Multiscale geometric approach to continuum mechanics and thermodynamics

(Habilitation Thesis)

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Víceškálový geometrický přístup k mechanice a termodynamice kontinua

(Habilitační práce)

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Contents

1 Introduction

"The generality that I embrace, instead of dazzling our lights, will reveal to us rather the true laws of Nature in all their splendor, and we will find there even stronger reasons to admire its beauty and simplicity."

— Leonhard Euler[1]

Non-equilibrium thermodynamics has a very general ambition to systematically describe evolution of any macroscopic system. Instead of making up a particular theory for each particular type of systems, the goal is to have a general structure capable to describe all systems, although such a goal might not be achievable. There are three main routes in non-equilibrium thermodynamics: (i) classical non-equilibrium thermodynamics based on balance laws, entropic closures, and constitutive relations, (ii) non-equilibrium statistical mechanics, using ensemble averaging or maximization of entropy, (iii) and geometric mechanics in connection with thermodynamics, described by cotangent bundles, Lie groups, and Lie algebras [Arnold, 1966]. In this habilitation, I advocate the third route.

What are the difficulties of classical non-equilibrium thermodynamics? Let us consider for instance complex fluids, fluids with some additional internal structures (for instance chains of polymeric molecules). Despite some early observations of complex fluids, the need for a systematic description of their motion rose with the advent of plastics. Since then, flows of complex fluids have been ubiquitous in chemical industry (fluids in reactors), processing industry (flowing foods and paints), or even electrochemistry (redox flow batteries). But traditional fluid mechanics based on the Navier-Stokes equations fails to predict behavior of complex fluids and it is necessary to add extra state variables expressing the internal structures of the fluids (for instance correlations of orientations of polymeric molecules) [Bird et al., 1987, Müller and Ruggeri, 1998].

Classical non-equilibrium thermodynamics proceeds in four steps: First the

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[1] *"La généralité que j'embrasse, au lieu d'éblouïr nos lumieres, nous découvrira plutôt les véritables loix de la Nature dans tout leur éclat, et on y trouvera des raisons encore plus fortes, d'en admirer la beauté et la simplicité."* [Dugas and de Broglie, 1950]

state variables are identified (typically mass, momentum, energy, and an extra state variable). Second, their balance laws are written (time derivative of a quantity equals to the divergence of flux of the quantity plus a production term). The balance laws involve some unknown quantities like the stress tensor or heat flux. Third, the evolution equation for entropy is obtained from the balance laws, still containing the undetermined quantities. Fourth, constitutive relations are chosen, expressing the unknown quantities in terms of the state variables while obeying the second law of thermodynamics [Truesdell, 1984, Müller, 1985, Jou et al., 2010, Berezovski and Ván, 2017].

But the second step (writing the balance laws) has little physical relevance for quantities that are not supposed to be conserved. Indeed, any partial differential equation can be written in the form of balance law if it contains only the first time derivative of a quantity and higher derivatives only with respect to space. There are only eight basic conserved quantities in classical mechanics: mass, three components of momentum, three components of angular momentum, and energy [Landau and Lifshitz, 1976]. Therefore, densities of mass, momentum, and energy obey conservation laws, although their evolution equations contain an a priori unknown stress tensor and heat flux (expressing Newton's laws and collecting non-mechanical macroscopic fluxes of energy). The state variables encoding some internal structure of the complex fluid, however, are typically not conserved and thus their balance laws are merely an arbitrary way of writing the equations. Moreover, the fourth step (identification of the constitutive relations) is often not unique, since one can choose any constitutive relations that do not violate the second law of thermodynamics; anything that neither increases nor decreases the entropy can be added. Classical non-equilibrium thermodynamics does not provide any general and unique way towards evolution equations of complex fluids.

On the other hand, Newtonian mechanics can be seen as a consequence of the principle of stationary action, and this principle leads also to continuum mechanics of complex fluids. A geometric formulation of the principle of stationary action is Hamiltonian mechanics on a cotangent bundle, and continuum mechanics can be formulated in a geometric way as well. The state variables are then equipped with geometric structures like Poisson brackets, and once the energy is determined, the evolution equations are implied in a unique way with no need of balance laws or constitutive relations. The conservation laws become consequences of geometry instead of being postulated.

In other words, geometric mechanics is an alternative and advantageous approach towards continuum mechanics [Grmela and Carreau, 1987].

Another route in non-equilibrium thermodynamics is based on statistical mechanics. It starts with a detailed description, for instance by means of distribution functions of classical particles, and evolution equations of some less detailed state variables are then obtained by averaging the detailed evolution equations. Although the process of averaging is feasible in simple cases, it becomes difficult in more complex nonlinear cases. The averaging is typically carried out with respect to space (BBGKY hierarchy) or momentum (Grad hierarchy) [Kirkwood, 1946, Grad, 1958, Struchtrup, 2005, Gorban and Karlin, 2005, Ruggeri and Sugiyama, 2015]. Geometric formulation of the averaging makes the process more tractable in some cases, since it splits the equations into several building blocks that can be treated separately. However, many parts of statistical mechanics are still waiting to be geometrized, provided that it is possible at all.

This habilitation summarizes a part of my research related to multiscale Hamiltonian mechanics and continuum thermodynamics. From the mathematical point of view, I work with cotangent bundles, infinite-dimensional Lie groups, and with the related Poisson geometry [Arnold, 1966] in combination with generalized gradient dynamics [Otto, 2001]. From the physical point of view, the Poisson geometry can be seen as Hamiltonian mechanics (reversible evolution), while gradient dynamics, evolution along the gradient of a dissipation potential, provides thermodynamic behavior (growth of entropy and irreversibility). This combination is a key idea of the General Equation for Non-Equilibrium Reversible-Irreversible Coupling (GENERIC), where the evolution is prescribed as the sum of reversible Hamiltonian mechanics and irreversible gradient dynamics [Grmela and Öttinger, 1997, Öttinger and Grmela, 1997].

The Hamiltonian part of GENERIC is given by two building blocks, a Poisson bracket and an energy functional, while the gradient part by another two building blocks, a dissipation potential and entropy. This decomposition to building blocks allows GENERIC to better express the multiscale character of non-equilibrium thermodynamics, where a single physical system can be described by various sets of state variables, differing in the amount of details. Such different levels of description should be compatible with each other so that building blocks on less detailed levels of description can be derived from the building blocks on more detailed levels. Moreover, it is possible to equip the deterministic GENERIC equations with stochastic terms whose compatibility with the deterministic evolution is guaranteed by a generalized fluctuation-dissipation theorem [Öttinger, 2005].

How to construct continuum mechanics geometrically? Why is continuum mechanics (disregarding the dissipative terms) often described by hyperbolic evolution equations? Is it possible to construct dissipative dynamics from purely Hamiltonian mechanics? Can dissipation potential be non-convex? From where does irreversible evolution emerge, if motion of classical particles is purely reversible? Having detailed evolution equations for a physical system, how to derive a less detailed description? Answers to these questions can be found in our monograph [Pavelka et al., 2018b] and the six recent papers attached to this thesis.[2]

Section 2 focuses on geometric continuum mechanics constructed from Poisson brackets. First, canonical Hamiltonian mechanics is derived from the stationary action principle in both finite-dimensional systems (mechanics of classical particles) and infinite-dimensional systems (Lagrangian continuum mechanics). The principle of stationary action also gives the evolution equations of the rigid body, which is a prototype of non-canonical Hamiltonian mechanics (degenerate, with non-empty kernel). Subsequently, canonical Lagrangian continuum mechanics is reduced to non-canonical Eulerian continuum mechanics, suitable for both solids and complex fluids. Kinetic theory is another example of non-canonical Hamiltonian mechanics. It is obtained by a lift of classical particle mechanics to the level of distribution functions (mathematically to a Lie algebra dual), and it can be reduced to fluid mechanics. Moreover, fluid mechanics can be extended by a semidirect product to a Hamiltonian theory of electrodynamics of moving media. All these mechanical equations are reversible with respect to the time-reversal transformation, they automatically satisfy Onsager-Casimir reciprocal relations, and they typically consist of quasilinear hyperbolic partial differential equations of the first order.

Section 3 equips reversible mechanics with irreversible terms, forming the GENERIC structure. GENERIC automatically satisfies a nonlinear generalization Onsager-Casimir reciprocal relations. The dissipation potentials (gen-

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[2] In all the attached papers I am either the first author or the corresponding author, or the main author was my student writing the paper as a part of his thesis.

erating the irreversible evolution) are usually convex, but they can be also non-convex without violating the second law of thermodynamics. Such non-convexity results in a kind of phase transitions in behavior of complex fluids (for instance, jumps of the stress tensor when increasing strain rate). Moreover, reversible mechanical equations can be equipped with irreversible dynamics constructed from the mechanics (for instance dissipative rigid body mechanics). Finally, a detailed GENERIC description (in particular purely Hamiltonian mechanics) can be reduced to a less detailed GENERIC evolution. Such compatibility between various levels of description is the essence of multiscale non-equilibrium thermodynamics, illustrated in Figure 1.

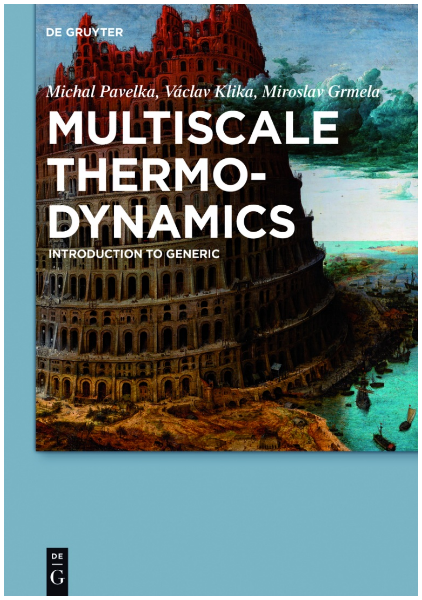

Figure 1: On the cover of monograph [Pavelka et al., 2018b], we would like to demonstrate several features of non-equilibrium thermodynamics. First, thermodynamics is an inherently multiscale theory. Each level of description differs in the amount of contained information, and neighboring levels should be compatible with each other. Second, there are many approaches (languages) towards non-equilibrium thermodynamics. Finally, since non-equilibrium thermodynamics aims to eventually describe all macroscopic physical systems within a single framework, it will probably never be finished.

2 Multiscale geometric continuum mechanics

"The aim of Mathematical Physics is not only to facilitate for the physicist the numerical calculation of certain constants or the integration of certain differential equations. It is besides, it is above all, to reveal to him the hidden harmony of things in making him see them in a new way."

— Henri Poincaré [Poincaré, 2012]

Instead of working directly with the evolution equations in Newtonian mechanics, we prefer to reveal the geometric structure under the hood (Poisson brackets and energy). Poisson brackets are skew-symmetric bilinear operators that take two functionals of chosen state variables and give another functional, and together with energy they give the reversible evolution equations of the state variables. In classical mechanics of particles, the Poisson bracket is canonical, see Section 2.1, but for other state variables (for instance rigid body mechanics), they are different and non-canonical (having non-zero kernel). A feature of Poisson brackets is the Jacobi identity, thanks to which the evolution equations preserve the Poisson bracket, and skew-symmetry of the brackets ensures conservation of energy. Poisson brackets and energy express a self-consistent internal structure of equations in mechanics.

From the mathematical point of view, a Poisson bracket and an energy constitute a Poisson geometry, which is a generalization of symplectic geometry (canonical) to the non-canonical case. Poisson brackets can be derived from the principle of stationary action or by reduction from more detailed Poisson brackets. Figure 2 shows a hierarchy of Poisson brackets that contains the Lagrangian continuum mechanics (elasticity with large deformations), the Eulerian theory of with distortion (unifying the motion of fluids and solids), mechanics of non-Newtonian fluids, fluid mechanics, kinetic theory, and electrodynamics of moving media. Further realizations of Poisson geometry can be found in [Pavelka et al., 2018b], including a theory of charged mixtures. But let us start from the beginning, recalling the Hamiltonian formulation of classical mechanics of particles.

2.1 Classical Hamiltonian mechanics

The geometric character of classical mechanics goes back to Lagrange, Bernoulli, Euler, Poisson, d'Alambert, Jacobi, and Hamilton [Lagrange, 1811, Lagrange

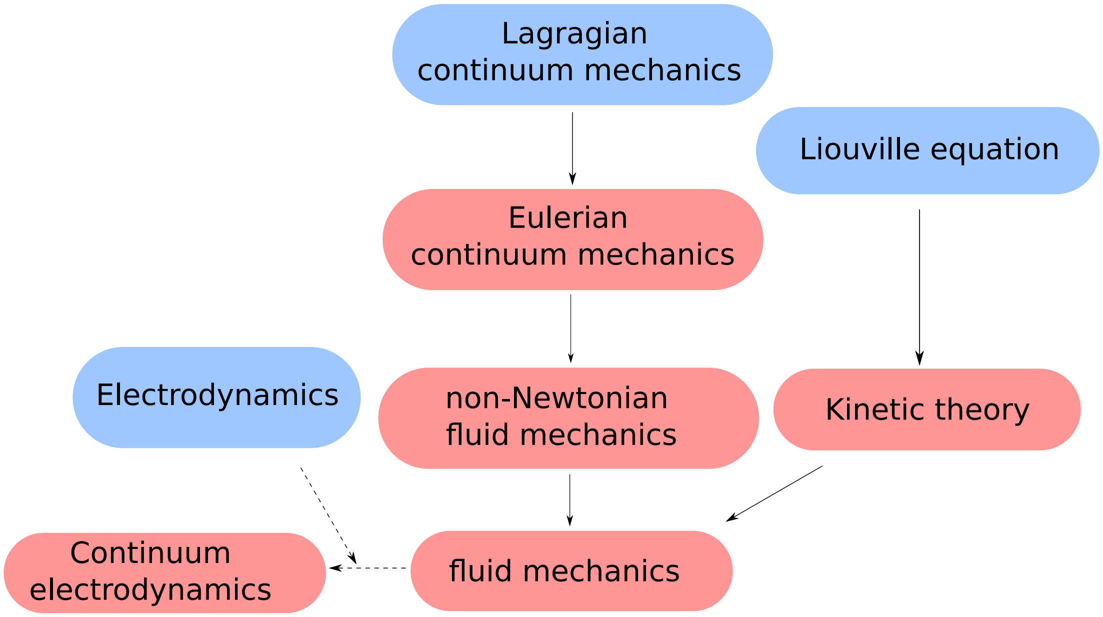

Figure 2: A hierarchy of levels of description in Hamiltonian continuum mechanics. The principle of stationary actions leads to the starting points in the diagram (blue): (i) the Lagrangian continuum mechanics (state variables $\mathbf{x}$ and $\mathbf{M}$), (ii) the Liouville equation (state variable f_N), and (iii) Hamiltonian electrodynamics (state variables $\mathbf{D}$ and $\mathbf{B}$). From the Poisson brackets at those starting points, one can derive less detailed Poisson brackets expressing kinematics on less detailed levels of description (red). Solid arrows indicate such projections. This way we get Eulerian continuum mechanics (with state variables ρ, $\mathbf{m}$, s, and $\mathbf{A}$) and kinetic theory (state variable f). From the latter two, one gets the fluid mechanics (state variables ρ, $\mathbf{m}$, and s). Finally, coupling of electrodynamics and fluid mechanics by means of the semidirect product theory leads to electrodynamics of moving media (state variables ρ, $\mathbf{m}$, s, $\mathbf{D}$, and $\mathbf{B}$).

and Bertrand, 1855, Poisson, 1809, Jacobi, 1840, Hamilton, 1834, 1835]. Now we only briefly recall the classical finite-dimensional Hamiltonian mechanics [Landau and Lifshitz, 1976, Goldstein, 2002].

