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2^{nd}-grade elasticity revisited

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Dedicated to the memory of Ioannis Vardoulakis, Professor of Mechanics at N.T.U. Athens, who initiated this research and contributed significantly to it till his untimely death. Working with him was a rare privilege.

Abstract

We present a compact, linearized theory for the quasi-static deformation of elastic materials whose stored energy depends on the first two gradients of the displacement (2^{nd}-grade elastic materials). The theory targets two main issues: (i) the mechanical interpretation of the boundary conditions and (ii) the analytical form and physical interpretation of the relevant stress fields in the sense of Cauchy. Since the pioneering works of Toupin [1,2] and Mindlin et al. [3-5], a major difficulty has been the lack of a convincing mechanical interpretation of the boundary conditions, causing 2^{nd}-grade theories to be viewed as "perturbations" of constitutive laws for simple (1^{st}-grade) materials. The first main contribution of this work is the provision of such an interpretation based on the concept of *ortho-fiber*. This approach enables us to circumvent some difficulties of a well known "reduction" of 2^{nd}-grade materials to continua with micro-structure (in the sense of Mindlin [3]) with internal constraints. A second main contribution is the deduction of the form of the linear- and angular-momentum balance laws, and related stress fields in the sense of Cauchy, as they should appear in a consistent Newtonian formulation. The viewpoint expressed in this work is substantially different from the one of Mindlin and Ehshel [5], while affinities can be found with recent studies by Dell'Isola et al. [6-8]. The merits of the new formulation and the associated numerical approach are demonstrated by stating and solving three example boundary value problems in isotropic elasticity. A general finite element discretization of the governing equations is presented, using C1-continuous interpolation, while the numerical results show excellent convergence even for relatively coarse meshes.

Keywords: Gradient theories · Linearized formulation · Boundary conditions · Higher-order stresses · Linear isotropic constitutive law

1 Introduction

Major contributions were given, in the late 50's, 60's and 70's to the development of continuum theories of elasticity that incorporate the second or higher-order gradients of the displacement in the expression of the elastic energy. We may call these theories "2nd-grade elasticity theories". These efforts should be placed in the wider framework of the rebirth, at that time, of continuum micro-mechanics. The basic kinematic and static concepts of the "Cosserat continuum" were reworked in a milestone paper by the late Professor Günther in 1958 [9], almost fifty years after the first publication of the original work of Eugène and François Cosserat [10]. A remarkable number of contributions were published thereafter on the subject of micro-mechanics, often as further variants of Cosserat elasticity or of the concept of couple-stress (e.g., [1-5,11-21]). The historical "IUTAM Symposium on the Mechanics of Generalized Continua", in Freudenstadt and Stuttgart in 1967, can be acknowledged as the most representative picture of the state-of-the art at that time [22].

Despite the fact that they were developed in the same intellectual environment, a clear distinction should be made between 2nd-grade elasticity and theories of elastic continua with micro-structure. By 2nd-grade elasticity we mean the classical, Hooke's elasticity framework, extended in the sense of a finer description of the elastic energy

$$\mathcal{W} = \int_V W \, dV \tag{1.1}$$

whose density W at material point X_i is now assumed to depend on the first and second gradients of the displacement:[1]

$$W = W(X_i; u_{i,j}; u_{i,jk}) \tag{1.2}$$

On the other hand, when invoking elastic continua with micro-structure we refer mainly to their extended kinematics. Most theories of the latter kind may be

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[1] The symbol $u_{i,j}$ denotes herein the *i-j* components of the displacement gradient, i.e. $(\cdot)_{,i} := \partial/\partial X_i$.

grossly grouped under the assumption that the degrees of freedom available at each material point are those of a "micro-cell" undergoing affine deformation, e.g. [3,13,14]. In the linearized framework, this extended kinematics can be expressed by introducing an antisymmetric tensor field Θ_{ij} and a symmetric tensor field Ξ_{ij}, both unrelated to u_i, as measures of the micro-cell rotation and of the micro-cell strain, respectively. Keeping in mind the above distinction, we mention the possibility of treating 2nd-grade models as a particular case of continua with micro-structure. One can assume, for example,

$$W = W(X_i; u_{i,j};\ \Theta_{ij,k}; \Xi_{ij,k}) \tag{1.3}$$

and impose the internal constraints[2]

$$\Theta_{ij} - u_{[i,j]} = 0, \qquad \Xi_{ij} - u_{(i,j)} = 0 \tag{1.4}$$

By differentiation of (1.4) in (1.3) one recovers, "essentially", Equation (1.2). Not surprisingly, as effectively summarized by late Prof. Germain in [21] (see Section 6 therein), it has been suggested that the additional boundary conditions arising for 2nd-grade materials (in particular those involving components of the gradient of the displacement) should be interpreted by reducing these models to continua with micro-structure under internal constrains. However, as reported in the same paper, this procedure introduces a certain degree of indeterminacy. An alternative approach is therefore proposed herein, based on the concept of *ortho-fiber* [23]. Namely, the derivations presented below in Section 2 prove that natural boundary conditions with a straightforward mechanical interpretation can be identified, for 2nd-grade materials, without resorting to extended kinematics of any kinds.

Theories of continua with microstructure have influenced the genesis and understanding of 2nd-grade models in other respects as well. We notice in particular that the derivatives of the elastic energy density (1.3) with respect to its three tensorial arguments are identified as stress-like fields, the first two of which are alike to the Cauchy-stress tensor field and to the (Cosserat) couple-stress tensor field respectively. Internal actions for 2nd-grade materials have therefore

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[2] We adopt in this paper the notation $a_{(i}b_{j)} = (a_ib_j + a_jb_i) / 2$ and $a_{[i}b_{j]} = (a_ib_j - a_jb_i) / 2$ for the symmetric and the anti-symmetric part of dyadic product a_ib_j, respectively. Consistently, when referring to the symmetric or to the antisymmetric part of the displacement gradient we use $u_{(i,j)} = (u_{i,j} + u_{j,i}) / 2$ and $u_{[i,j]} = (u_{i,j} - u_{j,i}) / 2$.

been interpreted in terms of Cauchy-stress, couple-stress, etc. Following this line, in the paper by Mindlin and Eshel [5] one can find an influential attempt to bridge the gap between the variational and the Newtonian approach to 2nd-grade linear elasticity. Nonetheless, some aspects in that paper are misleading and have motivated the derivations presented herein.

The outline of the rest of the paper is as follows. In Section 2 we develop a linear 2nd grade elasticity theory starting from first principles. In Section 3 we distinguish between stress fields in the sense of analytical mechanics (i.e. generalized forces) and stress fields in the strict sense (i.e. in the sense of Cauchy, as generalized reactive forces along internal separation surfaces). We provide an original proof that the stress- and higher-order-stress fields in the sense of Cauchy do not obey, for 2nd-grade models, the classical requirement of "linearity" with respect to the unit-normal. The actual dependence of the Cauchy stress vector on the geometrical descriptors of the internal surface it acts on is treated in detail. Finally, after showing that a non-standard form of couple-stress can be identified along with an additional, self-equilibrating higher-order stress, we deduce the corresponding balance laws. More elements on the mechanical interpretation of the boundary conditions are given in Section 4, by solving three basic boundary value problems in isotropic 2nd-grade elasticity. The respective solutions are identified with reference to the constitutive parameters resulting from an original representation of the constitutive law [23], previously discussed in the same section. In Section 5 we present a finite element treatment of the governing equations based on the displacement formulation, which requires C^1 interpolation, along with the numerical solution of example problems. Finally, some conclusions are drawn in Section 6.

2 Linear 2nd-grade elasticity

2.1 Geometry and kinematics

We call *V* the reference configuration and *S* its piece-wise smooth, outward-oriented boundary. Two connected smooth portions of *S* are joined along a curve. One can represent the edge *E* of *V* as the (possibly disconnected) path resulting from the union of such curves. n_i denotes the unit-normal vector of *S*. We employ a fixed system of Cartesian axes, using X_i (i=1,2,3) for the position of a material particle in the reference configuration. A generic deformed configuration is identified by a displacement field $u_i(X_j) = \chi_i(X_j) - X_i$ in which $\chi_i(X_j)$ represents the position of material particle X_i in the deformed configuration. We assume that the displacement gradients are small and therefore refer to the classical *linearized* measures of deformation: *e.g.*, the infinitesimal strain tensor $u_{(i,j)}$ and the infinitesimal rotation tensor $u_{[i,j]}$.

We define an *ortho-fiber* for the oriented surface *S* at its regular point X_i to be an oriented segment of material points having X_i as its reference (end) point, lying on the negative (internal) side of *S* and oriented according to the unit normal n_i. An ortho-fiber at $X_i \in S$ is therefore defined as the locus

$$\left\{ \hat{X}_i \in V \mid \hat{X}_i = X_i - \alpha\, n_i(X_j),\ 0 \le \alpha \le l \right\} \tag{2.1}$$

where l is generally considered much smaller than the dimensions of *V*. The *ortho-fiber stretch* can be identified with the stretch at X_i along the direction n_i:

$$\varsigma := n_i\, u_{(i,j)}\, n_j \tag{2.2}$$

where, as in the rest of the paper, Einstein's summation convention is used.

A further kinematic feature of interest is the linearized measure of the rotation of the ortho-fiber in (2.1). We calculate its orientation $\hat{n}_i$ in the deformed configuration as the limit for $l \to 0$ of the orientation of the cord joining the start- and end points of the ortho-fiber:

$$\hat{n}_i = \lim_{l \to 0} \frac{\chi_i(X_j) - \chi_i(X_j - l n_j)}{\left|\chi_i(X_j) - \chi_i(X_j - l n_j)\right|} = \frac{\chi_{i,j}\, n_j}{\left|\chi_{l,m}\, n_n\right|} \tag{2.3}$$

We want now to characterize the rotation transforming n_i into $\hat{n}_j$ in terms of a rotation of angle ϑ ($0 \le \vartheta \le \pi$) about an axis r_i, $|r_i| = 1$, orthogonal to n_i. By imposing a priori that $r_i n_i = 0$ we exclude rotation components about n_i, which would leave the orientation of the ortho-fiber unchanged and therefore provide no information. As usual, the corresponding (finite) rotation tensor Ω_{ij} can be conveniently expressed in terms of Beatty's formula [24]:

$$\Omega_{ij} = \delta_{ij} + (\sin\vartheta) r_k e_{kji} + (1-\cos\vartheta)(r_i r_j - \delta_{ij}) \tag{2.4}$$

where

$$r_i = \frac{e_{ijk} n_j \hat{n}_k}{\left| e_{lmn} n_m \hat{n}_n \right|}, \qquad \sin\vartheta = \left| e_{lmn} n_m \hat{n}_n \right|, \qquad \cos\vartheta = n_i \hat{n}_j \tag{2.5}$$

By substituting (2.3) in (2.5)[3] and calculating

$$n_i \chi_{i,j} n_j = 1 + n_i u_{i,j} n_j \tag{2.6}$$

and

$$\frac{1}{\left|\chi_{i,j} n_j\right|} = 1 - n_k u_{k,l} n_l + o(\varepsilon) \tag{2.7}$$

for $\varepsilon \to 0$, one finally obtains

$$(1-\cos\vartheta)(r_i r_j - \delta_{ij}) = o(\varepsilon) \tag{2.8}$$

Substitution of (2.5) and (2.8) in (2.4) gives

$$\Omega_{ij} - \delta_{ij} = e_{kpq} n_p \chi_{q,r} n_r e_{kji} + o(\varepsilon) = n_j u_{i,r} n_r - n_i u_{j,r} n_r + o(\varepsilon) \tag{2.9}$$

Consistently with (2.9) and the assumption of small displacement-gradients, we call *ortho-fiber rotation tensor* the anti-symmetric tensor

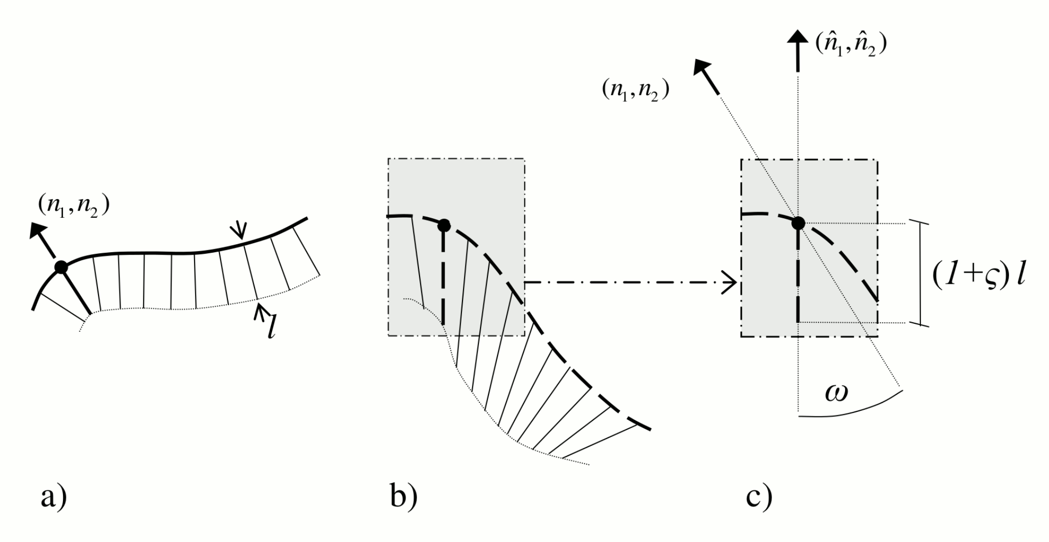


Figure 2.1: Two-dimensional interpretation of the ortho-fiber kinematics: material surface a) before and b) after deformation, along with c) a representation of the ortho-fiber stretch ς and of the ortho-fiber rotation ω.

$$\omega_{ij} := n_j u_{i,k} n_k - n_i u_{j,k} n_k \tag{2.10}$$

More compact expressions for ς and ω_{ij} can be written by introducing the *normal-derivative* operator $D := n_i \left(\partial / \partial X_i\right)$. One obtains

$$\varsigma = n_i \, Du_i \tag{2.11}$$

and

$$\omega_{ij} = n_j Du_i - n_i Du_j = -2n_{[i} Du_{j]} \tag{2.12}$$

The physical interpretation of the ortho-fiber stretch and rotation is given in Figure 2.1.

