q}}$ . We say that closure conditions (50) are satisfied, if there exist functionals  $\tilde{\mathcal{E}}, \tilde{\mathcal{S}} : \tilde{\mathcal{Q}} \rightarrow \mathbb{R}$  and geometric structures  $\tilde{\mathbb{J}}, \tilde{\mathbb{K}} : \tilde{\mathcal{Q}} \times \tilde{\mathcal{Q}}^* \rightarrow \tilde{\mathcal{Q}}$ , such that for all  $\hat{\mathbf{q}} \in \hat{\mathcal{Q}}$  there holds

$$\tilde{\mathcal{A}}(T(\hat{\mathbf{q}})) = \hat{\mathcal{A}}(\hat{\mathbf{q}}), \quad (50a)$$

$$\tilde{\mathbb{J}}(T(\hat{\mathbf{q}})) = \mathbb{L}(\hat{\mathbf{q}})\hat{\mathbb{J}}(\hat{\mathbf{q}})\mathbb{L}(\hat{\mathbf{q}})^*, \quad (50b)$$

$$\tilde{\mathbb{K}}(T(\hat{\mathbf{q}})) = \mathbb{L}(\hat{\mathbf{q}})\hat{\mathbb{K}}(\hat{\mathbf{q}})\mathbb{L}(\hat{\mathbf{q}})^*, \quad (50c)$$

with  $\mathbb{L}(\hat{\mathbf{q}}) := D_{\hat{\mathbf{q}}}T(\hat{\mathbf{q}})$  the Fréchet derivative of  $T$  in  $\hat{\mathbf{q}}$  and  $\mathbb{L}(\hat{\mathbf{q}})^*$  the adjoint of the linear operator  $\mathbb{L}(\hat{\mathbf{q}})$ , and for  $\tilde{\mathcal{A}} \in \{\tilde{\mathcal{E}}, \tilde{\mathcal{S}}\}$  in (50a), optionally also for  $\tilde{\mathcal{A}} = \tilde{\mathcal{M}}$ .

The closure condition also requires the validity of the chain rule for partial time derivatives with above  $\mathbb{L}$ , i.e., for all  $\hat{\mathbf{q}} : [0, T] \rightarrow \hat{\mathcal{Q}}$  and  $\tilde{\mathbf{q}}(t) := T(\hat{\mathbf{q}}(t))$  it is

$$\partial_t \tilde{\mathbf{q}} = \mathbb{L}(\hat{\mathbf{q}})\partial_t \hat{\mathbf{q}}. \quad (51)$$

Note that conditions (50) are straight-forward to satisfy if  $T$  is a diffeomorphism. For example, by (49) we automatically satisfy (50a). This is usually the case for a change of thermodynamic variables via  $T_V$ , cf. Sec. 3.4.2. Instead, for a change of coordinates, in particular from the Lagrangian to Eulerian frame, cf. Sec. 3.4.1, the map  $T_{LE} : \tilde{\mathcal{Q}} \rightarrow \mathcal{Q}$  need not be invertible and then (50) provide a fundamental, nontrivial requirement. Here, w.r.t. the chain rule for time derivatives (51), note that partial time derivatives are transformed according to (23), i.e.,

$$\partial_t \mathbf{q} = D_{\bar{\mathbf{q}}}T_{LE}(\boldsymbol{\chi}; \bar{\mathbf{q}})\partial_t \bar{\mathbf{q}} + D_{\boldsymbol{\chi}}T_{LE}(\boldsymbol{\chi}; \bar{\mathbf{q}})\dot{\boldsymbol{\chi}}, \quad (52)$$

with the expressions given in (22) for intensive and extensive variables. We point out that (52) results in a linear operator  $\mathbb{L}(\bar{\mathbf{q}}(t)) : \tilde{\mathcal{Q}} \rightarrow \mathcal{Q}$  with respect to  $\partial_t \bar{\mathbf{q}}(t) \in \tilde{\mathcal{Q}}$ , only if  $\boldsymbol{\chi}$  is a component of the state vector  $\bar{\mathbf{q}} \in \tilde{\mathcal{Q}}$ . Then, assuming (51) and with the corresponding adjoint operator  $\mathbb{L}^*$  we define the transformed structures  $\tilde{\mathbb{J}} = \mathbb{L}\hat{\mathbb{J}}\mathbb{L}^*$  and  $\tilde{\mathbb{K}} = \mathbb{L}\hat{\mathbb{K}}\mathbb{L}^*$ , so that it remains to check the validity of the closure assumptions (50b) and (50c), i.e., that the transformed operators only depend on the transformed state variables.

In the following we investigate how closure conditions (50) and (51) allow it to transform GENERIC systems into GENERIC systems, including their evolution equations (45). In fact, given the validity of condition (50a), by the chain rule and by the definition of the adjoint operator we identify the following transformation relation for the Fréchet derivatives of functionals  $\tilde{\mathcal{A}}$  and  $\hat{\mathcal{A}}$ .

**Lemma 3.8** Let  $\hat{\mathcal{Q}}$  and  $\tilde{\mathcal{Q}}$  be Banach spaces with dual spaces  $\hat{\mathcal{Q}}^*$ ,  $\tilde{\mathcal{Q}}^*$ , and  $\langle \cdot, \cdot \rangle_{\hat{\mathcal{Q}}}$ , resp.  $\langle \cdot, \cdot \rangle_{\tilde{\mathcal{Q}}}$  the dual pairing. Let  $T : \hat{\mathcal{Q}} \rightarrow \tilde{\mathcal{Q}}$  be Fréchet-differentiable with  $D_{\hat{\mathbf{q}}}T(\hat{\mathbf{q}}) : \hat{\mathcal{Q}} \rightarrow \tilde{\mathcal{Q}}$  denoting its Fréchet



derivative in  $\hat{q} \in \hat{Q}$ . Furthermore, let  $\tilde{A} : T(\hat{Q}) \subset \tilde{Q} \rightarrow \mathbb{R}$  be Fréchet-differentiable and related to  $\hat{A} : \hat{Q} \rightarrow \mathbb{R}$  by (50a). Then, also  $\hat{A}$  is Fréchet-differentiable and for all  $\hat{v} \in \hat{Q}$  it is

$$\langle D_{\hat{q}}\hat{A}(\hat{q}), \hat{v} \rangle_{\hat{Q}} = \langle D_{\tilde{q}}\tilde{A}(T(\hat{q})), D_{\hat{q}}T(\hat{q})\hat{v} \rangle_{\tilde{Q}} = \langle D_{\hat{q}}T(\hat{q})^*D_{\tilde{q}}\tilde{A}(\tilde{q}), \hat{v} \rangle_{\hat{Q}}, \quad (53)$$

where  $D_{\hat{q}}T(\hat{q})^* : \tilde{Q}^* \rightarrow \hat{Q}^*$  denotes the adjoint of the linear operator  $D_{\hat{q}}T(\hat{q}) : \hat{Q} \rightarrow \tilde{Q}$ .

If a transformed system fails to be of GENERIC/Onsager/Hamiltonian structure, then usually this is because the closure conditions are not satisfied [49]. However, assuming the validity of the closure conditions (50b) and (50c) the properties of geometric structures  $\hat{\mathbb{J}}, \hat{\mathbb{K}}$  carry over to the transformed structures  $\tilde{\mathbb{J}}, \tilde{\mathbb{K}}$ , see Lemmata 3.9 and 3.10.

**Lemma 3.9** *Let  $\hat{Q}, \tilde{Q}$  as in Lemma 3.8 and such that their dual pairings comply with Remark 3.1. Let  $\hat{\mathcal{X}}, \tilde{\mathcal{X}}$  as in (25). Consider a smooth map  $T : \hat{Q} \rightarrow \tilde{Q}$ . Then, we have the following statements 1.-3. which lead to the main result 4.:*

- 1 Let  $\tilde{A} \in \tilde{\mathcal{X}}$ . Then  $\hat{A} := (\tilde{A} \circ T) \in \hat{\mathcal{X}}$ .
- 2 Let  $\tilde{\mathcal{F}}, \tilde{\mathcal{G}} \in \tilde{\mathcal{X}}, T$  as above, and  $\hat{\mathbb{J}}$  as in (32). Then we have

$$\hat{\Psi} := \langle D_{\hat{q}}(\tilde{\mathcal{F}} \circ T), \hat{\mathbb{J}}D_{\hat{q}}(\tilde{\mathcal{G}} \circ T) \rangle_{\hat{Q}} \in \hat{\mathcal{X}}.$$

- 3 Let the assumptions of 2. hold true and assume that  $\tilde{\mathbb{J}} : \tilde{Q} \times \tilde{Q}^* \rightarrow \tilde{Q}$  satisfies (50b) with  $\mathbb{L} = D_{\tilde{q}}T$ . Then, for all  $\hat{q} \in \hat{Q}$  and  $\tilde{q} = T(\hat{q}) \in \tilde{Q}$  there holds

$$\langle D_{\tilde{q}}\tilde{\mathcal{F}}(\tilde{q}), \tilde{\mathbb{J}}(\tilde{q})D_{\tilde{q}}\tilde{\mathcal{G}}(\tilde{q}) \rangle_{\tilde{Q}} = \langle D_{\hat{q}}\hat{\mathcal{F}}(\hat{q}), \hat{\mathbb{J}}(\hat{q})D_{\hat{q}}\hat{\mathcal{G}}(\hat{q}) \rangle_{\hat{Q}}$$

with  $\hat{\mathcal{F}}, \hat{\mathcal{G}}$  defined like  $\hat{A}$  in 1.

- 4 Let the assumptions of 3. hold true and assume that also  $\tilde{\mathbb{J}}(\cdot)$  complies with (32). Further assume that  $\hat{\mathbb{J}}(\hat{q}) : \hat{Q}^* \rightarrow \hat{Q}$  generates a bracket via (27a) that satisfies Jacobi's identity (26c) for all  $\hat{q} \in \hat{Q}$ . Then also the bracket generated by  $\tilde{\mathbb{J}}(\tilde{q}) : \tilde{Q}^* \rightarrow \tilde{Q}$  satisfies Jacobi's identity for all  $\tilde{q} = T(\hat{q}) \in T(\hat{Q}) \subset \tilde{Q}$ .

**Proof:** Statements 1. & 2. are straight-forward to see, also thanks to the statements in Remark 3.1, and 1. gives (50a), so that (53) is true. Then Statement 3. is obtained as follows:

$$\begin{aligned} \langle D_{\hat{q}}\hat{\mathcal{F}}(\hat{q}), \hat{\mathbb{J}}(\hat{q})D_{\hat{q}}\hat{\mathcal{G}}(\hat{q}) \rangle_{\hat{Q}} &\stackrel{1.}{=} \langle D_{\tilde{q}}\tilde{\mathcal{F}}(T(\hat{q})), \hat{\mathbb{J}}(\hat{q})D_{\hat{q}}\tilde{\mathcal{G}}(T(\hat{q})) \rangle_{\hat{Q}} \\ &\stackrel{(53)}{=} \langle D_{\hat{q}}T(\hat{q})^*D_{\tilde{q}}\tilde{\mathcal{F}}(T(\hat{q})), \hat{\mathbb{J}}(\hat{q})D_{\hat{q}}T(\hat{q})^*D_{\tilde{q}}\tilde{\mathcal{G}}(T(\hat{q})) \rangle_{\hat{Q}} \\ &= \langle D_{\tilde{q}}\tilde{\mathcal{F}}(T(\hat{q})), D_{\hat{q}}T(\hat{q})\hat{\mathbb{J}}(\hat{q})D_{\hat{q}}T(\hat{q})^*D_{\tilde{q}}\tilde{\mathcal{G}}(T(\hat{q})) \rangle_{\hat{Q}} \\ &\stackrel{(50b)}{=} \langle D_{\tilde{q}}\tilde{\mathcal{F}}(\tilde{q}), \tilde{\mathbb{J}}(\tilde{q})D_{\tilde{q}}\tilde{\mathcal{G}}(\tilde{q}) \rangle_{\tilde{Q}}. \end{aligned}$$

Observe now that the smoothness of  $\tilde{\mathbb{J}}$  given by (32) ensures that  $\tilde{\Psi} := \langle D_{\tilde{q}}\tilde{\mathcal{F}}, \tilde{\mathbb{J}}D_{\tilde{q}}\tilde{\mathcal{G}} \rangle_{\tilde{Q}} \in \tilde{\mathcal{X}}$ . Then above calculation also shows that  $\{\tilde{\mathcal{H}}, \{\tilde{\mathcal{F}}, \tilde{\mathcal{G}}\}_{\tilde{Q}}\}_{\tilde{Q}} = \{\hat{\mathcal{H}}, \{\hat{\mathcal{F}}, \hat{\mathcal{G}}\}_{\hat{Q}}\}_{\hat{Q}}$  holds for all  $\tilde{\mathcal{H}}, \tilde{\mathcal{F}}, \tilde{\mathcal{G}} \in \tilde{\mathcal{X}}$  and  $\hat{\mathcal{H}}, \hat{\mathcal{F}}, \hat{\mathcal{G}}$  defined like  $\hat{A}$  in 1. and for any  $\tilde{q} \in T(\hat{Q})$ . Thus Statement 4. follows.  $\square$

With similar simpler arguments, one can also verify the remaining properties of the GENERIC structure.

**Lemma 3.10** *Let  $\hat{Q}, \tilde{Q}$ , and  $T : \hat{Q} \rightarrow \tilde{Q}$  as in Lemma 3.8. Further assume that  $\mathbb{L}(\hat{q}) : \hat{Q} \rightarrow \tilde{Q}$  is a linear, continuous operator for all  $\hat{q} \in \hat{Q}$ , and  $\mathbb{L}(\hat{q})^* : \tilde{Q}^* \rightarrow \hat{Q}^*$  its adjoint with the transformation properties (50). Then, the following statements hold true:*

- 1 Let  $\hat{\mathbb{J}}(\hat{q}) : \hat{Q}^* \rightarrow \hat{Q}$  be skewsymmetric. Then  $\tilde{\mathbb{J}}(\tilde{q})$  obtained via (50b) is skewsymmetric as well.
- 2 Let  $\hat{\mathbb{K}}(\hat{q}) : \hat{Q}^* \rightarrow \hat{Q}$  be symmetric. Then  $\tilde{\mathbb{K}}(\tilde{q})$  obtained via (50c) is symmetric as well.
- 3 Let  $\hat{\mathbb{K}}(\hat{q}) : \hat{Q}^* \rightarrow \hat{Q}$  be positively (semi)definite. Then also  $\tilde{\mathbb{K}}(\tilde{q})$  obtained via (50c) is positively (semi)definite.

In addition, the following statements can be made with regard to the transformation of GENERIC systems.

**Theorem 3.11** *Let the assumptions of Lemma 3.9 hold true for the state spaces  $\hat{Q}$ ,  $\tilde{Q}$  and for the map  $T : \hat{Q} \rightarrow \tilde{Q}$ . Denote by  $\mathbb{L}(\hat{q}) := D_{\hat{q}}T(\hat{q})$  its Fréchet derivative in  $\hat{q} \in \hat{Q}$ .*

- 1 Let  $(\hat{Q}, \hat{\mathcal{E}}, \hat{\mathcal{S}}, \hat{\mathbb{J}}, \hat{\mathbb{K}})$  be a GENERIC system and assume that closure conditions (50) are satisfied. Then also  $(\tilde{Q}, \tilde{\mathcal{E}}, \tilde{\mathcal{S}}, \tilde{\mathbb{J}}, \tilde{\mathbb{K}})$  is a GENERIC system, i.e., in particular the NIC (44) hold true.
- 2 Let the prerequisites of 1. hold true and assume that also condition (51) is satisfied. For all  $t \in [0, T]$  let  $\hat{q} : [0, T] \rightarrow \hat{Q}$  be a solution of

$$\partial_t \hat{q} = \hat{\mathbb{J}}(\hat{q})D_{\hat{q}}\hat{\mathcal{E}}(\hat{q}) + \hat{\mathbb{K}}(\hat{q})D_{\hat{q}}\hat{\mathcal{S}}(\hat{q}) \text{ in } \hat{Q} \quad (54a)$$

Then, for all  $t \in [0, T]$  the transformed function  $\tilde{q} := T(\hat{q}) : [0, T] \rightarrow \tilde{Q}$  is a solution of

$$\partial_t \tilde{q} = \tilde{\mathbb{J}}(\tilde{q})D_{\tilde{q}}\tilde{\mathcal{E}}(\tilde{q}) + \tilde{\mathbb{K}}(\tilde{q})D_{\tilde{q}}\tilde{\mathcal{S}}(\tilde{q}) \text{ in } \tilde{Q}, \quad (54b)$$

where the operators  $\tilde{\mathbb{J}}, \tilde{\mathbb{K}}$  are related to  $\hat{\mathbb{J}}, \hat{\mathbb{K}}$  by (50).

**Proof:** *To 1.:* Thanks to the smoothness of  $T$ , for all  $\hat{q} \in \hat{Q}$  the operator  $\mathbb{L}(\hat{q}) = D_{\hat{q}}T(\hat{q}) : \hat{Q} \rightarrow \tilde{Q}$  is a linear and continuous operator. Also thanks to the smoothness of  $\hat{\mathbb{J}}, \hat{\mathbb{K}}$  all statements of Lemmata 3.9 & 3.10 hold true.

To verify the NIC (44) we make use of transformation relation (53) for the Fréchet derivatives of  $\hat{\mathcal{E}}, \hat{\mathcal{S}}$ , and  $\hat{\mathcal{M}}$ . In view of (50) we thus have

$$\begin{aligned} \tilde{\mathbb{M}}(\tilde{q})D_{\tilde{q}}\tilde{\mathcal{A}}(\tilde{q}) &= \mathbb{L}(\hat{q})\hat{\mathbb{M}}(\hat{q})\mathbb{L}(\hat{q})^*D_{\hat{q}}\hat{\mathcal{A}}(\hat{q}) \\ &= \mathbb{L}(\hat{q})\hat{\mathbb{M}}(\hat{q})D_{\hat{q}}\hat{\mathcal{A}}(\hat{q}) \end{aligned}$$

with  $\hat{\mathbb{M}}$  as a placeholder for  $\hat{\mathbb{J}}, \hat{\mathbb{K}}$  and  $\hat{\mathcal{A}}$  as a placeholder for  $\hat{\mathcal{E}}, \hat{\mathcal{S}}, \hat{\mathcal{M}}$ . Hence, if  $\hat{\mathbb{M}}(\hat{q})D_{\hat{q}}\hat{\mathcal{A}}(\hat{q}) = 0$  by NIC (44) for the GENERIC system  $(\hat{Q}, \hat{\mathcal{E}}, \hat{\mathcal{S}}, \hat{\mathbb{J}}, \hat{\mathbb{K}})$ , then also  $\tilde{\mathbb{M}}(\tilde{q})D_{\tilde{q}}\tilde{\mathcal{A}}(\tilde{q}) = 0$  by the linearity of  $\mathbb{L}(\hat{q}) : \hat{Q} \rightarrow \tilde{Q}$ .

*To 2.:* In view of condition (51) for the partial time derivatives, to find relation (54b) from property (54a) we apply  $\mathbb{L}(\hat{q}(t)) = D_{\hat{q}}T(\hat{q}(t))$  to both sides of (54a) and use (53) to transform the Fréchet derivative of the functional. This results in (54b) and confirms the transformation relation (50b) & (50c) for the operators  $\hat{\mathbb{J}}, \hat{\mathbb{K}}$ .  $\square$

### 3.4.1 Reduction and extension maps for GENERIC structures

We now discuss non-invertible transformations in more detail. Prototypes of non-invertible maps  $T$  are given by reductions and extensions defined as follows.

**Definition 3.12 (Reduction and extension)** Let  $\hat{\mathcal{Q}}$  and  $\tilde{\mathcal{Q}}$  either be finite-dimensional normed vector spaces of dimension  $\hat{n}$  and  $\tilde{n}$  or Banach spaces over domains  $\hat{\Omega}, \tilde{\Omega} \subset \mathbb{R}^d$  such that  $\hat{\mathcal{Q}} \subset \{\hat{\mathbf{q}} : \hat{\Omega} \rightarrow \mathbb{R}^{\hat{n}}\}$  and  $\tilde{\mathcal{Q}} \subset \{\tilde{\mathbf{q}} : \tilde{\Omega} \rightarrow \mathbb{R}^{\tilde{n}}\}$ . Let  $(\hat{\mathcal{Q}}, \hat{\mathcal{E}}, \hat{\mathcal{S}}, \hat{\mathcal{J}}, \hat{\mathcal{K}})$  and  $(\tilde{\mathcal{Q}}, \tilde{\mathcal{E}}, \tilde{\mathcal{S}}, \tilde{\mathcal{J}}, \tilde{\mathcal{K}})$  be GENERIC systems and  $\mathbb{T} : \hat{\mathcal{Q}} \rightarrow \tilde{\mathcal{Q}}$  a smooth map that satisfies closure conditions in Def. 3.7. If  $\tilde{n} < \hat{n}$  we call  $\mathbb{T}$  a reduction map and  $(\tilde{\mathcal{Q}}, \tilde{\mathcal{E}}, \tilde{\mathcal{S}}, \tilde{\mathcal{J}}, \tilde{\mathcal{K}})$  is the reduction of  $(\hat{\mathcal{Q}}, \hat{\mathcal{E}}, \hat{\mathcal{S}}, \hat{\mathcal{J}}, \hat{\mathcal{K}})$ . Vice versa, if  $\tilde{n} > \hat{n}$  we call  $\mathbb{T}$  an extension map and  $(\tilde{\mathcal{Q}}, \tilde{\mathcal{E}}, \tilde{\mathcal{S}}, \tilde{\mathcal{J}}, \tilde{\mathcal{K}})$  is the extension of  $(\hat{\mathcal{Q}}, \hat{\mathcal{E}}, \hat{\mathcal{S}}, \hat{\mathcal{J}}, \hat{\mathcal{K}})$ .

The distinction of reduction and extension has its reason in the satisfiability of the closure condition. For invertible transformations the closure conditions (50) are satisfied uniquely, e.g., (50a) is valid using (49). However, for the reduction the closure condition is a nontrivial constraint that needs to be confirmed. Nevertheless, we show in Example 3.14 that the reduction map is often motivated by symmetries and invariances that generate conservation laws and thereby motivate the closure condition. Instead, for extensions to a larger space the closure condition can sometimes even lead to an ambiguity. For example, if the extension contains the old state as a component  $\tilde{\mathbf{q}} := \mathbb{T}(\hat{\mathbf{q}}) = (\hat{\mathbf{q}}, \tilde{v}(\hat{\mathbf{q}}))$ , then setting  $\tilde{\mathcal{A}}(\tilde{\mathbf{q}}) := \hat{\mathcal{A}}(\hat{\mathbf{q}})$  provides one possibility to satisfy the closure condition.

Different notions of reduction are considered in literature and the review by Morrison [52] gives a general introduction to the subject in the context of Hamiltonian descriptions of fluid flow. For fluids the reduction formalism was used in the derivation of the Euler equation from their Lagrangian formulation [2, 18, 52] and has also been extended to GENERIC structures [26]. For this purpose we now discuss the Lagrangian-Eulerian transformation of coordinates  $\mathbb{T} = \mathbb{T}_{\text{LE}} : \bar{\mathcal{Q}} \rightarrow \mathcal{Q}$  as a special case of a reduction. Based on the previous considerations for the partial time derivative calculated by (52) in case that the flow map  $\chi$  is an element of the state vector  $\bar{\mathbf{q}} \in \bar{\mathcal{Q}}$  we deduce the following transformation behavior  $\mathbb{L}$ .

**Lemma 3.13 (Fréchet derivative of  $\mathbb{T}_{\text{LE}}$ )** Consider two Banach spaces  $\bar{\mathcal{Q}}, \mathcal{Q}$  such that

$$\begin{aligned} \bar{\mathcal{Q}} &\subset \{\bar{\mathbf{q}} = (\chi, \bar{\alpha}, \bar{A}, \bar{\mathbf{A}}) : \bar{\Omega} \rightarrow \mathbb{R}^d \times \mathbb{R} \times \mathbb{R} \times \mathbb{R}^N\}, \\ \mathcal{Q} &\subset \{\mathbf{q} = (\alpha, A, \mathbf{A}) : \Omega \rightarrow \mathbb{R} \times \mathbb{R} \times \mathbb{R}^N\} \end{aligned}$$

and  $\mathbb{T}_{\text{LE}} : \bar{\mathcal{Q}} \rightarrow \mathcal{Q}$  the Lagrangian-Eulerian transformation given by (20a) for the scalar-valued extensive variable  $\bar{A}$  (energy or entropy) or component-wise for vector-valued extensive variables  $\bar{\mathbf{A}}$  (concentration or momentum) and by (20b) for the scalar-valued intensive variable  $\bar{\alpha}$  (temperature, pressure, or chemical potential). Then for all  $\bar{\mathbf{q}} \in \bar{\mathcal{Q}}$  the linear transformation operator  $\mathbb{L}(\bar{\mathbf{q}}) : \bar{\mathcal{Q}} \rightarrow \mathcal{Q}$  in closure condition (50) is given by the Fréchet derivative  $\mathbb{L}(\bar{\mathbf{q}}) = \mathbb{D}_{\bar{\mathbf{q}}} \mathbb{T}_{\text{LE}}(\bar{\mathbf{q}})$  and takes the form

$$\mathbb{L}(\bar{\mathbf{q}}) = \begin{pmatrix} -\square \cdot \nabla \alpha & \square & 0 & 0 \\ -\nabla \cdot (A \square) & 0 & \frac{\square}{V} & 0 \\ -\nabla \cdot (\mathbf{A} \otimes \square) & 0 & 0 & \frac{\square}{V} \end{pmatrix}_{\bar{x}=\chi^{-1}(x)}, \quad (55)$$

and  $\square$  indicates where an argument has to be put. Moreover, also closure condition (51) for the partial time derivatives holds true and gives the transformation relations (22) for time derivatives from the Lagrangian to the Eulerian frame, i.e.,

$$\dot{\mathbf{q}} = \begin{pmatrix} \dot{\alpha} \\ \dot{A} \\ \dot{\mathbf{A}} \end{pmatrix} = \mathbb{L}(\bar{\mathbf{q}}) \begin{pmatrix} \dot{\chi} \\ \dot{\bar{\alpha}} \\ \dot{\bar{A}} \\ \dot{\bar{\mathbf{A}}} \end{pmatrix} = \begin{pmatrix} \dot{\alpha} - \dot{\chi} \nabla \alpha \\ \frac{\dot{A}}{V} - \nabla \cdot (A \dot{\chi}) \\ \frac{\dot{\mathbf{A}}}{V} - \nabla \cdot (\mathbf{A} \otimes \dot{\chi}) \end{pmatrix},$$

evaluated in  $\bar{x} = \chi^{-1}(t, x)$  and spatial  $x$ -derivatives also act on the  $x$ -dependence of  $\chi^{-1}$ .

**Example 3.14 (Reduction in finite dimensions)** In the following we discuss the reduction of the finite-dimensional Hamiltonian system from Ex. 3.3. Let now  $d = 2$ , so that

$$\bar{\mathbf{q}} = (\bar{x}_1, \bar{x}_2, \bar{p}_1, \bar{p}_2)^\top \in \bar{\mathcal{Q}} \equiv \mathbb{R}^4,$$

and consider an Hamiltonian of the form

$$\bar{\mathcal{E}}(\bar{\mathbf{q}}) = \frac{\bar{p}_1^2 + \bar{p}_2^2}{2M} + \bar{U}_{\text{pot}}(\bar{x}_1 - \bar{x}_2),$$

where the potential energy  $\bar{U}_{\text{pot}} : \mathbb{R} \rightarrow \mathbb{R}$  depends only on the variable  $r = \bar{x}_1 - \bar{x}_2$ . For the system  $(\bar{\mathcal{Q}}, \bar{\mathcal{E}}, \bar{\mathbb{J}}_{\text{can}})$  with  $\bar{\mathbb{J}}_{\text{can}}$  from (34a) Hamilton's equations then are

$$\begin{aligned} \dot{\bar{x}}_1 &= \frac{\bar{p}_1}{M}, & \dot{\bar{p}}_1 &= -\bar{U}'_{\text{pot}}(\bar{x}_1 - \bar{x}_2), \\ \dot{\bar{x}}_2 &= \frac{\bar{p}_2}{M}, & \dot{\bar{p}}_2 &= +\bar{U}'_{\text{pot}}(\bar{x}_1 - \bar{x}_2). \end{aligned}$$

Due to the symmetry of the energy we define the reduction map  $T : \bar{\mathcal{Q}} \rightarrow \mathcal{Q}$  by

$$\mathbf{q} = \begin{pmatrix} r \\ p_1 \\ p_2 \end{pmatrix} = T(\bar{\mathbf{q}}) = \begin{pmatrix} \bar{x}_1 - \bar{x}_2 \\ \bar{p}_1 \\ \bar{p}_2 \end{pmatrix} \in \mathcal{Q} \equiv \mathbb{R}^3,$$

and compute  $\mathbb{L} = DT(\bar{\mathbf{q}}) \in \mathbb{R}^{3 \times 4}$  and  $\mathbb{L}^* \in \mathbb{R}^{4 \times 3}$  as

$$\mathbb{L} = \begin{pmatrix} +1 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad \mathbb{L}^* = \begin{pmatrix} +1 & 0 & 0 \\ -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Via (50b) we obtain the non-canonical Poisson operator

$$\mathbb{J} = \mathbb{L} \begin{pmatrix} 0 & +\mathbb{I}_2 \\ -\mathbb{I}_2 & 0 \end{pmatrix} \mathbb{L}^* = \begin{pmatrix} 0 & +1 & -1 \\ -1 & 0 & 0 \\ +1 & 0 & 0 \end{pmatrix} \in \mathbb{R}^{3 \times 3},$$

and via (50a) the reduced Hamiltonian

$$\mathcal{E}(\mathbf{q}) = \frac{p_1^2 + p_2^2}{2M} + \bar{U}_{\text{pot}}(r),$$

where the closure conditions are obviously satisfied. With the reduced structure  $\{\mathcal{Q} \simeq \mathbb{R}^3, \mathcal{E}, \mathbb{J}\}$  this gives the reduced system of Hamilton's equations

$$\dot{r} = \frac{p_1 - p_2}{M}, \quad \dot{p}_1 = -\bar{U}'_{\text{pot}}(r), \quad \dot{p}_2 = +\bar{U}'_{\text{pot}}(r),$$

which could be further reduced by momentum conservation  $\dot{p}_1 + \dot{p}_2 = 0$ . \*

### 3.4.2 Change of thermodynamical variables and role of free energies and entropies as driving potentials

In the following we specialize the mapping to a transformation  $T_v : \hat{\mathcal{Q}} \rightarrow \tilde{\mathcal{Q}}$  that realizes a change of thermodynamical variables; again we write  $\tilde{\mathbf{q}} = T_v(\hat{\mathbf{q}}) \in \tilde{\mathcal{Q}}$  for  $\hat{\mathbf{q}} \in \hat{\mathcal{Q}}$ . For Fréchet differentiable  $T_v$  the transformation operator  $\mathbb{L}$  in the closure condition (50) is obtained assuming the chain rule (51), i.e., for  $\hat{\mathbf{q}} : [0, T] \rightarrow \hat{\mathcal{Q}}$

$$\partial_t \tilde{\mathbf{q}} = \partial_t T_v(\hat{\mathbf{q}}) = D_{\hat{\mathbf{q}}} T_v(\hat{\mathbf{q}}) \partial_t \hat{\mathbf{q}} =: \mathbb{L}(\hat{\mathbf{q}}) \partial_t \hat{\mathbf{q}}. \quad (57)$$

Hence, for smooth  $T_v$ , all the results of L. 3.9–Thm. 3.11 hold true. Let us further assume that there is a set of state variables  $w$ , that remains unchanged by the transformation, whereas the set of state variables  $\hat{v}$  will be mapped by  $T_v$  to new states  $\tilde{v}$ . As we explained in Sec. 2.1, at least one of the new state variables needs to be extensive. In this way, the mapping can be written

$$T_v : \hat{\mathcal{Q}} \rightarrow \tilde{\mathcal{Q}}, \quad \hat{\mathbf{q}} = (w, \hat{v}) \mapsto \tilde{\mathbf{q}} = (w, \tilde{v}) = (w, \tilde{v}(\hat{\mathbf{q}})). \quad (58)$$

As a characteristic property of a change of thermodynamic variables, we assume that  $T_v$  is a diffeomorphism, i.e.,  $T_v$  is a smooth, bijective map and also its inverse  $T_v^{-1}$  is smooth. For shorter notation we write

$$\tilde{T}_v := T_v^{-1} : \tilde{\mathcal{Q}} \rightarrow \hat{\mathcal{Q}}. \quad (59)$$

With this notation the operator  $\mathbb{L}(\hat{\mathbf{q}}) = D_{\hat{\mathbf{q}}} T_v(\hat{\mathbf{q}}) : \hat{\mathcal{Q}} \rightarrow \tilde{\mathcal{Q}}$  from (57) takes the form

$$\mathbb{L}(\hat{\mathbf{q}}) = D_{\hat{\mathbf{q}}} T_v(\hat{\mathbf{q}}) = \begin{pmatrix} \mathbb{I}_w & 0 \\ \mathbb{D}_w \tilde{v}(\hat{\mathbf{q}}) & \mathbb{D}_{\hat{v}} \tilde{v}(\hat{\mathbf{q}}) \end{pmatrix}, \quad (60a)$$

and accordingly  $\mathbb{L}(\hat{\mathbf{q}})^* : \tilde{\mathcal{Q}}^* \rightarrow \hat{\mathcal{Q}}^*$ ,

$$\mathbb{L}(\hat{\mathbf{q}})^* = D_{\hat{\mathbf{q}}} T_v(\hat{\mathbf{q}})^* = \begin{pmatrix} \mathbb{I}_w & \mathbb{D}_w^* \tilde{v}(\hat{\mathbf{q}}) \\ 0 & \mathbb{D}_{\hat{v}}^* \tilde{v}(\hat{\mathbf{q}}) \end{pmatrix}. \quad (60b)$$

Here,  $\mathbb{I}_w$  is the identity operator on  $\hat{\mathcal{Q}}_w$ . Moreover, the operator  $\mathbb{L}$  in (60a) carries the entries  $\mathbb{D}_w \tilde{v}(\hat{\mathbf{q}})$ ,  $\mathbb{D}_{\hat{v}} \tilde{v}(\hat{\mathbf{q}})$ , which denotes the Fréchet derivative of  $\tilde{v}$  with respect to  $w$  and  $\hat{v}$ . In turn,  $\mathbb{D}_w^* \tilde{v}(\hat{\mathbf{q}})$  and  $\mathbb{D}_{\hat{v}}^* \tilde{v}(\hat{\mathbf{q}})$  in (60b) denote their adjoints. This distinction is of relevance if the new thermodynamic state  $\tilde{v}$  also depends on gradients of  $\hat{\mathbf{q}}$ , as can be seen in Example 3.15 below.