Once a manifold $\mathbf{Q}$ with coordinates $\mathbf{q}$ is defined, a Lagrangian $\mathcal{L}(\mathbf{q}, \dot{\mathbf{q}})$ is used to construct an action integral,

$$\int_{t_0}^{t_1} \mathcal{L}(\mathbf{q}, \dot{\mathbf{q}}) dt. \tag{2.1}$$

The stationary points (curves) of the action, which describe motion of the physical system parametrized by coordinates $\mathbf{q}$, are solutions to the Euler-Lagrange equations, which can be rewritten as Hamilton canonical equations,

$$\begin{pmatrix} \dot{\mathbf{q}} \\ \dot{\mathbf{p}} \end{pmatrix} = \underbrace{\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}}_{=\mathbf{L}} \cdot \begin{pmatrix} H_{\mathbf{q}} \\ H_{\mathbf{p}} \end{pmatrix}. \tag{2.2}$$

Momentum $\mathbf{p} = \frac{\partial L}{\partial \dot{\mathbf{q}}}$ and the Hamiltonian $H(\mathbf{q}, \mathbf{p}) = -L(\mathbf{q}, \dot{\mathbf{q}}(\mathbf{q}, \mathbf{p})) + \dot{\mathbf{q}}(\mathbf{q}, \mathbf{p}) \cdot \mathbf{p}$ come from the velocity $\dot{\mathbf{q}}$ and Lagrangian $\mathcal{L}$ by Legendre transformation. From Equation (2.2), we can see that the evolution of position and momentum is given by an operator $\mathbf{L}$ (here just a matrix) and by derivatives of the Hamiltonian (here denoted by subscripts). The operator $\mathbf{L}$ is called a Poisson bivector, it is skew-symmetric and twice contravariant on the manifold $\mathcal{M} = T^*\mathbf{Q}$ (the cotangent bundle of $\mathbf{Q}$). In the inertial reference frames, the Hamiltonian coincides with the energy of the system[3].

Time evolution of any functional F of the state variables $\mathbf{q}$ and $\mathbf{p}$ can be expressed as

$$\dot{F}(\mathbf{q}(t), \mathbf{p}(t)) = \{F, E\}^{(CM)}, \tag{2.3}$$

where $\{\bullet, \bullet\}^{(CM)}$ is the canonical Poisson bracket of classical mechanics,

$$\{F, G\}^{(CM)} = F_{q^i} G_{p_i} - G_{q^i} F_{p_i}. \tag{2.4}$$

Equation (2.3) looks different from the Hamilton canonical equations (2.2), both are equivalent.

Poisson bivector $\mathbf{L}$ in classical mechanics can be also seen as the inverse of the symplectic two-form, and Hamilton canonical equations represent evolution

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[3] Note that in non-inertial reference frames, the connection between energy and Hamiltonian is less direct[Strocchi, 2018].

within symplectic geometry [Fecko, 2006]. However, the Poisson bivectors in continuum mechanics will typically be non-invertible, breaking the direct connection with symplectic geometry. Therefore, we have to introduce the more general Poisson geometry.

2.2 Hamiltonian mechanics and Poisson geometry

Poisson geometry can be seen as a generalization of symplectic geometry, allowing for non-invertible Poisson bivectors and for additional conserved quantities than those obtained by the Noether theorem [Goldstein, 2002]. From the geometric perspective, the reason is that the manifold of state variables is typically not a cotangent bundle, but rather a Lie group, Lie algebra, or its dual.

Consider a space $\mathcal{M}$ (or manifold) with local coordinates $\mathbf{x}$ (state variables). Kinematics of the state variables is expressed by a Poisson bracket, which may be different from the Poisson bracket of classical mechanics (2.4). In general, a Poisson bracket is a bilinear mapping taking two functionals from a space of functionals over $\mathcal{M}$, $\mathcal{F}(\mathcal{M})$, and giving another functional from $\mathcal{F}(\mathcal{M})$, $\{\mathcal{F}(\mathcal{M}),\mathcal{F}(\mathcal{M})\} \mapsto \mathcal{F}(\mathcal{M})$. Moreover, it has the following properties:

$$\text{skew-symmetry}: \quad \{F,G\} = -\{G,F\}, \tag{2.5a}$$

$$\text{Leibniz rule}: \quad \{FG,H\} = F\{G,H\} + \{F,H\}G, \tag{2.5b}$$

$$\text{and Jacobi identity}: \quad \{F,\{G,H\}\} + \{G,\{H,F\}\} + \{H,\{F,G\}\} = 0 \tag{2.5c}$$

for all admissible[4] functionals F, G, and H. Evolution of any functional $F \in \mathcal{F}(\mathcal{M})$ and the evolution of the state variables are then prescribed as[5]

$$\dot{F} = \{F,E\} \quad \text{and} \quad \dot{x}^i = L^{ij} E_{x^j}, \tag{2.6}$$

and the relations between a Poisson bivector and the corresponding Poisson bracket are

$$\{F,G\} = \langle F_{\mathbf{x}} | \mathbf{L} | G_{\mathbf{x}} \rangle \quad \text{and} \quad L^{ij} = \{x^i, x^j\}. \tag{2.7}$$

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[4] Admissible so that the mathematical operations are well defined [Ebin and Marsden, 1970].

[5] The equivalence between the evolution of functionals and evolution of state variables can be shown by the chain rule, as long as we have solutions in the classical sense [Evans, 1998].

The right hand side of the latter equation in (2.6) can be interpreted as components of the Hamiltonian vector field

$$\mathbb{X} = X^i \frac{\delta}{\delta x^i} = L^{ij} E_{x^j} \frac{\delta}{\delta x^i} = \mathbf{L}|dE\rangle, \tag{2.8}$$

which can be also seen as the action of the Poisson bivector $\mathbf{L} = L^{ij} \frac{\delta}{\delta x^i} \otimes \frac{\delta}{\delta x^j}$ on the differential of energy $dE = E_{x^i} dx^i$. In order to cover also field theories, we use the functional derivatives $\delta \bullet / \delta \bullet$ and the contraction between two indexes then stands for integration (L^2 scalar product) or the duality in the sense of distributions [Courant and Hilbert, 2008, Roubíček, 2005, Evans, 1998].

What is the meaning of properties (2.5), that any Poisson bracket has to satisfy? From the skew-symmetry of the Poisson bracket, one obtains the first law of thermodynamics,

$$\dot{E} = \{E, E\} = -\{E, E\} = 0, \tag{2.9}$$

the law of conservation of energy. Therefore, we shall be restricted to isolated systems in inertial Galilean reference frames, where the Hamiltonian coincides with the energy [Strocchi, 2018] and where energy is conserved. The second property (Leibniz rule) tells that biasing energy by a constant has no effect on the evolution equations. Finally, Jacobi identity can be interpreted as a requirement of self-consistency of the Hamiltonian evolution. Indeed, it is equivalent to the equation $\mathcal{L}_{\mathbb{X}} \mathbf{L} = 0$, expressing that the Lie derivative of the Poisson bivector field with respect to the Hamiltonian vector field is zero, or that the Poisson bivector is passively advected by the Hamiltonian flow [Fecko, 2006].

Due to the possible degeneracy of the Poisson bivector, Poisson brackets admit additional conserved quantities, Casimirs (here denoted by S), for which it holds that

$$\{S, G\} = 0 \quad \forall G \in \mathcal{F}(\mathcal{M}). \tag{2.10}$$

For instance entropy is a typical Casimir of the Poisson brackets, as we shall see later. Poisson brackets admitting Casimirs are non-canonical (they can not be transformed to the canonical form).

The Poisson bracket of classical mechanics originates from the principle of least action and subsequent interpretation of the Euler-Lagrange equations as dynamics on the cotangent bundle. Where do non-canonical Poisson brackets come from? They can be obtained by variation of action on a Lie group, where only variations respecting the Lie group are allowed [Arnold, 1966], and by reduction from more detailed Poisson brackets [Pavelka et al., 2016]. Let us first discuss the former possibility.

2.3 Rigid body motion

In this section we show how a non-canonical Poisson bracket is brought up when describing a freely rotating rigid body. Motion of the rigid body can be seen as motion within the Lie group $SO(3)$, which consists of all rotations in the three-dimensional Euclidean space [Poincaré, 1901]. Let us denote by $\mathbf{X}$ (Lagrangian coordinates) the position of a material point in a frame co-rotating with the rigid body (body frame). The position of the point in the laboratory space (Eulerian coordinates) can be then expressed as $\mathbf{x} = \mathbf{R} \cdot \mathbf{X}$ where $\mathbf{R} \in SO(3)$ is an (orthogonal) rotation matrix. When we differentiate this relation with respect to time, we obtain the velocity $\dot{\mathbf{x}} = \mathbf{v}$ in terms of the rotation matrix,

$$\mathbf{v} = \dot{\mathbf{R}} \cdot \mathbf{X} = \underbrace{\dot{\mathbf{R}} \cdot \mathbf{R}^{-1}}_{=\hat{\boldsymbol{\omega}}} \cdot \mathbf{x}, \tag{2.11}$$

where $\hat{\boldsymbol{\omega}}$ is a skew-symmetric angular velocity matrix (an element of the Lie algebra $\mathfrak{so}(3)$). Transformation of this matrix into the body frame,

$$\hat{\boldsymbol{\Omega}} = \mathbf{R}^{-1} \cdot \hat{\boldsymbol{\omega}} \cdot \mathbf{R} = \mathbf{R}^{-1}\dot{\mathbf{R}}, \tag{2.12}$$

is called the body angular velocity. Because this matrix is skew-symmetric, it can be represented by the pseudovector of body angular velocity $\boldsymbol{\Omega}$ such that $\hat{\boldsymbol{\Omega}} \cdot \mathbf{X} = \boldsymbol{\Omega} \times \mathbf{X}$, which leads to formula

$$\mathbf{R}^{-1} \cdot \dot{\mathbf{R}} \cdot \mathbf{X} = \boldsymbol{\Omega} \times \mathbf{X} \qquad \forall \mathbf{X}. \tag{2.13}$$

Varying $\mathbf{R}$ and Ω in formula (2.13), we obtain that the variations of $\boldsymbol{\Omega}$ are constrained to

$$\delta\Omega = \dot{\boldsymbol{\Sigma}} + \Omega \times \boldsymbol{\Sigma}, \tag{2.14}$$

where $\boldsymbol{\Sigma}$ is the pseudovector corresponding to the skew-symmetric matrix $\hat{\boldsymbol{\Sigma}} = \mathbf{R}^{-1} \cdot \delta\mathbf{R} \in \mathfrak{so}(3)$. Details of the calculation can be found in [Marsden and Scheurle, 1993], and an introduction to Lie groups and algebras in [Fecko, 2006]. So far we have recalled kinematics on the group $SO(3)$, including the form of admissible variations within the Lie algebra $\mathfrak{so}(3)$.

Let us now proceed to the variational principle. The kinetic energy of the rotating rigid body,

$$T = \int \frac{1}{2}\rho_0 \mathbf{v}^2 d\mathbf{X}, \tag{2.15}$$

can be also expressed in terms of the angular velocity, using equation (2.11), as

$$T = \frac{1}{2} I^{ij}\Omega_i\Omega_j, \quad \text{where} \quad I^{ij} = \int \left(\mathbf{X}^2\delta^{ij} - X^i X^j\right) d\mathbf{x} \tag{2.16}$$

is the tensor of inertia. Because we have the freedom to choose the body reference frame, we choose it so that the tensor of inertia becomes diagonal, $\mathbf{I} = \mathrm{diag}(I_x, I_y, I_z)$ with $I_x \leq I_y \leq I_z$. Variation of action

$$\delta \int_{t_0}^{t_1} T(\mathbf{\Omega}) dt \tag{2.17}$$

respecting constraint (2.14) leads to the Euler-Lagrange equation

$$\frac{d}{dt}\left(\mathbf{I}\cdot\mathbf{\Omega}\right) = \left(\mathbf{I}\cdot\mathbf{\Omega}\right) \times \mathbf{\Omega}, \tag{2.18}$$

where $\mathbf{I}$ is the tensor of inertia.