2.2 Elastic energy

The *elastic energy density* W in the generic configuration is assumed to be a function of the variables in (1.2), i.e. it depends on the first and second gradient of the displacement. The requirement that the elastic energy density be *objective* can be expressed directly by prescribing, according to (1.2), that

$$W\,(X_i; u_{i,j}; u_{i,jk}) - W\,(X_i; u^*_{i,j}; u^*_{i,jk}) = 0 \tag{2.13}$$

where the starred quantities are those measured by a second observer. It is convenient to deduce the implications of (2.13) for arbitrary *infinitesimal changes of the observer*, i.e., when the two measurements are related by

$$u^*_i - u_i = W_{ij} X_j + a_i\,, \qquad u^*_{i,j} - u_{i,j} = W_{ij}\,, \qquad u^*_{i,jk} - u_{i,jk} = 0 \tag{2.14}$$

where $W_{ij} = -W_{ji}$ and a_i are constants that characterize the change of observer (see Appendix A). By virtue of (2.13), (2.14) and of the arbitrariness of the second observer, one obtains

$$W\,(\,\cdot\,; u_{i,j}; u_{i,jk}) = W\,(\,\cdot\,, u_{(i,j)}; u_{i,jk}) \tag{2.15}$$

i.e, that the deformation gradient enters the expression of the elastic energy density only through its symmetric part.

The variation of the elastic energy functional is expressed as

$$\delta\mathcal{W} = \int_V \left(\tau_{ij}\delta u_{i,j} + \xi_{ijk}\delta u_{i,jk}\right) dV \tag{2.16}$$

where the functional derivatives

$$\tau_{ij} := \frac{\partial W}{\partial u_{i,j}}, \qquad \xi_{ijk} := \frac{\partial W}{\partial u_{i,jk}} \tag{2.17}$$

are stress-like quantities dual in energy to the variations $\delta u_{i,j}$ and $\delta u_{i,jk}$ of the first and second gradient of the displacement, respectively. Finally we remark that one can deduce the symmetry $\xi_{ijk} = \xi_{ikj}$ directly from $(2.17)^2$ and from the corresponding symmetry of $\delta u_{i,jk}$, while $\tau_{ij} = \tau_{ji}$ is an implication of the objectivity requirement on W in the form (2.15).

Remark 2.1: The quantities τ_{ij} and ξ_{ijk}, after a change of sign, acquire the meaning of generalized forces in the sense of analytical mechanics. In the attempt to frame 2nd-grade models in the realm of Newtonian mechanics, τ_{ij} is often confused in the literature with Cauchy's stress tensor and ξ_{ijk} is depicted as a higher-order stress tensor in the sense of Cauchy. The reasons why this practice is incorrect and misleading are discussed in Section 3.

We now carry out the usual procedure of integration of the elastic energy functional, through which we aim at identifying energetically-meaningful degrees of freedom active at the boundary S. Using $\delta u_{i,j} = (\delta u_i)_{,j}$ and $\delta u_{i,jk} = (\delta u_{i,j})_{,k}$ for the respective terms in (2.16) and applying integration by parts one obtains

$$\begin{aligned}\delta\mathcal{W} = &-\int_V \tau_{ij,j}\,\delta u_i\,dV - \int_V \xi_{ijk,k}\,\delta u_{i,j}\,dV + \int_S \tau_{ij} n_j\,\delta u_i\,dS \\ &+ \int_S \xi_{ijk} n_k\,\delta u_{i,j}\,dS\end{aligned} \tag{2.18}$$

A new integration by parts on the second integral in (2.18) gives

$$\begin{aligned}\delta\mathcal{W} = &-\int_V \tau_{ij,j}\,\delta u_i\,dV + \int_V \xi_{ijk,kj}\,\delta u_i\,dV + \int_S \tau_{ij} n_j\,\delta u_i\,dS \\ &- \int_S \xi_{ijk,k} n_j\,\delta u_i\,dS + \int_S \xi_{ijk} n_k\,\delta u_{i,j}\,dS\end{aligned} \tag{2.19}$$

Following the treatment in [3] we write the last term on the r.h.s. of (2.19) as

$$\begin{aligned}\int_S \xi_{ijk} n_k\,\delta u_{i,j}\,dS = &\int_S \xi_{ijk} n_k n_j\,\delta(Du_i)\,dS - \int_S D_j(\xi_{ijk} n_k)\,\delta u_i dS \\ &+ \int_S (D_l n_l)\;\xi_{ijk} n_k n_j\;\delta u_i\,dS + \int_E \xi_{ijk}\left[\!\left[m_j n_k \right]\!\right]\delta u_i\,dE\end{aligned} \tag{2.20}$$

where $D_j := (\delta_{ij} - n_i n_j)\left(\partial / \partial X_i\right)$ is the *surface-gradient* operator and the *edge tensor* $[\![m_i n_j]\!]$ characterizes the edge E as a discontinuity of S (see Appendix B). Following the notation in Figure 2.2, the expression for the edge tensor is

$$[\![m_i n_j]\!] = m_i n_j + m_i' n_j' \tag{2.21}$$

where the unit vectors n_i and m_i refer to one of the two half-planes tangent to the surface S at each regular point of the edge E. n_i has the usual meaning while m_i is orthogonal to n_i and to the edge E, and outward-oriented with respect to the

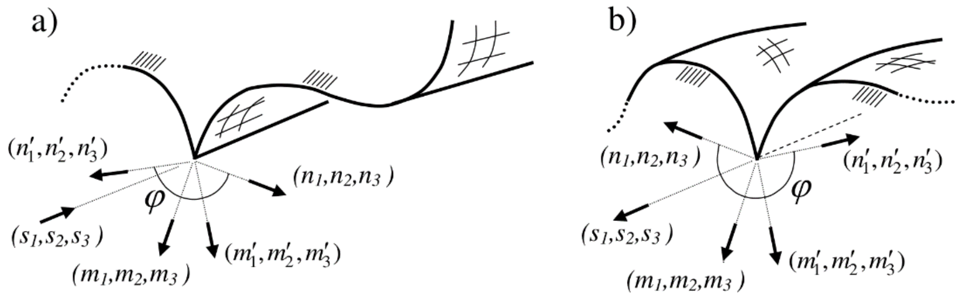


Figure 2.2: Geometrical characterization of the edge tensor at a) a convex and b) a concave edge

relevant half-plane.[3] Similar definitions hold for n_i' and m_i' on the second half-plane.

Substitution of (2.20) in (2.19) gives

$$\begin{aligned}\delta\mathcal{W} &= \int_V (-\tau_{ij,j} + \xi_{ijk,kj})\,\delta u_i\, dV \\ &+ \int_S \left((\tau_{ij} - \xi_{ijk,k}) n_j - D_j(\xi_{ijk} n_k) + (D_l n_l)\, \xi_{ijk} n_k n_j \right) \delta u_i\, dS \\ &+ \int_S \xi_{ijk} n_j n_k\, \delta(D u_i)\, dS \\ &+ \int_E \xi_{ijk} [\![m_j n_k]\!] \delta u_j\, dE .\end{aligned} \tag{2.22}$$

A major advantage of the treatment leading to (2.22) is the separation of the variations of u_i and Du_i in the surface integrals. It is a result known as Hadamard's lemma that knowledge of u_i on S gives no information on Du_i, and vice-versa [25]. In this sense, u_i and Du_i on S can be regarded as independent

[3] In referring to regular points of the edge E we exclude the vertices contained therein.

degrees of freedom available at the surface. To provide a less abstract picture of the normal derivative Du_i as a degree of freedom we write the identity

$$Du_i = (n_j Du_j)n_i + (n_j Du_i - n_i Du_j)n_j \tag{2.23}$$

and substitute (2.11) and (2.12), leading to

$$Du_i = \varsigma n_i + \omega_{ij} n_j \tag{2.24},$$

i.e. the normal derivative of the displacement carries information on the stretch and rotation of the ortho-fiber. Motivated by the above we express the fourth term on the r.h.s. of (2.22) as

$$\int_S \xi_{ijk} n_k n_j \,\delta(Du_i)\, dS = \int_S \xi_{ijk} n_k n_j n_i \,\delta\varsigma\, dS + \int_S \xi_{[ijk} n_{l]}\, n_k n_j \,\delta\omega_{il}\, dS \tag{2.25}$$

where we have exploited the antisymmetry of ω_{ij} and introduced

$$\xi_{[ijk} n_{l]} := \frac{1}{2}\left(\xi_{ijk} n_l - \xi_{ljk} n_i\right) \tag{2.26}$$

Substitution of (2.25) in (2.22) gives a new expression for the variation of the elastic energy functional:

$$\begin{aligned}
\delta\mathcal{W} = &\int_V (-\tau_{ij,j} + \xi_{ijk,kj})\,\delta u_i\, dV \\
&+ \int_S \Big((\tau_{ij} - \xi_{ijk,k}) n_j - D_j(\xi_{ijk} n_k) + (D_l n_l)\,\xi_{ijk} n_k n_j \Big)\delta u_i\, dS \\
&+ \int_S \xi_{ijk} n_k n_j n_i \,\delta\varsigma\, dS \\
&+ \int_S \xi_{[ijk} n_{l]}\, n_k n_j \,\delta\omega_{il}\, dS \\
&+ \int_E \xi_{ijk} \left[\!\left[m_j n_k \right]\!\right] \delta u_j\, dE
\end{aligned} \tag{2.27}$$

The improvement with respect to the classical expression (2.22) is in that all the kinematic fields in the surface integrals in (2.27) have a clear mechanical interpretation.

Remark 2.2: Equation (2.27) should be placed in the context of previous attempts to establish a convincing form of the boundary conditions for 2nd-grade materials. One should compare this result to Equation (12.12) in [3], obtained for Form III of Mindlin's theory. The very long analytical derivation in that paper arguably obscures the physical significance of the surface terms, and probably encouraged the widespread misbelief that physically-different types of boundary conditions might be considered depending on the chosen form of the expression of the elastic energy density, i.e. if Form I, Form II or Form III. A second relevant attempt is that of Bluenstein [26]: Equation (18) in that paper proposes essentially the same interpretation of the boundary term coupled to the ortho-fiber stretch as the one appearing herein in (2.27).

2.3 External actions

We restrict ourselves, for the sake of simplicity, to the case of a body submitted to self-equilibrating external actions in the absence of external constraints, i.e., to the free-body problem.

We have implicitly assumed in the previous sections that the internal actions (i.e., the generalized forces preserving the integrity of the system) are conservative, by virtue of assuming that a *potential of the internal actions*, namely the elastic energy $\mathcal{W}$, is a function of the current configuration only. Its current value is equal to minus the work done by the internal actions on the deformation leading to the current configuration. Analogously, we now introduce a system of conservative external actions by assuming that the work they expend is a function of the current configuration only. We assume they work on the same kinematic measures that the elastic energy function depends on: the displacement u_i, the ortho-fiber stretch ς and the ortho-fiber rotation ω_{ij}. Finally, we assume the *work of the external actions* to have the form

$$\mathcal{P}[u_i] := \int_V U_V^u dV + \int_S U_S^u dS + \int_E U_E^u dE + \int_S U_S^\varsigma dE + \int_S U_S^\omega dE \qquad (2.28)$$

where

$$U_V^u = U_V^u(X_i; u_i) \qquad (2.29)$$

is a volume field, while

$$U_S^u = U_S^u(X_i; u_i), \qquad U_S^\varsigma = U_S^\varsigma(X_i; \varsigma), \qquad U_S^\omega = U_S^\omega(X_i; \omega_{ij}) \qquad (2.30)$$

are surface fields and

$$U_E^u = U_E^u(X_i; u_i) \qquad (2.31)$$

is a lineal field on E. For consistency, all fields in (2.29)-(2.31) are assumed to vanish on the reference configuration, so that $\mathcal{P}[0]=0$.

We work under the assumption of *small deformations*, which we generalize as follows for a 2nd-grade material:

$$\frac{|u_i|}{C^u} \ll 1, \qquad \frac{|\varsigma|}{C^\varsigma} \ll 1, \qquad \frac{|\omega_{ij}|}{C^\omega} \ll 1 \tag{2.32}$$

In the above, C^u is an external characteristic length that represents the order of magnitude for a displacement to cause non-negligible increments of U_V^u. Similar definitions hold for the dimensionless quantities C^ς and C^ω, referred to the densities U_S^u and U_E^u respectively. We can therefore refer to the McLaurin expansions

$$U_V^u(\,\cdot\,;u_i) = F_j u_j + o(|u_i|) \tag{2.33}$$

$$U_S^u(\,\cdot\,;u_i) = t_j u_j + o(|u_i|) \tag{2.34}$$

$$U_E^u(\,\cdot\,;u_i) = s_j u_j + o(|u_i|) \tag{2.35}$$

$$U_S^\varsigma(\cdot\,;\varsigma) = f\varsigma + o(|\varsigma|) \tag{2.36}$$

$$U_S^\Sigma(\cdot\,;\omega_{ij}) = m_{ij}\omega_{ij} + o(|\omega_{ij}|) \tag{2.37}$$

in which the various force-like terms are defined as

$$F_i = \left.\frac{\partial U_V^u}{\partial u_i}\right|_{u_i=0}, \; t_i = \left.\frac{\partial U_S^u}{\partial u_i}\right|_{u_i=0}, \; s_i = \left.\frac{\partial U_E^u}{\partial u_i}\right|_{u_i=0}, \; f = \left.\frac{\partial U_S^\varsigma}{\partial \varsigma}\right|_{u_i=0}, \; m_{ij} = \left.\frac{\partial U_S^\omega}{\partial \omega_{ij}}\right|_{u_i=0} \tag{2.38}$$

and depend in general on the position X_i. These are called herein the *volume force*, the *surface traction*, the *edge*- or *line traction*, the *ortho-fiber tension* and the *ortho-fiber couple* respectively. The physical meaning of the volume force and the surface traction is the same as in classical elasticity, in the sense that they are vector quantities energy conjugate to the displacement. Line traction is also energy conjugate to the displacement, however it only appears along surface edges. This quantity is reminiscent of surface tension as applicable to fluids, in the sense that it has units of force per length and acts along lines, rather than on surfaces or points. The ortho-fiber tension corresponds to localized, self-equilibrating force doublets energy conjugate to the ortho-fiber stretch. Finally, ortho-fiber couples correspond to surface couples energy conjugate to the ortho-fiber rotation.

