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Which Kind of External Loading Second Gradient Materials Can Sustain?

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Abstract. In this communication, materials are considered whose deformation energy depends on both first and second gradient of placement map. When deriving the equilibrium equations by a variational approach, through integration by parts and the reiterated application of the divergence theorem, the class of external loading which are admissible for second gradient materials can be easily identified. Discrepancies with respect to Cauchy's first gradient continua are highlighted, with special reference to the double forces acting over the boundary faces and the edge loading.

INTRODUCTION

Cauchy's first gradient theory [1] represented for more than one century the dominant paradigm of continuum mechanics [2]. In the academic community, the main assumption of Cauchy's theory, namely the dependence of traction vector on the point and on the local normal vector, was exhibited along several decades as the unique valid choice to model every material regardless of the length scale, concealing its true nature of constitutive hypothesis, see e.g. [3, 4]. However, in some pioneering works of Gabrio Piola (1794-1850), see e.g. [5], the equilibrium problem for a continuous medium was investigated with reference to general expressions of stored energy density W , depending not only on local deformation gradient $\mathbf{F} = \partial\chi/\partial\mathbf{X}$, but also on its spatial derivatives of higher order $\nabla^{(k)}\mathbf{F}$, with $k \geq 1$. Symbol $\mathbf{x} = \chi(\mathbf{X})$ denotes as usual the placement map defined in the Lagrangian (material, referential) domain $\Omega_\star \subset \mathcal{R}^3$ and valued in the Eulerian (spatial, current) domain $\Omega \subset \mathcal{R}^3$. In this communication focus is posed on second gradient materials, with Lagrangian energy densities in the form $W(\mathbf{F}, \nabla\mathbf{F})$. Of course, such densities must be nonnegative and objective. Explicit dependence of the energy expression on right Cauchy-Green tensor \mathbf{C} (or on its inverse) guarantees frame invariance, but makes prohibitive the analytical developments through integration by parts. Therefore in the results which follow partial derivatives of energy must be intended as those of the composite function $W(\mathbf{C}(\mathbf{F}))$. Recourse was made to two diverse orthonormal bases for the Lagrangian and the Eulerian domain, implying unit metric tensors \mathbf{G} and \mathbf{g} and Christoffel symbols identically vanishing, respectively. As far as possible, Lagrangian and Eulerian variables and relevant indices were denoted by uppercase and lowercase symbols, respectively.

APPROACH À LA PIOLA

Before than Menabrea and Castigliano, Gabrio Piola was hugely impressed by Lagrange's mechanics for discrete systems and understood that also the equilibrium configuration of a continuum body can be derived by minimizing the total energy functional over a suitable functional set K including essential boundary conditions, namely

$$\hat{\chi} = \arg \min_K \left\{ \mathcal{E}^{\text{TOT}}(\chi) = \int_{\Omega_\star} W(\mathbf{F}, \nabla \mathbf{F}) d\Omega_\star - \mathcal{E}^{\text{EXT}}(X, \chi) \right\} \quad (1)$$

The field which makes minimum the above functional can be sought by prescribing the first variation to vanish. As for the inner work contribution, one has (see [6, 7])

$$\delta \int_{\Omega_\star} W(\mathbf{F}, \nabla \mathbf{F}) d\Omega_\star = \int_{\Omega_\star} \left(\frac{\partial W}{\partial \mathbf{F}} : \delta \mathbf{F} + \frac{\partial W}{\partial \nabla \mathbf{F}} : \delta (\nabla \mathbf{F}) \right) d\Omega_\star = \quad (2)$$

$$= \int_{\Omega_\star} \frac{\partial W}{\partial F_A^i} \delta F_A^i d\Omega_\star + \int_{\Omega_\star} \frac{\partial W}{\partial F_{AB}^i} \delta F_{AB}^i d\Omega_\star = \int_{\Omega_\star} P_{1i}^A \delta F_A^i d\Omega_\star + \int_{\Omega_\star} P_{2i}^{AB} \delta F_{AB}^i d\Omega_\star; \quad (3)$$

where symbols $:$ and \cdot denote the usual double dot product and the triple contraction, respectively, and

$$\delta F_A^i = \frac{\partial}{\partial X^A} \delta \chi^i(\mathbf{X}); \quad \delta F_{AB}^i = \frac{\partial^2}{\partial X^A \partial X^B} \delta \chi^i(\mathbf{X}); \quad (4)$$

It is worth noting that the first variation commutes with both the partial derivative and the integral operator. In Eq. (3) $P_{1i}^A(\mathbf{X})$ indicates a second rank stress-like tensor, referred to as first Piola-Kirchhoff stress, with an Eulerian and a Lagrangian index, whilst $P_{2i}^{AB}(\mathbf{X})$ represents a third rank tensor, two times contravariant (Lagrangian indices) and one time covariant (Eulerian). We will refer to it as Piola hyper-stress or double stress, see e.g. [8, 9]. Subscripts 1 and 2 remark that relevant tensors were provided by derivative wrt the first and the second gradient, respectively. It is worth emphasizing that the above equation equals the inner contribution to the virtual work equation, which by itself is more general and does not requires a constitutive relationship to be previously defined as above.

