Numerical simulations of classical problems in two-dimensional (non) linear second gradient elasticity

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Abstract

A two-dimensional solid consisting of a linear elastic isotropic material is considered in this paper. The strain energy is expressed as a function of the strain and of the gradient of strain. The balance equations and the boundary conditions have been derived and numerically simulated for those classical problems for which an analytical solution is available in the literature. Numerical simulations have been developed with a commercial code and a perfect overlap between the results and the analytical solution has been found. The role of external edge double forces and external wedge forces has also been analyzed. We investigate a mesh-size independency of second gradient numerical solutions with respect to the classical first gradient one. The necessity of a second gradient modelling is finally shown. Thus, we analyse a non-linear anisotropic problem, for which experimental evidence of internal boundary layer is shown and we prove that this can be related to the second gradient modelling.

Keywords: Second gradient, Elasticity, Variational approach, Isotropy, Anisotropy, Numerical solution, Two-dimensional problems
1. Introduction

The introduction of higher order gradients of the strain into the constitutive law for the internal energy leads to a partial differential equation of higher orders and the Galerkin method requires a higher regularity of the interpolation scheme, see e.g. [14]. The reason of introducing higher-order gradient theories is based on different points of view, see e.g. [6, 7, 8, 9]. The first example is referred to the case related to strongly localized deformation features [3, 21, 59, 60, 65] and references therein. In such cases, it is reasonable to complement the displacement field with some additional kinematical descriptors [34, 35, 36, 55, 56, 58, 63], which leads to the so-called micromorphic models, see also [38, 43, 44, 51]. Another possibility is to consider higher order gradient theories, in which the deformation energy depends on second and/or higher gradients of the displacement [27, 31, 42]. This is done in the literature for both monophasic systems (see [12, 64], in which continuous systems are investigated, and [2, 70] for cases of lattice/woven structures) and for bi-phasic (see e.g. [10, 26, 49, 69]) or granular materials [50, 74]. The second example is referred to the fact that, unlike classical Cauchy continua, second and higher order continua can respond to concentrated forces and generalized contact actions (see e.g. in [17, 23]). It is worth to be noted that it is also possible to conceive a framework in classical elasticity (see, e.g., [16, 47] and references therein) in which concentrated forces are possible. However, with a greater theoretical and numerical efforts. The third example is becoming increasingly important for practical and applicative reasons in the last years, as the novelties in manufacturing procedures (due to, e.g., 3D printing, self assembly etc.) are making possible the realization of a much wider class of new architected materials [24, 46]. In these cases, the deficiencies of classical approaches when the material behaviour exhibits size-scale effects is investigated in [66, 67, 68], and in [52] a novel invariance requirement (micro-randomness) in addition to isotropy is formulated, which implies conformal invariance of the curvature. In general, new theories are put into place when existing theories prove to be inadequate to describe some observed phenomenon. Such new theories however have to lead to well posed problems in the sense that the governing equations and boundary conditions lead to solvable problems. The papers [2, 45, 57] already proved that the problems we study here is indeed well-posed.

A survey of variational principles, which form the basis for computational methods in both
continuum mechanics and multi-rigid body dynamics is presented in [5] and numerical investigation
of structures of the type considered also requires special attention and the development of novel
techniques [4, 15, 18, 19, 20, 37, 39] or the proper employment of the existing ones (see for instance
[71], where Galerkin Boundary Element Method is used to address a class of strain gradient elastic
materials). The objective of the contribution [41] is to formulate a geometrically nonlinear theory
of higher-gradient elasticity accounting for boundary (surface and curve) energies. To reduce the
computational costs and avoid the macroscopic grid sensitivity, an adaptive multiscale technique is
developed for strain localization analysis of periodic lattice truss materials in [79]. In [75] a general
finite element discretization of micromorphic Mindlin’s elasticity is presented. The behaviour of all
elements is also examined at the limiting case of strain gradient elasticity. The numerical solution of
second gradient elasticity equations with a displacement-based finite element method requires the
use of C1-continuous elements, that motivates the implementation of the concept of isogeometric
analysis in [32]. In [54] a new C1 hexahedral element which is the first three-dimensional C1
element ever constructed and give excellent rates of convergence in a benchmark (without edge
forces) boundary value problem of gradient elasticity. In [53] a methodology by which C1 elements,
such as the TUBA 3 element proposed by Argyris et al. [11], can be constructed is presented. This
kind of elements are largely present in the literature of strain gradient elasticity [1, 22, 33, 76, 77, 78].