Equations (2.33)-(2.37), by virtue of the assumption (2.32) of small deformations, suggest the use of the approximation

$$\mathcal{P}[u_i] \approx \int_V F_i u_i dV + \int_S t_i u_i dS + \int_E s_i u_i dE + \int_S f \varsigma dS + \int_S m_{ij} \omega_{ij} dS \qquad (2.39)$$

by which we replace from now on (2.28).

Remark 2.3: The ortho-fiber couple m_{ij} cannot be arbitrarily chosen in the space of antisymmetric tensors, as ordinary couples can (e.g. in Cosserat continuum theory). This is an immediate consequence of its duality in energy to the ortho-fiber rotation tensor ω_{ij}: once the unit normal n_i is assigned, these two quantities vary in a tensor space of dimension 2 assigned by

$$\left\{ a_{ij} \mid a_{ij} = b_{[i} n_{j]},\ n_i b_i = 0 \right\} \qquad (2.40)$$

The couple m_{ij} is therefore dual to rotations about axes orthogonal to n_i.

Remark 2.4: One can alternatively describe the concept of ortho-fiber couple stress by using the axial vector $\hat{m}_i$ associated to m_{ij}, i.e. $\hat{m}_i$ such that

$$m_{ij} c_j = e_{ijk} \hat{m}_j c_k \qquad (2.41)$$

for all vectors c_j. The argument of Cauchy’s tetrahedron would eventually lead to the result that the stress tensor in the sense of Cauchy, associated to the (couple) stress vector $\hat{m}_i$, is deviatoric; this would translate the fact that surface couples dual to rotations about the local unit normal cannot be absorbed by the model. This scenario is the one envisaged in Form-III Mindlin’s theory [3,5]. Our derivations in Section 3 prove this conjecture unphysical, the weak point being the presumed applicability of the argument of Cauchy's tetrahedron, at least in its usual format.

As previously for the elastic energy, we now require that the work of the external actions be objective, in the sense that

$$\mathcal{P}(u_i^*) - \mathcal{P}(u_i) = 0 \tag{2.42}$$

whenever the displacement field u_i^* is related to u_i by an infinitesimal change of the observer (see Section 2.2 and Appendix A; cf. [27]). According to (2.39) one can write (2.42) as

$$\begin{aligned} &\int_V F_i(u_i^* - u_i)\,dV + \int_S t_i(u_i^* - u_i)\,dS + \int_E s_i(u_i^* - u_i)\,dE \\ &\quad + \int_S f(\varsigma^* - \varsigma)\,dS + \int_S m_{ij}(\omega_{ij}^* - \omega_{ij})\,dS = 0 \end{aligned} \tag{2.43}$$

where u_i^* and u_i are related by (2.14) while

$$\varsigma^* - \varsigma = 0, \qquad \omega_{ij}^* - \omega_{ij} = n_j W_{ik} n_k - n_i W_{jk} n_k \tag{2.44}$$

can be deduced from (2.11) and (2.12). (2.43) is therefore replaced by

$$\begin{aligned} &a_j\left(\int_V F_i dV + \int_S t_i dS + \int_E s_i dE\right) + \\ &W_{ij}\left(\int_V X_{[i}F_{j]}dV + \int_S X_{[i}t_{j]}dS + \int_E X_{[i}s_{j]}dE + \int_S m_{ij}dS\right) = 0 \end{aligned} \tag{2.45}$$

and the arbitrariness of a_j and W_{ij} gives

$$\int_V F_i dV + \int_S t_i dS + \int_E s_i dE = 0 \tag{2.46}$$

$$\int_V X_{[i}F_{j]}dV + \int_S X_{[i}t_{j]}dS + \int_E X_{[i}s_{j]}dE + \int_S m_{ij}dS = 0 \tag{2.47}$$

(cf. (52) in Fried and Gurtin [28]). Equation (2.46) is identified as a force balance equation, and (2.47) as a force-moment balance equation for the external actions.

2.4 Principle of virtual work

We seek the set of all possible configurations of the system that can be maintained under a set of admissible external actions, i.e. for a self-equilibrating quintuplet $\left\{F_i, t_i, s_i, f, m_{ij}\right\}$ for which (2.46) and (2.47) hold true. *The principle of virtual work* identifies such configurations as those satisfying the condition

$\delta\mathcal{P} - \delta\mathcal{W} = 0$ for arbitrary variations of the kinematic fields. From (2.39) one has

$$\begin{aligned}\delta\mathcal{P} = &\int_V F_i\,\delta u_i\,dV + \int_S t_i\,\delta u_i\,dS + \int_E s_i\,\delta u_i\,dE \\ &+ \int_S f\,\delta\varsigma\,dS + \int_S m_{ij}\,\delta\omega_{ij}\,dS\end{aligned} \tag{2.48}$$

and the principle of virtual work can be expressed requiring that, for all δu_i,

$$\begin{aligned}&\int_V F_i\,\delta u_i\,dV + \int_S t_i\,\delta u_i\,dS + \int_E s_i\,\delta u_i\,dE + \int_S f\,\delta\varsigma\,dS + \int_S m_{ij}\,\delta\omega_{ij}\,dS \\ &\quad - \int_V (-\tau_{ij,j} + \xi_{ijk,kj})\,\delta u_i\,dV \\ &\quad - \int_S \Big((\tau_{ij} - \xi_{ijk,k})n_j - D_j(\xi_{ijk}n_k) + (D_l n_l)\,\xi_{ijk}n_k n_j\Big)\delta u_i\,dS \\ &\quad - \int_S \xi_{ijk}n_k n_j n_i\,\delta\varsigma\,dS - \int_S \xi_{[ijk}n_{l]}\,n_k n_j\,\delta\omega_{il}\,dS \\ &\quad - \int_E \xi_{ijk}\,[\![m_j n_k]\!]\,\delta u_i\,dE = 0\end{aligned} \tag{2.49}$$

Exploiting the arbitrariness of the variations of the displacement field one obtains the following system of Euler's equations for the mechanical system:

$$\tau_{ij,j} - \xi_{ijk,kj} + F_i = 0 \tag{2.50}$$

$$(\tau_{ij} - \xi_{ijk,k})n_j - D_j(\xi_{ijk}n_k) + (D_l n_l)\,\xi_{ijk}n_k n_j = t_i \tag{2.51}$$

$$\xi_{ijk}n_k n_j n_i = f \tag{2.52}$$

$$\xi_{[ijk}n_{l]}\,n_k n_j = m_{il} \tag{2.53}$$

$$\xi_{ijk}\,[\![m_j n_k]\!] = s_i \tag{2.54}$$

3 Generalized stress fields in the sense of Cauchy

3.1 Continuity constraints

We consider an arbitrary decomposition of the reference configuration into two regular regions, V^- and V^+, separated by a piecewise-smooth internal surface Σ (i.e. $V = V^- \cup V^+$, $\Sigma = V^- \cap\ V^+$). The symbols S^- and E^- (S^+ and E^+) are used with reference to $V^{-}\,(V^{+})$ with the same meaning as S and E for V. The internal surface Σ is assumed part of S^{-}, i.e. are both outward-oriented with respect to V^{-}. We denote by $-\Sigma$ the corresponding part of S^{+}.

In Section 2 we implicitly assumed, as is customary, that u_i is differentiable with continuity up to an order *d*, which is high enough to carry out the relevant calculations. We temporarily drop this assumption and allow discontinuities across Σ for the displacement field and its first *d* gradients. Continuity can be restored by enforcing

$$u_i\big|_{\Sigma} - u_i\big|_{-\Sigma} = 0 \tag{3.1}$$

$$u_{i,j}\big|_{\Sigma} - u_{i,j}\big|_{-\Sigma} = 0\,, \qquad u_{i,jk}\big|_{\Sigma} - u_{i,jk}\big|_{-\Sigma} = 0 \tag{3.2}$$

up to

$$u_{i,\,j_1 j_2 \ldots j_d}\big|_{\Sigma} - u_{i,\,j_1 j_2 \ldots j_d}\big|_{-\Sigma} = 0 \tag{3.3}$$

at each point of Σ. It comes as a further implication of Hadamard's lemma (cf. Section 2.2) that the set of kinematic constraints (3.1)-(3.3) can be equivalently expressed by requiring (3.1) at each point of Σ, along with the following constraints on the normal derivatives of order 1 to *d*:

$$D^{(N)}u_i\big|_{\Sigma} - (-1)^{(N)}\, D^{(N)}u_i\big|_{-\Sigma} = 0 \qquad (1 \le N \le d) \tag{3.4}$$

at each regular point of Σ, with

$$D^{(1)}u_i := Du_i = u_{i,j}n_j\,, \qquad D^{(2)}u_i := u_{i,jk}n_k n_j \tag{3.5}$$

up to

$$D^{(d)}u_i := u_{i,\,j_1 j_2 \ldots j_d}\, n_{j_d} n_{j_{d-1}} \ldots n_{i_1} \tag{3.6}$$

To investigate the internal actions arising through these kinematic constraints, we express (3.4)-(3.6) in integral form, i.e. require that

$$\mathcal{P}^{(0)} := \int_{\Sigma} \lambda_i^{(0)} \left(u_i\big|_{\Sigma} - u_i\big|_{-\Sigma} \right) dS = 0 \tag{3.7}$$

$$\mathcal{P}^{(N)} := \int_{\Sigma \backslash E^{-}} \lambda_i^{(N)} \left(D^{(N)}u_i\big|_{\Sigma} - (-1)^{N}\, D^{(N)}u_i\big|_{-\Sigma} \right) dS = 0 \qquad (1 \le N \le d) \tag{3.8}$$

for arbitrary Lagrangian multiplier fields $\lambda_i^{(0)}$ on Σ and $\lambda_i^{(1)}$, …, $\lambda_i^{(d)}$ on $\Sigma \setminus E^-$. These are generalized functions in the sense of the theory of distributions, serving as reactive, force-like quantities that preserve continuity, up to order d, across Σ. Accordingly, we express the principle of virtual work as

$$\delta\mathcal{P} + \delta\mathcal{P}^{(0)} + \delta\mathcal{P}^{(1)} + ... + \delta\mathcal{P}^{(d)} - \delta\mathcal{W} = 0 \tag{3.9}$$

for arbitrary variations of the displacement field.

Due to the discontinuous kinematics, divergence theorems now apply to V^- and V^+ separately. As concerns the variations of the elastic energy, integration by parts gives

$$\begin{aligned}\delta\mathcal{W} &= \int_{V^-} (-\tau_{ij,j} + \xi_{ijk,kj})\,\delta u_i\,dV + \int_{V^+} (-\tau_{ij,j} + \xi_{ijk,kj})\,\delta u_i\,dV \\ &+ \int_{S^-} \Big((\tau_{ij} - \xi_{ijk,k})n_j - D_j(\xi_{ijk}n_k) + (D_l n_l)\,\xi_{ijk}n_k n_j\Big)\delta u_i\,dS \\ &+ \int_{S^+} \Big((\tau_{ij} - \xi_{ijk,k})n_j - D_j(\xi_{ijk}n_k) + (D_l n_l)\,\xi_{ijk}n_k n_j\Big)\delta u_i\,dS \\ &+ \int_{S^-} \xi_{ijk}n_k n_j\,\delta(Du_i)\,dS + \int_{S^+} \xi_{ijk}n_k n_j\,\delta(Du_i)\,dS \\ &+ \int_{E^-} \xi_{ijk}\,[\![m_j n_k]\!]\,\delta u_i\,dE + \int_{E^+} \xi_{ijk}\,[\![m_j n_k]\!]\,\delta u_i\,dE\end{aligned} \tag{3.10}$$

cf. (2.22), which could be also expressed in terms of ortho-fiber stretch and rotations, cf. (2.27). It is also convenient to split the work of the constraints as

$$\mathcal{P}^{(0)} = \int_{\Sigma} \lambda_i^{(0)} u_i dS - \int_{-\Sigma} \lambda_i^{(0)} u_i dS \tag{3.11}$$

$$\mathcal{P}^{(N)} = \int_{\Sigma\setminus E^-} \lambda_i^{(N)} D^{(N)} u_i dS + (-1)^N \int_{-\Sigma\setminus E^+} \lambda_i^{(N)} D^{(N)} u_i dS \qquad (1 \le N \le d) \tag{3.12}$$

Substituting (3.10), (3.11) and (3.12) in (3.9), Euler's equations are obtained, as usual, by exploiting the arbitrariness of the variations of the displacement fields. Taking δu_i to vanish in V^+ but remain arbitrary in V^- yields[4]

$$(\tau_{ij} - \xi_{ijk,k})n_j - D_j(\xi_{ijk}n_k) + (D_l n_l)\,\xi_{ijk}n_k n_j = \hat{\lambda}_i^{(0)} \tag{3.13}$$

$$\xi_{ijk}\,[\![m_j n_k]\!] = \hat{\lambda}_i^{(0)} \tag{3.14}$$

$$\xi_{ijk}n_k n_j n_i = \lambda_i^{(1)} n_i \tag{3.15}$$

[4] Sign alternation under square brackets in (3.16) applies only to the indices i and l.

$$\xi_{[ijk}n_k n_j n_{l]} = \lambda^{(1)}_{[i}n_{l]} \tag{3.16}$$

$$\lambda_i^{(2)} = ... = \lambda_i^{(d)} = 0 \tag{3.17}$$

where $\widehat{\lambda}_i^{(0)}$ on $E^- \cap \Sigma$ and $\hat{\lambda}_i^{(0)}$ on $\Sigma \setminus E^-$ are a convenient replacement for $\lambda_i^{(0)}$.

