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GENERIC*, AN ALTERNATIVE FORMULATION OF NONEQUILIBRIUM CONTINUUM MECHANICS?

Abstract.

During the last 15 years a bracket formalism of dissipative continuum physics has been developed which resulted in a formulation which is shortly denoted as GENERIC. GENERIC has been applied to different problems of continuum thermodynamics, often in this way, that a well-known problem was reformulated in GENERIC formalism. So in 1997 the GENERIC form of the equations of motion of a Navier-Stokes fluid was formulated. To learn some more about the GENERIC procedure we consider here a general 5-field theory of fluids. Usually GENERIC is formulated for an isolated system, but here we will discuss the facility to formulate GENERIC for an open system.

1. Introduction

The phenomenological theories of thermodynamics are divided into continuumtheoretical ones and into those of discrete systems. There is a variety of phenomenological non-equilibrium continuum theories which are similar, but differ in basic concepts [10]. These are the Linear Irreversible Thermodynamics [2], Rational and Extended Thermodynamics ([14] to [7]), Non-Classical Thermodynamics [9], and theories using evolution criteria [11] and variational principles [6]. These well-known thermodynamical theories are now added by a special dissipative continuum procedure which was developped during the last 15 years starting out with a bracket formalism originated by an extension of Hamiltonian mechanics [3]. One result of this bracket approach is the GENERIC formalism [4, 5] which is totally different from the theories mentioned above, but is claimed by its investigators to be generally valid for all discrete systemsall theories in field formulation. In GENERIC the balance equations are generated by total energy and total entropy both acting as potentials and being only dependent on the wanted fields and not on the state space. The GENERIC balances are splitted additively into a reversible and an irreversible part. Beyond the balance equations there are so-called degeneracy conditions which are unknown in conventional, rational, and extended thermodynamics. Jacobi identities stemming from the antisymmetric bracket of the reversible part of the balance equations and calling to mind the Hamiltonian mechanics background of the GENERIC formalism are also unknown in the other approaches [1].

The distinctions between GENERIC and the usual approach demand for a possibility to compare them in a way as general as possible. Here a general 5-field formulation for fluids is considered in GENERIC treatment. First of all we report on general the GENERIC setting which is independent of special constitutive assumptions. Then we will extend the GENERIC

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formalism to open systems. The structure of GENERIC can be motivated by a microscopic foundation [12],[13].

2. GENERIC setting

The fundamental structure of GENERIC is determined by six building blocks [3] to [12].

1. The set of the basic or wanted fields $\mathbf{Z}$ of the system which is presupposed to be open,
2. the total energy $E^{tot}(\mathbf{Z})$ of the open system and
3. its total entropy $S(\mathbf{Z})$, as two global potentials which depend only of the basic fields
4. two, in general operator-valued matrices $\mathcal{L}(\mathbf{Z})$ and
5. the dissipation operator $\mathcal{M}(\mathcal{Z})$ which depend on the state space $\mathcal{Z}$ which is not identical to the basic fields $\mathbf{Z}$,
6. the supply of the wanted fields $\mathbf{f}_e$ wich is vanishing for an isolated system.

The *equations of motion* of the basic fields $\mathbf{Z}$ have the special GENERIC form

$$\partial_t \mathbf{Z} = \mathcal{L} \cdot \frac{\delta E^{tot}}{\delta \mathbf{Z}} + \mathcal{M} \cdot \frac{\delta S}{\delta \mathbf{Z}} + \mathbf{f}_e, \tag{1}$$

which always can be split into its reversible, its irreversible and its supply part

$$\partial_t \mathbf{Z}^{rev} := \mathcal{L} \cdot \frac{\delta E^{tot}}{\delta \mathbf{Z}}, \qquad \partial_t \mathbf{Z}^{irr} := \mathcal{M} \cdot \frac{\delta S}{\delta \mathbf{Z}}, \qquad \partial_t \mathbf{Z}^{sup} := \mathbf{f}_e. \tag{2}$$

Here δ/δ is the functional derivative which maps global quantities to local ones, as we will see in the GENERIC treatment.

