

# Rheology of solids: internal variable approach in the GENERIC framework

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## Abstract

The internal variable methodology of nonequilibrium thermodynamics, with a symmetric tensorial internal variable, provides an important rheological model family for solids, the so-called Kluitenberg–Verhás model family [1]. This model family is distinguished not only from theoretical aspects but also on experimental grounds (see [2] for plastics and [3, 4, 5] for rocks). In this article, we present and discuss how the internal variable formulation leading to the Kluitenberg–Verhás model family can be presented in the nonequilibrium thermodynamical framework GENERIC (General Equation for the Non-Equilibrium Reversible–Irreversible Coupling) [6, 7], for the benefit of both thermodynamical methodologies as well as for promising practical applications.

## 1 Introduction

The internal variable approach of nonequilibrium thermodynamics, with a symmetric tensorial internal variable, provides a distinguished model family – the Kluitenberg–Verhás model family [1] (covering the Hooke, Kelvin–Voigt, Maxwell and Jeffrey models as special cases) – for the rheology of solids. This family is significant not only from theoretical perspective but also for experimental applications [2, 3, 4, 5]. GENERIC (General Equation for Nonequilibrium Reversible–Irreversible Coupling) is an attractive general framework for nonequilibrium thermodynamical models (see, *e.g.*, [6, 7]). Whenever a new nonequilibrium thermodynamical model emerges, it is advantageous and recommended to check how it suits the frame of GENERIC. Here, we investigate how the internal variable formulation leading to the Kluitenberg–Verhás model family can be represented in GENERIC.

For the main part of the paper, specific entropy is treated as one of the state variables—a choice natural from principal aspects. Later, in an alternative version, temperature is used, instead—which formulation may be more convenient for certain engineering applications.

We believe that the relationship between the internal variable framework and GENERIC may be fruitful for both approaches, providing

- insight concerning the theoretical side,
- wider applicability,
- suggestions for novel numerical methods (see, *e.g.*, [8, 9] for such a promising direction), and
- beneficial connection of such numerical approaches with analytical results (*e.g.*, [10]).

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## 2 Necessary elements I: The internal variable formulation of rheology of solids

We start with a summary and generalization of the internal variable approach that leads to the Kluitenberg–Verhás rheological model family of solids [1]. The discussion is generalized in that the derivation in [1] neglected thermal expansion and started from Hookean elasticity, while the version here is free of those restrictions, only isotropy of the material being assumed.

The small-strain regime is considered, where strain  $\boldsymbol{\varepsilon}$  is small ( $|\boldsymbol{\varepsilon}| \ll 1$ ), there is no need to distinguish spacetime and material manifold variables and vectors/tensors—accordingly, aspects of objectivity and space-time compatibility [11, 12] are not addressed here—, mass density  $\varrho$  is constant, and one can relate time derivative (partial coinciding with substantial) of strain with the symmetrized gradient<sup>1</sup> of the velocity field  $\mathbf{v}$ ,

$$\dot{\boldsymbol{\varepsilon}} = \left( \mathbf{v} \otimes \overleftarrow{\nabla} \right)^S. \quad (1)$$

The balance of linear momentum is

$$\varrho \dot{\mathbf{v}} = \boldsymbol{\sigma}_0 \cdot \overleftarrow{\nabla} \quad (2)$$

with the divergence of stress  $\boldsymbol{\sigma}_0$  on the rhs, where stress is related to a specific internal energy  $e_{\text{int}}(\mathbf{x}_0)$  of variables

$$\mathbf{x}_0 = (\mathbf{v}, \boldsymbol{\varepsilon}^d, \boldsymbol{\varepsilon}^s, s_0) \quad (3)$$

as shown by the partial derivatives

$$\frac{\partial e_{\text{int}}}{\partial \boldsymbol{\varepsilon}^d} = \frac{1}{\varrho} \boldsymbol{\sigma}_0^d, \quad \frac{\partial e_{\text{int}}}{\partial \boldsymbol{\varepsilon}^s} = \frac{1}{\varrho} \boldsymbol{\sigma}_0^s, \quad \frac{\partial e_{\text{int}}}{\partial s_0} = T; \quad (4)$$

due to the isotropy of the material, the deviatoric–spherical decomposition of symmetric tensors plays here an important role (the spherical part of, *e.g.*, strain is proportional to the identity tensor,  $\boldsymbol{\varepsilon}^s = \frac{1}{3}(\text{tr } \boldsymbol{\varepsilon}) \mathbf{1}$ , while  $\boldsymbol{\varepsilon}^d = \boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^s$  is its deviatoric part), moreover,  $s_0$  and  $T$  denote specific entropy and temperature, respectively.

Rheology is a behaviour most manifest in the mechanical aspect so, for an internal variable description of it, in conform with that strain and stress are second order symmetric tensors, we introduce a symmetric tensorial internal variable  $\boldsymbol{\xi}$ . Mechanical effects of rheology are to be embodied by a  $\boldsymbol{\xi}$  dependent extension of stress:

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}_0 + \hat{\boldsymbol{\sigma}}, \quad (5)$$

$$\varrho \dot{\mathbf{v}} = \boldsymbol{\sigma} \cdot \overleftarrow{\nabla}. \quad (6)$$

We conceive rheology as irreversibility-related so specific entropy is also assumed to be influenced; concavity concerns (and Morse’s lemma [13]) suggest the variable transformation  $s_0 \rightarrow s$ ,

$$s = s_0 - \frac{1}{2} \text{tr} \left( \boldsymbol{\xi}^d \boldsymbol{\xi}^d \right) - \frac{1}{2} \text{tr} \left( \boldsymbol{\xi}^s \boldsymbol{\xi}^s \right). \quad (7)$$

Correspondingly, specific internal energy expressed in terms of the extended collection of variables,

$$\mathbf{x} = \left( \mathbf{v}, \boldsymbol{\varepsilon}^d, \boldsymbol{\varepsilon}^s, s, \boldsymbol{\xi}^d, \boldsymbol{\xi}^s \right), \quad (8)$$

is of the form

$$e_{\text{int}}(\mathbf{x}) = e_{\text{int}} \left( \boldsymbol{\varepsilon}^d, \boldsymbol{\varepsilon}^s, s_0(s, \boldsymbol{\xi}^d, \boldsymbol{\xi}^s) \right). \quad (9)$$

The balance of internal energy is

$$\varrho \dot{e}_{\text{int}} = -\mathbf{j}_e \cdot \overleftarrow{\nabla} + \text{tr}(\boldsymbol{\sigma} \dot{\boldsymbol{\varepsilon}}), \quad (10)$$

where  $\mathbf{j}_e$  denotes heat current density, and the only source term considered is related to mechanical power. Substituting (4), (5) and (7) into (10), on the one hand we obtain

$$\begin{aligned} \varrho \dot{e}_{\text{int}} &= \varrho \left\{ \text{tr} \left( \frac{\partial e_{\text{int}}}{\partial \boldsymbol{\varepsilon}^d} \dot{\boldsymbol{\varepsilon}}^d \right) + \text{tr} \left( \frac{\partial e_{\text{int}}}{\partial \boldsymbol{\varepsilon}^s} \dot{\boldsymbol{\varepsilon}}^s \right) + \frac{\partial e_{\text{int}}}{\partial s_0} \left[ \frac{\partial s_0}{\partial s} \dot{s} + \text{tr} \left( \frac{\partial s_0}{\partial \boldsymbol{\xi}^d} \dot{\boldsymbol{\xi}}^d \right) + \text{tr} \left( \frac{\partial s_0}{\partial \boldsymbol{\xi}^s} \dot{\boldsymbol{\xi}}^s \right) \right] \right\} = \\ &= \text{tr} \left( \boldsymbol{\sigma}_0^d \dot{\boldsymbol{\varepsilon}}^d \right) + \text{tr} \left( \boldsymbol{\sigma}_0^s \dot{\boldsymbol{\varepsilon}}^s \right) + \varrho T \dot{s} + \varrho T \text{tr} \left( \boldsymbol{\xi}^d \dot{\boldsymbol{\xi}}^d \right) + \varrho T \text{tr} \left( \boldsymbol{\xi}^s \dot{\boldsymbol{\xi}}^s \right), \end{aligned} \quad (11)$$

