Chapter 2

FROM MATHEMATICAL PHYSICS TO ENGINEERING SCIENCE

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Abstract The theory of configurational - or material - forces smells good of its mathematical-physical origins. This contribution outlines this characteristic trait with the help of a four-dimensional formalism in which energy and canonical momentum go along, with sources that prove to be jointly consistent in a dissipation inequality. This is what makes the formulation so powerful while automatically paving the way for an exploitation of irreversible thermodynamics, e.g., in the irreversible progress of a defect throughout matter

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1. INTRODUCTION

Although it now finds applications in typical engineering settings such as the application of finite-element and finite-volume computational techniques, the theory of configurational - or material - forces smells good of its **mathematical-physical origin**. This was transparent in Eshelby's original works but even more so in the author's works. The newly entertained relationship with computational techniques based on mathematical formulations akin to **general conservation laws** (weak form such as the principle of virtual power, classical volume balance laws) is not so surprising.

In fact, both the deep physical meaning and the practical usefulness of the critical expressions (e.g., of thermodynamical driving forces) obtained within this framework stem from the intimate relationship built from the start between these expressions and a **field-theoretical invariance** or lack of invariance. Symmetries and their eventual breaking are the physically most profound and intellectually puzzling tenets in modern physics. That engineering applications fit into this general picture is a comforting view of the **mutual enrichment** of pure science and modern engineering. This contribution outlines these features with the help of a four-(3+1) dimensional formalism in which energy and canonical momentum go along, with sources that prove to be jointly consistent in a dissipation inequality. This is what makes the formulation so powerful while automatically paving the way for an exploitation of **irreversible thermodynamics**, e.g., in the irreversible progress of a defect throughout matter.

The wealth and wide range of applications opened by the configurational vision of mechanics or mathematical physics is extremely impressive. Among the now traditional applications we find:

i.) The study of the progress of "**defects**" or objects considered as such, or even macroscopic physical manifestations of the like. Among these we have: dislocations, disclinations ; cracks, growth, phase transformations, plasticity (pseudo-material inhomogeneities). This is exemplified and documented in several synthetic works, e. g., [1]-[5].

ii.) The applications to **dynamical systems** rewritten in the appropriate form : Canonical balance laws applied to the perturbed motion of soliton complexes (solitonic systems governed by systems of partial differential equations - works by Maugin-Pouget-Sayadi-Kosevich et al in both continuous and discrete frameworks - *etc*) representing localized solutions, cf. [6]-[8];

and more recently

iii.) Applications to **various numerical schemes**, e.g., in *Finite-differences* (e.g., Christov and Maugin [6]; in *Finite-elements* (e.g., Braun [9], Mueller, Gross, Maugin [10]-[11], Steinmann *et al* [12], *etc*, and in *Finite-volumes /continuous cellular automata* (e.g., works by: Berezovski and Maugin [13].

Points (i) and (iii) above are richly illustrated by other contributions in this volume. We shall focus attention on the original field-theorretical framework (already exposed in lecture notes, Maugin and Trimarco [14]), and the thermomechanical formulation that contains the essence of the subject matter.

In a different style but of great interest are also the presentation and applications developed by Kienzler and Herrmann [15] - also these authors' contributions in the lecture notes mentioned in ref. 14).

2. THE FIELD-THEORETICAL FRAMEWORK

Basic fields are noted $\phi^{\alpha}, \alpha = 1,2,3,...$ They depend on a space-time parametrization (X^K, t) where in the classical continuum physics of deformable solids X^K, K=1,2,3 are material coordinates and t is Newton's absolute time. Examples of such fields are the classical *direct* motion $x^i = \bar{x}^i(X^K, t)$, the micromotion $\chi^i = \bar{\chi}^i(X^K, t)$ of micromorphic media, and electromagnetic potentials $(\phi, \mathbf{A})(X^K, t)$. Note in the latter case that the fields are what are called "potentials" by physicists. It is essential here to clearly distinguish between the fields *per se* and the space-time parametrization. In standard continuum mechanics the placement $\mathbf{x}$ in the actual configuration at time t is the three-dimensional field. In the absence of dissipation, relying on a Hamiltonian variational formulation, the basic Euler-Lagrange equations of "motion", (one for each field or for each component of multidimensional field) read formally

$$\delta \phi^{\alpha} : \; E_{\alpha} = 0 \quad , \quad \alpha = 1,2,3,.. \tag{1}$$