Taking δu_i to vanish in V^- but remain arbitrary in V^+ one obtains the equivalent form of (3.13)-(3.16) for $-\Sigma$:

$$(\tau_{ij} - \xi_{ijk,k})n_j - D_j(\xi_{ijk}n_k) + (D_l n_l)\xi_{ijk}n_k n_j = -\widehat{\lambda}_i^{(0)} \tag{3.18}$$

$$\xi_{ijk}\left[\!\left[m_j n_k \right]\!\right] = -\hat{\lambda}_i^{(0)} \tag{3.19}$$

$$\xi_{ijk}n_k n_j n_i = -\lambda_i^{(1)}n_i \tag{3.20}$$

$$\xi_{[ijk}n_k n_j n_{l]} = -\lambda^{(1)}_{[i}n_{l]} \tag{3.21}$$

Remark 3.1: From (3.17) it follows that, for the prescribed expression of the elastic energy, constraints on second- or higher-order derivatives of the displacement field do not give rise to reactive internal actions across Σ. Conversely, for 1st-grade materials the same procedure would show $\hat{\lambda}_i^{(0)}$ and $\lambda_i^{(1)}$ to be zero.

3.2 Generalized Cauchy stress-vector fields

It is interesting to note how the concept of stress in classical continuum mechanics was originally shaped by A. Cauchy [29,30] through a generalization of the concept of pressure for ideal fluids. As expressed by *Cauchy's postulate,* the generalization consisted in allowing, at material point X_i, distinct values of the stress vector $\widehat{t}_i$ depending on the relevant internal surface, with the unit normal n_i as the sole geometrical descriptor:

$$\widehat{t}_i = \widehat{t}_i(X_j; n_j) \tag{3.22}$$

This postulate is unfortunately regarded in continuum mechanics as almost a physical principle, rather than a restrictive assumption (though one of very general scope). In what respects the framework established by Cauchy's postulate is not general enough to cover 2nd-grade materials is discussed in the following. The appropriate generalization is given, derived from the variational formulation and based on the idea that internal actions in the sense of Cauchy can be regarded as generalized reactive forces granting for the “constraint of continuity” assumed for the displacement field and its derivatives. Similarities can be identified with the deductive procedure and the results of dell’Isola et al. [6-8], although there is no complete agreement.

By virtue of being a surface force density that prevents separation or interpenetration of parts V^+ and V^- across Σ, the internal action $\widehat{\lambda}_i^{(0)}$ in Section 3.1 can be identified with Cauchy’s stress vector field. Therefore, in order to assess the validity of Cauchy’s postulate for 2nd-grade materials, we investigate the dependence of $\widehat{\lambda}_i^{(0)}$ on the local properties of Σ and express (3.13) as

$$\widehat{\lambda}_i^{(0)} = (\tau_{ij} - 2\xi_{ijk,k})n_j + \xi_{ijk,l}n_l n_k n_j - \xi_{ijk}(\delta_{jl}\delta_{km} + n_j n_k \delta_{lm}) D_l n_m \qquad (3.23)$$

Clearly, the r.h.s. of (3.23) does not fit (3.22), whose relevant generalization is

$$\widehat{t}_i = \widehat{t}_i(X_i; n_i; D_i n_j) \qquad (3.24)$$

It also appears from (3.23) that the dependence on the unit normal in (3.24) is “cubic” rather than “linear”. In this sense, one should not expect the classical argument of Cauchy tetrahedron to lead to the existence of a 2nd-order tensor with the same properties as Cauchy’s stress tensor.

Further information on the dependence on the geometrical descriptors of the internal surface in (3.24) can be obtained by expressing

$$D_i n_j = \kappa' s_i' s_j' + \kappa'' s_i'' s_j'' \qquad (3.25)$$

where κ' and κ'' are the principal normal curvatures at a given regular point of Σ , with s_i' and s_i'' the relevant curvature directions[5]. In (3.25), κ' and κ'' are oriented quantities (i.e. take either negative or positive values depending on n_i pointing towards or opposite to the relevant centers of curvature, respectively.). Finally, for appropriate s_j' and s_k'' one has

$$n_i = e_{ijk} s_j' s_k'' \qquad (3.26)$$

[5] This is an implication of the *formulae of O. Rodrigues* (see Theorem 45.1 in [31]).

According to (3.25) and (3.26) it makes sense to use

$$\widehat{t}_i = \widehat{t}_i(X_j; s'_j; s''_j; \kappa'; \kappa'') \tag{3.27}$$

in place of (3.24) as a pertinent generalization of Cauchy's postulate.

As concerns the internal action $\hat{\lambda}_i^{(0)}$, Equation (3.14) can be expressed as

$$\hat{\lambda}_i^{(0)} = \xi_{ijk}\left(\frac{(n'_j n_k + n_j n'_k) - \cos(\varphi)(n_j n_k + n'_j n'_k)}{\sin(\varphi)}\right) \tag{3.28}$$

(see Figure 2.3 and the calculation in Appendix B). How (3.28) is a degenerate form of (3.23) can be inferred by computing the surface integral of the latter equation at the limit where one of the two principal curvatures tends to infinity. Therefore, according to (3.28), a complete generalization of Cauchy's concept of stress must include a line-traction term of type

$$\hat{t}_i = \hat{t}_i(X_i; n_i; n'_i) \tag{3.29}$$

along the edges of the internal surface Σ.

Finally, the relevant format of the action-reaction laws can be deduced directly from (3.23) and (3.28):

$$\widehat{t}_i(X_i; n_i; D_i n_i) = -\widehat{t}_i(X_i; -n_i; D_i(-n_j)), \tag{3.30}$$

$$\hat{t}_i(X_i; n_i; n'_i) = -\hat{t}_i(X_i; -n_i; -n'_i) \tag{3.31}$$

Remark 3.2: Readers familiar with the axiomatics of continuum mechanics pioneered by Noll [32] will have noticed an important but apparent contradiction. In particular, a classical theorem in that paper (Theorem IV) seems to exclude the possibility for the stress vector to depend on the curvature of the surface at the relevant point. Prof. Noll commented in a footnote that: *"[...] It has been proposed occasionally that one should weaken this assumption and allow the stress to depend not only on the tangent plane at x but also on the curvature of the surface c at x. The theorem given here shows that such dependence on the curvature, or any other local property of the surface at x, is impossible."* We clarify that 2nd-grade materials do not comply with the assumptions of that theorem, despite its great generality, due to lineal force densities along the edges of internal surfaces, as in (3.29) (a similar viewpoint is expressed in [8]). For the same reasons, the concept of Cauchy flux [33-35] does not apply here either, while it is appropriate for other non-simple materials, e.g. Cosserat continua (e.g. [36]).

3.3 Higher-order stress fields

The proper form of further generalized internal actions in the sense of Cauchy can be inferred from the force-like field $\lambda_i^{(1)}$, instead of $\widehat{\lambda}_i^{(0)}$ and $\hat{\lambda}_i^{(0)}$ as in Section 3.2. In (3.15) one can interpret the term $\lambda_i^{(1)} n_i$ as the ortho-fiber tension exerted by V^+ on V^- across Σ. Similarly, $\lambda_{[i}^{(1)} n_{l]}$ in (3.16) can be interpreted as an ortho-fiber couple. We now introduce an *ortho-fiber-tension stress field*

$$\psi = \psi(X_i; n_i) \tag{3.32}$$

and an *ortho-fiber-couple stress field*

$$\mu_{ij} = \mu_{ij}(X_k; n_k) \tag{3.33}$$

in agreement with (3.15) and (3.16), respectively. The relevant action-reaction laws can be deduced by comparison of (3.15) and (3.16) with (3.20) and (3.21) respectively:

$$\psi(X_i; n_i) = -\psi(X_i; -n_i) \tag{3.34}$$

$$\mu_{ij}(X_k; n_k) = -\mu_{ij}(X_k; -n_k) \tag{3.35}$$

where the ortho-fiber couple μ_{ij} is an antisymmetric tensor of the type shown by (2.40).

Remark 3.3: For both the ψ and μ_{ij} fields, one cannot expect the existence of related tensors with properties analogous to the classical Cauchy stress-tensor. This is once more because the dependence on n_i in (3.32) and (3.33) is “cubic” and not “linear” (see the l.h.s. terms of (3.15) and (3.16)).

3.4 Balance laws for generalized stress fields

We focus on part V^- and regard the actions exerted by the exterior of V and by V^+ as external. The work of such actions on a displacement u_i of V^- can be obtained by isolating the respective contributions from $\mathcal{P}$, $\mathcal{P}^{(0)}$ and $\mathcal{P}^{(1)}$. Using the quantities $\widehat{t}_i$, $\hat{t}_i$, μ_{ij} and ψ introduced in Sections 3.2 and 3.3 instead of the Lagrangian multiplier fields defined in (3.7) and (3.8) one can write the work of external actions on V^- in the form

$$\begin{aligned}\mathcal{P}^- = \int_V F_i u_i \, dV + \int_S t_i u_i \, dS + \int_E s_i u_i \, dE + \int_S f \varsigma dS + \int_S m_{ij} \omega_{ij} \, dS \\ + \int_\Sigma \widehat{t}_i u_i \, dS \ + \int_{E^- \cap \Sigma} \hat{t}_i u_i \, dS \ + \int_\Sigma \psi \, \varsigma \, dS + \int_\Sigma \mu_{ij} \omega_{ij} \, dS \ .\end{aligned} \tag{3.36}$$

We now require $\mathcal{P}^-$ to be objective. By the same procedure as in Section 2.3, we obtain

$$\int_{V^-} F_i dV + \int_{S^- \cap S} t_i \, dS + \int_{E^- \cap S} s_i \, dE + \int_{S^- \cap \Sigma} \widehat{t}_i \, dS + \int_{E^- \cap \Sigma} \hat{t}_i \, dE = 0 \tag{3.37}$$

and

$$\begin{aligned}\int_{V^-} X_{[i} F_{j]} \, dV + \int_{S^- \cap S} X_{[i} t_{j]} \, dS + \int_{E^- \cap S} X_{[i} s_{j]} \, dE + \int_{S^- \cap S} m_{ij} \, dS \\ + \int_{S^- \cap \Sigma} X_{[i} \, \widehat{t}_{j]} \, dS + \int_{E^- \cap \Sigma} X_{[i} \, \hat{t}_{j]} \, dE + \int_{S^- \cap \Sigma^-} \mu_{ij} \, dS = 0\end{aligned} \tag{3.38}$$

which are the linear- and angular momentum balance laws for the actions on V^-. The above equations suggest

$$\int_\Sigma \widehat{t}_i \, dS + \int_{E^- \cap \Sigma} \hat{t}_i \, dE \tag{3.39}$$

as the generalized form of the resultant force on the internal surface Σ, and

$$\int_\Sigma X_{[i} \, \widehat{t}_{j]} \, dS + \int_{E^- \cap \Sigma} X_{[i} \, \hat{t}_{j]} \, dE + \int_\Sigma \mu_{ij} \, dS \tag{3.40}$$

as the relevant force-moment computed at the origin of the reference system. Notably, the ortho-fiber-tension stress field ψ does not enter the balance laws (3.37) and (3.38), i.e. is self-equilibrating.