Beyond the equations of motion (1) the complementary degeneracy conditions

$$\mathcal{L} \cdot \frac{\delta S(\mathbf{Z})}{\delta \mathbf{Z}} = \mathbf{0}, \qquad \mathcal{M} \cdot \frac{\delta E^{tot}(\mathbf{Z})}{\delta \mathbf{Z}} = \mathbf{0} \tag{3}$$

are satisfied by $\mathcal{L}$ and $\mathcal{M}$. Therefore the degeneracy conditions (3) describe the reversible-irreversible coupling which is meant in the name of GENERIC. The two contributions (3) to the time evolution of $\mathbf{Z}$ generated by the total energy E^{tot} and by the total entropy S are called the reversible and irreversible contributions to dynamics, respectively.

General properties of $\mathcal{L}$ and $\mathcal{M}$ are discussed easily in terms of two brackets, one is anti-symmetric, the other one symmetric

$$\begin{aligned} &[A, B] := \left\langle \frac{\delta A}{\delta \mathbf{Z}}, \mathcal{L} \cdot \frac{\delta B}{\delta \mathbf{Z}} \right\rangle \doteq -[B, A] + \frac{1}{2}(\mathcal{O}^{rev}(A, B) + \mathcal{O}^{rev}(B, A)), \\ &[A, A] = \mathcal{O}^{rev}(A, A), \end{aligned} \tag{4}$$

$$\{A, B\} := \left\langle \frac{\delta A}{\delta \mathbf{Z}}, \mathcal{M} \cdot \frac{\delta B}{\delta \mathbf{Z}} \right\rangle \doteq \{B, A\} + \frac{1}{2}(\mathcal{O}^{irr}(B, A) - \mathcal{O}^{irr}(A, B)), \tag{5}$$

$$\{A, A\} + \mathcal{O}^{irr}(A, A) \dot{\geq} 0. \tag{6}$$

Here $\langle\ ,\ \rangle$ denotes a scalar product, especially

$$\left\langle \frac{\delta A}{\delta \mathbf{Z}}, \mathcal{L} \cdot \frac{\delta B}{\delta \mathbf{Z}} \right\rangle := \int_{\mathcal{G}} \left[\frac{\delta A}{\delta \mathbf{Z}} \cdot \mathcal{L} \cdot \frac{\delta B}{\delta \mathbf{Z}} \right] d^3x, \tag{7}$$

A and B are sufficiently regular and real-valued functionals on $\mathbf{Z}$, $\mathcal{O}^{rev}$ is the reversible part, and $\mathcal{O}^{irr}$ is the irreversible part of the flux through the surface of the Volume $\mathcal{G}$. From the setting (4) follows, that $\mathcal{L}$ is antisymmetric, whereas we have to demand the symmetry of $\mathcal{M}$ which cannot be concluded from (5). Now we can express the degeneracy conditions (3) with the brackets, we find

$$[S, E^{tot}] - \mathcal{O}^{rev}(E^{tot}, S) = 0, \qquad \{E^{tot}, S\} + \mathcal{O}^{irr}(E^{tot}, S) = 0 \tag{8}$$

The antisymmetric bracket is presupposed to satisfy the Jacobi identity for closed systems, i.e all the surface terms vanish

$$[A, [B, C]] + [B, [C, A]] + [C, [A, B]] \doteq 0. \tag{9}$$

According to (1), (4) and (5) we can write the time evolution of A as

$$A = \int a(\mathbf{Z})\, d^3x, \ \longrightarrow\ \frac{\delta A}{\delta \mathbf{Z}} = \frac{\partial a}{\partial \mathbf{Z}}, \tag{10}$$

and because the system is an open one, we obtain

$$\frac{d}{dt} A = \int \partial_t a(\mathbf{Z})\, d^3x = [A, E^{tot}] + \{A, S\} + \int \frac{\partial a}{\partial \mathbf{Z}} \cdot \mathbf{f_e}\, d^3x. \tag{11}$$