Since  $T_v$  is a diffeomorphism, by the rule for the derivative of the inverse function the transformation matrix  $\mathbb{L}$  can equivalently be expressed through the inverse map  $\tilde{T}_v$  from (59), i.e.,  $\mathbb{L}(\hat{\mathbf{q}}) = D_{\hat{\mathbf{q}}} T_v(\hat{\mathbf{q}}) = D_{\tilde{\mathbf{q}}} \tilde{T}_v(\tilde{\mathbf{q}})^{-1}$ , hence, equivalently to (60) it is

$$\mathbb{L}(\hat{\mathbf{q}}) = D_{\tilde{\mathbf{q}}} \tilde{T}_v(\tilde{\mathbf{q}})^{-1} = \begin{pmatrix} \mathbb{I}_w & 0 \\ \mathbb{D}_w \hat{v}(\tilde{\mathbf{q}}) & \mathbb{D}_{\tilde{v}} \hat{v}(\tilde{\mathbf{q}}) \end{pmatrix}^{-1}, \quad (61a)$$

and accordingly

$$\mathbb{L}(\hat{\mathbf{q}})^* = (D_{\tilde{\mathbf{q}}} \tilde{T}_v(\tilde{\mathbf{q}})^{-1})^*. \quad (61b)$$

**Example 3.15** For given constant concentration  $\bar{C}$  and mass density  $\bar{\rho}$ , consider a thermomechanical system characterized in Lagrangian coordinates by the state vector  $\hat{\mathbf{q}} = \bar{\mathbf{q}}_{\bar{S}} := (\boldsymbol{\chi}, \bar{\mathbf{P}}, \bar{S}) \in \bar{\mathcal{Q}}_{\bar{S}} = \hat{\mathcal{Q}}$ . With the map  $T_v$  the state vector  $\bar{\mathbf{q}}_{\bar{S}}$  is mapped to the new Lagrangian state vector  $\tilde{\mathbf{q}} = \bar{\mathbf{q}}_{\bar{E}} :=$

$(\boldsymbol{\chi}, \bar{\mathbf{P}}, \bar{E}) \in \bar{Q}_{\bar{E}} = \bar{Q}$ . Thus, here  $w = (\boldsymbol{\chi}, \bar{\mathbf{P}})$ , whereas  $\hat{v} = \bar{S}$  and  $\tilde{v} = \bar{E}$ . For shorter notation we abbreviate the kinetic energy density by

$$\bar{E}_{\text{kin}}(\bar{\mathbf{P}}) := \frac{|\bar{\mathbf{P}}|^2}{2\bar{\varrho}}. \quad (62)$$

Then, the total energy of the system is given by

$$\bar{\mathcal{E}}(\bar{\mathbf{q}}_{\bar{E}}) = \int_{\bar{\Omega}} \bar{E} \, d\bar{x} = \bar{\mathcal{E}}_{\bar{S}}(\bar{\mathbf{q}}_{\bar{S}}) = \int_{\bar{\Omega}} \bar{E}_{\bar{S}}(\bar{\mathbf{q}}_{\bar{S}}) \, d\bar{x} = \int_{\bar{\Omega}} \left( \bar{E}_{\text{kin}}(\bar{\mathbf{P}}) + \bar{U}(\bar{\mathbf{C}}, \bar{T}_{\bar{V}}(\boldsymbol{\chi}), \bar{S}) \right) d\bar{x}, \quad (63)$$

with  $\bar{T}_{\bar{V}}(\boldsymbol{\chi}) = \det(\bar{\mathbf{F}}) = \bar{V}$  the volume density and  $\bar{\mathbf{F}} = \bar{\nabla}\boldsymbol{\chi}$  as in (18b). We assume that the system is thermodynamically closed, so that all state variables satisfy homogeneous boundary conditions. Thus, by the chain rule, in view of (18d), and using integration by parts, the Fréchet derivative  $\mathbb{D}_{\boldsymbol{\chi}}\bar{\mathcal{E}}_{\bar{S}}(\bar{\mathbf{q}}_{\bar{S}})$  is given by

$$\begin{aligned} \langle \mathbb{D}_{\boldsymbol{\chi}}\bar{\mathcal{E}}_{\bar{S}}(\bar{\mathbf{q}}_{\bar{S}}), \bar{\mathbf{v}}_{\boldsymbol{\chi}} \rangle &= \int_{\bar{\Omega}} (\partial_{\bar{V}}\bar{U}(\bar{\mathbf{C}}, \bar{V}, \bar{S}) \text{Cof}(\bar{\mathbf{F}}) : \bar{\nabla}\bar{\mathbf{v}}_{\boldsymbol{\chi}}) \, d\bar{x} \\ &= \int_{\bar{\Omega}} -\left( \bar{\nabla} \cdot (\partial_{\bar{V}}\bar{U}(\bar{\mathbf{C}}, \bar{V}, \bar{S}) \text{Cof}(\bar{\mathbf{F}})) \right) \cdot \bar{\mathbf{v}}_{\boldsymbol{\chi}} \, d\bar{x}, \end{aligned}$$

again with  $\bar{\mathbf{F}} := \bar{\nabla}\boldsymbol{\chi}$ . Using that  $\partial_{\bar{V}}\bar{U}(\bar{\mathbf{C}}, \bar{V}, \bar{S}) = -\bar{\pi}$  and  $\partial_{\bar{S}}\bar{U}(\bar{\mathbf{C}}, \bar{V}, \bar{S}) = \bar{\theta}$  by (5) yields

$$\mathbb{D}_{\boldsymbol{\chi}}\bar{E}_{\bar{S}}(\bar{\mathbf{q}}_{\bar{S}})\square = \mathbb{D}_{\boldsymbol{\chi}}\bar{U}(\bar{\mathbf{q}}_{\bar{S}})\square = -\bar{\pi}\text{Cof}(\bar{\mathbf{F}}) : \bar{\nabla}\square, \quad (64a)$$

$$\mathbb{D}_{\bar{\mathbf{P}}}\bar{E}_{\bar{S}}(\bar{\mathbf{q}}_{\bar{S}})\square = \mathbb{D}_{\bar{\mathbf{P}}}\bar{E}_{\text{kin}}(\bar{\mathbf{q}}_{\bar{S}})\square = \frac{\bar{\mathbf{P}}}{\bar{\varrho}} \cdot \square, \quad (64b)$$

$$\mathbb{D}_{\bar{S}}\bar{E}_{\bar{S}}(\bar{\mathbf{q}}_{\bar{S}})\square = \mathbb{D}_{\bar{S}}\bar{U}(\bar{\mathbf{q}}_{\bar{S}})\square = \bar{\theta}\square, \quad (64c)$$

here  $\square$  indicates the placement of the function the operator acts on. Additionally we have the adjoints

$$\mathbb{D}_{\boldsymbol{\chi}}^*\bar{E}_{\bar{S}}(\bar{\mathbf{q}}_{\bar{S}})\square = \mathbb{D}_{\boldsymbol{\chi}}^*\bar{U}(\bar{\mathbf{q}}_{\bar{S}})\square = \bar{\nabla} \cdot (\bar{\pi}\square\text{Cof}(\bar{\mathbf{F}})), \quad (64d)$$

$$\mathbb{D}_{\bar{\mathbf{P}}}^*\bar{E}_{\bar{S}}(\bar{\mathbf{q}}_{\bar{S}})\square = \mathbb{D}_{\bar{\mathbf{P}}}^*\bar{E}_{\text{kin}}(\bar{\mathbf{q}}_{\bar{S}})\square = \frac{\bar{\mathbf{P}}}{\bar{\varrho}} \cdot \square, \quad (64e)$$

$$\mathbb{D}_{\bar{S}}^*\bar{E}_{\bar{S}}(\bar{\mathbf{q}}_{\bar{S}})\square = \mathbb{D}_{\bar{S}}^*\bar{U}(\bar{\mathbf{q}}_{\bar{S}})\square = \bar{\theta}\square. \quad (64f)$$

This produces as the linearization the operator

$$\mathbb{L}(\bar{\mathbf{q}}_{\bar{S}}) = \begin{pmatrix} \mathbb{I}_{\boldsymbol{\chi}} & 0 & 0 \\ 0 & \mathbb{I}_{\bar{\mathbf{P}}} & 0 \\ \mathbb{D}_{\boldsymbol{\chi}}\bar{E}_{\bar{S}} & \mathbb{D}_{\bar{\mathbf{P}}}\bar{E}_{\bar{S}} & \mathbb{D}_{\bar{S}}\bar{E}_{\bar{S}} \end{pmatrix}, \quad \mathbb{L}^*(\bar{\mathbf{q}}_{\bar{S}}) = \begin{pmatrix} \mathbb{I}_{\boldsymbol{\chi}} & 0 & \mathbb{D}_{\boldsymbol{\chi}}^*\bar{E}_{\bar{S}} \\ 0 & \mathbb{I}_{\bar{\mathbf{P}}} & \mathbb{D}_{\bar{\mathbf{P}}}^*\bar{E}_{\bar{S}} \\ 0 & 0 & \mathbb{D}_{\bar{S}}^*\bar{E}_{\bar{S}} \end{pmatrix},$$

using the derivatives of  $\bar{E}_{\bar{S}}$  given above. \*

**Preservation of fundamental thermodynamic relations under  $\bar{T}_{\bar{V}}$ .** Following the ideas of Mielke [44, Sec. 2.3] we explain now how the particular choice of variables enters the fundamental thermodynamic relations, such as the definition of temperature, pressure, and chemical potential given in (5). For this, the case that the map  $\bar{T}_{\bar{V}}$  only transforms one single, scalar thermodynamic variable is of particular importance. We indicate this variable by  $\hat{v} = \hat{\tau}$  and it concerns the map

$$\bar{T}_{\bar{V}} : (w, \hat{v} \equiv \hat{\tau}) \mapsto (w, \tilde{v} \equiv \tilde{\tau}), \quad (65)$$

with  $\hat{\tau}, \tilde{\tau} \in \{\bar{S}, \bar{U}, \bar{\theta}, \bar{E}\}$ . Here, the set of variables  $w = (\boldsymbol{\chi}, \bar{\mathbf{P}}, \bar{\mathbf{C}}, \bar{V})$  is not affected by the transformation. To point out the mapping property of  $\bar{T}_{\bar{V}}$  for the component  $\hat{\tau}$  we now set  $\tilde{\tau} := \bar{T}_{\hat{\tau} \rightarrow \tilde{\tau}}(w, \hat{\tau})$ .

To indicate that a state function  $A$  is a function of  $\hat{\tau}$ , resp.  $\tilde{\tau}$  we write  $A_{\hat{\tau}}$ , resp.  $A_{\tilde{\tau}}$ . With this notation we have

$$A_{\tilde{\tau}}(w, \tilde{\tau}) = A_{\hat{\tau}}(w, \mathbb{T}_{\hat{\tau} \rightarrow \tilde{\tau}}(w, \hat{\tau})) = A_{\hat{\tau}}(w, \hat{\tau}). \quad (66a)$$

By the chain rule, there holds

$$\left(\frac{\partial A_{\tilde{\tau}}}{\partial \hat{\tau}}\right)_w = \left(\frac{\partial A_{\tilde{\tau}}}{\partial \tilde{\tau}}\right)_w \left(\frac{\partial \mathbb{T}_{\hat{\tau} \rightarrow \tilde{\tau}}}{\partial \hat{\tau}}\right)_w, \quad (66b)$$

$$\left(\frac{\partial A_{\tilde{\tau}}}{\partial w}\right)_{\hat{\tau}} = \left(\frac{\partial A_{\tilde{\tau}}}{\partial w}\right)_{\tilde{\tau}} + \left(\frac{\partial A_{\tilde{\tau}}}{\partial \tilde{\tau}}\right)_w \left(\frac{\partial \mathbb{T}_{\hat{\tau} \rightarrow \tilde{\tau}}}{\partial w}\right)_{\hat{\tau}}. \quad (66c)$$

From this we obtain the following invariance relations for the fundamental thermodynamic relations, such as (5):

**Lemma 3.16** *Let  $\bar{U}_{\tilde{\tau}} = \bar{U}_{\tilde{\tau}}(w, \tilde{\tau})$  and  $\bar{S}_{\tilde{\tau}} = \bar{S}_{\tilde{\tau}}(w, \tilde{\tau})$  be continuously differentiable with respect to  $(w, \tilde{\tau})$ . Then, for any choice of  $\tilde{\tau} \in \{\bar{S}, \bar{U}, \bar{\theta}, \bar{E}\}$  there holds*

$$\bar{\theta} = \left(\frac{\partial \bar{U}_{\tilde{\tau}}}{\partial \tilde{\tau}} / \frac{\partial \bar{S}_{\tilde{\tau}}}{\partial \tilde{\tau}}\right)_w = \left(\frac{\partial \bar{E}_{\tilde{\tau}}}{\partial \tilde{\tau}} / \frac{\partial \bar{S}_{\tilde{\tau}}}{\partial \tilde{\tau}}\right)_w, \quad (67a)$$

$$\begin{aligned} \left(\frac{\partial(\bar{E}_{\text{kin}} + \bar{U}_{\tilde{\tau}})}{\partial w}\right)_{\tilde{\tau}} - \mathbb{T}_{\tilde{\tau} \rightarrow \bar{\theta}}(w, \tilde{\tau}) \left(\frac{\partial \bar{S}_{\tilde{\tau}}}{\partial w}\right)_{\tilde{\tau}} \\ = \left(\frac{\partial(\bar{E}_{\text{kin}} + \bar{F}(w, \bar{\theta}))}{\partial w}\right)_{\bar{\theta}}, \end{aligned} \quad (67b)$$

$$\begin{aligned} \left(\frac{\partial \bar{S}_{\tilde{\tau}}}{\partial w}\right)_{\tilde{\tau}} - \frac{1}{\mathbb{T}_{\tilde{\tau} \rightarrow \bar{\theta}}(w, \tilde{\tau})} \left(\frac{\partial(\bar{E}_{\text{kin}} + \bar{U}_{\tilde{\tau}})}{\partial w}\right)_{\tilde{\tau}} \\ = \left(\frac{\partial(-\frac{1}{\bar{\theta}} \bar{E}_{\text{kin}} + \bar{J}(w, \bar{\theta}))}{\partial w}\right)_{\bar{\theta}}, \end{aligned} \quad (67c)$$

using  $\bar{\theta} = \mathbb{T}_{\tilde{\tau} \rightarrow \bar{\theta}}(w, \tilde{\tau})$  in (67b) and (67c), the kinetic energy  $\bar{E}_{\text{kin}}$  from (62), and the thermodynamic potentials  $\bar{F}$  and  $\bar{J}$  as in Tab. 1.

**Special form of GENERIC by  $\tilde{\mathbb{T}}_{\tilde{\tau}}$  and thermodynamic driving forces.** We discuss here the special form of GENERIC that directly ensures the validity of the noninteraction conditions (44). This special form makes use of changes of variables as discussed above, but separately for the reversible and the irreversible driving force of a GENERIC system. More precisely, a GENERIC system characterized by the states  $\tilde{\mathbf{q}}_{\tilde{\tau}} = (w, \tilde{\tau})$  with evolution

$$\partial_t \tilde{\mathbf{q}}_{\tilde{\tau}} = \mathbb{J}_{\tilde{\tau}}(\tilde{\mathbf{q}}_{\tilde{\tau}}) \mathbb{D}\mathcal{E}(\tilde{\mathbf{q}}_{\tilde{\tau}}) + \mathbb{K}_{\tilde{\tau}}(\tilde{\mathbf{q}}_{\tilde{\tau}}) \mathbb{D}\mathcal{S}(\tilde{\mathbf{q}}_{\tilde{\tau}}) \quad (68)$$

is rewritten by suitable changes of variables in the form

$$\begin{aligned} \mathbb{J}_{\tilde{\tau}}(\tilde{\mathbf{q}}_{\tilde{\tau}}) &= \mathbb{L}_{\bar{S}}(\hat{\mathbf{q}}_{\bar{S}}) \mathbb{J}_{\bar{S}}(\hat{\mathbf{q}}_{\bar{S}}) \mathbb{L}_{\bar{S}}(\hat{\mathbf{q}}_{\bar{S}})^*, \\ \mathbb{K}_{\tilde{\tau}}(\tilde{\mathbf{q}}_{\tilde{\tau}}) &= \mathbb{L}_{\bar{E}}(\hat{\mathbf{q}}_{\bar{E}}) \mathbb{K}_{\bar{E}}(\hat{\mathbf{q}}_{\bar{E}}) \mathbb{L}_{\bar{E}}(\hat{\mathbf{q}}_{\bar{E}})^*. \end{aligned} \quad (69)$$

To obtain (69), the reversible part of the GENERIC system (68) is transformed by the map

$$\mathbb{T}_{\tilde{\tau}} \equiv \mathbb{T}_{\bar{S}}: \hat{\mathbf{Q}}_{\bar{S}} \rightarrow \tilde{\mathbf{Q}}_{\tilde{\tau}}, \quad \hat{\mathbf{q}}_{\bar{S}} = (w, \bar{S}) \mapsto \tilde{\mathbf{q}}_{\tilde{\tau}} = (w, \tilde{\tau}), \quad (70a)$$

whereas for the irreversible part of system (68) a change of variables is done by

$$\mathbb{T}_{\tilde{\tau}} \equiv \mathbb{T}_{\bar{E}}: \hat{\mathbf{Q}}_{\bar{E}} \rightarrow \tilde{\mathbf{Q}}_{\tilde{\tau}}, \quad \hat{\mathbf{q}}_{\bar{E}} = (w, \bar{E}) \mapsto \tilde{\mathbf{q}}_{\tilde{\tau}} = (w, \tilde{\tau}). \quad (70b)$$

Using  $\bar{A}$  as a placeholder for the scalar state functions  $\bar{S}$  and  $\bar{E}$  we now determine the transformation map  $\mathbb{L}_{\bar{A}}(\hat{\mathbf{q}}_{\bar{A}})$  based on relations (60) and (61). Since above changes of variables (70) are of the type (65), where only the scalar “thermal”-variable  $\tau$  is changed,  $\mathbb{L}_{\bar{A}}(\hat{\mathbf{q}}_{\bar{A}})$  can be sometimes determined through  $\tilde{\Gamma}_{\bar{A}} = \Gamma_{\bar{A}}^{-1}$  more explicitly than indicated in (61), i.e., in the present case of (70) relation (61) yields

$$\mathbb{L}_{\bar{A}}(\hat{\mathbf{q}}_{\bar{A}}) = D_{\tilde{\mathbf{q}}_{\bar{A}}} \tilde{\Gamma}_{\bar{A}}(\tilde{\mathbf{q}}_{\bar{A}})^{-1} = \begin{pmatrix} \mathbb{I}_w & 0 \\ \mathbb{D}_w \bar{A}(\tilde{\mathbf{q}}_{\bar{A}}) & \partial_{\tilde{\tau}} \bar{A}(\tilde{\mathbf{q}}_{\bar{A}}) \end{pmatrix}^{-1} = \begin{pmatrix} \mathbb{I}_w & 0 \\ -\frac{1}{\partial_{\tilde{\tau}} \bar{A}} \mathbb{D}_w \bar{A}(\tilde{\mathbf{q}}_{\bar{A}}) & \frac{0}{\partial_{\tilde{\tau}} \bar{A}(\tilde{\mathbf{q}}_{\bar{A}})} \end{pmatrix}. \quad (71)$$

Here we wrote  $\square$  in order to emphasize how the operator is applied to components of a vector, i.e.,  $\square$  has to be replaced by this component. Additionally,

$$\mathbb{L}_{\bar{A}}(\hat{\mathbf{q}}_{\bar{A}})^* = \begin{pmatrix} \mathbb{I}_w & \mathbb{D}_w^* \bar{A}(\tilde{\mathbf{q}}_{\bar{A}}) [-\frac{\square}{\partial_{\tilde{\tau}} \bar{A}}] \\ 0 & \frac{\square}{\partial_{\tilde{\tau}} \bar{A}(\tilde{\mathbf{q}}_{\bar{A}})} \end{pmatrix} \quad (72a)$$

$$\text{with } \mathbb{D}_w^* \bar{A}(\tilde{\mathbf{q}}_{\bar{A}}) [\bar{\xi}] := \bar{\xi} \partial_w \bar{A}(\tilde{\mathbf{q}}_{\bar{A}}) - \bar{\nabla} \cdot (\bar{\xi} \partial_{\bar{v}_w} \bar{A}(\tilde{\mathbf{q}}_{\bar{A}})) \quad (72b)$$

for some scalar test function  $\bar{\xi}$ . Observe with (72a) that we used  $\mathbb{D}_{\tilde{\tau}} \bar{A}[\bar{\xi}] = (\partial_{\tilde{\tau}} \bar{A}) \bar{\xi}$ , since  $\bar{A}$  does not depend on gradients of the thermal variable  $\tilde{\tau}$ . This is also motivated in Example 3.17 below. From (72a) it is easy to see that  $\mathbb{L}_{\bar{A}}(\hat{\mathbf{q}}_{\bar{A}})^* D_{\tilde{\mathbf{q}}_{\bar{A}}} \bar{\mathcal{A}}(\tilde{\mathbf{q}}) = (0, 1)^\top$ , hence specifically

$$\mathbb{L}_{\bar{S}}(\hat{\mathbf{q}}_{\bar{S}})^* D_{\tilde{\mathbf{q}}_{\bar{S}}} \bar{\mathcal{S}}(\tilde{\mathbf{q}}_{\bar{S}}) = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad \mathbb{L}_{\bar{E}}(\hat{\mathbf{q}}_{\bar{E}})^* D_{\tilde{\mathbf{q}}_{\bar{E}}} \bar{\mathcal{E}}(\tilde{\mathbf{q}}_{\bar{E}}) = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

Thus, in order to guarantee the noninteraction condition (44a) it has to be ensured that

$$\bar{\mathbb{J}}_{\bar{S}}(\tilde{\mathbf{q}}_{\bar{S}}) \begin{pmatrix} 0 \\ 1 \end{pmatrix} = 0 \quad \text{and} \quad \bar{\mathbb{K}}_{\bar{E}}(\tilde{\mathbf{q}}_{\bar{E}}) \begin{pmatrix} 0 \\ 1 \end{pmatrix} = 0; \quad (73)$$

see, (97) and (104) for examples of operators  $\bar{\mathbb{J}}_{\bar{S}}(\tilde{\mathbf{q}}_{\bar{S}})$  and  $\bar{\mathbb{K}}_{\bar{E}}(\tilde{\mathbf{q}}_{\bar{E}})$  complying with (73).

In addition, the special form of GENERIC characterizes the Helmholtz free energy as the driving potential for reversible processes and the Helmholtz free entropy as the driving potential for irreversible, dissipative processes by

$$\mathbb{L}_{\bar{S}}^* D_{\tilde{\mathbf{q}}_{\bar{S}}} \bar{\mathcal{E}}(\tilde{\mathbf{q}}_{\bar{S}}) = \begin{pmatrix} \mathbb{D}_w^* \bar{E}(\tilde{\mathbf{q}}_{\bar{S}}) [1] - \mathbb{D}_w^* \bar{S}(\tilde{\mathbf{q}}_{\bar{S}}) [\bar{\theta}] \\ \bar{\theta} \end{pmatrix}, \quad (74a)$$

$$\mathbb{L}_{\bar{E}}^* D_{\tilde{\mathbf{q}}_{\bar{E}}} \bar{\mathcal{S}}(\tilde{\mathbf{q}}_{\bar{E}}) = \begin{pmatrix} \mathbb{D}_w^* \bar{S}(\tilde{\mathbf{q}}_{\bar{E}}) [1] - \mathbb{D}_w^* \bar{E}(\tilde{\mathbf{q}}_{\bar{E}}) [\frac{1}{\bar{\theta}}] \\ 1/\bar{\theta} \end{pmatrix}, \quad (74b)$$

since the first components of the vectors in (74a) & (74b) coincide with (67b) & (67c).

With regard to the noninteraction condition (44b) for the Fréchet derivative of the total mass we observe

$$\mathbb{L}_{\bar{A}}(\hat{\mathbf{q}}_{\bar{A}})^* D_{\tilde{\mathbf{q}}_{\bar{A}}} \bar{\mathcal{M}}(\tilde{\mathbf{q}}_{\bar{A}}) = \begin{pmatrix} D_w \bar{\mathcal{M}} \\ 0 \end{pmatrix}$$

for  $\bar{A} \in \{\bar{E}, \bar{S}\}$  and spatially constant  $D_w \bar{\mathcal{M}}$  emerging from derivatives w.r.t. concentration according to (24b) & (24c). Hence (44b) can be ensured if  $\bar{\mathbb{J}}_{\bar{S}}(\tilde{\mathbf{q}}_{\bar{S}})$  and  $\bar{\mathbb{K}}_{\bar{E}}(\tilde{\mathbf{q}}_{\bar{E}})$  additionally also satisfy

$$\bar{\mathbb{J}}_{\bar{S}}(\tilde{\mathbf{q}}_{\bar{S}}) \begin{pmatrix} D_w \bar{\mathcal{M}} \\ 0 \end{pmatrix} = 0 \quad \text{and} \quad \bar{\mathbb{K}}_{\bar{E}}(\tilde{\mathbf{q}}_{\bar{E}}) \begin{pmatrix} D_w \bar{\mathcal{M}} \\ 0 \end{pmatrix} = 0.$$

We refer to Sec. 4–6 for more details on the implementation of NIC (44b).



**Example 3.17** Let  $\bar{\xi}_{\bar{U}} : \bar{\Omega} \rightarrow \mathbb{R}$  and  $\bar{v}_{\chi} : \bar{\Omega} \rightarrow \mathbb{R}^d$  smooth functions and  $\bar{U}(\bar{C}, \bar{V} = \det \bar{F}, \bar{S})$  the internal energy. In the setting of Example 3.15 we then have

$$\begin{aligned} \int_{\bar{\Omega}} \bar{\xi}_{\bar{U}} \mathbb{D}_{\chi} \bar{U}[\bar{v}_{\chi}] dx &= \int_{\bar{\Omega}} -\bar{\xi}_{\bar{U}} \bar{\pi} \text{Cof}(\bar{F}) : \bar{\nabla} \bar{v}_{\chi} dx \\ &= \int_{\bar{\Omega}} \bar{\nabla} \cdot (\bar{\xi}_{\bar{U}} \bar{\pi} \text{Cof}(\bar{F})) \cdot \bar{v}_{\chi} dx = \int_{\bar{\Omega}} (\mathbb{D}_{\chi}^* \bar{U}[\bar{\xi}_{\bar{U}}]) \cdot \bar{v}_{\chi} dx, \end{aligned}$$

where  $\mathbb{D}_{\chi} \bar{U}[\bar{v}_{\chi}] \equiv \mathbb{D}_{\chi} \bar{U}(\bar{q}) \bar{v}_{\chi}$ . Thus, writing  $\mathbb{D}_{\chi}^* \bar{U}[\bar{\xi}_{\bar{U}}]$  implies that the divergence, which arises in presence of gradients, also has to be applied to the function  $\bar{\xi}_{\bar{U}}$ . Given an arbitrary functional  $\bar{A}$ , the first variation is defined by

$$\langle \mathbb{D} \bar{A}, \bar{v} \rangle = \int_{\bar{\Omega}} \frac{\delta \bar{A}}{\delta \bar{q}} \cdot \bar{v} d\bar{x}, \quad (76)$$

so that setting  $\bar{\xi}_{\bar{U}} = 1$  above yields

$$\mathbb{D}_{\chi} \bar{A}(\bar{q}) \equiv \delta_{\chi} \bar{A}(\bar{q}) \equiv \mathbb{D}_{\chi}^* \bar{A}(\bar{q})[1] = -\bar{\nabla} \cdot (\partial_{\bar{V}} \bar{A} \text{Cof}(\bar{F})).$$

This identification of the functional derivative  $\mathbb{D} \bar{A}$  with  $\delta \bar{A} / \delta \bar{q}$  relies on the assumption of homogeneous boundary conditions. \*

## 4 Application to fluid dynamics

In this section we combine the thermomechanical fundamentals introduced in Sec. 2 with the GENERIC framework presented in Sec. 3 in order to provide a variational approach to model fluid flows in terms of GENERIC systems. In addition to the GENERIC structure and the resulting evolution equations, we will also discuss boundary conditions, conserved quantities, and transformations between different sets of variables and coordinates.

In Sec. 4.1 we provide the Hamiltonian system  $(\bar{Q}, \bar{\mathcal{E}}, \bar{\mathbb{J}})$  for the flow of an ideal compressible fluid in Lagrangian coordinates and carry out the formal transformation of the structure from the Lagrangian to Eulerian frame. Here we use the reduction approach introduced in Sec. 3.4.1 to obtain the corresponding Eulerian Hamiltonian system  $(\mathcal{Q}, \mathcal{E}, \mathbb{J})$ . Then, in Sec. 4.2 we discuss the GENERIC structure  $(\bar{Q}, \bar{\mathcal{E}}, \bar{\mathcal{S}}, \bar{\mathbb{J}}, \bar{\mathbb{K}})$  of the Navier-Stokes system. Finally, in Sec. 4.3 we derive the Onsager structure for a compressible Stokes flow as a formal asymptotic limit of the GENERIC system.

Throughout Sec. 4 we consider a single species,  $N = 1$ , of concentration  $\bar{C}$ , which is locally conserved in the sense of Lemma 2.9 and again we shall assume that all quantities involved are sufficiently smooth. The only irreversible process will be viscous dissipation, whereas chemical reactions, heat conduction, and diffusion will be discussed in Sec. 5 and 6.

### 4.1 Hamiltonian description of ideal fluids

In the following, we provide the Hamiltonian description of reversible dynamics for the flow of an ideal fluid, i.e., the compressible Euler equations. A complete description of the underlying geometrical structures is beyond the scope of this work and can be found in literature [52, 6]. We consider an isentropic flow, i.e., both the particle concentration  $\bar{C}$  and the entropy density  $\bar{S}$  are constant in time, i.e., locally conserved. This reflects the reversible nature of the process.

Now we construct the triple  $(\bar{\mathcal{Q}}, \bar{\mathcal{E}}, \bar{\mathbb{J}})$  that yields the compressible Euler equations. The dynamics is driven by the total energy  $\bar{\mathcal{E}} : \bar{\mathcal{Q}} \rightarrow \mathbb{R}$ ,

$$\bar{\mathcal{E}}(\bar{\mathbf{q}}) = \int_{\bar{\Omega}} \left( \frac{1}{2\bar{\varrho}} |\bar{\mathbf{P}}|^2 + \bar{U}(\bar{C}, \bar{V}, \bar{S}) \right) d\bar{x}, \quad (77)$$

given as the sum of kinetic energy and internal energy. The volume density  $\bar{V} = T_{\bar{V}}(\bar{\mathbf{q}}) = \det(\bar{\nabla} \chi)$  is not an independent state variable, but a function of the flow map. In the Lagrangian description, we thus consider the state variables

$$\bar{\mathbf{q}} = \begin{pmatrix} \chi : \bar{\Omega} \rightarrow \mathbb{R}^d \\ \bar{\mathbf{P}} : \bar{\Omega} \rightarrow \mathbb{R}^d \end{pmatrix} \in \bar{\mathcal{Q}}, \quad (78)$$

with the flow map  $\chi$  as in Def. 2.4, the linear momentum  $\bar{\mathbf{P}}$ , both defined on the reference domain  $\bar{\Omega} \subset \mathbb{R}^d$ . Similar to Ex. 3.3, also here the Poisson operator in Lagrangian coordinates is in canonical form

$$\bar{\mathbb{J}}(\bar{\mathbf{q}}) \equiv \bar{\mathbb{J}}_{\text{can}} = \begin{pmatrix} 0 & \mathbb{I}_d \\ -\mathbb{I}_d & 0 \end{pmatrix}. \quad (79a)$$

Following (27a),  $\bar{\mathbb{J}}$  generates the Poisson bracket

$$\begin{aligned} \{\bar{\mathcal{G}}, \bar{\mathcal{H}}\}(\bar{\mathbf{q}}) &= \langle D\bar{\mathcal{G}}(\bar{\mathbf{q}}), \bar{\mathbb{J}}(\bar{\mathbf{q}}) D\bar{\mathcal{H}}(\bar{\mathbf{q}}) \rangle_{\bar{\mathcal{Q}}} \\ &= \int_{\bar{\Omega}} \frac{\delta \bar{\mathcal{G}}(\bar{\mathbf{q}})}{\delta \bar{\mathbf{q}}} \cdot \bar{\mathbb{J}}(\bar{\mathbf{q}}) \frac{\delta \bar{\mathcal{H}}(\bar{\mathbf{q}})}{\delta \bar{\mathbf{q}}} d\bar{x} \stackrel{(79a)}{=} \int_{\bar{\Omega}} \sum_{i=1}^d \left( \frac{\delta \bar{\mathcal{G}}}{\delta \chi_i} \frac{\delta \bar{\mathcal{H}}}{\delta \bar{\mathbf{P}}_i} - \frac{\delta \bar{\mathcal{G}}}{\delta \bar{\mathbf{P}}_i} \frac{\delta \bar{\mathcal{H}}}{\delta \chi_i} \right) d\bar{x} \end{aligned}$$

for all functionals  $\bar{\mathcal{G}}(\bar{\mathbf{q}}) = \int_{\bar{\Omega}} \bar{G}(\bar{\mathbf{q}}) d\bar{x}$ ,  $\bar{\mathcal{H}}(\bar{\mathbf{q}}) = \int_{\bar{\Omega}} \bar{H}(\bar{\mathbf{q}}) d\bar{x}$  such that  $\bar{\mathcal{G}}, \bar{\mathcal{H}} \in \bar{\mathcal{X}}$ , cf. (25), and for all  $\bar{\mathbf{q}} \in \bar{\mathcal{Q}}$ .

The Fréchet derivative  $D\bar{\mathcal{E}}(\bar{\mathbf{q}}) \in \bar{\mathcal{Q}}^*$  of the total energy (77) is characterized by

$$\langle D\bar{\mathcal{E}}(\bar{\mathbf{q}}), \bar{\mathbf{v}} \rangle_{\bar{\mathcal{Q}}} = \int_{\bar{\Omega}} \mathbb{D}_{\bar{\mathbf{q}}} \bar{E}(\bar{\mathbf{q}}) \bar{\mathbf{v}} d\bar{x} = \int_{\bar{\Omega}} \left( \frac{\bar{\mathbf{P}}}{\bar{\varrho}} \cdot \bar{\mathbf{v}}_{\bar{\mathbf{P}}} + \mathbb{D}_{\bar{\mathbf{q}}} \bar{U}(\bar{\mathbf{q}}) \bar{\mathbf{v}} \right) d\bar{x} \quad (80a)$$

for all  $\bar{\mathbf{v}} = (\bar{\mathbf{v}}_{\chi}, \bar{\mathbf{v}}_{\bar{\mathbf{P}}}) \in \bar{\mathcal{Q}}$ . Since  $\bar{U}$  only depends on  $\bar{\mathbf{q}}$  through the volume  $\bar{V}$ , while  $\bar{C}$  and  $\bar{S}$  are locally conserved, for the Fréchet derivative of the internal energy density we have  $\mathbb{D}_{\bar{\mathbf{q}}} \bar{U}(\bar{\mathbf{q}}) \bar{\mathbf{v}} = \mathbb{D}_{\chi} \bar{U}(\bar{\mathbf{q}}) \bar{\mathbf{v}}_{\chi}$  with the linear operator  $\mathbb{D}_{\chi} \bar{U}(\bar{\mathbf{q}})$  determined in Ex. 3.15 as

$$\mathbb{D}_{\chi} \bar{U}(\bar{\mathbf{q}}) \bar{\mathbf{v}}_{\chi} = -\bar{\pi} \text{Cof}(\bar{\mathbf{F}}) : \bar{\nabla} \bar{\mathbf{v}}_{\chi}. \quad (80b)$$

for any sufficiently smooth  $\bar{\mathbf{v}}_{\chi} : \bar{\Omega} \rightarrow \mathbb{R}^d$ . Moreover, as discussed in Ex. 3.17, the coupling to other intensive variables  $\bar{z} : \bar{\Omega} \rightarrow \mathbb{R}$ , will involve the adjoint operator

$$\mathbb{D}_{\chi}^* \bar{U}(\bar{\mathbf{q}}) [\bar{\xi}_{\bar{z}}] = \bar{\nabla} \cdot (\bar{\pi} \bar{\xi}_{\bar{z}} \text{Cof}(\bar{\mathbf{F}})) \quad (80c)$$

with  $\text{Cof}(\bar{\mathbf{F}}) := \bar{V} \bar{\mathbf{F}}^{-\top}$  and  $\bar{\mathbf{F}} := \bar{\nabla} \chi$ . In addition, we shall use the identification

$$D_{\chi} \bar{U}(\bar{\mathbf{q}}) \equiv \delta_{\chi} \bar{U}(\bar{\mathbf{q}}) \equiv \mathbb{D}_{\chi}^* \bar{U}(\bar{\mathbf{q}}) [1] = \bar{\nabla} \cdot (\bar{\pi} \text{Cof}(\bar{\mathbf{F}})). \quad (80d)$$

The derivative of the total energy is thus identified as

$$D\bar{\mathcal{E}}(\bar{\mathbf{q}}) \equiv \delta_{\bar{\mathbf{q}}} \bar{E}(\bar{\mathbf{q}}) = \begin{pmatrix} \delta_{\chi} \bar{U}(\bar{\mathbf{q}}) \\ \bar{\mathbf{P}}/\bar{\varrho} \end{pmatrix}. \quad (80e)$$

For the triple  $(\bar{Q}, \bar{\mathcal{E}}, \bar{\mathbb{J}})$  given by (77)–(79) and the driving forces (80), the evolution law  $\partial_t \bar{q} = \bar{\mathbb{J}}(\bar{q}) D\bar{\mathcal{E}}(\bar{q})$  yields the compressible Euler equation in the Lagrangian frame

$$\dot{\chi} = \frac{\bar{P}}{\bar{\rho}}, \quad (81a)$$

$$\dot{\bar{P}} = -\bar{\nabla} \cdot (\bar{\pi} \text{Cof}(\bar{F})). \quad (81b)$$

We emphasize once more that  $\bar{C} = \bar{C}(\bar{x})$  and  $\bar{S} = \bar{S}(\bar{x})$  are not variables, as they are locally conserved quantities and therefore do not have an evolution in the Lagrangian frame. Instead, they can be understood as space-dependent parameters in the internal energy  $\bar{U}$ . System (81) is complemented with initial conditions  $\bar{q}(0) = \bar{q}_0 \in \bar{Q}$  and boundary conditions on  $\partial\bar{\Omega}$ .

**Remark 4.1 (Boundary conditions)** The Hamiltonian formulation of the Euler equations can be supplemented by either of the following boundary conditions:

- i) vanishing normal flow  $\dot{\chi} \cdot \bar{F}^{-\top} \bar{n} = 0$  as an essential Dirichlet boundary condition enforced in  $\bar{Q}$ ,
- ii) vanishing pressure  $\bar{\pi} = 0$  as the natural boundary condition following from  $\bar{\mathbb{J}}$ .

The natural boundary condition follows from the integration by parts when passing from  $\mathbb{D}\bar{U}$  to  $\mathbb{D}^*\bar{U}$ . Using the chain rule and (18h), one finds that the internal energy density of this system evolves according to

$$\partial_t \bar{U} = \frac{\partial \bar{U}}{\partial \bar{V}} \dot{\bar{V}} = \mathbb{D}_{\chi} \bar{U}(\bar{q}) \dot{\chi} = -\bar{\pi} \bar{V} \text{Cof}(\bar{F}) : \bar{\nabla} \dot{\chi}. \quad (82a)$$

By (81) one has for the kinetic energy density

$$\partial_t \frac{|\bar{P}|^2}{2\bar{\rho}} = \dot{\chi} \cdot \dot{\bar{P}} = \dot{\chi} \cdot (-\bar{\nabla} \cdot (\bar{\pi} \text{Cof}(\bar{F}))), \quad (82b)$$

so that the total energy density evolves as

$$\partial_t \bar{E} = -\bar{\nabla} \cdot (\bar{\pi} \text{Cof}(\bar{F})^{\top} \dot{\chi}). \quad (82c)$$

Now, energy conservation can be shown by integrating  $\bar{E}$  over the Lagrangian domain and using either i) or ii) as boundary conditions when applying Gauss's theorem. On the formal level, energy conservation already follows directly from the evolution equation using the chain rule and the skew-symmetry of  $\bar{\mathbb{J}}(\bar{q})$ , cf. (30). \*

Next, we consider the transformation of the PDE-system (81) to the Eulerian frame of reference by exploiting transformation behavior (22b) of extensive quantities and of their derivatives as in (21g),(21h). This yields the common form of the compressible Euler equations

$$\partial_t \mathbf{P} + \nabla \cdot (\rho \mathbf{v} \otimes \mathbf{v}) = -\nabla \pi, \quad (83a)$$

$$\partial_t C + \nabla \cdot (C \mathbf{v}) = 0, \quad (83b)$$

$$\partial_t S + \nabla \cdot (S \mathbf{v}) = 0, \quad (83c)$$

for the Eulerian momentum density  $\mathbf{P} = \rho \mathbf{v}$ , particle density  $C$ , and entropy density  $S$ . The (intensive) Eulerian fluid pressure  $\pi$  is given by

$$\bar{\pi}(\bar{C}, \bar{V}, \bar{S}) = -\partial_{\bar{V}} \bar{U}(\bar{C}, \bar{V}, \bar{S}) = C \partial_C U + S \partial_S U - U = C \mu + \theta S - U = \pi(C, S) \quad (84)$$

with  $\bar{U}(\bar{C}, \bar{V}, \bar{S}) = \bar{V}U(C, S)$ ,  $C = \bar{C}/\bar{V}$ , and  $S = \bar{S}/\bar{V}$ . Note that now the continuity equation for the entropy (83c) has to be taken into account in order to be able to compute  $\pi$  via (84).