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<sup>1</sup> $\overleftarrow{\nabla}$  and  $\overrightarrow{\nabla}$  act to the left and to the right, respectively, reflecting proper tensorial order.

and on the other hand

$$\varrho \dot{e}_{\text{int}} = -\mathbf{j}_e \cdot \overleftarrow{\nabla} + \text{tr}(\boldsymbol{\sigma}_0^{\text{d}} \dot{\boldsymbol{\varepsilon}}^{\text{d}}) + \text{tr}(\boldsymbol{\sigma}_0^{\text{s}} \dot{\boldsymbol{\varepsilon}}^{\text{s}}) + \text{tr}(\hat{\boldsymbol{\sigma}}^{\text{d}} \dot{\boldsymbol{\varepsilon}}^{\text{d}}) + \text{tr}(\hat{\boldsymbol{\sigma}}^{\text{s}} \dot{\boldsymbol{\varepsilon}}^{\text{s}}). \quad (12)$$

The rhs of (11) is to be equal to the rhs of (12), which leads to

$$\varrho \dot{s} = -\frac{1}{T} \mathbf{j}_e \cdot \overleftarrow{\nabla} + \frac{1}{T} \text{tr}(\hat{\boldsymbol{\sigma}}^{\text{d}} \dot{\boldsymbol{\varepsilon}}^{\text{d}}) + \frac{1}{T} \text{tr}(\hat{\boldsymbol{\sigma}}^{\text{s}} \dot{\boldsymbol{\varepsilon}}^{\text{s}}) - \varrho \text{tr}(\boldsymbol{\xi}^{\text{d}} \dot{\boldsymbol{\varepsilon}}^{\text{d}}) - \varrho \text{tr}(\boldsymbol{\xi}^{\text{s}} \dot{\boldsymbol{\varepsilon}}^{\text{s}}). \quad (13)$$

Since the balance of the extended entropy is to be of the form

$$\varrho \dot{s} = -\mathbf{j}_s \cdot \overleftarrow{\nabla} + \pi_s \quad (14)$$

with entropy current density  $\mathbf{j}_s$  chosen to be the usual  $\mathbf{j}_s = \frac{1}{T} \mathbf{j}_e$ , and entropy production  $\pi_s$ , in the light of (13), we can write

$$\pi_s = \varrho \dot{s} + \mathbf{j}_s \cdot \overleftarrow{\nabla} = \mathbf{j}_e \cdot \left( \frac{1}{T} \otimes \overleftarrow{\nabla} \right) + \frac{1}{T} \text{tr}(\hat{\boldsymbol{\sigma}}^{\text{d}} \dot{\boldsymbol{\varepsilon}}^{\text{d}}) + \frac{1}{T} \text{tr}(\hat{\boldsymbol{\sigma}}^{\text{s}} \dot{\boldsymbol{\varepsilon}}^{\text{s}}) - \varrho \text{tr}(\boldsymbol{\xi}^{\text{d}} \dot{\boldsymbol{\varepsilon}}^{\text{d}}) - \varrho \text{tr}(\boldsymbol{\xi}^{\text{s}} \dot{\boldsymbol{\varepsilon}}^{\text{s}}). \quad (15)$$

Positive definiteness of entropy production can be ensured for the first term via  $\mathbf{j}_e = \lambda \left( \frac{1}{T} \otimes \overleftarrow{\nabla} \right)$ ,  $\lambda > 0$  (Fourier heat conduction, a vectorial part that cannot isotropically couple to the remaining, tensorial, terms<sup>2</sup>), and via Onsagerian equations concerning the further terms, with independent deviatoric and spherical parts because of isotropy:

$$\hat{\boldsymbol{\sigma}}^{\text{d}} = l_{11}^{\text{d}} \dot{\boldsymbol{\varepsilon}}^{\text{d}} + l_{12}^{\text{d}} \left( -\varrho T \boldsymbol{\xi}^{\text{d}} \right), \quad \hat{\boldsymbol{\sigma}}^{\text{s}} = l_{11}^{\text{s}} \dot{\boldsymbol{\varepsilon}}^{\text{s}} + l_{12}^{\text{s}} \left( -\varrho T \boldsymbol{\xi}^{\text{s}} \right), \quad (16)$$

$$\dot{\boldsymbol{\varepsilon}}^{\text{d}} = l_{21}^{\text{d}} \dot{\boldsymbol{\varepsilon}}^{\text{d}} + l_{22}^{\text{d}} \left( -\varrho T \boldsymbol{\xi}^{\text{d}} \right), \quad \dot{\boldsymbol{\varepsilon}}^{\text{s}} = l_{21}^{\text{s}} \dot{\boldsymbol{\varepsilon}}^{\text{s}} + l_{22}^{\text{s}} \left( -\varrho T \boldsymbol{\xi}^{\text{s}} \right), \quad (17)$$

with appropriate conditions on the deviatoric coefficients  $l_{ij}^{\text{d}}$  and the spherical ones  $l_{ij}^{\text{s}}$ , each of which are going to be assumed constant for simplicity<sup>3</sup>. These conditions can be read off from the quadratic form obtained by substituting (16)–(17) into (15), which yields<sup>4</sup>

$$T\pi_s = \begin{pmatrix} \dot{\boldsymbol{\varepsilon}}^{\text{d}} & -\varrho T \boldsymbol{\xi}^{\text{d}} & \dot{\boldsymbol{\varepsilon}}^{\text{s}} & -\varrho T \boldsymbol{\xi}^{\text{s}} \end{pmatrix} \begin{pmatrix} l_{11}^{\text{d}} & l_{12}^{\text{d}} & 0 & 0 \\ l_{12}^{\text{d}} & l_{22}^{\text{d}} & 0 & 0 \\ 0 & 0 & l_{11}^{\text{s}} & l_{12}^{\text{s}} \\ 0 & 0 & l_{12}^{\text{s}} & l_{22}^{\text{s}} \end{pmatrix} \begin{pmatrix} \dot{\boldsymbol{\varepsilon}}^{\text{d}} \\ -\varrho T \boldsymbol{\xi}^{\text{d}} \\ \dot{\boldsymbol{\varepsilon}}^{\text{s}} \\ -\varrho T \boldsymbol{\xi}^{\text{s}} \end{pmatrix} \quad (18)$$

with  $l_{\text{S}}^{\text{d}} = \frac{1}{2} (l_{12}^{\text{d}} + l_{21}^{\text{d}})$  and  $l_{\text{S}}^{\text{s}} = \frac{1}{2} (l_{12}^{\text{s}} + l_{21}^{\text{s}})$ . Hence, the four-by-four coefficient matrix in the middle is required to be positive definite, which necessitates for the coefficients, using Sylvester's criteria,

$$l_{11}^{\text{d}} \geq 0, \quad l_{22}^{\text{d}} \geq 0, \quad \det l_{\text{S}}^{\text{d}} \geq 0, \quad (19)$$

$$l_{11}^{\text{s}} \geq 0, \quad l_{22}^{\text{s}} \geq 0, \quad \det l_{\text{S}}^{\text{s}} \geq 0. \quad (20)$$