According to (11), (8), (4) and (5) we obtain the time rate of the total energy and that of the total entropy of the isolated system

$$\begin{aligned} \frac{d}{dt} E^{tot} &= [E^{tot}, E^{tot}] + \{E^{tot}, S\} + \int \frac{\partial e^{tot}}{\partial \mathbf{Z}} \cdot \mathbf{f_e}\, d^3x \\ &= \mathcal{O}^{rev}(E^{tot}, E^{tot}) - \mathcal{O}^{irr}(E^{tot}, S) + \int \frac{\partial e^{tot}}{\partial \mathbf{Z}} \cdot \mathbf{f_e}\, d^3x, \end{aligned} \tag{12}$$

$$\begin{aligned} \frac{d}{dt} S &= [S, E^{tot}] + \{S, S\} + \int \frac{\partial \varrho s}{\partial \mathbf{Z}} \cdot \mathbf{f_e}\, d^3x \\ &= \mathcal{O}^{rev}(E^{tot}, S) + \{S, S\} + \int \frac{\partial \varrho s}{\partial \mathbf{Z}} \cdot \mathbf{f_e}\, d^3x. \end{aligned} \tag{13}$$

with the entropy production

$$\sigma = \{S, S\} + \mathcal{O}^{irr}(S, S) \geq 0.$$

This inequality represents the second law of thermodynamics of an open system in global formulation, where the surface term represents the flux of the entropy through the surface of the system. It is also clear, that all the surface terms have to vanish, if we want to describe an isolated system.

To go on with the GENERIC treatment we now have to introduce constitutive assumptions, that means, we have to proceed beyond the general setting of GENERIC.

3. GENERIC treatment

We consider an one-component simple fluid which is decribed by five basic fields: Mass density ϱ, material velocity $\mathbf{v}$, and specific internal energy ε. Therefore is the set of the wanted field given by

$$\mathbf{Z}(\mathbf{x},t) = (\varrho,\ \mathbf{p} := \varrho\mathbf{v},\ \eta := \varrho\varepsilon)(\mathbf{x},t). \tag{14}$$

Then we can introduce the global potentials, as the total energy of the system

$$E^{tot}(\mathbf{Z}) = \int \left[\frac{\mathbf{p}^2(\mathbf{x},t)}{2\varrho(\mathbf{x},t)} + \eta(\mathbf{x},t)\right] d^3x, \tag{15}$$

and the global entropy of the system is by setting a functional on $\mathbf{Z}$

$$S(\mathbf{Z}) = \int \varrho s(\varrho,\mathbf{p},\eta)\, d^3x. \tag{16}$$

More over, we know about a five field theorie, that the fields have to satisfy the following balance equation for the wanted fields

$$\begin{array}{llll} & \text{reversible part} & \text{irreversible part} & \text{supply} \\ \partial_t\rho = & -\nabla\cdot\rho\mathbf{v} & +0 & +0 \\ \partial_t\mathbf{p} = & -\nabla\cdot\mathbf{p}\mathbf{v} - \nabla P & +\nabla\cdot\mathbf{V} & +\mathbf{f} \\ \partial_t\eta = & -\nabla\cdot\eta\mathbf{v} - P\nabla\cdot\mathbf{v} & +\nabla\mathbf{v}:\mathbf{V} - \nabla\cdot\mathbf{q} & +r \end{array} \tag{17}$$

where P is the pressure, $\mathbf{V}$ is the traceless viscous pressure tensor, $\mathbf{q}$ is the heat flux density, $\mathbf{f}$ is the supply of the momentum and r is the supply of the internal energy. We have also performed a split into a reversible and an irreversible part, respectively. But this is an unsolved problem in GENERIC, how to do the right split. Until now it is only possible to see that the split has been found correct, if the resulting entropy production is the right one. But for knowing the entropy production you have to treat the five field theory by another theory, for example by Rational Thermodynamics and by exploiting the Liu-procedure [9].