Similarly as in the case of classical mechanics in Section 2.1, we interpret the Euler-Lagrange equation in terms of a state variable dual to the velocity, the angular momentum in the body frame, $\mathbf{M} = \frac{\partial T}{\partial \mathbf{\Omega}}$. Because the angular velocity Ω is an element of the Lie algebra $\mathfrak{so}(3)$, derivative of a functional with respect to the angular velocity is in the dual space, $\mathbf{M} \in \mathfrak{so}(3)^*$. Euler-Lagrange equation (2.18) then becomes

$$\dot{\mathbf{M}} = \mathbf{M} \times \frac{\partial E}{\partial \mathbf{M}} = \{\mathbf{M}, E\}^{(SO(3)}, \tag{2.19}$$

with Hamiltonian

$$E = \frac{1}{2}\left(\frac{M_x^2}{I_x} + \frac{M_y^2}{I_y} + \frac{M_z^2}{I_z}\right) \tag{2.20}$$

obtained from the Lagrangian T by Legendre transformation. The Poisson bracket of rigid body mechanics is

$$\{F, G\}^{(SO(3))} = -\mathbf{M}\cdot\left(\frac{\partial F}{\partial \mathbf{M}} \times \frac{\partial G}{\partial \mathbf{M}}\right) \qquad \forall F(\mathbf{M}) \quad \text{and} \quad G(\mathbf{M}). \tag{2.21}$$

From the geometrical point of view, bracket (2.21) is a prototype of so called Lie-Poisson brackets, which provide Hamiltonian evolution on Lie algebra duals [Marsden and Ratiu, 1999].

Similarly as the Poisson bracket of classical mechanics corresponds to the canonical Poisson bivector, Poisson bracket (2.21) corresponds to Poisson bivector

$$L^{ij} = -M_k \varepsilon^{kij}. \tag{2.22}$$

In contrast with the canonical case, however, this bivector is not constant. Moreover, the rigid body Poisson bracket allows for conserved quantities that are not connected with symmetries of the Hamiltonian through the Noether theorem [Landau and Lifshitz, 1976]. When we consider a function of the magnitude of $\mathbf{M}$, $S(\mathbf{M}^2)$, the value of the function is conserved,

$$\dot{S} = \{S, E\}^{(SO(3))} = -M_i \varepsilon_{ijk} \frac{\partial S}{\partial(\mathbf{M}^2)} 2 M_j E_{m_k} = 0, \tag{2.23}$$

as follows from the simultaneous symmetry and skew-symmetry with respect to swapping $i \leftrightarrow j$. Bracket (2.21) has thus Casimir functions $S(\mathbf{m}^2)$, which are conserved regardless the choice of energy. This means that the angular momentum observed from the body frame does not change its magnitude[6]

In summary, variation of action on Lie groups leads to non-canonical Poisson brackets, which can have Casimir functionals. Let us now explore another way towards Poisson brackets. We shall start with a Poisson bracket on a detailed level of description, define a mapping to a less detailed level, and obtain another Poisson bracket on the less detailed level.

2.4 Lagrangian continuum mechanics

In Lagrangian continuum mechanics, each material point has a Lagrangian label $\mathbf{X}$. These labels then form a continuous manifold of Lagrangian points. The position of each Lagrangian point within the laboratory frame is expressed by the Lagrange$\mapsto$Euler mapping $\mathbf{x}(t, \mathbf{X})$, and the Lagrangian then depends on the position mapping $\mathbf{x}$ and its derivatives, $L(\mathbf{x}, \partial_t \mathbf{x}, \partial_{\mathbf{X}} \mathbf{x})$. Similarly as in classical particle mechanics, the principle of stationary action then

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[6] Notice, however, that the direction of $\mathbf{M}$ varies in time. It is the angular momentum in the laboratory frame stays constant while the angular momentum in the body frame evolves [Landau and Lifshitz, 1976].

leads to the Hamilton canonical equations on the Lagrangian manifold,

$$\partial_t x^i = E_{M_i} \tag{2.24a}$$

$$\partial_t M_i = - E_{x^i}, \tag{2.24b}$$

where the Lagrangian momentum density $\mathbf{M}(t, \mathbf{X})$ is the Legendre conjugate of the velocity $\partial_t \mathbf{x}$. Note that the subscripts stand for the functional derivatives. Hamilton canonical Equations (2.24) are also generated by the canonical Poisson bracket of Lagrangian mechanics,

$$\{F, G\}^{(\text{Lagrange})} = \int \left(\frac{\delta F}{\delta x^i} \frac{\delta G}{\delta M_i} - \frac{\delta G}{\delta x^i} \frac{\delta F}{\delta M_i} \right), \tag{2.25}$$

which can be seen as the infinite-dimensional version of the Poisson bracket of classical mechanics.

The energy consists of the kinetic energy and elastic energy,

$$E = \int \left(\frac{\mathbf{M}^2(t, \mathbf{X})}{2\rho_0(\mathbf{X})} + \rho_0(\mathbf{X}) W \left(\frac{\partial \mathbf{x}(t, \mathbf{X})}{\partial \mathbf{X}} \right) \right) d\mathbf{X}, \tag{2.26}$$

where $\rho_0(\mathbf{X})$ is a constant-in-time reference mass density. Finally, by plugging this energy into Hamilton canonical equations (2.24), we get

$$\partial_t x^i = \frac{M^i}{\rho_0} \tag{2.27a}$$

$$\partial_t M_i = \frac{\partial}{\partial X^I} \left(\rho_0 \frac{\partial W}{\partial \frac{\partial x^i}{\partial X^I}} \right), \tag{2.27b}$$

which are the evolution equations for Lagrangian elasticity in large deformations with position and momentum density as the state variables. Although these equations might appear simple, they contain a large amount of information because position of each material point is known. Instead, we can focus on some overall properties of the continuum like mass and momentum densities, which is the point of the following section.

2.5 Eulerian continuum mechanics

In Eulerian continuum mechanics, we no longer track each material point. Moreover, it is easier in this setting to introduce dissipation because the Eulerian equations are formulated in the laboratory frame, not in the abstract

Lagrangian frame. The Hamiltonian structure of Lagrangian mechanics is translated to a Hamiltonian structure in the Eulerian frame, as shown for instance by Beris and Edwards [Beris and Edwards, 1994]. Here, however, we choose more detailed Eulerian state variables, namely mass density, momentum density, entropy density, and the distortion field, which are defined in terms of the Lagrangian variables as

$$\begin{aligned}
\rho(\mathbf{x}) &= \rho_0(\mathbf{X}(\mathbf{x})) \cdot \det \frac{\partial \mathbf{X}}{\partial \mathbf{x}} && \text{(2.28a)}\\
\mathbf{m}(\mathbf{x}) &= \mathbf{M}(\mathbf{X}(\mathbf{x})) \cdot \det \frac{\partial \mathbf{X}}{\partial \mathbf{x}} && \text{(2.28b)}\\
s(\mathbf{x}) &= s_0(\mathbf{X}(\mathbf{x})) \cdot \det \frac{\partial \mathbf{X}}{\partial \mathbf{x}} && \text{(2.28c)}\\
A^I{}_i(\mathbf{x}) &= \frac{\partial X^I}{\partial x^i}, && \text{(2.28d)}
\end{aligned}$$

respectively. For simplicity, we do not write the explicit dependence on time. Distortion is the inverse of the deformation gradient evaluated at the Eulerian coordinate and thus it measures the deformation [Landau et al., 1986]. With these state variables, we can express the conservation laws of mass, momentum, and energy, the second law of thermodynamics (after introducing dissipation), as well as the deformations of the continuum. Moreover, both fluids and solids can be described using the same set of state variables and their evolution equations thus share the same structure [Godunov and Romenskii, 2003].

Plugging functionals dependent only on the Eulerian fields (2.28) into Poisson bracket (2.25), we obtain the Eulerian Poisson bracket

$$\begin{aligned}
\{F,G\}^{(A)} &= \{F,G\}^{(FM)} - \int A^L{}_i (F_{A^L{}_l} \partial_l G_{m_i} - G_{A^L{}_l} \partial_l F_{m_i})\, d\mathbf{x}\\
&\quad - \int \partial_i A^L{}_l (F_{A^L{}_l} G_{m_i} - G_{A^L{}_l} F_{m_i})\, d\mathbf{x}, \qquad \text{(2.29)}
\end{aligned}$$

which consists of the Poisson bracket of fluid mechanics,

$$
\begin{aligned}
\{F,G\}^{(FM)} = \int \rho(\partial_i F_\rho G_{m_i} - \partial_i G_\rho F_{m_i})\, d\mathbf{x} \\
+ \int m_i(\partial_j F_{m_i} G_{m_j} - \partial_j G_{m_i} F_{m_j})\, d\mathbf{x} \\
+ \int s(\partial_i F_s G_{m_i} - \partial_i G_s F_{m_i})\, d\mathbf{x},
\end{aligned}
\tag{2.30}
$$

and a part expressing kinematics of the distortion field $\mathbf{A}$ [Pavelka et al., 2020b]. The evolution equations given by bracket (2.29) are

$$
\begin{aligned}
\partial_t \rho &= -\partial_i(\rho E_{m_i}) && (2.31a)\\
\partial_t m_i &= -\partial_j(m_i E_{m_j}) - \rho\partial_i E_\rho - m_j \partial_i E_{m_j} - s\partial_i E_s - A^L{}_l \partial_i E_{A^L{}_l} \\
&\quad +\partial_i(A^L{}_l E_{A^L{}_l}) - \partial_l(A^L{}_i E_{A^L{}_l}) && (2.31b)\\
\partial_t s &= -\partial_i(s E_{m_i}), && (2.31c)\\
\partial_t A^L{}_l &= -\partial_l(A^L{}_i E_{m_i}) + (\partial_l A^L{}_i - \partial_i A^L{}_l) E_{m_i} && (2.31d)
\end{aligned}
$$

and they can be used to describe for instance Eulerian elasticity in large deformations or non-Newtonian fluids. Equations (2.31) represent the reversible part of the Symmetric Hyperbolic Thermodynamically Compatible (SHTC) equations [Godunov, 1972, Godunov and Romensky, 1995, Dumbser et al., 2016, Peshkov et al., 2018], which is an approach towards continuum thermodynamics suitable large scale numerical computations [Reinarz et al., 2020] including shock waves and acoustic waves. It is also possible to transform the distortion to its inverse, which leads to evolution equation for the Eulerian deformation gradient [Hütter and Tervoort, 2009].

If the energy depends only on the left Cauchy-Green tensor, $B^{ij} = F^i{}_I F^j{}_J G^{IJ}$, where $\mathbf{F} = \mathbf{A}^{-1}$ and G^{IJ} is the inverse material metric (typically identity), Poisson bracket (2.29) can be reduced to a Poisson bracket with the left Cauchy-Green tensor (6 independent components) instead of distortion (9 components). For functionals that depend only on variables $(\rho, \mathbf{m}, s, \mathbf{B})$, we then obtain Poisson bracket

$$
\begin{aligned}
\{F,G\}^{(LCG)} &= \{F,G\}^{(FM)} \\
&\quad + \int \left(F_{B^{ik}}(B^{jk}\partial_j G_{m_i} + B^{ji}\partial_j G_{m_k}) - G_{B^{ik}}(B^{jk}\partial_j G_{m_i} + B^{ji}\partial_j F_{m_k})\right)\, d\mathbf{x} \\
&\quad - \int \partial_j B^{ik}(F_{B^{ik}} G_{m_j} - G_{B^{ik}} F_{m_j})\, d\mathbf{x},
\end{aligned}
\tag{2.32}
$$

which gives evolution equations

$$\partial_t \rho = -\partial_i(\rho E_{m_i}) \tag{2.33a}$$

$$\begin{aligned}\partial_t m_i = {} & -\partial_j(m_i E_{m_j}) - \rho\partial_i E_\rho - m_j \partial_i E_{m_j} - s\partial_i E_s - B^{jk}\partial_i E_{B^{jk}} \\ & +\partial_i(B^{jk}E_{B^{jk}}) + \partial_j(B^{jk}(E_{B^{ik}} + E_{B^{ki}}))\end{aligned} \tag{2.33b}$$

$$\partial_t B^{ik} = -E_{m_j}\partial_j B^{ik} + B^{jk}\partial_j E_{m_i} + B^{ji}\partial_j E_{m_k} \tag{2.33c}$$

$$\partial_t s = -\partial_i(s E_{m_i}). \tag{2.33d}$$

The equation for distortion in the SHTC equations (2.31) is replaced by an equation for $\mathbf{B}$ containing the upper-convected derivative (note that the velocity is $\mathbf{v} = E_{\mathbf{m}}$). In contrast to the traditional non-equilibrium continuum thermodynamics [Truesdell, 1984], the upper-convected derivative does not need to be assumed; it follows directly from Hamiltonian mechanics.

Equations (2.31) can be also interpreted in the context of the natural configurations framework [Rajagopal and Srinivasa, 2004, Málek et al., 2018, Leonov, 1976], where evolution of continuum is described using three configurations: a reference configuration, a natural configuration, and an actual configuration. Here, the reference configuration is the manifold of Lagrangian labels $\mathbf{X}$, and the actual configuration is the Eulerian laboratory frame $\mathbf{x}$. After introducing dissipation, which is done in Section 3 below, distortion can cease to be the gradient of the mapping from the actual configuration to the reference, $\mathbf{X}(t, \mathbf{x})$, but it goes from the actual configuration to the natural one [Pelech et al., 2020].

Moreover, when the functionals depend neither on the distortion field nor the left Cauchy-Green tensor, the kinematics is expressed only by the Poisson bracket of fluid mechanics (2.30) and the evolution equations are the compressible Euler equations,

$$\partial_t \rho = -\partial_i(\rho E_{m_i}) \tag{2.34a}$$

$$\partial_t m_i = -\partial_j(m_i E_{m_j}) - \rho\partial_i E_\rho - m_j \partial_i E_{m_j} - s\partial_i E_s \tag{2.34b}$$

$$\partial_t s = -\partial_i(s E_{m_i}). \tag{2.34c}$$

When we change the variables from the energetic representation (having entropy as a state variable) to the entropic representation (taking energy density $e(\rho, \mathbf{m}, s)$ instead), these equations become the laws of conservation of mass (or the continuity equation), momentum, and energy. The Poisson bracket of fluid mechanics can be also interpreted as the Lie-Poisson bracket on the Lie-algebra dual of volume diffeomorphisms, combined with the two vector spaces of the mass density and entropy density fields by means of semidirect products [Marsden et al., 1984].