For the engineering structures of common interest, the outer boundary of the bulk material (in the Lagrangian configuration denoted by Ω_\star) is constituted of the union of disjoint regular *faces*, separated by piecewise regular curves, referred to as *edges*, which represent discontinuity loci for their normal vectors. In turn, discontinuity points for the tangent vector along the *edges*, are referred to as *wedges*. Any edge is shared by two contiguous faces as a part of their border, whilst at least three faces concur to each *wedge*. For the additivity of Lebesgue integral, surface integral over the volume boundary can be split into the sum of addends extended to a unique face, and the same occurs for the line integrals along the face border.

Through integration by parts and the reiterated applications of the divergence theorem, extended to curved surfaces with border, after several manipulations facing important difficulties we could express the above virtual work equation as a sum of volume, surface and edge contributions. Test functions are represented not only by variation of placement map $\delta \chi$, but also by their normal derivative $\partial \delta \chi / \partial N$ with respect to the boundary face. Developing the inner work contribution over the boundary face, the contact pressure for such class of materials turned out to be the sum of expressions with a complex dependence on normal components (e.g. see [10]), including, besides the linear term shared with Cauchy's theory, an algebraic polynomial of third degree (through the triple product of normal components), a differential expression (through the gradient of the normal vector), and a combination of them (through the product of two normal components with the derivative of the normal vector). In particular, the derivative of normal vector coincides with the local mean curvature of the face, namely the trace of the Weingarten shape operator (see the next section). For the sake of brevity, herein only the virtual work contributions including normal derivative of virtual displacement over the boundary face Σ_\star and that concerning the boundary edges L_\star are reported. For the former, one has (see [11])

$$\int_{\Sigma_\star} \frac{\partial W}{\partial F_{AB}^i} N_B N_A \left[N^C \frac{\partial}{\partial X^C} \delta \chi^i \right] d\Sigma_\star = \int_{\Sigma_\star} \frac{\partial W}{\partial F_{AB}^i} N_B N_A \left[\frac{\partial}{\partial N} \delta \chi^i \right] d\Sigma_\star \quad (5)$$

In the above surface integral we can recognize the hyperstress tensor contracted with two components of the normal vector (as for the Lagrangian indices). Such Eulerian vector (index i being free) has been referred to in the literature

as inner double force (in Italian *biforza*). Dimensionally it is an energy per unit surface, equivalently a force per unit length, or also a pressure multiplied by a length (which better suggests the analogy with a dipole). For the latter, one has

$$\int_{L_\star} \frac{\partial W}{\partial F_{CD}^i} N_D B_C \delta \chi^i dL_\star \quad (6)$$

where symbol B_C denotes the components of the unit outward normal to the face border, which is tangent also to the face. We can recognize the same hyperstress tensor but this time its Lagrangian valences are contracted with two different unit vectors: due to the Schwarz' theorem, only the symmetric part of the product $N_{(D} B_{C)}$ can play a role. The outward normal to the boundary face can be obtained through cross product as $\mathbf{N} = \mathbf{B} \times \mathbf{T}$.

EXTERNAL WORK AND STRONG FORM

Since the inner and the external virtual works must balance for any test function, we can specify consistently the contributions of external loading for a second gradient material, namely

$$\delta \mathcal{E}^{\text{EXT}} = \int_{\Omega_\star} \mathcal{F}_{\Omega_\star i}^{\text{ext}} \delta \chi^i d\Omega_\star + \int_{\Sigma_\star} \mathcal{F}_{\Sigma_\star i}^{\text{ext}} \delta \chi^i d\Sigma_\star + \int_{\Sigma_\star} \mathcal{F}_{\perp \Sigma_\star i}^{\text{ext}} \frac{\partial \delta \chi^i}{\partial N} d\Sigma_\star + \int_{L_\star} \mathcal{F}_{L_\star i}^{\text{ext}} \delta \chi^i dL_\star; \quad (7)$$

Above symbols possess the following meaning: $\mathcal{F}_{\Omega_\star i}^{\text{ext}}(\mathbf{X})$, $\mathcal{F}_{\Sigma_\star i}^{\text{ext}}(\mathbf{X})$ and $\mathcal{F}_{L_\star i}^{\text{ext}}(\mathbf{X})$ denote Eulerian vectors defined in the Lagrangian domain, over its boundary face and along its edges, dimensionally equal to force densities per unit volume, per unit surface and per unit length, respectively; $\mathcal{F}_{\perp \Sigma_\star i}^{\text{ext}}(\mathbf{X})$ indicates an Eulerian vector defined over the Lagrangian boundary faces, referred to as external double force, dimensionally equal to a force per unit length, work conjugate of vector $\partial \delta \chi^i / \partial N$.