3.1. State space

In 5-field theory the wanted basic fields (14) are those of a fluid and because we consider dissipative fluids, we choose as a state space one includes the gradients of the basic fields

$$\mathcal{Z}^+ := (\varrho,\eta,\mathbf{v},\nabla\varrho,\nabla\eta,\nabla\mathbf{v}). \tag{18}$$

Taking into account, that state spaces are spanned by objective quantities we have to change (18) into

$$\mathcal{Z} := (\varrho,\eta,\nabla\varrho,\nabla\eta,(\nabla\mathbf{v})^s). \tag{19}$$

Here $()^s$ is the symmetric part of a tensor. Because of (14) the constitutive quantities in the balances (17) are

$$\mathbf{V} = \mathcal{V}(\mathcal{Z}(\mathbf{x},t)), \qquad \mathbf{q}(\mathbf{x},t) = \mathcal{Q}(\mathcal{Z}(\mathbf{x},t)). \tag{20}$$

(21)

The viscous pressure tensor is symmetric

$$\mathbf{V}(\mathbf{x},t) = \mathbf{V}^\top(\mathbf{x},t), \tag{22}$$

because we only consider fluids without internal spin.

3.2. Reversible part

Because in GENERIC the equations of motions for the basic fields (1) can be split into their reversible and irreversible part (2), we start out with the reversible part of (1) which is as represented in the first column in (17). The first step is that we have to calculate the functional derivative from the global total energy (15). According to (14) the functional derivative in $(2)_1$ generates from (15) the local fields

$$\left(\frac{\delta E^{tot}}{\delta \mathbf{Z}}\right)^T = \left(-\frac{1}{2}\mathbf{v}^2(\mathbf{x},t),\ \mathbf{v}(\mathbf{x},t),\ 1\right), \tag{23}$$

which inserted in $(2)_1$ result in the reversible part of the equations of motion

$$\begin{pmatrix} \partial_t \varrho \\ \partial_t \mathbf{p} \\ \partial_t \eta \end{pmatrix}_{rev} = \mathcal{L} \cdot \begin{pmatrix} -\frac{1}{2}\mathbf{v}^2 \\ \mathbf{v} \\ 1 \end{pmatrix} = \begin{pmatrix} -\nabla \cdot (\mathbf{v}\varrho) \\ -\nabla \cdot (\mathbf{v}\mathbf{p}) - \nabla P \\ -\nabla \cdot (\mathbf{v}\eta) - P\nabla \cdot \mathbf{v} \end{pmatrix}. \tag{24}$$

These five equations are not sufficient to determine the 13 components of the antisymmetric $\mathcal{L}$. Concerning the balances (17) this undetermination is not important, because all the different $\mathcal{L}$ result in the same balances. Concerning the degeneracy conditions $(3)_1$ it is not evident that all these different $\mathcal{L}$ have the same kernel. On the other hand $\mathcal{L}$ is also not determined by the kernel $\delta S/\delta \mathbf{Z}$. The consequences of this undetermination of $\mathcal{L}$ are not fully discussed up to now.

Now we can show, that one operator-valued matrix satisfying (24) is the following one

$$\mathcal{L} = -\begin{pmatrix} 0 & \nabla\varrho\cdot & 0 \\ \varrho\nabla & [\nabla\mathbf{p} + \mathbf{p}\nabla]^\top\cdot & \nabla P + \eta\nabla \\ 0 & (P\nabla + \nabla\eta)\cdot & 0 \end{pmatrix}. \tag{25}$$

The degeneracy conditions $(3)_1$ are now used to determine the kernel $\delta S/\delta \mathbf{Z}$ of $\mathcal{L}$. As already remarked, it is not evident, that this kernel is unique. The global entropy of the system depending only on $\mathbf{Z}$ is given by (16) and the functional derivative of S generates local quantities

$$\left(\frac{\delta S}{\delta \mathbf{Z}}\right)^T = \left(\frac{\partial(\varrho s)}{\partial \varrho} =: -\frac{g}{T}(\mathbf{x},t),\ \frac{\partial(\varrho s)}{\partial \mathbf{p}}(\mathbf{x},t),\ \frac{\partial(\varrho s)}{\partial \eta} =: \frac{1}{T}(\mathbf{x},t)\right). \tag{26}$$