In order to transform the Hamiltonian triple  $(\bar{Q}, \bar{\mathcal{E}}, \bar{\mathbb{J}})$  generating (81) into the corresponding triple  $(Q, \mathcal{E}, \mathbb{J})$  in the Eulerian frame, the method of reduction by symmetry [40, 52] explained in Sec. 3.4.1 will be applied. This provides an alternative approach to derive the Eulerian PDE-system (83). For this, we introduce the transformation  $T_{LE} : \bar{Q} \rightarrow Q$ ,

$$\mathbf{q} = \begin{pmatrix} \mathbf{P} : \Omega \rightarrow \mathbb{R}^d \\ C : \Omega \rightarrow \mathbb{R} \\ S : \Omega \rightarrow \mathbb{R} \end{pmatrix} = T_{LE}(\bar{\mathbf{q}}) \in Q, \quad (85a)$$

where each of these extensive variables is defined on  $\Omega$  and generated by  $\bar{\mathbf{q}}$  according to relation (20a), i.e.,

$$\mathbf{P} \circ \boldsymbol{\chi} = \frac{\bar{\mathbf{P}}}{\bar{V}}, \quad (85b)$$

$$C \circ \boldsymbol{\chi} = \frac{\bar{C}}{\bar{V}}, \quad (85c)$$

$$S \circ \boldsymbol{\chi} = \frac{\bar{S}}{\bar{V}}, \quad (85d)$$

keeping in mind that  $\bar{C}$  and  $\bar{S}$  are locally conserved, i.e., parameters in the Lagrangian frame, but that the volume  $\bar{V}$  depends on time. The transformation operator  $\mathbb{L}(\bar{\mathbf{q}}) : \bar{Q} \rightarrow Q$  maps partial time derivatives of states in  $\bar{Q}$  to partial time derivatives of states in  $Q$ . According to Lemma 3.13 we have

$$\mathbb{L}(\bar{\mathbf{q}}) = DT_{LE}(\bar{\mathbf{q}}) = \begin{pmatrix} -\nabla \cdot \left( \frac{\bar{\mathbf{P}}}{\bar{V}} \otimes \square \right) & \frac{\square}{\bar{V}} \\ -\nabla \cdot \left( \frac{\bar{C}}{\bar{V}} \square \right) & 0 \\ -\nabla \cdot \left( \frac{\bar{S}}{\bar{V}} \square \right) & 0 \end{pmatrix}, \quad (86)$$

and indeed, this gives

$$\begin{pmatrix} \dot{\bar{\mathbf{P}}} \\ \dot{\bar{C}} \\ \dot{\bar{S}} \end{pmatrix} = \mathbb{L}(\bar{\mathbf{q}}) \begin{pmatrix} \dot{\boldsymbol{\chi}} \\ \dot{\bar{\mathbf{P}}} \\ \dot{\bar{P}} \end{pmatrix} = \begin{pmatrix} \frac{\dot{\bar{\mathbf{P}}}}{\bar{V}} - \nabla \cdot \left( \frac{\dot{\bar{\mathbf{P}}}}{\bar{V}} \otimes \dot{\boldsymbol{\chi}} \right) \\ -\nabla \cdot \left( \bar{V}^{-1} \bar{C} \dot{\boldsymbol{\chi}} \right) \\ -\nabla \cdot \left( \bar{V}^{-1} \bar{S} \dot{\boldsymbol{\chi}} \right) \end{pmatrix} \quad (87)$$

with the Eulerian gradient acting on the Lagrangian variables evaluated at  $\bar{x} = \boldsymbol{\chi}^{-1}(x)$ , so that equivalently (85) can be used. From (86) we calculate the adjoint operator  $\mathbb{L}(\bar{\mathbf{q}})^* : Q^* \rightarrow \bar{Q}^*$  for any smooth  $\bar{\mathbf{v}} = (\bar{\mathbf{v}}_{\boldsymbol{\chi}}, \bar{\mathbf{v}}_{\bar{\mathbf{P}}}) \in \bar{Q}$  and  $\boldsymbol{\xi} = (\boldsymbol{\xi}_{\mathbf{P}}, \xi_C, \xi_S) \in Q^*$  via integration by parts

$$\begin{aligned} \langle \boldsymbol{\xi}, \mathbb{L}\bar{\mathbf{v}} \rangle_Q &= \int_{\Omega} \xi_C \left[ -\nabla \cdot \left( \frac{\bar{C}}{\bar{V}} \bar{\mathbf{v}}_{\boldsymbol{\chi}} \right) \right] + \xi_S \left[ -\nabla \cdot \left( \frac{\bar{S}}{\bar{V}} \bar{\mathbf{v}}_{\boldsymbol{\chi}} \right) \right] + \boldsymbol{\xi}_{\mathbf{P}} \cdot \left[ \bar{V}^{-1} \bar{\mathbf{v}}_{\bar{\mathbf{P}}} - \nabla \cdot \left( \frac{\bar{\mathbf{P}}}{\bar{V}} \otimes \bar{\mathbf{v}}_{\boldsymbol{\chi}} \right) \right] dx \\ &= \int_{\bar{\Omega}} \left\{ \left[ \bar{C} \nabla \xi_C + (\nabla \boldsymbol{\xi}_{\mathbf{P}})^{\top} \bar{\mathbf{P}} + \bar{S} \nabla \xi_S \right] \cdot \bar{\mathbf{v}}_{\boldsymbol{\chi}} + \boldsymbol{\xi}_{\mathbf{P}} \cdot \bar{\mathbf{v}}_{\bar{\mathbf{P}}} \right\} d\bar{x} = \langle \mathbb{L}^* \boldsymbol{\xi}, \bar{\mathbf{v}} \rangle_{\bar{Q}}, \end{aligned} \quad (88)$$

where  $\nabla \boldsymbol{\xi} = (\bar{\nabla} \bar{\boldsymbol{\xi}}) \bar{\mathbf{F}}^{-1}$  by (21g). From (88) one can identify the adjoint operator  $\mathbb{L}(\bar{\mathbf{q}})^* : Q^* \rightarrow \bar{Q}^*$ ,

$$\mathbb{L}(\bar{\mathbf{q}})^* = DT_{LE}(\bar{\mathbf{q}})^* = \begin{pmatrix} (\nabla \square)^{\top} \bar{\mathbf{P}} & \bar{C} \nabla \square & \bar{S} \nabla \square \\ \square & 0 & 0 \end{pmatrix}. \quad (89)$$

With the transformation operators  $\mathbb{L}, \mathbb{L}^*$  from (86)–(89) together with the Lagrangian Poisson structure  $\mathbb{J}$  from (79a), the Eulerian Poisson structure  $\mathbb{J}$  is obtained by direct calculation

$$\mathbb{J}(\mathbf{q}) = \mathbb{L}(\bar{\mathbf{q}})\mathbb{J}(\bar{\mathbf{q}})\mathbb{L}(\bar{\mathbf{q}})^* = - \begin{pmatrix} ((\nabla\Box)^\top \mathbf{P} + \nabla \cdot (\mathbf{P} \otimes \Box) & C\nabla\Box & S\nabla\Box \\ \nabla \cdot (C\Box) & 0 & 0 \\ \nabla \cdot (S\Box) & 0 & 0 \end{pmatrix}, \quad (90)$$

and results in the corresponding Poisson bracket

$$\begin{aligned} \{\mathcal{F}, \mathcal{G}\}(\mathbf{q}) = \langle D\mathcal{F}(\mathbf{q}), \mathbb{J}(\mathbf{q})D\mathcal{G}(\mathbf{q}) \rangle_{\mathcal{Q}} = & - \int_{\Omega} \sum_{i,j=1}^d \left[ \mathbf{P}_i \left( \frac{\delta F}{\delta \mathbf{P}_j} \partial_{x_j} \frac{\delta G}{\delta \mathbf{P}_i} - \frac{\delta G}{\delta \mathbf{P}_j} \partial_{x_j} \frac{\delta F}{\delta \mathbf{P}_i} \right) \right. \\ & + C \left( \frac{\delta F}{\delta \mathbf{P}_j} \partial_{x_j} \frac{\delta G}{\delta C} - \frac{\delta G}{\delta \mathbf{P}_j} \partial_{x_j} \frac{\delta F}{\delta C} \right) \\ & \left. + S \left( \frac{\delta F}{\delta \mathbf{P}_j} \partial_{x_j} \frac{\delta G}{\delta S} - \frac{\delta G}{\delta \mathbf{P}_j} \partial_{x_j} \frac{\delta F}{\delta S} \right) \right] dx, \end{aligned}$$

where the derivatives  $\delta F/\delta \mathbf{q}, \delta G/\delta \mathbf{q}$  are evaluated at  $\mathbf{q} \in \mathcal{Q}$ . This form of the Poisson bracket is well-known in literature [52]. Note that this reduced Poisson operator satisfies closure condition (50b) and only depends on  $\mathbf{q}$ .

Now consider the Eulerian energy  $\mathcal{E} : \mathcal{Q} \rightarrow \mathbb{R}$

$$\mathcal{E}(\mathbf{q}) = \int_{\Omega} \frac{1}{2\varrho} |\mathbf{P}|^2 + U(C, S) dx, \quad (91)$$

with the Eulerian mass density  $\varrho = MC$  and the given, constant particle mass  $M > 0$ . Notice the difference to the Lagrangian mass density  $\bar{\varrho} = M\bar{C} = \bar{V}\varrho$ . In accordance with closure condition (50a) we notice that indeed  $\mathcal{E}(\mathbf{q}) = \bar{\mathcal{E}}(\bar{\mathbf{q}})$  for any  $\mathbf{q} = \mathbb{T}_{LE}(\bar{\mathbf{q}})$  and  $\bar{\mathbf{q}} \in \bar{\mathcal{Q}}$  by the definition of the transformation (85), the change of coordinates formula (20a) for extensive quantities, and the transformation of integrals. Moreover, (91) yields the driving force for reversible dynamics

$$D\mathcal{E}(\mathbf{q}) = \begin{pmatrix} \partial_C U - \frac{1}{2\varrho} |\mathbf{P}|^2 \\ \partial_S U \end{pmatrix} = \begin{pmatrix} \mu - \frac{1}{2\varrho} |\mathbf{P}|^2 \\ \theta \end{pmatrix}.$$

With this one checks that the evolution  $\dot{\mathbf{q}} = \mathbb{J}(\mathbf{q})D\mathcal{E}(\mathbf{q})$  of the Hamiltonian system  $(\mathcal{Q}, \mathcal{E}, \mathbb{J})$  in Eulerian coordinates provided by (90) and (91) indeed leads to the compressible Euler equations (83). For this, one exploits the relation  $\varrho = MC$  and the definition of the pressure (84). Moreover, one makes use of the identity

$$(\nabla \boldsymbol{\nu})^\top \mathbf{P} = \varrho \nabla \left( \frac{|\mathbf{P}|^2}{2\varrho^2} \right) = \varrho \nabla \frac{|\boldsymbol{\nu}|^2}{2} \quad (92)$$

to cancel two terms emerging in the momentum balance from the entries  $\mathbb{J}_{PP}$  and  $\mathbb{J}_{PC}$  of  $\mathbb{J}(\mathbf{q})$  in (90).

Multiplying the mapping relation for the concentration rates in (87), resp. (83b), with the constant particle mass  $M > 0$ , results in the continuity equation

$$\partial_t \varrho + \nabla \cdot (\varrho \boldsymbol{\nu}) = 0. \quad (93)$$

However, replacing (83b) with (93) in the Hamiltonian structure requires to define Eulerian extensive quantities to be mass-specific rather than volume-specific. We discuss this alternative in Example 4.2 and more general perspectives in Remark 4.3 below.

**Example 4.2 (Hamiltonian structure in  $d = 1$ )** The Hamiltonian structure of the compressible Euler equations in Eulerian coordinates is simpler in 1D when using the velocity  $\nu : [0, T] \times \mathbb{R} \rightarrow \mathbb{R}$  and the mass density  $\varrho : [0, T] \times \mathbb{R} \rightarrow \mathbb{R}$  as variables. With the mass-specific internal energy density  $\tilde{U} = \tilde{U}(\varrho)$  the total energy and the Poisson structure are defined as

$$\mathcal{E}(\mathbf{q}) = \int_{\mathbb{R}} \frac{\varrho}{2} \nu^2 + \varrho \tilde{U}(\varrho) dx, \quad \mathbb{J} = - \begin{pmatrix} 0 & \partial_x \\ \partial_x & 0 \end{pmatrix},$$

and result in the PDE-system

$$\begin{aligned} \partial_t \varrho + \partial_x(\varrho \nu) &= 0, \\ \partial_t \nu + \nu \partial_x \nu &= -\varrho^{-1} \partial_x \pi, \end{aligned}$$

with the pressure  $\pi = \varrho^2 \partial_\varrho \tilde{U}$ . A relevant choice of internal energy may be that of an ideal gas (14), i.e.,

$$\bar{U}(\bar{q}) = \bar{C} \left( \frac{\bar{C}}{\bar{V}} \right)^{\frac{2}{3}} \bar{W} \left( \frac{\bar{S}}{\bar{C}} \right),$$

for a function  $\bar{W} : \mathbb{R} \rightarrow \mathbb{R}$ . Then,

$$\bar{U}(\bar{q}) d\bar{x} = \bar{V} \varrho \tilde{U}(\varrho) d\bar{x} = \varrho \tilde{U} dx$$

with  $\tilde{U}(\varrho) = \bar{W} \varrho^{2/3}$  and  $\varrho = M \bar{C} / \bar{V}$ . For the pressure this gives  $\pi = \frac{2}{3} \bar{W} \varrho^{5/3}$  for the isentropic evolution. In literature [66] one usually finds  $\pi(\varrho) \sim \varrho^\gamma$  with  $\gamma > 1$ . \*

Compared to (83) and in a more general setting, different choices of the Eulerian state variables are possible and we here discuss the choice of Eulerian mass-specific concentrations instead of the Eulerian concentrations.

**Remark 4.3** As an alternative to the mapping (85) for extensive variables in general, in literature [21, 52, 50] the 1-homogeneity of the Gibbs-Duhem relation can be represented by scaling of the extensive quantities by the mass density instead of scaling by the volume, i.e.,

$$\bar{U}(\bar{C}, \bar{V}, \bar{S}) = \bar{\varrho} \tilde{U} \left( \frac{\bar{C}}{\bar{\varrho}}, \frac{\bar{V}}{\bar{\varrho}}, \frac{\bar{S}}{\bar{\varrho}} \right),$$

and  $\tilde{C} = \bar{C} / \bar{\varrho}$ ,  $\tilde{S} = \bar{S} / \bar{\varrho}$ , and  $\tilde{V} = \bar{V} / \bar{\varrho} = \tilde{\varrho}^{-1}$ . This naturally leads to  $\tilde{\mathbf{q}} = (\tilde{C}, \tilde{V}, \tilde{S})$  as natural Eulerian state variables and to the intensive state variables

$$\tilde{\theta} = \frac{\partial \bar{U}}{\partial \bar{S}} = \frac{\partial \tilde{U}}{\partial \tilde{S}} \tag{94a}$$

$$\tilde{\pi} = -\frac{\partial \bar{U}}{\partial \bar{V}} = -\frac{\partial \tilde{U}}{\partial \tilde{\varrho}^{-1}} \tag{94b}$$

$$\tilde{\mu} = \frac{\partial \bar{U}}{\partial \bar{C}} = \frac{\partial \tilde{U}}{\partial \tilde{C}} \tag{94c}$$

Introducing the Eulerian internal energy  $\mathcal{U}_{\tilde{\mathbf{q}}}$  with a mass-specific density  $\tilde{U}$  as

$$\mathcal{U}_{\tilde{\mathbf{q}}}(\tilde{\mathbf{q}}) = \int_{\Omega} \tilde{\varrho} \tilde{U}(\tilde{\mathbf{q}}) dx,$$

suggests the definition of a mass-specific integration measure  $d\tilde{m} = \tilde{\varrho} dx$ , so that

$$\mathcal{U}_{\tilde{\mathbf{q}}}(\tilde{\mathbf{q}}) = \int_{\Omega} \tilde{U}(\tilde{\mathbf{q}}) d\tilde{m} = \int_{\Omega} U(\mathbf{q}) dx = \mathcal{U}(\mathbf{q}),$$

and similarly for any other extensive variable. \*

## 4.2 Navier-Stokes equations as a GENERIC system

Next, we discuss the GENERIC description for a viscous fluid, i.e., a thermodynamic description of the compressible Navier-Stokes equations. These differ from the Navier-Stokes-Fourier system in that heat conduction is not included. For this we couple a non-canonical version of the Poisson structure from Sec. 4.1 with an Onsager structure that accounts for irreversible processes due to changes of entropy and volume by shear and compression. Again we consider a single species  $N = 1$  which is locally conserved in the sense of Lemma 2.9 and assume that all quantities are smooth. We point out that the results of this section represent a generalization of the finite-dimensional mechanical system from Ex. 3.6.

We start in the Lagrangian frame with reference configuration  $\bar{\Omega} \subset \mathbb{R}^d$  and the state vector

$$\bar{\mathbf{q}}_{\bar{S}} = \begin{pmatrix} \chi \\ \bar{\mathbf{P}} \\ \bar{S} \end{pmatrix} \in \bar{\mathcal{Q}}_{\bar{S}}, \quad (95)$$

i.e., compared to (78) the state vector is now augmented by the entropy density  $\bar{S} : \bar{\Omega} \rightarrow \mathbb{R}$  as an additional independent extensive state variable. The total energy and the total entropy of the system are given by

$$\bar{\mathcal{E}}_{\bar{S}}(\bar{\mathbf{q}}_{\bar{S}}) = \int_{\bar{\Omega}} \frac{1}{2\bar{\varrho}} |\bar{\mathbf{P}}|^2 + \bar{U}(\bar{C}, \bar{V}, \bar{S}) \, d\bar{x}, \quad (96a)$$

$$\bar{\mathcal{S}}_{\bar{S}}(\bar{\mathbf{q}}_{\bar{S}}) = \int_{\bar{\Omega}} \bar{S} \, d\bar{x}, \quad (96b)$$

with the internal energy density  $\bar{U}$  in terms of its natural variables. Note that  $\bar{\mathcal{E}}_{\bar{S}}(\bar{\mathbf{q}}_{\bar{S}})$  coincides with  $\bar{\mathcal{E}}(\bar{\mathbf{q}})$  from (77) if we replace the locally conserved entropy with the entropy from  $\bar{\mathbf{q}}_{\bar{S}}$ . However, we use the subscript  $\bar{S}$  as explained in Sec. 3.4.2 to highlight the dependence on  $\bar{S}$  as a state variable. This notation will be important in the upcoming discussion on changes of variables.

**Reversible contribution to dynamics.** In order to account for the additional dissipative state variable  $\bar{S}$ , the canonical Poisson operator from (79a) is augmented by additional entries, leading to the non-canonical operator

$$\bar{\mathbb{J}}_{\bar{S}}(\bar{\mathbf{q}}_{\bar{S}}) := \begin{pmatrix} 0 & \mathbb{I}_d & 0 \\ -\mathbb{I}_d & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \quad (97)$$

In this form  $\bar{\mathbb{J}}_{\bar{S}}(\bar{\mathbf{q}}_{\bar{S}})$  obviously satisfies the NIC (44a),

$$\bar{\mathbb{J}}_{\bar{S}}(\bar{\mathbf{q}}_{\bar{S}}) \text{D}\bar{\mathcal{S}}_{\bar{S}}(\bar{\mathbf{q}}_{\bar{S}}) \equiv 0 \quad \text{with} \quad \text{D}\bar{\mathcal{S}}_{\bar{S}}(\bar{\mathbf{q}}_{\bar{S}}) = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

for the entropy defined in (96b). Conservation of mass is ensured with the locally conserved particle density  $\bar{C}$ , hence  $\bar{\varrho}(\bar{x}) \equiv M\bar{C}(\bar{x})$  with constant, specific particle mass  $M > 0$ . Thus,  $\text{D}_{\bar{\mathbf{q}}_{\bar{S}}} \bar{\mathcal{M}}(\bar{\mathbf{q}}_{\bar{S}}) = 0$  so that the NIC (44b) for mass conservation is trivially satisfied.

To simplify the coupling with irreversible dynamics later on, we carry out a change of variables as outlined in Sec. 3.4.2. Here we change from the entropy density  $\bar{S}$  to the internal energy density  $\bar{U}$  as a state variable. More precisely, we consider the mapping  $\text{T}_v : \bar{\mathcal{Q}}_{\bar{S}} \rightarrow \bar{\mathcal{Q}}_{\bar{U}}$ ,

$$\text{T}_v(\bar{\mathbf{q}}_{\bar{S}}) = \bar{\mathbf{q}}_{\bar{U}} = \begin{pmatrix} \chi \\ \bar{\mathbf{P}} \\ \bar{U} \end{pmatrix} \in \bar{\mathcal{Q}}_{\bar{U}} \quad (98)$$

by setting  $\bar{U} = \bar{U}(\bar{C}, \mathbb{T}_{\bar{V}}(\boldsymbol{\chi}), \bar{S})$  using (18b) and the equation of state  $\bar{U}(\bar{C}, \bar{V}, \bar{S})$ . Here,  $w = (\boldsymbol{\chi}, \bar{\mathbf{P}})$  remains unchanged in the sense of (58). Following (60a), we determine the transformation operator  $\mathbb{L}(\bar{\mathbf{q}}_{\bar{S}}) = \text{DT}_{\bar{V}}(\bar{\mathbf{q}}_{\bar{S}}) : \bar{\mathcal{Q}}_{\bar{S}} \rightarrow \bar{\mathcal{Q}}_{\bar{U}}$ ,

$$\mathbb{L}^*(\bar{\mathbf{q}}_{\bar{S}}) = \begin{pmatrix} \mathbb{I}_d & 0 & 0 \\ 0 & \mathbb{I}_d & 0 \\ \mathbb{D}_{\boldsymbol{\chi}}\bar{U} & \mathbb{D}_{\bar{\mathbf{P}}}\bar{U} & \mathbb{D}_{\bar{S}}\bar{U} \end{pmatrix} = \begin{pmatrix} \mathbb{I}_d & 0 & 0 \\ 0 & \mathbb{I}_d & 0 \\ \mathbb{D}_{\boldsymbol{\chi}}\bar{U} & 0 & \bar{\theta} \end{pmatrix},$$

with  $\mathbb{D}_{\boldsymbol{\chi}}\bar{U}(\bar{\mathbf{q}}_{\bar{S}})\bar{\mathbf{v}}_{\boldsymbol{\chi}} = -\bar{\pi}\text{Cof}(\bar{\mathbf{F}}) : \bar{\nabla}\bar{\mathbf{v}}_{\boldsymbol{\chi}}$  as in (80b). This gives the adjoint operator  $\mathbb{L}^* : \bar{\mathcal{Q}}_{\bar{U}}^* \rightarrow \bar{\mathcal{Q}}_{\bar{S}}^*$ ,

$$\mathbb{L}^*(\bar{\mathbf{q}}_{\bar{S}}) = \begin{pmatrix} \mathbb{I}_d & 0 & \mathbb{D}_{\boldsymbol{\chi}}^*\bar{U}(\bar{\mathbf{q}}_{\bar{S}}) \\ 0 & \mathbb{I}_d & 0 \\ 0 & 0 & \bar{\theta} \end{pmatrix},$$

with  $\mathbb{D}_{\boldsymbol{\chi}}^*\bar{U}(\bar{\mathbf{q}}_{\bar{S}})\bar{\xi}_{\bar{U}} = \bar{\nabla} \cdot (\bar{\xi}_{\bar{U}}\bar{\pi}\text{Cof}(\bar{\mathbf{F}}))$  from (80c) for  $\bar{z} = \bar{U}$ . Thus, the Poisson operator  $\bar{\mathbb{J}}_{\bar{S}}$  from (97) transforms to

$$\bar{\mathbb{J}}_{\bar{U}} = \mathbb{L}\bar{\mathbb{J}}_{\bar{S}}\mathbb{L}^* = \begin{pmatrix} 0 & \mathbb{I}_d & 0 \\ -\mathbb{I}_d & 0 & -\mathbb{D}_{\boldsymbol{\chi}}^*\bar{U} \\ 0 & \mathbb{D}_{\boldsymbol{\chi}}\bar{U} & 0 \end{pmatrix}. \quad (99)$$

For the transformed total energy functional  $\bar{\mathcal{E}}_{\bar{U}}$  with density  $\bar{E}_{\bar{U}}(\bar{\mathbf{q}}_{\bar{U}}) = \frac{1}{2\bar{\rho}}|\bar{\mathbf{P}}|^2 + \bar{U}$  the Fréchet derivative reads

$$\text{D}\bar{\mathcal{E}}_{\bar{U}}(\bar{\mathbf{q}}_{\bar{U}}) = \delta_{\bar{\mathbf{q}}_{\bar{U}}}\bar{E}_{\bar{U}}(\bar{\mathbf{q}}_{\bar{U}}) = \begin{pmatrix} 0 \\ \frac{\bar{\mathbf{P}}}{\bar{\rho}} \\ 1 \end{pmatrix}. \quad (100)$$

Recalling the results of Thm. 3.11 and (73) we conclude that the NIC (44a), i.e.,  $\bar{\mathbb{J}}_{\bar{U}}(\bar{\mathbf{q}}_{\bar{U}})\text{D}\bar{\mathcal{E}}_{\bar{U}}(\bar{\mathbf{q}}_{\bar{U}}) = 0$  is satisfied also for the transformed system. This can also be directly checked taking into account that

$$\text{D}_{\bar{\mathbf{q}}_{\bar{U}}}\bar{\mathcal{S}}_{\bar{q}} = \begin{pmatrix} \delta_{\boldsymbol{\chi}}\bar{S}_{\bar{U}} \\ 0 \\ 1/\bar{\theta} \end{pmatrix} = \begin{pmatrix} \mathbb{D}_{\boldsymbol{\chi}}^*\bar{U}[-1/\bar{\theta}] \\ 0 \\ 1/\bar{\theta} \end{pmatrix}, \quad (101)$$

since  $\mathbb{D}_{\boldsymbol{\chi}}^*\bar{S}_{\bar{U}}(\bar{\mathbf{q}}_{\bar{U}})[1] = -\bar{\nabla} \cdot (\frac{\bar{\pi}}{\bar{\theta}}\text{Cof}(\bar{\mathbf{F}})) = \mathbb{D}_{\boldsymbol{\chi}}^*\bar{U}(\bar{\mathbf{q}}_{\bar{U}})[-1/\bar{\theta}]$  for  $\bar{\mathbf{F}} = \bar{\nabla}\boldsymbol{\chi}$  by (7b) and (80c).

**Example 4.4 (External forces)** Conservative external mechanical forces can be generated by a potential energy  $\bar{U}_{\text{ext}}(\boldsymbol{\chi})$ . Then, the total energy is replaced by  $\bar{\mathcal{E}}_{\text{ext}}(\bar{\mathbf{q}}_{\bar{U}})$  with density  $E_{\text{ext}}(\bar{\mathbf{q}}_{\bar{U}}) := \frac{1}{2\bar{\rho}}|\bar{\mathbf{P}}|^2 + \bar{U} + \bar{U}_{\text{ext}}(\boldsymbol{\chi})$ . This gives the driving force  $\text{D}\bar{\mathcal{E}}_{\text{ext}}(\bar{\mathbf{q}}_{\bar{U}}) = (\delta_{\boldsymbol{\chi}}\bar{U}_{\text{ext}}, \frac{\bar{\mathbf{P}}}{\bar{\rho}}, 1)$  and  $\dot{\bar{\mathbf{q}}} = \bar{\mathbb{J}}_{\bar{U}}(\bar{\mathbf{q}})\text{D}\bar{\mathcal{E}}_{\text{ext}}(\bar{\mathbf{q}})$  extends the previous dynamics to the new conserved energy  $\bar{\mathcal{E}}_{\text{ext}}$ . This allows for a reduction if the closure condition  $\mathcal{E}_{\text{ext}}(\mathbf{q}) = \bar{\mathcal{E}}_{\text{ext}}(\bar{\mathbf{q}})$  is satisfied. Gravitational energies  $\bar{U}_{\text{ext}} = \bar{\rho}\mathbf{g} \cdot \boldsymbol{\chi}$  with gravitational acceleration vector  $\mathbf{g} \in \mathbb{R}^d$  can be reduced since  $U_{\text{ext}}(\mathbf{q}) = \underline{\rho}\mathbf{g} \cdot \mathbf{x}$  for  $\mathbf{q} = (\underline{\rho}, \mathbf{P}, U)$ . In the presence of irreversible dynamics, when checking the NIC  $\bar{\mathbb{K}}\text{D}\bar{\mathcal{E}} = 0$  the extra contribution from  $\bar{U}_{\text{ext}}$  needs to be taken into account. The reduction in the way explained before would fail for hyperelastic energies  $\bar{U}_{\text{ext}}(\boldsymbol{\chi}) = W_{\text{elast}}(\nabla\boldsymbol{\chi})$ , since the closure condition is not satisfied in general. \*



**Dissipative contribution to dynamics.** Now we construct the Onsager operator  $\bar{\mathbb{K}}^S$  for viscous flows in terms of a Stokes dissipation and we have to take care that the corresponding NIC (44a), i.e.,  $\bar{\mathbb{K}}^S D\bar{\mathcal{E}} = 0$  is satisfied. For the state vector

$$\bar{q}_{\bar{U}} = \begin{pmatrix} \bar{\chi} \\ \bar{P} \\ \bar{U} \end{pmatrix} \in \bar{Q}_{\bar{U}}, \quad (102)$$

and the corresponding, sufficiently smooth dual variables  $\bar{\xi} = (\bar{\xi}_{\bar{\chi}}, \bar{\xi}_{\bar{P}}, \bar{\xi}_{\bar{U}}) \in \bar{Q}_{\bar{U}}^*$ , we define a quadratic dual dissipation potential as follows

$$\bar{\Psi}_S^*(\bar{q}; \bar{\xi}) = \langle \bar{\xi}, \frac{1}{2} \bar{\mathbb{K}}_{\bar{U}}^S \bar{\xi} \rangle_{\bar{Q}_{\bar{U}}} = \int_{\bar{\Omega}} \frac{1}{2} [2\bar{\lambda} |\bar{\mathbf{w}}|^2 + \bar{\zeta} \text{tr}(\bar{\mathbf{w}})^2] \bar{V} d\bar{x}, \quad (103a)$$

with  $\bar{\lambda} = \bar{\theta} \lambda$ ,  $\bar{\zeta} = \bar{\theta} \zeta$ ,  $\bar{\mathbf{w}} = \bar{\nabla}_s \bar{\xi}_{\bar{P}} - \bar{\xi}_{\bar{U}} \bar{\nabla}_s \bar{\nu}$ , and the symmetric gradient  $\bar{\nabla}_s \bar{\mathbf{a}} = \frac{1}{2} (\bar{\nabla} \bar{\mathbf{a}} \bar{F}^{-1} + \bar{F}^{-T} \bar{\nabla} \bar{\mathbf{a}}^T)$ . The viscous material properties are characterized by the shear viscosity  $\lambda > 0$  and the volume viscosity  $\xi = \zeta + \frac{2\lambda}{d} > 0$ . The integrand of (103a) can be rewritten as

$$\begin{aligned} 2\bar{\lambda} |\bar{\mathbf{w}}|^2 + \bar{\zeta} \text{tr}(\bar{\mathbf{w}})^2 &= [2\bar{\lambda} \bar{\mathbf{w}} + \bar{\zeta} \text{tr}(\bar{\mathbf{w}}) \mathbb{I}_d] : \bar{\mathbf{w}} \\ &= (2\bar{\lambda} \bar{\mathbf{w}} + \bar{\zeta} \text{tr}(\bar{\mathbf{w}}) \mathbb{I}_d) : (\bar{\nabla} \bar{\xi}_{\bar{P}} - \bar{\xi}_{\bar{U}} \bar{\nabla} \bar{\nu}) \bar{F}^{-1} \\ &= ((2\bar{\lambda} \bar{\mathbf{w}} + \bar{\zeta} \text{tr}(\bar{\mathbf{w}}) \mathbb{I}_d) \bar{F}^{-T}) : (\bar{\nabla} \bar{\xi}_{\bar{P}} - \bar{\xi}_{\bar{U}} \bar{\nabla} \bar{\nu}) \end{aligned} \quad (103b)$$

by the orthogonality  $(\mathbf{A} + \mathbf{A}^T) : (\mathbf{B} - \mathbf{B}^T) = 0$  and the identity  $(\mathbf{A}\mathbf{B}) : \mathbf{C} = \mathbf{A} : (\mathbf{C}\mathbf{B}^T)$  for general matrices  $\mathbf{A}, \mathbf{B}, \mathbf{C} \in \mathbb{R}^{d \times d}$ . Note that  $\bar{\Psi}_S^*$  and the Onsager operator  $\bar{\mathbb{K}}_{\bar{U}}^S = D_{\bar{\xi}} \bar{\Psi}_S^*$  depend on the state  $\bar{q}_{\bar{U}}$  through velocity  $\bar{\nu} = \bar{P}/\bar{\rho}$ , temperature  $\bar{\theta}$ , deformation gradient  $\bar{F}$ , and volume  $\bar{V} = \det \bar{F}$ . Additionally,  $\bar{\Psi}_S^*$  only depends on  $\bar{\xi}_{\bar{P}}$  and  $\bar{\xi}_{\bar{U}}$ . Therefore, the Onsager operator has the form

$$\bar{\mathbb{K}}_{\bar{U}}^S = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \bar{\mathbb{K}}_{\bar{P}\bar{P}}^S & \bar{\mathbb{K}}_{\bar{P}\bar{U}}^S \\ 0 & \bar{\mathbb{K}}_{\bar{U}\bar{P}}^S & \bar{\mathbb{K}}_{\bar{U}\bar{U}}^S \end{pmatrix}, \quad (104a)$$

with the entries determined from (103b)

$$\bar{\mathbb{K}}_{\bar{P}\bar{P}}^S \bar{\xi}_{\bar{P}} = -\bar{\nabla} \cdot ((2\bar{\lambda} \bar{\nabla}_s \bar{\xi}_{\bar{P}} + \bar{\zeta} \text{tr}(\bar{\nabla}_s \bar{\xi}_{\bar{P}}) \mathbb{I}_d) \text{Cof} \bar{F}), \quad (104b)$$

$$\bar{\mathbb{K}}_{\bar{U}\bar{U}}^S \bar{\xi}_{\bar{U}} = (2\bar{\lambda} |\bar{\nabla}_s \bar{\nu}|^2 + \bar{\zeta} \text{tr}(\bar{\nabla}_s \bar{\nu})^2) \bar{\xi}_{\bar{U}} \bar{V}, \quad (104c)$$

$$\bar{\mathbb{K}}_{\bar{U}\bar{P}}^S \bar{\xi}_{\bar{P}} = -((2\bar{\lambda} \bar{\nabla}_s \bar{\xi}_{\bar{P}} + \bar{\zeta} \text{tr}(\bar{\nabla}_s \bar{\xi}_{\bar{P}}) \mathbb{I}_d) \text{Cof} \bar{F}) : \bar{\nabla} \bar{\nu}, \quad (104d)$$

$$\bar{\mathbb{K}}_{\bar{P}\bar{U}}^S \bar{\xi}_{\bar{U}} = \bar{\nabla} \cdot ((2\bar{\lambda} \bar{\nabla}_s \bar{\nu} + \bar{\zeta} \text{tr}(\bar{\nabla}_s \bar{\nu}) \mathbb{I}_d) \bar{\xi}_{\bar{U}} \text{Cof} \bar{F}), \quad (104e)$$

where integration by parts was applied for (104b) and (104e). Making in (104) the choice  $\bar{\xi} = D\bar{\mathcal{E}}_{\bar{U}}$  as in (100) one can directly check the NIC  $\bar{\mathbb{K}}_{\bar{U}}^S D_{\bar{q}_{\bar{U}}} \bar{\mathcal{E}}_{\bar{U}} = 0$ . Dissipative dynamics is driven by  $D\bar{S}_{\bar{U}}$  from (101).

**GENERIC Lagrangian Navier-Stokes system.** From the above considerations we conclude that the system  $(\bar{Q}_{\bar{U}}, \bar{\mathcal{E}}_{\bar{U}}, \bar{S}_{\bar{U}}, \bar{\mathbb{J}}_{\bar{U}}, \bar{\mathbb{K}}_{\bar{U}}^S)$  with the reversible and irreversible operators and driving forces introduced in (99)-(101) and (104) indeed provides a GENERIC system in Lagrangian coordinates.

The evolution law  $\partial_t \bar{q}_{\bar{U}} = \bar{\mathbb{J}}_{\bar{U}} D \bar{\mathcal{E}}_{\bar{U}} + \bar{\mathbb{K}}_{\bar{U}}^S D \bar{\mathcal{S}}_{\bar{U}}$  results in the PDE-system

$$\dot{\chi} = +\delta_{\bar{P}} \bar{E}_{\bar{U}} = \frac{1}{\bar{\theta}} \bar{\mathbf{P}}, \quad (105a)$$

$$\begin{aligned} \partial_t \bar{\mathbf{P}} &= -\mathbb{D}_{\chi}^* \bar{U} [1] + \bar{\mathbb{K}}_{\bar{P}\bar{U}}^S \left[ \frac{1}{\bar{\theta}} \right] \\ &= -\bar{\nabla} \cdot (\bar{\pi} \text{Cof}(\bar{\mathbf{F}})) + \bar{\nabla} \cdot \bar{\Sigma}_{\text{visc}}, \end{aligned} \quad (105b)$$

$$\begin{aligned} \partial_t \bar{U} &= +\mathbb{D}_{\chi} \bar{U} \left[ \frac{1}{\bar{\theta}} \bar{\mathbf{P}} \right] + \bar{\mathbb{K}}_{\bar{U}\bar{U}}^S \left[ \frac{1}{\bar{\theta}} \right] \\ &= -\bar{\pi} \text{Cof}(\bar{\mathbf{F}}) : \bar{\nabla} \bar{\nu} + \bar{\Sigma}_{\text{visc}} : \bar{\nabla} \bar{\nu}, \end{aligned} \quad (105c)$$

with the first Piola-Kirchhoff stress tensor

$$\bar{\Sigma}_{\text{visc}} = (2\lambda(\bar{\nabla}_s \bar{\nu}) + \zeta \text{tr}(\bar{\nabla}_s \bar{\nu}) \mathbb{I}_d) \text{Cof}(\bar{\mathbf{F}}) \quad (105d)$$

obtained by comparison with (104). Here we have set  $\lambda = \bar{\lambda}/\bar{\theta}$  and  $\zeta = \bar{\zeta}/\bar{\theta}$ . The viscous stress accounts for heat generation by fluid viscosity in (105c),

$$\bar{\Sigma}_{\text{visc}} : \bar{\nabla} \bar{\nu} = 2\lambda |\bar{\nabla}_s \bar{\nu}|^2 + \zeta \text{tr}(\bar{\nabla}_s \bar{\nu})^2 \geq 0.$$

(105c) can be transformed to an evolution equation for  $\bar{S}$  with locally conserved  $\bar{C}$  as follows:

$$\begin{aligned} \partial_t \bar{S} &= \frac{\partial \bar{S}}{\partial \bar{V}} \mathbb{D}_{\chi} \bar{V}(\bar{q}_{\bar{U}}) \dot{\chi} + \frac{\partial \bar{S}}{\partial \bar{U}} \dot{\bar{U}} \stackrel{(18h)}{=} \frac{\bar{\pi}}{\bar{\theta}} \text{Cof}(\bar{\mathbf{F}}) : \bar{\nabla} \dot{\chi} + \frac{1}{\bar{\theta}} \dot{\bar{U}} \\ &\stackrel{(105c)}{=} \bar{\theta}^{-1} \bar{\mathbb{K}}_{\bar{U}\bar{U}}^S \bar{\theta}^{-1} = \bar{\theta}^{-1} (\bar{\Sigma}_{\text{visc}} : \bar{\nabla} \bar{\nu}) \geq 0, \end{aligned}$$

which shows indeed a positive entropy production. A more systematic change of variables for the GENERIC structure for reactive fluid flow based on the methods of Sec. 3.4 will be performed in Sec. 6.