Noether's identity - that we prefer to refer to as Noether-Ericksen identity [16] - is written as (note the summation over α; $\nabla_R = \partial / \partial \mathbf{X}$)

$$\sum_{\alpha} E_{\alpha} . (\nabla_R \phi^{\alpha})^T = 0 \tag{2}$$

This is a co-vectorial equation on the material manifold M^3. It is referred to as the equation of *canonical* or *material momentum* because, according to d'Alembert's principle, it is clearly generated by a variation of the material coordinates X^K. Equation (2), unlike (1), governs the whole set of fields α. That is, it has the same ontological status as the following "theorem of kinetic energy" that is obtained from the set (1) by an equivalent time-like operation:

$$\sum_{\alpha} E_{\alpha} . \left(\frac{\partial \phi^{\alpha}}{\partial t} \right) = 0 \tag{3}$$

Although this clearly is the time-like equation associated with the space-like equation (2), this is not exactly the *energy theorem*, for it should be combined with a statement of the first law of thermodynamics in order to introduce the notions of internal energy and heat. Ultimately, this manipulation will yield a *balance of entropy*, perhaps for an energy quantity such as entropy multiplied by temperature: $\theta\, S$, where θ is the absolute temperature and S is the entropy per unit reference volume (see below). Both this equation and eqn. (2) are canonical (of a general ever realized form) and, in the presence of dissipative processes, do not refer to necessarily strictly conserved quantities. This will be seen hereafter. For the time being, in order to emphasize the role of this type of equation as governing the *whole* physical system under consideration and not only the classical degrees of translation of a standard deformable medium, we note a few examples of expressions of the canonical (or material) momentum:

- general analytical-mechanics formula:

$$P = -\rho_0 \sum_{\alpha} \left(\frac{\partial \phi^{\alpha}}{\partial t} \right) . \left(\nabla_R \phi_{\alpha} \right) \tag{4}$$

- classical deformable solid:

$$P = -\rho_0 \mathbf{F}^T . \mathbf{v} \;\; ; \;\; \mathbf{v} = \frac{\partial}{\partial t} \overline{\mathbf{x}} \;\; , \;\; \mathbf{F} = \nabla_R \overline{\mathbf{x}} \; . \tag{5}$$

where $\rho_0(\mathbf{X})$ is the matter density at the reference configuration, $\mathbf{v}$ is the physical velocity, and $\mathbf{F}$ is the direct motion gradient. Here the canonical or material momentum simply is the pullback, changed of sign, of the physical (mechanical) momentum $\mathbf{p} = \rho_0 \mathbf{v}$.

- deformable solid with a rigid microstructure (micropolar medium) [17]

$$P = -\rho_0 \left(\mathbf{F}^T . \mathbf{v} + \left(\nabla_R \overline{\chi} \right) . \mathbf{I} . \frac{\partial}{\partial \mathrm{t}} \dot{\overline{\chi}} \right) \tag{6}$$

where $\mathbf{I}$ is some kind of rotational inertia tensor.

- * *deformable electromagnetic solid* (full electrodynamics) [1],[14]

$$P = -\left(\rho_0 \mathbf{F}^T . \mathbf{v} - \frac{1}{c} \Pi \times \mathbf{B} \right) = \rho_0 \mathbf{C} . \mathbf{V} + \frac{1}{c} \Pi \times \mathbf{B} \tag{7}$$

where Π and $\mathbf{B}$ are *material* electric polarization and magnetic induction. In this case the "physical" electromagnetic electromagnetic momentum is $\mathbf{p}^{em} = \frac{1}{c}\mathbf{E}\times\mathbf{B}$, where $\mathbf{E}$ and $\mathbf{B}$ are "physical" electric field and magnetic induction).

This series of examples emphasizes the global-system nature of the canonical balance laws of continuum physics insofar as the balance of canonical momentum is concerned.