According to the fundamental lemma of the calculus of variations, the strong form of Lagrangian equilibrium equations can be derived by selecting test functions with their compact support localized within the open part of the domains (i.e. deprived of the borders) to which are restricted for the diverse integrals. In particular for $\delta \chi$ the compact support was localized in turn within the volume interior, over the boundary faces (excluding their border edges) and along the edges (excluding wedges, if any), whilst for $\partial \delta \chi / \partial N$ it was localized within the boundary faces, excluding their border. For the sake of simplicity, with a slight abuse of notation the difference (in the sense of set theory) between such domains and their differential border was herein denoted by symbol \mathring{D} . Hence, one can write

$$-\frac{\partial}{\partial X^A} (P_{1i}^A) + \frac{\partial}{\partial X^B} \frac{\partial}{\partial X^A} (P_{2i}^{AB}) - \mathcal{F}_{\Omega_\star i}^{\text{ext}}(\mathbf{X}) = 0 \quad \mathbf{X} \in \mathring{\Omega}_\star; \quad (8)$$

$$P_{1i}^A N_A - \frac{\partial P_{2i}^{AB}}{\partial X_B} N_A - \frac{\partial P_{2i}^{AB}}{\partial X_A} N_B - P_{2i}^{AB} \frac{\partial N_A}{\partial X^B} + \frac{\partial P_{2i}^{AB}}{\partial X_C} N_B N^C N_A + P_{2i}^{AB} N_B N_A \frac{\partial N^D}{\partial X^D} - \mathcal{F}_{\Sigma_\star i}^{\text{ext}}(\mathbf{X}) = 0 \quad \mathbf{X} \in \mathring{\Sigma}_\star; \quad (9)$$

$$P_{2i}^{AB} N_A N_B - \mathcal{F}_{\perp \Sigma_\star i}^{\text{ext}}(\mathbf{X}) = 0 \quad \mathbf{X} \in \mathring{\Sigma}_\star; \quad (10)$$

$$P_{2i}^{AB} ([B^+]_A [N^+]_B + [B^-]_A [N^-]_B) - \mathcal{F}_{L_\star i}^{\text{ext}}(\mathbf{X}) = 0 \quad \mathbf{X} \in \mathring{L}_\star; \quad (11)$$

In the last equation, symbol $[\bullet^+]$ (and $[\bullet^-]$) denotes that vector \bullet belongs to the face at the left of the edge (resp. at the right), with respect to one orientation of the tangent selected by the user. In fact, the line integral relevant to the support of each edge gives rise to two possible contributions: vector quantities B_A and N_B are discontinuous across the edge and depend on which of the contiguous faces one is considering, implying two diverse orientations for the border edge. If two contiguous faces are parallel, i.e. they possess the same outward normal, the edge normal vectors are opposite equal and the expression of Eq. (11) vanishes. Actually, in that scenario the edge as discontinuity locus does not exist, and the two contiguous faces represent a unique regular surface. The second equation Eq. (9) is often expressed through the tangential projectors and the surface divergence, namely

$$\left(P_{1i}^A - \frac{\partial P_{2i}^{AB}}{\partial X_B} \right) N_A - \frac{\partial}{\partial X^C} (P_{2i}^{AB} N_A [M_{\parallel B}^E]) [M_{\parallel E}^C] - \mathcal{F}_{\Sigma_\star i}^{\text{ext}}(\mathbf{X}) = 0 \quad \mathbf{X} \in \mathring{\Sigma}_\star; \quad (12)$$

The first two equations Eqs. (8) and (9) can assume a slightly shorter form by defining an effective Lagrangian stress

$$P_i^{\text{eff}A} = P_{1i}^A - \frac{\partial P_{2i}^{AB}}{\partial X_B} \quad (13)$$

CLOSING REMARKS AND FUTURE PROSPECTS

The variational approach utilized in this study for second gradient materials has allowed us to derive naturally non-standard equilibrium equations over the boundary face and along the border edges. Moreover, it has led to define a third rank hyperstress tensor, needed to govern the inner virtual work, and has provided a complex expression for the contact pressures, involving addends with multiple product of normal components, their gradient and a combination of both. In this framework, the class of admissible loading implied by Cauchy's first order theory and consisting of volume and surface densities, dual of virtual placement map, was enriched up to comprehend double forces over the boundary faces, work conjugate to the normal derivative of virtual placement map, and edge loading along the face border, work conjugate to the virtual placement map. Any other kind of loading turns out to be not consistent with the present formulation and must be rejected. Topics still under development concern the transport of external loading from the Lagrangian to the Eulerian configuration (and vice versa), a priori conditions on the energy density under which loading contributions satisfy prescribed requirements, mixed numerical-experimental methodologies capable of distinguishing kinematic fields at different scales, see e.g. [12, 13, 14].

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