From a general point of view a comparison between analytical and numerical solution is needed to
check the quality of the used code. In other words, it means that the code has good performances and
there is a degree of reliability to be assigned to it. In this paper a two-dimensional solid consisting
of a linear elastic isotropic material is considered. The strain energy is expressed as a function
of the strain and of the gradient of strain. The aim of the paper is to present the possibility to
numerically simulate general strain gradient elasticity by the use of a commercial code that includes
the Argyris shape functions. This is done with the use of benchmark boundary value problem for
which an analytical solution exist. We remark that in such a 2-dimensional benchmark boundary
value problem wedge forces are present. We remark a perfect overlap between the numerical results
and the analytical solution of the benchmark classical boundary value problem. The role of external
edge double forces and external wedge forces has also been analyzed. We also investigate a mesh-
size independence of second gradient numerical solutions with respect to the classical first gradient one. Finally, we show an experimental evidence of the necessity of second gradient modelling. We show the experimental results [25] of a bias test on a pantographic structure. In particular, we show that the boundary layer experimentally observed can be numerically achieved by a non-null second gradient constitutive coefficient and the largeness of such a boundary layer can be used to identify such a second gradient parameter. For a better representation of the state of the art of material identification of second gradient coefficients the reader is invited to see [13, 61, 62].

2. Formulation of the problem

2.1. The general case

The coordinates $X$, in the reference configuration, are those of the 2-dimensional body $B$. The internal energy density functional $U (G, \nabla G)$ depends not only on the strain $G = (F^T F - I) / 2$ but also on its gradient $\nabla G$, where $F = \nabla \chi$, $\chi$ is the placement function. In Mindlin [48] a general form of the density of the strain energy functional of a linear isotropic second gradient elastic material is given, for the sake of simplicity, in indicial notation,

$$U (G, \nabla G) = \frac{\lambda}{2} G_{ij}G_{jj} + \mu G_{ij}G_{ij} +$$

$$+4\alpha_1 G_{aa,b}G_{bc,c} + \alpha_2 G_{aa,b}G_{cc,b} + 4\alpha_3 G_{ab,a}G_{ab,c} + 2\alpha_4 G_{ab,c}G_{ab,c} + 4\alpha_5 G_{ab,c}G_{ac,b},$$

where subscript $j$ after comma indicates derivative with respect to $X_j$ and a general rule for index notation is the following: the subscript-indeces of a symbol denoting a vector or a tensor quantity denote the components of that quantity. In the 2-dimensional case we have

$$U (G, \nabla G) = \bar{U} (u) = (\lambda + 2\mu) (u_{1,1}^2 + u_{2,2}^2) + \mu (u_{1,1}^2 + u_{2,2}^2) + 2\lambda u_{1,1}u_{2,2} + 2\mu u_{1,2}u_{2,1}$$

$$+ \frac{1}{2} A (u_{1,22}^2 + u_{2,11}^2) + \frac{1}{2} B (u_{1,11}^2 + u_{2,22}^2) + C (u_{1,12}^2 + u_{2,21}^2) + 2D (u_{1,11}u_{2,12} + u_{2,22}u_{1,12})$$

$$+ \frac{1}{2} (A + B - 2C) (u_{1,11}u_{1,22} + u_{2,11}u_{2,22}) + (B - A - 2D) (u_{1,12}u_{2,11} + u_{1,22}u_{2,12})$$,
2.1 The general case

where

\[ A = 2\alpha_3 + 2\alpha_4 + 2\alpha_5, \quad B = 8\alpha_1 + 2\alpha_2 + 8\alpha_3 + 4\alpha_4 + 8\alpha_5. \]  (3)