4 Examples in isotropic elasticity

4.1 Linear isotropic constitutive law

We seek now to derive the expression of the elastic energy density for a linearly-elastic 2nd-grade material obeying isotropy. The latter assumption can be expressed as the requirement that

$$W(X_i;u_{i,j};u_{i,jk})=W(X_i;\hat{u}_{i,j};\hat{u}_{i,jk}) \tag{4.1}$$

where u_i is an arbitrary displacement field and $\hat{u}_i$ the same displacement field rotated about X_i, such that

$$\hat{u}_i = Q_{ij}^T u_j \tag{4.2}$$

where the orthogonal, unit-determinant tensor Q_{ij} represents the rotation to the new, arbitrary frame of reference. As concerns the gradients of $\hat{u}_i$, differentiation of (4.2) with respect to X_i yields

$$\hat{u}_{i,j} = Q_{ik}u_{k,l}Q_{lj}^T , \qquad \hat{u}_{i,jk} = Q_{il}u_{l,mn}Q_{mj}^T Q_{nk}^T \tag{4.3}$$

A general expression for the elastic energy density of a linearly-elastic 2nd-grade material (without pre-stress) is

$$W=\frac{1}{2}\alpha_{ij\,lm}\,u_{i,j}\,u_{l,m}+\beta_{ij\,lmn}u_{i,j}\,u_{l,mn}+\frac{1}{2}\gamma_{ijk\,lmn}u_{i,jk}\,u_{l,mn} \tag{4.4}$$

After (4.3) and (4.4), the isotropy requirement (4.1) becomes

$$\begin{aligned}&\alpha_{ij\,lm}u_{i,j}\,u_{l,m}+2\beta_{ij\,lmn}u_{i,j}\,u_{l,mn}+\gamma_{ijk\,lmn}u_{i,jk}\,u_{l,mn}\\&\quad=\alpha_{pq\,rs}Q_{pi}\,u_{i,j}Q_{qj}Q_{rl}\,u_{l,m}Q_{sm}+2\beta_{pq\,rst}Q_{pi}\,u_{i,j}Q_{qj}Q_{rl}\,u_{l,mn}Q_{sm}Q_{tn}\\&\quad+\gamma_{pqr\,stu}\,Q_{pi}\,u_{i,jk}Q_{qj}Q_{rk}Q_{sl}\,u_{l,mn}Q_{tm}Q_{un}\end{aligned} \tag{4.5}$$

To obtain an expression that is independent of Q_{ij} the constitutive coefficients in (4.5) must be combinations of Kroneker deltas whose product with Q_{ij} and its transpose equals a scalar constant. No such combination can be found for the coefficients $\beta_{ij\,klm}$, due to the fact that Q_{ij} appears an odd number of times in the relevant term in (4.5). In other words, isotropy implies $\beta_{ij\,lmn}=0$. Furthermore, demanding that $\alpha_{ijlm} = \alpha_{pqrs} Q_{pi} Q_{qj} Q_{rl} Q_{sm}$ and $\gamma_{ijklmn} = \gamma_{pqrstu} Q_{pi} Q_{qj} Q_{rk} Q_{sl} Q_{tm} Q_{un}$ yields

$$\alpha_{ijlm} = \alpha^{(1)} \delta_{ij}\delta_{lm} + \alpha^{(2)}\delta_{il}\delta_{jm} + \alpha^{(3)}\delta_{im}\delta_{jl} \tag{4.6}$$

and

$$\begin{aligned}\gamma_{ijklmn} = {} & \gamma^{(1)} \delta_{ij}\delta_{kl}\delta_{mn} + \gamma^{(2)} \delta_{ij}\delta_{km}\delta_{ln} + \gamma^{(3)} \delta_{ij}\delta_{kn}\delta_{lm} \\ & + \gamma^{(4)} \delta_{ik}\delta_{jl}\delta_{mn} + \gamma^{(5)} \delta_{ik}\delta_{jm}\delta_{ln} + \gamma^{(6)} \delta_{ik}\delta_{jn}\delta_{lm} \\ & + \gamma^{(7)} \delta_{il}\delta_{jk}\delta_{mn} + \gamma^{(8)} \delta_{il}\delta_{jm}\delta_{kn} + \gamma^{(9)} \delta_{il}\delta_{jn}\delta_{km} \\ & + \gamma^{(10)} \delta_{im}\delta_{jk}\delta_{ln} + \gamma^{(11)} \delta_{im}\delta_{jl}\delta_{kn} + \gamma^{(12)} \delta_{im}\delta_{jn}\delta_{kl} \\ & + \gamma^{(13)} \delta_{in}\delta_{jk}\delta_{lm} + \gamma^{(14)} \delta_{in}\delta_{jl}\delta_{km} + \gamma^{(15)} \delta_{in}\delta_{jm}\delta_{kl}\end{aligned} \tag{4.7}$$

respectively. The resulting set of 18 material constants $\alpha^{(1)}, \alpha^{(2)}$, $\alpha^{(3)}$, $\gamma^{(1)}$, $\gamma^{(2)}$, …, $\gamma^{(15)}$ can be reduced by exploiting (i) the minor symmetries $\alpha_{ijlm} = \alpha_{ijml}$, $\alpha_{ijlm} = \alpha_{jiml}$, $\gamma_{ijklmn} = \gamma_{ijklnm}$ and $\gamma_{ijklmn} = \gamma_{ikjlmn}$ that arise due to the symmetries of $u_{(i,j)}$, τ_{ij}, $u_{i,jk}$ and ξ_{ijk}, along with (ii) the major symmetries $\alpha_{ijlm} = \alpha_{lmij}$ and $\gamma_{ijklmn} = \gamma_{lmnijk}$ which hold true due to (4.4) being a quadratic form. The reduced set of material constants is:

$$\lambda = \alpha^{(1)}, \qquad \mu = \alpha^{(2)} = \alpha^{(3)} \tag{4.8}$$

where λ and μ are identified as the usual Lamé's constants, and

$$g^{(1)} = \gamma^{(7)}, \qquad g^{(2)} = \gamma^{(8)} = \gamma^{(9)} \tag{4.9}$$

$$g^{(3)} = \gamma^{(1)} = \gamma^{(4)} = \gamma^{(10)} = \gamma^{(13)} \tag{4.10}$$

$$g^{(4)} = \gamma^{(2)} = \gamma^{(3)} = \gamma^{(5)} = \gamma^{(6)} \tag{4.11}$$

$$g^{(5)} = \gamma^{(11)} = \gamma^{(12)} = \gamma^{(14)} = \gamma^{(15)} \tag{4.12}$$

We can now express α_{ijlm} and γ_{ijklmn} as

$$\alpha_{ijlm} = \lambda \delta_{ij}\delta_{lm} + \mu\left(\delta_{il}\delta_{jm} + \delta_{im}\delta_{jl}\right) \tag{4.13}$$

$$
\begin{aligned}
\gamma_{ijklmn} = {} & g^{(1)}\,\delta_{il}\delta_{jk}\delta_{mn} + g^{(2)}(\,\delta_{il}\delta_{jm}\delta_{kn} + \delta_{il}\delta_{jn}\delta_{km}) \\
& + g^{(3)}(\delta_{ij}\delta_{kl}\delta_{mn} + \delta_{ik}\delta_{jl}\delta_{mn} + \delta_{im}\delta_{jk}\delta_{ln} + \delta_{in}\delta_{jk}\delta_{lm}) \\
& + g^{(4)}(\,\delta_{ij}\delta_{km}\delta_{ln} + \delta_{ij}\delta_{kn}\delta_{lm} + \delta_{ik}\delta_{jm}\delta_{ln} + \delta_{ik}\delta_{jn}\delta_{lm}) \\
& + g^{(5)}(\,\delta_{im}\delta_{jl}\delta_{kn} + \delta_{im}\delta_{jn}\delta_{kl} + \delta_{in}\delta_{jl}\delta_{km} + \delta_{in}\delta_{jm}\delta_{kl})
\end{aligned}
\tag{4.14}
$$

Substituting (4.13) and (4.14) in (4.4), exploiting the symmetry of $u_{i,jk}$ and carrying out the calculations we finally arrive to the following general form of the elastic energy density for linearly-isotropic, 2nd-grade elastic materials:

$$
\begin{aligned}
W = {} & \frac{1}{2}\lambda\, u_{i,i}u_{j,j} + \mu\, u_{(i,j)}u_{(i,j)} + \frac{1}{2}g^{(1)}\,u_{i,jj}u_{i,kk} + g^{(2)}u_{i,jk}u_{i,jk} \\
& + 2g^{(3)}u_{j,ji}u_{i,kk} + 2g^{(4)}u_{j,ji}u_{k,ki} + 2g^{(5)}u_{i,jk}u_{j,ki}
\end{aligned}
\tag{4.15}
$$

Employing (2.17) further yields

$$
\tau_{ij} = \lambda\,\delta_{ij}u_{l,l} + 2\mu\,u_{(i,j)} \tag{4.16}
$$

and

$$
\begin{aligned}
\xi_{ijk} = {} & g^{(1)}\,\delta_{jk}u_{i,ll} + 2g^{(2)}u_{i,jk} + g^{(3)}(\delta_{ij}u_{k,ll} + \delta_{ik}u_{j,ll} + 2\delta_{jk}u_{l,li}) \\
& + 2g^{(4)}(\,\delta_{ij}u_{l,lk} + \delta_{ik}u_{l,lj}) + 2g^{(5)}(u_{j,ki} + u_{k,ij})
\end{aligned}
\tag{4.17}
$$

4.2 Positive definiteness of the elastic energy density

The decomposition of the linear space of symmetric 2nd-order tensors in the direct sum of the linear subspaces of spherical and deviatoric tensors is the starting point for deriving the positive definiteness conditions of the elastic energy density for linearly-elastic isotropic 1st-grade materials. Successful attempts to extend this procedure, in whole or in part, to 2nd-grade materials can be found in [3,28,37,38]. We provide herein a complete description of the original decomposition procedure already mentioned in [23], based on Spencer's minimal integrity base for isotropic 3rd-order tensors (see [39]).

We define the mutually-orthogonal projections

$$
a_{ijk} := \frac{1}{3}\left(u_{i,jk} + u_{j,ki} + u_{k,ij}\right), \qquad b_{ijk} := u_{i,jk} - a_{ijk} \tag{4.18}
$$

of $u_{i,jk}$ onto the linear space of fully-symmetric 3rd-order tensors, i.e. such that $a_{ijk} = a_{jki} = a_{kij}$. We decompose further as

$$a^s_{ijk} := \frac{1}{5}\left(a_{ill}\delta_{jk} + a_{ljl}\delta_{ki} + a_{llk}\delta_{ij}\right), \qquad a^d_{ijk} := a_{ijk} - a^s_{ijk} \tag{4.19}$$

$$b^s_{ijk} := \frac{1}{2}\left(b_{ill}\delta_{jk} + b_{ljl}\delta_{ki} + b_{llk}\delta_{ij}\right), \qquad b^d_{ijk} := b_{ijk} - b^s_{ijk} \tag{4.20}$$

where the superscripts "s" for "spherical" and "d" for "deviatoric" should be understood as follows:

$$a^s_{ijj} = a^s_{jij} = a^s_{jji}, \qquad a^d_{ijj} = a^d_{jij} = a^d_{jji} = 0 \tag{4.21}$$

$$b^s_{ijj} = -2b^s_{jij} = -2b^s_{jji}, \qquad b^d_{ijj} = b^d_{jij} = b^d_{jji} = 0 \tag{4.22}$$

The resulting decomposition

$$u_{i,jk} = a^s_{ijk} + a^d_{ijk} + b^s_{ijk} + b^d_{ijk} \tag{4.23}$$

is still in terms of mutually orthogonal components, i.e.

$$a^s_{ijk}a^d_{ijk} = a^s_{ijk}b^s_{ijk} = a^s_{ijk}b^d_{ijk} = a^d_{ijk}b^s_{ijk} = a^d_{ijk}b^d_{ijk} = b^s_{ijk}b^d_{ijk} = 0 \tag{4.24}$$

Remark 4.1: The identities

$$b_{ijk} = \frac{1}{3}e_{lij}B_{lk} + \frac{1}{3}e_{lik}B_{lj} \tag{4.25}$$

$$b^s_{ijk} = \frac{1}{3}e_{lij}B_{[lk]} + \frac{1}{3}e_{lik}B_{[lj]}, \qquad b^d_{ijk} = \frac{1}{3}e_{lij}B_{(lk)} + \frac{1}{3}e_{lik}B_{(lj)} \tag{4.26}$$

with $B_{ij} := e_{lmi}u_{l,mj}$ disclose the inner structure of b_{ijk}, b^s_{ijk} and b^d_{ijk}.[6] They also provide equivalent definitions for the respective terms, as elements of minimal integrity bases for isotropic 3rd-order tensors [39].[7]

Equations (4.23) and (4.24) refer to a decomposition in direct sum for the linear space of 3rd-order tensors with symmetry in the last two indices. Similar to the classical procedure for 1st-grade materials, we now introduce the above

[6] The tensor B_{ij} is closely related to the *rotation gradient* $\bar{\kappa}_{ij}$ in Mindlin et al. [3,5]. In particular: $\bar{\kappa}_{ij} = -2B_{ji}$.

[7] We acknowledge Dr. S.-A. Papanicolopulos [40] for bringing to our attention the possibility of using the definitions in (4.20) as alternatives to the usual ones, in (4.26).

definitions in (4.27), to obtain a suitable expression for the elastic energy density. Use of the identities (4.21)-(4.22), along with

$$a^s_{ijk}\,a^s_{ijk} = \frac{3}{5}a^s_{ijj}a^s_{ikk}\,, \qquad b^s_{ijk}\,b^s_{ijk} = \frac{3}{4}b^s_{ijj}\,b^s_{ikk} \tag{4.28}$$

$$b^s_{ijk}\,b^s_{ijk} = -2b^s_{ijk}\,b^s_{jki}\,, \qquad b^s_{ijk}\,b^d_{jki} = b^s_{ijk}\,b^d_{kij} = 0 \tag{4.29}$$

lead to

$$\begin{aligned} W = {} & \frac{3\lambda + 2\mu}{2} s_{ij}s_{ij} + \mu\, d_{ij}d_{ij} + \frac{1}{2}G^{(1)}\, a^s_{ijk}a^s_{ijk} + \frac{1}{2}G^{(2)}\, a^d_{ijk}a^d_{ijk} \\ & + \frac{1}{2}G^{(3)}\, b^s_{ijk}b^s_{ijk} + \frac{1}{2}G^{(4)}\, b^d_{ijk}b^d_{ijk} + G^{(5)}\, a^s_{ijj}b^s_{ikk} \end{aligned} \tag{4.30}$$

in which

$$G^{(1)} := \frac{5}{3}g^{(1)} + 2g^{(2)} + \frac{20}{3}g^{(3)} + \frac{20}{3}g^{(4)} + 4g^{(5)} \tag{4.31}$$

$$G^{(2)} := 2g^{(2)} + 4g^{(5)} \tag{4.32}$$

$$G^{(3)} := \frac{4}{3}g^{(1)} + 2g^{(2)} - \frac{8}{3}g^{(3)} + \frac{4}{3}g^{(4)} - 2g^{(5)} \tag{4.33}$$

$$G^{(4)} := 2g^{(2)} - 2g^{(5)} \tag{4.34}$$

$$G^{(5)} := g^{(1)} + g^{(3)} - 2g^{(4)} \tag{4.35}$$

and where s_{ij} and d_{ij} are the spherical and deviatoric part of the infinitesimal strain tensor, respectively.