The total entropy,

$$S = \int s \, d\mathbf{x}, \tag{2.35}$$

is a Casimir of the above Poisson brackets, that is $\{S, G\}^{(A)} = \{S, G\}^{(LCG)} = \{S, G\}^{(FM)} = 0$ for any functional G. Therefore, entropy is conserved by the Hamiltonian evolution regardless of the choice of energy. The second law of thermodynamics, which dictates that entropy of an isolated system must grow, will be satisfied after we add dissipative dynamics in Section 3.

So far, we have seen passages the from the Lagrangian continuum mechanics and bracket $\{\bullet, \bullet\}^{(\text{Lagrange})}$ to the Eulerian continuum mechanics with distortion and bracket $\{\bullet, \bullet\}^{(A)}$, and from the latter to fluid mechanics with Poisson bracket $\{\bullet, \bullet\}^{(FM)}$. Those two passages are reductions of Poisson brackets because they can not be carried out in the opposite directions. In the next section, we show another way towards Hamiltonian fluid mechanics, based on a reduction from kinetic theory.

2.6 Hamiltonian kinetic theory

Systems with many particles can be described for instance by means of positions $\mathbf{r}$ and momenta $\mathbf{p}$ of the particles, or by the probability distribution function dependent on those coordinates, $f(t, \mathbf{r}, \mathbf{p})$. The former way leads to molecular dynamics while the latter to kinetic theory. Similarly as particle mechanics is a Hamiltonian theory, kinetic theory, when disregarding the dissipative dynamics like inelastic collisions, is also Hamiltonian.

When the one-particle distribution function $f(t, \mathbf{r}, \mathbf{p})$ is the state variable, the Poisson bracket expressing evolution of the distribution function is

$$\{F, G\}^{(B)} = \int\int f \cdot \left(\frac{\partial F_f}{\partial r^i} \frac{\partial G_f}{\partial p_i} - \frac{\partial G_f}{\partial r^i} \frac{\partial F_f}{\partial p_i} \right) \mathrm{d}\mathbf{r}\mathrm{d}\mathbf{p}. \tag{2.36}$$

How to derive this bracket? From the geometric perspective, the bracket acts on the Lie algebra dual of the Lie group of canonical transformations [Marsden, 1982, Esen et al., 2019]. Alternatively, bracket (2.36) can be seen as the average of the canonical Poisson bracket (2.4) [Pavelka et al., 2018b].

The evolution equation given by the Boltzmann Poisson bracket is the reversible part of the Boltzmann equation,

$$\partial_t f = -\frac{\partial E_f}{\partial p_i}\frac{\partial f}{\partial r^i} + \frac{\partial E_f}{\partial r^i}\frac{\partial f}{\partial p_i}. \tag{2.37}$$

Similarly as in fluid mechanics, the total entropy[7]

$$S = \int\int \eta(f) \mathrm{d}\mathbf{r}\mathrm{d}\mathbf{p}, \tag{2.38}$$

is a Casimir of the Boltzmann Poisson bracket and is thus conserved. The Boltzmann Poisson bracket is non-canonical.

The Boltzmann Poisson bracket provides an alternative way towards Hamiltonian fluid mechanics by reduction to the state variables of fluid mechanics

$$\rho(t,\mathbf{r}) = \int m f \mathrm{d}\mathbf{p} \tag{2.39a}$$

$$\mathbf{m}(t,\mathbf{r}) = \int p_i f \mathrm{d}\mathbf{p} \tag{2.39b}$$

$$s(t,\mathbf{r}) = \int \eta(f) \mathrm{d}\mathbf{p}, \tag{2.39c}$$

where m is the mass of one particle. Plugging functionals dependent only on the state variables of fluid mechanics into Poisson bracket (2.36), we obtain the Poisson bracket of fluid mechanics (2.30), see [Pavelka et al., 2016]. Let us now consider an extension of fluid mechanics by coupling with the electromagnetic fields.

2.7 Hamiltonian electrodynamics of moving media

Electrodynamics of moving media combines electrodynamics with motion of matter, for instance with Hamiltonian fluid mechanics. The Poisson bracket for electromagnetic fields $\mathbf{D}$ and $\mathbf{B}$, which are the state variables in Hamiltonian electrodynamics, can be constructed from the canonical Poisson bracket for the electric displacement field $\mathbf{D}$ and the vector potential $\mathbf{A}$,

$$\{F,G\}^{(\mathbf{D},\mathbf{A})} = \int \left(F_{\mathbf{D}} \cdot G_{\mathbf{A}} - G_{\mathbf{D}} \cdot F_{\mathbf{A}}\right) \mathrm{d}\mathbf{r}, \tag{2.40}$$

---

[7] For instance, $\eta(f) = -k_B f(\ln(h^3 f) - 1)$ for ideal gases Callen [1960], Pavelka et al. [2018b].

by letting the functionals depend only on the $\mathbf{D}$ field and the magnetic field $\mathbf{B} = \nabla \times \mathbf{A}$ [Marsden and Weinstein, 1982]. Poisson bracket (2.40) then turns to

$$\{F, G\}^{(\mathrm{EM})} = \int \left(F_{D^i} \varepsilon^{ijk} \partial_j G_{B^k} - G_{D^i} \varepsilon^{ijk} \partial_j F_{B^k} \right) \mathrm{d}\mathbf{r}, \tag{2.41}$$

which is the electromagnetic Poisson bracket, leading to the vacuum Maxwell equations

$$(\partial_t D^i)_{\mathrm{rev}} = \varepsilon^{ijk} \partial_j E_{B^k} \tag{2.42a}$$

$$(\partial_t B^i)_{\mathrm{rev}} = -\, \varepsilon^{ijk} \partial_j E_{D^k}. \tag{2.42b}$$

Electric field and magnetic intensity in these evolution equations are defined as derivatives of energy,

$$\mathbf{E} = \frac{\delta E}{\delta \mathbf{D}} \qquad \text{and} \qquad \mathbf{H} = \frac{\delta E}{\delta \mathbf{B}}, \tag{2.43}$$

respectively. Finally, to complete the set of Maxwell equations, we have to add the other pair telling that $\nabla \cdot \mathbf{B} = 0$ and $\nabla \cdot \mathbf{D} = 0$ in vacuum. These equations follow from equations (2.42) by applying the divergence operator by subsequent integration in time.

How to combine Hamiltonian electrodynamics with fluid mechanics? A geometric way towards electrodynamics of moving media uses the theory of semidirect products [Marsden et al., 1984], letting the cotangent bundle of $\mathbf{D}$ and $\mathbf{A}$ be advected by the motion of the fluid [Esen et al., 2016, Vágner et al., 2021]. This results into Poisson bracket

$$
\begin{aligned}
\{F,G\}^{(\mathrm{mEMHD})}(\rho,\mathbf{m},s,\mathbf{D},\mathbf{B}) = {} & \{F,G\}^{(\mathrm{FM})} + \{F,G\}^{(\mathrm{EM})} \\
& + \int D^i \left(\partial_j F_{D^i} G_{m_j} - \partial_j G_{D^i} F_{m_j}\right) \mathrm{d}\mathbf{r} \\
& + \int \partial_j D^j (F_{m_i} G_{D^i} - G_{m_i} F_{D^i}) \mathrm{d}\mathbf{r} \\
& + \int D^j (F_{m_i} \partial_j G_{D^i} - G_{m_i} \partial_j F_{D^i}) \mathrm{d}\mathbf{r} \\
& + \int B^i \left(\partial_j F_{B^i} G_{m_j} - \partial_j G_{B^i} F_{m_j}\right) \mathrm{d}\mathbf{r} \\
& + \int \partial_j B^j (F_{m_i} G_{B^i} - G_{m_i} F_{B^i}) \mathrm{d}\mathbf{r} \\
& + \int B^j (F_{m_i} \partial_j G_{B^i} - G_{m_i} \partial_j F_{B^i}) \mathrm{d}\mathbf{r},
\end{aligned}
\tag{2.44}
$$

which expresses kinematics of electrodynamics in coupling with moving charged matter [Holm, 1986]. The evolution equations implied by this bracket contain for instance the Lorentz force, which is a consequence of the geometric coupling Pavelka et al. [2018b]. Moreover, this Hamiltonian mechanics may be enriched by including the polarization and magnetization as state variables [Vágner et al., 2021].

In order to write the equations in a closed form, we have to provide a formula for energy. In this case, the energy is

$$
E_{EMHD} = \int \left(\frac{1}{2}\rho\mathbf{v}^2 + \frac{1}{2}\mathbf{D}\cdot\boldsymbol{\epsilon}^{-1}\cdot\mathbf{D} + \frac{1}{2}\mathbf{B}\cdot\boldsymbol{\mu}^{-1}\cdot\mathbf{B} + \mathbf{v}\cdot(\mathbf{D}\times\mathbf{B}) + \varepsilon(\rho_\alpha, s)\right) \mathrm{d}\mathbf{r}.
\tag{2.45}
$$

The set evolution equations obtained from bracket (2.44) is invariant with respect to the to Galilean transformations [Le Bellac and Lévy-Leblond, 1973, Matolcsi, 1993]. In other words, Hamiltonian electrodynamics with matter seems to lead to a Galilean invariant theory of electromagnetism. In contrast with the old Hertz's theory [Hertz, 1890], no aether seems to be necessary.

Apart from the free charge ($\nabla \cdot \mathbf{D}$), polarization charge, its conjugate momentum, and magnetization can be also added to this geometric theory by means of semidirect products. This results in a system of evolution equations for deformable dielectrics admitting polarization waves and for deformable magnetic media [Vágner et al., 2021].

So far we have discussed several examples of Hamiltonian continuum mechanics and connections between them. The next section defines in which sense the mechanical equations are called reversible.

2.8 Reversibility and Onsager-Casimir reciprocal relations

What is the meaning of reversibility of evolution equations? Imagine a bunch of classical particles moving according to the Hamilton canonical equations. When we record a video of their motion, we can play it backwards, flipping the momenta and the time stepping. Such flipping is called the time-reversal transformation (TRT). Motion of the particles on the backward movie is described by the same equations as when playing the movie forwards. In other words, Hamilton canonical equations are invariant with respect to the time-reversal transformation. Quantities that are not affected by TRT are called even (for instance position, mass, energy, entropy, or electric field) while quantities that get an minus sign are called odd (for example momentum, velocity, or magnetic field). Even quantities are said to have parity $\mathcal{P}$ equal to one while odd quantities have $\mathcal{P} = -1$.

We have already seen that Hamilton canonical equations (2.2) are constructed from a Poisson bivector and energy. Since the canonical Poisson bivector is a constant matrix, it is even with respect to TRT and the following formula holds for the bivector,

$$TRT(L^{ij}) = -\mathcal{P}(x^i)\mathcal{P}(x^j)L^{ij} \qquad \forall i, j. \tag{2.46}$$

Note that in classical Hamiltonian mechanics $\mathbf{x} = (\mathbf{r}, \mathbf{p})$. Energy is not affected by TRT and is thus also even. Once condition (2.46) is satisfied for a Poisson bivector, the Hamiltonian evolution transforms under TRT as

$$\begin{aligned} \dot{x}^i = L^{ij}E_{x^j} \quad \overset{\text{TRT}}{\Rightarrow} \quad -\mathcal{P}(x^i)\dot{x}^i =& -\mathcal{P}(x^i)\mathcal{P}(x^j)L^{ij}\mathcal{P}(x^j)E_{x^j} \\ =& -\mathcal{P}(x^i)L^{ij}E_{x^j} \end{aligned} \tag{2.47}$$

and the image of Hamiltonian evolution under TRT is equivalent with the original equations.[8] Condition (2.46) can be thus seen as the condition of reversibility of Hamiltonian evolution.

---

[8] Note, however, that the TRT applies only infinitesimally in time.

Reversibility condition (2.46) is fulfilled by the canonical Poisson bivector, from which the reversibility is inherited by the Boltzmann Poisson bracket (2.36). Moreover, the condition of reversibility is valid in the case of mechanics of multiple particles, which similarly yields the reversibility of the Liouville equation (and of the underlying Poisson bracket). The Lagrangian Poisson bracket for continuum mechanics (2.25), which also fulfills condition (2.46), yields reversibility of all the implied Poisson brackets for Eulerian continuum mechanics with distortion, (2.29), with the left Cauchy-Green tensor, (2.30), as well as reversibility of the fluid mechanics Poisson bracket, (2.32). In other words, a Poisson bracket producing reversible evolution (satisfying condition (2.46)) generates a hierarchy of reversible Poisson brackets obtained by reductions from the original bracket.

Another consequence of the reversibility condition (2.46) are the Onsager-Casimir reciprocal relations (OCRR) [Onsager, 1931a,b, Casimir, 1945, Grmela, 1990],

(i) variables with the same parities, $\mathcal{P}(x^i) = \mathcal{P}(x^j)$, (2.48a)
are coupled through an symmetric operator,
(ii) but variables with opposite parities, $\mathcal{P}(x^i) = -\mathcal{P}(x^j)$,
are coupled through an skew-symmetric operator (2.48b)

with respect to simultaneous TRT and transposition [Öttinger, 2005, Esen et al., 2016, Pavelka et al., 2018b]. This might seem surprising, since OCRR are typically assigned to the irreversible part of the evolution [de Groot and Mazur, 1984], so we will illustrate OCRR for instance on the Poisson bivector of fluid mechanics,

$$L(\mathbf{r},\mathbf{r}') = \begin{pmatrix} 0 & \rho(\mathbf{r}')\frac{\partial\delta}{\partial\mathbf{r}'} & 0 \\ -\rho(\mathbf{r})\frac{\partial\delta}{\partial\mathbf{r}} & \mathbf{m}(\mathbf{r}')\frac{\partial\delta}{\partial\mathbf{r}'} - \mathbf{m}(\mathbf{r})\frac{\partial\delta}{\partial\mathbf{r}} & -\epsilon(\mathbf{r})\frac{\partial\delta}{\partial\mathbf{r}} + \frac{\partial\delta}{\partial\mathbf{r}'}p(\mathbf{r}') \\ 0 & \epsilon(\mathbf{r}')\frac{\partial\delta}{\partial\mathbf{r}'} - \frac{\partial\delta}{\partial\mathbf{r}}p(\mathbf{r}) & 0 \end{pmatrix}, \quad (2.49)$$

where $\delta = \delta(\mathbf{r} - \mathbf{r}')$. This operator is skew-symmetric, as each Poisson bivector. The terms coupling density with momentum (and vice versa) are even with respect to TRT. Therefore, the coupling between density (even) and momentum (odd) is skew-symmetric with respect to simultaneous TRT and transposition (using the adjoint operator). On the other hand, the terms coupling momentum with itself are odd and thus they provide symmetric coupling. Onsager-Casimir reciprocal relation are present already in purely Hamiltonian mechanics.

