Carlo Sansour
Sebastian Skatulla
Editors

International Centre for Mechanical Sciences

Generalized Continua and Dislocation Theory

Theoretical Concepts, Computational Methods and Experimental Verification

CISM Courses and Lectures, vol. 537

SpringerWienNewYork

SpringerWienNewYork

CISM COURSES AND LECTURES

The series presents lecture notes, monographs, edited works and proceedings in the field of Mechanics, Engineering, Computer Science and Applied Mathematics.
Purpose of the series is to make known in the international scientific and technical community results obtained in some of the activities organized by CISM, the International Centre for Mechanical Sciences.

INTERNATIONAL CENTRE FOR MECHANICAL SCIENCES

COURSES AND LECTURES - No. 537

GENERALIZED CONTINUA AND DISLOCATION THEORY

THEORETICAL CONCEPTS, COMPUTATIONAL METHODS AND EXPERIMENTAL VERIFICATION

EDITED BY

CARLO SANSOUR
UNIVERSITY OF NOTTINGHAM, NOTTINGHAM, GREAT BRITAIN

SEBASTIAN SKATULLA
CERECAM, DEPARTMENT OF CIVIL ENGINEERING,
UNIVERSITY OF CAPE TOWN, SOUTH AFRICA

SpringerWienNewYork

This volume contains 76 illustrations

Printed in Italy
SPIN 86085123

All contributions have been typeset by the authors.

ISBN 978-3-7091-1221-2 SpringerWienNewYork

PREFACE

The term generalised continua was coined in the proceedings of the IUTAM conference held in Freudenstadt in 1967; a remarkable gathering of some of the most influential names in mechanics at the time. The term generalisation was meant as an extension of the concept of the Cosserat continuum. In fact some hundred years ago, the Cosserat brothers introduced their concept of a continuum which not only was revolutionary, it made complete the ideas itself involved in the definition of a continuum. The angular momentum equation was treated on equal footing as that of linear momentum. It was explicitly used instead of being reduced to a symmetry statement of the stress tensor. Notwithstanding the appeal of the concept it was only after a paper by Ericksen and Truesdell in 1957 that the ideas of the Cosserat brothers were revived. In this paper the original concept was modified in two ways. On the one hand the idea of directors, the rotation of which provided the characteristic new degree of freedom, was introduced and on the other hand these directors where also allowed to deform to describe a micro deformation as well. Later, Eringen and associates coined the term micromorphic for such continua. They also used the term micropolar to describe the Cosserat continua. Moreover, unlike Ericksen and Truesdell and other early contributors in the field, they derived the strain measures based on the notion of the group element itself. That is the group of rotation tensors was directly introduced in the case of the Cosserat continuum and that of the linear transformations in the case of the micromorphic continuum. In spite of the quite advanced state of this kind of theories, in the following decades applications of generalised formulations were more or less restricted to rod and shell theories as, with few exceptions such as the dispersion relation in wave propagation, no real understanding of scale effects incorporated in these theories was available. Further, these theories were restricted to elastic material behaviour. With the progress in material sciences in understanding the material behaviour at micro and nano scales and beyond, scale effects became of common interest and so the interest in generalised formulations resurfaced. Also the availability of computer power meant that solutions of problems based on these theories became accessible albeit numerical ones. Moreover, computations at smaller scales allows to address the source of scale ef-

fects and provides much needed understanding as to the background of such generalised theories. In fact much of these sources lie in defects and dislocations at a much smaller scale which mannifest themselves in scale effects and inelastic deformations.

This book contains some of the lectures presented at the CISM Centre in Udine on generalised continua and dislocation theory.

The first contribution by Gérard Maugin deals with the driving forces on different types of "defects" such as, dislocations, disclinations, point defects, cracks, phase-transition fronts and shock waves in micropolar and micromorphic materials. Exploiting modern notions of mathematical physics (Noether's theorem, Lie groups, Cartan geometry) these so-called material or configurational *forces are related to the* Eshelby stress tensor *and a corresponding dissipative energy approach.*

The following chapter by Carlo Sansour and Sebastian Skatulla starts with a compact treatment of linear transformation groups (Lie Groups), associated Lie algebras and the role of the exponential map. Rules of differentiations and variations are discussed and many relevant formulas for the rotation group are derived. The subsequent excursion into the continuum theory of generalised continua sets out motivating the inclusion of the angular momentum equation within a framework of classical deformations. The Cosserat formulation comes as a natural extension of the classical formulation. After a critical assessment of the micromorphic theory by Eringen and associates, a unified framework of generalised continua based on the notion of fibre bundle is presented. It puts all formulations including higher gradient ones on a common ground and allows for a rational treatment of inelastic and non-linear material behaviour. Numerical results based on finite elements and meshfree methods illustrate the relevance of the framework.

The next contribution by Samuel Forest gives an account on continuum crystal plasticity starting from the classical theory and providing the transition to Cosserat, strain-gradient and micromorphic continuum-based formulations where the material hardening and evolution of dislocations and damage are related to the lattice curvature captured in the higher-order strains. The generalised theories are embedded in an energy balance equation and an entropy principle to derive the state laws and residual dissipation. The application to dam-

ages mechanics addresses the deficiency of classical crystal plasticity to realisticly predict crack tip behaviour, especially in fatigue. Moreover, plastic strain heterogeneities and scale effects can be addressed, e.g. found in thin polycrystal coatings. The resulting properties of the polycrystal material are obtained by homogenization scheme making use of Hill-Mandel's approach periodic Dirichlet boundary conditions.

The final chapter by Hussein Zbib is devoted to dislocation dynamics and its fundamental importance to describe irreversible deformations of crystalline materials linked to the motion of the constituent defects. The complex governing mechanisms located at micro- and nano scales and the associated local quantities such as plastic distortion and internal stresses are exhaustively treated. Moreover, their embedment into continuum mechanical frameworks which can be exploited computationally are given particular attention. It is demonstrated that the coupling of continuum mechanical analysis with suitable computational algorithms represents a powerful technique in material engineering analysis.

Finally, a word of clarification and gratitude. Regrettably there have been serious delays in publication of the book. However, the present contributions have been brought up to date and reflect state of the art in the field, also regarding the literature. In spite of the delay, Generalised Continua have lost nothing of their relevance to today's research in the broader field of solid mechanics and so we hope that this book provides a valuable contribution to introduce researchers to this active field of research. In this regard the editor is indebted to the authors for their patience and to Prof. Serafini for his encouragement and support to bring this book to a completion.

Carlo Sansour and Sebastian Skatulla

CONTENTS

Defects, Dislocations and the General Theory of Material Inhomogeneity
by G. A. Maugin 1

Approaches to Generalized Continua
by C. Sansour and S. Skatulla 85

Generalized Continuum Modelling of Crystal Plasticity
by S. Forest 181

Introduction to Discrete Dislocation Dynamics
by H.M. Zbib 289

Defects, Dislocations and the General Theory of Material Inhomogeneity

G. A. Maugin

Institut Jean Le Rond d'Alembert
Université Pierre et Marie Curie, Paris, France

Abstract The present lecture notes have for main purpose to introduce the reader to the notion of driving forces acting on defects in various classes of materials. These classes include elasticity, the standard case in its pure homogeneous form, and more complex behaviors including inhomogeneous and dissipative materials. A typical such driving force is the Peach–Koehler force acting on a dislocation line. More generally, these forces of a non-Newtonian nature are so-called *material or configurational* forces which are contributors to the canonical equation of momentum, here the momentum equation completely, canonically projected onto the material manifold. The latter indeed is the arena of all material defects and the essential ingredient then becomes the so-called material *Eshelby stress tensor*. This stress is the driving force behind various types of local matter rearrangements such as plasticity, damage, growth, and phase transformations. Its material divergence provides the sought driving force on different types of "defects" such as, dislocations, disclinations, point defects, cracks, phase-transition fronts and shock waves. Here the emphasis is placed on defects more particularly related to materials science and for materials presenting a microstructure such as polar materials and micromorphic ones. Of importance is the fact that the concept of driving force is always accompanied by a parallel energy approach, so that the dissipation (energy release rate) occurring during the progress of a defect is exactly the non-negative product of the driving force by the velocity of progress. Modern notions of mathematical physics (Noether's theorem, Lie groups, Cartan geometry) as well as efficiently adapted mathematical tools (*e.g.*, generalized functions or "distributions") are exploited where necessary. The three great heroes of the reported story are J. D. Eshelby, E. Kroener and J. Mandel.