As apparent in (4.30), the independent deformation modes s_{ij} , d_{ij}, a^s_{ijk}, a^d_{ijk}, b^s_{ijk} and b^s_{ijk} are pairwise-orthogonal in energy, but the pair composed of a^s_{ijk} and b^s_{ijk}. Therefore, a first set of independent positive-definiteness conditions for the elastic energy density can be inferred directly as

$$\mu > 0\,, \qquad 3\lambda + 2\mu > 0 \tag{4.36}$$

$$G^{(1)} > 0\,, \qquad G^{(2)} > 0\,, \qquad G^{(3)} > 0\,, \qquad G^{(4)} > 0 \tag{4.37}$$

A last, seventh positive-definiteness condition arises in the form

$$-\sqrt{\frac{G^{(1)}G^{(3)}}{5}} < \frac{2}{3}G^{(5)} < \sqrt{\frac{G^{(1)}G^{(3)}}{5}} \tag{4.38}$$

as soon as, in (4.30), the sum of quadratic terms in a^s_{ijk} and b^s_{ijk} is expressed as

$$\frac{1}{2}(\begin{bmatrix} 3/5\, G^{(1)} & G^{(5)} \\ G^{(5)} & 3/4\, G^{(3)} \end{bmatrix}\begin{bmatrix} a^s_{ikk} \\ b^s_{ikk} \end{bmatrix}) \cdot \begin{bmatrix} a^s_{ill} \\ b^s_{ill} \end{bmatrix} \tag{4.39}$$

as allowed by (4.28).

In the remainder of this paper we restrict ourselves to the case where the conditions (4.36)-(4.38) are satisfied, i.e. to strictly-convex, non-negative elastic energy densities. Under the same assumption the elastic energy functional $\mathcal{W}$ is also strictly-convex and non-negative, when the linear space of admissible displacement fields is restricted so as to exclude non-trivial, infinitesimal rigid motions. The same then holds for the work functional $\mathcal{P} - \mathcal{W}$, according to the definition (2.39). Uniqueness of the solution to the displacement problem for an unconstrained body then follows, up to pairs of displacement fields that differ by non-trivial infinitesimal rigid motions. In the example boundary value problems solved in Section 4.3, 4.4 and 4.5, the relevant kinematic constraints exclude non-trivial infinitesimal rigid motions, leading to unique solutions.

4.3 Oedometric compression with interlocked boundaries

We consider the compression in direction 3 of a layer of height H, extending infinitely along directions 1 and 2. We isolate a periodic parallelepipedal element (see Figure 4.1) with rectangular section and finite dimensions in the 1-2 plane. We separate the outward-oriented boundary S in six portions: $S^{[1]}$, $S^{[2]}$, $S^{[3]}$, $S^{[-1]}$, $S^{[-2]}$ and $S^{[-3]}$, with unit normal δ_{i1}, δ_{i2}, δ_{i3}, $-\delta_{i1}$, $-\delta_{i2}$ and $-\delta_{i3}$ respectively. Periodicity is expressed by the kinematic constraints

$$u_i(0,\cdot,\cdot) = u_i(L_1,\cdot,\cdot), \qquad u_i(\cdot,0,\cdot) = u_i(\cdot,L_2,\cdot) \tag{4.40}$$

$$\varsigma\big|_{\delta_{i1}}(0,\cdot,\cdot) = \varsigma\big|_{\delta_{i1}}(L_1,\cdot,\cdot), \qquad \varsigma\big|_{\delta_{i2}}(\cdot,0,\cdot) = \varsigma\big|_{\delta_{i2}}(\cdot,L_2,\cdot) \tag{4.41}$$

$$\omega_{ij}\big|_{\delta_{i1}}(0,\cdot,\cdot) = \omega_{ij}\big|_{\delta_{i1}}(L_1,\cdot,\cdot), \qquad \omega_{ij}\big|_{\delta_{i2}}(0,\cdot,\cdot) = \omega_{ij}\big|_{\delta_{i2}}(L_2,\cdot,\cdot) \tag{4.42}$$

where $\varsigma|_{\delta_{i1}}(X_j)$ denotes the ortho-fiber stretch for a material surface with the unit normal δ_{i1} at material point X_i, and similar definitions hold for the remaining terms in (4.41) and (4.42) . We apply a constant surface traction $t_i = -\bar{F} n_i$, with $\bar{F} > 0$, on the top and the bottom plane ($S^{[3]}$ and $S^{[-3]}$, resp.). In addition, we assume that $\bar{F}$ is applied through contact with a loading agent, in such a way that no vertical strain can develop at the interface. This situation can be explained if contact is imagined taking place through the interlocking of matching surface asperities. This type of boundary condition implies zero ortho-fiber stretch fields:

$$\varsigma|_{\delta_3}(\cdot,\cdot,H/2) = 0, \qquad \varsigma|_{-\delta_3}(\cdot,\cdot,-H/2) = 0 \tag{4.43}$$

The characteristics of the problem (i.e. its symmetry and periodicity) justify the use of the semi-inverse method, according to which a class of displacement/strain fields with some general properties is assumed beforehand and a solution fulfilling the boundary conditions is constructed. Here we choose the class

$$u_i(X_1, X_2, X_3) = \delta_{i3}\, y(X_3) \tag{4.44}$$

where $y(X_3)$ is an antisymmetric function. If such a solution exists, uniqueness is enforced by the fact that (4.44) excludes non-trivial rigid-body motions (see Section 4.2). Introducing a field of the above type in (2.50), noting also (4.16) and

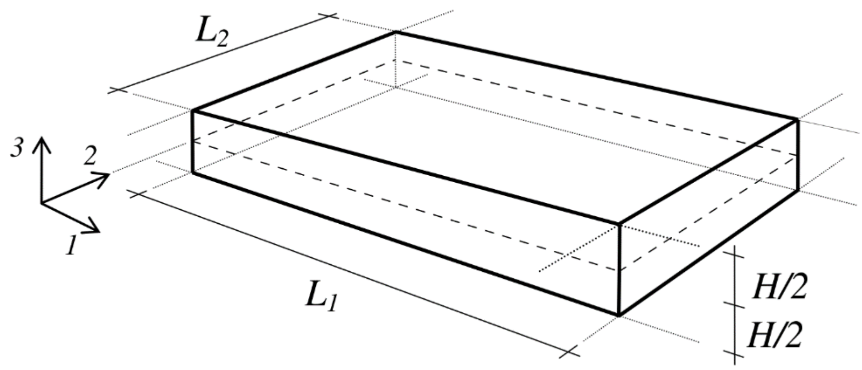


Figure 4.1: Periodic element of an infinite layer of height *H*.

using a prime to denote differentiation with respect to X_3, eventually leads to the governing equation

$$y'' - \bar{l}^2 y'''' = 0 \tag{4.45}$$

whose general solution for antisymmetric $y(X_3)$ is

$$y = C_1 \sinh\left(\frac{X_3}{\bar{l}}\right) + C_2 X_3 \tag{4.46}$$

In the above expression, $\bar{l}$ is identified as the characteristic internal length of the problem and is given by

$$\bar{l} := \sqrt{\frac{g^{(1)} + 2g^{(2)} + 4g^{(3)} + 4g^{(4)} + 4g^{(5)}}{\lambda + 2\mu}} = \sqrt{\frac{3G^{(1)} + 2G^{(2)}}{5(\lambda + 2\mu)}} \tag{4.47}$$

where the arguments of the square roots are positive due to the positive-definiteness assumptions in Section 4.2.

According to (4.50), the boundary conditions of type (2.53) and (4.43) can be expressed on the top plane as

$$y'(H/2) - \bar{l}^2 y'''(H/2) = -\frac{\bar{F}}{E_{oed}}, \qquad y'(H/2) = 0 \tag{4.48}$$

where $E_{oed} = \lambda + 2\mu$ is the oedometric modulus. The relevant integration constants are retrieved by solving the linear system resulting from the substitution of (4.46) into (4.48). The so-obtained displacement fields is

$$u_i = \delta_{i3} \frac{\bar{F}}{E_{ed}} \left(\bar{l} \, \frac{\sinh\left(\frac{X_3}{\bar{l}}\right)}{\cosh\left(\frac{H}{2\bar{l}}\right)} - X_3 \right) \tag{4.49}$$

which can now be verified to fulfill the complete set of boundary conditions, i.e. of type (2.51), (2.53) and (4.43) on both $S^{[3]}$ and $S^{[-3]}$, and of type (4.40)-(4.42) on $S^{[1]}$ $S^{[-1]}$, $S^{[2]}$ and $S^{[-2]}$.

A plot of the corresponding vertical strain $u_{3,3}$ vs. the vertical position X_3 is shown in Figure 5.3. The solution of the 2nd-grade problem differs from that of the classical, 1st-grade problem in that the former predicts the existence of localized boundary layers that decay exponentially with the distance from the boundaries.

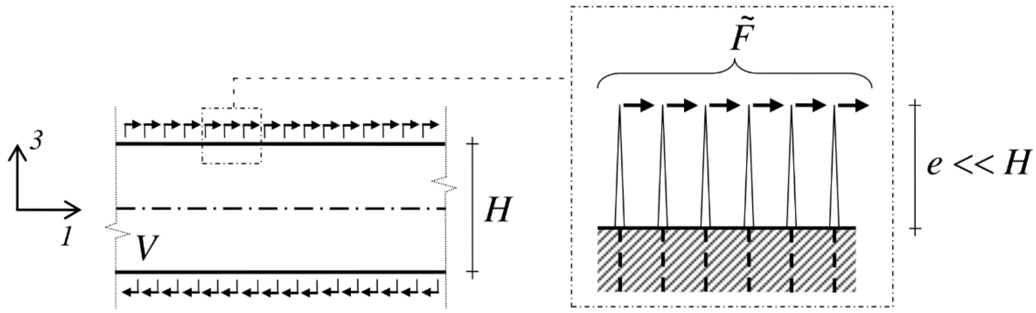


Figure 4.2: External actions for simple shear with eccentric boundaries

4.4 Simple shear with eccentric boundaries

As a second example on the infinite layer configuration in Figure 4.1, we examine the case of simple shearing, i.e. application of a uniform shear force $\tilde{F}$ at the top and the bottom plane. As shown in Figure 4.2, we assume that $\tilde{F}$ is applied through a layer of embedded stiff asperities, with characteristic length e small compared to the height of the periodic element. The shear traction $t_i = \tilde{F}\delta_{i1}$ on $S^{[3]}$ is therefore accompanied by a parasitic ortho-fiber couple $m_{ij} = e\, t_{[i}n_{j]}$. The same holds for the equilibrating shear traction $t_i = -\tilde{F}\delta_{i1}$ on $S^{[-3]}$.

Following again the semi-inverse method, we consider now a displacement fields of the type

$$u_i(X_1, X_2, X_3) = \delta_{i1}\, y(X_3) \tag{4.50}$$

where $y(X_3)$ is an antisymmetric function. This choice leads again to a governing equation in the form (4.45), with a solution of type (4.46), provided the internal length $\bar{l}$ of Section 4.3 is replaced here by

$$\tilde{l} = \sqrt{\frac{g^{(1)} + 2g^{(2)}}{\mu}} = \sqrt{\frac{\frac{1}{5}G^{(1)} + \frac{4}{5}G^{(2)} + G^{(3)} + G^{(4)} + \frac{4}{3}G^{(5)}}{3\mu}} \tag{4.51}$$

where positive arguments of the square roots are granted by the positive-definiteness assumptions for the elastic energy density.

According to (4.50), the boundary conditions of type (2.51) and (2.53) can be expressed on $S^{[3]}$ as

$$y'(H/2)-\tilde{l}^2 y'''(H/2)-\frac{\tilde{F}}{\mu}=0\,, \qquad \tilde{l}^2 y''(H/2)-\frac{e\tilde{F}}{\mu}=0 \tag{4.52}$$

The relevant integration constants are then obtained by substitution of (4.46), taken with $\tilde{l}$ instead of $\overline{l}$, into (4.52). The procedure finally leads to the displacement field

$$u_i=\delta_{i1}\frac{\tilde{F}}{\mu}\left(e\frac{\sinh\left(\dfrac{X_3}{\tilde{l}}\right)}{\sinh\left(\dfrac{H}{2\tilde{l}}\right)}+X_3\right) \tag{4.53}$$

which fulfills the complete set of boundary conditions, i.e. of type (2.51)-(2.53) on both $S^{[3]}$ and $S^{[-3]}$ and the periodic conditions on $S^{[1]}$ $S^{[-1]}$, $S^{[2]}$ and $S^{[-2]}$.

A plot of the corresponding engineering shear strain $\gamma_{13}:=u_{1,3}+u_{3,1}$ will be found in Section 5 (Figure 5.4) compared to the numerical solution treated therein. Similar to the oedometric compression example, one can observe the exponential decay for the perturbation of the classical solution about the boundary layers.

4.5 Bolted layer

The external actions considered in this last example are described in Figure 4.3. as resulting from regular arrays of bolts, anchored at small depth in the vicinity of the top and of the bottom plane of the periodic element in Figure 4.1. The bolts and properly tensioned by screwing the externally accessible nuts, causing local compression of the top and the bottom planes, in the direction of the unit normal. We model this physical situation by assuming a constant ortho-fiber stress, acting on $S^{[3]}$ and $S^{[-3]}$, computed as $f=-\hat{F}d$. Namely, $\hat{F}$ is the magnitude of the force per unit surface transferred by both the nut and the head of the bolts to the interposed layer of thickness d (small compared to H).