We remark that, both in (19) and (20), the three conditions are not independent: the third one and either of the first two ones imply the remaining one. It is important to notice that the antisymmetric part of the coefficient matrix does not contribute to entropy production but only its symmetric part creates irreversibility. We can emphasize this by dividing the Onsagerian equations (16)–(17) into presumably reversible and irreversible parts:

$$\hat{\boldsymbol{\sigma}}^{\text{d}} = \left[ l_{\text{A}}^{\text{d}} \left( -\varrho T \boldsymbol{\xi}^{\text{d}} \right) \right] + \left[ l_{11}^{\text{d}} \dot{\boldsymbol{\varepsilon}}^{\text{d}} + l_{\text{S}}^{\text{d}} \left( -\varrho T \boldsymbol{\xi}^{\text{d}} \right) \right], \quad \hat{\boldsymbol{\sigma}}^{\text{s}} = \left[ l_{\text{A}}^{\text{s}} \left( -\varrho T \boldsymbol{\xi}^{\text{s}} \right) \right] + \left[ l_{11}^{\text{s}} \dot{\boldsymbol{\varepsilon}}^{\text{s}} + l_{\text{S}}^{\text{s}} \left( -\varrho T \boldsymbol{\xi}^{\text{s}} \right) \right], \quad (21)$$

$$\dot{\boldsymbol{\varepsilon}}^{\text{d}} = \left[ -l_{\text{A}}^{\text{d}} \dot{\boldsymbol{\varepsilon}}^{\text{d}} \right] + \left[ l_{\text{S}}^{\text{d}} \dot{\boldsymbol{\varepsilon}}^{\text{d}} + l_{22}^{\text{d}} \left( -\varrho T \boldsymbol{\xi}^{\text{d}} \right) \right], \quad \dot{\boldsymbol{\varepsilon}}^{\text{s}} = \left[ -l_{\text{A}}^{\text{s}} \dot{\boldsymbol{\varepsilon}}^{\text{s}} \right] + \left[ l_{\text{S}}^{\text{s}} \dot{\boldsymbol{\varepsilon}}^{\text{s}} + l_{22}^{\text{s}} \left( -\varrho T \boldsymbol{\xi}^{\text{s}} \right) \right] \quad (22)$$

with  $l_{\text{A}}^{\text{d}} = \frac{1}{2} (l_{12}^{\text{d}} - l_{21}^{\text{d}})$  and  $l_{\text{A}}^{\text{s}} = \frac{1}{2} (l_{12}^{\text{s}} - l_{21}^{\text{s}})$ .

<sup>2</sup>Correspondingly, heat conduction is ignored in what follows—it can be added later without any complication.

<sup>3</sup>No principal difficulties are expected when these coefficients are  $\mathbf{x}$  dependent, and here we intend to keep formulae relatively short.

<sup>4</sup>The upper right and lower left two-by-two submatrices contain only zero elements due to the isotropic decoupling of deviatoric and spherical parts.

It is to be noted that, in general, the coefficient matrices  $l^d$ ,  $l^s$  need not be symmetric nor antisymmetric, corresponding to that the concrete physical interpretation of  $\xi$  may not be available and the behaviour of  $\xi$  under time reflection might not be purely sign preserving/flipping.<sup>5</sup>

For the Hookean special case, eliminating the internal variable leads, in the isothermal approximation, to the Kluitenberg–Verhás model family [1],

$$\sigma^d + \tau^d \dot{\sigma}^d = E_0^d \epsilon^d + E_1^d \dot{\epsilon}^d + E_2^d \ddot{\epsilon}^d, \quad (23)$$

$$\sigma^s + \tau^s \dot{\sigma}^s = E_0^s \epsilon^s + E_1^s \dot{\epsilon}^s + E_2^s \ddot{\epsilon}^s, \quad (24)$$

with necessary and sufficient thermodynamical inequality conditions on the coefficients  $\tau^d, E_0^d, E_1^d, E_2^d, \dots$  stemming from (19)–(20) (for closer details, see [1]).

### 3 Necessary elements II: Summary of the GENERIC framework

In GENERIC [6, 7], time evolution of the collection of state variables (fields, in case of continuum models like ours here),  $\mathbf{x}$ , is formulated as

$$\frac{d\mathbf{x}}{dt} = \mathbf{L}(\mathbf{x}) \frac{\delta E}{\delta \mathbf{x}} + \mathbf{M}(\mathbf{x}) \frac{\delta S}{\delta \mathbf{x}}, \quad (25)$$

where the so-called reversible operator matrix  $\mathbf{L}$  acts on the column vector that is the functional derivative of the energy functional  $E$  of  $\mathbf{x}$ , and the irreversible operator matrix  $\mathbf{M}$  acts on the column vector that is the functional derivative of the entropy functional  $S$  of  $\mathbf{x}$ .  $\mathbf{L}$  is required to be antisymmetric,

$$\mathbf{L} = -\mathbf{L}^T \quad (26)$$

(<sup>T</sup> denoting transpose which, for operators, means not merely matrix index transposition but includes operator adjoint). Thanks to this and the degeneracy condition

$$\mathbf{M} \frac{\delta E}{\delta \mathbf{x}} = \mathbf{0}, \quad (27)$$

energy is conserved,  $\frac{dE}{dt} = 0$ . In parallel, the other degeneracy requirement

$$\mathbf{L} \frac{\delta S}{\delta \mathbf{x}} = \mathbf{0} \quad (28)$$

ensures that the first term on the rhs of (25) does not increase entropy, and  $\mathbf{M}$  is demanded to be positive definite to lead to  $\frac{dS}{dt} \geq 0$  eventually. That  $\mathbf{L} \frac{\delta E}{\delta \mathbf{x}}$  is related to reversible dynamics is manifested further by also prescribing the Jacobi identity

$$\{A, \{B, C\}\} + \{B, \{C, A\}\} + \{C, \{A, B\}\} = 0 \quad (29)$$

( $A, B, C$  arbitrary functionals) for the bilinear generalized Poisson bracket

$$\{A, B\} := \int_V \frac{\delta A}{\delta \mathbf{x}} \mathbf{L} \frac{\delta B}{\delta \mathbf{x}} dV. \quad (30)$$

Consequently, the first term on the rhs of (25) can be interpreted as a reversible—generalized Hamiltonian—time evolution contribution (vector field) while the second term (another vector field) embodies irreversible time evolution contribution to dynamics.

Analogously to (26) and (30), imposing symmetricity for  $\mathbf{M}$ ,

$$\mathbf{M} = \mathbf{M}^T, \quad (31)$$

induces that the bilinear product

$$[A, B] := \int_V \frac{\delta A}{\delta \mathbf{x}} \mathbf{M} \frac{\delta B}{\delta \mathbf{x}} dV \quad (32)$$

is positive definite,  $[A, A] \geq 0$ . The latter bracket (32) completes the former one (30) in the sense that time evolution for any functional  $A$  can be expressed as

$$\frac{dA}{dt} = \{A, E\} + [A, S]. \quad (33)$$

A constructive and productive way to generate the irreversible contribution to dynamics is to derive it from a dissipation potential [7, 14, 15]. Assuming a dissipation potential is, on the other side, not necessary and reduces the level of generality of the GENERIC framework [16].

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<sup>5</sup>Rocks are one example of complex enough materials that may require such a description.

## 4 Internal variable rheology of solids realized in the GENERIC formulation

Section 2 has actually been given in a form to provide preparations for the present one, where we establish GENERIC form for the  $\xi$ -described rheology of solids. The set of variables  $\mathbf{x}$  is (8), the energy functional consists of the internal energy contribution (9) supplemented by the kinetic energy related one, and the entropy functional is straightforward:

$$E = \int_V \varrho e dV = \int_V \varrho \left[ \frac{1}{2} \mathbf{v} \cdot \mathbf{v} + e_{\text{int}}(\boldsymbol{\varepsilon}^d, \boldsymbol{\varepsilon}^s, s_0(s, \boldsymbol{\xi}^d, \boldsymbol{\xi}^s)) \right] dV, \quad (34)$$

$$S = \int_V \varrho s dV. \quad (35)$$

The corresponding functional derivatives are

$$\frac{\delta E}{\delta \mathbf{x}} = \begin{pmatrix} \varrho \mathbf{v} \\ \boldsymbol{\sigma}_0^d \\ \boldsymbol{\sigma}_0^s \\ \varrho T \\ \varrho T \boldsymbol{\xi}^d \\ \varrho T \boldsymbol{\xi}^s \end{pmatrix}, \quad \frac{\delta S}{\delta \mathbf{x}} = \begin{pmatrix} \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \\ \varrho \\ \mathbf{0} \\ \mathbf{0} \end{pmatrix}. \quad (36)$$