1 Lecture 1: The Eshelby–Kroener View of Defects and their Driving Force: Peach–Koehler Force, Incompatibility, Eshelby Stress

1.1 The Case of a Dislocation Line (Peach–Koehler Force; Eshelby's Derivation)

We start with the evaluation of a material force acting on one singular line. This was first developed by Peach and Koehler (1950)) in a celebrated paper, a true landmark in dislocation theory. A dislocation line L is seen in continuum physics as a line along which the displacement vector of elasticity suffers, in a certain sense, a finite discontinuity, called the *Burgers vector*, that we shall note $\tilde{\mathbf{b}}$ in order to avoid any confusion with the Eshelby stress (although there exists a relation between these two notions). The magnitude and direction of $\tilde{\mathbf{b}}$ characterize the different types of dislocations (see Lardner, 1974). In discrete crystals $\tilde{\mathbf{b}}$ can only be equal to a finite number of the vectors of the lattice. What exactly occurs is that in the presence of a dislocation line L the displacement vector $\mathbf{u}$ is no longer a single-valued function of the coordinates: it receives a finite increment $\tilde{\mathbf{b}}$ in going along a circuit S around the dislocation line L. With a definite choice of sign, this is expressed by

$$\oint_S \mathrm{d}\mathbf{u} = \oint_S \frac{\mathrm{d}\mathbf{u}}{\mathrm{d}s}\,\mathrm{d}s = -\tilde{\mathbf{b}}, \tag{1}$$

where s is a line coordinate along the circuit S. A dislocation is called a screw dislocation when $\tilde{\mathbf{b}}$ is parallel to the unit tangent τ to L. It follows from this a singularity in the distortion $\beta = \nabla\mathbf{u}$. On subjecting an elastic crystal containing dislocations to an appropriate external loading, some of the atoms in the discrete view will move and the dislocation line will seem to move in the opposite direction. The dislocation is thus subjected to a "displacement" and the true mechanician will associate with that motion a "force". This is the *driving force* on the dislocation, not a force in the classical Newtonian sense, since the dislocation line is not a massive object but a mathematical notion (a singularity of the field). This force is called the *Peach–Koehler force* after its creators, the qualification of *creators* – *not* discoverers – being here justified since this force does not belong to the physical space. However, this "force" can be computed if we know the field solution of the problem at hand outside the singularity. Its original derivation goes as follows.

In the continuum elastic description of a defective crystal the interaction energy between a dislocation D characterized by an elastic displacement field $\mathbf{u}^D$ and an applied stress field σ^A is given by

$$E(D,A) = -\int_S \mathbf{n}\cdot\boldsymbol{\sigma}^A\cdot\mathbf{u}^D\,\mathrm{d}a = -\int_S \mathbf{u}^D\cdot\mathbf{T}^A\,\mathrm{d}a, \tag{2}$$

where $\mathbf{T}^A$ is the traction associated with stress $\boldsymbol{\sigma}^A$ and S is the boundary of the region containing the dislocation line L. Equation (2) is the expression of a *potential energy*. The dislocation itself is supposed *not* to produce any traction at S. Thus we may add the vanishing contribution $-\mathbf{n}\cdot\boldsymbol{\sigma}^D\cdot\mathbf{u}^A = -\mathbf{u}^A\cdot\mathbf{T}^D$ to the integrand in (2), and we obtain

$$E(D,A) = -\int_S (\mathbf{u}^D\cdot\mathbf{T}^A - \mathbf{u}^A\cdot\mathbf{T}^D)\,\mathrm{d}a. \tag{3}$$

According to the statement of the well-known *Rayleigh–Betti reciprocity theorem* of linear (isotropic or anisotropic) elasticity – *cf.* Maugin, 1992, p. 87, eqn. (A.16) – for any closed surface $\partial\Omega$ that does not embrace any body force or singularity, we have

$$\int_{\partial\Omega} (\mathbf{u}^1\cdot\mathbf{T}^2 - \mathbf{u}^2\cdot\mathbf{T}^1)\,\mathrm{d}a = 0, \tag{4}$$

for two elastic solutions labelled 1 and 2. Accordingly, the vector

$$\mathbf{g} := \mathbf{u}^1\cdot\boldsymbol{\sigma}^2 - \mathbf{u}^2\cdot\boldsymbol{\sigma}^1, \tag{5}$$

is divergence free in that enclosed surface $\partial\Omega$. Applying this reasoning to our dislocation case, the surface S can be replaced by any other surface enclosing the line L as the difference between (3) and the new integral will be zero. In particular, we may choose a surface such as in Figure 1 made up of an open tube enclosing L and the top Σ_+ and bottom Σ_- of an arbitrary discontinuity surface Σ leaning on the dislocation line L. Here Eshelby (1982, p. 211) proposes an ingenious argument that is often bypassed (compared to the treatments of Nabarro, 1967, p. 83, or Kosevich, 1979, p. 63). Suppose, to simplify the reasoning (but this is really immaterial) that the cross-section of the small tube that provides a jacket for the loop, is everywhere along L a circle of radius a. Then divide the tube into a large number of short cylindrical beads threaded by the dislocation (*i.e.*, somewhat like a necklace). While integrating the second contribution in (4) over one bead we may take the comparatively slowly spatially varying field $\mathbf{u}^A$ outside the integral. The stress field $\boldsymbol{\sigma}^D$ of a dislocation is of the order of the inverse, $1/r$, of the distance r from the dislocation (for this, see Nabarro, 1967, or Kosevich, 1979). Thus, the total traction exerted on the curved surface of the cylinder will be of the order of $a^2\,a^{-1} = a$, while each bead is in static

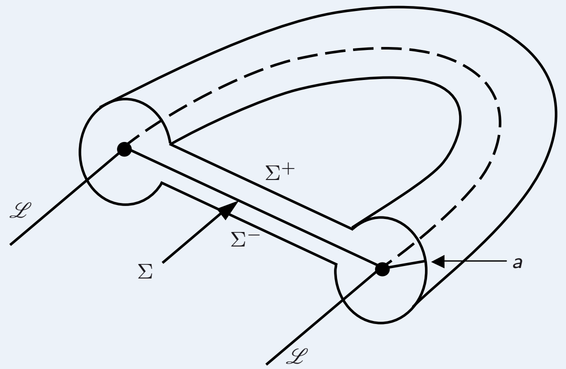

Figure 2.3 *Shrinking of $\mathscr{S}$ to a surface englobing $\mathscr{L}$ and a singularity surface Σ.*

Figure 1. Shrinking of $\mathcal{S}$ to a surface englobing $\mathcal{L}$ and a singularity Σ (Maugin, 1993).

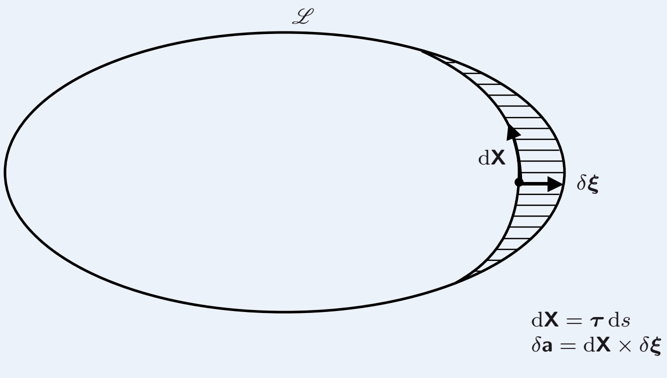

Figure 2.4 *Slight change in the dislocation loop $\mathscr{L}$ generating the Peach–Koehler force.*

Figure 2. Slight change in the dislocation loop $\mathcal{L}$ generating the Peach-Köhler force(Maugin, 1993).

equilibrium. Accordingly, we are now sure that the second contribution in (4) will go to zero with a. As to the first contribution, according to a classical evaluation of dislocation theory (see Nabarro, 1967, or Kosevich, 1979), we have $|\mathbf{u}^D| = \mathcal{O}(\ln(r))$ for small r, so that this contribution causes no trouble. As a result, we shall be left in (4) with the integral over the two sides Σ_+ and Σ_- of the cut Σ. The second contribution from (4) is continuous across Σ while $\mathbf{u}^D$ has a discontinuity of a value equal to the Burgers vector $\tilde{\mathbf{b}}$. Therefore, expression (4) is now reduced to

$$E(D,A) = -\tilde{\mathbf{b}} \int_{\Sigma=\Sigma_+} \mathbf{T}^A \,\mathrm{d}a, \tag{6}$$

where Σ_+ is oriented as Σ. To complete the proof, we consider that when the dislocation loop L suffers a little change of shape, say by an infinitesimal vectorial displacement $\delta\xi$ (*cf.* Figure 2), then the corresponding change in (6), δE is just the value of the integral in the right-hand side of (6) taken over the freshly formed portion of the cut. This additional infinitesimal surface element can be written in vector form as

$$\delta\mathbf{a} = \mathrm{d}\mathbf{X} \times \delta\boldsymbol{\xi}, \quad \mathrm{d}\mathbf{X} \equiv \boldsymbol{\tau}\,\mathrm{d}s, \tag{7}$$

where $\boldsymbol{\tau}$ is the unit tangent vector to L.

We can now write δE as

$$\delta E = -\int_L \mathbf{f}^{(PK)} \cdot \delta\boldsymbol{\xi}\,\mathrm{d}s, \tag{8}$$

where the Peach–Koehler "force" acting on the dislocation line L per unit length, due to an applied stress field $\boldsymbol{\sigma}^A$ is given by

$$\mathbf{f}^{(PK)} = (\tilde{\mathbf{b}} \cdot \boldsymbol{\sigma}^A) \times \tau. \tag{9}$$

Like other "configurational" material forces in other paragraphs, the Peach–Koehler force is generated in a *thought experiment* by a displacement of the defect, the dislocation loop L, in material space.