**Lagrangian-Eulerian reduction of (105).** We consider the GENERIC system  $(\bar{Q}_{\bar{U}}, \bar{\mathcal{E}}_{\bar{U}}, \bar{\mathcal{S}}_{\bar{U}}, \bar{\mathbb{J}}_{\bar{U}}, \bar{\mathbb{K}}_{\bar{U}}^S)$  and perform a change of coordinates from the Lagrangian to the Eulerian frame via reduction by symmetry, cf. Sec. 3.4.1. As in Sec. 4.1 we introduce a map

$$\mathbb{T}_{\text{LE}}(\bar{q}_{\bar{U}}) = \mathbf{q}_U = \begin{pmatrix} \mathbf{P} : \Omega \rightarrow \mathbb{R}^d \\ C : \Omega \rightarrow \mathbb{R} \\ U : \Omega \rightarrow \mathbb{R} \end{pmatrix} \in \mathcal{Q}_U, \quad (106a)$$

with each of the above extensive variables transformed as in Definition 2.6, by

$$\mathbf{P} \circ \chi = \frac{\bar{\mathbf{P}}}{\bar{V}}, \quad (106b)$$

$$C \circ \chi = \frac{\bar{C}}{\bar{V}}, \quad (106c)$$

$$U \circ \chi = \frac{\bar{U}}{\bar{V}}. \quad (106d)$$

Compared to the purely Hamiltonian case (85) now only  $\bar{C}$  is locally conserved but both entropy  $\bar{S}$  and internal energy  $\bar{U}$  are nontrivial state variables. In accordance with Lemma 3.13 and in particular with (86) we have the following transformation operator  $\mathbb{L}_{\text{LE}}(\bar{q}_{\bar{U}}) = D\mathbb{T}_{\text{LE}}(\bar{q}_{\bar{U}}) : \bar{Q}_{\bar{U}} \rightarrow \mathcal{Q}_U$ ,

$$\mathbb{L}_{\text{LE}}(\bar{q}_{\bar{U}}) = \begin{pmatrix} -\bar{\nabla} \cdot (\bar{V}^{-1} \bar{\mathbf{P}} \otimes \square) & \frac{\square}{\bar{V}} & 0 \\ -\bar{\nabla} \cdot (\bar{V}^{-1} \bar{C} \square) & 0 & 0 \\ -\bar{\nabla} \cdot (\bar{V}^{-1} \bar{U} \square) & 0 & \frac{\square}{\bar{V}} \end{pmatrix}. \quad (107)$$

The operator transforms rates  $(\dot{\chi}, \dot{\mathbf{P}}, \dot{U}) \in \bar{\mathcal{Q}}_{\bar{U}}$  to rates  $(\dot{\mathbf{P}}, \dot{C}, \dot{U}) \in \mathcal{Q}_U$  as follows

$$\begin{pmatrix} \dot{\mathbf{P}} \\ \dot{C} \\ \dot{U} \end{pmatrix} = \mathbb{L}_{\text{LE}}(\bar{\mathbf{q}}_{\bar{U}}) \begin{pmatrix} \dot{\chi} \\ \dot{\mathbf{P}} \\ \dot{U} \end{pmatrix} = \begin{pmatrix} \frac{\dot{\mathbf{P}}}{\bar{V}} - \nabla \cdot \left( \frac{\bar{\mathbf{P}}}{\bar{V}} \otimes \dot{\chi} \right) \\ -\nabla \cdot \left( \frac{\bar{C}}{\bar{V}} \dot{\chi} \right) \\ \frac{\dot{U}}{\bar{V}} - \nabla \cdot \left( \frac{\bar{U}}{\bar{V}} \dot{\chi} \right) \end{pmatrix}.$$

Adapting the calculation in (88), we determine the adjoint operator  $\mathbb{L}_{\text{LE}}(\bar{\mathbf{q}}_{\bar{U}})^* : \mathcal{Q}_U^* \rightarrow \bar{\mathcal{Q}}_{\bar{U}}^*$ ,

$$\mathbb{L}_{\text{LE}}(\bar{\mathbf{q}}_{\bar{U}})^* = \begin{pmatrix} ((\nabla \square)^\top \bar{\mathbf{P}} & \bar{C} \nabla \square & \bar{U} \nabla \square) \\ \square & 0 & 0 \\ 0 & 0 & \square \end{pmatrix}. \quad (108)$$

This allows us to transform the Lagrangian Poisson operator  $\bar{\mathbb{J}}_{\bar{U}}$  from (99) to the Eulerian frame as follows

$$\mathbb{J}_U = \mathbb{L}_{\text{LE}} \bar{\mathbb{J}}_{\bar{U}} \mathbb{L}_{\text{LE}}^* = - \begin{pmatrix} ((\nabla \square)^\top \mathbf{P} + \nabla \cdot (\mathbf{P} \otimes \square) & C \nabla \square & U \nabla \square + \nabla(\pi \square) \\ \nabla \cdot (C \square) & 0 & 0 \\ \nabla \cdot (U \square) + \pi \nabla \cdot \square & 0 & 0 \end{pmatrix}. \quad (109)$$

Herein, the terms involving the pressure  $\pi$  arise by the transformation of the Lagrangian terms according to the composition of the operators as follows:

$$\frac{1}{\bar{V}} \mathbb{D}_{\chi} \bar{U} \square = -\frac{\bar{\pi}}{\bar{V}} \text{Cof}(\bar{\mathbf{F}}) : \bar{\nabla} \square = -\pi \nabla \cdot \square, \quad (110a)$$

$$\frac{-1}{\bar{V}} \mathbb{D}_{\chi}^* \bar{U} [\square] = \frac{-1}{\bar{V}} \bar{\nabla} \cdot (\square \bar{\pi} \text{Cof}(\bar{\mathbf{F}})) = -\nabla(\pi \square), \quad (110b)$$

where we used (80b) and (80c) together with the transformation rules for derivatives (21g), (21h), and the Piola identity (18g). Similarly, we transform the Onsager operator  $\bar{\mathbb{K}}_{\bar{U}}^{\text{S}}$  for the Stokes problem from (104)

$$\mathbb{K}_U^{\text{S}} = \mathbb{L}_{\text{LE}} \bar{\mathbb{K}}_{\bar{U}}^{\text{S}} \mathbb{L}_{\text{LE}}^* = \frac{1}{\bar{V}} \begin{pmatrix} \bar{\mathbb{K}}_{\bar{\mathbf{P}}\bar{\mathbf{P}}}^{\text{S}} & 0 & \bar{\mathbb{K}}_{\bar{\mathbf{P}}\bar{U}}^{\text{S}} \\ 0 & 0 & 0 \\ \bar{\mathbb{K}}_{\bar{U}\bar{\mathbf{P}}}^{\text{S}} & 0 & \bar{\mathbb{K}}_{\bar{U}\bar{U}}^{\text{S}} \end{pmatrix} = \begin{pmatrix} \mathbb{K}_{\mathbf{P}\mathbf{P}}^{\text{S}} & 0 & \mathbb{K}_{\mathbf{P}U}^{\text{S}} \\ 0 & 0 & 0 \\ \mathbb{K}_{U\mathbf{P}}^{\text{S}} & 0 & \mathbb{K}_{UU}^{\text{S}} \end{pmatrix},$$

corresponding to the Eulerian dual dissipation potential

$$\Psi_{\text{S}}^*(\mathbf{q}_U; \boldsymbol{\xi}) = \langle \boldsymbol{\xi}, \frac{1}{2} \mathbb{K}_U^{\text{S}} \boldsymbol{\xi} \rangle_{\mathcal{Q}_U} = \int_{\Omega} \frac{1}{2} [2\bar{\lambda} |\mathbf{w}|^2 + \bar{\zeta} \text{tr}(\mathbf{w})^2] dx, \quad (111a)$$

similar to (103a), with  $\mathbf{P} = \rho \boldsymbol{\nu}$ ,  $\mathbf{w} = \nabla_s \boldsymbol{\xi}_{\mathbf{P}} - \xi_U \nabla_s \boldsymbol{\nu}$ , and  $\nabla_s \boldsymbol{\xi} = \frac{1}{2} (\nabla \boldsymbol{\xi} + \nabla \boldsymbol{\xi}^\top)$  the symmetric gradient. The operators in (111) is derived as for (104b), i.e.,

$$\mathbb{K}_{\mathbf{P}\mathbf{P}}^{\text{S}} \boldsymbol{\xi}_{\mathbf{P}} = -\nabla \cdot (2\bar{\lambda} \nabla_s \boldsymbol{\xi}_{\mathbf{P}} + \bar{\zeta} \text{tr}(\nabla_s \boldsymbol{\xi}_{\mathbf{P}}) \mathbb{I}_d), \quad (111b)$$

$$\mathbb{K}_{UU}^{\text{S}} \xi_U = (2\bar{\lambda} |\nabla_s \boldsymbol{\nu}|^2 + \bar{\zeta} \text{tr}(\nabla_s \boldsymbol{\nu})^2) \xi_U, \quad (111c)$$

$$\mathbb{K}_{U\mathbf{P}}^{\text{S}} \boldsymbol{\xi}_{\mathbf{P}} = -(2\bar{\lambda} \nabla_s \boldsymbol{\xi}_{\mathbf{P}} + \bar{\zeta} \text{tr}(\nabla_s \boldsymbol{\xi}_{\mathbf{P}}) \mathbb{I}_d) : \nabla \boldsymbol{\nu}, \quad (111d)$$

$$\mathbb{K}_{\mathbf{P}U}^{\text{S}} \xi_U = \nabla \cdot ((2\bar{\lambda} \nabla_s \boldsymbol{\nu} + \bar{\zeta} \text{tr}(\nabla_s \boldsymbol{\nu}) \mathbb{I}_d) \xi_U). \quad (111e)$$

The Eulerian driving functionals are

$$\mathcal{E}_U(\mathbf{q}_U) = \int_{\Omega} \frac{1}{2\varrho} |\mathbf{P}|^2 + U dx, \quad \mathcal{S}_U(\mathbf{q}_U) = \int_{\Omega} S(C, U) dx$$

with  $\varrho = MC$  the mass density. This results in the driving forces for reversible and irreversible dynamics

$$D\mathcal{E}_U = \begin{pmatrix} \frac{1}{\varrho} \mathbf{P} \\ -\frac{M}{2\varrho^2} |\mathbf{P}|^2 \\ 1 \end{pmatrix} \quad \text{and} \quad D\mathcal{S}_U = \frac{1}{\theta} \begin{pmatrix} 0 \\ -\mu \\ 1 \end{pmatrix},$$

and leads to the Eulerian Navier-Stokes system

$$\begin{aligned} \dot{\mathbf{P}} + \nabla \cdot (\boldsymbol{\nu} \otimes \mathbf{P}) &= -\nabla \pi + \mathbb{K}_{\mathbf{P}U}^S \theta^{-1}, \\ &= -\nabla \pi + \nabla \cdot \boldsymbol{\sigma}_{\text{visc}}, \end{aligned} \quad (112a)$$

$$\dot{C} + \nabla \cdot (C\boldsymbol{\nu}) = 0, \quad (112b)$$

$$\begin{aligned} \dot{U} + \nabla \cdot (U\boldsymbol{\nu}) &= -\pi \nabla \cdot \boldsymbol{\nu} + \mathbb{K}_{UU}^S \theta^{-1}, \\ &= -\pi \nabla \cdot \boldsymbol{\nu} + \boldsymbol{\sigma}_{\text{visc}} : \nabla \boldsymbol{\nu}. \end{aligned} \quad (112c)$$

with the Cauchy stress tensor

$$\boldsymbol{\sigma}_{\text{visc}} = 2\lambda(\nabla_s \boldsymbol{\nu}) + \zeta(\nabla \cdot \boldsymbol{\nu}) \mathbb{I}_d. \quad (112d)$$

The viscosity parameters  $\lambda, \zeta$  may also depend on state variables, i.e.,  $\lambda, \zeta : Q_U \rightarrow \mathbb{R}$ . With the entropy density  $S = S(C, U)$  the pressure  $\pi$  is given by the relations

$$\frac{\pi}{\theta} = S - C \partial_C S - U \partial_U S, \quad \text{and} \quad \frac{1}{\theta} = \partial_U S.$$

This shows that the closure conditions Def. 3.7 for the reduction are satisfied. Also the NIC (44) hold true for system  $(Q_U, \mathcal{E}_U, \mathcal{S}_U, \mathbb{J}_U, \mathbb{K}_U^S)$  thanks to Thm. 3.11.

**Remark 4.5 (Stress tensors)** The first Piola-Kirchhoff stress tensor  $\bar{\boldsymbol{\Sigma}}_{\text{visc}}$  from (105d) in Lagrangian coordinates and the Cauchy stress tensor  $\boldsymbol{\sigma}_{\text{visc}}$  in Eulerian coordinates are related by the Piola transform

$$\bar{\boldsymbol{\Sigma}}_{\text{visc}} \text{Cof}(\bar{\mathbf{F}})^{-1}(t, \bar{x}) = \boldsymbol{\sigma}_{\text{visc}}(t, x). \quad *$$

**Remark 4.6 (Boundary conditions)** System (112) is complemented by one of the following boundary conditions:

- i) *impermeability*: Set  $\boldsymbol{\nu} \cdot \mathbf{n} = 0$ , so that no flow in/out the boundary is possible.
- ii) *no condition on  $\boldsymbol{\nu}$* : If no (essential) boundary condition is specified for the velocity  $\boldsymbol{\nu}$ , then the boundary can move and a force balance holds.
- iii) *natural boundary conditions*: If the normal velocity is set by the impermeability condition, then we obtain for all tangential vectors  $\mathbf{t}$  that

$$\mathbf{t} \cdot \boldsymbol{\sigma}_{\text{visc}} \mathbf{n} = 0,$$

when integrating by parts the Stokes operator. If no essential boundary condition is specified for  $\boldsymbol{\nu}$ , then we additional get the normal force balance

$$\mathbf{n} \cdot \boldsymbol{\sigma}_{\text{visc}} \mathbf{n} = \pi.$$

One might include  $\pi$  into the Cauchy stress tensor. However, this obscures the different origin of  $\pi$  being a thermodynamic driving force in contrast to the viscous stress  $\boldsymbol{\sigma}_{\text{visc}}$  generated by the Onsager operator. \*

### 4.3 Onsager structure of compressible Stokes flows

Now we discuss the Onsager structure of the compressible Stokes equations, i.e., the overdamped slow evolution of a compressible highly viscous fluid. In order to derive the model from the Lagrangian Navier-Stokes system (105), we formally introduce scaling assumptions for time  $T$ , length  $L$  and viscosity coefficients  $\zeta, \lambda$  such that

$$[L] = \mathcal{O}(1), \quad [T] = [L/v] = \mathcal{O}(\varepsilon^{-1}), \quad [\zeta, \lambda] = \mathcal{O}(\varepsilon^{-1}),$$

and assume  $\varepsilon \ll 1$ . In this way, (105) becomes

$$\begin{aligned} \varepsilon \dot{\boldsymbol{\chi}} &= +\varepsilon \frac{1}{\varrho} \bar{\mathbf{P}}, \\ \varepsilon^2 \dot{\bar{\mathbf{P}}} &= -\bar{\nabla} \cdot (\bar{\pi} \text{Cof}(\bar{\mathbf{F}})) + \bar{\mathbb{K}}_{\bar{\mathbf{P}}\bar{U}}^S \bar{\theta}^{-1}, \\ \varepsilon \dot{\bar{U}} &= -\varepsilon \bar{\pi} \text{Cof}(\bar{\mathbf{F}}) : \bar{\nabla} \bar{\boldsymbol{\nu}} + \varepsilon \bar{\Sigma}_{\text{visc}} : \bar{\nabla} \bar{\boldsymbol{\nu}}, \end{aligned}$$

which suggests that the acceleration  $\dot{\bar{\mathbf{P}}}$  in the momentum balance is of lower order. With  $\dot{\boldsymbol{\chi}} = \bar{\boldsymbol{\nu}} = \frac{1}{\varrho} \bar{\mathbf{P}}$  we rewrite

$$\begin{aligned} \mathbf{0} &= -\bar{\nabla} \cdot (\bar{\pi} \text{Cof}(\bar{\mathbf{F}})) + \bar{\nabla} \cdot (2\lambda \bar{\nabla}_s \dot{\boldsymbol{\chi}} + \zeta \text{tr}(\bar{\nabla}_s \dot{\boldsymbol{\chi}}) \mathbb{I}_d) \text{Cof}(\bar{\mathbf{F}}), \\ \dot{\bar{U}} &= -\bar{\pi} \text{Cof}(\bar{\mathbf{F}}) : \bar{\nabla} \dot{\boldsymbol{\chi}} + 2\lambda |\bar{\nabla}_s \dot{\boldsymbol{\chi}}|^2 + \zeta \text{tr}(\bar{\nabla}_s \dot{\boldsymbol{\chi}})^2. \end{aligned}$$

The second equation can be transformed to entropy

$$\bar{\theta} \dot{\bar{S}} = 2\lambda |\bar{\nabla}_s \dot{\boldsymbol{\chi}}|^2 + \zeta \text{tr}(\bar{\nabla}_s \dot{\boldsymbol{\chi}})^2. \quad (113)$$

The entropy equation (113) does not have an Onsager structure in the variables  $\bar{\mathbf{q}} = (\boldsymbol{\chi}, \bar{S})$ , as the heat source term can not be expressed in the state variables. The evolution of the deformation itself can be written in the form of an Onsager structure. With the dissipation potential

$$\bar{\Psi}(\bar{\mathbf{q}}; \bar{\boldsymbol{\nu}}) = \frac{1}{2} \int_{\bar{\Omega}} \left[ 2\lambda |\bar{\nabla}_s \bar{\boldsymbol{\nu}}|^2 + \zeta \text{tr}(\bar{\nabla}_s \bar{\boldsymbol{\nu}})^2 \right] \bar{V} \, d\bar{x} = \frac{1}{2} \langle \bar{\mathbb{G}}(\bar{\mathbf{q}}) \bar{\boldsymbol{\nu}}, \bar{\boldsymbol{\nu}} \rangle. \quad (114a)$$

and the metric operator  $\bar{\mathbb{G}}(\bar{\mathbf{q}}) : \bar{\mathcal{Q}}_{\boldsymbol{\chi}} \rightarrow \bar{\mathcal{Q}}_{\boldsymbol{\chi}}^*$  the evolution can be written as

$$\dot{\boldsymbol{\chi}} = \bar{\mathbb{G}}^{-1}(\bar{\mathbf{q}}) D_{\boldsymbol{\chi}} \bar{\mathcal{U}}(\bar{\mathbf{q}}), \quad (114b)$$

with the internal energy  $\bar{\mathcal{U}}(\bar{\mathbf{q}})$  with density  $\bar{U}(\bar{\mathbf{q}}) = \bar{U}(\bar{C}, \bar{V}, \bar{S})$  for  $\bar{\mathbf{q}} = (\boldsymbol{\chi}, \bar{S})$  and  $\bar{V} = \det(\bar{\nabla} \boldsymbol{\chi})$ . Then  $\bar{S}$  evolves according to equation (113) and clearly increases. If the viscosity coefficients  $\lambda, \zeta$  do not depend on temperature or for other reasons the dependence can be neglected, then the evolution of the system can be written in terms of the mechanical Onsager structure (114b).

**Lagrangian-Eulerian reduction.** The reduction from Lagrangian to Eulerian coordinates is performed analogously to the procedure for the Navier-Stokes equation. The driving potential now is the internal energy

$$\mathcal{U}(\mathbf{q}) = \int_{\Omega} U(C, S) \, dx,$$

where the Eulerian variables and equation of state are defined as before by

$$C \circ \boldsymbol{\chi} = \frac{\bar{C}}{\bar{V}}, \quad S \circ \boldsymbol{\chi} = \frac{\bar{S}}{\bar{V}}, \quad U(C, S) = \frac{1}{\bar{V}} \bar{U}(\bar{C}, \bar{V}, \bar{S}),$$

with  $\bar{V} = \det(\bar{\nabla}\chi)$ . This gives rise to the Eulerian Onsager operator  $\mathbb{G}$ , the Cauchy stress tensor  $\sigma$

$$\langle \bar{\mathbb{G}}(\bar{\mathbf{q}})\bar{\boldsymbol{\nu}}, \bar{\boldsymbol{\nu}} \rangle = \int_{\Omega} \left[ 2\lambda |\nabla_s \boldsymbol{\nu}|^2 + \zeta \operatorname{tr}(\nabla_s \boldsymbol{\nu})^2 \right] dx = \int_{\Omega} \boldsymbol{\sigma}_{\text{visc}} : \nabla \boldsymbol{\nu} dx,$$

and the evolution equations

$$-\nabla \cdot \boldsymbol{\sigma}_{\text{visc}} = -\nabla \pi, \quad (115a)$$

$$\partial_t C + \nabla \cdot (C\boldsymbol{\nu}) = 0, \quad (115b)$$

$$\partial_t S + \nabla \cdot (S\boldsymbol{\nu}) = \theta^{-1} \boldsymbol{\sigma}_{\text{visc}} : \nabla \boldsymbol{\nu}, \quad (115c)$$

where  $\pi = U - C\partial_C U - S\partial_S U$  and  $\theta = \partial_S U$ . By multiplying (115b) with the particle mass  $M$  one finds the continuity equation for the (conserved) mass density.

## 5 Reactions, diffusion, heat transport

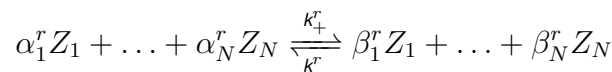
In this section we provide a detailed description of dissipative reaction-diffusion processes and heat transport, for which dynamics is driven by the entropy as a function of the internal energy and particle number density. We assume that mechanics is in equilibrium, so that the pressure is constant and  $\bar{V} \equiv 1$ . The coupling to mechanics can be achieved using, e.g., the Stokes operator from Sec. 4.2. We introduce mass-action type reaction kinetics in Sec. 5.1. Next, we consider heat conduction without transport of matter in Sec. 5.2. In Sec. 5.3 we consider diffusion in a multicomponent system. In all these cases we focus on purely dissipative processes without cross coupling such that the NIC (44) are satisfied. Thus, in Sec. 5.4 we address cross-coupling in Onsager systems. The description of these dissipative processes is performed in the Lagrangian frame, as deformations can be taken into account using the reduction formalism presented in Sec.s 3.4 & 4. Also, similar to Sec. 4.2 for the Stokes operator, Lagrangian gradients and volume elements in the Onsager operator are to be replaced by their Eulerian versions, i.e.,

$$\bar{\nabla} \mapsto \bar{\mathbf{F}}^{-\top} \bar{\nabla} \equiv \nabla, \quad d\bar{x} \mapsto \det(\bar{\mathbf{F}}) d\bar{x} \equiv dx. \quad (116)$$

This section presents pure Onsager systems in a way suitable for their coupling to reversible dynamics in a GENERIC system. Detailed description of the thermodynamic and geometric structure of reaction-diffusion processes can also be found in literature [22, 70, 15, 25, 45, 7, 23].

### 5.1 Reaction kinetics

Consider  $\bar{\mathbf{q}} = (\bar{\mathbf{C}}, \bar{V}, \bar{U}) \in \bar{\mathcal{Q}}$  with  $\bar{\mathbf{C}}(t) : \bar{\Omega} \rightarrow \mathbb{R}^N$  being the particle number densities of  $N$  different chemical species  $Z_1, \dots, Z_N$  that react according to



in  $r = 1, \dots, R$  elementary reactions. For each reaction  $r$  we have the vectors of stoichiometric coefficients  $\boldsymbol{\alpha}^r, \boldsymbol{\beta}^r \in \mathbb{N}_0^N$ , and the forward and backward reaction rates  $k_+^r, k_-^r : \bar{\mathcal{Q}} \rightarrow \mathbb{R}$ , cf. also Ex. 5.2. The positive rates depend on  $\bar{\mathbf{q}}$  and we assume that all reactions are reversible, i.e.,  $k_{\pm}^r > 0$ . The corresponding reaction kinetics is of mass-action type and given by the ODE-system

$$\dot{\bar{\mathbf{C}}} = \sum_{r=1}^R \left( k_-^r(\bar{\mathbf{C}}) \bar{\mathbf{C}}^{\boldsymbol{\beta}^r} - k_+^r(\bar{\mathbf{C}}) \bar{\mathbf{C}}^{\boldsymbol{\alpha}^r} \right) (\boldsymbol{\alpha}^r - \boldsymbol{\beta}^r) \quad (117)$$

with the multi-index notation  $\bar{\mathbf{C}}^\alpha := \bar{\mathbf{C}}_1^{\alpha_1} \dots \bar{\mathbf{C}}_N^{\alpha_N}$ . Furthermore, we assume a detailed balance condition, i.e., there exists a steady state  $\bar{\mathbf{C}}_{\text{ref}}$ , such that

$$k^r(\bar{\mathbf{q}}) = k_+^r(\bar{\mathbf{C}})\bar{\mathbf{C}}_{\text{ref}}^{\alpha^r} = k_-^r(\bar{\mathbf{C}})\bar{\mathbf{C}}_{\text{ref}}^{\beta^r} \quad (118)$$

for all  $r = 1, \dots, R$ . Under this condition, the reaction kinetics (117) can be written as an Onsager system. With the general entropy functional  $\bar{\mathcal{S}}(\bar{\mathbf{q}})$  of a multicomponent system, in view of (7b), we have the driving force

$$D\bar{\mathcal{S}}(\bar{\mathbf{q}}) = \begin{pmatrix} \frac{\partial \bar{\mathcal{S}}}{\partial \bar{\mathbf{C}}} \\ \frac{\partial \bar{\mathcal{S}}}{\partial \bar{V}} \\ \frac{\partial \bar{\mathcal{S}}}{\partial \bar{U}} \end{pmatrix} = \begin{pmatrix} \frac{-\bar{\mu}}{\theta} \\ \frac{\bar{\pi}}{\theta} \\ \frac{1}{\theta} \end{pmatrix}. \quad (119)$$

Dissipative dynamics is generated by the dual dissipation potential  $\bar{\Psi}_{\text{reac}}^*(\bar{\mathbf{q}}; \bar{\boldsymbol{\xi}}) = \frac{1}{2} \langle \bar{\boldsymbol{\xi}}, \bar{\mathbb{K}}_{\text{reac}}(\bar{\mathbf{q}}) \bar{\boldsymbol{\xi}} \rangle$ ,

$$\bar{\Psi}_{\text{reac}}^*(\bar{\mathbf{q}}; \bar{\boldsymbol{\xi}}) := \int_{\bar{\Omega}} \frac{1}{2} \begin{pmatrix} \bar{\boldsymbol{\xi}}_{\bar{\mathbf{C}}} \\ \bar{\xi}_{\bar{V}} \\ \bar{\xi}_{\bar{U}} \end{pmatrix} \cdot \bar{\mathbb{H}}(\bar{\mathbf{q}}) \begin{pmatrix} \bar{\boldsymbol{\xi}}_{\bar{\mathbf{C}}} \\ \bar{\xi}_{\bar{V}} \\ \bar{\xi}_{\bar{U}} \end{pmatrix} d\bar{x}, \quad (120a)$$

for any  $\bar{\boldsymbol{\xi}} = (\bar{\boldsymbol{\xi}}_{\bar{\mathbf{C}}}, \bar{\xi}_{\bar{V}}, \bar{\xi}_{\bar{U}}) \in \bar{\mathcal{Q}}^*$ . Here  $\bar{\mathbb{H}}$  is multiplicative and of  $3 \times 3$  block structure

$$\bar{\mathbb{H}} := \begin{pmatrix} \bar{\mathbb{H}}_{\bar{\mathbf{C}}\bar{\mathbf{C}}} & \bar{\mathbb{H}}_{\bar{\mathbf{C}}\bar{V}} & \bar{\mathbb{H}}_{\bar{\mathbf{C}}\bar{U}} \\ \bar{\mathbb{H}}_{\bar{\mathbf{C}}\bar{V}}^* & \bar{\mathbb{H}}_{\bar{V}\bar{V}} & \bar{\mathbb{H}}_{\bar{V}\bar{U}} \\ \bar{\mathbb{H}}_{\bar{\mathbf{C}}\bar{U}}^* & \bar{\mathbb{H}}_{\bar{V}\bar{U}}^* & \bar{\mathbb{H}}_{\bar{U}\bar{U}} \end{pmatrix} \quad \text{with} \quad (120b)$$

$$\bar{\mathbb{H}}_{\bar{\mathbf{C}}\bar{\mathbf{C}}}(\bar{\mathbf{q}}) := \sum_{r=1}^R \frac{k^r(\bar{\mathbf{q}})}{k_{\text{B}}} \ell\left(\left(\frac{\bar{\mathbf{C}}}{\bar{\mathbf{C}}_{\text{ref}}}\right)^{\alpha^r}, \left(\frac{\bar{\mathbf{C}}}{\bar{\mathbf{C}}_{\text{ref}}}\right)^{\beta^r}\right) \bar{\mathbb{S}}^r, \quad (120c)$$

$$\bar{\mathbb{S}}^r := (\boldsymbol{\alpha}^r - \boldsymbol{\beta}^r) \otimes (\boldsymbol{\alpha}^r - \boldsymbol{\beta}^r), \quad (120d)$$

$$\ell(u, v) := \begin{cases} \frac{u-v}{\log u - \log v} & \text{for } u \neq v, \\ v & \text{for } u = v. \end{cases} \quad (120e)$$

While the possibility of non-zero components  $\bar{\mathbb{H}}_{\bar{V}\bar{V}}, \bar{\mathbb{H}}_{\bar{\mathbf{C}}\bar{V}}$  of reactive nature can not be excluded per se, it seems that these cross-coupling terms are of mechanical nature and would appear in a corresponding contribution to the dual dissipation. In the following we assume  $\bar{\mathbb{H}}_{\bar{V}\bar{V}} = 0, \bar{\mathbb{H}}_{\bar{\mathbf{C}}\bar{V}} = 0$ . The couplings to the internal energy are also assumed to be zero, i.e.,  $\bar{\mathbb{H}}_{\bar{\mathbf{C}}\bar{U}} = \bar{\mathbb{H}}_{\bar{V}\bar{U}} = \bar{\mathbb{H}}_{\bar{U}\bar{U}} = 0$ , in order to satisfy the noninteraction condition  $\bar{\mathbb{H}} D\bar{\mathcal{U}} = 0$ . The related Onsager operator for reactions  $\bar{\mathbb{K}}_{\text{reac}}$  can be directly identified from (120a) as

$$\bar{\mathbb{K}}_{\text{reac}}(\bar{\mathbf{q}}) = \begin{pmatrix} \bar{\mathbb{H}}_{\bar{\mathbf{C}}\bar{\mathbf{C}}}(\bar{\mathbf{q}}) & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \quad (121)$$

Due to this block structure, the absence of coupling to  $\bar{\xi}_{\bar{U}}$ , and the choice of variables, the noninteraction condition for the internal energy is automatically satisfied, i.e.,  $\bar{\mathbb{K}} D\bar{\mathcal{U}}$ , since  $D\bar{\mathcal{U}}(\bar{\mathbf{q}}) \equiv (0, 0, 1)^\top$  for all  $\bar{\mathbf{q}} \in \bar{\mathcal{Q}}$ . Thus, the internal energy is locally conserved and here it also coincides with the total energy of the system. Applying (121) to  $D\bar{\mathcal{S}}$  yields the reaction kinetics

$$\begin{aligned} \dot{\bar{\mathbf{C}}} &= -\bar{\mathbb{H}}_{\bar{\mathbf{C}}\bar{\mathbf{C}}}(\bar{\mathbf{q}}) \frac{\bar{\mu}}{\theta}, \\ \dot{\bar{V}} &= 0, \\ \dot{\bar{U}} &= 0. \end{aligned}$$

Additionally, conservation of mass  $\bar{M}$  is ensured if the vector of particle masses  $\mathbf{M} = (\mathbf{M}_i)_{i=1,\dots,N}$  is orthogonal to the linear space generated by stoichiometric coefficients for each reaction [15], i.e.,

$$\mathbf{M} \cdot (\boldsymbol{\alpha}^r - \boldsymbol{\beta}^r) = 0 \quad \text{for all } r = 1, \dots, R. \quad (123)$$

This is one of the main ingredients for stoichiometry. For the entropy evolution this implies

$$\dot{\bar{S}} = \frac{\partial \bar{S}(\bar{q})}{\partial \bar{\mathbf{C}}} \cdot \dot{\bar{\mathbf{C}}} = \frac{\bar{\mu}}{\theta} \cdot \bar{\mathbb{H}}_{\bar{\mathbf{C}}\bar{\mathbf{C}}}(\bar{q}) \frac{\bar{\mu}}{\theta} \geq 0.$$

Even though cross coupling is not included in our choice for  $\bar{\mathbb{K}}_{\text{reac}}$ , nonetheless  $\bar{\Psi}^*$  provides a general ansatz compatible with GENERIC.

**Example 5.1 (Reaction kinetics)** We consider the the entropy density (15) of an ideal gas and define

$$\bar{S}(\bar{q}) = \int_{\bar{\Omega}} \bar{S}(\bar{q}) \, d\bar{x},$$

with  $\bar{q} = (\bar{\mathbf{C}}, \bar{V}, \bar{\theta})$  as natural variables. The driving force for reactions is obtained from the Helmholtz free energy

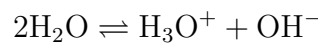
$$\frac{\bar{\mu}_i}{\theta} = \frac{1}{\bar{\theta}} \frac{\partial \bar{F}}{\partial \bar{\mathbf{C}}_i} = k_B \log \left( \frac{\bar{\mathbf{C}}_i}{\bar{\mathbf{C}}_{\text{ref},i}} \right), \quad (124a)$$

for the multi-component system with  $i = 1, \dots, N$  and the reference density

$$\bar{\mathbf{C}}_{\text{ref},i} = \frac{\bar{V}}{\lambda_{i,\theta}^3}, \quad (124b)$$

for the detailed balance condition (118). When inserting this expression into (120), one immediately recovers the mass-action type reaction kinetics (117). \*

**Example 5.2** Consider the self-ionization of water



as an example for a single reaction with three species corresponding to water  $Z_1=\text{H}_2\text{O}$ , hydronium  $Z_2=\text{H}_3\text{O}^+$ , and hydroxide  $Z_3=\text{OH}^-$ . The vector of masses is  $\mathbf{M} = (18.015, 19.02, 17.01)\text{g mol}^{-1}$  with stoichiometric coefficients  $\boldsymbol{\alpha} = (2, 0, 0)$  and  $\boldsymbol{\beta} = (0, 1, 1)$ . Note that conservation of mass is ensured by  $\mathbf{M} \cdot (\boldsymbol{\alpha} - \boldsymbol{\beta}) = 0$ . The Onsager operator for reactions,  $\bar{\mathbb{H}}$  will then result in the system of ODEs

$$\partial_t \begin{pmatrix} \bar{\mathbf{C}}_1 \\ \bar{\mathbf{C}}_2 \\ \bar{\mathbf{C}}_3 \end{pmatrix} = k(\bar{q}) \begin{pmatrix} \bar{\mathbf{C}}_2 \bar{\mathbf{C}}_3 \\ \bar{\mathbf{C}}_{2,\text{ref}} \bar{\mathbf{C}}_{3,\text{ref}} \\ \frac{(\bar{\mathbf{C}}_1)^2}{(\bar{\mathbf{C}}_{1,\text{ref}})^2} \end{pmatrix} \begin{pmatrix} +2 \\ -1 \\ -1 \end{pmatrix}$$

where the reaction rate  $k$  and reference densities  $\bar{\mathbf{C}}_{\text{ref}}$  depend on the state, e.g., on temperature and pressure as in (124b) of Example 5.1. \*



## 5.2 Heat conduction

Heat conduction is the irreversible process of redistribution of internal energy inside a material. This process is neither diffusive nor convective in the sense that it does not involve diffusive or convective transport of particles or changes in the concentration due to reactions. For the mathematical description consider the Lagrangian domain  $\bar{\Omega} \subset \mathbb{R}^d$  and the state variables  $\bar{\mathbf{q}} = (\bar{C}, \bar{V}, \bar{U}) \in \bar{\mathcal{Q}}$ . Heat conduction is an irreversible process driven by the entropy  $\bar{S}(\bar{\mathbf{q}})$ . We define the dual dissipation potential  $\bar{\Psi}_{\text{heat}}^* : \bar{\mathcal{Q}} \times \bar{\mathcal{Q}}^* \rightarrow \mathbb{R}$ ,

$$\bar{\Psi}_{\text{heat}}^*(\bar{\mathbf{q}}; \bar{\boldsymbol{\xi}}) := \int_{\bar{\Omega}} \frac{1}{2} \nabla \bar{\xi}_{\bar{U}} \cdot \bar{\theta}^2 \bar{k}_{\text{heat}}(\bar{\mathbf{q}}) \nabla \bar{\xi}_{\bar{U}} \, d\bar{x} \quad (125a)$$

for all  $\bar{\boldsymbol{\xi}} = (\bar{\xi}_{\bar{C}}, \bar{\xi}_{\bar{V}}, \bar{\xi}_{\bar{U}})$ , with  $\bar{k}_{\text{heat}} : \bar{\mathcal{Q}} \rightarrow \mathbb{R}^{d \times d}$  symmetric, positive definite, resulting in the Onsager operator

$$\bar{\mathbb{K}}_{\text{heat}} := \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \bar{\mathbb{K}}_{\bar{U}\bar{U}}^{\text{heat}} \end{pmatrix} \quad \text{with} \quad (125b)$$

$$\bar{\mathbb{K}}_{\bar{U}\bar{U}}^{\text{heat}}(\bar{\mathbf{q}}) \bar{\xi}_{\bar{U}} := -\nabla \cdot (\bar{\theta}^2 \bar{k}_{\text{heat}}(\bar{\mathbf{q}}) \nabla \bar{\xi}_{\bar{U}}). \quad (125c)$$

Also the noninteraction condition  $\bar{\mathbb{K}}_{\text{heat}} D\bar{\mathbf{U}} \equiv 0$  is satisfied. With the driving forces

$$D\bar{S}(\bar{\mathbf{q}}) = \begin{pmatrix} \frac{\partial \bar{S}}{\partial \bar{C}} \\ \frac{\partial \bar{S}}{\partial \bar{V}} \\ \frac{\partial \bar{S}}{\partial \bar{U}} \end{pmatrix} = \begin{pmatrix} \frac{-\bar{\mu}}{\bar{\theta}} \\ \frac{\bar{\pi}}{\bar{\theta}} \\ \frac{1}{\bar{\theta}} \end{pmatrix},$$

the evolution of the internal energy  $\bar{U}(t) : \bar{\Omega} \rightarrow \mathbb{R}$  reads

$$\dot{\bar{U}} = \bar{\nabla} \cdot (\bar{k}_{\text{heat}}(\bar{\mathbf{q}}) \bar{\nabla} \bar{\theta}),$$

where the positive coefficient function  $\bar{k}_{\text{heat}} = \bar{k}_{\text{heat}}(\bar{\mathbf{q}})$  is the *thermal conductivity*, relating temperature gradients and heat flux by Fourier's law, i.e.,  $\bar{\mathbf{J}}_{\text{heat}} = -\bar{k}_{\text{heat}} \bar{\nabla} \bar{\theta}$ . The temperature is expressed in terms of the other state variables using the equation of state  $\bar{\theta}^{-1} = \partial_{\bar{U}} \bar{S}(\bar{\mathbf{q}})$  for the ideal gas, i.e.,  $\bar{\theta} = \bar{C}_{\bar{V}}^{-1} \bar{U}$ .