The nontrivial task is to identify  $\mathbf{L}$  and  $\mathbf{M}$ . Concerning the time evolution of the state variables, we know (6), (1), (13) and (16)–(17) so we conjecture the decomposition to reversible and irreversible parts as<sup>6</sup>

$$\begin{pmatrix} \dot{\mathbf{v}} \\ \dot{\boldsymbol{\varepsilon}}^d \\ \dot{\boldsymbol{\varepsilon}}^s \\ \dot{s} \\ \dot{\boldsymbol{\xi}}^d \\ \dot{\boldsymbol{\xi}}^s \end{pmatrix} = \begin{pmatrix} \frac{1}{\varrho} [\boldsymbol{\sigma}_0^d + \boldsymbol{\sigma}_0^s] \cdot \overleftarrow{\nabla} \\ \left[ (\mathbf{v} \otimes \overleftarrow{\nabla})^S \right]^d \\ \left[ (\mathbf{v} \otimes \overleftarrow{\nabla})^S \right]^s \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \end{pmatrix} + \begin{pmatrix} \frac{1}{\varrho} \left[ l_{11}^d \dot{\boldsymbol{\varepsilon}}^d + l_{12}^d (-\varrho T \boldsymbol{\xi}^d) + l_{11}^s \dot{\boldsymbol{\varepsilon}}^s + l_{12}^s (-\varrho T \boldsymbol{\xi}^s) \right] \cdot \overleftarrow{\nabla} \\ \mathbf{0} \\ \mathbf{0} \\ \left( \frac{l_{11}^d}{\varrho T} \text{tr}(\dot{\boldsymbol{\varepsilon}}^d \dot{\boldsymbol{\varepsilon}}^d) - 2l_{12}^d \text{tr}(\boldsymbol{\xi}^d \dot{\boldsymbol{\varepsilon}}^d) + l_{22}^d \varrho T \text{tr}(\boldsymbol{\xi}^d \boldsymbol{\xi}^d) + \right. \\ \left. + \frac{l_{11}^s}{\varrho T} \text{tr}(\dot{\boldsymbol{\varepsilon}}^s \dot{\boldsymbol{\varepsilon}}^s) - 2l_{12}^s \text{tr}(\boldsymbol{\xi}^s \dot{\boldsymbol{\varepsilon}}^s) + l_{22}^s \varrho T \text{tr}(\boldsymbol{\xi}^s \boldsymbol{\xi}^s) \right) \\ l_{21}^d \dot{\boldsymbol{\varepsilon}}^d + l_{22}^d (-\varrho T \boldsymbol{\xi}^d) \\ l_{21}^s \dot{\boldsymbol{\varepsilon}}^s + l_{22}^s (-\varrho T \boldsymbol{\xi}^s) \end{pmatrix}. \quad (37)$$

The governing principle for this decision for decomposition is that, since dissipation and irreversibility is related to entropy production and to the internal variable, the reversible vector field should not contain them but only pure fluid mechanics.

Then  $\mathbf{L}$  can directly read off from the first term on the rhs of (37):

$$\mathbf{L} = \begin{pmatrix} 0 & \frac{1}{\varrho} \bullet \cdot \overleftarrow{\nabla} & \frac{1}{\varrho} \bullet \cdot \overleftarrow{\nabla} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \frac{1}{\varrho} \left[ (\bullet \otimes \overleftarrow{\nabla})^S \right]^d & 0 & 0 & \mathbf{0} & 0 & 0 \\ \frac{1}{\varrho} \left[ (\bullet \otimes \overleftarrow{\nabla})^S \right]^s & 0 & 0 & \mathbf{0} & 0 & 0 \\ \mathbf{0} \cdot & \mathbf{0} : & \mathbf{0} : & 0 & \mathbf{0} : & \mathbf{0} : \\ \mathbf{0} \otimes & 0 & 0 & \mathbf{0} & 0 & 0 \\ \mathbf{0} \otimes & 0 & 0 & \mathbf{0} & 0 & 0 \end{pmatrix}, \quad (38)$$

with  $\bullet$  denoting the ‘slot’ where the operator acts. This  $\mathbf{L}$  apparently fulfils the degeneracy condition  $\mathbf{L} \frac{\delta S}{\delta \mathbf{x}} = \mathbf{0}$ .

To prove antisymmetry of  $\mathbf{L}$ , let us take the corresponding bracket (30):

$$\{A, B\} = \int_V \frac{1}{\varrho} \left[ A_{\mathbf{v}} \cdot (B_{\boldsymbol{\varepsilon}^d} \cdot \overleftarrow{\nabla} + B_{\boldsymbol{\varepsilon}^s} \cdot \overleftarrow{\nabla}) + \text{tr} \left\{ A_{\boldsymbol{\varepsilon}^d} \left[ (B_{\mathbf{v}} \otimes \overleftarrow{\nabla})^S \right]^d \right\} + \text{tr} \left\{ A_{\boldsymbol{\varepsilon}^s} \left[ (B_{\mathbf{v}} \otimes \overleftarrow{\nabla})^S \right]^s \right\} \right] dV, \quad (39)$$

<sup>6</sup>Beware that, if we prefer to write  $\mathbf{x}$  and  $\dot{\mathbf{x}}$  as column vectors then (36) should contain row vectors, as being covectors with respect to the vector space of  $\mathbf{x}$ . However, then  $\mathbf{L}$  and  $\mathbf{M}$  could not be displayed as customary square matrices. The misleading double meaning of column vectors could be resolved by writing  $\mathbf{x}$ -covectors like in (36) as column vectors but within  $[ \ ]$  instead of  $( \ )$ . Then, correspondingly,  $\mathbf{L}$ ,  $\mathbf{M}$  were to be written within  $[ \ ]$ . Here, we decided not to use this convention but at least to draw attention to that distinction between vectors and covectors is not only principally important but also avoids considerable confusion during calculations.

where  $A$  and  $B$  are arbitrary functionals of the state variables, and abbreviations of the kind

$$A_{\mathbf{v}} := \frac{\delta A}{\delta \mathbf{v}}, \quad A_{\boldsymbol{\varepsilon}^d} := \frac{\delta A}{\delta \boldsymbol{\varepsilon}^d}, \quad A_{\boldsymbol{\varepsilon}^s} := \frac{\delta A}{\delta \boldsymbol{\varepsilon}^s}, \quad A_s := \frac{\delta A}{\delta s}, \quad A_{\boldsymbol{\xi}^d} := \frac{\delta A}{\delta \boldsymbol{\xi}^d}, \quad A_{\boldsymbol{\xi}^s} := \frac{\delta A}{\delta \boldsymbol{\xi}^s} \quad (40)$$

have been introduced. Using indices (with Einstein convention and the Kronecker symbol  $\delta_{ij}$ ), we have

$$\left[ \left( B_{\mathbf{v}} \otimes \overleftarrow{\nabla} \right)^S \right]^S = \frac{1}{3} \text{tr} \left[ \left( B_{\mathbf{v}} \otimes \overleftarrow{\nabla} \right)^S \right] \mathbf{1} = \frac{1}{3} \partial_k (B_{\mathbf{v}})_k \delta_{ij}, \quad (41)$$

$$\left[ \left( B_{\mathbf{v}} \otimes \overleftarrow{\nabla} \right)^S \right]^d = \left( B_{\mathbf{v}} \otimes \overleftarrow{\nabla} \right)^S - \left[ \left( B_{\mathbf{v}} \otimes \overleftarrow{\nabla} \right)^S \right]^S = \frac{1}{2} \left[ \partial_j (B_{\mathbf{v}})_i + \partial_i (B_{\mathbf{v}})_j \right] - \frac{1}{3} \partial_k (B_{\mathbf{v}})_k \delta_{ij}, \quad (42)$$

leading to

$$\begin{aligned} \{A, B\} = \int_V \frac{1}{\varrho} & \left[ (A_{\mathbf{v}})_i \left[ \partial_j (B_{\boldsymbol{\varepsilon}^d})_{ij} + \partial_j (B_{\boldsymbol{\varepsilon}^s})_{ij} \right] + (A_{\boldsymbol{\varepsilon}^d})_{ij} \left\{ \frac{1}{2} \left[ \partial_j (B_{\mathbf{v}})_i + \partial_i (B_{\mathbf{v}})_j \right] - \frac{1}{3} \partial_k (B_{\mathbf{v}})_k \delta_{ij} \right\} + \right. \\ & \left. + (A_{\boldsymbol{\varepsilon}^s})_{ij} \frac{1}{3} \partial_k (B_{\mathbf{v}})_k \delta_{ij} \right] dV. \end{aligned} \quad (43)$$