Several remarks are in order. First, there exists a discussion whether it is the whole of $\boldsymbol{\sigma}^A$ or just its deviatoric part that should be involved in the computation of $\mathbf{f}^{(PK)}$ – *cf.* Nabarro, 1967, p. 84. Second, expression (9) is very similar to that of the force acting on a current-carrying wire in applied electromagnetism. Third, a generalization of (9) based on *nonlinear elasticity* was given by Zorski (1981). Finally, a dynamical equation was derived when velocities are involved. This was achieved by Kosevich (1962, 1964) by using an analogy with Lorentz's derivation of the equation of motion of an electron accounting for its self-action (*cf.* Lorentz, 1952). The resulting equation reads

$$\mathbf{f}^{(PK)} = (\mathbf{p} \cdot \tilde{\mathbf{b}})\,(\mathbf{V} \times \tau), \tag{10}$$

where the left-hand side is given by expression (9), $\mathbf{p} = \rho_0\,\mathbf{v}$ is the linear momentum corresponding to a displacement rate due to both the external field and the self-field of the dislocation, and $\mathbf{V}$ is the velocity field of the position of the dislocation loop L. A field-theoretic derivation of (10) was given by Rogula (1977, p. 709). The right-hand side of (10) can be further transformed to give it the appearance of the product of a "mass" (so-called effective mass of a dislocation) and an "acceleration", so that (10) takes a "Newtonian" form – see Kosevich (1979, pp. 104–109) for this. Remarkably, the right-hand side of (10) is of second order jointly in the physical velocity of the material and the dislocation velocity. More recently a connection between $\mathbf{f}^{(PK)}$ and the *Eshelby stress* has been established.

1.2 Kroener's Approach to Incompatibility

In small strains the compatibility equations for integrating a displacement gradient (in general nine independent components) into a displacement vector (three components) are written as the set of six celebrated Saint-Venant conditions (ε_{ajk} is the Levi–Civita completely skewsymmetric alternating symbol)

$$S_{ab} \equiv -\varepsilon_{ajk}\,\varepsilon_{bli}\,\frac{\partial^2 \varepsilon_{ki}}{\partial x^j\,\partial x^l} = 0, \tag{11}$$

where $\varepsilon_{ki} = u_{(k,i)}$ or $\varepsilon = (\nabla \mathbf{u})_S$ in direct notation. Kroener (1958) introduced the source of elastic incompatibility $\boldsymbol{\eta}$ as the negative of the quantity defined in the first part of (11), *i.e.*,

$$S_{ab} + \eta_{ab} = 0. \tag{12}$$

Accordingly, in the absence of elastic incompatibility, we recover the integrability condition given by the second part of (11). We may conceive of (12) as a *balance* equation between the Einstein curvature tensor (this is what is S_{ab} in three dimensions) and Kroener's incompatibility tensor. But this is in fact related to a "defect of closure" and the concept of Burgers vector in a theory of continuous distributions of dislocations.

Indeed, equation (1) can also be written as

$$\oint_S \mathrm{d}x_j\,\beta_{ji} = -\tilde{b}_i, \tag{13}$$

where $\beta_{ji} = u_{i,j}$ is the distortion (displacement gradient). Using Stokes' theorem for a surface A leaning on S, we can rewrite this as

$$\int_A \mathrm{d}a_p \, \varepsilon_{pmi} \, \beta_{ij,m} = -\int_A \mathrm{d}a_p \, \tau_p \, \tilde{b}_j \, \delta(\xi), \tag{14}$$

where $\delta(\xi)$ is Dirac's distribution and ξ is the two-dimensional radius vector taken from the axis of the dislocation in the plane perpendicular to the unit vector τ at the given point. For arbitrary contour S and surface A, (13) yields

$$\varepsilon_{pmi} \, \beta_{ij,m} = -\tau_p \, \tilde{b}_j \, \delta(\xi). \tag{15}$$

As ξ goes to zero this relation becomes meaningless due to the obvious singularity arising in the limit. Passing now to the *continuous theory of dislocations*, (13) is generalized by introducing a tensor of dislocation density $\boldsymbol{\alpha}$, of components α_{ik}, such that

$$\int_A \mathrm{d}a_i \, \alpha_{ik} = \tilde{b}_k, \tag{16}$$

so that (1.15) is replaced by

$$\varepsilon_{ilm} \, \beta_{mk,l} = -\alpha_{ik}. \tag{17}$$

From this there follows immediately a **conservation law**:

$$\operatorname{div} \alpha = \mathbf{0}, \quad \text{or} \quad \frac{\partial \alpha_{ik}}{\partial x_i} = 0. \tag{18}$$

For a single dislocation this would be equivalent to the statement: "The Burgers vector is constant along the dislocation line". Furthermore, applying the operator $\varepsilon_{jpk} \, \partial/\partial x_p$ to (17) and symmetrizing with respect to i and j we obtain (12) in the form

$$\eta_{ij} = \frac{1}{2} \left(\varepsilon_{ipl} \, \frac{\partial \alpha_{jl}}{\partial x_p} + \varepsilon_{jpl} \, \frac{\partial \alpha_{il}}{\partial x_p} \right). \tag{19}$$

1.3 Passing to the Material Framework

For reasons to become clear later on we are interested in formulating some of the above-given elements in the material framework. We remind the reader of a few notations. Here a nondefective material body is a simply connected region B of a three-dimensional Euclidean manifold M^3, or simply M, called the *material manifold.* The elements of this manifold are so-called material points X. In (possibly but not necessarily) curvilinear coordinates X^K, $K = 1, 2, 3$, this point is simply represented by the bold-face letter $\mathbf{X}$. To each point X on M is attached a density, the matter density ρ_0, which is the density of matter at the reference configuration K_R. This may be a function of X, as is the case in materially inhomogeneous bodies, and perhaps, but rarely, a function of Newtonian time t itself. The latter scalar parameter belongs to an ordered one-dimensional continuum, the positive real line R which presents no defects. *I.e.*, time itself cannot be "fractured". With this we have introduced the *basic space-time parametrization* of the classical mechanics of deformable solids, the set $(\mathbf{X}, t)$. The motion (or deformation) of the material body B of M is the time ordered sequence of the positions, sometimes called *placements*, occupied by the point X in Euclidean physical space E^3, the arena of classical phenomenological physics. This is expressed by the sufficiently (as needed) regular space-time parametrized mapping

$$\mathbf{x} = \chi(\mathbf{X}, t). \tag{20}$$

This is often (but not necessarily) reported to a Cartesian system of coordinates x^i, $i = 1, 2, 3$.

Note that physical space here is always Euclidean, since we work in Newtonian physics, while M could be non-Euclidean (as would be the case in a *defective* material body). The set of geometrical points $\mathbf{x}(B, t$ fixed) constitutes the *actual* or *current configuration* K_t of the body at time t. Usually, an origin of time, say t_0, is chosen such that $t_0 < t$, and (20) then reads $\mathbf{x}_0 = \chi(\mathbf{X}, t_0)$. When this one and (20) are sufficiently smooth, and in particular, invertible, we can rewrite (20) as

$$\mathbf{x} = \chi\big(\chi^{-1}(\mathbf{x}_0, t_0), t\big) = \bar{\chi}(\mathbf{x}_0, t; t_0) = \tilde{\chi}(\mathbf{x}_0, t). \tag{21}$$

This representation of the direct motion is called Lagrangian, the $\mathbf{x}_0$ being Lagrangian coordinates. The configuration $K_0 = K_t(t = t_0)$ of the body, the *initial configuration* at $t = t_0$, belongs to the sequence of "actual" configurations. This is the motion description preferred in fluid mechanics. Many authors identify the two representations (20) and (21) by identifying $\mathbf{X}_0$ and $\mathbf{x}_0$. But the motion representation (20) is somewhat more abstract and is essentially due to Gabrio Piola (1848) in a paper of far reaching insight. Indeed, the consideration of the material configuration K_R that corresponds to an ideally unstrained and unloaded configuration, corresponding usually to a minimizer of the energy (*cf.* Lardner, 1974), is essential in studying the material symmetry of solid bodies and defining material properties in a general manner. While (20) is called *the direct motion mapping* $K_R \to K_t$ *at* t, in the same smoothness conditions as above, the *inverse* motion is given by

$$\mathbf{X} = \chi^{-1}(\mathbf{x}, t). \tag{22}$$

The direct $\mathbf{F}$ and inverse $\mathbf{F}^{-1}$ motion **gradients** are defined thus

$$\mathbf{F} := \nabla_R \chi \equiv \frac{\partial \chi}{\partial \mathbf{X}}, \quad \mathbf{F}^{-1} := \nabla_R \chi^{-1} \equiv \frac{\partial \chi^{-1}}{\partial \mathbf{x}}. \tag{23}$$