Another unusual consequence of Hamiltonian mechanics is a Riemannian structure on the state space of the state variables, discussed in the following section.

2.9 Riemannian structure of Hamiltonian mechanics of hydrodynamic type

Although Hamiltonian mechanics is generated by a skew-symmetric bivector while the metric tensor in Riemannian geometry is symmetric, these two concepts are intimately related. When the Poisson bivector contains only ultralocal terms (proportional to Dirac δ) and weakly non-local terms (proportional to $\nabla\delta$), it can be written in the following form,

$$L^{ij} = \{x^i(\mathbf{r}), x^j(\mathbf{r}')\} = g^{ij}(\mathbf{x}(\mathbf{r}))\partial_{\mathbf{r}}\delta(\mathbf{r}-\mathbf{r}') + b^{ij}_k(\mathbf{x}(\mathbf{r}))\partial_{\mathbf{r}}x^k\delta(\mathbf{r}-\mathbf{r}'). \quad (2.50)$$

If, moreover, the energy does not depend on gradients of the state variables, the Hamiltonian system is called of hydrodynamic type, and the Hamiltonian evolution equations can be rewritten as a system of quasilinear first-order equations,

$$\partial_t x^i = \left(g^{ik}\frac{\partial^2 e}{\partial x^k \partial x^j} + b^{ik}_j \frac{\partial e}{\partial x^k}\right)\partial_{\mathbf{r}} x^j. \quad (2.51)$$

Any Hamiltonian system of hydrodynamic type generates a pseudo-Riemannian geometry on the manifold of state variables and the inverse metric tensor g^{ij} can be read from the formula for the Poisson bivector (2.50) [Tsarëv, 1991, Dubrovin and Novikov, 1983].

If the metric tensor is non-degenerate ($\det g \neq 0$), then $b^{ij}_k = -g^{il}\Gamma^j_{lk}$ and Γ^j_{lk} are the Christoffel symbols of an affine connection. Moreover, the connection is then metric-compatible and Jacobi identity of the Poisson bracket yields zero curvature and torsion. Equations (2.51) can be then rewritten as

$$\partial_t x^i = g^{ij} e_{jk} \partial_{\mathbf{r}} x^k, \quad (2.52)$$

where $e_{ij} = \nabla_i \nabla_j e$ is the second covariant gradient of the energy density e. After multiplication of these equations by the second covariant gradient, which is symmetric and positive definite in the case non-degenerate metric and convex energy, the set of equations becomes symmetric hyperbolic [Friedrichs, 1978, Pavelka et al., 2020b]. Indeed, the matrix in front of the time-derivative is positive definite and the matrix in front of the spatial derivative is symmetric.

So far we have discussed the Hamiltonian structure of continuum mechanics. In the following text, Hamiltonian mechanics will be equipped with irreverible dynamics responsible for thermodynamic behavior.

3 Mutliscale non-equilibrium thermodynamics

"Thermodynamics is a funny subject. The first time you go through it, you don't understand it at all. The second time you go through it, you think you understand it, except for one or two small points. The third time you go through it, you know you don't understand it, but by that time you are so used to it, it doesn't bother you anymore."

— Arnold Sommerfeld [Angrist and Helper, 1967]

By thermodynamics, one often means classical equilibrium thermodynamics and its applications in heat engines. However, equilibrium thermodynamics is just a part of non-equilibrium thermodynamics, which describes also systems out of thermodynamic equilibrium. Is there a general structure behind non-equilibrium thermodynamics? And how to derive a less detailed non-equilibrium thermodynamic description from a more detailed theory? None of these questions has been answered satisfactorily so far, but we will discuss at least some partial answers.

3.1 Classical and multiscale non-equilibrium thermodynamics

Classical equilibrium thermodynamics stems from works of Carnot, Clausius, Joule, Kelvin, and others, and was given a geometric meaning by Gibbs [Carnot, 1824, Clausius et al., 1867, Gibbs, 1984]. A key concept in thermodynamics is the entropy, which has emerged when studying heat engines. Once the dependence of entropy on energy, volume, and number of moles of chemical constituents (the fundamental thermodynamic relation) is known, the equilibrium behavior of the macroscopic physical system is determined. Regarding evolution of the system, processes in classical thermodynamics are typically quasi-static, moving from one equilibrium state to another with infinitesimal velocity [Callen, 1960].

But what if the processes are faster than the time necessary for the equilibration of the system? The equilibrium description then turns inadequate, leading to *non-equilibrium thermodynamics*. In non-equilibrium thermodynamics, physical systems are described by more detailed state variables than the equilibrium variables (energy, volume, composition, and entropy). The state variables are then equipped with evolution equations, and future states of the system are determined by solving the equations [de Groot and Mazur, 1984].

Consider an isolated system in equilibrium (for instance a gas in a box), described by the equilibrium state variables. When it is brought out of the equilibrium by an external force, additional state variables on top of the equilibrium ones (for instance velocity of matter) start to play an important role. Which set of state variables is appropriate for description of the system? If the distribution of the velocities of particles of the gas is non-Maxwellian initially, the kinetic theory is most likely the appropriate level of description. However, after the time sufficient for restoring the Maxwellian distribution, hydrodynamics becomes compatible with the observed phenomena although it contains less details than the kinetic theory. And equilibrium thermodynamics will eventually become appropriate as the system reaches the equilibrium. In other words, any isolated physical system can be described on various levels of description and the less detailed levels become appropriate as the system gradually reaches the equilibrium. This is the *multiscale* character of non-equilibrium thermodynamics [Pavelka et al., 2018b].

The microscopic origin of classical equilibrium thermodynamics can be seen in statistical physics, where by maximization of entropy we obtain the equilibrium distribution function and the equilibrium fundamental thermodynamic relation [Landau and Lifschitz, 1969, Pavelka et al., 2018b]. And because classical equilibrium thermodynamics can be seen as the final stage of multiscale non-equilibrium thermodynamics, we can expect that non-equilibrium thermodynamics also follows from statistical physics. Statistical physics is actually a reduction method from more detailed levels (for instance from the knowledge of distribution function) to less detailed levels (for instance to the hydrodynamic fields). But in non-equilibrium thermodynamics there can still be some evolution on the less detailed level of description (unlike on the equilibrium level of description). Therefore, apart from the fundamental thermodynamic relation, we have to derive also the evolution equations on the less detailed level. Reduction of a detailed description to a fundamental thermodynamic relation on a less detailed level is called *static reduction* while reduction to the less detailed evolution equations is called *dynamic reduction.*

In contrast to mechanics, which is invariant with respect to the time-reversal transformation and thus reversible, thermodynamic behavior is irreversible [Pavelka et al., 2014]. Non-equilibrium thermodynamics thus contains both the reversible and irreversible dynamics. Splitting the evolution to reversible and irreversible is a cornerstone of the *General Equation for Non-Equilibrium Reversible-Irreversible Coupling (GENERIC)* [Grmela and Öttinger, 1997, Öttinger and Grmela, 1997], summarized in monographs [Öttinger, 2005, Pavelka et al., 2018b]. In GENERIC, the evolution equations of chosen state variables have two ingredients: Hamiltonian mechanics and gradient dynamics. The former, which is reversible and keeps both energy and entropy, was discussed in Section 2, while the latter, which is irreversible and produces entropy or diminishes energy, will be discussed now.

3.2 General Equation for Non-Equilibrium Reversible-Irreversible Coupling (GENERIC)

GENERIC was developed in 1997 by Grmela and Öttinger [Grmela and Öttinger, 1997, Öttinger and Grmela, 1997] as a non-equilibrium thermodynamic framework unifying fluid mechanics, kinetic theory, and mechanics of non-Newtonian fluids. The main idea is to combine Hamiltonian mechanics (given by a Poisson bracket and energy) and dissipative gradient dynamics (generated by a dissipation potential and entropy) [Dzyaloshinskii and Volovick, 1980, Grmela, 1984, Kaufman, 1984, Morrison, 1984, Gyarmati, 1970]. A connection between GENERIC and fluctuations, turning GENERIC to stochastic differential equations, was shown in monograph [Öttinger, 2005], and the hierarchical geometric structure of GENERIC was summarized in monograph [Pavelka et al., 2018b].[9]

To construct a model within GENERIC, one first needs to define a manifold $\mathcal{M}$ (or a vector space) of state variables $\mathbf{x} \in \mathcal{M}$ and four building blocks:

1. Poisson bracket $\{\bullet, \bullet\}$
2. energy functional $E(\mathbf{x})$
3. dissipation potential $\Xi(\mathbf{x}, \mathbf{x}^*)$

---

[9] Instead of a dissipation potential, it is also possible to use a bilinear positive semi-definite operator called dissipative bracket [Morrison, 1984, Öttinger, 2005]. When the dissipative bracket is symmetric, it is equivalent to a quadratic dissipation potential. The question whether non-symmetric dissipative brackets are necessary has been long debated [Hütter and Svendsen, 2013, Grmela, 2018].

4. entropy functional $S(\mathbf{x})$.

The former two blocks constitute the Hamiltonian (reversible) part while the latter two form the gradient (irreversible) part. Moreover, conjugate variables $\mathbf{x}^*$ are introduced as the derivatives of entropy, $\mathbf{x}^* = S_{\mathbf{x}}$. Within GENERIC, evolution on manifold $\mathcal{M}$ is given as the sum of the Hamiltonian part and the gradient part,

$$\partial_t \mathbf{x} = \{\mathbf{x}, E\} + \Xi_{\mathbf{x}^*}\Big|_{\mathbf{x}^*=S_{\mathbf{x}}}, \tag{3.1}$$

and since the Hamiltonian part has already been discussed in Section 2.2, we shall now focus on the gradient part.

To be consistent with the thermodynamics, the dissipation potential must satisfy the following conditions: (i) $\langle \mathbf{x}^*, \Xi_{\mathbf{x}^*}\rangle \geq 0 \quad \forall \mathbf{x}, \mathbf{x}^*$, (ii) $\Xi(\mathbf{x}, \bullet)$ has a minimum at $\mathbf{x}^* = 0$, and (iii) $\left\langle E_{\mathbf{x}}, \Xi_{\mathbf{x}^*}\Big|_{\mathbf{x}^*=S_{\mathbf{x}}}\right\rangle = 0$. Condition (i) expresses consistency with the second law of thermodynamics,

$$\dot{S} = \underbrace{\{S, E\}}_{=0} + \left\langle S_{\mathbf{x}}, \Xi_{\mathbf{x}^*}\Big|_{\mathbf{x}^*=S_{\mathbf{x}}}\right\rangle \geq 0, \tag{3.2}$$

noting that $\{S, E\} = 0$ because S is assumed to be a Casimir of the Poisson bracket. Condition (ii) expresses that the irreversible evolution disappears in the thermodynamic equilibrium, where $S_{\mathbf{x}} = 0$. Condition (iii) ensures the first law of thermodynamics,

$$\dot{E} = \underbrace{\{E, E\}}_{=0} + \left\langle E_{\mathbf{x}}, \Xi_{\mathbf{x}^*}\Big|_{\mathbf{x}^*=S_{\mathbf{x}}}\right\rangle = 0. \tag{3.3}$$

Entropy increases in GENERIC while energy is kept constant.[10]

Condition (i), expressing the second law of thermodynamics, is automatically satisfied for convex dissipation potentials [Pavelka et al., 2020a, Roubíček, 2005], which is why dissipation potentials are usually assumed convex. Due to condition (ii) (minimum at the origin), dissipation potentials can be considered quadratic near the equilibrium. A quadratic dissipation potential can

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[10] Note that for simplicity we assume only isolated or boundary-less systems, where fluxes of energy and entropy through the boundary disappear.

be expressed by a symmetric positive semi-definite operator $\mathbf{M}$, called the dissipative matrix,

$$\Xi = \frac{1}{2}\langle \mathbf{x}^* | \mathbf{M} | \mathbf{x}^* \rangle = \frac{1}{2} x^*_i M^{ij} x^*_j, \quad \mathbf{M} = \mathbf{M}^T, \quad \mathbf{M} \geq 0, \tag{3.4}$$

and GENERIC evolution (3.1) then becomes

$$\partial_t x^i = L^{ij} E_{x^j} + M^{ij} S_{x^j}, \tag{3.5}$$

where L^{ij} is the Poisson bivector corresponding to the Poisson bracket. Condition (ii) is then satisfied automatically and condition (i) follows from the positive semi-definiteness of the dissipative matrix. Condition (iii) is translated into the requirement that $M^{ij} E_{x^j} = 0 \quad \forall i$. This quadratic form of gradient dynamics has been developed by Landau and Ginzburg [Ginzburg and Landau, 1950] in the context of physics and by Otto in the context of mathematics [Otto, 2001].