Here the usual abbreviations *specific free enthalpy* g and *absolute equilibrium temperature* T for the derivatives of the entropy are introduced. The degeneracy condition $(3)_1$ results in the following equations

$$\frac{\partial \varrho s}{\partial \mathbf{p}} = \mathbf{0}, \tag{27}$$

$$-\varrho\nabla\frac{g}{T} + \nabla\frac{P}{T} + \eta\nabla\frac{1}{T} = 0. \tag{28}$$

As (27) shows, the GENERIC setting allows to derive that the entropy density does not depend on the velocity $\mathbf{v}$. From (28) follows immediately by use of (26) and (27) that the following equation yields

$$-\varrho s = \frac{1}{T}(\varrho g - P - \eta) + const \longrightarrow \tag{29}$$

$$\longrightarrow g = \varepsilon + \frac{P}{\varrho} - Ts\,, \quad const = 0, \tag{30}$$

because (30) is the definition of the specific free enthalpy g.

The exploitation of the reversible part of the GENERIC equations of motion (1) results in (25), (27), and (28). Now we investigate its irreversible part in the next section.

3.3. Irreversible part

We now have to generate one $\mathcal{M}$ by use of the irreversible part of the equations of motion $(2)_2$ and by the degeneracy condition $(3)_2$

$$\mathcal{M}\cdot\frac{\delta S(\mathbf{Z})}{\delta\mathbf{Z}} = \mathcal{M}\cdot\begin{pmatrix}-\frac{g}{T}\\ \mathbf{0}\\ \frac{1}{T}\end{pmatrix} = \begin{pmatrix}0\\ \nabla\cdot\mathbf{V}\\ \nabla\mathbf{v}:\mathbf{V}-\nabla\cdot\mathbf{q}\end{pmatrix}, \tag{31}$$

$$\mathcal{M}\cdot\frac{\delta E^{tot}(\mathbf{Z})}{\delta\mathbf{Z}} = \mathcal{M}\cdot\begin{pmatrix}-(1/2)\mathbf{v}^2\\ \mathbf{v}\\ 1\end{pmatrix} = \begin{pmatrix}0\\ \mathbf{0}\\ 0\end{pmatrix}. \tag{32}$$

From (6) and (31) we can immediately read off the entropy production without any knowledge of $\mathcal{M}$

$$\begin{aligned}\sigma &= \left\langle\frac{\delta S(\mathbf{Z})}{\delta\mathbf{Z}},\mathcal{M}\cdot\frac{\delta S(\mathbf{Z})}{\delta\mathbf{Z}}\right\rangle+\int\nabla\cdot\frac{\mathbf{q}}{T}d^3x\\ &= \int\left(\frac{1}{T}[\nabla\mathbf{v}:\mathbf{V}-\nabla\cdot\mathbf{q}]+\nabla\cdot\frac{\mathbf{q}}{T}\right)d^3x\\ &= \int[\frac{1}{T}\nabla\mathbf{v}:\mathbf{V}+\mathbf{q}\cdot\nabla\frac{1}{T}]\,d^3x = \int\pi^s\,d^3x \geq 0 \end{aligned} \tag{33}$$

Because the last equal sign is valid for all domains of integration, we obtain for the local entropy production density

$$\pi^s = \frac{1}{T}\nabla\mathbf{v}:\mathbf{V}+\mathbf{q}\cdot\nabla\frac{1}{T}. \tag{34}$$

This is the same result as in the conventional procedure like in rational thermodynamics [9] and has the usual form of a product between fluxes and forces.