It is immediately checked that

$$\mathbf{F} \cdot \mathbf{F}^{-1} = \mathbf{1}, \quad \mathbf{F}^{-1} \cdot \mathbf{F} = \mathbf{1}_R, \tag{24}$$

where the symbols $\mathbf{1}$ and $\mathbf{1}_R$ represent the unit dyadics in E^3 and on M, respectively. It must be emphasized that both $\mathbf{F}$ and $\mathbf{F}^{-1}$ are *not* tensors in the traditional sense because they are geometric objects defined on two different manifolds simultaneously. In a picturesque language, we can say that they have one foot in K_t and another in K_R. Such objects are so-called *two-point tensor fields.* They have components

$$\mathbf{F} = \left\{ F^i_{\ K} \equiv F_{iK} \right\}, \quad \mathbf{F}^{-1} = \left\{ (\mathbf{F}^{-1})^K_{\ i} = (\mathbf{F}^{-1})^{Ki} \right\}, \tag{25}$$

where the upward or downward position of lower Latin indices is irrelevant by virtue of the Cartesian representation chosen in K_t. Speaking of an *a priori* symmetry of $\mathbf{F}$ and $\mathbf{F}^{-1}$ is a mathematical nonsense since one must specify with respect to what metric is tensorial symmetry defined. The Jacobian determinant of $\mathbf{F}$ is noted

$$J_F = \det \mathbf{F}. \tag{26}$$

Of course, $J_{F^{-1}} = \det \mathbf{F}^{-1} = (J_F)^{-1}$. If ρ_0, the *matter density* at $\mathbf{X}$, does not depend on time, the actual mass density ρ is related to ρ_0 by the change of volume between configurations, *i.e.*,

$$\rho(\mathbf{x}, t) = \rho_0(\mathbf{X})\, J_F^{\ -1}. \tag{27}$$

Since densities are always positive, only deformation mappings such that J_F *is positive and never vanishes*, are considered. In physical terms this signifies the *impenetrability* of matter.

Deformation measures are typical "metrics" (truly symmetric tensors). Some of them can be defined thus (here the superscript T denotes the operation of *transposition*, δ's are Kronecker symbols):

$$\mathbf{C}(\mathbf{X}, t) := \mathbf{F}^T \mathbf{F} = \left\{ C_{KL} = F^i_{\ K}\, \delta_{ij}\, F^j_{\ L} \right\}, \tag{28}$$

and

$$\mathbf{C}^{-1} := (\mathbf{F}^{-1})\,(\mathbf{F}^{-1})^T = \left\{ (\mathbf{C}^{-1})^{KL} = (\mathbf{F}^{-1})^K_{\ i}\, \delta^{ij}\, (\mathbf{F}^{-1})^L_{\ j} \right\}. \tag{29}$$

These are defined over M, and are called the *Cauchy–Green* finite (material) strain tensor and the *Piola* finite (material) strain tensor, respectively. They are inverse to one another. These two measures are *absolute* ones. They are not compared to an undeformed metric. A natural *relative* strain measure is given by

$$\mathbf{E} := \frac{1}{2}\,(\mathbf{C} - \mathbf{1}_R). \tag{30}$$

A more general definition than this allows one to introduce a series of material strain measures such that, $m = \ldots, -2, -1, +1, +2, \ldots$,

$$\mathbf{E}^{(m)} := \frac{1}{m}\,(\mathbf{U}^m - \mathbf{1}_R). \tag{31}$$

Here $\mathbf{U}$ is the *right stretch (material) tensor* introduced in the polar decomposition of any non singular $\mathbf{F}$ – non vanishing $\det \mathbf{F}$ – according to a theorem due to Cauchy:

$$\mathbf{F} = \mathbf{R}\,\mathbf{U} = \mathbf{V}\,\mathbf{R}, \tag{32}$$

where $\mathbf{V}$ is the left stretch (spatial) tensor, and $\mathbf{R}$ is a rotation that belong to $SO(3)$, *i.e.* $\mathbf{R}^T = \mathbf{R}^{-1}$, $\det \mathbf{R} = +1$. Both $\mathbf{U}$ and $\mathbf{V}$ are positive definite. We immediately check that $\mathbf{C} = \mathbf{U}^2$, $J_F = \det \mathbf{U}$, and thus from (31), in particular,

$$\mathbf{E}^{(2)} \equiv \mathbf{E}, \quad \mathbf{E}^{(-2)} = \frac{1}{2}\,(\mathbf{1}_R - \mathbf{C}^{-1}). \tag{33}$$

Note that finding $\mathbf{U}$ from $\mathbf{C}$ is an awkward operation (finding the square root of a tensor).

The *displacement field* is the field $\mathbf{u}(\mathbf{X}, t)$ or $\bar{\mathbf{u}}(\mathbf{x}, t)$ defined by

$$\mathbf{x} = \mathbf{X} + \mathbf{u}(\mathbf{X}, t) \quad \text{or } \mathbf{x} = \mathbf{X} + \bar{\mathbf{u}}(\mathbf{x}, t), \tag{34}$$

On taking the material gradient ∇_R of the first of these and the spatial gradient ∇ of the second we obtain with (23),

$$\mathbf{F} = \mathbf{1} + \mathbf{H}, \;\; \mathbf{H} \equiv \nabla_R \mathbf{u} \quad ; \quad \mathbf{F}^{-1} = \mathbf{1} - \mathbf{h}, \;\; \mathbf{h} \equiv \nabla \bar{\mathbf{u}}. \tag{35}$$

It follows that we have the following *exact* formulas:

$$\mathbf{E} = \frac{1}{2}\,\left(\mathbf{H} + \mathbf{H}^T + \mathbf{H}^T\,\mathbf{H}\right), \quad \mathbf{e} = \frac{1}{2}\,\left(\mathbf{h} + \mathbf{h}^T - \mathbf{h}^T\,\mathbf{h}\right). \tag{36}$$

In *small strain theory* for which $\mathbf{H}$ and $\mathbf{h}$ are small in the sense that $|\mathbf{H}| \equiv (\mathit{trace}\,\mathbf{H}^T\mathbf{H})^{1/2}$ or $|\mathbf{h}| \equiv (\mathit{trace}\,\mathbf{h}^T\,\mathbf{h})^{1/2}$ is considered as an infinitesimal quantity of the first order, neglecting terms of second order in the "small" displacement gradients, we obtain the following approximation

$$\begin{aligned} \mathbf{E} = \mathbf{e} = \varepsilon = (\nabla \mathbf{u})_S \equiv \frac{1}{2}\left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T\right), \\ \mathbf{R} - \mathbf{1} = \omega = (\nabla \mathbf{u})_A \equiv \frac{1}{2}\left(\nabla \mathbf{u} - (\nabla \mathbf{u})^T\right), \end{aligned} \tag{37}$$

where the subscripts S and A denote the operations of symmetrization and skew (anti)- symmetrization, respectively. The true tensors ε and ω are called the infinitesimal strain and rotation. Furthermore, to the same degree of approximation (tr = trace),

$$J_F \cong 1 + \operatorname{tr} \varepsilon, \quad J_F^{-1} \cong 1 - \operatorname{tr} \varepsilon. \tag{38}$$

Then we are back to the notion of **integrability** of the displacementh field. **Question**: Find a unique displacement $\mathbf{u}$ corresponding to a given deformed metric $\mathbf{C}$. Of course there must exist six so-called compatibility conditions in order to extract the three components of $\mathbf{u}$ from the nine components of $\mathbf{C}$ or $\mathbf{E}$. These were originally derived in the 19$^{\text{th}}$ century by Navier and Saint–Venant in small strain theory. For finite strain theory, it is noticed that in the absence of defects, the material manifold is *flat* (in the sense of Riemannian differential geometry) and must remain so in the course of the deformation. Accordingly, the Riemann curvature associated with $\mathbf{C}$ or $\mathbf{E}$ must always vanish (see, for instance, Maugin, 1993, pp. 54–57, for these developments). In three-dimensional space which is our concern, the Riemann curvature tensor reduces to the so-called *Einstein tensor*. For small strains this tensor, in term of the deformed metric ε, is given by

$$S_{ab} = -\varepsilon_{ajk}\, \varepsilon_{bli}\, \varepsilon_{ki,jl}, \tag{39}$$

which is none other than $(11)_1$.