**Example 5.3 (Temperature)** We change variables from  $\bar{\mathbf{q}} = (\bar{C}, \bar{V}, \bar{U})$  to  $\bar{\mathbf{q}}_{\bar{\theta}} = (\bar{C}, \bar{V}, \bar{\theta})$  and assume that volume and concentration remain constant. Using the definition of the heat capacity (10) we can directly transform the heat equation to

$$\dot{\bar{U}} = \left( \frac{\partial \bar{U}}{\partial \bar{\theta}} \right)_{\bar{V}} \dot{\bar{\theta}} \equiv \bar{C}_{\bar{V}} \dot{\bar{\theta}} = \bar{\nabla} \cdot (\bar{k}_{\text{heat}}(\bar{\mathbf{q}}) \bar{\nabla} \bar{\theta}). \quad (126)$$

The transformation on the level of the Onsager structure in terms of a change of variables following Sec. 3.4 is accomplished with

$$\mathbb{L} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \frac{\partial \bar{\theta}(\bar{\mathbf{q}})^{\top}}{\partial \bar{C}} & \frac{\partial \bar{\theta}(\bar{\mathbf{q}})}{\partial \bar{V}} & \frac{\partial \bar{\theta}(\bar{\mathbf{q}})}{\partial \bar{U}} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \frac{\partial \bar{\theta}(\bar{\mathbf{q}})^{\top}}{\partial \bar{C}} & \frac{\partial \bar{\theta}(\bar{\mathbf{q}})}{\partial \bar{V}} & \frac{1}{\bar{C}_{\bar{V}}} \end{pmatrix},$$

again using the relation  $\frac{\partial \bar{\theta}(\bar{\mathbf{q}})}{\partial \bar{U}} = 1/\bar{C}_V$ . This yields the transformed Onsager operator  $\bar{\mathbb{K}}_{\bar{\theta}} = \bar{\mathbb{K}}(\bar{\mathbf{q}}_{\bar{\theta}})$

$$\bar{\mathbb{K}}_{\bar{\theta}} = \mathbb{L} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \bar{\mathbb{K}}_{\text{heat}}(\bar{\mathbf{q}}) \end{pmatrix} \mathbb{L}^* = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \bar{\mathbb{K}}_{\text{heat}}(\bar{\mathbf{q}}_{\bar{\theta}}) \end{pmatrix} \quad (127a)$$

$$\text{with } \bar{\mathbb{K}}_{\text{heat}}(\bar{\mathbf{q}}_{\bar{\theta}})\xi_{\bar{\theta}} = \frac{-1}{\bar{C}_V} \bar{\nabla} \cdot \left( \bar{\theta}^2 \bar{k}_{\text{heat}} \bar{\nabla} \left( \frac{\xi_{\bar{\theta}}}{\bar{C}_V} \right) \right). \quad (127b)$$

For  $\xi_{\bar{\theta}} = D\bar{\mathcal{S}}(\bar{\mathbf{q}}_{\bar{\theta}}) = \bar{C}_V \bar{\theta}^{-1}$  we recover (126) from the transformed Onsager operator (127b). \*

**Example 5.4 (Entropy as the variable)** The evolution of the entropy for heat conduction is given by

$$\dot{\mathcal{S}} = \frac{\partial \bar{\mathcal{S}}(\bar{\mathbf{q}})}{\partial \bar{U}} \dot{\bar{U}} = \frac{1}{\bar{\theta}} \bar{\nabla} \cdot (\bar{k}_{\text{heat}} \bar{\nabla} \bar{\theta}) = \bar{\nabla} \cdot \left( \frac{\bar{k}_{\text{heat}}}{\bar{\theta}} \bar{\nabla} \bar{\theta} \right) + \frac{\bar{k}_{\text{heat}}}{\bar{\theta}^2} |\bar{\nabla} \bar{\theta}|^2.$$

This shows that the entropy is increasing in time, in case of natural boundary conditions  $\bar{\mathbf{n}} \cdot \bar{k}_{\text{heat}} \bar{\nabla} \bar{\theta} = 0$ , i.e.,

$$\frac{d}{dt} \bar{\mathcal{S}}(\bar{\mathbf{q}}(t)) = \int_{\bar{\Omega}} \frac{\bar{k}_{\text{heat}}}{\bar{\theta}^2} |\bar{\nabla} \bar{\theta}|^2 d\bar{x} + \int_{\partial \bar{\Omega}} \bar{\mathbf{n}} \cdot \frac{\bar{k}_{\text{heat}}}{\bar{\theta}} \bar{\nabla} \bar{\theta} d\bar{s} \geq 0.$$

Next, we change variables from the internal energy  $\bar{\mathbf{q}} = (\bar{C}, \bar{V}, \bar{U})$  to the entropy  $\bar{\mathbf{q}}_{\bar{\mathcal{S}}} = (\bar{C}, \bar{V}, \bar{\mathcal{S}})$  with driving force  $D\bar{\mathcal{S}}(\bar{\mathbf{q}}_{\bar{\mathcal{S}}}) = (0, 0, 1)^\top$ . Similar to Ex. 5.4, we find

$$\bar{\mathbb{K}}_{\text{heat}}(\bar{\mathbf{q}}_{\bar{\mathcal{S}}})\xi_{\bar{\mathcal{S}}} = \frac{-1}{\bar{\theta}} \bar{\nabla} \cdot \left( \bar{\theta}^2 \bar{k}_{\text{heat}} \bar{\nabla} \left( \frac{\xi_{\bar{\mathcal{S}}}}{\bar{\theta}} \right) \right).$$

for the transformed Onsager operator. \*

Both Onsager systems, i.e., for  $\bar{\theta}$  and  $\bar{\mathcal{S}}$ , are generally valid for any chosen equation of state. With the natural boundary condition  $\bar{\mathbf{n}} \cdot \bar{k}_{\text{heat}} \bar{\nabla} \bar{\theta} = 0$  we make sure that the entropy is increasing. While the internal energy is not a locally conserved quantity, with the above natural boundary condition, we have

$$\frac{d}{dt} \bar{\mathcal{U}}(\bar{\mathbf{q}}(t)) = \int_{\partial \bar{\Omega}} \bar{\mathbf{n}} \cdot \bar{k}_{\text{heat}}(\bar{\mathbf{q}}) \bar{\nabla} \bar{\theta} d\bar{s} \equiv 0.$$

### 5.3 Diffusion processes

We consider diffusion of a multicomponent system as an irreversible process driven by entropy and with state variables  $\bar{\mathbf{q}} = (\bar{C}, \bar{V}, \bar{U}) \in \bar{\mathcal{Q}}$ . In conjunction with reactions, the same entropy expression serves as a driving functional for reactions and for diffusion of components. The standard form of single-component diffusion is

$$\dot{\bar{C}} = \bar{\nabla} \cdot (\bar{D} \bar{\nabla} \bar{C}) \quad (128)$$

with diffusion constant  $\bar{D} \in \mathbb{R}$ . We introduce a quadratic, dual dissipation potential  $\bar{\Psi}_{\text{diff}}^* : \bar{\mathcal{Q}} \times \bar{\mathcal{Q}}^* \rightarrow [0, \infty]$ ,

$$\bar{\Psi}_{\text{diff}}^*(\bar{\mathbf{q}}, \bar{\xi}) = \frac{1}{2} \sum_{i,j=1}^N \int_{\bar{\Omega}} \bar{\nabla} \bar{\xi}_i \cdot \bar{\mathbb{M}}_{ij}(\bar{\mathbf{q}}) \bar{\nabla} \bar{\xi}_j d\bar{x}, \quad (129a)$$

for all  $\bar{\mathbf{q}} \in \bar{\mathcal{Q}}$  and any  $\bar{\boldsymbol{\xi}} = (\bar{\boldsymbol{\xi}}_{\bar{C}}, \bar{\boldsymbol{\xi}}_{\bar{V}}, \bar{\boldsymbol{\xi}}_{\bar{U}}) \in \bar{\mathcal{Q}}^*$ , and with the symmetric, positively semidefinite mobility matrix

$$\bar{\mathbb{M}}(\bar{\mathbf{q}}) = \begin{pmatrix} \bar{\mathbb{M}}_{\bar{C}\bar{C}}(\bar{\mathbf{q}}) & \bar{\mathbb{M}}_{\bar{C}\bar{V}}(\bar{\mathbf{q}}) & \bar{\mathbb{M}}_{\bar{C}\bar{U}}(\bar{\mathbf{q}}) \\ \bar{\mathbb{M}}_{\bar{C}\bar{V}}^*(\bar{\mathbf{q}}) & \bar{\mathbb{M}}_{\bar{V}\bar{V}}(\bar{\mathbf{q}}) & \bar{\mathbb{M}}_{\bar{V}\bar{U}}(\bar{\mathbf{q}}) \\ \bar{\mathbb{M}}_{\bar{C}\bar{U}}^*(\bar{\mathbf{q}}) & \bar{\mathbb{M}}_{\bar{V}\bar{U}}^*(\bar{\mathbf{q}}) & \bar{\mathbb{M}}_{\bar{U}\bar{U}}(\bar{\mathbf{q}}) \end{pmatrix}. \quad (129b)$$

This results in the Onsager operator

$$\bar{\mathbb{K}}_{\text{diff}}(\bar{\mathbf{q}})\bar{\boldsymbol{\xi}} = -\bar{\nabla} \cdot (\bar{\mathbb{M}}(\bar{\mathbf{q}})\bar{\nabla}\bar{\boldsymbol{\xi}}), \quad (129c)$$

which satisfies the noninteraction condition  $\bar{\mathbb{K}}_{\text{diff}}D\bar{\mathcal{U}} \equiv 0$  for any matrix  $\bar{\mathbb{M}}$ , since  $\bar{\mathbb{M}}\bar{\nabla}(0, 0, 1)^\top = 0$ .

In what follows we set  $\bar{\mathbb{M}}_{ij} = 0$  if  $i, j \in \{\bar{V}, \bar{U}\}$ , since these terms are rather of mechanical origin. Yet, these terms must not be excluded per se, but they are not connected to diffusion. In particular  $\bar{\mathbb{M}}_{\bar{U}\bar{U}} = 0$  since it corresponds to heat conduction.

Let us discuss the NIC (44b) for the total mass, i.e.,

$$\sum_{i=1}^N \dot{\bar{C}}_i \mathbf{M}_i = 0,$$

as it emerges from (24) and needs to be satisfied for the reaction-diffusion system

$$\partial_t \bar{C}_i + \bar{\nabla} \cdot \bar{\mathbf{J}}_i = \bar{\mathbf{R}}_i, \quad i = 1, \dots, N.$$

One requires that reactions and diffusion satisfy the mass conservation separately [15, 8], i.e.,

$$\sum_{i=1}^N \mathbf{M}_i \bar{\mathbf{R}}_i = 0, \quad (130a)$$

$$\sum_{i=1}^N \mathbf{M}_i \bar{\mathbf{J}}_i = \mathbf{0}, \quad (130b)$$

where (130a) is satisfied for each reaction by construction  $\bar{\mathbf{R}}(\bar{\mathbf{q}}) = -\bar{\mathbb{H}}_{\bar{C}\bar{C}}(\bar{\mathbf{q}})\frac{\bar{\mu}}{\theta}$  using (123), as shown in Ex. 5.2. Note that condition (130b) for a diffusion system in Onsager form with  $\bar{\mathbb{M}}(\bar{\mathbf{q}}) = \bar{\mathbb{M}}_{\bar{C}\bar{C}}(\bar{\mathbf{q}})$  is given as

$$\mathbf{0} = -(\bar{\mathbb{M}}(\bar{\mathbf{q}})\bar{\nabla}\partial_{\bar{C}}\bar{S}(\bar{\mathbf{q}}))^\top \mathbf{M}, \quad (130c)$$

saying that  $\mathbf{M}$  is in the kernel of the matrix product  $(\bar{\nabla}\bar{\mathbf{q}})^\top (\partial_{\bar{q}}\partial_{\bar{C}}\bar{S}(\bar{\mathbf{q}}))^\top \bar{\mathbb{M}}(\bar{\mathbf{q}})$  along solutions. There are different ways to construct a variational formulation for diffusion processes [13, 15, 60] that obey (130b), resp. (130c). Here, we exemplarily consider *local modifications* [60]. For the special case of diagonal diffusion  $\bar{\mathbb{M}}_{\bar{C}\bar{C}} = \text{diag}(\bar{D}_1, \dots, \bar{D}_N)$  and equal masses,  $\mathbf{M}_i = M$  for all  $i \in \{1, \dots, N\}$ , one can modify the flux with a local force  $\mathbf{f}$ , resulting in  $\bar{\mathbf{J}}_i = -\bar{D}_i(\bar{\nabla}\bar{\boldsymbol{\xi}}_i + \mathbf{f})$ . Requiring (130b) to be satisfied by  $\bar{\mathbf{J}}_i$  and solving for  $\mathbf{f}$ , gives

$$\bar{\mathbf{J}}_i = -\sum_{j=1}^N \tilde{\mathbb{M}}_{ij} \bar{\nabla}\bar{\boldsymbol{\xi}}_j, \quad \tilde{\mathbb{M}}_{ij} = \bar{D}_i \delta_{ij} - \frac{\bar{D}_i \bar{D}_j}{\sum_{k=1}^N \bar{D}_k},$$

ensuring that (130b) holds true for all thermodynamical forces  $\bar{\boldsymbol{\xi}} = (\bar{\boldsymbol{\xi}}_j)_{j=1}^N \in \bar{\mathcal{Q}}^*$ , hence in particular (130c). For a general vector  $\mathbf{M} \in \mathbb{R}^N$  of particle masses, condition (130c) can also be ensured by requiring [8] one of

$$\mathbf{0} = (\partial_{\bar{q}}\partial_{\bar{C}}\bar{S}(\bar{\mathbf{q}}))^\top \bar{\mathbb{M}}(\bar{\mathbf{q}})\mathbf{M}, \quad (131a)$$

$$\mathbf{0} = \bar{\mathbb{M}}(\bar{\mathbf{q}})\mathbf{M} \quad (131b)$$

to hold for all  $\bar{\mathbf{q}} \in \bar{\mathcal{Q}}_{\bar{v}}$ . Enforcing (131b) also ensures (131a) and (130b) to hold for all  $\bar{\boldsymbol{\xi}} = (\bar{\xi}_j)_{j=1}^N \in \bar{\mathcal{Q}}^*$ , since  $\sum_{i=1}^N \mathbf{M}_i \bar{\mathbf{J}}_i = -(\bar{\nabla} \bar{\boldsymbol{\xi}})^\top \bar{\mathbb{M}} \mathbf{M} = 0$ . Given a symmetric, positively (semi-)definite matrix  $\hat{\mathbb{M}}(\bar{\mathbf{q}})$ , one can construct such a symmetric matrix  $\bar{\mathbb{M}}(\bar{\mathbf{q}})$  satisfying property (131b) with the aid of a projection  $\mathbb{P}$  by

$$\bar{\mathbb{M}}(\bar{\mathbf{q}}) = \mathbb{P}^\top \hat{\mathbb{M}}(\bar{\mathbf{q}}) \mathbb{P} \quad \text{with } \mathbb{P} = \mathbb{I}_N - \frac{\mathbf{M} \mathbf{M}^\top}{|\mathbf{M}|^2}. \quad (132)$$

See also Remark 5.7 for further discussion of the NIC.

**Example 5.5 (Diffusion equation)** Let  $\bar{\mathbb{M}}_{\bar{C}\bar{v}} = 0$ . A multicomponent ideal gas has the driving force  $D_{\bar{C}} \bar{S} = -\bar{\mu}/\bar{\theta} = -k_B \log(\bar{C}/\bar{C}_{\text{ref}})$ , cf. (124a). This gives

$$\dot{\bar{C}} = -\bar{\nabla} \cdot \bar{\mathbf{J}}, \quad \bar{\mathbf{J}} = -\bar{\mathbb{M}}_{\bar{C}\bar{C}}(\bar{\mathbf{q}}) \bar{\nabla} \log \left( \frac{\bar{C}}{\bar{C}_{\text{ref}}} \right).$$

When neglecting the NIC (44b) for the mass density, then it makes sense to consider a single component. Setting  $\bar{\mathbb{M}}_{\bar{C}\bar{C}} = \bar{D} \bar{D}(\bar{\mathbf{q}})$  it results in the diffusion equation

$$\dot{\bar{C}} = -\bar{\nabla} \cdot \bar{\mathbf{J}}, \quad \bar{\mathbf{J}} = -\bar{D} \bar{C}_{\text{ref}} \bar{\nabla} \left( \frac{\bar{C}}{\bar{C}_{\text{ref}}} \right).$$

This gives the usual diffusion equation if  $\bar{C}_{\text{ref}}$  does not depend on space through a state. The entropy in this case evolves according to

$$\dot{\bar{S}} = \frac{\partial \bar{S}}{\partial \bar{C}} \cdot \dot{\bar{C}} = -\frac{\bar{\mu}}{\bar{\theta}} \bar{\nabla} \cdot (\bar{\mathbb{M}}_{\bar{C}\bar{C}} \bar{\nabla} \frac{\bar{\mu}}{\bar{\theta}}).$$

In case of natural boundary conditions  $\bar{\mathbf{n}} \cdot \bar{\nabla}(\bar{\mu}/\bar{\theta}) = 0$  one finds entropy increase, i.e.,

$$\frac{d}{dt} \bar{S}(\bar{\mathbf{q}}(t)) = \int_{\bar{\Omega}} (\bar{\nabla} \frac{\bar{\mu}}{\bar{\theta}}) \cdot \bar{\mathbb{M}}_{\bar{C}\bar{C}}(\bar{\mathbf{q}}) (\bar{\nabla} \frac{\bar{\mu}}{\bar{\theta}}) d\bar{x} \geq 0.$$

\*

**Example 5.6 (Two-component systems)** For a two-component system,  $N = 2$ , with different masses, e.g., heavy and light particles  $M_2 = \varepsilon M_1$  with  $0 < \varepsilon \ll 1$ , the matrices in (132) are given by

$$\bar{\mathbb{M}}_{\bar{C}\bar{C}} = \bar{D}(\bar{\mathbf{q}}) \mathbb{P}, \quad \mathbb{P} = \frac{1}{1+\varepsilon^2} \begin{pmatrix} +\varepsilon^2 & -\varepsilon \\ -\varepsilon & 1 \end{pmatrix}$$

and the resulting Onsager operator satisfies NIC (44a). The general diffusion flux for a two-component system is

$$\mathbf{J}_i = - \sum_{j=1}^2 \bar{D}(\bar{\mathbf{q}}) \mathbb{P}_{ij} \bar{\nabla} \frac{\bar{\mu}_j}{\bar{\theta}},$$

with a positive state-dependent  $\bar{D} : \bar{\mathcal{Q}} \rightarrow \mathbb{R}$ .

\*

## 5.4 Cross-coupling in Onsager systems

All the dissipative processes discussed in this section are driven by the same entropy functional  $\bar{\mathcal{S}}(\bar{\mathbf{q}})$  and most constructions were performed for the state vector  $\bar{\mathbf{q}} = (\bar{\mathbf{C}}, \bar{V}, \bar{U})$ . For a thermodynamical system, where reactions, heat conduction, and diffusion occur simultaneously, then the coupled dynamics is

$$\dot{\bar{\mathbf{q}}} = \bar{\mathbb{K}}(\bar{\mathbf{q}})D\bar{\mathcal{S}}(\bar{\mathbf{q}}), \quad (133a)$$

and, as discussed in Sec. 3.2, the Onsager operator  $\bar{\mathbb{K}}$  now encodes all the processes according to

$$\bar{\mathbb{K}}(\bar{\mathbf{q}}) = \bar{\mathbb{K}}_{\text{reac}}(\bar{\mathbf{q}}) + \bar{\mathbb{K}}_{\text{heat}}(\bar{\mathbf{q}}) + \bar{\mathbb{K}}_{\text{diff}}(\bar{\mathbf{q}}) = \begin{pmatrix} \bar{\mathbb{K}}_{\bar{\mathbf{C}}\bar{\mathbf{C}}}^{\text{diff}} + \bar{\mathbb{K}}_{\bar{\mathbf{C}}\bar{\mathbf{C}}}^{\text{reac}} & 0 & \bar{\mathbb{K}}_{\bar{\mathbf{C}}\bar{U}} \\ 0 & 0 & 0 \\ \bar{\mathbb{K}}_{\bar{\mathbf{C}}\bar{U}}^* & 0 & \bar{\mathbb{K}}_{\bar{U}\bar{U}}^{\text{heat}} \end{pmatrix}. \quad (133b)$$

Here we assumed mechanical equilibrium, so that all coupling- and cross-coupling terms related to volume changes are neglected. Heat conduction is encoded in  $\bar{\mathbb{K}}_{\bar{U}\bar{U}}^{\text{heat}}$  and reactions based on detailed balance are encoded in  $\bar{\mathbb{K}}_{\bar{\mathbf{C}}\bar{\mathbf{C}}}^{\text{reac}}$ . Ex. 5.5 for diffusion only treated the scalar case  $\bar{\mathbf{C}} = \bar{C}$ . Above, the operator  $\bar{\mathbb{K}}_{\bar{\mathbf{C}}\bar{\mathbf{C}}}^{\text{reac}}$  is not diagonal and its internal substructure is basically determined by the stoichiometric coefficients contributing to  $\bar{\mathcal{S}}^r$  in (120d). Diffusion  $\bar{\mathbb{K}}_{\bar{\mathbf{C}}\bar{\mathbf{C}}}^{\text{diff}}$  with off-diagonal contributions is generally known as cross-diffusion. This has been discussed in the context pattern formation in biological systems or for complex polymer systems [33, 72]. These systems have been studied from an application and also mathematical point of view [48, 38] and also more recently using energetic-variational mathematical methods [32].

Cross-coupling effects in diffusion processes are, e.g., due to the Soret effect [15, 34] (thermodiffusion, thermophoresis), which describes diffusion caused by temperature gradients. The consistent cross-coupling due to Onsager's reciprocal relations is called the Dufour effect. The above ansatz leads to the reaction-diffusion-heat conduction system

$$\begin{aligned} \dot{\bar{\mathbf{C}}} &= -\bar{\nabla} \cdot [\bar{\mathbb{M}}_{\bar{\mathbf{C}}\bar{\mathbf{C}}} \bar{\nabla} \left( \frac{-\bar{\mu}}{\bar{\theta}} \right) + \bar{\mathbb{M}}_{\bar{\mathbf{C}}\bar{U}} \bar{\nabla} \frac{1}{\bar{\theta}}] - \bar{\mathbb{H}}_{\bar{\mathbf{C}}\bar{\mathbf{C}}} \frac{\bar{\mu}}{\bar{\theta}}, \\ \dot{\bar{U}} &= -\bar{\nabla} \cdot [\bar{\mathbb{M}}_{\bar{\mathbf{C}}\bar{U}}^* \bar{\nabla} \left( \frac{-\bar{\mu}}{\bar{\theta}} \right) + \bar{\mathbb{M}}_{\bar{U}\bar{U}} \bar{\nabla} \frac{1}{\bar{\theta}}], \\ \dot{\bar{V}} &= 0. \end{aligned}$$

It satisfies the NIC (44a) for the internal energy and entropy increase  $\frac{d}{dt}\bar{\mathcal{S}} \geq 0$ . The construction of  $\bar{\mathbb{M}}_{\bar{\mathbf{C}}\bar{U}}$  is similar to  $\bar{\mathbb{M}}_{\bar{\mathbf{C}}\bar{\mathbf{C}}}$ , but more restrictive due to the NIC (44) for energy and mass. Hence, in the following we shall set  $\bar{\mathbb{M}}_{\bar{\mathbf{C}}\bar{U}}, \bar{\mathbb{M}}_{\bar{U}\bar{\mathbf{C}}} = 0$ .

**Remark 5.7 (NIC (44a) and cross-coupling)** For a general reaction-diffusion process with heat conduction we consider the state vector  $\bar{\mathbf{q}}_{\bar{E}} = (\bar{\mathbf{C}}, \bar{V}, \bar{E})^\top \in \bar{\mathcal{Q}}_{\bar{E}}$ , i.e., we use the total energy density  $\bar{E} = \frac{1}{2}\bar{\mathbf{C}} \cdot \bar{\mathbf{M}}|\bar{\mathbf{v}}|^2 + \bar{U}$  including the kinetic energy instead of the internal energy density  $\bar{U}$  as a thermodynamical variable. If we assume

$$\bar{\mathbb{K}}_{\bar{E}} = \begin{pmatrix} \bar{\mathbb{K}}_{\bar{\mathbf{C}}\bar{\mathbf{C}}} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \bar{\mathbb{K}}_{\bar{E}\bar{E}} \end{pmatrix},$$

with  $\bar{\mathbb{K}}_{\bar{E}\bar{E}} = -\nabla \bar{\theta}^2 \bar{k}_{\text{heat}} \nabla \square$  we immediately infer that the NIC (44a)  $\bar{\mathbb{K}}_{\bar{E}}(\bar{\mathbf{q}}_{\bar{E}})D\bar{\mathcal{E}}(\bar{\mathbf{q}}_{\bar{E}}) = 0$  is satisfied with  $D\bar{\mathcal{E}}(\bar{\mathbf{q}}_{\bar{E}}) \equiv (0, 0, 1)^\top$ .

By the transformation  $\mathbb{T}_{\bar{E} \rightarrow \bar{U}} : \bar{\mathcal{Q}}_{\bar{E}} \rightarrow \bar{\mathcal{Q}}_{\bar{U}}, \bar{\mathbf{q}}_{\bar{E}} \mapsto \bar{\mathbf{q}}_{\bar{U}} = (\bar{\mathbf{C}}, \bar{V}, \bar{U})^\top$  we perform a change of variables along the lines of (71–73) using

$$\mathbb{L}_{\bar{U}}(\bar{\mathbf{q}}_{\bar{E}}) = \text{DT}_{\bar{E} \rightarrow \bar{U}} = \begin{pmatrix} \mathbb{I}_N & 0 & 0 \\ 0 & 1 & 0 \\ -\partial_{\bar{\mathbf{C}}}\bar{E} & 0 & 1 \end{pmatrix},$$

where we already exploited  $\partial_{\bar{U}}\bar{E} = 1$  and  $\partial_{\bar{V}}\bar{E} = 0$ . This results in the transformed reaction-diffusion-heat Onsager operator

$$\bar{\mathbb{K}}_{\bar{U}}^{\text{rdh}}(\bar{\mathbf{q}}_{\bar{U}}) = \mathbb{L}_{\bar{U}}(\bar{\mathbf{q}}_{\bar{E}}) \bar{\mathbb{K}}_{\bar{E}}(\bar{\mathbf{q}}_{\bar{E}}) \mathbb{L}_{\bar{U}}(\bar{\mathbf{q}}_{\bar{E}})^* \quad (135)$$

$$= \begin{pmatrix} \bar{\mathbb{K}}_{\bar{\mathbf{C}}\bar{\mathbf{C}}}(\square) & 0 & \bar{\mathbb{K}}_{\bar{\mathbf{C}}\bar{\mathbf{C}}}(-\partial_{\bar{\mathbf{C}}}\bar{E}\square) \\ 0 & 0 & 0 \\ -\partial_{\bar{\mathbf{C}}}\bar{E}^\top \bar{\mathbb{K}}_{\bar{\mathbf{C}}\bar{\mathbf{C}}}(\square) & 0 & -\partial_{\bar{\mathbf{C}}}\bar{E}^\top \bar{\mathbb{K}}_{\bar{\mathbf{C}}\bar{\mathbf{C}}}(-\partial_{\bar{\mathbf{C}}}\bar{E}\square) + \bar{\mathbb{K}}_{\bar{E}\bar{E}}(\square) \end{pmatrix} \quad (136)$$

displaying the cross-coupling terms indicated in (133b). In view of Thm. 3.11 we conclude that the non-interaction condition (44a), i.e.,  $\bar{\mathbb{K}}_{\bar{U}}(\bar{\mathbf{q}}_{\bar{U}}) \text{D}\bar{\mathcal{E}}_{\bar{U}}(\bar{\mathbf{q}}_{\bar{U}}) = 0$  is also satisfied with the derivative  $\text{D}\bar{\mathcal{E}}_{\bar{U}}(\bar{\mathbf{q}}_{\bar{U}}) \equiv (-\frac{1}{2}|\bar{\nu}|^2 \mathbf{M}, 0, 1)$ . In (135), the term  $\bar{\mathbb{K}}_{\bar{\mathbf{C}}\bar{\mathbf{C}}} = \bar{\mathbb{K}}_{\bar{\mathbf{C}}\bar{\mathbf{C}}}^{\text{diff}} + \bar{\mathbb{K}}_{\bar{\mathbf{C}}\bar{\mathbf{C}}}^{\text{reac}}$  may comprise both diffusion as in (129c) and chemical reactions as in (120). For the force term  $-\frac{1}{2}|\bar{\nu}|^2 \mathbf{M}$  induced by the kinetic energy we observe that  $\bar{\mathbb{K}}_{\bar{\mathbf{C}}\bar{\mathbf{C}}}^{\text{reac}}(\frac{1}{2}|\bar{\nu}|^2 \mathbf{M}) = 0$  thanks to (123). The same holds true also for diffusion, i.e.,  $\bar{\mathbb{K}}_{\bar{\mathbf{C}}\bar{\mathbf{C}}}^{\text{diff}}(\frac{1}{2}|\bar{\nu}|^2 \mathbf{M}) = 0$  given that the mobility matrix  $\bar{\mathbb{M}}_{\bar{\mathbf{C}}\bar{\mathbf{C}}}$  enjoys property (131b). If this property is not satisfied, then the cross-coupling terms ensure the NIC  $\bar{\mathbb{K}}_{\bar{U}}^{\text{rdh}}(\bar{\mathbf{q}}_{\bar{U}}) \text{D}\bar{\mathcal{E}}_{\bar{U}}(\bar{\mathbf{q}}_{\bar{U}}) = 0$  and lead to additional terms in the evolution equation

$$\begin{aligned} \partial_t \bar{\mathbf{C}} &= -\bar{\mathbb{K}}_{\bar{\mathbf{C}}\bar{\mathbf{C}}} \left[ \frac{\bar{\mu}}{\bar{\theta}} + \frac{1}{2} |\bar{\nu}|^2 \mathbf{M} \bar{\theta}^{-1} \right], \\ \partial_t \bar{U} &= \frac{1}{2} |\bar{\nu}|^2 \mathbf{M}^\top \bar{\mathbb{K}}_{\bar{\mathbf{C}}\bar{\mathbf{C}}} \left[ \frac{\bar{\mu}}{\bar{\theta}} + \frac{1}{2} |\bar{\nu}|^2 \mathbf{M} \bar{\theta}^{-1} \right] + \bar{\mathbb{K}}_{\bar{E}\bar{E}}[\bar{\theta}^{-1}]. \end{aligned}$$

However, in the following we assume that (131b) is valid, so that these terms do not appear. \*

## 6 Application to reactive viscous flows

In this part we combine the variational approach for compressible viscous fluid flows presented in Sec. 4 with dissipative processes like reactions, diffusion, and heat conduction from Sec. 5. First, in Sec. 6.1 we present a GENERIC quintuple for reactive flows in Lagrangian coordinates and map the system to Eulerian coordinates for different sets of thermodynamic variables. In Sec. 6.2 we provide an alternative formulation using the pressure and the temperature as variables and combine reactive flows with a Darcy-type dissipation as an example.

### 6.1 GENERIC formulation of reactive fluid flows

To couple the Hamiltonian system for the compressible Euler equations from Sec. 4.1 with the Onsager systems from Sec. 5 we use the Lagrangian state vector

$$\bar{\mathbf{q}}_{\bar{\tau}} = \begin{pmatrix} \chi : \bar{\Omega} \rightarrow \mathbb{R}^d \\ \bar{\mathbf{P}} : \bar{\Omega} \rightarrow \mathbb{R}^d \\ \bar{\mathbf{C}} : \bar{\Omega} \rightarrow \mathbb{R}^N \\ \bar{\tau} : \bar{\Omega} \rightarrow \mathbb{R} \end{pmatrix} \in \bar{\mathcal{Q}}_{\bar{\tau}}$$

with the placeholder  $\bar{\tau} \in \{\bar{S}, \bar{U}, \bar{\theta}\}$  as in (65). Similar to Sec. 4.1 we carry out this coupling in the Lagrangian frame and then transform the obtained GENERIC system to its Eulerian version using the ideas of Sec. 3.4.1. Subsequently, we discuss the evolution of the Eulerian thermodynamic variable  $\tau \in \{S, U, \theta\}$  by performing changes of thermodynamic variables along the lines of Sec. 3.4.2.

**Reversible contribution to dynamics.** Consider the state vector  $\bar{q}_{\bar{U}} \in \bar{Q}_{\bar{U}}$ , i.e., now  $\bar{\tau} = \bar{U}$ . Compared to Sec. 4.1, where the flow of one single component with concentration  $\bar{C}$  was discussed, we now treat the flow of  $N$  components with a vector of concentrations  $\bar{C}$ . This generalization of the Hamiltonian system is straight-forward when assuming that no reversible processes among the components of  $\bar{C}$  occur. Accordingly, the Poisson structure from (99) can be adapted as

$$\bar{\mathbb{J}}_{\bar{U}}(\bar{q}_{\bar{S}}) = \begin{pmatrix} 0 & \mathbb{I}_d & 0 & 0 \\ -\mathbb{I}_d & 0 & 0 & -\mathbb{D}_{\chi}^* \bar{U} \\ 0 & 0 & 0 & 0 \\ 0 & \mathbb{D}_{\chi} \bar{U} & 0 & 0 \end{pmatrix}, \quad (137)$$

with  $\mathbb{D}_{\chi} \bar{U}(\bar{q}_{\bar{S}})$  and  $\mathbb{D}_{\chi}^* \bar{U}(\bar{q}_{\bar{S}})$  as in (80b) and (80c).

**Dissipative contribution to dynamics.** We now couple the Stokes flow from Sec. 4.2 with reaction-diffusion and heat conduction from Sec. 5. As discussed in Sec. 3.2, thanks to the additive nature of Onsager operators, the operator  $\bar{\mathbb{K}}_{\bar{U}}$  for the coupled processes is the sum of the operators for the single effects, i.e.,

$$\bar{\mathbb{K}}_{\bar{U}} := \bar{\mathbb{K}}^S + \bar{\mathbb{K}}_{\bar{U}}^{\text{rdh}} = \bar{\mathbb{K}}^S + \bar{\mathbb{K}}^{\text{react}} + \bar{\mathbb{K}}^{\text{heat}} + \bar{\mathbb{K}}^{\text{diff}}, \quad (138)$$

with  $\bar{\mathbb{K}}^S$  from (104) and  $\bar{\mathbb{K}}_{\bar{U}}^{\text{rdh}}$  from (135), both depending on  $\bar{q}_{\bar{U}} \in \bar{Q}_{\bar{U}}$ . We further recall from Sec. 3.2 that the Onsager operators  $\bar{\mathbb{K}}$  acting on an element  $\bar{\xi} = (\bar{\xi}_{\chi}, \bar{\xi}_{\bar{P}}, \bar{\xi}_{\bar{C}}, \bar{\xi}_{\bar{U}}) \in \bar{Q}_{\bar{U}}^*$  are given as the functional derivatives of the corresponding dual dissipation potentials  $\bar{\mathbb{K}} = \mathbb{D}_{\bar{\xi}} \bar{\Psi}^*(\bar{q}_{\bar{S}}; \bar{\xi})$ . For the Stokes flow this is

$$\bar{\Psi}_{\bar{S}}^*(\bar{q}_{\bar{U}}; \bar{\xi}) := \int_{\bar{\Omega}} \frac{1}{2} [2\bar{\lambda} |\bar{w}|^2 + \bar{\zeta} \text{tr}(\bar{w})^2] \bar{V} d\bar{x},$$

with  $\bar{w} = \bar{\nabla}_s \bar{\xi}_{\bar{P}} - \bar{\xi}_{\bar{U}} \bar{\nabla}_s \bar{\nu}$  as introduced in (103a).

Chemical reactions are modeled by

$$\bar{\Psi}_{\text{react}}^*(\bar{q}_{\bar{U}}; \bar{\xi}) := \int_{\bar{\Omega}} \frac{1}{2} \bar{\xi}_{\bar{C}} \cdot \bar{\mathbb{H}}_{\bar{C}\bar{C}}(\bar{q}) \bar{\xi}_{\bar{C}} \bar{V} d\bar{x},$$

with  $\bar{\mathbb{H}}_{\bar{C}\bar{C}}$  as in (120a). Heat conduction and diffusion are described by the dual dissipation potentials

$$\bar{\Psi}_{\text{heat}}^*(\bar{q}_{\bar{U}}; \bar{\xi}) := \frac{1}{2} \int_{\bar{\Omega}} \bar{\theta}^2 \bar{w}_{\bar{U}} \cdot \bar{k}_{\text{heat}}(\bar{q}) \bar{w}_{\bar{U}} \bar{V} d\bar{x},$$

$$\bar{\Psi}_{\text{diff}}^*(\bar{q}_{\bar{U}}; \bar{\xi}) := \frac{1}{2} \int_{\bar{\Omega}} \bar{w}_{\bar{C}} : \bar{\mathbb{M}}_{\bar{C}\bar{C}}(\bar{q}) \bar{w}_{\bar{C}} \bar{V} d\bar{x}$$

with  $\bar{k}_{\text{heat}}$  and  $\bar{w}_{\bar{U}} = \bar{F}^{-\top} \bar{\nabla} \bar{\xi}_{\bar{U}}$  as in (125) as well as  $\bar{\mathbb{M}}_{\bar{C}\bar{C}}$  and  $\bar{w}_{\bar{C}} = \bar{\nabla} \bar{\xi}_{\bar{C}} \bar{F}^{-1}$  as in (129) with adjustments of derivatives as outlined in (116). Observe that there is no dissipative effect explicitly connected to  $\bar{\xi}_{\chi}$ . We further point out that the Lagrangian potentials defined above have an explicit dependence on  $\bar{V}$  and on  $\bar{F}$  in the gradient terms. This choice is made such that the resulting Eulerian Onsager operators do not depend on  $\bar{V}$  and  $\bar{F}$  and thus satisfy closure condition (50c). Above

considerations thus allow us to deduce that

$$\bar{\mathbb{K}}_{\bar{U}} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \bar{\mathbb{K}}_{\bar{P}\bar{P}}^S & 0 & \bar{\mathbb{K}}_{\bar{P}\bar{U}}^S \\ 0 & 0 & \bar{\mathbb{K}}_{\bar{C}\bar{C}} & 0 \\ 0 & \bar{\mathbb{K}}_{\bar{U}\bar{P}}^S & 0 & \bar{\mathbb{K}}_{\bar{U}\bar{U}} \end{pmatrix} \quad \text{with} \quad \begin{aligned} \bar{\mathbb{K}}_{\bar{C}\bar{C}} &:= \bar{\mathbb{K}}_{\bar{C}\bar{C}}^{\text{reac}} + \bar{\mathbb{K}}_{\bar{C}\bar{C}}^{\text{diff}}, \\ \bar{\mathbb{K}}_{\bar{U}\bar{U}} &:= \bar{\mathbb{K}}_{\bar{U}\bar{U}}^S + \bar{\mathbb{K}}_{\bar{U}\bar{U}}^{\text{heat}}. \end{aligned} \quad (140a)$$

Notice that the contributions for the reaction-diffusion process are slightly different compared to (133) because now we set  $\bar{\mathbb{K}}_{\bar{U}\bar{C}} = 0$  and  $\bar{\mathbb{K}}_{\bar{C}\bar{U}} = 0$  for the off-diagonal contributions, cf. also the discussion in Rem. 5.7

In addition  $\bar{V} = \det(\bar{\nabla}\chi)$  is not constant anymore and terms involving pressure gradients may appear. The total energy  $\bar{\mathcal{E}}(\bar{q}_{\bar{U}})$  and total entropy  $\bar{\mathcal{S}}(\bar{q}_{\bar{U}})$  of the system with densities  $\bar{E}(\bar{q}_{\bar{U}}) = \frac{|\bar{P}|^2}{2\bar{\theta}} + \bar{U}$  and  $\bar{S}(\bar{q}_{\bar{U}}) = \bar{S}(\bar{C}, \bar{V}, \bar{U})$  generate the driving forces

$$D\bar{\mathcal{E}}(\bar{q}_{\bar{U}}) = \left( 0, \frac{\bar{P}}{\bar{\theta}}, -M \frac{|\bar{v}|^2}{2}, 1 \right)^\top, \quad D\bar{\mathcal{S}}(\bar{q}_{\bar{U}}) = \left( \delta_\chi \bar{S}, 0, -\frac{\bar{\mu}}{\bar{\theta}}, \frac{1}{\bar{\theta}} \right)^\top,$$

with  $\delta_\chi \bar{S} = -\bar{\nabla} \cdot \left( \frac{\bar{\pi}}{\bar{\theta}} \text{Cof}(\bar{F}) \right)$  by the chain rule together with (7b), (18d), and integration by parts, similar to Ex. 3.15. For the above driving forces and the geometric structures  $\bar{\mathbb{J}}_{\bar{U}}$  and  $\bar{\mathbb{K}}_{\bar{U}}$  from (137) and (140) it can be readily checked that the NIC (44a) hold true. Indeed, the NIC  $\bar{\mathbb{J}}_{\bar{U}} D\bar{\mathcal{S}}(\bar{q}_{\bar{U}}) = 0$  is straight-forward to see, whereas  $\bar{\mathbb{K}}_{\bar{U}} D\bar{\mathcal{E}}(\bar{q}_{\bar{U}}) = 0$  follows from Remark 5.7.

**Evolution of system**  $(\bar{Q}_{\bar{U}}, \bar{\mathcal{E}}_{\bar{U}}, \bar{\mathcal{S}}_{\bar{U}}, \bar{\mathbb{J}}_{\bar{U}}, \bar{\mathbb{K}}_{\bar{U}})$ . Combining reversible and dissipative contributions in (45), we obtain the Lagrangian formulation of reactive flows

$$\partial_t \chi = \bar{P} \bar{\theta}^{-1}, \quad (141a)$$

$$\begin{aligned} \partial_t \bar{P} &= -\mathbb{D}_\chi^* \bar{U}[1] + \bar{\mathbb{K}}_{\bar{P}\bar{U}}^S[\bar{\theta}^{-1}] \\ &= \bar{\nabla} \cdot \left( \bar{\pi} \text{Cof}(\bar{F}) \right) + \bar{\nabla} \cdot \bar{\Sigma}_{\text{visc}}, \end{aligned} \quad (141b)$$

$$\begin{aligned} \partial_t \bar{C} &= - \left( \bar{\mathbb{K}}_{\bar{C}\bar{C}}^{\text{reac}} + \bar{\mathbb{K}}_{\bar{C}\bar{C}}^{\text{diff}} \right) \left[ \frac{\bar{\mu}}{\bar{\theta}} \right] \\ &= \bar{\nabla} \cdot \left( \bar{\mathbb{M}}_{\bar{C}\bar{C}} \left( \bar{\nabla} \frac{\bar{\mu}}{\bar{\theta}} \right) \bar{F}^{-1} \text{Cof}(\bar{F}) \right) - \bar{V} \bar{\mathbb{H}}_{\bar{C}\bar{C}} \frac{\bar{\mu}}{\bar{\theta}}, \end{aligned} \quad (141c)$$

$$\begin{aligned} \partial_t \bar{U} &= \mathbb{D}_\chi \bar{U} \left[ \frac{\bar{P}}{\bar{\theta}} \right] + \left( \bar{\mathbb{K}}_{\bar{U}\bar{U}}^{\text{heat}} + \bar{\mathbb{K}}_{\bar{U}\bar{U}}^S \right) \left[ \frac{1}{\bar{\theta}} \right] \\ &= -\bar{\pi} \text{Cof}(\bar{F}) : \bar{\nabla} \bar{v} + \bar{\nabla} \cdot \left( \text{Cof}(\bar{F})^\top \bar{k}_{\text{heat}} \bar{F}^{-\top} \bar{\nabla} \bar{\theta} \right) + \bar{\Sigma}_{\text{visc}} : \bar{\nabla} \bar{v} \end{aligned}$$

with the viscous stress tensor  $\bar{\Sigma}_{\text{visc}}$  from (105d). A similar set of PDEs with entropy as the thermodynamic variable has been constructed by using a more geometric approach by Gay-Balmaz and Yoshimura [23].

