An effective strategy to transform second-gradient equilibrium equations from the Eulerian to the Lagrangian configuration

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Abstract. In this communication the problem of transforming the equilibrium equations from the Eulerian to the Lagrangian form is discussed with reference to materials governed by second-gradient energy densities. In particular, novel theoretical achievements are outlined, which represent intermediate steps to attain the purpose: the transformation of edge vectors and of complementary orthogonal projectors over the boundary surface; a novel formula based on the divergence theorem for curved surfaces with boundary, relating material and spatial expressions; a remarkable relationship between Lagrangian and Eulerian (hyper-)stress tensors of different orders.

Introduction

Higher gradient materials constitute a wide class of materials for which the stored energy density depends not only on the deformation gradient but also on its higher order derivatives. In the last decade, such kind of mathematical models have attracted an increasing number of researchers in continuum and computational mechanics. This circumstance is mainly due to the fact that higher gradient modelling is capable of describing complex phenomena which cannot be predicted by the conventional Cauchy approach. Among others, we can mention size effects taking into account characteristic length scales, boundary layers, corner and surface effects, which are crucial in all those scenarios in which the separation of scales is not sharp. Moreover, higher gradient materials admit "exotic" loading which cannot be sustained by a Cauchy medium, such as double forces, expending work under the normal derivative of the virtual placement, edge or wedge loading (see e.g. [1-2]): these generalized forces represent versatile tools when investigating surface tension in fluids or other interface issues, wave propagation in crystals, fiber nets interacting with the matrix in composites and more in general the mechanical behaviour of the so called metamaterials.

In this study a strategy is proposed, to transport the governing equations for second-gradient materials from the Eulerian to the Lagrangian form. Such a study revealed important differential geometric features of the equilibrium problem, and is expected to play an important role for the formulation and the implementation of advanced mechanical theories.

Variational approach

In the present approach, the deformation process of a continuum body is described as a bijection between two configurations, namely a reference configuration $\Omega_{å} \subseteq \mathsf{R}^3$, referred to as material or Lagrangian, and another one, usually referred to as spatial or Eulerian $\Omega \subseteq \mathsf{R}^3$. Such a map is continuous and differentiable, being its inverse also continuous and differentiable, and is denoted by the symbol $\boldsymbol{\chi}: \mathbf{X} \in \Omega_{å} \rightarrow \mathbf{x} \in \Omega$. It represents a diffeomorphism between submanifolds with boundary, for which we have $J = \det(\mathbf{F}) > 0$, where symbol $\mathbf{F} = \partial\boldsymbol{\chi} / \partial\mathbf{X}$ denotes the deformation gradient. We assume moreover that the (differential and topological) boundary of the above domains is constituted of the union of regular *faces*, having in common two by two parts of their border, referred to as *edges*, which represent discontinuity loci for the face normals. In this study we consider an energy density depending on the first and second gradient of the placement map, namely $\mathrm{W}(\mathbf{X}, \mathbf{F}, \nabla\mathbf{F})$, see [1]. The objectivity of such an energy is guaranteed by prescribing the dependence on the right Cauchy-Green tensor $\mathbf{C} = \mathbf{F}^T\mathbf{F}$. The equilibrium configuration corresponds to the placement minimizing the total potential energy functional [3], namely

$$\hat{\boldsymbol{\chi}} = \arg\min_K \left\{ \mathsf{E}^{\mathrm{TOT}}(\boldsymbol{\chi}) = \int_{\Omega_{å}} \mathrm{W}\left(\mathbf{F}, \nabla\mathbf{F}\right) d\Omega_{å} - \mathsf{E}^{\mathrm{EXT}}(\boldsymbol{\chi}, \nabla\boldsymbol{\chi}) \right\} \tag{1}$$