Among the important operations involving deformation, we have those of convection, of a tensorial object, called *pull back* or *push forward* depending on whether the operation carries a tensorial object from the actual configuration to the reference one, or from the latter to the former. They are tensorial transformations effected with help of the motion mapping itself since these operations are conducted between two different manifolds. Historically first, but also endowed with a definite relevance in continuum mechanics, is the convection operation introduced by Piola, the *Piola transformation*. Let $\mathbf{A}$ be a vector field in the actual configuration. Then the material contravector defined by

$$\overline{\mathbf{A}} = J_F\, \mathbf{F}^{-1}\, \mathbf{A} = \left\{ \overline{A}^K = J_F (\mathbf{F}^{-1})^{Ki}\, A_i \right\}, \tag{40}$$

is the *Piola transform* of $\mathbf{A}$. Conversely,

$$\mathbf{A} = J_F^{-1}\,\mathbf{F}\,\overline{\mathbf{A}} = \left\{ A = J_F^{-1}\,F^i_K\,\overline{A}^K \right\}. \tag{41}$$

We easily verify the following identities

$$\nabla_R (J_F\,\mathbf{F}^{-1}) = \mathbf{0}, \quad \nabla (J_F^{-1}\,\mathbf{F}) = \mathbf{0}, \tag{42}$$

from which there follows that

$$\nabla_R \cdot \overline{\mathbf{A}} = J_F\,\mathbf{F} \cdot (\nabla_R \mathbf{A}) = J_F\,\nabla \cdot \mathbf{A}. \tag{43}$$

This reminds us of the formula for the change of elementary volume, dv and dV, between the actual and reference configurations:

$$dv = J_F\,dV, \tag{44}$$

so that

$$(\nabla_R \cdot \overline{\mathbf{A}})\,dV = (\nabla \cdot \mathbf{A})\,dv. \tag{45}$$

By the same token it is salient to remind the reader of the so-called Nanson's formula for the change between oriented surface elements $\mathbf{n}\,ds$ and $\mathbf{N}\,dS$ of the same surface with respective unit normals $\mathbf{n}$ and $\mathbf{N}$ in the actual and reference configurations:

$$\mathbf{n}\,ds = J_F\,\mathbf{N} \cdot \mathbf{F}^{-1}\,dS, \quad \mathbf{N}\,dS = J_F^{-1}\,\mathbf{n} \cdot \mathbf{F}\,ds. \tag{46}$$

If $\boldsymbol{\sigma}$ is a spatial tensor defined per unit area in K_t, then we readily check that

$$\mathbf{n} \cdot \boldsymbol{\sigma}\,ds = \mathbf{N} \cdot \mathbf{T}\,dS, \tag{47}$$

where the two-point tensor field $\mathbf{T}$ is such that

$$\mathbf{T} = J_F\,\mathbf{F}^{-1}\,\boldsymbol{\sigma} = \left\{ T_i^K = J_F\,(\mathbf{F}^{-1})^{Kj}\,\sigma_{ji} \right\}, \quad \boldsymbol{\sigma} = J_F^{-1}\,\mathbf{F}\,\mathbf{T}. \tag{48}$$

Note that eq. (47) still has a foot in the actual configuration (physical space). The object $\mathbf{T}$ is the Piola transformed of $\boldsymbol{\sigma}$, but on the first index only. Of course, if one takes the material divergence to the left, noted div_R, of $\mathbf{T}$, one gets immediately (compare to (45))

$$\mathrm{div}_R\,\mathbf{T} = J_F\,\mathrm{div}\,\boldsymbol{\sigma} = J_F\,\nabla \cdot \boldsymbol{\sigma}, \tag{49}$$

where the symbol ∇ denotes the spatial divergence taken at the left of a tensorial object. Equation (49), just like (46), still has a foot in the actual configuration. Now we can revisit some of the notions introduced in Paragraphs 1.1 and 1.2.

1.4 Local Rearrangement of Matter

For the sake of illustration we consider the case of finite-strain pure elasticity for which the equilibrium equations in the *Cauchy format* in the *actual configuration* read

$$\operatorname{div} \boldsymbol{\sigma} = \mathbf{0} \text{ in } B, \quad \mathbf{n} \cdot \boldsymbol{\sigma} = \mathbf{T}^d \text{ at } \partial B, \tag{50}$$

if $\boldsymbol{\sigma}$ is the Cauchy stress tensor. Applying the operations (40) through (49) we also have the so-called *Piola–Kirchhoff* format of these equations

$$\operatorname{div}_R \mathbf{T} = 0 \text{ in } B_R, \quad \mathbf{N} \cdot \mathbf{T} = \overline{\mathbf{T}}^d \text{ at } \partial B_R, \tag{51}$$

where $\mathbf{T}$, a two-point tensor field, is called the first *Piola–Kirchhoff stress.* The two equations in (51) still have components in the actual configuration and, therefore, are *not completely material.* In pure, possibly anisotropic and inhomogeneous, elasticity in finite-strains, $\mathbf{T}$ is derived from an elastic energy per unit of the reference configuration $W = \overline{W}(\mathbf{F}; \mathbf{X})$ by

$$\mathbf{T} = \frac{\partial \overline{W}}{\partial \mathbf{F}}. \tag{52}$$

In the case when $\mathbf{T}$ is function of $\mathbf{F}$ and $\mathbf{F}$ *only*, where $\mathbf{F}$ is a true gradient, (52) represents the essence of *pure homogeneous elasticity* – a paradigmatic case as we shall see herein after – with

$$\mathbf{T} = \overline{\mathbf{T}}(\mathbf{F}) = \frac{\partial W(\mathbf{F})}{\partial \mathbf{F}}. \tag{53}$$

This plays the role of a *standard* with which any other situation in a solid is compared (case of more complicated functional dependences of W). Indeed, as soon as W becomes an explicit function of additional arguments, we are no longer in this ideal framework. This happens whether the additional argument is another field variable such as temperature in thermoelasticity, or electric polarization or magnetization in electro-magneto-elasticity (*cf.* Maugin, 1988), or else any variables such as so-called internal variables of state supposed to account for the hidden complexity of microscopic processes which have a macroscopic manifestation in the form of thermodynamic irreversibility (*i.e.*, dissipation; *cf.* Maugin, 1999a). Another frequent possibility (such as above) is that the energy W depends explicitly on the material particle X, in which case $W = \overline{W}(\mathbf{F}; \mathbf{X})$ and the elastic material is said to be *materially inhomogeneous.* We have called *material force of inhomogeneity* the material co-vector defined by

$$\mathbf{f}^{inh} := - \left. \frac{\partial \overline{W}}{\partial \mathbf{X}} \right|_{expl}, \tag{54}$$

if $\overline{W}$ is a sufficiently smooth function of $\mathbf{X}$, and where the subscript *expl* means that the material gradient is taken at fixed field (here $\mathbf{F}$). In composite materials where inhomogeneities manifest abruptly by jumps in material properties, (54) must be replaced by a distributional (generalized function) definition. The *force* $\mathbf{f}^{inh}$ belongs in the world of **material forces** (*cf.* Maugin, 1993, 1995) since it is a co-vector on the material manifold. It is a *directional indicator* of the changes of elastic properties as it is oriented opposite to the direct explicit gradient of W.

Now we can exploit the *thought experiment* of Epstein and Maugin (1990a,b). To that purpose, imagine that at *each material point* $\mathbf{X}$ we can give to the material deformation energy the appearance of that of a pure homogeneous elastic body (dependence on one deformation only and nothing else) by applying the appropriate *local* (at $\mathbf{X}$) *change*, here noted $\mathbf{K}$, of reference configuration, a so-called *uniformity map* in the language of Noll (1967) and Wang (1967). We consider this along with the concomitant change of volume and write

$$W = \overline{W}(\mathbf{F};\mathbf{X}) = J_K^{-1}\, W(\mathbf{F}\,\mathbf{K}(\mathbf{X})) = \widetilde{W}(\mathbf{F},\mathbf{K}). \tag{55}$$

We can compute the partial derivatives of the last function by obtaining thus

$$\mathbf{T} = \frac{\partial \overline{W}(\mathbf{F};\mathbf{X})}{\partial \mathbf{F}}, \quad \mathbf{b} = -\frac{\partial \widetilde{W}(\mathbf{F},\mathbf{K})}{\partial \mathbf{K}}\,\mathbf{K}^T = W\,\mathbf{1}_R - \mathbf{T}\,\mathbf{F}. \tag{56}$$

Thus there exits a relationship between the notion of material inhomogeneity and that of *configurational or Eshelby material (here quasi-static) stress tensor* $\mathbf{b}$. This is made more visible by applying the definition (54):

$$\begin{aligned} \mathbf{f}^{inh} &= -\left.\frac{\partial \overline{W}(\mathbf{F};\mathbf{K})}{\partial \mathbf{X}}\right|_{expl} = -\frac{\partial \widetilde{W}(\mathbf{F},\mathbf{K})}{\partial \mathbf{K}} \cdot \frac{\partial \mathbf{K}}{\partial \mathbf{X}} \\ &= \mathbf{b}\cdot\mathbf{K}^{-T}\cdot\frac{\partial \mathbf{K}}{\partial \mathbf{X}} = \mathbf{b}\cdot\left(\mathbf{K}^{-T}\cdot(\nabla_R \mathbf{K})^T\right) \end{aligned} \tag{57}$$