Via partial integration and omitting surface terms,

$$\begin{aligned} \{A, B\} = - \int_V \frac{1}{\varrho} & \left[ \partial_j (A_{\mathbf{v}})_i (B_{\boldsymbol{\varepsilon}^d})_{ij} + \partial_j (A_{\mathbf{v}})_i (B_{\boldsymbol{\varepsilon}^s})_{ij} + \frac{1}{2} \left[ \partial_j (A_{\boldsymbol{\varepsilon}^d})_{ij} (B_{\mathbf{v}})_i + \partial_i (A_{\boldsymbol{\varepsilon}^d})_{ij} (B_{\mathbf{v}})_j \right] - \right. \\ & \left. - \frac{1}{3} \partial_k (A_{\boldsymbol{\varepsilon}^d})_{ij} (B_{\mathbf{v}})_k \delta_{ij} + \frac{1}{3} \partial_k (A_{\boldsymbol{\varepsilon}^s})_{ij} (B_{\mathbf{v}})_k \delta_{ij} \right] dV. \end{aligned} \quad (44)$$

Now, taking into consideration that the functional derivative of a scalar functional with respect to a symmetric tensor is symmetric, with respect to a deviatoric tensor is deviatoric, and with respect to a spherical tensor is spherical, the first term in the integrand can be reformulated as

$$\text{tr} \left\{ B_{\boldsymbol{\varepsilon}^d} \left[ \left( A_{\mathbf{v}} \otimes \overleftarrow{\nabla} \right)^S \right]^d \right\}, \quad (45)$$

and the second term can be treated analogously. Next, it is easy to show that the third term is  $B_{\mathbf{v}} \cdot \left( A_{\boldsymbol{\varepsilon}^d} \cdot \overleftarrow{\nabla} \right)$ . Further, in the terms that contain  $\delta_{ij}$ , the  $j$  index can be changed to  $i$ , hence, in these terms we find the gradient of the trace of a tensor. Therefore, the fourth term contains trace of a deviatoric tensor—which is traceless—so this term gives zero contribution. Finally, the fifth term contains a spherical tensor and thus can be rewritten as  $\frac{1}{3} \partial_k (A_{\boldsymbol{\varepsilon}^s})_{ii} (B_{\mathbf{v}})_k = \partial_k (A_{\boldsymbol{\varepsilon}^s})_{ik} (B_{\mathbf{v}})_i$ . To sum up, we find

$$\begin{aligned} \{A, B\} = - \int_V \frac{1}{\varrho} & \left[ B_{\mathbf{v}} \cdot \left( A_{\boldsymbol{\varepsilon}^d} \cdot \overleftarrow{\nabla} + A_{\boldsymbol{\varepsilon}^s} \cdot \overleftarrow{\nabla} \right) + \text{tr} \left\{ B_{\boldsymbol{\varepsilon}^d} \left[ \left( A_{\mathbf{v}} \otimes \overleftarrow{\nabla} \right)^S \right]^d \right\} + \right. \\ & \left. + \text{tr} \left\{ B_{\boldsymbol{\varepsilon}^s} \left[ \left( A_{\mathbf{v}} \otimes \overleftarrow{\nabla} \right)^S \right]^s \right\} \right] dV = - \{B, A\}, \end{aligned} \quad (46)$$

antisymmetry is revealed.

Since  $\mathbf{L}$  is independent of the state variables and is antisymmetric, the generalized Poisson bracket also satisfies the Jacobi identity [6].

Now let us turn towards the irreversible side: the operator matrix  $\mathbf{M}$  can be constructed from the second term of the time evolution equation (37) and the degeneracy condition (27); we find

$$\mathbf{M} = \begin{pmatrix} M_{11} & \mathbf{0} \cdot & \mathbf{0} \cdot & M_{14} & M_{15} & M_{16} \\ \mathbf{0} \otimes & 0 & 0 & \mathbf{0} & 0 & 0 \\ \mathbf{0} \otimes & 0 & 0 & \mathbf{0} & 0 & 0 \\ M_{41} & \mathbf{0} : & \mathbf{0} : & M_{44} & M_{45} & M_{46} \\ M_{51} & 0 & 0 & M_{54} & M_{55} & 0 \\ M_{61} & 0 & 0 & M_{64} & 0 & M_{66} \end{pmatrix} \quad (47)$$

with

$$\begin{aligned}
M_{11} &= -\frac{l_{11}^d}{\varrho^2} \left\{ T \left[ \left( \bullet \otimes \overleftarrow{\nabla} \right)^{\mathbb{S}^d} \right]^d \right\} \cdot \overleftarrow{\nabla} - \frac{l_{11}^s}{\varrho^2} \left\{ T \left[ \left( \bullet \otimes \overleftarrow{\nabla} \right)^{\mathbb{S}^s} \right]^s \right\} \cdot \overleftarrow{\nabla}, \\
M_{14} &= \frac{1}{\varrho^2} \left\{ \left[ l_{11}^d \left[ \left( \mathbf{v} \otimes \overleftarrow{\nabla} \right)^{\mathbb{S}^d} \right]^d + l_{12}^d (-\varrho T \boldsymbol{\xi}^d) + l_{11}^s \left[ \left( \mathbf{v} \otimes \overleftarrow{\nabla} \right)^{\mathbb{S}^s} \right]^s + l_{12}^s (-\varrho T \boldsymbol{\xi}^s) \right] \bullet \right\} \cdot \overleftarrow{\nabla}, \\
M_{15} &= \frac{l_{12}^d}{\varrho} (T \bullet) \cdot \overleftarrow{\nabla}, & M_{16} &= \frac{l_{12}^s}{\varrho} (T \bullet) \cdot \overleftarrow{\nabla}, \\
M_{41} &= -\frac{l_{11}^d}{\varrho^2} \text{tr} \left\{ \left[ \left( \mathbf{v} \otimes \overleftarrow{\nabla} \right)^{\mathbb{S}^d} \right]^d \left[ \left( \bullet \otimes \overleftarrow{\nabla} \right)^{\mathbb{S}^d} \right]^d \right\} + \frac{l_{21}^d}{\varrho} \text{tr} \left\{ T \boldsymbol{\xi}^d \left[ \left( \bullet \otimes \overleftarrow{\nabla} \right)^{\mathbb{S}^d} \right]^d \right\} - \\
&\quad - \frac{l_{11}^s}{\varrho^2} \text{tr} \left\{ \left[ \left( \mathbf{v} \otimes \overleftarrow{\nabla} \right)^{\mathbb{S}^s} \right]^s \left[ \left( \bullet \otimes \overleftarrow{\nabla} \right)^{\mathbb{S}^s} \right]^s \right\} + \frac{l_{21}^s}{\varrho} \text{tr} \left\{ T \boldsymbol{\xi}^s \left[ \left( \bullet \otimes \overleftarrow{\nabla} \right)^{\mathbb{S}^s} \right]^s \right\}, \\
M_{44} &= \frac{l_{11}^d}{\varrho^2 T} \text{tr} \left\{ \left[ \left( \mathbf{v} \otimes \overleftarrow{\nabla} \right)^{\mathbb{S}^d} \right]^d \left[ \left( \mathbf{v} \otimes \overleftarrow{\nabla} \right)^{\mathbb{S}^d} \right]^d \right\} - \frac{2l_{12}^d}{\varrho} \text{tr} \left\{ \boldsymbol{\xi}^d \left[ \left( \mathbf{v} \otimes \overleftarrow{\nabla} \right)^{\mathbb{S}^d} \right]^d \right\} + l_{22}^d T \text{tr} (\boldsymbol{\xi}^d \boldsymbol{\xi}^d) + \\
&\quad + \frac{l_{11}^s}{\varrho^2 T} \text{tr} \left\{ \left[ \left( \mathbf{v} \otimes \overleftarrow{\nabla} \right)^{\mathbb{S}^s} \right]^s \left[ \left( \mathbf{v} \otimes \overleftarrow{\nabla} \right)^{\mathbb{S}^s} \right]^s \right\} - \frac{2l_{12}^s}{\varrho} \text{tr} \left\{ \boldsymbol{\xi}^s \left[ \left( \mathbf{v} \otimes \overleftarrow{\nabla} \right)^{\mathbb{S}^s} \right]^s \right\} + l_{22}^s T \text{tr} (\boldsymbol{\xi}^s \boldsymbol{\xi}^s), \\
M_{45} &= \frac{l_{12}^d}{\varrho} \text{tr} \left\{ \left[ \left( \mathbf{v} \otimes \overleftarrow{\nabla} \right)^{\mathbb{S}^d} \right]^d \bullet \right\} - l_{22}^d T \text{tr} (\boldsymbol{\xi}^d \bullet), & M_{46} &= \frac{l_{12}^s}{\varrho} \text{tr} \left\{ \left[ \left( \mathbf{v} \otimes \overleftarrow{\nabla} \right)^{\mathbb{S}^s} \right]^s \bullet \right\} - l_{22}^s T \text{tr} (\boldsymbol{\xi}^s \bullet), \\
M_{51} &= -\frac{l_{21}^d}{\varrho} T \left[ \left( \bullet \otimes \overleftarrow{\nabla} \right)^{\mathbb{S}^d} \right]^d, & M_{54} &= \frac{l_{21}^d}{\varrho} \left[ \left( \mathbf{v} \otimes \overleftarrow{\nabla} \right)^{\mathbb{S}^d} \right]^d - l_{22}^d T \boldsymbol{\xi}^d, & M_{55} &= l_{22}^d T, \\
M_{61} &= -\frac{l_{21}^s}{\varrho} T \left[ \left( \bullet \otimes \overleftarrow{\nabla} \right)^{\mathbb{S}^s} \right]^s, & M_{64} &= \frac{l_{21}^s}{\varrho} \left[ \left( \mathbf{v} \otimes \overleftarrow{\nabla} \right)^{\mathbb{S}^s} \right]^s - l_{22}^s T \boldsymbol{\xi}^s, & M_{66} &= l_{22}^s T.
\end{aligned} \tag{48}$$