An example of quadratic gradient dynamics in continuum thermodynamics is the Fourier heat conduction. The state variable is the field of total energy density e, the total entropy is a functional of e, typically $S = \int s(e(\mathbf{r})) d\mathbf{r}$, and dissipation potential is

$$\Xi^{(\text{Fourier})} = \int \frac{\lambda}{2} (\nabla e^*)^2 d\mathbf{r}. \tag{3.6}$$

Gradient dynamics generated by this dissipation potential then reads

$$\partial_t e = -\nabla \cdot (\lambda \nabla e^*) \Big|_{e^* = S_e} = -\nabla \cdot \left(\lambda \nabla T^{-1} \right), \tag{3.7}$$

where the inverse temperature is identified with the derivative of entropy with respect to the energy density. Heat flux is equal to $J_{\mathbf{q}} = \lambda \nabla T^{-1}$ and heat thus flows against the gradient of temperature. The non-negative material coefficient λ can depend on energy and is proportional to the thermal conductivity. The implied evolution equation for entropy density $s(e)$ is

$$\partial_t s = T^{-1} \partial_t e = -\nabla \cdot (\lambda T^{-1} \nabla T^{-1}) + \lambda (\nabla T^{-1})^2. \tag{3.8}$$

The former term on the right hand side represents negative divergence of the entropy flux $\mathbf{J}_s = J_{\mathbf{q}}/T$, which is the classical relation between heat and entropy fluxes [Landau and Lifschitz, 1969, Callen, 1960]. This relation can be seen as a consequence of gradient dynamics, but notice that it needs to be generalized in the context of hyperbolic heat conduction [Pavelka et al., 2018b], [Szücs et al., 2021]. The second term on the right hand side of Equation (3.8) is the entropy production, which is clearly non-negative and ensures the second law of thermodynamics.

Another quadratic example is the isothermal viscous dissipation.[11] It represents irreversible evolution in the equation for momentum density $\mathbf{m}$ and is generated by dissipation potential

$$\Xi^{(\text{viscous})} = \int \mu \mathbb{D}^2 d\mathbf{r}, \tag{3.9}$$

where $\mathbb{D} = \frac{T}{2}\left(\nabla \mathbf{m}^* + (\nabla \mathbf{m}^*)^T\right)$. Once evaluated at $\mathbf{m} = S_{\mathbf{m}} = -\mathbf{v}/T$, we obtain that $\mathbb{D} = \frac{1}{2}\left(\nabla \mathbf{v} + (\nabla \mathbf{v})^T\right)$, which is the usual symmetric velocity gradient (or strain rate). The full GENERIC evolution for momentum density in isothermal fluids is the combination of the Hamiltonian part (Equation (2.34b)) and derivative of dissipation potential (3.9),

$$\begin{aligned} \partial_t m_i &= -\partial_j(m_i E_{m_j}) - \partial_i p + \frac{\delta \Xi^{(\text{viscous})}}{\delta m^{*i}} \\ &= -\partial_j(m_i v^j) - \partial_i p + \partial_j\left(\mu(\partial_i v^j + \partial_j v^i)\right), \end{aligned} \tag{3.10}$$

where the pressure is equal to

$$p = -e + \rho\frac{\partial e}{\partial \rho} + m_j\frac{\partial e}{\partial m_j} + s\frac{\partial e}{\partial s}. \tag{3.11}$$

This formula is actually equivalent with the usual notion of pressure in systems with the local thermodynamic equilibrium Pavelka et al. [2018b].

Dissipation potentials for Fourier heat conduction and viscous dissipation involve spatial gradients, which is why they are called weakly non-local. Apart from these weakly non-local dissipation potentials, we often meet also ultralocal dissipation potentials, that involve no spatial gradients. Such dissipation potentials occur in chemical reactions [Grmela, 2012, Ajji et al., 2021], electrochemical reactions [Pavelka et al., 2015a], hyperbolic heat conduction, or plasticity [Dumbser et al., 2016, Godunov et al., 1996]. For instance the SHTC

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[11] For simplicity we neglect the bulk viscosity, treatment of which can be found in [Pavelka et al., 2018b], as well as the non-isothermal case.

equations have ultralocal dissipation potentials, where an irreversible term appears in the equation for distortion **A** and another term (entropy production) in the equation for entropy [Peshkov et al., 2018]. Similarly, in the case of dynamics of the left Cauchy-Green tensor **B**, an ultralocal dissipation potential can be used to formulate the Maxwell model of non-Newtonian fluids [Pelech et al., 2020]. An advantage of ultralocal dissipation potentials is that they do not alter the hyperbolic character of the evolution equations, but a disadvantage is that mathematical analysis (like proof of large-time existence and uniqueness of weak solutions) becomes difficult without the weakly non-local terms [Feireisl et al., 2016]. Anyway, gradient dynamics is responsible for dissipative behavior (raising entropy) and it produces irreversible evolution. Let us have a closer look at the meaning of irreversibility.

3.3 Time-reversal transformation and Onsager-Casimir reciprocal relations

The time-reversal transformation (TRT) is a tool that distinguishes between reversible and irreversible transformation, and we have already discussed it in the context of Hamiltonian mechanics in Section 2.8. We have already seen that Onsager-Casimir reciprocal relations (OCRR) are satisfied by Hamiltonian mechanics and now we will discuss TRT and OCRR in relation with the gradient dynamics. Both dissipation potentials and entropy are required to be even with respect to TRT, since flipping velocities of all particles could otherwise violate the second law of thermodynamics. Gradient dynamics then gets an extra minus sign under TRT with respect to the time derivative of the state variables,

$$\dot{x}^i = \frac{\delta \Xi}{\delta x^*_i} \quad \overset{\mathrm{TRT}}{\Rightarrow} \quad -\mathcal{P}(x^i)\dot{x}^i = \frac{\delta \Xi}{\delta x^*_i}\mathcal{P}(x^i), \tag{3.12}$$

while the reversible part was invariant with respect to TRT.

When the dissipation potential is quadratic, its evenness leads to the condition

$$\mathcal{P}(M^{ij}) = \mathcal{P}(x^i)\mathcal{P}(x^j). \tag{3.13}$$

For instance the Fourier dissipation potential (3.6) corresponds to the dissipative matrix

$$M^{(e(\mathbf{r}),e(\mathbf{r}'))} = \frac{\partial}{\partial r'^i}\frac{\partial}{\partial r^i}\left(\lambda T^2 \delta(\mathbf{r}-\mathbf{r}')\right), \tag{3.14}$$

which is symmetric with respect to swapping $e(\mathbf{r})$ and $e(\mathbf{r}')$ and even with respect to TRT. It is thus compatible with OCRR (2.48) because it provides coupling between state variables of the same parity (energy and energy). Both parts of GENERIC are automatically compatible with OCRR.

Dissipation potentials can typically be expressed in terms is their density ξ, where $\Xi = \int \xi d\mathbf{r}$, and the density is a function of *thermodynamic forces* $\boldsymbol{\mathfrak{X}}$. For instance, in the case of Fourier heat conduction we have $\xi^F = \frac{\lambda}{2}(\mathfrak{X}^F)^2$ and $\mathfrak{X} = \nabla e^*$. By interchanging the second derivatives, we obtain that

$$\frac{\partial^2 \xi}{\partial \mathfrak{X}_i \partial \mathfrak{X}_j} = \frac{\partial^2 \xi}{\partial \mathfrak{X}_j \partial \mathfrak{X}_i}, \tag{3.15}$$

which is a generalization of OCRR to the case of non-quadratic dissipation potentials. *Thermodynamic fluxes* corresponding to the thermodynamic forces are defined as $\mathfrak{J}^i = \frac{\partial \xi}{\partial \mathfrak{X}_i}$. One can then obtain additional Maxwell relations between the forces and fluxes, for example $\left(\frac{\partial \mathfrak{J}^1}{\partial \mathfrak{J}^2}\right)_{\mathfrak{X}_1} = \left(\frac{\partial \mathfrak{X}_2}{\partial \mathfrak{X}_1}\right)_{\mathfrak{J}^2}$ [Grmela et al., 2015], as well as a generalization of the Braun-Le Chatelier principle for gradient dynamics [Chatelier, 1884, Pavelka and Grmela, 2019]. Instead of expressing dissipation potentials in terms of the thermodynamic forces, we can carry out the Legendre transformation to the dual dissipation potentials, which depend on the thermodynamic fluxes. This brings us to the concept of dual gradient dynamics, studied in the following section.

3.4 Dual gradient dynamics and non-convex dissipation potentials

In dual gradient dynamics the dual dissipation potentials are expressed in terms of the thermodynamic fluxes rather than in terms of the forces, which provides a tool for analyzing non-convex dissipation potentials. The definition of thermodynamic fluxes can be also interpreted as a solution $\boldsymbol{\mathfrak{J}}(\boldsymbol{\mathfrak{X}})$ to the equation

$$\frac{\partial}{\partial \mathfrak{X}_i}\left(-\xi + \mathfrak{J}^i \mathfrak{X}_\mathrm{i}\right) = 0, \tag{3.16}$$

which is actually the Legendre transformation from $\xi(\boldsymbol{\mathfrak{X}})$ to the dual dissipation potential density,

$$\xi^*(\boldsymbol{\mathfrak{J}}) = -\xi(\boldsymbol{\mathfrak{X}}(\boldsymbol{\mathfrak{J}})) + \mathfrak{J}^i \mathfrak{X}_i(\boldsymbol{\mathfrak{J}}). \tag{3.17}$$

The inverse Legendre transformation, from ξ^* to ξ, reads

$$\frac{\partial}{\partial \mathfrak{J}^i}\left(-\xi^* + \mathfrak{J}^i \mathfrak{X}_i\right) = 0, \quad \text{or} \quad \frac{\partial \xi^*}{\partial \mathfrak{J}^i} = \mathfrak{X}_i. \tag{3.18}$$

If we have gradient dynamics

$$\dot{x}^i = \frac{\partial \xi}{\partial \mathfrak{X}_i}, \tag{3.19a}$$

then the dual gradient dynamics is

$$\frac{\partial \xi^*}{\partial \dot{x}^i} = \mathfrak{X}_i. \tag{3.19b}$$

Dual gradient dynamics is used for instance when describing the austenite-martensite transformations [Tůma et al., 2018] and the Legendre transformation is also behind the formulation of continuum thermodynamics based on the Gibbs energy [Průša et al., 2020].

Let us now turn to the possibility of non-convex dissipation potentials in non-Newtonian fluids. Convexity of the dissipation potential is a sufficient condition for fulfillment of the second law of thermodynamics, but not necessary. The irreversible part of the Cauchy stress can be obtained similarly as in the Newtonian case, as the irreversible term under the divergence in the momentum equation,

$$\mathbb{T} = \frac{\partial \xi}{\partial \mathbb{D}}. \tag{3.20}$$

This relation is a particular realization of gradient dynamics in terms of the forces and fluxes (3.19a).[12] While in the Newtonian case the stress is proportional to the strain rate, a nonlinear relation has been observed in non-Newtonian fluids [Olmsted, 2008]. In [Boltenhagen et al., 1997], the stress-strain rate relation for a non-Newtonian fluid was acquired (Figure 3) by putting the fluid between two concentric cylinders, one of which is static while the other rotating, and by measuring the angular velocity and forces exerted on the cylinders. They observed that when varying the shear stress

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[12] Note that the divergence operator in front of the stress tensor can be put into equation (3.19a), but we do not include it explicitly, for simplicity. Note also that we assume incompressibility until the end of this section. Therefore, we do not need to distinguish between $\mathbb{T}$ and its deviatoric part and between $\mathbb{D}$ and its deviatoric part explicitly. More details can be found in [Janečka and Pavelka, 2018].

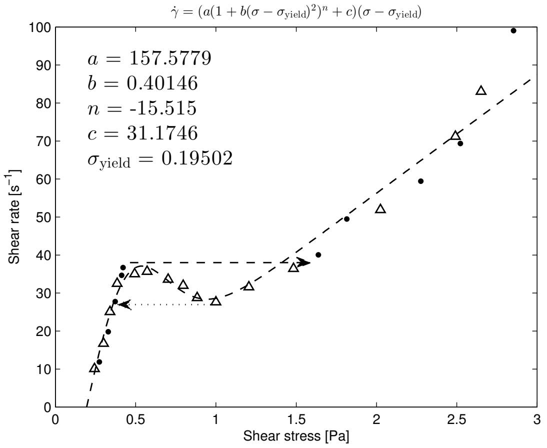

Figure 3: Steady-state stress/shear–rate behavior for a 7.5/7.5 mM TTAA/NaSal solution from the controlled shear stress (Δ) and controlled shear–rate (●) experiments [Boltenhagen et al., 1997]. The dashed arrow indicates the experimentally observed jump in shear stress while the dotted arrow indicates the expected jump when lowering shear rates (hysteresis), based on the theoretical analysis. Figure adapted from [Janečka and Pavelka, 2018].

(slowly increasing the external force rotating the outer cylinder), the shear rate behaves continuously. On the other hand, when varying the shear rate (slowly increasing the rotation rate), the shear stress exhibits a jump. What is the reason for such asymmetry? Let us answer this question by phenomenological means.

The strain–stress relation $\mathbb{D}(\mathbb{T})$ in Figure 3 can be obtained as dual gradient dynamics (3.19b)

$$\mathbb{D} = \frac{\partial \xi^*}{\partial \mathbb{T}} \tag{3.21}$$

with a dissipation potential motivated by Le Roux and Rajagopal [Le Roux and Rajagopal, 2013]. The dependence $\mathbb{D}(\mathbb{T})$, replacing $\mathbb{T}(\mathbb{D})$, is sometimes called an implicit constitutive relation [Málek et al., 2010, Perlácová and Průša, 2015]. Figure 4 shows the dual dissipation potential while Figure 5 displays dissipation potential ξ (obtained by the Legendre transformation of ξ^*). Since ξ is multi-valued (not being a function), it has to be split into several branches that are functions. On the other hand, the dual dissipation potential ξ^* is not multi-valued, which makes it easier to use than ξ. In the dissipation potential ξ in Figure 5, however, we can see an unstable branch ($C-D$), two metastable branches ($B-C$ and $D-E$), and two stable branches $A-B$ and $E-F$. Stability of the branches can be analyzed in a similar way as in classical thermodynamics [Callen, 1960] although here it is not caused

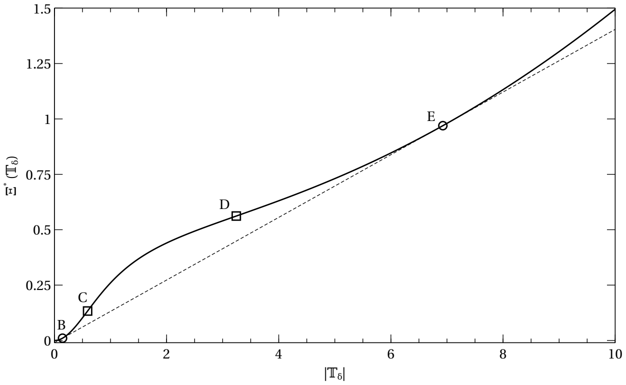

Figure 4: Dual dissipation potential $\xi^*(\mathbb{T})$. The region $C-D$ is not convex. The dashed tangent line $B-E$ indicates the convex hull of the potential and coincides with the Maxwell lever rule construction. The region $B-C$ and $D-E$ are convex. Figure adapted from [Janečka and Pavelka, 2018].