On the other hand, if we compute the material divergence of $\mathbf{b}$ in the case of quasi-statics in the absence of body force, for which the equilibrium at $\mathbf{X}$ is simply given by $(51)_1$, we have

$$\begin{aligned} \mathrm{div}_R\,\mathbf{b} &= \nabla_R W - (\mathrm{div}_R\,\mathbf{T})\cdot\mathbf{F} - \mathbf{T}\cdot(\nabla_R \mathbf{F})^T \\ &= \left(\frac{\partial W}{\partial \mathbf{F}} - \mathbf{T}\right)\cdot(\nabla_R \mathbf{F})^T + \left.\frac{\partial W}{\partial \mathbf{X}}\right|_{expl}, \end{aligned} \tag{58}$$

or, on account of $(56)_1$ and (57),

$$\mathrm{div}_R\,\mathbf{b} = -\mathbf{f}^{inh}. \tag{59}$$

Here the material force of inhomogeneity is deduced from (or balanced by) the material divergence of the configurational stress. It is justified to call **configurational forces** these forces that are deduced through an operation acting on the configurational stress, whether by differentiation or integration (*e.g.*, over a material surface, along a material contour in 2D). If we combine the results of (57) and (59), we also obtain an equation for $\mathbf{b}$ which involves the local transformation $\mathbf{K}$ in a source term, that is,

$$\operatorname{div}_R \mathbf{b} + \mathbf{b} \cdot \Gamma = \mathbf{0}, \tag{60}$$

where we have defined a *material connection* $\Gamma(\mathbf{K})$ by

$$\Gamma(\mathbf{K}) = (\nabla_R \mathbf{K}^{-1}) \cdot \mathbf{K} = -\mathbf{K}^{-1} \cdot (\nabla_R \mathbf{K})^T. \tag{61}$$

The result (60) is due to Epstein and Maugin (1990a,b). If $\mathbf{K}$ is the same for all points $\mathbf{X}$, then $\nabla_R \mathbf{K} = \mathbf{0}$, and (60) reduces to the strict conservation law

$$\operatorname{div}_R \mathbf{b} = \mathbf{0}, \tag{62}$$

in the case (we remind the reader) of the absence of body force and neglect of inertia (quasi-statics). Otherwise, we can write

$$\mathbf{f}^{inh} = \mathbf{b} \cdot \Gamma(\mathbf{K}), \tag{63}$$

Then the above-reported intellectual construct means that the operation carried out (introduction of $\mathbf{K}$) brings the neighborhood of each material point $\mathbf{X}$ into a *prototypical situation* of the pure elastic type which allows one to compare the response of different points. Since this is *point-like*, the operation will not result in an overall smooth manifold, but in a collection of non-fitting neighborhoods or infinitesimal chunks of materials, and $\mathbf{K}$ will not, accordingly, be itself a gradient. It may at most be a *Pfaffian form.* Of course, if $\mathbf{K}$ is not integrable, so is the case of $\overline{\mathbf{F}} = \mathbf{F}\,\mathbf{K}$. With eqns. (60)–(61) we enter the *geometrization of continuum mechanics* that was started in the mid 1950s by scientists such as Kondo (1952), Kroener (1958), Noll (1967) and Wang (1967) among others. This was thoroughly reviewed in Maugin (2003a,b). This ambitious program belongs in the Hilbertian–Einsteinian tradition of geometrization of physics. Of course, in this line of thought, the writing (60) does not fulfill the whole program because the two sides of (60) contain contributions of a different nature, the non-Riemannian geometry being contained only in the right-hand side through the notion of connection based on $\mathbf{K}$. However, there is progress here compared to other approaches in the sense that the whole equation (60) is written on the material manifold, which indeed is the arena of what may happen to the material in its intimacy (*e.g.*, defects). Let us examine the source term (60) more thoroughly and discuss more deeply the geometrical connotations.

First of all, in components, (60) reads

$$b^{J}_{.I,J} + b^{K}_{.J}(\mathbf{K}^{-1})^{\alpha}_{.K}\, K^{J}_{.\alpha,I} = 0. \tag{64}$$

This is a first-order differential equation which is identically satisfied by the tensor $\mathbf{b}$ associated with a solution of an elastic boundary-value problem. But generally speaking the $\mathbf{K}$ transformation creates a so-called *distant parallelism* (called in the past *absolute parallelism or Fernparallelismus*), and thus a (generally non-metric) *connection* (*cf.* Choquet–Bruhat, 1968 or Lichnerowicz, 1976) as defined by (61). In words and following Elie Cartan (probably the main contributor to this field of geometry), distant parallelism in a Riemannian space is materialized by the fact that, if we attach to each point in space a reference frame, and this in some arbitrary manner, then it is sufficient to agree that two vectors of any origin, $\boldsymbol{A}$ and $\boldsymbol{B}$, are parallel or equipollent if they have equal projections (components) on the rectangular frames at $\boldsymbol{A}$ and $\boldsymbol{B}$. Then the reference frames themselves are parallel to each other in that sense! In this process it is clear that the metric of the relevant space and the parallelism are dependent on one another, but for each given metric there is an infinity of distant parallelisms compatible with that metric and, conversely, given a distant parallelism there exists an infinity of metrics compatible with it. Of course, in a Riemannian space, the notion of *Riemannian curvature* plays a fundamental role: it is related to the deviation undergone by a vector when the latter is transported in a *parallel* manner around a closed circuit. This notion disappears in the condition of distant parallelism, *i.e.*, a Riemannian space with distant parallelism has *no* curvature. Still, something distinguishes it from a Euclidean space, and that is *torsion.* As a consequence all the intrinsic geometric properties which characterize a Riemannian space with distant parallelism derive from its torsion (E. Cartan, in some uncontrolled enthusiasm, once said that "*if physics can be geometrized at all, then all physical laws must be expressible in terms of partial differential equations governing the torsion of the relevant space*" (Cartan, 1931, translation from the French by GAM)). This was very far-sighted in so far as unified gravitational theories are concerned. But in a way it also applies to continuum mechanics on the material manifold, our present concern.

To be more specific, define a *moving crystallographic frame* over the material body B by

$$\mathbf{E}_{\alpha} = K^{K}_{.\alpha}\,\frac{\partial}{\partial X^{K}}. \tag{65}$$

Two vectors at different points in the reference configuration are, by definition, **K**-parallel if they have the same components in their respective crystallographic bases. This leads to the introduction of a covariant derivative (here denoted ";") of a vector **V** of components V^I:

$$V^I_{.;J}\,\frac{\partial}{\partial X^I}\otimes dX^J = V^\alpha_{.,J}\,\mathbf{E}_\alpha\otimes dX^J = \left((\mathbf{K}^{-1})^\alpha_{,I}\,V^I\right)_{,J}K^K_{.\alpha}\,\frac{\partial}{\partial X^K}\otimes dX^J, \quad (66)$$

or

$$V^I_{.;J} = V^I_{.,J} + \Gamma^I_{KJ}\,V^K, \quad (67)$$

with a connection $\mathbf{\Gamma}$ defined by (61).

Similarly, for a *one-form* (co-vector) **W**, working in the dual basis, we classically obtain

$$W_{I;J} = W_{I,J} - \Gamma^K_{IJ}\,W_K, \quad (68)$$

while for a mixed tensor **b**, we will have

$$b^J_{.I;K} = b^J_{.I,K} - \Gamma^L_{IK}\,b^J_{.L} + \Gamma^J_{LK}\,b^L_{.I}. \quad (69)$$

The connection symbol $\mathbf{\Gamma}$ is *not necessarily* symmetric (as is, in contrast, the Christoffell symbol based on a metric). It is the skew part of this connection which defines the *torsion* $\widetilde{\mathbf{T}}$ by

$$\widetilde{T}^I_{JK} := \Gamma^I_{JK} - \Gamma^I_{KJ}. \quad (70)$$

This allows one (Epstein and Maugin, 1990a) to show that (64) can be rewritten in the following remarkable form

$$\bar{b}^J_{.I;J} = \bar{b}^J_{.K}\,\widetilde{T}^K_{JI} + \bar{b}^J_{.I}\,\widetilde{T}^K_{JK}, \quad \bar{\mathbf{b}} \equiv J_K\,\mathbf{b}, \quad (71)$$

or

$$\mathrm{div}_{\mathbf{K}}\bar{\mathbf{b}} = B(\bar{\mathbf{b}}, \widetilde{\mathbf{T}}), \quad (72)$$

where $\mathrm{div}_{\mathbf{K}}$ denotes the covariant divergence based on **K**, and $B(.,.)$ denotes the specific bi-linear form introduced in the first of (71). The formula for the divergence of a determinant has been employed in writing this on account of the introduction of the weighted Eshelby stress $\bar{\mathbf{b}}$. Particular cases of (72) are easily discussed: (i) if the reference configuration itself is homogeneous, then the **K**-parallelism reduces to the Euclidean one and we simply have $\mathrm{div}_R\,\mathbf{b} = \mathbf{0}$. This corresponds to the absence of physical (material) inhomogeneity and of any configurational inhomogeneity (*i.e.*, artificial inhomogeneity due to the special choice of a reference configuration); (ii) if the body is materially homogeneous but the reference configuration is arbitrary, then we have the *material conservation law* $\mathrm{div}_{\mathbf{K}}\bar{\mathbf{b}} = \mathbf{0}$. We may say that an observer adapted to the crystallographic frame sees no inhomogeneity (somewhat like a geodesic observer does not feel any gravitational field in general relativity as we need two neighboring observers (notion of *geodesic separation*) to place that field in evidence); (iii) the general case is represented by (72) where not even an adapted observer can remove the inhomogeneity as the material is "*intrinsically dislocated*" (see next section). In any case, we say that the so-called *uniformity map* (in the language of Noll (1967) and Wang (1967)), $\mathbf{K}$ helps us define a local *prototype reference crystal* at each material point $\mathbf{X}$ on the material manifold.