**Lagrangian-Eulerian change of coordinates.** Next, we perform a change to Eulerian coordinates based on the method developed in Section 3.4 and already applied in Section 4. This transforms Navier-Stokes-Fourier system for reactive flows (141) in Lagrangian coordinates to its more familiar Eulerian version. The reduction map  $T_{\text{LE}} : \bar{Q}_{\bar{U}} \rightarrow Q_U$  from Lagrangian to Eulerian coordinates was introduced in (106) as

$$T_{\text{LE}}(\bar{q}_{\bar{U}}) = \mathbf{q}_U = \begin{pmatrix} \mathbf{P} : \Omega \rightarrow \mathbb{R}^d \\ \mathbf{C} : \Omega \rightarrow \mathbb{R}^N \\ U : \Omega \rightarrow \mathbb{R} \end{pmatrix} \in Q_U. \quad (142)$$



Under this transformation, the total energy  $\mathcal{E}_U(\mathbf{q}_U)$  and total entropy  $\mathcal{S}_U(\mathbf{q}_U)$  of the system are obtained from the densities  $E_U(\mathbf{q}_U) = \frac{|\mathbf{P}|^2}{2\varrho} + U$  and  $S_U(\mathbf{q}_U) = S(\mathbf{C}, U)$  and they generate the driving forces

$$D\mathcal{E}_U(\mathbf{q}_U) = \left( \frac{\mathbf{P}}{\varrho}, -\frac{M}{2\varrho^2} |\mathbf{P}|^2, 1 \right)^\top, \quad (143a)$$

$$D\mathcal{S}_U(\mathbf{q}_U) = \left( 0, -\frac{\boldsymbol{\mu}}{\theta}, \frac{1}{\theta} \right)^\top. \quad (143b)$$

Closure condition (50a) for the functionals  $\mathcal{E}_U(\mathbf{q}_U) = \bar{\mathcal{E}}(\bar{\mathbf{q}}_{\bar{U}})$  and  $\mathcal{S}_U(\mathbf{q}_U) = \bar{\mathcal{S}}(\bar{\mathbf{q}}_{\bar{U}})$  is apparently valid if we express  $\theta = \theta(\mathbf{q}_U)$ ,  $\boldsymbol{\mu} = \boldsymbol{\mu}(\mathbf{q}_U)$ . The derivative  $D\mathbb{T}_{LE}$  is similar to (107) but now  $\bar{\mathbf{C}}$  is not locally conserved anymore, so that

$$\mathbb{L}_{LE}(\bar{\mathbf{q}}_{\bar{U}}) = \begin{pmatrix} -\nabla \cdot (\bar{V}^{-1} \bar{\mathbf{P}} \otimes \square) & \frac{\square}{\bar{V}} & 0 & 0 \\ -\nabla \cdot (\bar{V}^{-1} \bar{\mathbf{C}} \otimes \square) & 0 & \frac{\square}{\bar{V}} & 0 \\ -\nabla \cdot (\bar{V}^{-1} \bar{U} \square) & 0 & 0 & \frac{\square}{\bar{V}} \end{pmatrix}.$$

The adjoint  $\mathbb{L}_{LE}^*$  is computed using the duality product as in (88) and reads

$$\mathbb{L}_{LE}(\bar{\mathbf{q}}_{\bar{U}})^* = \begin{pmatrix} (\nabla \square)^\top \bar{\mathbf{P}} & (\nabla \square)^\top \bar{\mathbf{C}} & \bar{U} \nabla \square \\ \mathbb{I}_d & 0 & 0 \\ 0 & \mathbb{I}_N & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Thus, the transformed Poisson operator  $\mathbb{J}_U = \mathbb{J}_U(\mathbf{q}_U)$  is

$$\begin{aligned} \mathbb{J}_U &= \mathbb{L}_{LE} \bar{\mathbb{J}}_{\bar{U}} \mathbb{L}_{LE}^* \\ &= \begin{pmatrix} \mathbb{J}_{PP} & \mathbb{J}_{PC} & \mathbb{J}_{PU} \\ \mathbb{J}_{CP} & 0 & 0 \\ \mathbb{J}_{UP} & 0 & 0 \end{pmatrix} \quad \text{with} \end{aligned} \quad \begin{aligned} \mathbb{J}_{PP} \square &= -(\nabla \square)^\top \bar{\mathbf{P}} - \nabla \cdot (\bar{\mathbf{P}} \otimes \square), \\ \mathbb{J}_{PC} \square &= -(\nabla \square)^\top \bar{\mathbf{C}}, \\ \mathbb{J}_{PU} \square &= -U \nabla \square + \nabla \cdot (\square \pi), \\ \mathbb{J}_{CP} \square &= -\nabla \cdot (\bar{\mathbf{C}} \otimes \square), \\ \mathbb{J}_{UP} \square &= -\nabla \cdot (U \square) + \pi \nabla \cdot \square. \end{aligned} \quad (145)$$

Similarly, the Onsager operator is transformed via  $\mathbb{K}_U = \mathbb{L}_{LE} \bar{\mathbb{K}}_{\bar{U}} \mathbb{L}_{LE}^*$  resulting in

$$\mathbb{K}_U := \begin{pmatrix} \mathbb{K}_{PP}^S & 0 & \mathbb{K}_{PU}^S \\ 0 & \mathbb{K}_{CC} & 0 \\ \mathbb{K}_{UP}^S & 0 & \mathbb{K}_{UU} \end{pmatrix} = \frac{1}{\bar{V}} \begin{pmatrix} \bar{\mathbb{K}}_{\bar{P}\bar{P}}^S & 0 & \bar{\mathbb{K}}_{\bar{P}\bar{U}}^S \\ 0 & \bar{\mathbb{K}}_{\bar{C}\bar{C}} & 0 \\ \bar{\mathbb{K}}_{\bar{U}\bar{P}}^S & 0 & \bar{\mathbb{K}}_{\bar{U}\bar{U}} \end{pmatrix} \quad (146a)$$

with  $\bar{\mathbb{K}}_{\bar{C}\bar{C}}$ ,  $\bar{\mathbb{K}}_{\bar{U}\bar{U}}$  from (140) and  $\mathbb{K}_{CC} = \mathbb{K}_{CC}^{\text{react}} + \mathbb{K}_{CC}^{\text{diff}}$ ,  $\mathbb{K}_{UU} = \mathbb{K}_{UU}^S + \mathbb{K}_{UU}^{\text{heat}}$  with  $\mathbb{K}_{UU}^S$  from (104c). Explicit computations lead to the following Eulerian expressions

$$\mathbb{K}_{CC}^{\text{react}} \square = \mathbb{H}_{CC} \square, \quad (146b)$$

$$\mathbb{K}_{CC}^{\text{diff}} \square = -\nabla \cdot (\bar{\mathbb{M}}_{CC} \nabla \square), \quad (146c)$$

$$\mathbb{K}_{UU}^{\text{heat}} \square = -\nabla \cdot (\theta^2 k_{\text{heat}} \nabla \square), \quad (146d)$$

and the coefficient functions  $\bar{\mathbb{H}}_{CC}$ ,  $\bar{\mathbb{M}}_{CC}$ ,  $\bar{k}_{\text{heat}}$  must satisfy closure condition (50c), i.e., they are only functions of  $U = \bar{U}/\bar{V}$  and  $\mathbf{C} = \bar{\mathbf{C}}/\bar{V}$  such that

$$\begin{aligned} \bar{\mathbb{H}}_{CC}(\mathbb{T}_{LE}(\bar{\mathbf{q}}_{\bar{U}})) &= \bar{\mathbb{H}}_{\bar{C}\bar{C}}(\bar{\mathbf{q}}_{\bar{U}}), \\ \bar{\mathbb{M}}_{CC}(\mathbb{T}_{LE}(\bar{\mathbf{q}}_{\bar{U}})) &= \bar{\mathbb{M}}_{\bar{C}\bar{C}}(\bar{\mathbf{q}}_{\bar{U}}), \\ k_{\text{heat}}(\mathbb{T}_{LE}(\bar{\mathbf{q}}_{\bar{U}})) &= \bar{k}_{\text{heat}}(\bar{\mathbf{q}}_{\bar{U}}). \end{aligned} \quad (146e)$$

By virtue of Thm. 3.11 the Eulerian geometric structures  $\mathbb{J}_U$  and  $\mathbb{K}_U$  from (145) and (146) also satisfy the noninteraction conditions (44).

Applying the Poisson operator  $\mathbb{J}_U$  and the Onsager operator  $\mathbb{K}_U$  to their respective driving forces from (143), yields the Eulerian form of the reactive Navier-Stokes-Fourier system

$$\begin{aligned}\partial_t \mathbf{P} + \nabla \cdot (\mathbf{P} \otimes \boldsymbol{\nu}) &= -\nabla \pi + \mathbb{K}_{PU}^S \theta^{-1} \\ &= -\nabla \pi + \nabla \cdot \boldsymbol{\sigma}_{\text{visc}},\end{aligned}\quad (147a)$$

$$\begin{aligned}\partial_t \mathbf{C} + \nabla \cdot (\mathbf{C} \otimes \boldsymbol{\nu}) &= -\mathbb{K}_{CC} \frac{\boldsymbol{\mu}}{\theta} \\ &= -\mathbb{H}_{CC} \frac{\boldsymbol{\mu}}{\theta} + \nabla \cdot (\mathbb{M}_{CC} \nabla \frac{\boldsymbol{\mu}}{\theta}),\end{aligned}\quad (147b)$$

$$\begin{aligned}\partial_t U + \nabla \cdot (U \boldsymbol{\nu}) &= -\pi \nabla \cdot \boldsymbol{\nu} + \mathbb{K}_{UU} \theta^{-1} \\ &= -\pi \nabla \cdot \boldsymbol{\nu} + \nabla \cdot (k_{\text{heat}} \nabla \theta) + \boldsymbol{\sigma}_{\text{visc}} : \nabla \boldsymbol{\nu}.\end{aligned}\quad (147c)$$

An analogous set of equations has been discussed by Bothe and Dreyer [7] in the context of class-I-II-III models. Continuity equation (24a) for the total mass density  $\varrho = \mathbf{M} \cdot \mathbf{C}$  can be retrieved by multiplying (147b) by the vector of particle masses  $\mathbf{M}$ , thus  $\varrho$  is conserved.

The evolution (147c) shows that the internal energy is a non-conserved quantity due to the reversible conversion of kinetic and internal energy and irreversible viscous dissipation. In order to see the evolution laws of further thermodynamic variables  $\tau \in \{S, \theta\}$  we subsequently transform the GENERIC system  $(\mathcal{Q}_U, \mathcal{E}_U, \mathcal{S}_U, \mathbb{J}_U, \mathbb{K}_U)$  via a change of thermodynamic variables according to Sec. 3.4.2. Analogous considerations as in Remark 4.1 show that the total energy  $\mathcal{E}$  is conserved.

**Change of variables**  $U \mapsto S$ . We consider the transformation map  $T_{U \rightarrow S} : \mathcal{Q}_U \rightarrow \mathcal{Q}_S$ ,  $\mathbf{q}_U \mapsto \mathbf{q}_S$  based on the Eulerian densities  $U(\mathbf{C}, S)$  and  $S(\mathbf{C}, U)$ . In view of (60a) its Fréchet derivative  $DT_{U \rightarrow S}(\mathbf{q}_U)$  is given by

$$DT_{U \rightarrow S} = \begin{pmatrix} \mathbb{I}_d & 0 & 0 \\ 0 & \mathbb{I}_N & 0 \\ \mathbb{D}_{PS} & \mathbb{D}_{CS} & \mathbb{D}_{US} \end{pmatrix} = \begin{pmatrix} \mathbb{I}_d & 0 & 0 \\ 0 & \mathbb{I}_N & 0 \\ 0 & -\frac{\boldsymbol{\mu}^\top}{\theta} & \frac{1}{\theta} \end{pmatrix}.$$

It is used to transform  $\mathbb{J}_U$  from (145) into

$$\begin{aligned}\mathbb{J}_S &= DT_{U \rightarrow S} \mathbb{J}_U DT_{U \rightarrow S}^* \\ &= \begin{pmatrix} \mathbb{J}_{PP} & \mathbb{J}_{PC} & \mathbb{J}_{PS} \\ \mathbb{J}_{CP} & 0 & 0 \\ \mathbb{J}_{SP} & 0 & 0 \end{pmatrix} \quad \text{with} \quad \begin{aligned}\mathbb{J}_{SP} \square &= -\frac{\boldsymbol{\mu}}{\theta} \cdot (\mathbb{J}_{CP} \square) + \frac{1}{\theta} \mathbb{J}_{UP} \square \\ &= \frac{\boldsymbol{\mu}}{\theta} \nabla \cdot (\mathbf{C} \otimes \square) - \frac{1}{\theta} (\nabla \cdot (U \square) + \pi \nabla \cdot \square), \\ \mathbb{J}_{PS} \square &= -\mathbb{J}_{PC} \frac{\boldsymbol{\mu}}{\theta} \square + \mathbb{J}_{PU} \frac{\square}{\theta} \\ &= (\nabla (\frac{\boldsymbol{\mu}}{\theta} \square))^\top \mathbf{C} - U \nabla \frac{\square}{\theta} - \nabla (\frac{\square}{\theta} \pi).\end{aligned}\end{aligned}$$

Accordingly,  $\mathbb{K}_U$  from (146) is transformed into

$$\mathbb{K}_S = DT_{U \rightarrow S} \mathbb{K}_U DT_{U \rightarrow S}^* = \begin{pmatrix} \mathbb{K}_{PP}^S & 0 & \mathbb{K}_{PU}^S (\frac{\square}{\theta}) \\ 0 & \mathbb{K}_{CC} & -\mathbb{K}_{CC} (\frac{\boldsymbol{\mu}}{\theta} \square) \\ \frac{1}{\theta} \mathbb{K}_{UP}^S & -\frac{\boldsymbol{\mu}}{\theta} \cdot \mathbb{K}_{CC} \square & \mathbb{K}_{SS} \end{pmatrix},$$

where  $\mathbb{K}_{SS} = \frac{\boldsymbol{\mu}}{\theta} \cdot \mathbb{K}_{CC} (\frac{\boldsymbol{\mu}}{\theta} \square) + \frac{1}{\theta} \mathbb{K}_{UU} \frac{\square}{\theta}$ . The transformed total energy  $\mathcal{E}_S(\mathbf{q}_S)$  and entropy  $\mathcal{S}_S(\mathbf{q}_S)$  of the system with densities  $E_S(\mathbf{q}_S) = \frac{|\mathbf{P}|^2}{2\varrho} + U(\mathbf{C}, S)$  and  $S_S(\mathbf{q}_S) = S$  generate the driving forces

$$D\mathcal{E}_S(\mathbf{q}_S) = (\mathbf{P}/\varrho, \boldsymbol{\mu}, \theta)^\top, \quad D\mathcal{S}_S(\mathbf{q}_S) = (0, 0, 1)^\top.$$

The evolution laws (45) of the GENERIC system  $(\mathcal{Q}_S, \mathcal{E}_S, \mathcal{S}_S, \mathbb{J}_S, \mathbb{K}_S)$  are then given by equations (147a), (147b) for  $\mathbf{P}$  and  $\mathbf{C}$ , and equation (147c) is replaced by the evolution of entropy

$$\partial_t S + \nabla \cdot (S\mathbf{v}) = \mathbb{K}_{SS}[1] = \frac{\boldsymbol{\mu}}{\theta} \cdot (\mathbb{K}_{CC}^{\text{react}} + \mathbb{K}_{CC}^{\text{diff}}) \frac{\boldsymbol{\mu}}{\theta} + \frac{1}{\theta} (\mathbb{K}_{UU}^S + \mathbb{K}_{UU}^{\text{heat}}) \frac{1}{\theta},$$

where we have used the relation  $\pi + U = \theta S + \boldsymbol{\mu} \cdot \mathbf{C}$  in order to rewrite the reversible term  $\mathbb{J}_{SP}\mathbf{v} = -\nabla \cdot (S\mathbf{v})$ . Entropy is shown explicitly for the operator  $\mathbb{H}_{CC}$  for chemical reactions from (120) with (146e), i.e.,

$$\frac{\boldsymbol{\mu}}{\theta} \cdot \mathbb{H}_{CC} \frac{\boldsymbol{\mu}}{\theta} = \sum_{r=1}^R \frac{\kappa^r \ell(x, y)}{k_B} |(\boldsymbol{\alpha}^r - \boldsymbol{\beta}^r) \cdot \frac{\boldsymbol{\mu}}{\theta}|^2 \geq 0,$$

with  $x = (\mathbf{C}/\mathbf{C}_{\text{ref}})^{\boldsymbol{\alpha}^r}$ ,  $y = (\mathbf{C}/\mathbf{C}_{\text{ref}})^{\boldsymbol{\beta}^r}$  and positive rates  $\kappa^r, \ell$ . For diffusion we can rewrite the operators

$$\begin{aligned} \mathbb{K}_{SS}[1] &= \frac{\boldsymbol{\mu}}{\theta} \cdot \mathbb{K}_{CC} \frac{\boldsymbol{\mu}}{\theta} + \frac{1}{\theta} \mathbb{K}_{UU} \frac{1}{\theta} = -\frac{\boldsymbol{\mu}}{\theta} \cdot \nabla \cdot (\mathbb{M}\mathbf{w}) + \frac{\boldsymbol{\mu}}{\theta} \cdot \mathbb{K}_{CC}^{\text{react}} \frac{\boldsymbol{\mu}}{\theta} + \frac{1}{\theta} \mathbb{K}_{UU} \frac{1}{\theta} \\ &= -\underbrace{\nabla \cdot \left( \frac{\boldsymbol{\mu}^\top}{\theta} \mathbb{M}\mathbf{w} \right)}_{\text{conserved}} + \underbrace{\mathbf{w} \cdot \mathbb{M}\mathbf{w}}_{\geq 0} + \underbrace{\frac{\boldsymbol{\mu}}{\theta} \cdot \mathbb{K}_{CC}^{\text{react}} \frac{\boldsymbol{\mu}}{\theta}}_{\geq 0} + \frac{1}{\theta} \mathbb{K}_{UU} \frac{1}{\theta}, \end{aligned}$$

where  $\mathbf{w} = \nabla(\boldsymbol{\mu}/\theta)$ . The integral of this expression is non-negative for  $\mathbb{M}$  positively semidefinite and natural boundary conditions  $\mathbf{n} \cdot \mathbb{M}\mathbf{w} = 0$ . Similarly, the positivity of  $\mathbb{K}_{UU}$  can be shown and directly follows from the Lagrangian Onsager structure defined in (125).

**Change of variables**  $U \mapsto \theta$ . Now, the GENERIC system is transformed to the setting  $\tau = \theta$  via the transformation  $\mathbb{T}_{U \rightarrow \theta} : \mathcal{Q}_U \rightarrow \mathcal{Q}_\theta$ ,  $\mathbf{q}_U \mapsto \mathbf{q}_\theta$ . For this, consider the internal energy and entropy densities,  $U_\theta(\mathbf{C}, \theta)$  and  $S_\theta(\mathbf{C}, \theta)$ , defined via

$$U_\theta(\mathbf{C}, \theta(\mathbf{C}, S)) := U(\mathbf{C}, S), \quad S_\theta(\mathbf{C}, \theta(\mathbf{C}, S)) := S,$$

with  $\theta(\mathbf{C}, S) = \partial_S U(\mathbf{C}, S)$ . Calculating the partial derivatives of  $U_\theta$  and  $S_\theta$  gives

$$\begin{aligned} \partial_{\mathbf{C}} U_\theta^\top &= \boldsymbol{\mu} - \frac{\theta}{\beta} \boldsymbol{\gamma} \equiv \boldsymbol{\xi}_{\mathbf{C}}, & \partial_\theta U_\theta &= \frac{\theta}{\beta} \equiv \xi_\theta, \\ \partial_{\mathbf{C}} S_\theta^\top &= -\frac{1}{\beta} \boldsymbol{\gamma}, & \partial_\theta S_\theta &= \frac{1}{\beta} \end{aligned}$$

with the capacities  $\beta, \boldsymbol{\gamma}$  from (9b). This results in

$$\begin{aligned} D\mathcal{E}_\theta(\mathbf{q}_\theta) &= (\boldsymbol{\nu}, -\frac{1}{2}|\boldsymbol{\nu}|^2 \mathbf{M} + \partial_{\mathbf{C}} U_\theta, \partial_\theta U_\theta)^\top, \\ D\mathcal{S}_\theta(\mathbf{q}_\theta) &= (0, \partial_{\mathbf{C}} S_\theta, \partial_\theta S_\theta)^\top. \end{aligned} \tag{149}$$

The transformation of the Poisson and Onsager operators  $\mathbb{J}_U$  &  $\mathbb{K}_U$  is done according to (50) with the Fréchet derivative  $D\mathbb{T}_{U \rightarrow \theta} : \mathcal{Q}_U \rightarrow \mathcal{Q}_\theta$ ,

$$D\mathbb{T}_{U \rightarrow \theta} = \begin{pmatrix} \mathbb{I}_d & 0 & 0 \\ 0 & \mathbb{I}_N & 0 \\ \mathbb{D}_{\mathbf{P}\theta} & \mathbb{D}_{\mathbf{C}\theta} & \mathbb{D}_{U\theta} \end{pmatrix} = \begin{pmatrix} \mathbb{I}_d & 0 & 0 \\ 0 & \mathbb{I}_N & 0 \\ 0 & \partial_{\mathbf{C}} \theta^\top & \partial_U \theta \end{pmatrix},$$

with  $\partial_{\mathbf{C}} \theta^\top = (-\theta^2) \boldsymbol{\gamma}_S = \boldsymbol{\gamma} - \frac{\boldsymbol{\mu}}{\theta} \beta$  and  $\partial_U \theta = (-\theta^2) \beta_S = \frac{\beta}{\theta}$  defined in (9c). This leads to

$$\mathbb{J}_\theta = D\mathbb{T}_{U \rightarrow \theta} \mathbb{J}_U D\mathbb{T}_{U \rightarrow \theta}^* = \begin{pmatrix} \mathbb{J}_{PP} & \mathbb{J}_{PC} & \mathbb{J}_{P\theta} \\ \mathbb{J}_{CP} & 0 & 0 \\ \mathbb{J}_{\theta P} & 0 & 0 \end{pmatrix},$$

where  $\mathbb{J}_{\theta P} = (\gamma - \frac{\mu}{\theta}\beta) \cdot \mathbb{J}_{CP} + \frac{\beta}{\theta}\mathbb{J}_{UP}$  and  $\mathbb{J}_{P\theta} = -\mathbb{J}_{\theta P}^*$ . Similarly, the transformed Onsager operator reads

$$\mathbb{K}_{\theta} = \text{DT}_{U \rightarrow \theta} \mathbb{K}_U \text{DT}_{U \rightarrow \theta}^* \quad \text{with} \quad \mathbb{K}_{\theta P} \square = \frac{\beta}{\theta} \mathbb{K}_{UP} \square,$$

$$= \begin{pmatrix} \mathbb{K}_{PP} & 0 & \mathbb{K}_{P\theta} \\ 0 & \mathbb{K}_{CC} & \mathbb{K}_{C\theta} \\ \mathbb{K}_{\theta P} & \mathbb{K}_{\theta C} & \mathbb{K}_{\theta\theta} \end{pmatrix} \quad \mathbb{K}_{\theta C} \square = (\gamma - \frac{\mu}{\theta}\beta) \cdot (\mathbb{K}_{CC} \square),$$

$$\mathbb{K}_{\theta\theta} \square = (\gamma - \frac{\mu}{\theta}\beta) \cdot (\mathbb{K}_{CC} [(\gamma - \frac{\mu}{\theta}\beta) \square]) + \frac{\beta}{\theta} \mathbb{K}_{UU} [\frac{\beta}{\theta} \square].$$

Due to the fact that the untransformed equations are driven by the same forces, i.e.,

$$\text{DT}_{U \rightarrow \theta}^* \text{D}\mathcal{E}_{\theta} = \begin{pmatrix} \nu \\ -\frac{1}{2} \mathbf{M} |\nu|^2 + \partial_C U_{\theta} + (\gamma - \frac{\mu}{\theta}\beta) \partial_{\theta} U_{\theta} \\ \frac{\beta}{\theta} \partial_{\theta} U_{\theta} \end{pmatrix} = \begin{pmatrix} \nu \\ -\frac{1}{2} \mathbf{M} |\nu|^2 \\ 1 \end{pmatrix} = \text{D}\mathcal{E}_U,$$

$$\text{DT}_{U \rightarrow \theta}^* \text{D}\mathcal{S}_{\theta} = \begin{pmatrix} 0 \\ \partial_C S_{\theta} + (\gamma - \frac{\mu}{\theta}\beta) \partial_{\theta} S_{\theta} \\ \frac{\beta}{\theta} \partial_{\theta} S_{\theta} \end{pmatrix} = \begin{pmatrix} 0 \\ -\frac{\mu}{\theta} \\ \frac{1}{\theta} \end{pmatrix} = \text{D}\mathcal{S}_U,$$

the evolution of  $P$  and  $C$  is again governed by equations (147a) and (147b). The temperature evolves according to

$$\partial_t \theta = \mathbb{J}_{\theta P} \nu + \mathbb{K}_{\theta C} \partial_C S_{\theta} + \mathbb{K}_{\theta\theta} \partial_{\theta} S_{\theta},$$

with the reversible part

$$\mathbb{J}_{\theta P} \nu = -\nu \cdot \nabla \theta - (\beta S + \gamma \cdot C) \nabla \cdot \nu,$$

where  $\beta = \theta/C_V$  and  $\beta S + \gamma \cdot C = \Lambda_V/C_V$ , and with the dissipative part

$$\mathbb{K}_{\theta C} \partial_C S_{\theta} + \mathbb{K}_{\theta\theta} \partial_{\theta} S_{\theta} = (\gamma - \frac{\mu}{\theta}\beta) \cdot \mathbb{K}_{CC} (-\frac{\mu}{\theta}) + \frac{\beta}{\theta} \mathbb{K}_{UU} \frac{1}{\theta},$$

where  $\mathbb{K}_{CC} (-\frac{\mu}{\theta}) = \nabla \cdot (\mathbb{M}_{CC} \nabla \frac{\mu}{\theta}) - \mathbb{H}_{CC} \frac{\mu}{\theta},$

$$\mathbb{K}_{UU} (\frac{1}{\theta}) = \nabla \cdot (k_{\text{heat}} \nabla \theta) + \sigma_{\text{visc}} : \nabla \nu.$$

Combining these terms ultimately results in

$$C_V (\partial_t \theta + \nu \cdot \nabla \theta) + \Lambda_V \nabla \cdot \nu = (\mu - \frac{\gamma C_V}{\theta}) \cdot \mathbb{K}_{CC} \frac{\mu}{\theta} + \mathbb{K}_{UU} \frac{1}{\theta}.$$

We now give an expression for the entropy of a multi-component ideal gas.

**Example 6.1 (Multi-component ideal gas)** We consider a mono-atomic three-dimensional multi-component ideal gas. From equation (15) we get the following Eulerian entropy

$$S(C, \theta) = k_B \sum_{i=1}^N C_i \left( \frac{5}{2} - \log(C_i \lambda_{i,\theta}^3) \right),$$

with  $\lambda_{i,\theta} = \sqrt{\frac{h^2}{2\pi m_i k_B \theta}}$  the de Broglie wave length from (16), for  $i \in \{1, \dots, N\}$ . This results in the following expressions for pressure and chemical potentials

$$\pi = k_B \theta \sum_{j=1}^N C_j \quad \mu_i = k_B \theta \log \left( \frac{C_i}{C_{\text{ref},i}} \right),$$

with the reference density  $\mathbf{C}_{\text{ref},i} = \lambda_{i,\theta}^{-3}$ . By exploiting the equation of state (13) we rewrite the quantities in terms of the internal energy  $U$

$$\theta = \frac{2}{3k_B} \frac{U}{\sum_j \mathbf{C}_j}, \quad \pi = \frac{2}{3}U, \quad \mu_i = \frac{U}{\sum_j \mathbf{C}_j} \log \left( \frac{\mathbf{C}_i}{\mathbf{C}_{\text{ref},i}} \right)^{\frac{2}{3}}.$$

The entropy as a function of  $U$  reads

$$S(\mathbf{C}, U) = k_B \sum_{i=1}^N \mathbf{C}_i \left( \frac{5}{2} - \log(\mathbf{C}_i \lambda_{i,U}^3) \right),$$

with  $\lambda_{i,U} = \sqrt{\frac{3h^2 \sum_j \mathbf{C}_j}{4\pi M_i U}}$ . Expressions in terms of concentration and entropy are derived analogously. \*

## 6.2 Reactive fluid flows with pressure and temperature

In some applications pressure and temperature are the thermodynamic observables rather than volume and entropy. However, due to the special role of the volume as a dependent variable  $\bar{V} = \det(\bar{\nabla}\chi)$ , this reformulation is somewhat tricky. This can be done, for example, using an extension mapping  $T_{\text{ext}} : \bar{\mathcal{Q}} \rightarrow \bar{\mathcal{Q}}_{\text{ext}}$  to a larger space, which contains additional thermodynamic variables explicitly, such as  $\bar{V}$ ,  $\bar{\pi}$  or  $\bar{\theta}$ . We show this construction exemplarily for the Hamiltonian system of the Euler equations, map the extended equation to Eulerian coordinates, and then transfer the methodology to the viscous reactive Darcy flow.

**Compressible Euler equations.** Based on the Hamiltonian system for the compressible Euler equation in Lagrangian coordinates from Sec. 4.1 with state variable  $\bar{\mathbf{q}} = (\chi, \mathbf{P}) \in \bar{\mathcal{Q}}$ , we define the extension map  $T_{\text{ext}} : \bar{\mathcal{Q}} \rightarrow \bar{\mathcal{Q}}_{\text{ext}}$

$$T_{\text{ext}}(\bar{\mathbf{q}}) = \bar{\mathbf{q}}_{\text{ext}} = \begin{pmatrix} \chi \\ \mathbf{P} \\ \bar{\pi} \\ \bar{\theta} \end{pmatrix} \quad (150)$$

with  $\bar{\theta} = \partial_{\bar{S}} \bar{U}(\bar{\mathbf{C}}, \bar{V}, \bar{S})$  and  $\bar{\pi} = -\partial_{\bar{V}} \bar{U}(\bar{\mathbf{C}}, \bar{V}, \bar{S})$  evaluated at  $\bar{V} = \det \nabla \chi$  and  $\bar{\mathbf{C}}$  considered as a parameter. The closure relation for the extension  $T_{\text{ext}}$  can be satisfied trivially using the original variables. The same strategy can be employed to introduce evolution laws of any other thermodynamic variable within the variational framework. In accordance with (60) it is

$$DT_{\text{ext}} = \begin{pmatrix} \mathbb{I}_d & 0 \\ 0 & \mathbb{I}_d \\ \mathbb{D}_{\chi} \bar{\pi} & 0 \\ \mathbb{D}_{\chi} \bar{\theta} & 0 \end{pmatrix}, \quad DT_{\text{ext}}^* = \begin{pmatrix} \mathbb{I}_d & 0 & \mathbb{D}_{\chi}^* \bar{\pi} & \mathbb{D}_{\chi}^* \bar{\theta} \\ 0 & \mathbb{I}_d & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad (151)$$

where  $(\mathbb{D}_{\chi} \bar{f}) \bar{v}_{\chi} = (\partial_{\bar{V}} \bar{f}) \text{Cof } \bar{\mathbf{F}} : \bar{\nabla} \bar{v}_{\chi}$  with its adjoint  $(\mathbb{D}_{\chi}^* \bar{f}) \bar{\xi} = -\bar{\nabla} \cdot ((\partial_{\bar{V}} \bar{f}) \bar{\xi} \text{Cof } \bar{\mathbf{F}})$  for  $\bar{f} \in \{\bar{\pi}, \bar{\theta}\}$ . To determine these expressions we note that  $T_{\text{ext}} = T_{\text{v}} \circ T_{\text{o}}$  is the composition of the extension map  $T_{\text{o}}(\bar{\mathbf{q}}) = (\bar{\mathbf{q}}, \bar{V}, \bar{S})^{\top}$  and the change of variables  $T_{\text{v}}((\bar{\mathbf{q}}, \bar{V}, \bar{S})^{\top}) = (\bar{\mathbf{q}}, \bar{\pi}, \bar{\theta})^{\top}$ . By

(60a) the derivatives of these maps are given by

$$DT_v = \begin{pmatrix} \mathbb{I}_d & 0 & 0 & 0 \\ 0 & \mathbb{I}_d & 0 & 0 \\ 0 & 0 & \partial_{\bar{V}}\bar{\pi} & \partial_{\bar{S}}\bar{\pi} \\ 0 & 0 & \partial_{\bar{V}}\bar{\theta} & \partial_{\bar{S}}\bar{\theta} \end{pmatrix}, \quad DT_o = \begin{pmatrix} \mathbb{I}_d & 0 \\ 0 & \mathbb{I}_d \\ \mathbb{D}_{\chi}\bar{V} & 0 \\ \mathbb{D}_{\chi}\bar{S} & 0 \end{pmatrix}, \quad (152)$$

where the partial derivatives in  $DT_v$  can be expressed by the capacities from (9a) and with  $\mathbb{D}_{\chi}\bar{V}\square = \text{Cof}\bar{\mathbf{F}} : \nabla\square$  and  $\mathbb{D}_{\chi}\bar{S}\square = \frac{\bar{\pi}}{\bar{\theta}}\text{Cof}\bar{\mathbf{F}} : \nabla\square$ . In this way, the expressions in (151) are determined as  $DT_{\text{ext}} = DT_v DT_o$  and  $DT_{\text{ext}}^* = DT_o^* DT_v^*$ . This transformation results in the extended Poisson operator

$$\begin{aligned} \bar{\mathbb{J}}_{\text{ext}}(\bar{\mathbf{q}}_{\text{ext}}) &= DT_{\text{ext}}(\bar{\mathbf{q}}) \bar{\mathbb{J}}_{\text{can}} DT_{\text{ext}}(\bar{\mathbf{q}})^* = \begin{pmatrix} \mathbb{I}_d & 0 \\ 0 & \mathbb{I}_d \\ \mathbb{D}_{\chi}\bar{\pi} & 0 \\ \mathbb{D}_{\chi}\bar{\theta} & 0 \end{pmatrix} \begin{pmatrix} 0 & \mathbb{I}_d \\ -\mathbb{I}_d & 0 \end{pmatrix} \begin{pmatrix} \mathbb{I}_d & 0 & \mathbb{D}_{\chi}^*\bar{\pi} & \mathbb{D}_{\chi}^*\bar{\theta} \\ 0 & \mathbb{I}_d & 0 & 0 \end{pmatrix} \\ &= \begin{pmatrix} 0 & +\mathbb{I}_d & 0 & 0 \\ -\mathbb{I}_d & 0 & -\mathbb{D}_{\chi}^*\bar{\pi} & -\mathbb{D}_{\chi}^*\bar{\theta} \\ 0 & \mathbb{D}_{\chi}\bar{\pi} & 0 & 0 \\ 0 & \mathbb{D}_{\chi}\bar{\theta} & 0 & 0 \end{pmatrix} \end{aligned} \quad (153)$$

and in the extended total energy  $\bar{\mathcal{E}}_{\text{ext}}(\bar{\mathbf{q}}_{\text{ext}})$  with density  $\bar{E}_{\text{ext}}(\bar{\mathbf{q}}_{\text{ext}}) = \frac{1}{2\bar{\rho}}|\bar{\mathbf{P}}|^2 + \bar{U}_{\text{ext}}(\bar{\mathbf{C}}, \bar{\pi}, \bar{\theta})$ . Here it is assumed that the extended internal energy  $\bar{U}_{\text{ext}}$  does not depend explicitly on the flow map but only on the variables  $(\bar{\mathbf{C}}, \bar{\pi}, \bar{\theta})$  with  $\bar{\mathbf{C}}$  as a parameter. Thus, the driving force for the extended system is

$$D\bar{\mathcal{E}}_{\text{ext}} = (0, \bar{\mathbf{P}}/\bar{\rho}, \partial_{\bar{\pi}}\bar{U}_{\text{ext}}, \partial_{\bar{\theta}}\bar{U}_{\text{ext}})^{\top}. \quad (154)$$

Then, the extended Hamiltonian evolution of the compressible Euler equation  $\dot{\bar{\mathbf{q}}}_{\text{ext}} = \bar{\mathbb{J}}_{\text{ext}} D\bar{\mathcal{E}}_{\text{ext}}$  reads

$$\partial_t \chi = \frac{\bar{\mathbf{P}}}{\bar{\rho}}, \quad (155a)$$

$$\partial_t \bar{\mathbf{P}} = -\mathbb{D}_{\chi}^*\bar{\pi}(\partial_{\bar{\pi}}\bar{U}_{\text{ext}}) - \mathbb{D}_{\chi}^*\bar{\theta}(\partial_{\bar{\theta}}\bar{U}_{\text{ext}}) = -\bar{\nabla} \cdot (\bar{\pi} \text{Cof}\bar{\mathbf{F}}), \quad (155b)$$

$$\partial_t \bar{\pi} = +(\mathbb{D}_{\chi}\bar{\pi})\frac{\bar{\mathbf{P}}}{\bar{\rho}} = (\partial_{\bar{V}}\bar{\pi})\text{Cof}\bar{\mathbf{F}} : \bar{\nabla}\bar{\mathbf{v}}, \quad (155c)$$

$$\partial_t \bar{\theta} = +(\mathbb{D}_{\chi}\bar{\theta})\frac{\bar{\mathbf{P}}}{\bar{\rho}} = (\partial_{\bar{V}}\bar{\theta})\text{Cof}\bar{\mathbf{F}} : \bar{\nabla}\bar{\mathbf{v}}, \quad (155d)$$

where we exploited that  $DT_{\text{ext}}^* \delta \bar{E}_{\text{ext}} = \delta \bar{E}$  in order to arrive at (155b). At this point we could use the definition of the capacities

$$\partial_{\bar{V}}\bar{\pi} = -\partial_{\bar{V}}^2 \bar{U} = \frac{-1}{V\bar{\kappa}_{\bar{S}}}, \quad \partial_{\bar{V}}\bar{\theta} = \partial_{\bar{V}}\partial_{\bar{S}}\bar{U} = \frac{-\bar{\Lambda}_{\bar{V}}}{\bar{C}_{\bar{V}}},$$

from (10) to replace the partial derivatives in (155).