Symbol K denotes herein an admissible set of functions sufficiently regular (also as for their trace) which incorporate the essential boundary conditions on the placement map and its normal derivative. According to a variational approach, the stationarity condition follows by imposing the first variation of the above functional to vanish. As for the inner virtual work, one obtains

$$\begin{aligned} \delta \int_{\Omega_{å}} \mathrm{W}\left(\mathbf{F}, \nabla\mathbf{F}\right) d\Omega_{å} &= \int_{\Omega_{å}} \frac{\partial \mathrm{W}}{\partial \mathbf{F}} : \delta\mathbf{F} + \frac{\partial \mathrm{W}}{\partial \nabla\mathbf{F}} \vdots \delta\left(\nabla\mathbf{F}\right) d\Omega_{å} = \\ &= \underbrace{\int_{\Omega_{å}} \frac{\partial \mathrm{W}}{\partial F^i_A} \delta F^i_A \, d\Omega_{å}}_{=\delta\mathsf{E}^{\mathrm{DEF}}_I} + \underbrace{\int_{\Omega_{å}} \frac{\partial \mathrm{W}}{\partial F^i_{AB}} \delta F^i_{AB} \, d\Omega_{å}}_{=\delta\mathsf{E}^{\mathrm{DEF}}_{II}} = \\ &= \int_{\Omega_{å}} P^A_i \, \delta F^i_A \, d\Omega_{å} + \int_{\Omega_{å}} P^{AB}_i \, \delta F^i_{AB} \, d\Omega_{å} ; \end{aligned} \tag{2}$$

In the above equation the parts of the energy variation relevant to the first and second gradient were marked by subscript *I* and *II*. As a key ingredient of the present formulation for second-gradient materials, the inner work depends not only on the second-rank Piola stress tensor, denoted above by P^A_{1i}, but also on a third-rank tensor P^{AB}_{2i}, referred to as hyper-stress tensor (or double-stress), see [2]. The present variational approach (and the more general principle of the virtual work which does not require any constitutive assumptions, see [4]) leads naturally to nonstandard boundary conditions and allows one to specify the admissible classes of external actions not known a priori. By the reiterated application of the integration by parts and of the divergence theorem extended to curved surfaces with boundary, we obtain a representation of the inner virtual work as the sum of diverse terms, including a novel surface action expending work versus the normal derivative of the virtual placement, an edge term, and contact pressures over the surface in which the linear dependence on the normal (according to the Cauchy's postulate) is superseded by the sum of nonlinear expressions involving the product of normals and of their derivatives: in particular, the dependence on the local mean curvature is made explicit, see [5].

Work-conjugate variables

The above formulation, based on the definition of a suitable energy density, is truly Lagrangian. However, the equilibrium problem can be formulated in an abstract setting by a proper choice of

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work-conjugate variables: then the governing equations assume the same form in the Lagrangian and in the Eulerian configuration. In fact, after computing the Eulerian counterparts of the virtual placement gradients, namely

$$\begin{aligned} &\delta D^i_j = \frac{\partial}{\partial x^j}\delta\chi^i(\mathbf{x}) = \frac{\partial \delta\chi^i}{\partial X^A}\frac{\partial X^A}{\partial x^j} = \delta F^i_A \left(\mathbf{F}^{-1}\right)^A_j ; \\ &\delta D^i_{kj} = \frac{\partial^2}{\partial x^j x^k}\delta\chi^i(\mathbf{x}) = \frac{\partial}{\partial x^k}\left(\frac{\partial}{\partial x^j}\delta\chi^i(\mathbf{x})\right) = \\ &= \frac{\partial}{\partial x^k}\left(\mathbf{F}^{-1}\right)^A_j \delta F^i_A + \left(\mathbf{F}^{-1}\right)^A_j \delta F^i_{AB}\left(\mathbf{F}^{-1}\right)^B_k ; \end{aligned} \tag{3}$$

equating the expressions of the Lagrangian and of the Eulerian inner virtual work, one obtains remarkable relationships between the Eulerian and Lagrangian hyper-stress tensors [6], namely

$$\begin{aligned} T^j_{1i} &= J^{-1} P^A_{1i} F^j_A + J^{-1} P^{AB}_{2i} F^j_{AB} \\ T^{jk}_{2i} &= J^{-1} P^{AB}_{2i} F^j_A F^k_B \end{aligned} \tag{4}$$

These relationships highlight a top-down structure typical of higher gradient modelling: in fact, the Lagrangian hyperstress affects both lower order Eulerian tensors, whilst the Piola stress tensor affects only the Cauchy stress T^j_{1i}.