Remark 1.1. In standard treatises on continuum mechanics it is recalled that *material symmetry* consists in studying the possible isomorphisms of a particle onto itself which leave invariant the response of the material (*cf.* Noll). This materializes in changes of the reference configuration which belong to a certain group (a *crystallographic group* in general as studied in the Appendix of Eringen and Maugin (1990), the group of *orthogonal transformations* in the case of *isotropy*). For instance, for an elastic body in large strains, we would write the invariance

$$W = \overline{W}(\mathbf{F}) = \overline{W}(\mathbf{F}\,\mathbf{P}), \quad \mathbf{P} \in SO(3), \quad \det \mathbf{P} = +1. \tag{73}$$

The first of these looks somewhat like $(55)_2$, but for the determinant factor which is here equal to one. What occurs here (Epstein and Maugin, 1990b) is as follows. Although one often concentrates on a discrete symmetry group, here we may consider that the material is a solid with a continuous symmetry group. In a uniform body B the symmetry groups of W at different points, although generally different, are all conjugate, *via* the $\mathbf{K}$-mappings, with the symmetry group of the *reference crystal*. Let $\mathbf{G}_X(\lambda)$ be a one-parameter (λ real) subgroup of the symmetry group of the energy W at X with $\mathbf{G}_X(0) = \mathbf{I}$, the identity. From the material symmetry condition we have

$$\overline{W}(\mathbf{F};\mathbf{X}) = \overline{W}(\mathbf{F}\,\mathbf{G}_{\mathbf{X}}(\lambda), \mathbf{X}), \tag{74}$$

that is valid for all real λ's and all non-singular deformation gradients $\mathbf{F}$. The remarkable property pointed out by Epstein and Maugin (1990b) is that the Eshelby stress does not produce any work in any small change of reference which belongs, at each material point X, to the *Lie algebra* of the symmetry group, *i.e.*,

$$\operatorname{tr}\left(\mathbf{b} \cdot \left.\frac{\mathrm{d}\mathbf{G}_{\mathbf{X}}(\lambda)}{\mathrm{d}\lambda}\right|_{\lambda=0}\right) = 0. \tag{75}$$

[*i.e.*, (73) is not a local rearrangement of matter that costs energy]. When applied to the special case of isotropy, this reasoning says that for this case where point-wise symmetry groups are all conjugate *via* $\mathbf{K}(\mathbf{X})$ with the proper orthogonal group $SO(3)$, the Eshelby stress is symmetric with respect to a Riemannian metric induced by the uniformity map and defined by

$$\mathbf{G}_{\mathbf{K}} := \mathbf{K}^{-T} \cdot \mathbf{K}^{-1}. \tag{76}$$

In a stress-free configuration, this reduces to ordinary Euclidean symmetry. This should be contrasted with the $\mathbf{C}$-symmetry satisfied by $\mathbf{b}$ when the Cauchy stress is symmetric (Epstein and Maugin, 1990a,b):

$$\mathbf{C} \cdot \mathbf{b} = (\mathbf{C} \cdot \mathbf{b})^{T} = \mathbf{b}^{T} \cdot \mathbf{C}. \tag{77}$$

The above reasoning involves the theory of so-called $\mathbf{G}$-structures admitting $\mathbf{G}_{\mathbf{X}}(\lambda)$ subgroups as discussed by Elzanowski *et al.* (1990).

1.5 Back to the Continuous Distribution of Dislocations

Starting with papers by Kroener (1958, 1960) and Bilby (1968), it has been proposed that the torsion of the material connection be a measure of the *dislocation density* – a special type of material inhomogeneities – in an elastic continuum presenting a continuous distribution of dislocations. The original approach of Kroener considered only small strains (see Paragraph 1.2) but now we can easily reformulate his reasoning in the finite-strain framework. To that effect, we shall note, α^{QK}, $Q, K = 1, 2, 3$, the local material components of the dislocation density tensor. The natural way of comparing the defect of closure of a Burgers' circuit given in the material framework is to write the displacement jump in the form (compare to (16))

$$\Delta \mathbf{u} = \oint_{C} \mathrm{d}\mathbf{X} = \oint_{C} (\mathbf{K}^{-1})^{\alpha}_{.K} \, \mathbf{E}_{\alpha} \, \mathrm{d}X^{K}, \tag{78}$$

and the relation to dislocation density is written as

$$\Delta u^{Q} = \int_{S} \alpha^{QK} \, \mathrm{d}A_{K} = \int_{S} \alpha^{QK} \, N_{K} \, \mathrm{d}A, \tag{79}$$

where the surface S leans on the contour C. On using Stokes' theorem, this yields

$$\Delta \mathbf{u} = \int_{S} \varepsilon^{KLM} \, (\mathbf{K}^{-1})^{\alpha}_{.K,L} \, \mathbf{E}_{\alpha} \, \mathrm{d}A_{K} = \int_{S} \varepsilon^{KLM} \, (\mathbf{K}^{-1})^{\alpha}_{.K,L} \, K^{J}_{.\alpha} \, \mathbf{G}_{J} \, \mathrm{d}A_{M} \tag{80}$$

since $\mathbf{E}_{\alpha} = K^{J}_{.\alpha} \, \mathbf{G}_{J}$, where the $\mathbf{G}$'s are a local basis on the material manifold. On comparing (79) and (81), we see that the following relation holds:

$$\alpha^{QM} = \varepsilon^{KLM} \, \Gamma^{Q}_{KL} = \varepsilon^{KLM} \, \widetilde{T}^{Q}_{KL}. \tag{81}$$

As a result, either $\boldsymbol{\alpha}$ or $\widetilde{\mathbf{T}}$ can equally characterize the dislocation density. We may conclude this paragraph by noting that the right-hand side of the first of (71) can be expanded on account of the definition of the quasi-static Eshelby stress while accounting for the skewsymmetry of the Levi–Civita permutation symbol and the symmetry of α (without loss of generality). We thus obtain the Peach–Koehler force in finite strains as

$$f_I^{(PK)} = J_{\mathbf{K}}\, F^i_{.Q}\, T^J_{.i}\, \varepsilon_{IJM}\, \alpha^{QM} = J_K\, \varepsilon_{IJM}\, M^J_{.Q}\, \alpha^{QM}, \tag{82}$$

where $\mathbf{M}$ is the so-called *Mandel (material) stress* such that

$$\mathbf{M} = \mathbf{T} \cdot \mathbf{F} = \mathbf{S} \cdot \mathbf{C} = W\, \mathbf{1}_R - \mathbf{b}, \tag{83}$$

where $\mathbf{S}$ is the second (symmetric, material, contravariant) Piola–Kirchhoff stress. The Mandel stress plays an important role in plasticity. It is the *driving force* behind volume-preserving plastic deformations (or in defining a material measure of *resolved shear stress*). In small strains this reduces to

$$f_i^{(PK)} = \varepsilon_{ijp}\, \sigma_{jk}\, \alpha_{kp}. \tag{84}$$

This coincides with the usual Peach–Koehler force (9) for a unique dislocation of Burgers' vector $\tilde{b}_i$ and unit tangent vector τ_j to the dislocation line with $\alpha_{ij} = \tilde{b}_i\, \tau_j\, \delta(\xi)$. Mura (1981) has given a derivation of this type.

1.6 Conclusion of Lecture 1

In this lecture we have established the connection between the *geometrical* description of continuum mechanics (in the tradition of Bilby, Kroener and others) for a defective body, that of *finite-strain formulation* (following modern continuum mechanics, and Mandel in particular), and that of *configurational* (and driving) *forces* (in the manner of Eshelby and Peach and Koehler). This synthesis exhibited in three lines of converging research trends in the chart 1 probably is one of the main achievements in contemporary continuum mechanics. Furthermore, the connection with the general *theory of material inhomogeneities* is shown in the next two sections. We also note that all theories involving so-called *internal strains* and *stresses* ("Eigenspannungen" in the original language of Kroener), such as those due to thermal effects, anelasticity, electro- and magneto-mechanical couplings (piezoelectricity, magnetostriction), phase transformation, can be interpreted in terms of local structural rearrangements in the thought experiment outlined in Paragraph 1.4 above (*cf.* Maugin, 2003a). By duality, an Eshelby stress and a configurational-material force are associated with all these phenomena.