One can notice that this  $\mathbf{M}$  is not symmetric—see the elements that contain  $l_{12}^d$  vs.  $l_{21}^d$ , as well as the ones with  $l_{12}^s$  vs.  $l_{21}^s$ . As mentioned in Section 2, when we have no additional microscopic or experimental information about  $\boldsymbol{\xi}$  and about the corresponding coefficients  $l^d$ ,  $l^s$  then we cannot exclude that antisymmetric parts  $l_A^d$ ,  $l_A^s$  appear in the dynamics.

Positive definiteness can (nevertheless) be shown by reformulating the integrand of the irreversible bracket  $[A, A]$  to a quadratic expression. More closely, we can form a matrix that contains nonnegative elements and the Onsagerian coefficients, and (19)–(20) just prove to be the conditions that ensure positive definiteness. The calculation is straightforward but lengthy.

Actually, the whole realization of  $\boldsymbol{\xi}$ -based rheology provided above is straightforward (if lengthy), and is expected to work for nonconstant coefficient matrices  $l^d$ ,  $l^s$  as well. However, specifically for constant coefficients, an alternative version is also possible: implementing the antisymmetric part of the coefficient matrices, that is, the constants  $l_A^d$ ,  $l_A^s$ , in the reversible part of the time evolution.

For this case, let us use the prepared (21)–(22) form of the Onsagerian equations. Rearranging the time evolution equation is straightforward, and we find for the alternative reversible operator matrix  $\mathbf{L}'$

$$\mathbf{L}' = \begin{pmatrix} 0 & \frac{1}{\varrho} \bullet \cdot \overleftarrow{\nabla} & \frac{1}{\varrho} \bullet \cdot \overleftarrow{\nabla} & 0 & -\frac{l_A^d}{\varrho} \bullet \cdot \nabla & -\frac{l_A^s}{\varrho} \bullet \cdot \nabla \\ \frac{1}{\varrho} \left[ \left( \bullet \otimes \overleftarrow{\nabla} \right)^{\mathbb{S}^d} \right]^d & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{\varrho} \left[ \left( \bullet \otimes \overleftarrow{\nabla} \right)^{\mathbb{S}^s} \right]^s & 0 & 0 & 0 & 0 & 0 \\ \mathbf{0} \cdot & \mathbf{0} : & \mathbf{0} : & 0 & \mathbf{0} : & \mathbf{0} : \\ -\frac{l_A^d}{\varrho} \left[ \left( \bullet \otimes \overleftarrow{\nabla} \right)^{\mathbb{S}^d} \right]^d & 0 & 0 & 0 & 0 & 0 \\ -\frac{l_A^s}{\varrho} \left[ \left( \bullet \otimes \overleftarrow{\nabla} \right)^{\mathbb{S}^s} \right]^s & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \tag{49}$$

while the elements of the alternative irreversible operator matrix  $\mathbf{M}'$  are very similar to (48): we just have to change all  $l_{12}^d$  and  $l_{21}^d$  to  $l_{12}^d$  and, similarly,  $l_{12}^s$  and  $l_{21}^s$  to  $l_{12}^s$ .

The degeneracy criteria, antisymmetry of  $\mathbf{L}'$ , the Jacobi identity for the generalized Poisson brackets, and positive definiteness for  $\mathbf{M}'$  prove to be satisfied. Moreover, in this case the symmetric property of  $\mathbf{M}'$  also holds.

We repeat that this alternative realization is valid only for constant Onsagerian coefficients as otherwise the Jacobi identity were violated.

This latter variant appears ‘funny’ from principal point of view but may be beneficial for numerical solutions, e.g., to have as much symplectic part in the numerical scheme as possible—see [8, 9] about the importance of this.

## 5 Temperature as state variable

For mechanical engineering applications and evaluations of experiments (see, *e.g.*, [2]), it can be beneficial to use temperature, instead of entropy, as state variable. Then the collection of state variables is

$$\tilde{\mathbf{x}} = (\mathbf{v}, \boldsymbol{\varepsilon}^d, \boldsymbol{\varepsilon}^s, T, \boldsymbol{\xi}^d, \boldsymbol{\xi}^s). \quad (50)$$

To keep the discussion as concrete and basic as possible, let us choose the simplest constitutive equation for the internal energy, linear in temperature with constant specific heat  $c$ , containing elastic energy related to Hooke’s law,

$$\boldsymbol{\sigma}_0 = E^d \boldsymbol{\varepsilon}^d + E^s \boldsymbol{\varepsilon}^s, \quad E^d = 2G, \quad E^s = 3K, \quad (51)$$

and neglecting thermal expansion—which is manifested in the separation of strain dependence and temperature dependence—:

$$\tilde{e}_{\text{int}} = \tilde{e}_{\text{th}}(T) + \tilde{e}_{\text{el}}(\boldsymbol{\varepsilon}^d, \boldsymbol{\varepsilon}^s) = cT + \frac{E^d}{2\rho} \text{tr}(\boldsymbol{\varepsilon}^d \boldsymbol{\varepsilon}^d) + \frac{E^s}{2\rho} \text{tr}(\boldsymbol{\varepsilon}^s \boldsymbol{\varepsilon}^s). \quad (52)$$

Temperature has the same relationship to specific entropy as seen in Section 4, now utilized in the opposite direction (*i.e.*, what is a variable and what is a function): The thermodynamical consistency condition  $\frac{d\tilde{s}_0}{dT} = \frac{1}{T} \frac{d\tilde{e}_{\text{th}}}{dT}$  that follows from the Gibbs relation leads to

$$\tilde{s}_0(\tilde{\mathbf{x}}) = \tilde{s}_{\text{aux}} + c \ln \frac{T}{T_{\text{aux}}}, \quad (53)$$

with auxiliary constants  $\tilde{s}_{\text{aux}}$ ,  $T_{\text{aux}}$ , and the extension (7) induces

$$\tilde{s}(\tilde{\mathbf{x}}) = \tilde{s}_0(\tilde{\mathbf{x}}) - \frac{1}{2} \text{tr}(\boldsymbol{\xi}^d \boldsymbol{\xi}^d) - \frac{1}{2} \text{tr}(\boldsymbol{\xi}^s \boldsymbol{\xi}^s), \quad (54)$$

or, expressing temperature,

$$T(\tilde{s}_0(\tilde{s}, \boldsymbol{\xi}^d, \boldsymbol{\xi}^s)) = T_{\text{aux}} \exp\left(\frac{\tilde{s}_0(\tilde{s}, \boldsymbol{\xi}^d, \boldsymbol{\xi}^s) - \tilde{s}_{\text{aux}}}{c}\right). \quad (55)$$