3. CANONICAL BALANCE LAWS

We now consider a standard continuous solid (no microstructure, no electromagnetic fields) but in the presence of heat and dissipative processes. The canonical balance laws still are the fundamental balance laws of thermomechanics (momentum and energy) expressed **intrinsically in terms of a good space-time parametrization**. In a relativistic background this would be the conservation - or lack of conservation - of the canonical energy-momentum tensor first spelled out in 1915 and 1918 by David Hilbert and Emmy Noether on a variational basis. Here we consider free energies per unit reference volume such as

$$W = \overline{W}(\mathbf{F}, \theta, \alpha; \mathbf{X}) \tag{8}$$

for an anisotropic, *possibly anelastically inhomogeneous* material in finite strains, whose basic behavior is elastic, but it may present combined anelasticity. The arguments of the supposedly sufficiently smooth function W are: **F:** deformation gradient, θ: thermodynamical temperature, α: set of internal variable of state representative of a macroscopically manifested irreversible behavior; **X:** material coordinates. The so-called *laws of* thermodynamical *state* are given by

$$\mathbf{T} = \frac{\partial \overline{W}}{\partial \mathbf{F}}, S = -\frac{\partial \overline{W}}{\partial \theta}, A = -\frac{\partial \overline{W}}{\partial \alpha} \tag{9}$$

Then at any *regular* material point $\mathbf{X}$ in the body B, we have the following ***local balance equations for*** **mass, linear momentum, and energy**:

$$\left.\frac{\partial \rho_0}{\partial t}\right|_{\mathbf{X}} = 0, \tag{10}$$

$$\left.\frac{\partial \mathbf{p}}{\partial t}\right|_{\mathbf{X}} - div_R \mathbf{T} = \mathbf{0} , \tag{11}$$

$$\left.\frac{\partial (K+E)}{\partial t}\right|_{\mathbf{X}} - \nabla_R . (\mathbf{T}.\mathbf{v} - \mathbf{Q}) = 0 , \tag{12}$$

These equations are presented here in the so-called *Piola-Kirchhoff formulation*, with an $(\mathbf{X},t)$ space-time parametrization, but the components of eqn. (11) are still in **physical space**, so that it is not an intrinsic formulation. We remind the reader of the following definitions and relations:

$$\mathbf{x} = \chi(\mathbf{X},t), \tag{13}$$

$$\mathbf{F} = \left.\frac{\partial \chi}{\partial \mathbf{X}}\right|_t = \nabla_R \chi , \mathbf{v} = \left.\frac{\partial \chi}{\partial t}\right|_{\mathbf{X}} , \tag{14}$$

$$\mathbf{p} = \rho_0 \mathbf{v} , K = \frac{1}{2} \rho_0 \mathbf{v}^2 , \tag{15}$$

$$E = W + S\theta . \tag{16}$$

Equation (10)-(12) are **strict conservation laws** (no source terms), because we assume, for the sake of simplicity, that there are neither external body force acting nor energy input per unit volume. In these conditions the entropy equation and the dissipation inequality read [18]

$$\theta \left.\frac{\partial S}{\partial t}\right|_{\mathbf{X}} + \nabla_R . \mathbf{Q} = \Phi^{intr} \quad , \quad \Phi^{intr} := A\dot{\alpha} \quad , \quad \dot{\alpha} \equiv \left.\frac{\partial \alpha}{\partial t}\right|_{\mathbf{X}} , \tag{17}$$

and

$$\sigma_B = \theta^{-1} \left(\Phi^{Intr} - \mathbf{S}.\nabla_R \theta \right) \geq 0 \ ; \ \mathbf{S} \equiv \mathbf{Q}/\theta , \tag{18}$$

with the continuity condition

$$\mathbf{Q}(\mathbf{F},\theta,\alpha;\nabla_{\mathrm{R}}\theta;\mathbf{X})\to\mathbf{0} \quad as \quad \nabla_R\theta\to\mathbf{0}. \tag{19}$$

Canonical equation of linear momentum

This is obtained by *projecting canonically* eqn. (11) onto the material manifold M^3 of points $\mathbf{X}$ constituting the body. The now classical - but rather trivial - result (first obtained by the author and co-workers) is

$$\left.\frac{\partial \mathbf{P}}{\partial t}\right|_{\mathbf{X}} - \left(div_R\mathbf{b}+\mathbf{f}^{inh}\right)=\mathbf{f}^{th}+\mathbf{f}^{intr}, \tag{20}$$

where the ***canonical momentum*** (here of purely mechanical and translational nature- cf. eqns. (4)-(7)) is given by

$$\mathbf{P}=-\mathbf{p}.\mathbf{F}=\rho_0\mathbf{C}.\mathbf{V} \tag{21}$$

A *Lagrangian function* density is formally introduced by:

$$L=L^{th}=K-W\ , \tag{22}$$

and there have been defined the ***Eshelby material stress:***

$$\mathbf{b}=-\left(L^{th}\mathbf{1}_R+\mathbf{T}.\mathbf{F}\right)\ , \tag{23}$$