Additional bibliography: Anthony, 1970; Bilby *et al.*, 1957; Elzanowski and Epstein, 1990; Epstein and Maugin, 1992, 1995b, 1997; Friedel, 1979; Forest, 2006; Indenbom, 1965; Kosevich, 1999; Kroener and Seeger, 1959; Le, 1999; Maugin, 2011; Nabarro, 1967, Mura, 1981; Zorski, 1981

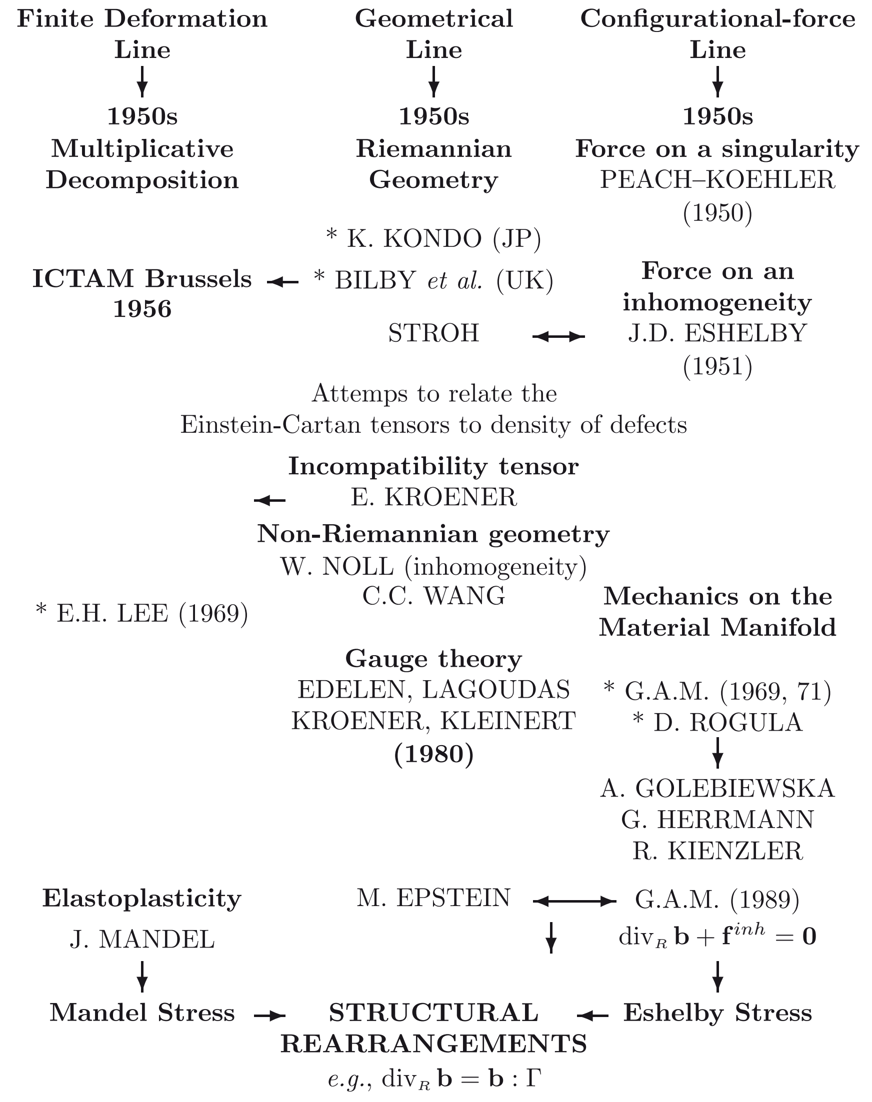

Table 1. FLOW CHART. Three converging lines of research (1950–2000).

2 Lecture 2: Canonical Momentum and Energy from a Variational Formulation (Noether's Theorem)

2.1 Elements of Field Theory

For a long time it has been thought that the notions of Eshelby stress and Eshelbian mechanics could be introduced and be meaningfully interpreted only after their introduction in the framework of a variational field-theoretical formulation. But this is blatantly erroneous as these notions should always exist as we shall show in further chapters. What is nonetheless true is that the field-theoretic formulation provides a hint to formulate dissipative cases (in the same way as Lagrange analytical mechanics suggests us how to introduce dissipative forces such as those related to friction). That is why we start with a standard variational formulation in order to introduce the celebrated Noether's theorem. In what follows it is understood that "variation" means "infinitesimal variation", and the symmetries involved are generated by infinitesimally small variations and parameters.

Here we are concerned with simple general features of field theories in a continuum with space-time parametrization $\{\mathbf{X}, t\}$, where $\mathbf{X}$ stands *for material coordinates* of classical continuum mechanics (*e.g.*, in Truesdell and Toupin, 1960), and t for a timelike scalar variable (Newton's absolute time). We consider *Hamiltonian actions* of the type

$$A(\phi; V) = \int_{V \times I} L(\phi^a, \partial_\mu \phi^a, \partial_\mu \partial_\nu \phi^a, ..; X^\mu)\, \mathrm{d}^4 X, \tag{85}$$

where ϕ^α, $\alpha = 1, 2, \ldots, N$, denotes the ordered array of fields, say the independent components of a certain geometric object, and $\mathrm{d}^4 X = \mathrm{d}V\, \mathrm{d}t$. This is a Cartesian-Newtonian notation, with

$$\left\{ \partial_\mu = \frac{\partial}{\partial X^\mu}; \mu = 1, 2, 3, 4 \right\} = \left\{ \frac{\partial}{\partial X^K}, K = 1, 2, 3; \frac{\partial}{\partial X^4} = \frac{\partial}{\partial t} \right\}. \tag{86}$$

The summation over dummy indices (Einstein convention) is enforced.

In agreement with the rather general expression (85), we say that we envisage the construction of an *n-th-order gradient theory* of the field ϕ^α when gradients of order n at most are considered in the functional dependence of the Lagrangian volume density L. Most of classical physics is based on first-order gradient theories (*cf.* Maugin, 1980). This is the case of classical elasticity which considers gradients of placement or displacement. But we note a recent attraction towards higher-order gradient theories in elasticity (a type of generalized continuum).

From expression (85) we can derive two types of equations: those relating to *each one* of the fields ϕ^α, and those which express a general *conservation* *law* of the system governing *all* fields simultaneously. The first group is obtained by imposing the requirement that the variation of the action A be zero when we perform a *small* variation $\delta\phi^\alpha$ of the field under well specified conditions at the boundary ∂V, of V (if V is not the whole of space), and at the end points of the time interval $I = [t_0, t_1]$ if such limitations are considered. However most field theories are developed for an infinite domain. The second group of equations are the result of the variation of the parametrization, and these results, on account of the former group, express the *invariance* or lack of invariance of the whole system under changes of this parametrization. To simplify the presentation we will assume an infinite domain V with vanishing fields at infinity, and an infinite time interval since our concern here is neither boundary conditions, nor initial conditions.

In order to perform these variations we consider ε-parametrized families of transformations of *both* coordinates (parametrization) and fields such as

$$(X^\mu, \phi^\alpha) \to (\overline{X}^\mu, \bar{\phi}^\alpha), \tag{87}$$

with

$$\overline{X}^\mu = \kappa^\mu(\mathbf{X}, \varepsilon), \quad \bar{\phi}^\alpha(\overline{\mathbf{X}}) = \Phi^\alpha(\phi^\beta(\mathbf{X}), \overline{\mathbf{X}}, \varepsilon), \tag{88}$$

where ε is an infinitesimal parameter such that for $\varepsilon = 0$ we have identically $\kappa^\mu(\mathbf{X}, 0) = X^\mu$, $\Phi^\alpha(\phi^\beta, \mathbf{X}, 0) = \phi^\alpha$. We assume that the quantity L in (85) transforms as a *scalar* quantity, *i.e.*,

$$L(\overline{\mathbf{X}}, \varepsilon) = \det\left(\frac{\partial \mathbf{X}}{\partial \overline{\mathbf{X}}}\right) L(\mathbf{X}). \tag{89}$$

We note that derivations with respect $\mathbf{X}$ and ε commute, and the same holds true of integration in $\mathbf{X}$ space and derivation with respect to ε. The variation of a field ϕ^α is then defined by

$$\delta\phi^\alpha := \left.\frac{\partial \Phi^\alpha}{\partial \varepsilon}\right|_{\varepsilon=0}. \tag{90}$$

With vanishing fields at infinity in space and vanishing variations at the ends of the time intervals, limiting ourselves to a first-order gradient theory, and applying an ε-parametrization to (85) we immediately have:

$$\delta A = \int \mathrm{d}^4 X \left(\sum_\alpha \left\{ \frac{\partial L}{\partial \phi^\alpha}\, \delta\phi^\alpha + \frac{\partial L}{\partial(\partial_\mu \phi^\alpha)}\, \delta(\partial_\mu \phi^\alpha) \right\} + \frac{\partial L}{\partial X^\mu}\, \delta X^\mu \right). \tag{91}$$

In order that δA vanish for all admissible $\delta\phi^\alpha(\mathbf{X})$, and any α, with $\mathbf{X}$ *fixed*, a classical computation yields the following *Euler–Lagrange equations*:

$$E_\alpha \equiv \frac{\delta L}{\delta \phi^\alpha} = \frac{\partial L}{\partial \phi^\alpha} - \partial_\mu \frac{\partial L}{\partial(\partial_\mu \phi^\alpha)} = 0 \tag{92}$$