For the sake of simplicity, we set here the first column and row equal to zero. Consequently we are looking for a symmetric matrix of the form

$$\mathcal{M} = \begin{pmatrix}0 & \mathbf{0} & 0\\ \mathbf{0} & \mathbf{M}^{22} & \mathbf{M}^{23}\\ 0 & \mathbf{M}^{32} & M^{33}\end{pmatrix}. \tag{35}$$

Now we can show, that one of the possible choice of the operator-valued matrix elements of the dissipation operator $\mathcal{M}$ have the following form due to the conditions (31) and (32)

$$M^{22}[*] = -\nabla\cdot\mathbf{V}T\frac{1}{(\nabla\cdot\mathbf{v})}\nabla * \tag{36}$$

$$M_k^{23}[*] = \nabla\cdot\mathbf{V}T * \tag{37}$$

$$M_k^{32}[*] = -(\mathbf{V}T\cdot\nabla)^T\cdot * \tag{38}$$

$$M^{33}[*] = \nabla\cdot\lambda\cdot\nabla+(\nabla\mathbf{v}:\mathbf{V})T*$$

with

$$\lambda_{ij} := \frac{q_i(\partial_j T)}{(\nabla T)^2}T^2.$$

The exploitation of the irrversible part results in (34) and (36) - (39).More over, we see that the generalized transport coefficients in (36) - (39) are not independent of each other. This is a result what is analogue to the Casimir Onsager recriprocal relations in TIP.

3.4. Balance equation for the global potentials

The last point, we have to discuss are the dynamic equations for both global potentials. The supply vector of the wanted fields is according to the last column in (15) is

$$\mathbf{f}_e^T = (0, \mathbf{f}, r), \tag{39}$$

and thus we get immediately from (13) using (29) and (33)

$$\frac{d}{dt}S(\mathbf{Z}) \quad = \quad [S, E^{tot}] + \{S, S\} + \int \frac{\partial \varrho s}{\partial \mathbf{Z}} \cdot \mathbf{f_e}\, d^3x \tag{40}$$

$$= \int \left[-\nabla \cdot \mathbf{v}\varrho s(\mathbf{Z}) + \pi^s - \nabla \cdot \frac{\mathbf{q}}{T} + \frac{r}{T} \right] d^3x. \tag{41}$$

Similiar we get from (12) using (4), (5) and $(3)_2$ the balance equation of the total energy

$$\begin{aligned}
\frac{d}{dt}E^{tot}(\mathbf{Z}) &= [E^{tot}, E^{tot}] + \{E^{tot}, S\} + \int \frac{\partial e^{tot}}{\partial \mathbf{Z}} \cdot \mathbf{f_e}\, d^3x \\
&= \int \left\{ -\nabla \cdot [(\mathbf{v}e^{tot}(\mathbf{Z}) + \mathbf{v}P) + (\mathbf{V}^T \cdot \mathbf{v} - \mathbf{q})] + \mathbf{v} \cdot \mathbf{f^e} + r \right\} d^3x \\
&= \dot{W} + \dot{Q}
\end{aligned} \tag{42}$$

with the work

$$\dot{W} := \int \left[-\nabla \cdot (\mathbf{v}e^{tot}(\mathbf{Z}) + \mathbf{v}P) + \nabla \cdot (\mathbf{V}^T \cdot \mathbf{v}) + \mathbf{v} \cdot \mathbf{f^e} + r \right] d^3x \tag{43}$$

and the heat exchange

$$\dot{Q} := \int \nabla \cdot \mathbf{q} d^3x. \tag{44}$$

4. Conclusion

An important statement of GENERIC is the fact, that the generalized transport coefficients of the dissipation operator are not independent. In GENERIC one derive a generalisation of Casimir-Onsager recriprocal relations. The structure of GENERIC provides, that the dissipation operator is positive definit and thus that a closed system decays to equilibrium.

It is also possible to give a microscopic foundation of the GENERIC formalism [12], [13] which gives us a powerfull argument for the validity of this structure. But nevertheless, we have the unsolved problem in GENERIC, that is a correct split into a reversible and an irreversible part is not achieved up to now. Although it seems to be possible to transform the whole GENERIC structure to open systems which was demonstrated here. Another important statement of GENERIC is, that we have to preassume local equilibrium, i.e the global potentials depend only on the wanted fields.

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