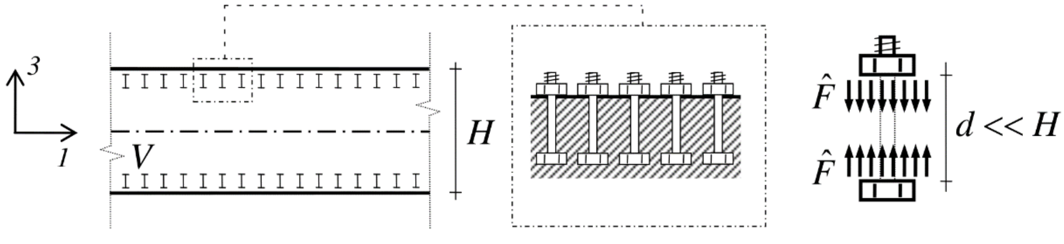


Figure 4.3: Externally applied ortho-fiber compression for a bolted layer

Given the similarities with the problem in Section 4.3, we proceed in the same manner and assume a solution of type (4.44), with $y(X_3)$ antisymmetric, leading to a governing equation in the form (4.45) with $\bar{l}$ as in (4.47). Expressing the boundary conditions (2.51) and (2.52) on $S^{[3]}$ accordingly, i.e. as

$$y'\left(\frac{H}{2\bar{l}}\right)-\bar{l}^{2}y'''\left(\frac{H}{2\bar{l}}\right)=0\,,\quad \bar{l}^{2}y''\left(\frac{H}{2}\right)=\frac{-\hat{F}d}{\lambda+2\mu} \tag{4.54}$$

the relevant integration constants are then identified after substitution of (4.54) in (4.46). The procedure leads to the displacement field

$$u_i=\delta_{i3}\,\frac{-\hat{F}d}{\lambda+2\mu}\,\frac{\sinh\left(\dfrac{X_3}{\bar{l}}\right)}{\sinh\left(\dfrac{H}{2\bar{l}}\right)} \tag{4.55}$$

which is found in agreement with the whole set of boundary conditions on $S^{[1]}$, $S^{[2]}$, $S^{[3]}$, $S^{[-1]}$, $S^{[-2]}$ and $S^{[-3]}$.

As for the two previous cases, a plot of the analytical solution can be found in Section 5 (Figure 5.5).

5 Outline of the finite element formulation

5.1 The weak form

We state the weak form of the boundary value problem of isotropic, linear 2nd-grade elasticity using the principle of virtual work, as is customarily done when using finite elements. First we rewrite (4.16) and (4.17) as

$$\tau_{ij}=\alpha_{ijkl}u_{k,l}\,,\qquad \xi_{ijk}=\gamma_{ijklmn}u_{l,mn} \tag{5.1}$$

Respectively. Combining the above with (2.16) and (2.48) yields

$$\begin{aligned}&\int_V\left(\delta u_{i,j}\,\alpha_{ijkl}\,u_{k,l}+\delta u_{i,jk}\,\gamma_{ijklmn}\,u_{l,mn}\right)dV\\&\quad=\int_V F_i\delta u_i\,dV+\int_S\left(t_i\delta u_i+f\,\delta\varsigma+m_{ij}\delta\omega_{ij}\right)dS+\int_E s_i\delta u_i\,dE\end{aligned} \tag{5.2}$$

Equation (5.2) can be treated numerically using a number of different strategies, depending on which quantities one chooses to discretize. Various schemes relevant to 2nd-grade elastic bodies can be found in the literature, with representative examples being the mixed formulation presented by Amanatidou and Aravas [41], the meshless approach used by Askes and Aifantis [42] and the penalty approach of Zervos [43]. Here we use the displacement formulation, i.e. we discretize the displacement field only, as was successfully done with gradient elasticity in [44,45] and gradient elastoplasticity in [46,47].

For the remainder of this section we adopt the standard matrix notation of the finite element method. We start by discretizing the displacement field $\mathbf{u}$ as

$$\mathbf{u} = \mathbf{N} \cdot \bar{\mathbf{u}} \tag{5.3}$$

where $\mathbf{N}$ is the matrix of shape functions and $\bar{\mathbf{u}}$ the vector of degrees of freedom. The components of the strain and the second derivative of the displacement can be arranged in vector form and written as

$$\boldsymbol{\varepsilon} = \mathbf{B_1} \cdot \bar{\mathbf{u}}\,, \qquad \boldsymbol{\kappa} = \mathbf{B}_2 \cdot \bar{\mathbf{u}} \tag{5.4}$$

where matrices $\mathbf{B_1}$ and $\mathbf{B_2}$ contain first and second derivatives of the shape functions respectively. Furthermore, the constitutive equations (5.1) are written as

$$\boldsymbol{\tau} = \boldsymbol{\alpha} \cdot \boldsymbol{\varepsilon}\,, \qquad \boldsymbol{\xi} = \boldsymbol{\gamma} \cdot \boldsymbol{\kappa} \tag{5.5}$$

where $\boldsymbol{\alpha}$ and $\boldsymbol{\gamma}$ are the α_{ijkl} and γ_{ijklmn} tensors in matrix form.

Substituting (5.3)-(5.5) into (5.2) and employing the arbitrariness of the virtual displacement field, the weak form becomes

$$\begin{aligned} &\int_V \left(\mathbf{B_1^T} \boldsymbol{\alpha} \mathbf{B_1} + \mathbf{B_2^T} \boldsymbol{\gamma} \mathbf{B_2} \right) dV \cdot \bar{\mathbf{u}} \\ &\quad = \int_V \mathbf{N^T F} dV + \int_S \mathbf{N^T t}\, dS + \int_S \left(\nabla_n \mathbf{N^T} \right) \mathbf{n}\, f\, dS + \int_S \mathbf{B_\omega^T m} dS + \int_E \mathbf{N^T s}\, dE \end{aligned} \tag{5.6}$$

where ∇_n is the matrix form of the normal derivative operator and the matrix $\mathbf{B_\omega}$ contains appropriate combinations of the first derivatives of the shape functions and the components of the unit-normal vector $\mathbf{n}$. The volume integral on the left hand side of (5.6) is identified as the stiffness matrix $\mathbf{K}$ and the right hand side as the load vector $\mathbf{f}$. The integrals in (5.6) can be calculated numerically using Gauss-Legendre quadrature schemes of appropriate order, and the resulting linear system solved for the degrees of freedom. Convergence can be ascertained by calculating the residual out-of-balance force $\mathbf{q}$:

$$\mathbf{q} = \int_{\mathbf{V}} \left(\mathbf{B}_1^{\mathbf{T}} \boldsymbol{\tau} + \mathbf{B}_2^{\mathbf{T}} \boldsymbol{\xi} \right) \mathbf{dV} - \mathbf{f} \tag{5.7}$$

5.2 Interpolation and continuity requirements

Using the displacement formulation leads to two constraints that an interpolation scheme must fulfill to be admissible: first, the shape functions should be at least quadratic, to guarantee non-vanishing second derivatives of displacement inside each finite element; second, due to the presence of second derivatives in the weak form given in (5.6), the first derivatives of displacements (i.e., the strains) should be continuous, i.e. C^1 continuity is required instead of C^0 that is sufficient for classical elasticity.

For one-dimensional problems, both constraints are fulfilled by the two-node element with four degrees of freedom (displacement and its derivative at each node) of the Hermite family.

For two-dimensional problems one can draw on the elements created in the 1960s for bending of thin plates. However, most of these are either non-conforming, i.e. continuity of first derivatives is limited at the nodes, or are C^1 only when undistorted and aligned with the global Cartesian reference frame [48], or require a structured mesh due to the special pre-processing necessary [44,49]. Two proper C^1 elements are the quintic triangles with 21 and 18 degrees of freedom respectively [50,51]. The first one is inconvenient to use, as its shape functions do not exist in analytical form, and also has mid-side nodes requiring special treatment [46]. Eliminating the degrees of freedom of the mid-side nodes leads to the second triangle [51], shown in Figure 5.1. Other C^1 triangles are possible to construct using the ideas and procedures outlined in [52,53].

Finally, to the authors' best knowledge, the only existing three-dimensional C^1 element is the brick presented in [54].

5.3 Numerical examples

As an example, we solve numerically the boundary value problems presented in Sections 4.3 to 4.5 and show that the numerical results converge to the closed-

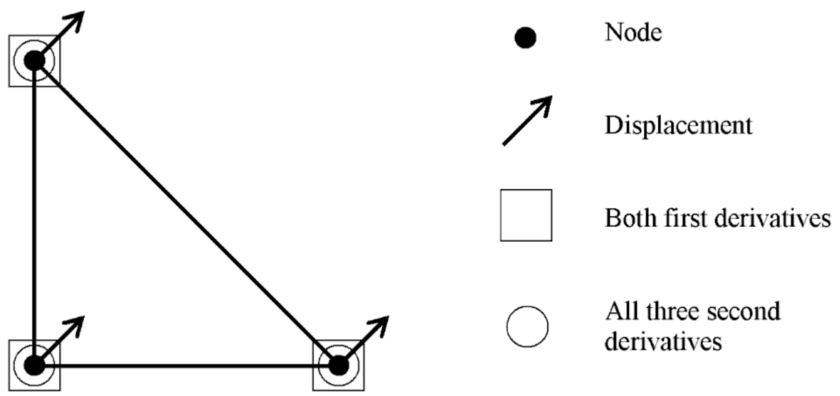


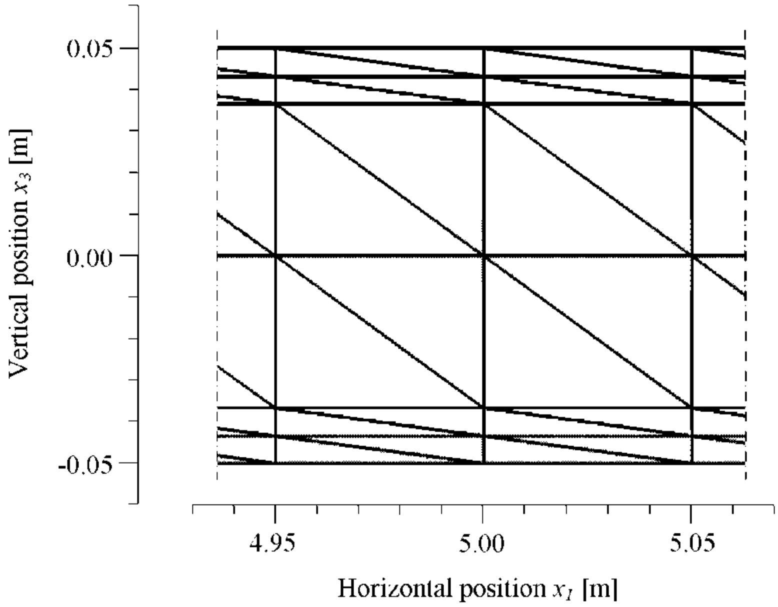
Figure 5.1: A C^1 triangle with 18 degrees of freedom.

form solution. We assume plane strain and use the C^1 triangle with 18 degrees of freedom discussed above.

In all cases, element stiffness is calculated numerically using Gauss-Legendre quadrature. Exact evaluation of the integrals requires an $O(h^9)$-accurate scheme, such as the one presented in [46]. However, $O(h^{2(P-M)+1})$-accuracy is sufficient to retain convergence [55], where P the degree of the complete polynomial used in the interpolation (here $P=5$), and M the highest order of the derivatives present in the problem (here $M=2$). Therefore an $O(h^7)$-accurate scheme suffices; here we use the well-known 13-point scheme [56].

Oedometric compression with interlocked boundaries

A numerical solution of the oedometric compression problem, presented in Section 4.3, is given below. To demonstrate the accuracy of the method and the element used, the very coarse mesh of Figure 5.2 is employed. The specimen is assumed to be $10\,cm$ high. To prevent the lateral boundaries of the model from influencing the solution, the specimen is assumed to be 10 m wide (i.e. an aspect ratio of 1:100). This extreme value was chosen arbitrarily during validation, and a lower aspect ratio would most probably suffice for practical purposes. The elastic properties are taken equal to $\lambda = 7000\,\text{kPa}$, $\mu = 3000\,\text{kPa}$, $g^{(1)} = g^{(3)} = 0$, $g^{(2)} = \frac{1}{2} l^2 \mu$, $g^{(4)} = g^{(5)} = \frac{1}{4} l^2 \lambda$ where $l = 0.5\,\text{cm}$ is an assumed internal length scale. The compressive stress applied at the top of the specimen is $40\,\text{kPa}$. The vertical displacement at the bottom is constrained and so is the horizontal displacement at the sides. Finally, we prescribe zero ortho-fiber stretch along the top and bottom boundaries by constraining the degrees of freedom corresponding



to $u_{3,3}$ and $u_{3,13}$ of the respective nodes.

Numerical results for the vertical strain $u_{3,3}$ along the vertical axis are compared with the closed-form solution, derived from (4.49), in Figure 5.3. They match it even for the very coarse mesh used, and capture the steep strain gradient close to the boundaries even though the boundary layer traverses only two to three elements. The high quality of the numerical results is due to the quintic interpolation used; also due to displacement derivatives being calculated directly at the nodes as degrees of freedom, rather than extrapolated from values calculated at the Gauss points as in classical elasticity.

Figure 5.2: Oedometric compression with interlocked boundaries: partial view of the finite element mesh.