**Lagrangian-Eulerian reduction of (155).** Next, the Lagrangian version (155) of the compressible Euler equations transformed to Eulerian coordinates. This transformation is a reduction since we abandon the flow map  $\chi$  as a variable. Additionally, we introduce the locally conserved Eulerian concentration  $\mathbf{C}$  as a further variable, as this will be needed later. For this, we consider the transformation to Eulerian coordinates

$$T_{\text{LE}}(\bar{\mathbf{q}}_{\text{ext}}) = \mathbf{q}_{\pi\theta} = \begin{pmatrix} \mathbf{P} : \Omega \rightarrow \mathbb{R}^d \\ \mathbf{C} : \Omega \rightarrow \mathbb{R}^N \\ \pi : \Omega \rightarrow \mathbb{R} \\ \theta : \Omega \rightarrow \mathbb{R} \end{pmatrix} \in \mathcal{Q}_{\pi\theta},$$

where the intensive pressure and temperature are defined by  $\pi \circ \chi = \bar{\pi}$  and  $\theta \circ \chi = \bar{\theta}$ . Using Lemma 3.13 we get

$$\text{DT}_{\text{LE}}(\bar{\mathbf{q}}_{\text{ext}}) = \begin{pmatrix} -\nabla \cdot \left( \frac{\bar{\mathbf{P}}}{\bar{V}} \otimes \square \right) & \frac{\square}{\bar{V}} & 0 & 0 \\ -\nabla \cdot \left( \frac{\bar{\mathbf{C}}}{\bar{V}} \otimes \square \right) & 0 & 0 & 0 \\ -\square \cdot \nabla \pi & 0 & \square & 0 \\ -\square \cdot \nabla \theta & 0 & 0 & \square \end{pmatrix} \quad (156a)$$

and correspondingly have its adjoint

$$\text{DT}_{\text{LE}}^* = \begin{pmatrix} (\nabla \square)^\top \bar{\mathbf{P}} & (\nabla \square)^\top \bar{\mathbf{C}} & -\bar{V} \square \nabla \pi & -\bar{V} \square \nabla \theta \\ \square & 0 & 0 & 0 \\ 0 & 0 & \bar{V} \square & 0 \\ 0 & 0 & 0 & \bar{V} \square \end{pmatrix}. \quad (156b)$$

The transformed Poisson operator  $\mathbb{J}_{\pi\theta} = \text{DT}_{\text{LE}} \bar{\mathbb{J}}_{\text{ext}} \text{DT}_{\text{LE}}^*$  computed from (153) then has the form

$$\mathbb{J}_{\pi\theta} = \begin{pmatrix} \mathbb{J}_{\mathbf{P}\mathbf{P}}^{\pi\theta} & \mathbb{J}_{\mathbf{P}\mathbf{C}}^{\pi\theta} & \mathbb{J}_{\mathbf{P}\pi}^{\pi\theta} & \mathbb{J}_{\mathbf{P}\theta}^{\pi\theta} \\ \mathbb{J}_{\mathbf{C}\mathbf{P}}^{\pi\theta} & 0 & 0 & 0 \\ \mathbb{J}_{\pi\mathbf{P}}^{\pi\theta} & 0 & 0 & 0 \\ \mathbb{J}_{\theta\mathbf{P}}^{\pi\theta} & 0 & 0 & 0 \end{pmatrix} \quad (157a)$$

with the individual components

$$\mathbb{J}_{\mathbf{P}\mathbf{P}}^{\pi\theta} \xi_{\mathbf{P}} = -\nabla \cdot (\mathbf{P} \otimes \xi_{\mathbf{P}}) - (\nabla \xi_{\mathbf{P}})^\top \mathbf{P}, \quad (157b)$$

$$\mathbb{J}_{\mathbf{P}\pi}^{\pi\theta} \xi_{\pi} = -\nabla \cdot (\kappa_S^{-1} \xi_{\pi}) + \xi_{\pi} \nabla \pi, \quad (157c)$$

$$\mathbb{J}_{\pi\mathbf{P}}^{\pi\theta} \xi_{\mathbf{P}} = -\kappa_S^{-1} \nabla \cdot \xi_{\mathbf{P}} - \xi_{\mathbf{P}} \cdot \nabla \pi, \quad (157d)$$

$$\mathbb{J}_{\mathbf{P}\mathbf{C}}^{\pi\theta} \xi_{\mathbf{C}} = -(\nabla \xi_{\mathbf{C}})^\top \mathbf{C}, \quad (157e)$$

$$\mathbb{J}_{\mathbf{C}\mathbf{P}}^{\pi\theta} \xi_{\mathbf{P}} = -\nabla \cdot (\mathbf{C} \otimes \xi_{\mathbf{P}}), \quad (157f)$$

$$\mathbb{J}_{\mathbf{P}\theta}^{\pi\theta} \xi_{\theta} = -\nabla \cdot \left( \frac{\Lambda_V}{C_V} \xi_{\theta} \right) + \xi_{\theta} \nabla \theta, \quad (157g)$$

$$\mathbb{J}_{\theta\mathbf{P}}^{\pi\theta} \xi_{\mathbf{P}} = -\frac{\Lambda_V}{C_V} \nabla \cdot \xi_{\mathbf{P}} - \xi_{\mathbf{P}} \cdot \nabla \theta, \quad (157h)$$

for  $\xi_{\mathbf{P}} : \Omega \rightarrow \mathbb{R}^d$ ,  $\xi_{\mathbf{C}} : \Omega \rightarrow \mathbb{R}^N$ ,  $\xi_{\theta}, \xi_{\pi} : \Omega \rightarrow \mathbb{R}$ .

The Eulerian total energy  $\mathcal{E}_{\pi\theta}(\mathbf{q}_{\pi\theta})$  and entropy  $\mathcal{S}_{\pi\theta}(\mathbf{q}_{\pi\theta})$  of the system are defined via the densities  $E_{\pi\theta}(\mathbf{q}_{\pi\theta}) = \frac{1}{2\varrho} |\bar{\mathbf{P}}|^2 + U_{\pi\theta}(\mathbf{C}, \pi, \theta)$  and  $S_{\pi\theta}(\mathbf{C}, \pi, \theta)$  with  $\varrho = \mathbf{C} \cdot \mathbf{M}$ . In order to comply with closure conditions (50) we here make the choice

$$U_{\pi\theta}(\mathbf{C}, \pi, \theta) := U_{\theta}(\mathbf{C}, \theta), \quad S_{\pi\theta}(\mathbf{C}, \pi, \theta) := S_{\theta}(\mathbf{C}, \theta), \quad (158)$$

based on the identities  $U_{\theta}(\mathbf{C}, \theta(\mathbf{C}, S)) := U(\mathbf{C}, S)$  and  $S_{\theta}(\mathbf{C}, \theta(\mathbf{C}, S)) := S$  for  $\theta(\mathbf{C}, S) = \partial_S U(\mathbf{C}, S)$ . Calculating the partial derivatives of  $U_{\pi\theta}$  and  $S_{\pi\theta}$  via the chain rule and using the capacities from (9b) results in

$$\partial_{\mathbf{C}} U_{\pi\theta} = \boldsymbol{\mu} - \frac{\theta}{\beta} \boldsymbol{\gamma} \equiv \boldsymbol{\xi}_{\mathbf{C}}, \quad \partial_{\theta} U_{\pi\theta} = \frac{\theta}{\beta} \equiv \xi_{\theta}, \quad (159a)$$

$$\partial_{\mathbf{C}} S_{\pi\theta} = -\frac{1}{\beta} \boldsymbol{\gamma} \equiv \boldsymbol{\xi}_{\mathbf{C}}, \quad \partial_{\theta} S_{\pi\theta} = \frac{1}{\beta} \equiv \xi_{\theta}, \quad (159b)$$

and  $\partial_{\pi} U_{\pi\theta} = \partial_{\pi} S_{\pi\theta} = 0$ . Thus, equivalent to (149)

$$\text{D}\mathcal{E}_{\pi\theta} = (\boldsymbol{\nu}, -\frac{1}{2} |\boldsymbol{\nu}|^2 \mathbf{M} + \boldsymbol{\xi}_{\mathbf{C}}, 0, \xi_{\theta})^\top. \quad (160)$$

With the thermodynamic relation  $\mathbf{C} \cdot \boldsymbol{\mu} + \theta S_{\pi\theta} = U_{\pi\theta} + \pi$ , the driving forces, and the capacities (9b) we observe

$$\begin{aligned} \partial_t \mathbf{P} &= \mathbb{J}_{\mathbf{P}\mathbf{P}}^{\pi\theta} \boldsymbol{\nu} + \mathbb{J}_{\mathbf{P}\mathbf{C}}^{\pi\theta} \left(-\frac{1}{2} |\boldsymbol{\nu}|^2 \mathbf{M} + \boldsymbol{\xi}_C\right) + \mathbb{J}_{\mathbf{P}\theta}^{\pi\theta} \xi_\theta \\ &= -\nabla \cdot (\mathbf{P} \otimes \boldsymbol{\nu}) - (\nabla \boldsymbol{\xi}_C)^\top \mathbf{C} - \nabla (\mathbf{C} \cdot \boldsymbol{\gamma} + S_{\pi\theta} \beta) \xi_\theta = -\nabla \cdot (\mathbf{P} \otimes \boldsymbol{\nu}) - \nabla \pi. \end{aligned}$$

For  $\mathbb{J}_{\pi\theta}$  from (157) and the driving forces from (160) the Euler equations  $\dot{\mathbf{q}} = \mathbb{J}_{\pi\theta} \text{D}\mathcal{E}_{\pi\theta}$  thus read

$$\partial_t \mathbf{P} + \nabla \cdot (\mathbf{P} \otimes \boldsymbol{\nu}) = -\nabla \pi, \quad (161a)$$

$$\partial_t \mathbf{C} + \nabla \cdot (\mathbf{C} \otimes \boldsymbol{\nu}) = 0, \quad (161b)$$

$$\partial_t \pi + \boldsymbol{\nu} \cdot \nabla \pi + \kappa_S^{-1} \nabla \cdot \boldsymbol{\nu} = 0, \quad (161c)$$

$$\partial_t \theta + \boldsymbol{\nu} \cdot \nabla \theta + \frac{\Lambda_V}{C_V} \nabla \cdot \boldsymbol{\nu} = 0, \quad (161d)$$

where similar to (92) the derivative of the kinetic energy w.r.t. the concentration is cancelled in (161a).

**Remark 6.2 (Role of pressure)** The role of the pressure in system (161) is ambiguous:

- i) With the relation  $\mathbf{C} \cdot \boldsymbol{\mu} + \theta S_{\pi\theta} - \pi = U_{\pi\theta}$  one can determine the pressure employing the equations of state  $U_{\pi\theta}(\mathbf{C}, \theta)$ ,  $S_{\pi\theta}(\mathbf{C}, \theta)$  for the state variables  $\mathbf{C}, \theta$ . This allows one to drop the evolution equation (161c) for the pressure.
- ii) Alternatively, one could also drop the evolution equation (161d) for the temperature and evolve the pressure independently from the equation of state via (161c). The concentration is always needed for the closure relation in order to relate momentum and velocity through  $\mathbf{P} = (\mathbf{M} \cdot \mathbf{C})\boldsymbol{\nu}$ . \*

**Darcy flow.** In the following we indicate the main steps in the construction of the Onsager operator for Darcy flows either using a GENERIC or a gradient structure. We start this consideration with the Onsager operator using the total energy as variable, i.e.,

$$\bar{\mathbb{K}}_E^D = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \bar{\mathbb{K}}_{\mathbf{P}\mathbf{P}}^D & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

which satisfies the NIC  $\bar{\mathbb{K}}_E^D \text{D}\bar{\mathcal{E}} = 0$  by construction. The Darcy Onsager operator is purely multiplicative, i.e.,  $\bar{\mathbb{K}}_{\mathbf{P}\mathbf{P}}^D = \bar{\theta} \bar{V} \bar{K}^D$  with a symmetric, positively definite, state-dependent matrix  $\bar{K}^D : \bar{\mathcal{Q}} \rightarrow \mathbb{R}^{d \times d}$ . Such a dissipative contribution is only material frame indifferent for multiphase flows, e.g., mixtures. Nevertheless, this example is valuable to show how GENERIC can be extended systematically to reactive multiphase flows. The transformation map for the change of variables to internal energy  $\bar{U} = \bar{E} - \frac{1}{2\bar{\rho}} |\bar{\mathbf{P}}|^2$  reads

$$\text{DT}_v(\bar{\mathbf{q}}) = \mathbb{L}(\bar{\mathbf{q}}) = \begin{pmatrix} \mathbb{I}_d & 0 & 0 \\ 0 & \mathbb{I}_d & 0 \\ \frac{\partial \bar{U}}{\partial \boldsymbol{\chi}} & \frac{\partial \bar{U}}{\partial \bar{\mathbf{P}}} & \frac{\partial \bar{U}}{\partial \bar{E}} \end{pmatrix} = \begin{pmatrix} \mathbb{I}_d & 0 & 0 \\ 0 & \mathbb{I}_d & 0 \\ 0 & -\bar{\boldsymbol{\nu}}^\top & 1 \end{pmatrix}$$

for states  $\bar{\mathbf{q}} = (\boldsymbol{\chi}, \bar{\mathbf{P}}, \bar{E})^\top \in \bar{\mathcal{Q}}$ , so that we have the transformed Onsager operator  $\bar{\mathbb{K}}_{\bar{U}}^D = \bar{\mathbb{K}}_{\bar{U}}^D(\bar{\mathbf{q}}_{\bar{U}})$ ,

$$\bar{\mathbb{K}}_{\bar{U}}^D = \mathbb{L} \bar{\mathbb{K}}_E^D \mathbb{L}^* = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \bar{\mathbb{K}}_{\mathbf{P}\mathbf{P}}^D & -\bar{\mathbb{K}}_{\mathbf{P}\mathbf{P}}^D \bar{\boldsymbol{\nu}} \\ 0 & -\bar{\boldsymbol{\nu}}^\top \bar{\mathbb{K}}_{\mathbf{P}\mathbf{P}}^D & \bar{\boldsymbol{\nu}}^\top \bar{\mathbb{K}}_{\mathbf{P}\mathbf{P}}^D \bar{\boldsymbol{\nu}} \end{pmatrix}, \quad (162)$$



now dependent on states  $\bar{\mathbf{q}}_{\bar{U}} = (\boldsymbol{\chi}, \bar{\mathbf{P}}, \bar{U})^\top \in \bar{\mathcal{Q}}_{\bar{U}}$  and again with  $\bar{\mathbb{K}}_{\bar{\mathbf{P}}\bar{\mathbf{P}}}^{\mathbb{D}} = \bar{\theta}\bar{V}\bar{K}^{\mathbb{D}}$ . Note that the form and the properties of  $\bar{\mathbb{K}}_{\bar{\mathbf{P}}\bar{\mathbf{P}}}^{\mathbb{D}}$  are very similar to the operator (47b) from the finite-dimensional Example 3.6. Using the same reversible contribution as in Section 4.2, we get the same Lagrangian formulation as in (105) but with  $\bar{\mathbb{K}}_{\bar{U}}^{\mathbb{S}}$  replaced by  $\bar{\mathbb{K}}_{\bar{U}}^{\mathbb{D}}$ . Using  $\mathbb{T}_{\text{LE}}$  from (142) for the Lagrangian-Eulerian transformation of a multi-component system and with  $\bar{\mathbb{K}}_{\bar{\mathbf{P}}\bar{\mathbf{P}}}^{\mathbb{D}} = \bar{V}^{-1}\bar{\mathbb{K}}_{\bar{\mathbf{P}}\bar{\mathbf{P}}}^{\mathbb{D}}$ , we obtain the Eulerian multi-component Darcy flow

$$\dot{\bar{\mathbf{P}}} + \nabla \cdot (\bar{\mathbf{P}} \otimes \boldsymbol{\nu}) = -\nabla \pi - K^{\mathbb{D}} \boldsymbol{\nu}, \quad (163a)$$

$$\dot{\bar{\mathbf{C}}} + \nabla \cdot (\bar{\mathbf{C}} \otimes \boldsymbol{\nu}) = 0, \quad (163b)$$

$$\dot{\bar{U}} + \nabla \cdot (U \boldsymbol{\nu}) = -\pi \nabla \cdot \boldsymbol{\nu} + \boldsymbol{\nu}^\top K^{\mathbb{D}} \boldsymbol{\nu}. \quad (163c)$$

with  $K^{\mathbb{D}}(\mathbf{q}_U) \equiv \bar{K}^{\mathbb{D}}(\bar{\mathbf{q}}_{\bar{U}}) \in \mathbb{R}^{d \times d}$ . Taking the overdamped limit of this equation we arrive at

$$K^{\mathbb{D}} \boldsymbol{\nu} = -\nabla \pi, \quad (164a)$$

$$\dot{\bar{\mathbf{C}}} + \nabla \cdot (\bar{\mathbf{C}} \otimes \boldsymbol{\nu}) = 0, \quad (164b)$$

$$\dot{\bar{U}} + \nabla \cdot (U \boldsymbol{\nu}) = -\nabla \cdot (\pi \boldsymbol{\nu}), \quad (164c)$$

where we multiplied the momentum balance by the velocity and used the resulting expression to replace  $\bar{\boldsymbol{\nu}}^\top \bar{K}^{\mathbb{D}} \bar{\boldsymbol{\nu}}$  in the evolution equation for the internal energy density. In this overdamped evolution, both  $\bar{\mathbf{C}}$  and the total energy  $\mathcal{E}(\mathbf{q}_U) = \int_{\Omega} U \, dx$  are conserved.

**Reactive multi-component Darcy flow.** We now augment the Lagrangian Darcy operator  $\bar{\mathbb{K}}_{\bar{U}}^{\mathbb{D}}$  from (162) by chemical reactions of an  $N$ -component system with concentrations  $\bar{\mathbf{C}} : \bar{\Omega} \rightarrow \mathbb{R}^N$ . With  $\bar{\mathbb{H}}_{\bar{\mathbf{C}}\bar{\mathbf{C}}}$  for chemical reactions from (120), the Lagrangian Onsager operator for the reactive  $N$ -component Darcy flow is given by

$$\bar{\mathbb{K}}^{\text{rD}}(\bar{\mathbf{q}}_{\bar{U}}) := \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \bar{\mathbb{K}}_{\bar{\mathbf{P}}\bar{\mathbf{P}}}^{\mathbb{D}} & 0 & -\bar{\mathbb{K}}_{\bar{\mathbf{P}}\bar{\mathbf{P}}}^{\mathbb{D}} \bar{\boldsymbol{\nu}} \\ 0 & 0 & \bar{V} \bar{\mathbb{H}}_{\bar{\mathbf{C}}\bar{\mathbf{C}}} & 0 \\ 0 & -\bar{\boldsymbol{\nu}}^\top \bar{\mathbb{K}}_{\bar{\mathbf{P}}\bar{\mathbf{P}}}^{\mathbb{D}} & 0 & \bar{\boldsymbol{\nu}}^\top \bar{\mathbb{K}}_{\bar{\mathbf{P}}\bar{\mathbf{P}}}^{\mathbb{D}} \bar{\boldsymbol{\nu}} \end{pmatrix} \quad (165)$$

for a state  $\bar{\mathbf{q}}_{\bar{U}} = (\boldsymbol{\chi}, \bar{\mathbf{P}}, \bar{\mathbf{C}}, \bar{U})^\top \in \bar{\mathcal{Q}}_{\bar{U}}$ . Similar to the compressible Euler case we are interested in a formulation of the system in terms of pressure and temperature as additional variables. Hence, alike (150), we introduce the extension map  $\mathbb{T}_{\text{ext}} : \bar{\mathcal{Q}}_{\bar{U}} \rightarrow \bar{\mathcal{Q}}_{\text{ext}}$ ,

$$\mathbb{T}_{\text{ext}}(\bar{\mathbf{q}}_{\bar{U}}) = \bar{\mathbf{q}}_{\text{ext}} = \begin{pmatrix} \boldsymbol{\chi} : \bar{\Omega} \rightarrow \mathbb{R}^d \\ \bar{\mathbf{P}} : \bar{\Omega} \rightarrow \mathbb{R}^d \\ \bar{\mathbf{C}} : \bar{\Omega} \rightarrow \mathbb{R}^N \\ \bar{\pi} : \bar{\Omega} \rightarrow \mathbb{R} \\ \bar{\theta} : \bar{\Omega} \rightarrow \mathbb{R} \end{pmatrix} \in \bar{\mathcal{Q}}_{\text{ext}},$$

where  $\bar{\theta} = (\partial_{\bar{U}} \bar{S})^{-1}$  and  $\bar{\pi} = \bar{\theta} \partial_{\bar{V}} \bar{S}$ , and with

$$\text{D}\mathbb{T}_{\text{ext}}(\bar{\mathbf{q}}_{\bar{U}}) = \begin{pmatrix} \mathbb{I}_d & 0 & 0 & 0 \\ 0 & \mathbb{I}_d & 0 & 0 \\ 0 & 0 & \mathbb{I}_N & 0 \\ \mathbb{D}_{\boldsymbol{\chi}} \bar{\pi} & 0 & \partial_{\bar{\mathbf{C}}} \bar{\pi}^\top & \partial_{\bar{U}} \bar{\pi} \\ \mathbb{D}_{\boldsymbol{\chi}} \bar{\theta} & 0 & \partial_{\bar{\mathbf{C}}} \bar{\theta}^\top & \partial_{\bar{U}} \bar{\theta} \end{pmatrix}, \quad (166)$$

where the partial derivatives and the adjoint  $DT_{\text{ext}}(\bar{\mathbf{q}}_{\bar{U}})^*$  are an adaption of (151) and (152). With the abbreviation  $\bar{w} := (\boldsymbol{\chi}, \bar{\mathbf{P}}, \bar{\mathbf{C}})$  this means in particular that the extension map  $T_{\text{ext}} = T_v \circ T_o$  is the composition of the extension map  $T_o((\bar{w}, \bar{V}, \bar{U})^\top) = (\bar{w}, \bar{V}, \bar{U})^\top$  and the change of variables  $T_v((\bar{w}, \bar{V}, \bar{U})^\top) = (\bar{w}, \bar{\pi}, \bar{\theta})^\top$ , with derivatives

$$DT_v = \begin{pmatrix} \mathbb{I}_d & 0 & 0 & 0 & 0 \\ 0 & \mathbb{I}_d & 0 & 0 & 0 \\ 0 & 0 & \mathbb{I}_N & 0 & 0 \\ 0 & 0 & \partial_{\bar{\mathbf{C}}}\bar{\pi}^\top & \partial_{\bar{V}}\bar{\pi} & \partial_{\bar{U}}\bar{\pi} \\ 0 & 0 & \partial_{\bar{\mathbf{C}}}\bar{\theta}^\top & \partial_{\bar{V}}\bar{\theta} & \partial_{\bar{U}}\bar{\theta} \end{pmatrix}, \quad DT_o = \begin{pmatrix} \mathbb{I}_d & 0 & 0 & 0 \\ 0 & \mathbb{I}_d & 0 & 0 \\ 0 & 0 & \mathbb{I}_N & 0 \\ \mathbb{D}_{\boldsymbol{\chi}}\bar{V} & 0 & \partial_{\bar{\mathbf{C}}}\bar{V}^\top & \partial_{\bar{U}}\bar{V} \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

with  $\mathbb{D}_{\boldsymbol{\chi}}\bar{V}\square = \text{Cof}\bar{\mathbf{F}} : \nabla\square$ . Thus, the partial derivatives in (166) are determined as  $DT_{\text{ext}}(\bar{\mathbf{q}}) = DT_v(\bar{\mathbf{q}})DT_o(\bar{\mathbf{q}})$  and  $DT_{\text{ext}}(\bar{\mathbf{q}})^* = DT_o(\bar{\mathbf{q}})^*DT_v(\bar{\mathbf{q}})^*$ . Transforming  $\bar{\mathbb{K}}^{\text{rD}}$  by  $DT_{\text{ext}}$  according to (50c) leads to

$$\begin{aligned} \bar{\mathbb{K}}_{\text{ext}}^{\text{rD}}(\bar{\mathbf{q}}_{\text{ext}}) &= DT_{\text{ext}}(\bar{\mathbf{q}})\bar{\mathbb{K}}^{\text{rD}}(\bar{\mathbf{q}})DT_{\text{ext}}(\bar{\mathbf{q}})^* \\ &= \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & \bar{\mathbb{K}}_{\bar{\mathbf{P}}\bar{\mathbf{P}}}^{\text{D}} & 0 & -\bar{\mathbb{K}}_{\bar{\mathbf{P}}\bar{\mathbf{P}}}\bar{\boldsymbol{\nu}}(\partial_{\bar{U}}\bar{\pi}) & -\bar{\mathbb{K}}_{\bar{\mathbf{P}}\bar{\mathbf{P}}}\bar{\boldsymbol{\nu}}(\partial_{\bar{U}}\bar{\theta}) \\ 0 & 0 & \bar{V}\bar{\mathbb{H}}_{\bar{\mathbf{C}}\bar{\mathbf{C}}} & \bar{V}\bar{\mathbb{H}}_{\bar{\mathbf{C}}\bar{\mathbf{C}}}(\partial_{\bar{\mathbf{C}}}\bar{\pi}) & \bar{V}\bar{\mathbb{H}}_{\bar{\mathbf{C}}\bar{\mathbf{C}}}(\partial_{\bar{\mathbf{C}}}\bar{\theta}) \\ 0 & -\partial_{\bar{U}}\bar{\pi}\bar{\boldsymbol{\nu}}^\top\bar{\mathbb{K}}_{\bar{\mathbf{P}}\bar{\mathbf{P}}}^{\text{D}} & (\partial_{\bar{\mathbf{C}}}\bar{\pi})^\top\bar{V}\bar{\mathbb{H}}_{\bar{\mathbf{C}}\bar{\mathbf{C}}} & \bar{\mathbb{K}}_{\bar{\pi}\bar{\pi}}^{\text{ext}} & \bar{\mathbb{K}}_{\bar{\pi}\bar{\theta}}^{\text{ext}} \\ 0 & -\partial_{\bar{U}}\bar{\theta}\bar{\boldsymbol{\nu}}^\top\bar{\mathbb{K}}_{\bar{\mathbf{P}}\bar{\mathbf{P}}}^{\text{D}} & (\partial_{\bar{\mathbf{C}}}\bar{\theta})^\top\bar{V}\bar{\mathbb{H}}_{\bar{\mathbf{C}}\bar{\mathbf{C}}} & \bar{\mathbb{K}}_{\bar{\theta}\bar{\pi}}^{\text{ext}} & \bar{\mathbb{K}}_{\bar{\theta}\bar{\theta}}^{\text{ext}} \end{pmatrix} \end{aligned}$$

with the bottom right components

$$\begin{aligned} \bar{\mathbb{K}}_{\bar{\pi}\bar{\pi}}^{\text{ext}} &= (\partial_{\bar{\mathbf{C}}}\bar{\pi})^\top\bar{V}\bar{\mathbb{H}}_{\bar{\mathbf{C}}\bar{\mathbf{C}}}(\partial_{\bar{\mathbf{C}}}\bar{\pi}) + (\partial_{\bar{U}}\bar{\pi})\bar{\boldsymbol{\nu}}^\top\bar{\mathbb{K}}_{\bar{\mathbf{P}}\bar{\mathbf{P}}}^{\text{D}}\bar{\boldsymbol{\nu}}(\partial_{\bar{U}}\bar{\pi}), \\ \bar{\mathbb{K}}_{\bar{\pi}\bar{\theta}}^{\text{ext}} &= (\partial_{\bar{\mathbf{C}}}\bar{\pi})^\top\bar{V}\bar{\mathbb{H}}_{\bar{\mathbf{C}}\bar{\mathbf{C}}}(\partial_{\bar{\mathbf{C}}}\bar{\theta}) + (\partial_{\bar{U}}\bar{\pi})\bar{\boldsymbol{\nu}}^\top\bar{\mathbb{K}}_{\bar{\mathbf{P}}\bar{\mathbf{P}}}^{\text{D}}\bar{\boldsymbol{\nu}}(\partial_{\bar{U}}\bar{\theta}), \\ \bar{\mathbb{K}}_{\bar{\theta}\bar{\pi}}^{\text{ext}} &= (\partial_{\bar{\mathbf{C}}}\bar{\theta})^\top\bar{V}\bar{\mathbb{H}}_{\bar{\mathbf{C}}\bar{\mathbf{C}}}(\partial_{\bar{\mathbf{C}}}\bar{\pi}) + (\partial_{\bar{U}}\bar{\theta})\bar{\boldsymbol{\nu}}^\top\bar{\mathbb{K}}_{\bar{\mathbf{P}}\bar{\mathbf{P}}}^{\text{D}}\bar{\boldsymbol{\nu}}(\partial_{\bar{U}}\bar{\pi}), \\ \bar{\mathbb{K}}_{\bar{\theta}\bar{\theta}}^{\text{ext}} &= (\partial_{\bar{\mathbf{C}}}\bar{\theta})^\top\bar{V}\bar{\mathbb{H}}_{\bar{\mathbf{C}}\bar{\mathbf{C}}}(\partial_{\bar{\mathbf{C}}}\bar{\theta}) + (\partial_{\bar{U}}\bar{\theta})\bar{\boldsymbol{\nu}}^\top\bar{\mathbb{K}}_{\bar{\mathbf{P}}\bar{\mathbf{P}}}^{\text{D}}\bar{\boldsymbol{\nu}}(\partial_{\bar{U}}\bar{\theta}), \end{aligned}$$

and with  $\bar{\mathbb{K}}_{\bar{\mathbf{P}}\bar{\mathbf{P}}}^{\text{D}}\square := \bar{\theta}\bar{V}\bar{K}^{\text{D}}\square$  with  $\bar{K}^{\text{D}} : \bar{\mathcal{Q}}_{\text{ext}} \rightarrow \mathbb{R}^{d \times d}$  defined by  $\bar{K}^{\text{D}}(\bar{\mathbf{q}}_{\text{ext}}) := \bar{K}^{\text{D}}(\bar{\mathbf{q}})$  for  $\bar{K}^{\text{D}} : \bar{\mathcal{Q}}_{\bar{U}} \rightarrow \mathbb{R}^{d \times d}$  symmetric and uniformly positively semidefinite for all  $\bar{\mathbf{q}} \in \bar{\mathcal{Q}}$  as in (162). In this way, closure condition (50c) is satisfied for the extended Darcy operator. Similarly, the operator  $\bar{\mathbb{H}}_{\bar{\mathbf{C}}\bar{\mathbf{C}}}$  for chemical reactions from (120) is defined for the extended states by setting  $\bar{\mathbb{H}}(\bar{\mathbf{q}}_{\text{ext}}) := \bar{\mathbb{H}}(\bar{\mathbf{q}})$ , so that closure condition (50c) holds true.

The total entropy  $\bar{\mathcal{S}}_{\text{ext}}(\bar{\mathbf{q}}_{\text{ext}})$  of the extended system is obtained from an extended density that we define via the identity

$$\bar{\mathcal{S}}_{\text{ext}}(\bar{\mathbf{C}}, \bar{\pi}(\bar{\mathbf{C}}, \bar{V}, \bar{U}), \bar{\theta}(\bar{\mathbf{C}}, \bar{V}, \bar{U})) = \bar{S}(\bar{\mathbf{C}}, \bar{V}, \bar{U}) \quad (167)$$

in order to satisfy closure condition (50a). The extended driving force is thus given by

$$D\bar{\mathcal{S}}_{\text{ext}} = (0, 0, \partial_{\bar{\mathbf{C}}}\bar{\mathcal{S}}_{\text{ext}}, \partial_{\bar{\pi}}\bar{\mathcal{S}}_{\text{ext}}, \partial_{\bar{\theta}}\bar{\mathcal{S}}_{\text{ext}})^\top,$$

where the components  $\partial_{\bar{\pi}}\bar{\mathcal{S}}_{\text{ext}}, \partial_{\bar{\theta}}\bar{\mathcal{S}}_{\text{ext}}$  are obtained by solving  $DT_v(\bar{\mathbf{q}}_{\text{ext}})^*\delta\bar{\mathcal{S}}_{\text{ext}}(\bar{\mathbf{q}}_{\text{ext}}) = \delta\bar{S}(\bar{\mathbf{q}}_{\bar{U}})$ .

Combining the Onsager system  $(\bar{\mathcal{Q}}_{\text{ext}}, \bar{\mathcal{S}}_{\text{ext}}, \bar{\mathbb{K}}_{\text{ext}}^{\text{rD}})$  for the reactive Darcy flow with the Hamiltonian system  $(\bar{\mathcal{Q}}_{\text{ext}}, \bar{\mathcal{E}}_{\text{ext}}, \bar{\mathbb{J}}_{\text{ext}})$  for the extended compressible Euler system (155) we arrive at a GENERIC

system  $(\bar{\mathcal{Q}}_{\text{ext}}, \bar{\mathcal{E}}_{\text{ext}}, \bar{\mathcal{S}}_{\text{ext}}, \bar{\mathbb{J}}_{\text{ext}}, \bar{\mathbb{K}}_{\text{ext}}^{\text{rD}})$  for a reactive flow of Darcy-type with thermal effects in Lagrangian coordinates.

$$\partial_t \chi = \frac{\bar{P}}{\bar{\varrho}}, \quad (168a)$$

$$\begin{aligned} \partial_t \bar{\mathbf{P}} &= -\bar{\nabla} \cdot (\bar{\pi} \text{Cof}(\bar{\mathbf{F}})) - \bar{\mathbb{K}}_{\bar{\mathbf{P}}\bar{\mathbf{P}}}^{\text{D}} \bar{\nu} \left( (\partial_{\bar{U}} \bar{\pi}) \partial_{\bar{\pi}} \bar{\mathcal{S}}_{\text{ext}} + (\partial_{\bar{U}} \bar{\theta}) \partial_{\bar{\theta}} \bar{\mathcal{S}}_{\text{ext}} \right) \\ &= -\bar{\nabla} \cdot (\bar{\pi} \text{Cof}(\bar{\mathbf{F}})) - \bar{V} \bar{K}^{\text{D}} \bar{\nu}, \end{aligned} \quad (168b)$$

$$\partial_t \bar{\mathbf{C}} = -\bar{\mathbb{H}}_{\bar{\mathbf{C}}\bar{\mathbf{C}}} \frac{\bar{\mu}}{\bar{\theta}}, \quad (168c)$$

$$\partial_t \bar{\pi} = \frac{1}{\bar{V} \bar{\kappa}_{\bar{S}}} \text{Cof}(\bar{\mathbf{F}}) : \bar{\nabla} \bar{\nu} + (\partial_{\bar{U}} \bar{\pi}) \bar{V} \bar{\nu}^{\text{T}} \bar{K}^{\text{D}} \bar{\nu} - (\partial_{\bar{C}} \bar{\pi})^{\text{T}} \bar{V} \bar{\mathbb{H}}_{\bar{\mathbf{C}}\bar{\mathbf{C}}} \frac{\bar{\mu}}{\bar{\theta}}, \quad (168d)$$

$$\partial_t \bar{\theta} = -\frac{\bar{\Lambda}_{\bar{V}}}{\bar{C}_{\bar{V}}} \text{Cof}(\bar{\mathbf{F}}) : \bar{\nabla} \bar{\nu} + (\partial_{\bar{U}} \bar{\theta}) \bar{V} \bar{\nu}^{\text{T}} \bar{K}^{\text{D}} \bar{\nu} - (\partial_{\bar{C}} \bar{\theta})^{\text{T}} \bar{V} \bar{\mathbb{H}}_{\bar{\mathbf{C}}\bar{\mathbf{C}}} \frac{\bar{\mu}}{\bar{\theta}}, \quad (168e)$$

where we have used in (168b) the relation  $(\partial_{\bar{U}} \bar{\pi})(\partial_{\bar{\pi}} \bar{\mathcal{S}}_{\text{ext}}) + (\partial_{\bar{U}} \bar{\theta})(\partial_{\bar{\theta}} \bar{\mathcal{S}}_{\text{ext}}) = \bar{\theta}^{-1}$ . The transformed system satisfies the NIC by virtue of (73) and since the closure conditions Def. 3.7 are valid. The remaining partial derivatives in (168) can be computed from the definition of the capacities (10) and from (9b)

$$\begin{aligned} \partial_{\bar{U}} \bar{\pi} &= \frac{\bar{\Lambda}_{\bar{V}}}{\bar{\theta} \bar{C}_{\bar{V}}}, & \partial_{\bar{C}} \bar{\pi}^{\text{T}} &= -\frac{\bar{S} \gamma + \alpha \bar{\mathbf{C}}}{\bar{V}^2} - \frac{\bar{\Lambda}_{\bar{V}}}{\bar{\theta} \bar{C}_{\bar{V}}} \bar{\mu}, \\ \partial_{\bar{U}} \bar{\theta} &= \frac{1}{\bar{C}_{\bar{V}}}, & \partial_{\bar{C}} \bar{\theta}^{\text{T}} &= \frac{\gamma}{\bar{V}} - \frac{\bar{\mu}}{\bar{C}_{\bar{V}}}. \end{aligned}$$

**Lagrangian-Eulerian reduction of** (168). We now transform the system  $(\bar{\mathcal{Q}}_{\text{ext}}, \bar{\mathcal{E}}_{\text{ext}}, \bar{\mathcal{S}}_{\text{ext}}, \bar{\mathbb{J}}_{\text{ext}}, \bar{\mathbb{K}}_{\text{ext}}^{\text{rD}})$  to the Eulerian frame using the map  $\text{T}_{\text{LE}} : \bar{\mathcal{Q}}_{\text{ext}} \rightarrow \mathcal{Q}_{\pi\theta}$ ,

$$\text{T}_{\text{LE}}(\bar{\mathbf{q}}_{\text{ext}}) = \mathbf{q}_{\pi\theta} = \begin{pmatrix} \mathbf{P} : \Omega \rightarrow \mathbb{R}^d \\ \mathbf{C} : \Omega \rightarrow \mathbb{R}^N \\ \pi : \Omega \rightarrow \mathbb{R} \\ \theta : \Omega \rightarrow \mathbb{R} \end{pmatrix} \in \mathcal{Q}_{\pi\theta}.$$

The intensive quantities pressure and temperature are mapped by  $\pi \circ \chi = \bar{\pi}$  and  $\theta \circ \chi = \bar{\theta}$ . In view of Lemma 3.13, the derivative of  $\text{T}_{\text{LE}}$  is given by

$$\text{DT}_{\text{LE}}(\bar{\mathbf{q}}_{\text{ext}}) = \begin{pmatrix} -\bar{\nabla} \cdot (\bar{\mathbf{P}} \otimes \square) & \frac{\square}{\bar{V}} & 0 & 0 & 0 \\ -\bar{\nabla} \cdot (\bar{\mathbf{C}} \otimes \square) & 0 & \frac{\square}{\bar{V}} & 0 & 0 \\ -\square \bar{\nabla} \pi & 0 & 0 & 1 & 0 \\ -\square \bar{\nabla} \theta & 0 & 0 & 0 & 1 \end{pmatrix}. \quad (169)$$

This similar to (156a), but now  $\bar{\mathbf{C}}$  is not locally conserved anymore. Yet, this has no influence on the form of the Poisson structure in Eulerian coordinates, i.e.,  $\mathbb{J}_{\pi\theta}(\mathbf{q}_{\pi\theta}) = \text{DT}_{\text{LE}}(\bar{\mathbf{q}}_{\text{ext}}) \bar{\mathbb{J}}_{\text{ext}} \text{DT}_{\text{LE}}(\bar{\mathbf{q}}_{\text{ext}})^*$  transformed by (169) coincides with  $\mathbb{J}_{\pi\theta}$  from (157). Similarly, the Eulerian Onsager operator is obtained as

$$\begin{aligned} \mathbb{K}_{\pi\theta}^{\text{rD}}(\mathbf{q}_{\pi\theta}) &= \text{DT}_{\text{LE}}(\bar{\mathbf{q}}_{\text{ext}}) \bar{\mathbb{K}}_{\text{ext}}^{\text{rD}}(\bar{\mathbf{q}}_{\text{ext}}) \text{DT}_{\text{LE}}(\bar{\mathbf{q}}_{\text{ext}})^* \\ &= \begin{pmatrix} \bar{V}^{-1} \bar{\mathbb{K}}_{\bar{\mathbf{P}}\bar{\mathbf{P}}}^{\text{D}} & 0 & \bar{\mathbb{K}}_{\bar{\mathbf{P}}\bar{\mathbf{P}}}^{\text{D}} \bar{\nu} (\partial_{\bar{U}} \bar{\pi}) & \bar{\mathbb{K}}_{\bar{\mathbf{P}}\bar{\mathbf{P}}}^{\text{D}} \bar{\nu} (\partial_{\bar{U}} \bar{\theta}) \\ 0 & \bar{\mathbb{H}}_{\bar{\mathbf{C}}\bar{\mathbf{C}}} & \bar{V} \bar{\mathbb{H}}_{\bar{\mathbf{C}}\bar{\mathbf{C}}} (\partial_{\bar{C}} \bar{\pi}) & \bar{V} \bar{\mathbb{H}}_{\bar{\mathbf{C}}\bar{\mathbf{C}}} (\partial_{\bar{C}} \bar{\theta}) \\ -(\partial_{\bar{U}} \bar{\pi}) \bar{\nu}^{\text{T}} \bar{\mathbb{K}}_{\bar{\mathbf{P}}\bar{\mathbf{P}}}^{\text{D}} & \bar{V} (\partial_{\bar{C}} \bar{\pi})^{\text{T}} \bar{\mathbb{H}}_{\bar{\mathbf{C}}\bar{\mathbf{C}}} & \bar{\mathbb{K}}_{\bar{\pi}\bar{\pi}}^{\text{ext}} \bar{V} & \bar{\mathbb{K}}_{\bar{\pi}\bar{\theta}}^{\text{ext}} \bar{V} \\ -(\partial_{\bar{U}} \bar{\theta}) \bar{\nu}^{\text{T}} \bar{\mathbb{K}}_{\bar{\mathbf{P}}\bar{\mathbf{P}}}^{\text{D}} & \bar{V} (\partial_{\bar{C}} \bar{\theta})^{\text{T}} \bar{\mathbb{H}}_{\bar{\mathbf{C}}\bar{\mathbf{C}}} & \bar{\mathbb{K}}_{\bar{\theta}\bar{\pi}}^{\text{ext}} \bar{V} & \bar{\mathbb{K}}_{\bar{\theta}\bar{\theta}}^{\text{ext}} \bar{V} \end{pmatrix}. \end{aligned} \quad (170)$$

The reactive and Darcy operators are mapped via  $\mathbb{H}(\mathbb{T}_{\text{LE}}(\bar{\mathbf{q}})) = \bar{\mathbb{H}}(\bar{\mathbf{q}})$  and  $\mathbb{K}^{\text{D}}(\mathbb{T}_{\text{LE}}(\bar{\mathbf{q}})) = \bar{\mathbb{K}}_{\bar{\mathbf{P}}\bar{\mathbf{P}}}^{\text{D}}(\bar{\mathbf{q}})$ , so that closure condition (50c) is satisfied. The Eulerian entropy  $\mathcal{S}(\mathbf{q}_{\pi\theta})$  is defined via the density  $S_{\pi\theta}(\mathbb{T}_{\text{LE}}(\bar{\mathbf{q}}_{\text{ext}}))$  chosen as in (158) such that  $S_{\pi\theta}(\mathbf{C}, \pi, \theta) := S_{\theta}(\mathbf{C}, \theta)$ . The driving force of dissipative dynamics is thus given by

$$\text{D}\mathcal{S}_{\pi\theta} = (0, \partial_{\mathbf{C}}S_{\pi\theta}, 0, \partial_{\theta}S_{\pi\theta})^{\top} = (0, \boldsymbol{\xi}_{\mathbf{C}}, 0, \xi_{\theta})^{\top}, \quad (171)$$

with  $\boldsymbol{\xi}_{\mathbf{C}}$  and  $\xi_{\theta}$  from (159b). The evolution equations (45) for the GENERIC system  $(\mathcal{Q}_{\pi\theta}, \mathcal{E}_{\pi\theta}, \mathcal{S}_{\pi\theta}, \mathbb{J}_{\pi\theta}, \mathbb{K}_{\pi\theta}^{\text{rD}})$  for a reactive flow of Darcy-type with thermal effects in Eulerian coordinates are then given by

$$\partial_t \mathbf{P} + \nabla \cdot (\mathbf{P} \otimes \boldsymbol{\nu}) = -\nabla \pi + \theta K^{\text{D}} \boldsymbol{\nu} \bar{V} \partial_{\bar{U}} \bar{\theta} \xi_{\theta} = -\nabla \pi + K^{\text{D}} \boldsymbol{\nu} \quad (172a)$$

$$\partial_t \mathbf{C} + \nabla \cdot (\mathbf{C} \otimes \boldsymbol{\nu}) = -\mathbb{H}_{\mathbf{C}\mathbf{C}} \frac{\boldsymbol{\mu}}{\theta}, \quad (172b)$$

$$\partial_t \pi + \boldsymbol{\nu} \cdot \nabla \pi + \kappa_S^{-1} \nabla \cdot \boldsymbol{\nu} = -(\partial_{\mathbf{C}} \pi)^{\top} \mathbb{H}_{\mathbf{C}\mathbf{C}} \frac{\boldsymbol{\mu}}{\theta} + (\partial_U \pi) \boldsymbol{\nu}^{\top} K^{\text{D}} \boldsymbol{\nu}, \quad (172c)$$

$$\partial_t \theta + \boldsymbol{\nu} \cdot \nabla \theta + \frac{\Lambda_V}{C_V} \nabla \cdot \boldsymbol{\nu} = -(\partial_{\mathbf{C}} \theta)^{\top} \mathbb{H}_{\mathbf{C}\mathbf{C}} \frac{\boldsymbol{\mu}}{\theta} + \frac{1}{C_V} \boldsymbol{\nu}^{\top} K^{\text{D}} \boldsymbol{\nu}. \quad (172d)$$

Here we used  $\pi = \pi(\mathbf{C}, U)$  and  $\theta = \theta(\mathbf{C}, U)$  and in order to arrive at (172a) we exploited that  $\bar{V} \partial_{\bar{U}} \bar{\theta} \xi_{\theta} = \theta^{-1}$ . This is obtained from the definition of the heat capacity (10) and the relation (158).