\[ C = 2\alpha_1 + \alpha_2 + 3\alpha_4 + 5\alpha_5, \quad D = 3\alpha_1 + \alpha_2 + 2\alpha_3, \]  (4)

where \( u \) is the displacement field, \( \lambda \) and \( \mu \) are the Lamè coefficients and \( \alpha_i \) with \( i = 1, 2, 3, 4, 5 \) are the 5 second gradient constitutive parameters. Note that here we use the Lamè coefficients \( \lambda \) and \( \mu \) to describe first-gradient, isotropic linear elasticity, but other choices could be made, e.g., the pair comprised of bulk modulus \( \kappa \) and shear modulus \( \mu \) [28, 29, 30, 40, 72, 73], which is particularly convenient, e.g., when treating quasi-incompressibility.

In Mindlin [48], in order to have the positive definiteness of \( U \), the following restrictions on the 7 constitutive parameters must be satisfied,

\[ \mu > 0, \quad 3\lambda + 2\mu > 0, \quad -4\alpha_1 + 2\alpha_2 + 2\alpha_3 + 6\alpha_4 - 6\alpha_5 > 0, \quad \alpha_4 > \alpha_5, \quad \alpha_4 + 2\alpha_5 > 0 \]  (5)

\[ 4\alpha_1 + \alpha_2 + 4\alpha_3 + 2\alpha_4 + 4\alpha_5 > 0, \quad \alpha_1 + \alpha_2 < \alpha_3, \quad 4\alpha_1 - 2\alpha_2 - 2\alpha_3 - 3\alpha_4 + 3\alpha_5 > 0. \]

In the 2-dimensional case the positive definiteness of \( U \) is implied again by the classical 2-dimensional restrictions

\[ \mu > 0, \quad \lambda + \mu > 0, \]

and by the positive definiteness of the following matrix

\[
\begin{pmatrix}
A & 0 & \frac{1}{2} (A + B - 2C) & 0 & 0 & B - A - 2D \\
0 & A & 0 & \frac{1}{2} (A + B - 2C) & B - A - 2D & 0 \\
\frac{1}{2} (A + B - 2C) & 0 & B & 0 & 0 & 2D \\
0 & \frac{1}{2} (A + B - 2C) & 0 & B & 2D & 0 \\
0 & B - A - 2D & 0 & 2D & 2C & 0 \\
B - A - 2D & 0 & 2D & 0 & 0 & 2C \\
\end{pmatrix}.
\]

Keeping this in mind, a classical variational procedure gives the following system of partial differ-
2.1 The general case

The general case

\[ u_{1,11} (\lambda + 2\mu) + u_{1,22}\mu + u_{2,12} (\lambda + \mu) = \\
= u_{1,1111}B + u_{1,2222}A + u_{1,1122} (A + B) + (u_{2,1222} + u_{2,1112}) (B - A) - b_{1}^{\text{ext}} \quad (6) \]

\[ u_{2,22} (\lambda + 2\mu) + u_{2,11}\mu + u_{1,12} (\lambda + \mu) = \\
= u_{2,2222}B + u_{2,1111}A + u_{2,1122} (A + B) + (u_{1,1222} + u_{1,1112}) (B - A) - b_{2}^{\text{ext}}, \quad (7) \]

and boundary conditions given \(\forall X_i \in \partial B\) from the following duality conditions

\[ \delta u_\alpha (t_\alpha - t_\alpha^{\text{ext}}) = 0, \; \delta u_\alpha, jn_j (\tau_\alpha - \tau_\alpha^{\text{ext}}) = 0, \; \int_{\partial B} \delta u_\alpha f_\alpha = \int_{\partial B} \delta u_\alpha f_\alpha^{\text{ext}}, \quad (8) \]