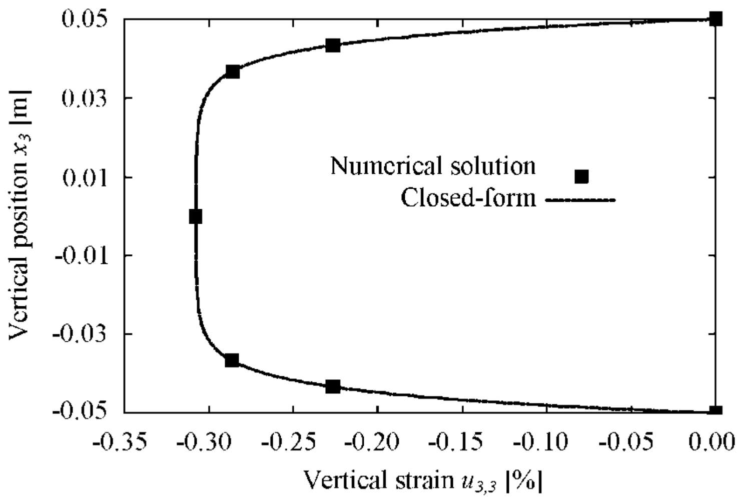


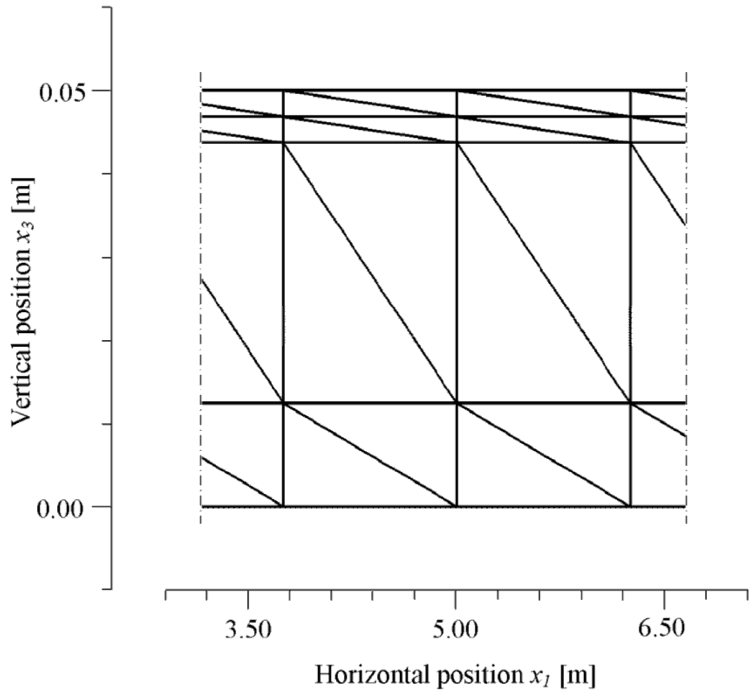
Figure 5.3: Oedometric compression with interlocked boundaries: predicted vertical strain profile vs. the closed-form solution.

Simple shear with eccentric boundaries

We present a numerical solution of the shear layer problem of Section 4.4, using the same numerical approach and elastic material parameters as in the example above. We assume the external length e to be equal to the internal length $\tilde{l}$, i.e. $e = \tilde{l} = 0.5\ \mathrm{cm}$.

As the solution is antisymmetric with respect to the horizontal axis passing through the middle of the specimen, it suffices to model the top half of the geometry of the layer. A portion of the mesh employed is shown in Figure 5.4. The specimen is again assumed to be $10\,\mathrm{cm}$ high with aspect ratio of 1:100. Numerical results are reported along the vertical symmetry axis. The surface traction applied at the top of the specimen is $t_1 = 40\,\mathrm{kPa}$ and the boundary couple is $m_{31} = 0.2\,\mathrm{kPa\,m}$. The bottom antisymmetry-boundary is constrained from moving vertically, the lateral sides of the model are free of constraints and loads, while ortho-fiber tension is zero everywhere.

Numerical results for the engineering shear strain γ_{13} are presented in Figure 5.5 and are compared with the closed-form solution, derived from (4.53).



They are again found to match it even for the very coarse mesh used, and capture accurately the steep strain gradient inside the shear boundary layer.

Bolted layer

Finally, the bolted layer problem is solved using the same numerical approach and elastic material parameters as in the previous examples. Due to symmetry it suffices to model the top half of the specimen, which is assumed to have the same dimensions and mesh as for oedometric compression.

The ortho-fiber tension applied by the bolts at the top of the specimen is taken as $f = 0.2\,\text{kPa m}$, corresponding to a compression of $40\,\text{kPa}$ imposed to a micro-layer of depth $d = l = 0.5\,\text{cm}$. The symmetry boundary at the bottom is constrained from moving vertically, while no surface tractions or couples act on any boundary.

Numerical results for the vertical strain $u_{3,3}$ along the vertical axis are presented in Figure 5.6 and are compared with the closed-form solution, derived from (4.55). Once more they match it and capture the boundary layer equally well with the other two solutions above.

Figure 5.4: Simple shear with eccentric boundaries: partial view of the finite element mesh.

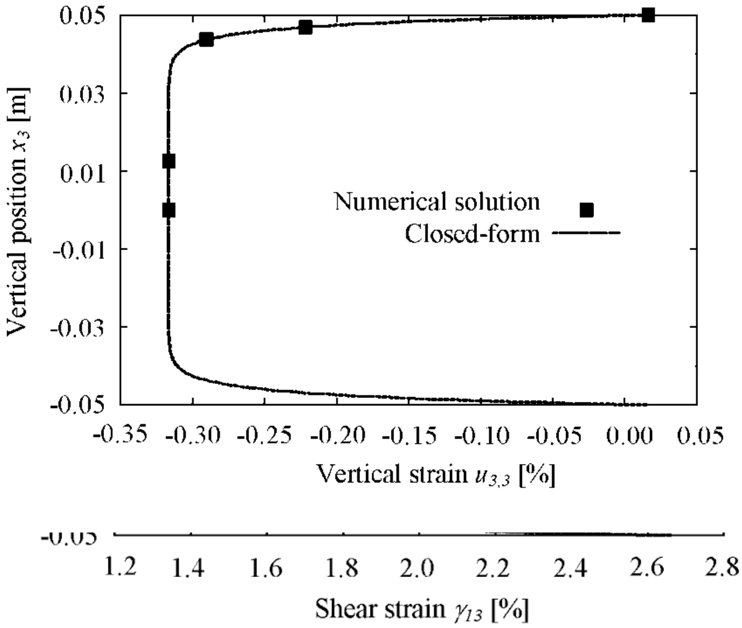


Figure 5.5: Simple shear with eccentric boundaries: predicted shear strain profile vs. the closed-form solution.

6 Conclusions

We presented a linearized theory for elastic materials whose stored energy depends on the first two gradients of the displacement. A clear mechanical interpretation of the boundary conditions was provided, based on the concepts of stretch and rotation of ortho-fibers, i.e. (infinitesimal) material fibers orthogonal to the boundary of the solid. Ortho-fiber stretch is conjugate to ortho-fiber tension, while ortho-fiber rotation is conjugate to ortho-fiber couples, where nevertheless rotation of a fiber about its own axis is inadmissible, and so are corresponding couples. This picture of the boundary conditions is completed by lineal traction allowed exclusively on the edges formed by the boundary of the body. These force-like quantities are subjected to balance laws that were deduced imposing objectivity of the potential of the external loads.

Furthermore, a mechanical interpretation was provided for the internal fields of traction-like quantities, i.e. stress fields in the sense of Cauchy, inherent in theories of this type (cf. [6-8]). In particular, these traction-like fields can be seen as preserving the continuity of the displacement and its first derivative across notional surfaces internal to the elastic body. A stress vector field holding the same physical meaning as the Cauchy stress vector field was identified for 2nd-grade materials. However, this stress vector field is remarkably different to Cauchy's, as the force density is a "cubic", not "linear", function of the unit normal; the force density depends on the curvature of the notional surface; the stress-vector field is in particular a generalized function in the sense of the theory of distributions, as lineal force-densities on the edges of the internal surface contribute, along with the classical surface densities, to the definition of the internal force. Lineal force densities can be seen as degenerate curvature-dependent surface densities at the limit where curvature tends to zero. As a result of the above, a stress tensor in the classical sense of Cauchy, i.e. a tensor whose projection on the unit normal equals the internal traction vector, *cannot be defined for 2nd-grade materials*. Additional stress-type fields in the sense of Cauchy were identified: an ortho-fiber-couple stress field and an ortho-fiber-tension stress fields. The ortho-fiber-couple stress field cannot be identified with the classical (Cosserat) couple-stress because no couples are allowed that work on rotations about the unit normal, and because the dependence on the unit normal is "cubic". This means that a corresponding couple-stress tensor cannot be postulated or deduced (cf., Toupin [1,2]). The linear- and angular momentum balance laws for these fields were identified as conditions of objectivity and found to be consistent with those exhibited by Fried and Gurtin [28]. The ortho-fiber-tension field is self-equilibrating in that it takes no part in the linear and angular momentum balance laws.

A finite element numerical discretization of linear 2nd-grade elasticity was presented, where the choice to discretize the displacement field only led to the need for C^1-continuous interpolation; appropriate elements were discussed.

Finally, closed-form and numerical solutions to three benchmark boundary value problems were produced and compared. All solutions lead to the identification of boundary layers of finite thickness, and are perturbations of the corresponding standard (1st-grade) solutions. In each problem, an internal length was identified on which the thickness of the boundary layer depends. The numerical results were shown to converge rapidly; accurate solutions were produced even for very coarse meshes.

Acknowledgements

This research was initiated by the late Ioannis Vardoulakis, Professor of Mechanics at N.T.U. Athens. It was carried out in close collaboration with him, and he had approved an earlier, longer version of the manuscript. Although the work was substantially complete at the time of his tragic death in 2009, we did not pursue it further after the event. We have since shortened the manuscript, both for clarity and to fit the length normally expected of a research journal paper, and updated the Introduction and References to include relevant work published in the meantime. However, the paper's substance remains unaltered and Vardoulakis's contribution was of a scale that would otherwise warrant co-authorship. In lieu of this, we dedicate the paper to his memory.

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7 Appendices

A. Infinitesimal change of the observer

We denote by X_i^*, χ_i^* and u_i^* the generic position, deformation and displacement according to a second “starred” observer (cf. X_i, χ_i and u_i for the first, standard observer, resp.). The measured deformation differs as

$$\chi_i^* = Q_{ij}^T \left(\chi_j - X_{0i} \right) \tag{A.1}$$

where x_i is the position of the second observer and Q_{ij} is the rotation of its frame of reference, at current time, as reported by the first observer. With no loss of generality, we assume that the two reference systems coincide at the time when the body occupies the reference configuration, i.e. $X_i^* = X_i$ for the same material point. The measured displacements are then related by

$$u_i^* = Q_{ij}^T u_j + \left(Q_{ij}^T - \delta_{ij} \right) X_j - Q_{ij}^T x_j \tag{A.2}$$

which also implies

$$u^*_{i,j} = Q^T_{ik} u_{k,j} + \left(Q^T_{ij} - \delta_{ij}\right), \qquad u^*_{i,jk} = Q^T_{il} u_{l,jk} \tag{A.3}$$

We particularize (A.2) and (A.3) to the case when the change of the observer is, in the following sense, “infinitesimal”. We express Q_{ij} in terms of the axis w_k, $\|w_k\| = 1$, and the angle θ of the relevant rotation and compute

$$Q_{ij} = \delta_{ij} + \theta w_k e_{kji} + o(\theta) \tag{A.4}$$

for $\theta \to 0$. Using (A.4) in (A.2) and (A.3) we obtain

$$u^*_i - u_i \approx W_{ij} X_j + a_i, \qquad u^*_{i,j} - u_{i,j} \approx W_{ij}, \qquad u^*_{i,jk} - u_{i,jk} \approx 0 \tag{A.5}$$

as the relevant approximations for $\theta << 1$, with

$$W_{ij} := -\theta w_k e_{kji}, \qquad a_i := -(\delta_{ij} + W_{ij})^T x_{xj} = -x_i + W_{ij} x_j \tag{A.6}$$

Assuming additionally that a_i is of the same order as u_i, Equations (A.5) can be received in the infinitesimal theory as equalities representative of a change of the observer.

B. Edge tensor

Figure 2.2 can be further commented by means of a simple computation that provides a simple geometrical description of the edge tensor $[\![m_i n_j]\!]$. In the same figure the unit vector m_i is orthogonal to unit-normal vector n_i and to the unit-tangent vector s_i for the edge *E*. We write in particular $m_i = e_{ijk}\, s_j\, n_k$ where s_i is chosen so that m_i is outward-oriented with respect to the relevant half-plane. As concerns the opposite half-plane, holds $m'_i = -e_{ijk}\, s_j\, n'_k$ with s_i as above and n'_i ,and m'_i both outward oriented.

We call φ the angle that characterizes a rotation about s_i transforming n_i into n'_i and compute

$$\begin{aligned} \sin(\varphi)\, m_i &= (s_n e_{nml} n_m n'_l)(e_{ijk} s_j n_k) = (s_j e_{jml} n_m n'_l)(e_{ijk} s_j n_k) \\ &= (\delta_{mk}\delta_{li} - \delta_{mi}\delta_{lk}) n_m n'_l n_k = (\delta_{il} - n_i n_l) n'_l \end{aligned} \tag{B.1}$$

where the tensor $(\delta_{ij} - n_i n_j)$ projects n'_i onto the plane orthogonal to n_i. Analogously, one obtains $\sin(\varphi)\, m'_i = (\delta_{ij} - n'_i n'_j) n_j$ and compute

$$
\begin{aligned}
\llbracket m_i n_j \rrbracket = m_i n_j + m'_i n'_j &= \frac{(\delta_{ik} - n_i n_k) n'_k n_j + (\delta_{ik} - n'_i n'_k) n_k n'_j}{\sin(\varphi)} \\
&= \frac{n'_i n_j - \left(n'_k n_k\right) n_i n_j + n_i n'_j - \left(n'_k n_k\right) n'_i n'_j}{\sin(\varphi)} \\
&= \frac{(n'_i n_j + n_i n'_j) - \cos(\varphi)(n_i n_j + n'_i n'_j)}{\sin(\varphi)}
\end{aligned}
\tag{B.2}
$$

It follows that $\llbracket m_i n_j \rrbracket$ is symmetric and vanishes in the limit for $\varphi \to 0$, as expected.