**Example 6.3 (Capacities for an ideal gas)** In view of the equation of state of the ideal gas (13), the Lagrangian pressure and temperature are

$$\bar{\theta} = \frac{2}{3} \frac{\bar{U}}{k_{\text{B}} \bar{C}}, \quad \bar{\pi} = \frac{2}{3} \frac{\bar{U}}{\bar{V}},$$

with  $\bar{C} = \sum_{i=1}^N \bar{C}_i$ . The Eulerian capacities in (172) are related to their Lagrangian counterparts and can be directly computed for the (monoatomic) ideal gas

$$\begin{aligned} \frac{\partial \theta}{\partial \bar{C}_i} &= \bar{V} \frac{\partial \bar{\theta}}{\partial \bar{C}_i} = -\frac{2}{3} \frac{U}{k_{\text{B}} C^2}, \\ \frac{\partial \pi}{\partial U} &= \bar{V} \frac{\partial \bar{\pi}}{\partial U} = \frac{2}{3}, \\ \frac{\partial \pi}{\partial \bar{C}} &= \bar{V} \frac{\partial \bar{\pi}}{\partial \bar{C}} = 0. \end{aligned}$$

Additionally, from (12) we compute the capacities

$$C_V = \frac{3}{2} k_{\text{B}} C, \quad \Lambda_V = k_{\text{B}} C \theta, \quad \kappa_S = \left(\frac{5}{3} k_{\text{B}} C \theta\right)^{-1},$$

which can be inserted into (172). \*

## Conclusion and Summary

We gave a detailed presentation for the GENERIC structure of fluid flows with a focus on the physical ingredients and the mathematical structures, i.e., thermodynamics, continuum mechanics, functionals, and operators. Based on the functional derivatives of the energy  $\text{D}\mathcal{E}$  and of the entropy  $\text{D}\mathcal{S}$  as generalized driving forces and suitable geometric structures  $\mathbb{J}$  and  $\mathbb{K}$  for reversible and dissipative dynamics, we established the evolution laws of Hamiltonian and Onsager systems. Their coupling in GENERIC systems via the noninteraction conditions  $\mathbb{J}\text{D}\mathcal{S} = 0$ ,  $\mathbb{K}\text{D}\mathcal{E} = 0$  ensures the laws of thermodynamics by construction and leads to the evolution  $\dot{\mathbf{q}} = \mathbb{J}\text{D}\mathcal{E} + \mathbb{K}\text{D}\mathcal{S}$ .

We showed how a fundamental thermodynamical description of fluids in Lagrangian coordinates using homogeneity assumptions can be transferred to a description in Eulerian coordinates. On the level of abstract state spaces, this leads to a nonlinear mapping  $\mathbb{T} : \bar{\mathcal{Q}} \rightarrow \mathcal{Q}$  between Banach spaces, of which the linearization  $\mathbb{L} = D\mathbb{T}$  is used to transform the operators via  $\mathbb{J} = \mathbb{L}\mathbb{J}\mathbb{L}^*$  and  $\mathbb{K} = \mathbb{L}\mathbb{K}\mathbb{L}^*$  and functionals via  $\mathcal{E} \circ \mathbb{T} = \bar{\mathcal{E}}$  and  $\mathcal{S} \circ \mathbb{T} = \bar{\mathcal{S}}$ . Assuming closure conditions for these transformations, cf. Def. 3.7, we proved that this construction remains valid even for non-invertible mappings, e.g., reductions and extensions, cf. L. 3.10 and Thm. 3.11. Making this connection between Lagrangian and Eulerian coordinates helps to reveal the origins and the assumptions behind certain thermodynamic relations in non-equilibrium thermodynamics, which usually stay hidden in the resulting system of partial differential equations. For example, many ingredients of this construction rely on the assumption of homogeneity of extensive and intensive quantities, see Def. 2.1, L. 2.8, and L. 3.13.

We presented examples for the Hamiltonian description of the ideal fluid, the Navier-Stokes equations, the Navier-Stokes-Fourier system, the reactive Navier-Stokes-Fourier system, and the reactive Navier-Stokes-Fourier-Darcy system with different sets of variables. In each of these cases we presented the system of partial differential equations and the underlying systems  $(\mathcal{Q}, \mathcal{E}, \mathcal{S}, \mathbb{J}, \mathbb{K})$  and discussed the validity of the noninteraction conditions. In particular the reactive Darcy flow shows how these structures can be extended to applications, e.g., soft matter, geophysical flows in ground water, or biological flows in tissue. In these applications, the coupling hyperelasticity should be considered.

Extensions of GENERIC structures for complex fluids have already been established in literature [28]. However, extensions to non-quadratic dissipation potentials, multiphysics and multiphase descriptions, multiscale limits, fluid-structure interaction, and interfacial thermomechanics offer many interesting avenues for future research. In particular for the latter two, the Eulerian-Lagrangian approach related by noninvertible reduction maps is appropriate.

## A Appendix

### A.1 Constitutive laws for fluids

Example 2.3 treats the ideal gas as the simplest constitutive relation of a fluid, neglecting particle interactions. Now we provide two further, more realistic examples.

**Example A.1 (Non-ideal fluids)** The equation of state of the Van der Waals fluid extends that of the ideal gas (12) by accounting for particle interaction via

$$\left( \bar{\pi} + a \left( \frac{\bar{C}}{\bar{V}} \right)^2 \right) (\bar{V} - \bar{C}b) = \bar{C}k_B\bar{\theta}, \quad (173)$$

where the empirical parameters  $a, b$  encode the particle interactions and excluded volume. The internal and free energy of the *Van der Waals gas* in natural variables are

$$\bar{U} = \frac{3h^2\bar{C}}{4\pi m} \left( \frac{\bar{C}}{\bar{V}-\bar{C}b} \right)^{\frac{2}{3}} \exp\left(\frac{2}{3}\frac{\bar{S}}{k_B\bar{C}} - \frac{5}{3}\right) + \bar{F}_{\text{mech}}, \quad (174a)$$

$$\bar{F} = \bar{C}k_B\bar{\theta} \left[ \log\left(\frac{\bar{C}}{\bar{V}-\bar{C}b}\lambda_\theta^3\right) - 1 \right] + \bar{F}_{\text{mech}}, \quad (174b)$$

with  $\lambda_\theta(\bar{\theta}) = C_{\text{therm}}/\sqrt{\bar{\theta}}$  the de Broglie wave length from (16) and  $\bar{F}_{\text{mech}} = -a\frac{\bar{C}^2}{\bar{V}}$ . From  $\bar{U}$  and  $\bar{F}$  all thermodynamic relations [3] and capacities can be deduced in terms of partial derivatives, e.g., we

have

$$\bar{\pi} = -\frac{\partial \bar{U}}{\partial \bar{V}} = -\frac{\partial \bar{F}}{\partial \bar{V}} = \frac{\bar{C} k_B \bar{\theta}}{\bar{V} - \bar{C} b} - a \frac{\bar{C}^2}{\bar{V}^2}, \quad (175a)$$

$$\bar{C}_{\bar{V}} = \bar{\theta} / \frac{\partial^2 \bar{U}}{\partial \bar{S}^2} = \frac{3}{2} k_B \bar{C}, \quad (175b)$$

$$\bar{\kappa}_{\bar{S}} = \frac{1}{\bar{V}} / \frac{\partial^2 \bar{U}}{\partial \bar{V}^2} = \left[ \frac{10 \bar{V} (\bar{U} - \bar{F}_{\text{mech}})}{9 (\bar{V} - \bar{C} b)^2} - 2a \left( \frac{\bar{C}}{\bar{V}} \right)^2 \right]^{-1}. \quad (175c)$$

We can also consider other types of mechanical energies contributing to the internal energy, e.g., for a compressible fluid

$$\bar{F}_{\text{mech}}(\bar{C}, \bar{V}) = \frac{1}{2\kappa} \frac{\bar{V}^2}{\bar{C}},$$

with  $\bar{F}_{\text{mech}}$  independent of  $\bar{\theta}$  and some parameter  $\kappa > 0$ . In this way, further energetic contributions are incorporated to the internal energy without modifying the original entropy expression which leave the heat capacity unchanged while pressure and compressibility become for example

$$\begin{aligned} \bar{\pi} &= \frac{\bar{C} k_B \bar{\theta}}{\bar{V}} - \frac{1}{\kappa} \frac{\bar{V}}{\bar{C}}, \\ \bar{C}_{\bar{V}} &= \frac{3}{2} k_B \bar{C}, \\ \bar{\kappa}_{\bar{S}} &= \left[ \frac{10}{9 \bar{V}} (\bar{U} - \bar{F}_{\text{mech}}) + \frac{\bar{V}}{\kappa \bar{C}} \right]^{-1}, \end{aligned}$$

\*

## A.2 Proof of Theorem 3.5: Consequences of the NIC (44)

The proofs of i) energy conservation, ii) entropy production, iii) mass conservation for GENERIC systems rely on the NIC (44), the chain rule for functionals, the GENERIC evolution equation (45), and properties (27), (37) of the geometric structures  $\bar{\mathbb{J}}$ ,  $\bar{\mathbb{K}}$ . Exemplarily, entropy production ii) is verified as follows

$$\begin{aligned} \frac{d}{dt} \bar{\mathcal{S}}(\bar{\mathbf{q}}(t)) &\stackrel{\text{chain rule}}{=} \langle D\bar{\mathcal{S}}(\bar{\mathbf{q}}), \partial_t \bar{\mathbf{q}} \rangle_{\bar{\mathcal{Q}}} \\ &\stackrel{(45)}{=} \langle D\bar{\mathcal{S}}(\bar{\mathbf{q}}), \bar{\mathbb{J}}(\bar{\mathbf{q}}) D\bar{\mathcal{E}}(\bar{\mathbf{q}}) + \bar{\mathbb{K}}(\bar{\mathbf{q}}) D\bar{\mathcal{S}}(\bar{\mathbf{q}}) \rangle_{\bar{\mathcal{Q}}} \\ &\stackrel{(27b)}{=} \langle D\bar{\mathcal{E}}, -\bar{\mathbb{J}} D\bar{\mathcal{S}} \rangle_{\bar{\mathcal{Q}}} + \langle D\bar{\mathcal{S}}, \bar{\mathbb{K}} D\bar{\mathcal{S}} \rangle_{\bar{\mathcal{Q}}} \\ &\stackrel{(44a)}{=} \langle D\bar{\mathcal{S}}(\bar{\mathbf{q}}), \bar{\mathbb{K}}(\bar{\mathbf{q}}) D\bar{\mathcal{S}}(\bar{\mathbf{q}}) \rangle_{\bar{\mathcal{Q}}} \stackrel{(37b)}{\geq} 0. \end{aligned}$$

Properties i) and iii) are shown with similar arguments.

For the proof of the maximum entropy principle iv) we maximize  $\bar{\mathcal{S}}(\bar{\mathbf{q}})$  subject to (46d), i.e.,  $\bar{\mathcal{E}}(\bar{\mathbf{q}}_*) = \bar{\mathcal{E}}_0$  and  $\bar{\mathcal{M}}(\bar{\mathbf{q}}_*) = \bar{\mathcal{M}}_0$ , by seeking critical points of

$$\Phi(\bar{\mathbf{q}}, \bar{\boldsymbol{\lambda}}) = -\bar{\mathcal{S}}(\bar{\mathbf{q}}) + \bar{\lambda}^{\bar{\mathcal{E}}} (\bar{\mathcal{E}}(\bar{\mathbf{q}}) - \bar{\mathcal{E}}_0) + \bar{\lambda}^{\bar{\mathcal{M}}} (\bar{\mathcal{M}}(\bar{\mathbf{q}}) - \bar{\mathcal{M}}_0),$$

with Lagrange multipliers  $\bar{\boldsymbol{\lambda}} = (\bar{\lambda}^{\bar{\mathcal{E}}}, \bar{\lambda}^{\bar{\mathcal{M}}}) \in \mathbb{R}^2$ . For a pair  $(\bar{\mathbf{q}}_*, \bar{\boldsymbol{\lambda}}_*) \in \bar{\mathcal{Q}} \times \mathbb{R}^2$  to be a critical point of  $\Phi : \bar{\mathcal{Q}} \times \mathbb{R}^2 \rightarrow \mathbb{R}$  the first order optimality conditions are  $D\Phi = 0$  with

$$D\Phi(\bar{\mathbf{q}}_*, \bar{\boldsymbol{\lambda}}_*) = \begin{pmatrix} -D\bar{\mathcal{S}}(\bar{\mathbf{q}}_*) + \bar{\lambda}_*^{\bar{\mathcal{E}}} D\bar{\mathcal{E}}(\bar{\mathbf{q}}_*) + \bar{\lambda}_*^{\bar{\mathcal{M}}} D\bar{\mathcal{M}}(\bar{\mathbf{q}}_*) \\ (\bar{\mathcal{E}}(\bar{\mathbf{q}}_*) - \bar{\mathcal{E}}_0) \\ (\bar{\mathcal{M}}(\bar{\mathbf{q}}_*) - \bar{\mathcal{M}}_0) \end{pmatrix}.$$

Then, by the NIC (44), there holds

$$\partial_t \bar{\mathbf{q}}_* = \bar{\mathbb{J}}(\bar{\mathbf{q}}_*) D\bar{\mathcal{E}}(\bar{\mathbf{q}}_*) + \bar{\mathbb{K}}(\bar{\mathbf{q}}_*) D\bar{\mathcal{S}}(\bar{\mathbf{q}}_*) = \frac{1}{\lambda_*^{\mathcal{E}}} \bar{\mathbb{J}}(\bar{\mathbf{q}}_*) D_{\bar{\mathbf{q}}} \Phi - \bar{\mathbb{K}}(\bar{\mathbf{q}}_*) D_{\bar{\mathbf{q}}} \Phi = 0,$$

i.e.,  $\bar{\mathbf{q}}_*$  is stationary.  $\square$

### A.3 Proof of Lemma 3.16: Preservation of thermodynamic relations

Suppose that  $\bar{U}_{\tilde{\tau}} = \bar{U}_{\tilde{\tau}}(w, \tilde{\tau})$  and  $\bar{S}_{\tilde{\tau}} = \bar{S}_{\tilde{\tau}}(w, \tilde{\tau})$  are continuously differentiable with respect to  $(w, \tilde{\tau})$ . In order to verify

$$\bar{\theta} = \left( \frac{\partial \bar{U}_{\tilde{\tau}}}{\partial \tilde{\tau}} / \frac{\partial \bar{S}_{\tilde{\tau}}}{\partial \tilde{\tau}} \right)_w = \left( \frac{\partial \bar{E}_{\tilde{\tau}}}{\partial \tilde{\tau}} / \frac{\partial \bar{S}_{\tilde{\tau}}}{\partial \tilde{\tau}} \right)_w, \quad (67a)$$

we consider the map that transforms the entropy, i.e.,  $\hat{\tau} = \bar{S}$  and  $\Gamma_{\bar{S} \rightarrow \tilde{\tau}}(w, \bar{S}) = \tilde{\tau}$ . Applying relation (66), i.e.,  $A_{\tilde{\tau}}(w, \tilde{\tau}) = A_{\tilde{\tau}}(w, \Gamma_{\tilde{\tau} \rightarrow \hat{\tau}}(w, \hat{\tau})) = A_{\tilde{\tau}}(w, \hat{\tau})$  for the internal energy densities  $\bar{U}_{\bar{S}}$ ,  $\bar{U}_{\tilde{\tau}}$  and the entropy density  $\bar{S}_{\tilde{\tau}}$  we obtain thanks to the fundamental relation (5a)

$$\bar{\theta} = \left( \frac{\partial \bar{U}_{\bar{S}}}{\partial \bar{S}} \right)_w \left( \frac{\partial \Gamma_{\bar{S} \rightarrow \tilde{\tau}}}{\partial \hat{\tau}} \right)_w = \left( \frac{\partial \bar{U}_{\bar{S}}}{\partial \bar{S}} \right)_w \left( \frac{\partial \bar{S}_{\tilde{\tau}}}{\partial \tilde{\tau}} \right)_w^{-1}.$$

This is (67a), also because  $\bar{E}_{\tilde{\tau}} = \bar{E}_{\text{kin}} + \bar{U}_{\tilde{\tau}}$  and  $\bar{E}_{\text{kin}}$  is independent of  $\tilde{\tau}$ . We also used  $\bar{S} = \Gamma_{\bar{S} \rightarrow \tilde{\tau}}^{-1}(w, \tilde{\tau}) = \bar{S}_{\tilde{\tau}}$ . Then  $\left( \frac{\partial \bar{S}_{\tilde{\tau}}}{\partial \tilde{\tau}} \right)_w = \left( \frac{\partial \Gamma_{\bar{S} \rightarrow \tilde{\tau}}^{-1}(w, \tilde{\tau})}{\partial \tilde{\tau}} \right)_w = \left( \frac{\partial \Gamma_{\bar{S} \rightarrow \tilde{\tau}}(w, \bar{S})}{\partial \bar{S}} \right)_w$  by the rule for the derivative of the inverse function. Hence we have  $\left( \frac{\partial \Gamma_{\bar{S} \rightarrow \tilde{\tau}}}{\partial \hat{\tau}} \right)_w = \left( \frac{\partial \bar{S}_{\tilde{\tau}}}{\partial \tilde{\tau}} \right)_w^{-1}$ .

Now we verify the relations

$$\left( \frac{\partial (\bar{E}_{\text{kin}} + \bar{U}_{\tilde{\tau}})}{\partial w} \right)_{\tilde{\tau}} - \Gamma_{\tilde{\tau} \rightarrow \bar{\theta}}(w, \tilde{\tau}) \left( \frac{\partial \bar{S}_{\tilde{\tau}}}{\partial w} \right)_{\tilde{\tau}} = \left( \frac{\partial (\bar{E}_{\text{kin}} + \bar{F}(w, \bar{\theta}))}{\partial w} \right)_{\bar{\theta}}, \quad (67b)$$

$$\left( \frac{\partial \bar{S}_{\tilde{\tau}}}{\partial w} \right)_{\tilde{\tau}} - \frac{1}{\Gamma_{\tilde{\tau} \rightarrow \bar{\theta}}(w, \tilde{\tau})} \left( \frac{\partial (\bar{E}_{\text{kin}} + \bar{U}_{\tilde{\tau}})}{\partial w} \right)_{\tilde{\tau}} = \left( \frac{\partial (-\frac{1}{\bar{\theta}} \bar{E}_{\text{kin}} + \bar{J}(w, \bar{\theta}))}{\partial w} \right)_{\bar{\theta}}, \quad (67c)$$

where  $\bar{\theta} = \Gamma_{\tilde{\tau} \rightarrow \bar{\theta}}(w, \tilde{\tau})$  and with  $\bar{E}_{\text{kin}}$  as in (62), and the thermodynamic potentials  $\bar{F}$  and  $\bar{J}$  as in Tab. 1. For this, observe that

$$\left( \frac{\partial (\bar{E}_{\text{kin}} + \bar{F})}{\partial w} \right)_{\bar{\theta}} = \left( \frac{\partial (\bar{E}_{\text{kin}} + \bar{U}_{\bar{\theta}})}{\partial w} - \bar{\theta} \frac{\partial \bar{S}_{\bar{\theta}}}{\partial w} \right)_{\bar{\theta}}, \quad (176a)$$

$$\left( \frac{\partial (-\frac{1}{\bar{\theta}} \bar{E}_{\text{kin}} + \bar{J})}{\partial w} \right)_{\bar{\theta}} = \left( \frac{\partial \bar{S}_{\bar{\theta}}}{\partial w} - \frac{1}{\bar{\theta}} \frac{\partial (\bar{E}_{\text{kin}} + \bar{U}_{\bar{\theta}})}{\partial w} \right)_{\bar{\theta}}, \quad (176b)$$

again with  $\bar{\theta} = \Gamma_{\tilde{\tau} \rightarrow \bar{\theta}}(w, \tilde{\tau})$ . Note that  $\Gamma_{\tilde{\tau} \rightarrow \bar{\theta}} = \Gamma_{\bar{\theta} \rightarrow \tilde{\tau}}^{-1}$ , so that now  $\tilde{\tau}$  plays the role of  $\hat{\tau}$  in (66) and  $\tilde{\tau} = \bar{\theta}$  (66). Hence, applying (66c) for  $\bar{U}_{\tilde{\tau}}$ ,  $\bar{U}_{\bar{\theta}}$  and for  $\bar{S}_{\tilde{\tau}}$ ,  $\bar{S}_{\bar{\theta}}$  gives

$$\begin{aligned} \left( \frac{\partial \bar{U}_{\tilde{\tau}}}{\partial w} \right)_{\tilde{\tau}} &= \left( \frac{\partial \bar{U}_{\bar{\theta}}}{\partial w} \right)_{\bar{\theta}} + \left( \frac{\partial \bar{U}_{\bar{\theta}}}{\partial \bar{\theta}} \right)_w \left( \frac{\partial \Gamma_{\tilde{\tau} \rightarrow \bar{\theta}}(w, \tilde{\tau})}{\partial w} \right)_{\tilde{\tau}}, \\ \left( \frac{\partial \bar{S}_{\tilde{\tau}}}{\partial w} \right)_{\tilde{\tau}} &= \left( \frac{\partial \bar{S}_{\bar{\theta}}}{\partial w} \right)_{\bar{\theta}} + \left( \frac{\partial \bar{S}_{\bar{\theta}}}{\partial \bar{\theta}} \right)_w \left( \frac{\partial \Gamma_{\tilde{\tau} \rightarrow \bar{\theta}}(w, \tilde{\tau})}{\partial w} \right)_{\tilde{\tau}}. \end{aligned}$$

Composing with this the linear combinations on the left of (67b), resp. (67c), leads to the expressions given (176) when taking into account that  $(\partial_w \Gamma_{\tilde{\tau} \rightarrow \bar{\theta}}(w, \tilde{\tau}))_{\tilde{\tau}} ((\partial_{\bar{\theta}} \bar{U}_{\bar{\theta}})_w - \Gamma_{\tilde{\tau} \rightarrow \bar{\theta}}(w, \tilde{\tau}) (\partial_{\bar{\theta}} \bar{S}_{\bar{\theta}})_w) = 0$  by (67a) due to  $\Gamma_{\tilde{\tau} \rightarrow \bar{\theta}}(w, \tilde{\tau}) = \bar{\theta}$ .  $\square$

## References

- [1] L. Ambrosio, N. Gigli, and G. Savaré. *Gradient Flows: In Metric Spaces and in the Space of Probability Measures*. Birkhäuser Basel, 2008.
- [2] V. Arnold. Sur la géométrie différentielle des groupes de Lie de dimension infinie et ses applications à l'hydrodynamique des fluides parfaits. *Ann. I. Fourier*, 16(1):319–361, 1966.
- [3] R. Balian. *From Microphysics to Macrophysics: Methods and Applications of Statistical Physics. Volume II*. Springer-Verlag Berlin Heidelberg, 2007.
- [4] G. K. Batchelor. *An Introduction to Fluid Dynamics*. Cambridge University Press, 2000.
- [5] D. Bensimon, L. P. Kadanoff, S. Liang, B. I. Shraiman, and C. Tang. Viscous flows in two dimensions. *Rev. Mod. Phys.*, 58(4):977–999, 1986.
- [6] A. N. Beris and B. J. Edwards. *Thermodynamics of Flowing Systems: with Internal Microstructure*. Number 36 in Oxford engineering science series. Oxford University Press on Demand, 1994.
- [7] D. Bothe and W. Dreyer. Continuum thermodynamics of chemically reacting fluid mixtures. *Acta Mech.*, 226(6):1757–1805, 2015.
- [8] M. Bulíček, A. Jüngel, M. Pokorný, and N. Zamponi. Existence analysis of a stationary compressible fluid model for heat-conducting and chemically reacting mixtures. *arXiv preprint arXiv:2001.06082*, 2020.
- [9] P. G. Ciarlet. *Mathematical Elasticity I: Three-Dimensional Elasticity*. North Holland, 1988.
- [10] B. D. Coleman. Thermodynamics of materials with memory. *Arch. Ration. Mech. Anal.*, 17(1):1–46, 1964.
- [11] M. C. Cross and P. C. Hohenberg. Pattern formation outside of equilibrium. *Rev. Mod. Phys.*, 65(3):851–1112, 1993.
- [12] E. C. D'Avignon. Physical Consequences of the Jacobi Identity. *arXiv preprint arXiv:1510.06455*, 2015.
- [13] P. G. de Gennes. Dynamics of fluctuations and spinodal decomposition in polymer blends. *J. Chem. Phys.*, 72(9):4756–4763, 1980.
- [14] P. G. de Gennes. Wetting: statics and dynamics. *Rev. Mod. Phys.*, 57(3):827–863, 1985.
- [15] S. R. de Groot and P. Mazur. *Non-equilibrium thermodynamics*. New York: Dover Publications, 1984.
- [16] M. Doi. Onsager's variational principle in soft matter. *J. Phys. Condens. Matter*, 23(28):284118, 2011.
- [17] M. H. Duong, M. A. Peletier, and J. Zimmer. GENERIC formalism of a Vlasov-Fokker-Planck equation and connection to large-deviation principles. *Nonlinearity*, 26(11):2951–2971, 2013.
- [18] D. G. Ebin and J. Marsden. Groups of diffeomorphisms and the motion of an incompressible fluid. *Ann. Math.*, 92(1):102–163, 1970.



- [19] C. Eck, H. Garcke, and P. Knabner. *Mathematische Modellierung*. Springer Spektrum, third edition, 2017.
- [20] C. Eckart. Variation principles of hydrodynamics. *Phys. Fluids*, 3(3):421–427, 1960.
- [21] L. C. Evans. *Partial Differential Equations*, volume 19. American Mathematical Society, 2010.
- [22] M. Feinberg and F. J. M. Horn. Chemical mechanism structure and the coincidence of the stoichiometric and kinetic subspaces. *Arch. Ration. Mech. Anal.*, 66(1):83–97, 1977.
- [23] F. Gay-Balmaz and H. Yoshimura. A Lagrangian variational formulation for nonequilibrium thermodynamics. Part II: Continuum systems. *J. Geom. and Phys.*, 111:194–212, 2017.
- [24] M.-H. Giga, A. Kirshtein, and C. Liu. *Variational Modeling and Complex Fluids*, pages 1–41. Springer, Cham, 2017.
- [25] A. Glitzky and A. Mielke. A gradient structure for systems coupling reaction-diffusion effects in bulk and interfaces. *Z. Angew. Math. Phys.*, 64(1):29–52, 2012.
- [26] M. Grmela, V. Klika, and M. Pavelka. Gradient and GENERIC time evolution towards reduced dynamics. *Phil. Trans. R. Soc. A.*, 378(2170):20190472, 2020.
- [27] M. Grmela and H. C. Öttinger. Dynamics and thermodynamics of complex fluids. I. Development of a general formalism. *Phys. Rev. E*, 56(6):6620–6632, 1997.
- [28] M. Grmela and H. C. Öttinger. Dynamics and thermodynamics of complex fluids. II. Illustrations of a general formalism. *Phys. Rev. E*, 56(6):6633–6655, 1997.
- [29] M. E. Gurtin. *An Introduction to Continuum Mechanics*. Academic Press, 1981.
- [30] M. Ishii and T. Hibiki. *Thermo-fluid Dynamics of Two-Phase Flow*. Springer, New York, NY, 2011.
- [31] D. Jou, J. Casas-Vázquez, and G. Lebon. Extended Irreversible Thermodynamics. In *Extended Irreversible Thermodynamics*, pages 41–74. Springer, Berlin, Heidelberg, 1996.
- [32] A. Jüngel. The boundedness-by-entropy method for cross-diffusion systems. *Nonlinearity*, 28(6):1963–2001, 2015.
- [33] K. Kawasaki, N. Shigesada, and E. Teramoto. Spatial segregation of interacting species. *J. Theor. Biol.*, 79(1):83–99, 1979.
- [34] W. Koehler and K. I. Morozov. The Soret effect in liquid mixtures-A review. *J. Non-Equil. Thermody.*, 41(3):151–197, 2016.
- [35] D. J. Korteweg. XVII. On a general theorem of the stability of the motion of a viscous fluid. *London Edinburgh Dublin Philos. Mag. J. Sci.*, 16(98):112–118, 1883.
- [36] L. D. Landau and E. M. Lifshitz. *Fluid Mechanics (Course of Theoretical Physics)*, volume 6. Pergamon Press, 1987.
- [37] G. Lebon, D. Jou, and J. Casas-Vázquez. *Understanding Non-equilibrium Thermodynamics*. Springer, Berlin, Heidelberg, 2008.
- [38] Y. Lou and W.-M. Ni. Diffusion, self-diffusion and cross-diffusion. *J. Differ. Equations*, 131(1):79–131, 1996.

- [39] J. Maas and A. Mielke. Modeling of Chemical Reaction Systems with Detailed Balance Using Gradient Structures. *J. Stat. Phys.*, 181(6):2257–2303, 2020.
- [40] J. Marsden and A. Weinstein. Reduction of symplectic manifolds with symmetry. *Rep. Math. Phys.*, 5(1):121–130, 1974.
- [41] J. E. Marsden and T. Ratiu. *Introduction to Mechanics and Symmetry: a Basic Exposition of Classical Mechanical Systems*, volume 17. Springer-Verlag, New York, 1999.
- [42] F. Massieu. *Thermodynamique: Mémoire sur les fonctions caractéristiques des divers fluides et sur la théorie des vapeurs*, volume 22 of *Mémoires présentés par divers savants à L'Académie des Sciences de L'Institut National de France*. Académie des Sciences de L'Institut National de France, Paris, 1876.
- [43] A. Mielke. A gradient structure for reaction-diffusion systems and for energy-drift-diffusion systems. *Nonlinearity*, 24(4):1329–1346, 2011.
- [44] A. Mielke. Formulation of thermoelastic dissipative material behavior using GENERIC. *Contin. Mech. Thermodyn.*, 23(3):233–256, 2011.
- [45] A. Mielke. Thermomechanical modeling of energy-reaction-diffusion systems, including bulk-interface interactions. *Discrete Contin. Dyn. Syst. Ser. S*, 6(2):479–499, 2013.
- [46] A. Mielke, M. A. Peletier, and D. R. M. Renger. On the Relation between Gradient Flows and the Large-Deviation Principle, with Applications to Markov Chains and Diffusion. *Potential Anal.*, 41(4):1293–1327, 2014.
- [47] A. Mielke, D. R. M. Renger, and M. A. Peletier. A generalization of Onsager's reciprocity relations to gradient flows with nonlinear mobility. *J. Non-Equil. Thermody.*, 41(2):141–149, 2016.
- [48] M. Mimura and K. Kawasaki. Spatial segregation in competitive interaction-diffusion equations. *J. Math. Biol.*, 9(1):49–64, 1980.
- [49] P. J. Morrison. Hamiltonian field description of two-dimensional vortex fluids and guiding center plasmas. Technical report, Princeton Univ., NJ (USA). Plasma Physics Lab., 1981.
- [50] P. J. Morrison. Poisson brackets for fluids and plasmas. *AIP Conf. Proc.*, 88(1):13–46, 1982.
- [51] P. J. Morrison. A paradigm for joined Hamiltonian and dissipative systems. *Physica D*, 18(1-3):410–419, 1986.
- [52] P. J. Morrison. Hamiltonian description of the ideal fluid. *Rev. Mod. Phys.*, 70(2):467–521, 1998.
- [53] A. Moses Badlyan and C. Zimmer. Operator-GENERIC Formulation of Thermodynamics of Irreversible Processes. *arXiv preprint arXiv:1807.09822*, 2018.
- [54] I. Müller and T. Ruggeri. *Rational extended thermodynamics*, volume 37. Springer-Verlag New York, 1998.
- [55] W. Muschik. Why so many “schools” of thermodynamics. *Forsch. Ingenieurwes.*, 71(149):149–161, 2007.
- [56] W. Nolting. *Theoretical Physics 5: Thermodynamics*. Springer International Publishing, 2017.

- [57] W. Nolting. *Theoretical Physics 8: Statistical Physics*. Springer International Publishing, 2018.
- [58] L. Onsager. Reciprocal relations in irreversible processes. I. *Phys. Rev.*, 37(4):405–426, 1931.
- [59] F. Otto. The geometry of dissipative evolution equations: the porous medium equation. *Commun. Partial Differ. Equ.*, 26(1-2):101–174, 2001.
- [60] F. Otto and W. E. Thermodynamically driven incompressible fluid mixtures. *J. Chem. Phys.*, 107(23):10177–10184, 1997.
- [61] M. Pavelka, V. Klika, and M. Grmela. *Multiscale Thermo-Dynamics*. De Gruyter, 2018.
- [62] M. Planck. *Vorlesungen über Thermodynamik*. Walter de Gruyter & Co, 1922.
- [63] I. Prigogine. *Introduction to Thermodynamics of Irreversible Processes*. John Wiley, 1968.
- [64] R. Salmon. Hamiltonian fluid mechanics. *Annu. Rev. Fluid Mech.*, 20(1):225–256, 1988.
- [65] J. Serrin. *Mathematical Principles of Classical Fluid Mechanics*, volume VIII, pages 125–263. Springer, Berlin, Heidelberg., 1959.
- [66] T. C. Sideris. Formation of singularities in three-dimensional compressible fluids. *Commun. Math. Phys.*, 101(4):475–485, 1985.
- [67] J. W. Strutt. Some general theorems relating to vibrations. *Proc. London Math. Soc.*, s1-4(1):357–368, 1871.
- [68] U. Thiele, D. V. Todorova, and H. Lopez. Gradient dynamics description for films of mixtures and suspensions: dewetting triggered by coupled film height and concentration fluctuations. *Phys. Rev. Lett.*, 111(11):117801, 2013.
- [69] C. Truesdell. Historical Introit. The origins of rational thermodynamics. In *Rational Thermodynamics*, pages 1–48. Springer, New York, NY, 1984.
- [70] C. Truesdell. *Rational Thermodynamics*. Springer-Verlag New York, 1984.
- [71] A. van der Schaft and D. Jeltsema. Port-Hamiltonian systems theory: An introductory overview. *Found. Trends Syst. Control*, 1(2-3):173–378, 2014.
- [72] V. K. Vanag and I. R. Epstein. Cross-diffusion and pattern formation in reaction-diffusion systems. *Phys. Chem. Chem. Phys.*, 11(6):897–912, 2009.
- [73] H. von Helmholtz. Zur Theorie der stationären Ströme in reibenden Flüssigkeiten. *Wiss. Abh.*, 1:223–230, 1868.