and various ***"material forces"*** (i.e., quantities having the physical dimension of forces but all co-vectors on the material manifild M^3):

$$\mathbf{f}^{inh}=\left.\frac{\partial L^{th}}{\partial \mathbf{X}}\right|_{expl}\ ;\ \mathbf{f}^{th}=S\nabla_R\theta\ ,\ \mathbf{f}^{intr}=A\left(\nabla_R\alpha\right)^T\ . \tag{24}$$

while the *Cauchy-Green finite strain* and the *material* velocity are defined by:

$$\mathbf{C}=\mathbf{F}^T.\mathbf{F}\quad ,\ \mathbf{V}=-\mathbf{F}^{-1}.\mathbf{v}=\left.\frac{\partial \chi^{-1}}{\partial t}\right|_x . \tag{25}$$

In particular, the first of eqn. (24) is explicitly given by

$$\mathbf{f}^{inh} = (\nabla_R \rho)\left(\frac{1}{2}\mathbf{v}^2\right) - \left.\frac{\partial \overline{W}}{\partial \mathbf{X}}\right|_{\mathbf{F},\theta,\alpha\ fixed} . \tag{26}$$

Thus the "force" $\mathbf{f}^{inh}$ captures indeed the explicit **X**-dependency and deserves its naming as *material force of inhomogeneity*, for short *inhomogeneity force*. This is the first cause for the momentum equation (20) to be *inhomogneous* (i.e., to have a source term) while the original - in physical space - momentum equation (11) was a true conservation law.

An inhomogeneity force is a *directional indicator* of the changes of material properties (this holds also at the sharp interface between components in a composite body). What is more surprising is that a *spatially nonuniform state of temperature* $(\nabla_R \theta \neq \mathbf{0})$ causes a similar effect, i.e., the *material* thermal force $\mathbf{f}^{th}$ acts just like a true material inhomogeneity in so far as the balance of canonical (material) momentum is concerned, cf. Epstein and Maugin [19]. It seems that Bui [20] was the first to uncover such a thermal term while studying fracture although in the small-strain framework and not in the material setting. Finally, any internal variable of state α that has not reached a spatially uniform state at point $\mathbf{X}$, $\nabla_R \alpha \neq \mathbf{0}$, has a similar effect in the equation of canonical momentum through the *intrinsic* material force $\mathbf{f}^{intr}$ [17]. We call such material forces, material forces of quasi- or *pseudo-inhomogeneity* [5]. Note that any additional variable put in the functional dependency of the free energy W will cause a similar effect. It is only in the pure materially homogeneous elastic case (W depending only on **F**) that the balance of canonical momentum is also a strict conservation law.

Note also that the material stress tensor **b** is not symmetric in a traditional sense. If the Cauchy stress is symmetric (that is the case in the present example), **b** is only symmetric with respect to **C** considered as the deformed metric on M^3, i.e.,

$$\mathbf{Cb} = \mathbf{b}^T \mathbf{C} . \tag{27}$$

Transformation of the energy equation (canonical form for dissipative processes)

Pushing the temperature under the time differentiation in the first of eqns. (17) we readily obtain the following enlightening form:

$$\left.\frac{\partial(S\theta)}{\partial t}\right|_{X} + \nabla_R.\mathbf{Q} = \Phi^{th} + \Phi^{int}, \ \Phi^{\mathrm{th}} := S\frac{\partial \theta}{\partial t}. \tag{28}$$

which is to be compared to eqn. (20), i.e.,

Comparing the source terms in the right-hand sides of eqns. $(28)_1$ and (29), we acknowledge that these two equations are none other than the time-like and space-like components of a unique four-dimensional Cartesian formulation in which **P** and θS are the space and time components of a unique four-vector [21]. This more generally hints at a true 4d analytical mechanics of dissipative continua.

4. CONCLUSION

This contribution had for purpose to emphasize the parallel and complementary roles played by the balance of canonical momentum and energy (the latter written in a specific way) in the mechanics of materials; It is this essentially four-(3+1) dimensional formalism, clearly inspired by mathematical physics, which shows that all reasonings made on the thermodynamics of driving forces in all types of applications (progress of defects, dynamics of nonlinear waves, improvement of numerical schemes) must be simultaneously carried out on the material forces of interest and the accompanying expended power. This, in particular, will guarantee that the corresponding dissipation, if any, is indeed the product of a material force and a material velocity, cf. [21].

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