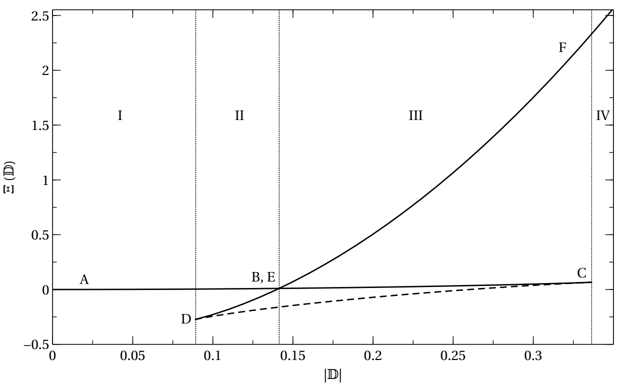

Figure 5: Dissipation potential $\xi(\mathbb{D})$ obtained by Legendre transformation of ξ^*. In regions II and III, the potential is multivalued and the dashed curve $C-D$ is an unstable branch. Curves $A-B$ and $E-F$ correspond to the convex hull of the dissipation potential ξ^*. Figure adapted from [Janečka and Pavelka, 2018].

by non-convexity entropy or free energy, but by the shape of the dissipation potential. Transition between the various branches can be then interpreted as a dissipative phase transition.

Let us now return to the question why behavior of the fluid is different when the stress is controlled from the case when the strain rate is controlled. When slowly raising the shear rate, we start in regime I in Figure 5, where shear stress is determined uniquely. After passing to regime II, another possible state appears, but the shear stress evolves continuously due to carefulness of the experimentalists (smallness of external perturbations). Passing also through regime III, point C (boundary between regimes III and IV) is reached, where the metastable state becomes unstable and the shear stress jumps to the stable state. That is why shear stress behaves discontinuously.

On the other hand, when slowly varying $\mathbb{T}$, there is always a unique value of $\mathbb{D}$, determined by slope of dissipation potential Ξ^* in Figure 4, and the slope varies continuously. That is why no jump in shear rate is observed in the experiment.

Moreover, it could be expected that when going back from high shear rates to the small ones, shear stress would fall as low as to point D, from which it would jump to the stable state on branch A. One should thus observe hysteresis in Figure 3, but no such experiment has been carried out.

The dual dissipation potential provides a phenomenological description of the observed experimental behavior. But how to derive such dissipation potential? Or how to derive dissipation potentials in general? There are several possibilities. If we know the statistical character of fluctuations of the state variables in terms of the theory of large deviations, a corresponding dissipation potential can be constructed [Mielke et al., 2014], using a generalized fluctuation-dissipation theorem [Mielke et al., 2016]. The dissipation potential can be also derived by a dynamic reduction from a more detailed dynamics, as in Section 3.6. Alternatively, if no such reduction is available, one can construct dissipation phenomenologically from purely Hamiltonian mechanics [Bloch et al., 1996, Pavelka et al., 2019b], which is discussed in the following section.

3.5 Ehrenfest regularization of Hamiltonian systems

Ehrenfest regularization is a method converting a purely Hamiltonian evolution to a partly dissipative evolution. Averaging Hamiltonian evolution (2.6) over time τ, we obtain, after an approximation, that

$$\frac{1}{\tau}\int_0^\tau \dot{x}^i dt = \frac{x^i(t+\tau)-x^i(t)}{\tau} \approx L^{ij}E_{x^j} + \frac{\tau}{2}\frac{\delta}{\delta x^k}\left(L^{ij}E_{x^j}\right)L^{kl}E_{x^l}. \tag{3.22}$$

Ehrenfest regularization [Pavelka et al., 2019a] is then the evolution equation

$$\dot{x}^i = L^{ij}E_{x^j} + \frac{\tau}{2}\frac{\delta}{\delta x^k}\left(L^{ij}E_{x^j}\right)L^{kl}E_{x^l}, \tag{3.23a}$$

which consists of the original Hamiltonian dynamics and an irreversible term (the second on the right hand side). The irreversible term increases all concave Casimirs of the underlying Poisson bracket, in particular the entropy ($\dot{S} \geq 0$), and reduces the energy ($\dot{E} \leq 0$).

Moreover, the irreversible term can be split into two contributions, leading to two other forms of Ehrenfest regularization. The entropic Ehrenfest regularization,

$$\dot{x}^i = L^{ij}E_{x^j} + \frac{\tau}{2}\frac{\delta}{\delta x^k}\left(L^{ij}\right)E_{x^j}L^{kl}E_{x^l}, \tag{3.23b}$$

conserves energy ($\dot{E} = 0$) and produces entropy ($\dot{S} \geq 0$), while the energetic Ehrenfest regularization,

$$\dot{x}^i = L^{ij} E_{x^j} + \frac{\tau}{2} L^{ij} E_{x^j x^k} L^{kl} E_{x^l}, \tag{3.23c}$$

reduces energy ($\dot{E} \leq 0$) and keeps the entropy ($\dot{S} = 0$).

Which form of Ehrenfest regularization to choose? It depends on the quantities that should be conserved. The energetic Ehrenfest regularization can be used for instance in the case of rigid body rotation, where the Casimir $\mathbf{M}^2$ (magnitude of angular momentum) is conserved while energy should decrease. We will explore this case in more detail below. On the other hand, the energetic Ehrenfest regularization can be used in the kinetic theory, providing growth of entropy while keeping the energy constant, which leads to kinetic equations with diffusion in space [Svärd, 2018].

The full Ehrenfest regularization (3.23a) is useful when constructing numerical schemes for non-canonical Hamiltonian mechanics. Indeed, using the forward Euler discretization of the full Ehrenfest regularization, (3.23a), while taking τ equal to the numerical time step dt, we obtain a numerical scheme conserving both energy and entropy up to the second order in dt. Numerical results for rigid body rotation are shown in Figure 6a.[13]

On the other hand, the energetic Ehrenfest regularization of rigid body mechanics leads to results in Figure 6b. While the magnitude of angular momentum is conserved, the energy is reduced. Although in the purely Hamiltonian case (without any regularization), rotations around both the axes with the lowest and the highest moments of inertia are stable, only the latter is stable after the regularization. Such behavior was observed for instance in the unexpected change of rotation of the Explorer 1 probe [Likins, 1966].

Although Ehrenfest regularization leads to systems with desired thermodynamic properties (entropy increasing or energy decreasing), it is only a phenomenological way to dissipative dynamics. Moreover, it does not provide any information about the value of the relaxation time τ. Ehrenfest regularization is, however, the first step in the Ehrenfest reduction, where dynamics on a detailed level of description is reduced to dynamics on a less detailed level [Gorban et al., 2001, Karlin et al., 2003, Pavelka et al., 2018a,b].

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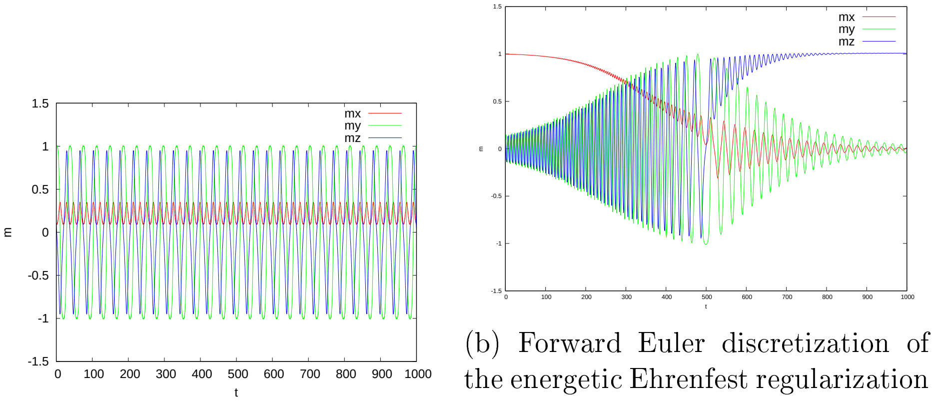
[13] The principal moments of inertia were chosen as $I_z > I_y > I_x$.



(a) Numerical results of the full Ehrenfest discretization (3.23a) for rigid body. The solution is periodic and preserves both energy and magnitude of angular momentum.

(b) Forward Euler discretization of the energetic Ehrenfest regularization (3.23c) of rigid body motion. Only pure rotation around the $z-$axis is stable (even asymptotically stable). Pure rotation around the minor $x-$axis becomes unstable because it has higher kinetic energy for given $\mathbf{M}^2$ than pure rotation around the major $z-$axis.

Figure 6: Evolution of components (m_x red, m_y green and m_z blue) of angular momentum of a rigid body observed from the body reference frame.

In the following section, we shall discuss another method that needs no a priori knowledge of the relaxation time.

3.6 Lack-of-fit reduction

The lack-of-fit reduction is a method of dynamic reduction, reducing a detailed level of description with the GENERIC structure to a less detailed GENERIC [Pavelka et al., 2020a]. Similar goal (albeit without the underlying GENERIC structure) is carried out for instance by the Chapman-Enskog reduction (requiring dissipative terms on the detailed level) [Chapman et al., 1990, de Groot and Mazur, 1984], projection operator techniques (often leading to integrodifferential equations) [Zwanzig, 2001], or the Ehrenfest reduction [Ehrenfest and Ehrenfest, 1990, Gorban et al., 2001, Karlin et al., 2003, Pavelka et al., 2018a]. A special feature of the lack-of-fit reduction, which was first proposed in [Turkington, 2013], is that it leads to the GENERIC structure and that dynamics on the lower level of description can be dissipative even if the detailed evolution is purely reversible. Moreover, the method contains no fitting parameters.

Let us consider an upper level (more detailed) with state variables $\mathbf{x} \in \mathcal{M}$, entropy ${}^{\uparrow}S(\mathbf{x})$, energy ${}^{\uparrow}E(\mathbf{x})$, Poisson bivector ${}^{\uparrow}\mathbf{L}(\mathbf{x})$, and dissipation potential ${}^{\uparrow}\Xi(\mathbf{x}, \mathbf{x}^*)$, which constitute the GENERIC building blocks for evolution

$$\dot{x}^i = {}^{\uparrow}L^{ij} \frac{\partial {}^{\uparrow}E}{\partial x^j} + \frac{\partial {}^{\uparrow}\Xi}{\partial x^*_i}\Big|_{\mathbf{x}^* = {}^{\uparrow}S_{\mathbf{x}}}. \tag{3.24}$$

A mapping $\boldsymbol{\pi}$ from the upper level $\mathcal{M}$ to a lower level $\mathcal{N}$ defines the less detailed state variables $\mathbf{y} = \boldsymbol{\pi}(\mathbf{x}) \in \mathcal{N}$. What is the autonomous dynamics on the less detailed level (expressed only in terms of state variables $\mathbf{y}$)?

First we have to carry out the static reduction which leads to the entropy and energy on the lower level (${}^{\downarrow}S(\mathbf{y})$ and ${}^{\downarrow}E(\mathbf{y})$). In the static reduction the lower-level entropy ${}^{\downarrow}S$ is obtained by evaluating the upper-level entropy ${}^{\uparrow}S$ at the MaxEnt values, $\mathbf{x}(\mathbf{y}^*(\mathbf{y}))$. The MaxEnt (maximum entropy) values are obtained by maximization of ${}^{\uparrow}S$ with the constraints that we know the value of $\mathbf{y}$, which gives the MaxEnt mapping $\mathbf{y} \mapsto \mathbf{y}^* \mapsto \mathbf{x}$. The image of the lower-level manifold $\mathcal{N}$ under this mapping is a submanifold of $\mathcal{M}$, called the MaxEnt submanifold. The MaxEnt mapping can be interpreted as a sequence of two Legendre transformations, a non-invertible one from $\mathbf{x}$ to $\mathbf{y}^*$ and an invertible from $\mathbf{y}^*$ to $\mathbf{y}$, as in Figure 7. Similarly, the lower-level energy ${}^{\downarrow}E(\mathbf{y}) = {}^{\uparrow}E(\mathbf{x}(\mathbf{x}^*(\mathbf{y})))$ is obtained by evaluating the upper-level energy at the MaxEnt image of $\mathbf{y}$.

$$\begin{tikzcd}
\mathbf{x} \arrow[r, leftrightarrow, "\text{LT}"] \arrow[d, "\boldsymbol{\pi}"'] & \mathbf{x}^* \\
\mathbf{y} \arrow[r, leftrightarrow, "\text{LT}"] & \mathbf{y}^* \arrow[ul, "\text{MaxEnt}"']
\end{tikzcd}$$

Figure 7: Relations between state variables on the upper level of description and the lower level and their conjugates. LT stands for Legendre transformations which are invertible. The MaxEnt mapping is not invertible.