Edge vectors

In the classical treatises of continuum mechanics a few formulae were already available to transform vectors defined over the boundary faces from the Lagrangian to the Eulerian configuration, such as those concerning the contravariant tangent vector and the covariant normal. However, the authors proposed novel relationships for the covariant and contravariant form of the border normal, namely the normal to the border edge which is orthogonal to the tangent and belongs to the face tangent plane. By assuming as ansatz an affine function of the Lagrangian variable, and exploiting the above mentioned orthogonality conditions the following relationship was derived for the contravariant form of the edge normal

$$b^r = \left\{ F^r_R B^R - \frac{\left(g_{rs} F^r_R B^R F^s_S T^S\right)}{\left(g_{rs} F^r_R T^R F^s_S T^S\right)} F^r_R T^R \right\} \frac{\| \mathbf{FT} \|}{\| J\mathbf{F}^{-T}\mathbf{N} \|} ; \tag{5}$$

An analogous formula can also be provided for the covariant form of the edge normal, see [6]. It is worth emphasizing that such transformations are not unique and alternative expressions may exist: not necessarily they are available in closed form for both the contravariant and covariant representation of the same vector. The above formula can be regarded as an application of Gram-Schmidt orthonormalization procedure, where a key role is played by the pull-back metric tensor.

Transport of surface projectors

As well known, at each point of a surface a pair of complementary orthogonal projectors can be defined, referred to as normal and tangential, and denoted by symbols $\left[M_\perp\right]^S_V = N^S N_V$ and $[M_\parallel]^S_V = \delta^S_V - N^S N_V$ respectively, apt to project any vector of the space environment onto the normal or the tangent space at that point. We provided effective transformation formulae for such projectors from the Lagrangian to the Eulerian configuration. For the normal projector, exploiting the transformation rule for the covariant normal we get

$$
\begin{aligned}
[m_\perp]^r_s = n^r n_s = g^{rt} \frac{\left(\mathbf{F}^{-1}\right)^Q_t N_Q}{\| \mathbf{F}^{-T}\mathbf{N} \|} \frac{\left(\mathbf{F}^{-1}\right)^V_s N_V}{\| \mathbf{F}^{-T}\mathbf{N} \|} = \\
= \frac{g^{rt}\left(\mathbf{F}^{-1}\right)^Q_t g_{QS}}{\| \mathbf{F}^{-T}\mathbf{N} \|^2} \left[N^W N_V \right] \left(\mathbf{F}^{-1}\right)^V_s = \\
= \frac{g^{rt}\left(\mathbf{F}^{-1}\right)^Q_t g_{QS}}{\| \mathbf{F}^{-T}\mathbf{N} \|^2} [M_\perp]^S_V \left(\mathbf{F}^{-1}\right)^V_s ;
\end{aligned}
\tag{6}
$$

whilst a more complex relationship is met for the tangential projector. It is worth underlying that the Eulerian tangential projector depends on both the Lagrangian projectors: hence, an Eulerian vector normal to an Eulerian surface when transported to the Lagrangian configuration is expected to possess non-vanishing components in both the normal and the tangent space at the corresponding point.

Divergence theorem revisited

In the present approach recourse is made to the divergence theorem formulated for submanifolds with boundary, which represents an important result of differential geometry, e.g. see [6]. Such a theorem was revisited, providing a novel relationship between spatial and material expressions extremely useful for the analytical developments, namely

$$
\begin{aligned}
[m_\parallel]^c_a \frac{\partial}{\partial x^c}([m_\parallel]^a_b w^b)\|J\mathbf{F}^{-T}\mathbf{N}\| = \\
= [M_\parallel]^A_S \frac{\partial}{\partial X^A}(\|J\mathbf{F}^{-T}\mathbf{N}\|(\mathbf{F}^{-1})^R_a([m_\parallel]^a_b w^b)[M_\parallel]^S_R);
\end{aligned}
\tag{7}
$$

In a sense, this formula generalizes Piola's bulk transformation, see [4].

Closing remarks and future prospects

In this study the transport from the Eulerian to the Lagrangian configuration of the equilibrium equations was addressed for the first time with reference to second-gradient modelling. To attain the purpose, novel theoretical results were achieved, which represent intermediate steps and however exhibit a general interest. The methodology proposed above can be easily extended to higher-order gradient materials (see e.g. [7]), possibly enriched by damage and plasticity. Moreover the novel results are expected to play a role for advanced mechanical theories and their implementation (see e.g. [8]), possibly concerning fracture propagation and contact mechanics.

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