Now the energy and entropy functionals are

$$\tilde{E} = \int_V \varrho \tilde{e} dV = \int_V \varrho \left[ \frac{1}{2} \mathbf{v} \cdot \mathbf{v} + cT + \frac{E^d}{2\rho} \text{tr}(\boldsymbol{\varepsilon}^d \boldsymbol{\varepsilon}^d) + \frac{E^s}{2\rho} \text{tr}(\boldsymbol{\varepsilon}^s \boldsymbol{\varepsilon}^s) \right] dV, \quad (56)$$

$$\tilde{S} = \int_V \varrho \tilde{s} dV = \int_V \varrho \left[ \tilde{s}_{\text{aux}} + c \ln \frac{T}{T_{\text{aux}}} - \frac{1}{2} \text{tr}(\boldsymbol{\xi}^d \boldsymbol{\xi}^d) - \frac{1}{2} \text{tr}(\boldsymbol{\xi}^s \boldsymbol{\xi}^s) \right] dV, \quad (57)$$

with corresponding functional derivatives

$$\frac{\delta \tilde{E}}{\delta \tilde{\mathbf{x}}} = \begin{pmatrix} \varrho \mathbf{v} \\ E^d \boldsymbol{\varepsilon}^d \\ E^s \boldsymbol{\varepsilon}^s \\ \varrho c \\ \mathbf{0} \\ \mathbf{0} \end{pmatrix}, \quad \frac{\delta \tilde{S}}{\delta \tilde{\mathbf{x}}} = \begin{pmatrix} \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \\ \frac{\varrho c}{T} \\ -\varrho \boldsymbol{\xi}^d \\ -\varrho \boldsymbol{\xi}^s \end{pmatrix}. \quad (58)$$

We perform a transformation of variables  $\mathbf{x} \rightarrow \tilde{\mathbf{x}}$ , to which the transformation (operator) matrix  $\mathbf{Q} = \frac{\delta \tilde{\mathbf{x}}}{\delta \mathbf{x}}$  is accompanied. This  $\mathbf{Q}$  can be used to establish the relationship between the original and transformed reversible and irreversible operator matrices [6]:

$$\tilde{\mathbf{L}} = \mathbf{Q} \mathbf{L} \mathbf{Q}^T, \quad \tilde{\mathbf{M}} = \mathbf{Q} \mathbf{M} \mathbf{Q}^T. \quad (59)$$



In the present current special case, we change only the fourth state variable (from  $s$  to  $T$ ), so only the fourth row of  $\mathbf{Q}$  contains nontrivial elements. Furthermore, since (55) does not contain nonlocal (gradient) terms, we can realize the transformation directly in the form

$$\mathbf{Q} = \frac{\partial \tilde{\mathbf{x}}}{\partial \mathbf{x}} = \begin{pmatrix} 1 & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{I} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \frac{1}{c}T & \frac{1}{c}T\xi^d & \frac{1}{c}T\xi^s \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{I} \end{pmatrix}, \quad (60)$$

where  $\mathbf{I}$  denotes the fourth order identity tensor [the identity that maps tensors to tensors, *i.e.*, themselves]. Then, using (59) we find<sup>7</sup>

$$\tilde{\mathbf{L}} = \mathbf{L}, \quad (61)$$

and that the structure of  $\tilde{\mathbf{M}}$  is the same as of  $\mathbf{M}$  [see (47)], with the elements

$$\begin{aligned} \tilde{M}_{11} &= -\frac{l_{11}^d}{\varrho^2} \left\{ T \left[ \left( \bullet \otimes \overleftarrow{\nabla} \right)^S \right]^d \right\} \cdot \overleftarrow{\nabla} - \frac{l_{11}^s}{\varrho^2} \left\{ T \left[ \left( \bullet \otimes \overleftarrow{\nabla} \right)^S \right]^s \right\} \cdot \overleftarrow{\nabla}, \\ \tilde{M}_{14} &= \frac{1}{\varrho^2 c} \left\{ l_{11}^d \left[ \left( \mathbf{v} \otimes \overleftarrow{\nabla} \right)^S \right]^d T \bullet + l_{11}^s \left[ \left( \mathbf{v} \otimes \overleftarrow{\nabla} \right)^S \right]^s T \bullet \right\} \cdot \overleftarrow{\nabla}, \\ \tilde{M}_{15} &= \frac{l_{12}^d}{\varrho} (T \bullet) \cdot \overleftarrow{\nabla}, & \tilde{M}_{16} &= \frac{l_{12}^s}{\varrho} (T \bullet) \cdot \overleftarrow{\nabla}, \\ \tilde{M}_{41} &= -\frac{T}{\varrho^2 c} \text{tr} \left\{ l_{11}^d \left[ \left( \mathbf{v} \otimes \overleftarrow{\nabla} \right)^S \right]^d \left[ \left( \bullet \otimes \overleftarrow{\nabla} \right)^S \right]^d + l_{11}^s \left[ \left( \mathbf{v} \otimes \overleftarrow{\nabla} \right)^S \right]^s \left[ \left( \bullet \otimes \overleftarrow{\nabla} \right)^S \right]^s \right\}, \\ \tilde{M}_{44} &= \frac{T}{\varrho^2 c^2} \text{tr} \left\{ l_{11}^d \left[ \left( \mathbf{v} \otimes \overleftarrow{\nabla} \right)^S \right]^d \left[ \left( \mathbf{v} \otimes \overleftarrow{\nabla} \right)^S \right]^d \bullet + l_{11}^s \left[ \left( \mathbf{v} \otimes \overleftarrow{\nabla} \right)^S \right]^s \left[ \left( \mathbf{v} \otimes \overleftarrow{\nabla} \right)^S \right]^s \bullet \right\}, \\ \tilde{M}_{45} &= \frac{l_{12}^d}{\varrho c} T \text{tr} \left\{ \left[ \left( \mathbf{v} \otimes \overleftarrow{\nabla} \right)^S \right]^d \bullet \right\}, & \tilde{M}_{46} &= \frac{l_{12}^s}{\varrho c} T \text{tr} \left\{ \left[ \left( \mathbf{v} \otimes \overleftarrow{\nabla} \right)^S \right]^s \bullet \right\}, \\ \tilde{M}_{51} &= -\frac{l_{21}^d}{\varrho} T \left[ \left( \bullet \otimes \overleftarrow{\nabla} \right)^S \right]^d, & \tilde{M}_{54} &= \frac{l_{21}^d}{\varrho c} T \left[ \left( \mathbf{v} \otimes \overleftarrow{\nabla} \right)^S \right]^d, & \tilde{M}_{55} &= l_{22}^d T, \\ \tilde{M}_{61} &= -\frac{l_{21}^s}{\varrho} T \left[ \left( \bullet \otimes \overleftarrow{\nabla} \right)^S \right]^s, & \tilde{M}_{64} &= \frac{l_{21}^s}{\varrho c} T \left[ \left( \mathbf{v} \otimes \overleftarrow{\nabla} \right)^S \right]^s, & \tilde{M}_{66} &= l_{22}^s T. \end{aligned} \quad (62)$$

The variable transformation is expected to preserve the structure of GENERIC [6]. Actually, by substituting (52) into (10) and rewriting it in terms of temperature, the evolution equation for  $T$  is obtained, and turns out to coincide with the fourth row of  $\tilde{\mathbf{M}}_{\delta\tilde{\mathbf{x}}}$ . However, as in the  $s$  variable case  $\mathbf{M}$  has proved nonsymmetric for nonzero  $l_A^d$  or  $l_A^s$ ,  $\tilde{\mathbf{M}}$  behaves the same way.