After the static reduction, we can turn to the dynamic reduction, actually comparing the evolution equations on both levels. We are looking for a vector field[14] expressing evolution of the lower conjugate variables, $\dot{\mathbf{y}}^*$, [Turkington, 2013]. Imagine that we have such a vector field. Then residuum

$$R^i = \dot{x}^i - \frac{\partial x^i}{\partial y^*_a}\dot{y}^*_a = {}^{\uparrow}L^{ij}\frac{\partial {}^{\uparrow}\bar{E}}{\partial x^j} + \frac{\partial {}^{\uparrow}\Xi}{\partial x^*_i} - \frac{\partial x^i}{\partial y^*_a}\dot{y}^*_a \tag{3.25}$$

expresses the difference between the known vector field on the upper level (the right hand side of Equation (3.24)) on the MaxEnt submanifold and the MaxEnt mapping of the sought reduced dual vector field $\dot{\mathbf{y}}^*$. The residuum measures the lack of fit between those two vector fields on the MaxEnt submanifold [Pavelka et al., 2020a]. The lack-of-fit Lagrangian is then defined using the entropic norm (see [Gorban and Karlin, 2005]) of the residuum as

$$\mathcal{L}(\mathbf{y}^*(t), \dot{\mathbf{y}}^*(t)) = -\frac{1}{2}R^i(x(\mathbf{y}^*))\frac{\partial^2 {}^{\uparrow}S}{\partial x^i \partial x^j}\Big|_{\mathbf{x}(\mathbf{y}^*)} R^j(x(\mathbf{y}^*)), \tag{3.26}$$

where the MaxEnt values of $\mathbf{x}$ were substituted into the expressions on the upper level of description. Action

$$\int_{t_0}^{t_1} \mathrm{d}t\, \mathcal{L}(\mathbf{y}^*(t), \dot{\mathbf{y}}^*(t)) \tag{3.27}$$

is then minimized[15], keeping the initial time t_0 and the final state $\mathbf{y}^*_1$ fixed while letting the final time and the initial state vary. The reason is that as the final time t_1 approaches infinity, the final state $\mathbf{y}^*_1$ is expected to approach the thermodynamic equilibrium, determined by the maximum of entropy. The minimum of the action (denoted as $\Psi(t_1, \mathbf{y}^*_0)$) then depends on the final time and initial state.

How to find the extremal trajectory $\mathbf{y}^*(t)$? It is obtained by means of the Hamilton-Jacobi equations [Gelfand and Fomin, 2012],

$$-\frac{\partial \Psi}{\partial y^*_a} = \frac{\partial \mathcal{L}}{\partial \dot{y}^*_a}, \tag{3.28a}$$

$$\frac{\partial \Psi}{\partial t} = \mathcal{H}\left(t, y^*_1, -\frac{\partial \Psi}{\partial y^*_a}\right), \tag{3.28b}$$

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[14] Note that the right hand side of an evolution equation $\dot{x}^i = X^i$ can be interpreted as components of vector field $\mathbb{X} = X^i \frac{\partial}{\partial x^i}$.

[15] Note that the minus sign makes the Lagrangian positive definite, since the second differential of entropy is negative definite (concave function).

where $\mathcal{H}$ is the Legendre transformation of $\mathcal{L}$,

$$\mathcal{H}(\mathbf{y}^*, \mathbf{z}) = -\mathcal{L}(\mathbf{y}^*, \dot{\mathbf{y}}^*(\mathbf{y}^*, \mathbf{z})) + z^a \dot{y}^*_a(\mathbf{y}^*, \mathbf{z}) \tag{3.29}$$

with the dependence $\dot{\mathbf{y}}^*(\mathbf{z})$ calculated from $z^a = \frac{\partial \mathcal{L}}{\partial \dot{y}^*_a}$. Since the Lagrangian does not explicitly depend on time, we can assume that the action is time-independent and the Hamilton-Jacobi equation (3.28b) turns to

$$\mathcal{H}\left(\mathbf{y}^*, -\frac{\partial \Psi}{\partial \mathbf{y}^*}\right) = 0. \tag{3.30}$$

The minimal action $\Psi(\mathbf{y}^*)$ is determined as the solution to this stationary Hamilton-Jacobi equation. Finally, equation (3.28a) can be rewritten, using the concrete form of Lagrangian (3.26), as

$$\dot{y}^a = {}^{\downarrow}\tilde{L}^{ab} \frac{\partial {}^{\downarrow}E}{\partial y^b} + \frac{\partial}{\partial y^*_a} \underbrace{\left({}^{\uparrow}\Xi(\mathbf{x}(\mathbf{y}), \mathbf{x}^*(\mathbf{y}^*)) + \Psi(\mathbf{y}^*)\right)}_{= {}^{\downarrow}\Xi(\mathbf{y}^*)}, \tag{3.31}$$

where ${}^{\downarrow}\tilde{L}^{ab} = \frac{\delta \pi^a}{\delta x^i} {}^{\uparrow}L^{ij} \frac{\delta \pi^b}{\delta x^j}\Big|_{\mathbf{x}(\mathbf{y}^*)}$ is the lower-level bivector[16]. A GENERIC evolution on the upper level (3.24) is reduced to a GENERIC evolution on the lower level of description (3.31) by minimization of the lack-of-fit action (3.27). In particular, even if the evolution on the upper level is purely Hamiltonian, the evolution on the lower level can contain dissipation.

While functionals ${}^{\downarrow}S$ and ${}^{\downarrow}E$ are obtained by the static reduction, the lower-level bivector ${}^{\downarrow}\tilde{\mathbf{L}}$ and dissipation potential ${}^{\downarrow}\Xi$ are obtained by the dynamic reduction, minimizing the lack of fit between the exact evolution on the MaxEnt submanifold and the MaxEnt mapping of the reduced evolution. Even in the case of purely Hamiltonian evolution on the upper level (${}^{\uparrow}\Xi = 0$), the reduced evolution can be dissipative. Indeed, the lower-level dissipation potential contains the minimum of the action, Ψ, which may be non-zero. In other words, dissipation can be interpreted as an emergent property brought up by disregarding some details of the upper level of description [Pavelka et al., 2020a].

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[16] Note that it is not guaranteed that the reduced bivector satisfies Jacobi identity and if it is the case, the reduced evolution is actually called pre-GENERIC [Kraaij et al., 2018].

4 Conclusion, my contribution, and outlook

GENERIC is a framework for non-equilibrium thermodynamics combining Hamiltonian mechanics and gradient dynamics. It is constructed from four building blocks: an energy, an entropy, a Poisson bracket, and a dissipation potential. GENERIC is compatible with the first law of thermodynamics, the second law, and generalized Onsager-Casimir reciprocal relations. In contrast to other forms of non-equilibrium thermodynamics [de Groot and Mazur, 1984, Truesdell, 1984, Müller, 1985, Jou et al., 2010, Berezovski and Ván, 2017], which are based on balance equations and subsequent entropic closures, the Hamiltonian part of GENERIC is based on geometric mechanics while balance laws come as a consequence. Moreover, the building blocks of GENERIC can be used to conveniently pass between various levels of description, for instance via the presented hierarchy of Poisson brackets.

My main contributions to the Hamiltonian part of GENERIC are: (i) Clarification of the time-reversal transformation also for state variables without parity (for instance the distribution function in kinetic theory) [Pavelka et al., 2014], (ii) a hierarchy of Poisson brackets starting with Liouville equation and going to weakly non-local extensions of fluid mechanics including entropy (geometric grandcanonical BBGKY hierarchy) [Pavelka et al., 2016], (iii) the Hamiltonian structure of Eulerian continuum mechanics with distortion [Peshkov et al., 2018], (iv) the Riemannian approach towards hyperbolicity of Hamiltonian systems [Pavelka et al., 2020b], and (v) the Hamiltonian structure of electrodynamics coupled with motion of matter [Esen et al., 2016, Vágner et al., 2021].

Regarding the irreversible part of GENERIC, my main contributions are: (i) the GENERIC version of Ehrenfest reduction [Gorban et al., 2001, Karlin et al., 2003, Pavelka et al., 2018a], which resulted in the Ehrenfest regularization of Hamiltonian systems [Pavelka et al., 2019b]. (ii) We have also shown how to use non-convex dissipation potentials in GENERIC [Janečka and Pavelka, 2018] and what are the physical implications (phase transitions in the dynamic behavior of complex fluids). (iii) Finally, we have generalized the method of lack-of-fit reduction to non-Boltzmann entropies and non-canonical Poisson brackets while allowing also full GENERIC evolution on the upper level of description (instead of being only purely Hamiltonian with only the Boltzmann entropy) [Pavelka et al., 2020a].

Another area of my research, standing out of the scope of this thesis, is theoretical electrochemistry (related to my Ph.D. thesis). My main contributions are: (i) Generalization of the exergy analysis in thermodynamic optimization [Hoffmann et al., 2003], where in the case of non-isothermal boundary it is not entropy production that cases efficiency losses, but a related quantity (map of losses) [Pavelka et al., 2015a, Vágner et al., 2017], (ii) explanation why desorption in Nafion membranes (in hydrogen fuel cells) is faster than absorption [Klika et al., 2017], and (iii) calculation of the open-circuit voltage in vanadium and zinc-air redox-flow batteries better explaining the experimental data [Pavelka et al., 2015b, del Olmo et al., 2021]. Although the GENERIC framework has only rarely been applied in electrochemistry because electrochemical processes are usually purely dissipative [Pavelka et al., 2015a, Bedeaux et al., 2014], it might enrich electrochemistry by inertial effects (adding Hamiltonian mechanics [Ajji et al., 2021]) and by improving the transition state theory (by multiscale thermodynamics [Gorban, 2021]).

In future, I would like to address for instance the following issues:

1. Where does GENERIC come from? Section 3.6 provides an answer by means of the lack-of-fit reduction, where GENERIC is derived from purely Hamiltonian mechanics by minimizing a discrepancy between evolutions on two levels of description. The method also reduces a full GENERIC evolution (including dissipation) to a less detailed GENERIC. However, the lack-of-fit reduction still contains several caveats. It has to be generalized to properly take into account boundary conditions, it remains unclear whether the method is transitive, and further numerical tests are needed to better understand where the method correctly approximates the detailed evolution. If successfull, the method could become a general tool for reductions in non-equilibrium thermodynamics [Gorban and Karlin, 2014].

2. The sum of Hamiltonian mechanics and gradient dynamics, on which GENERIC is based, is difficult to grasp from the geometrical point of view. Although each of the parts has its own well defined geometric setting, their sum lacks solid geometric formulation. So far the best choice for a geometry unifying both the reversible and irreversible parts of GENERIC seems to be the contact geometry [Arnold, 1989, Grmela, 2010, Pavelka et al., 2018b], but a comprehensive formulation of GENERIC including the infinite-dimensional case of fields is missing.

3. The Lagrangian continuum mechanics can be mapped to the Eulerian continuum mechanics with the distortion field, as in Section 2.5, and a further reduction leads to fluid mechanics. On the other hand, fluid mechanics can be also obtained by a reduction from kinetic theory (from the Liouville or Boltzmann equation). Can Eulerian continuum mechanics with distortion be obtained from kinetic theory as well? Answering this question would show how to add fluctuations to the equation for distortion, which should play a role for instance in simulations of colloidal solid particles by means of the dissipative particle dynamics method [Ellero et al., 2003, Hütter et al., 2018].

4. Superfluids, for instance liquid helium-4 at low temperatures, show remarkable behavior like flows through a very narrow capillary caused by a temperature difference [Landau, 1941]. The main approaches towards modeling of superfluids include the Landau-Tisza model, the Hall-Vinen-Bekarevich-Khalatnikov model (HVBK), the vortex filament model, and the Gross-Pitaevskii model [Landau et al., 1986]. Moreover, models for hyperbolic heat conduction have also been shown compatible with behavior of superfluids [Mongiovì et al., 2018]. Do all those models possess the GENERIC structure and are they related with each other via a hierarchy of Poisson brackets? Preliminary data indicate that GENERIC indeed provides a unifying framework at least for the Landau-Tisza, HVBK, and hyperbolic heat conduction models.

5. The equations describing processes in electrochemistry consist of purely dissipative drift-diffusion equations equipped at most with the Poisson equation for the electric potential. Such equations possess no inertial effects. On the other hand, inertial effects can affect rates of chemical reactions [Calef and Wolynes, 1983], and transport of charged species with inertia seems to be important on the nanoscale [Amatore et al., 2008]. The Hamiltonian electrodynamics of moving media, shortly presented in Section 2.7, should lead to a theory where both transport and electrochemical equations contain inertial effects, for instance wave-like propagation of polarization and magnetization, interacting with ultrafast electrochemical reactions. Moreover, this approach could lead to a fully Galilean invariant theory of electrodynamics of moving bodies approximating the Lorentz-invariant theory [Einstein, 1905] without the need of aether [Hertz, 1890].

6. Similarly as symplectic integrators exhibit superior numerical stability in simulations of particle mechanics, Poisson integrators should be advantageous when solving evolution equations of non-canonical Hamiltonian systems (for instance the Eulerian continuum mechanics) [Hairer et al., 2013, Leimkuhler et al., 2004]. Hamiltonian integrators should respect the Hamiltonian structure of the continuous equations. A way to derive them is the direct discretization of the action integral or of the underlying Lie group [Kraus, 2013, Gawlik and Gay-Balmaz, 2020]. On the other hand, GENERIC contains also irreversible evolution, which should be discretized as well, and several approaches have been proposed [Romero, 2009, Öttinger, 2018]. However, I believe that one should first derive a geometric framework covering both the reversible and irreversible parts of GENERIC, for instance the contact geometric approach above, and discretize that framework in order to obtain geometric integrators for GENERIC.

7. Finally, the multiscale character of non-equilibrium thermodynamics is closely related to pattern recognition. On the other hand, modern techniques of machine learning like autoencoders provide means of pattern recognition [Gorban et al., 2018]. Therefore, it seems that multiscale GENERIC could enrich machine learning by providing extra geometric structure while autoencoders could pave an alternative way for passing between levels of description [González et al., 2019, Chinesta et al., 2021].

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6 Attached papers

6.1 Ilya Peshkov, Michal Pavelka, Evgeniy Romenski, and Miroslav Grmela. Continuum Mechanics and Thermodynamics in the Hamilton and the Godunov-type Formulations. *Continuum Mechanics and Thermodynamics*, 30(6), 1343-1378, 2018.

6.2 Michal Pavelka, Ilya Peshkov, and Václav Klika. On Hamiltonian continuum mechanics. *Physica D: Nonlinear phenomena*, 408, 132510, 2020.

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6.4 Adam Janečka and Michal Pavelka. Non-convex dissipation potentials in multiscale non-equilibrium thermodynamics. *Continuum Mechanics and Thermodynamics*, 30(4), 917-941, 2018.

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