Now let us repeat moving the  $l_A^d$  and  $l_A^s$  related part of the dynamics to the reversible part. We find the antisymmetric

$$\tilde{\mathbf{L}}' = \begin{pmatrix} 0 & \frac{1}{\varrho} \bullet \cdot \overleftarrow{\nabla} & \frac{1}{\varrho} \bullet \cdot \overleftarrow{\nabla} & \tilde{L}'_{14} & -\frac{l_A^d}{\varrho} \bullet \cdot \overleftarrow{\nabla} & -\frac{l_A^s}{\varrho} \bullet \cdot \overleftarrow{\nabla} \\ \frac{1}{\varrho} \left[ \left( \bullet \otimes \overleftarrow{\nabla} \right)^S \right]^d & 0 & 0 & \mathbf{0} & 0 & 0 \\ \frac{1}{\varrho} \left[ \left( \bullet \otimes \overleftarrow{\nabla} \right)^S \right]^s & 0 & 0 & \mathbf{0} & 0 & 0 \\ \tilde{L}'_{41} & \mathbf{0} : & \mathbf{0} : & 0 & \mathbf{0} : & \mathbf{0} : \\ -\frac{l_A^d}{\varrho} \left[ \left( \bullet \otimes \overleftarrow{\nabla} \right)^S \right]^d & 0 & 0 & \mathbf{0} & 0 & 0 \\ -\frac{l_A^s}{\varrho} \left[ \left( \bullet \otimes \overleftarrow{\nabla} \right)^S \right]^s & 0 & 0 & \mathbf{0} & 0 & 0 \end{pmatrix} \quad (63)$$

<sup>7</sup>The same results (61)–(62) are found directly from the time evolution formula and the degeneracy conditions.

with

$$\begin{aligned}\tilde{L}'_{14} &= -\frac{1}{\rho c} \left( l_A^d T \boldsymbol{\xi}^d \bullet + l_A^s T \boldsymbol{\xi}^s \bullet \right) \cdot \tilde{\nabla}, \\ \tilde{L}'_{41} &= -\frac{T}{\rho c} \operatorname{tr} \left\{ l_A^d \boldsymbol{\xi}^d \left[ \left( \bullet \otimes \tilde{\nabla} \right)^S \right]^d + l_A^s \boldsymbol{\xi}^s \left[ \left( \bullet \otimes \tilde{\nabla} \right)^S \right]^s \right\},\end{aligned}\tag{64}$$

and that  $\tilde{\mathbf{M}}'$  can be obtained from  $\tilde{\mathbf{M}}$  like  $\mathbf{M}'$  from  $\mathbf{M}$ , *i.e.*, changing all  $l_{12}^d$  and  $l_{21}^d$  to  $l_S^d$  and  $l_{12}^s$  and  $l_{21}^s$  to  $l_S^s$ . The degeneracy criteria, as well as symmetry and positive definiteness of  $\tilde{\mathbf{M}}$ , are all satisfied. The surprising finding, however, is that  $\tilde{\mathbf{L}}'$  violates the Jacobi identity<sup>8</sup>. Why this is surprising is that, on general grounds, any variable transformation is expected to preserve the Jacobi property as well [6].

This result being so unexpected, we have checked it (for the one space dimensional version) with the application `jacobi.m` [17] as well, and while `jacobi.m` confirmed the Jacobi property for  $\mathbf{L}$ ,  $\mathbf{L}'$  and  $\tilde{\mathbf{L}}$ , it also found violation of it for  $\tilde{\mathbf{L}}'$ .

## 6 Conclusions

The results can be summarized according to Table 1.

	$s$ varied		$T$ varied	
	$l_A^d, l_A^s$ in $\mathbf{M}$	$l_A^d, l_A^s$ in $\mathbf{L}$	$l_A^d, l_A^s$ in $\mathbf{M}$	$l_A^d, l_A^s$ in $\mathbf{L}$
$\mathbf{L}$ fulfils Jacobi	✓	✓	✓	×
$\mathbf{M}$ is symmetric	×	✓	×	✓

Table 1: How the four versions behave with respect to generic GENERIC expectations.

The most apparent task for the future is to find the reason behind the violation of the Jacobi identity found in one of the four realizations. We suspect that it may be connected to the transformation of a specific extensive variable to an intensive one while having the small-strain related assumption of constant mass density, which together prohibit neglect of certain surface terms during partial integration for the space integrals. Whether the reason is this or not, the details should be worked out, and the outcome is expected to be something generally useful to know concerning GENERIC.

Next, a finite deformation version would be welcome. How deeply this will require to address objectivity and spacetime compatibility aspects [11, 12] is a question for the future.

In parallel, the current small-strain version could be numerically (*e.g.*, along the lines of [8, 9]) applied for concrete problems. For example, the recent analytical results in [10] promise methodologically useful outcome since those considerations are done in the force equilibrium approximation [zero lhs in (6), an approximation valuable for various engineering situations], which is a challenge for GENERIC with its explicite time evolution formulation. Principal as well as numerically working solutions to this compelling situation can provide fruitful contribution to both science and engineering.

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## References

- [1] Cs. Asszonyi, T. Fülöp and P. Ván, Distinguished rheological models for solids in the framework of a thermodynamical internal variable theory, *Continuum Mech. Thermodyn.* **27** (2015), 971–986.
- [2] Cs. Asszonyi, A. Csátár and T. Fülöp, Elastic, thermal expansion, plastic and rheological processes – theory and experiment, *Period. Polytech. Civil Eng.* **60** (2016), 591–601.

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<sup>8</sup>Recall that  $l_A^d, l_A^s$  are constants.

- [3] W. Lin, Y. Kuwahara, T. Satoh, N. Shigematsu, Y. Kitagawa, T. Kiguchi, *et al.*, A case study of 3D stress orientation determination in Shikoku Island and Kii Peninsula, Japan, in: *I. Vrkljan (ed.) Rock Engineering in Difficult Ground Conditions (Soft Rock and Karst), Proceedings of Eurock'09*, Cavtat, Croatia, 28-29 October, 2009, pp. 277–282.
- [4] K. Matsuki and K. Takeuchi, Three-dimensional in situ stress determination by anelastic strain recovery of a rock core, *Int. J. Rock Mech. Min. Sci. & Geomech. Abstr.* **30** (1993), 1019–1022.
- [5] K. Matsuki, Anelastic strain recovery compliance of rocks and its application to in situ stress measurement, *Int. J. Rock Mech. Min. Sci.* **45** (2008), 952–965.
- [6] H. C. Öttinger, *Beyond Equilibrium Thermodynamics*, John Wiley & Sons, Inc., Hoboken, New Jersey, 2005.
- [7] M. Grmela, Why GENERIC?, *J. Non-Newtonian Fluid Mech.* **165** (2010), 980–986.
- [8] H. C. Öttinger, GENERIC integrators: structure preserving time integration for thermodynamic systems, *J. Non-Equilib. Thermodyn.* **43** (2018) 89–100.
- [9] X. Shang and H. C. Öttinger, Structure-preserving integrators for dissipative systems based on reversible-irreversible splitting, preprint (2018), <https://arxiv.org/pdf/1804.05.pdf>.
- [10] T. Fülöp and M. Szücs, Analytical solution method for rheological problems of solids, preprint (2018), <https://arxiv.org/pdf/1810.06350.pdf>.
- [11] T. Fülöp and P. Ván, Kinematic quantities of finite elastic and plastic deformation, *Mathematical Methods in the Applied Sciences* **35** (2012) 1825–1841.
- [12] T. Fülöp, Objective thermomechanics, preprint (2015), <https://arxiv.org/pdf/1510.08038.pdf>.
- [13] J. Verhás, *Thermodynamics and rheology*, Akadémiai Kiadó and Kluwer Academic Publisher, Budapest, 1997; online version: [http://montavid.hu/materials/Verhas\\_Thermodynamics\\_and\\_Rheology\\_2017-05-17.pdf](http://montavid.hu/materials/Verhas_Thermodynamics_and_Rheology_2017-05-17.pdf), Society for the Unity of Science and Technology, Budapest, 2017.
- [14] A. Janečka and M. Pavelka, Non-convex dissipation potentials in multiscale non-equilibrium thermodynamics, *Continuum Mech. Thermodyn.* **30** (2018) 917–941.
- [15] M. Grmela, M. Pavelka, V. Klika, B.-Y. Cao and N. Bendian, Entropy and entropy production in multiscale dynamics, preprint (2018), <https://arxiv.org/pdf/1809.05412.pdf>.
- [16] M. Hütter and B. Svendsen, Quasi-linear versus potential-based formulations of force–flux relations and the GENERIC for irreversible processes: comparisons and examples, *Continuum Mech. Thermodyn.* **25** (2013), 803–816.
- [17] M. Kröger, M. Hütter and H. C. Öttinger, Symbolic test of the Jacobi identity for given generalized ‘Poisson’ bracket, *Comput. Phys. Commun.* **137** (2001), 325–340.