where \(b_\alpha^{\text{ext}}, t_\alpha^{\text{ext}}, \tau_\alpha^{\text{ext}}\) and \(f_\alpha^{\text{ext}}\) are the external actions: \(b_\alpha^{\text{ext}}\) is the external force per unit area and is applied on the whole 2-dimensional domain \(B\); \(t_\alpha^{\text{ext}}\) and \(\tau_\alpha^{\text{ext}}\) are the external force and double force (respectively) and are applied on (a part of) the one-dimensional boundary \(\partial B\) of the domain \(B\); and \(f_\alpha^{\text{ext}}\) is the external concentrated force applied on the set of points belonging to the boundary of the boundary \([\partial B]\), so that the last integral can be also represented as the sum of the external works made by the concentrated forces acting on each vertex of the domain. In other words, if we define the boundary \(\partial B\) as the union of \(m\) regular parts \(\Sigma_c\) with \(c = 1, \ldots, m\) and \([\partial B]\) as the union of the corresponding \(m\) vertex-points \(V_c\) with \(c = 1, \ldots, m\),

\[ \partial B = \bigcup_{c=1}^{m} \Sigma_c, \quad [\partial B] = \bigcup_{c=1}^{m} V_c, \]

then the line and vertex-integrals of a generic field \(g(X_i)\) are represented as follows,

\[ \oint_{\partial B} g(X_i) = \sum_{c=1}^{m} \int_{\Sigma_c} g(X_i), \quad \int_{[\partial B]} g(X_i) = \sum_{c=1}^{m} g(X_i^c) \quad (9) \]

where \(X_i^c\) is the coordinate of the vertex \(V_c\). Moreover, the so called contact force \(t_\alpha\), contact double
2.2 Rectangles

force $\tau_\alpha$ and contact wedge force $f_\alpha$ are defined,

\begin{align*}
    t_\alpha &= (S_{\alpha j} - T_{\alpha j,h,h}) n_j - P_{ka} (T_{\alpha hj} P_{ah} n_j)_k, \\
    \tau_\alpha &= T_{\alpha jk} n_j n_k, \\
    f_\alpha &= T_{ahk} V_{hk}
\end{align*}

where $n_j$ is the normal to the boundary $\partial \mathcal{B}$, $P_{ij}$ is its tangential projector operator ($P_{ij} = \delta_{ij} - n_i n_j$), $V$ is the vertex operator

$$V_{hk} = \nu^l h^l n_j^l + \nu^r h^r n_j^r,$$

where superscripts $l$ and $r$ refers (roughly speaking, left and right), respectively, to one and to the other sides that define a certain vertex-point $V_c$; $\nu$ is the external tangent unit vector. Stress and hyper stresses are defined,

\begin{align*}
    S_{ij} &= \frac{\partial U}{\partial G_{ij}}, \\
    T_{ij,h} &= \frac{\partial U}{\partial G_{ij,h}}.
\end{align*}
2.2. Rectangles

2.2.1. The general case of straight lines

In the case of boundaries \( \partial B \) composed of straight-lines, the contact force in (10), the contact double force in (11) and the contact wedge force (12) are

\[
t_\alpha = S_{\alpha j} n_j - (T_{\alpha j,h} + T_{\alpha j,\dot{h}}) n_j + T_{\alpha h,j,k} n_h n_k n_j, \quad \tau_\alpha = T_{\alpha j,k} n_k, \quad f_\alpha = T_{\alpha ij} V_{ij},
\]

that, in terms of the displacement fields, yield,

\[
t_\alpha = \lambda u_{a,a} n_a + \mu u_{a,j} n_j + \mu u_{j,a} n_j - u_{a,ab} n_a (6\alpha_1 + 2\alpha_2 + 4\alpha_3) - u_{a,aak} n_k (6\alpha_1 + 2\alpha_2 + 4\alpha_3 + 8\alpha_5) - u_{a,aak} n_k (2\alpha_3 + 4\alpha_4 + 6\alpha_5) - u_{k,aaa} n_k (2\alpha_1 + 2\alpha_3 + 2\alpha_4 + 6\alpha_5) + u_{a,aak} n_a n_j n_k (4\alpha_1 + 2\alpha_2 + 2\alpha_3) + u_{j,aak} n_a n_j n_k (2\alpha_1 + 2\alpha_3) + u_{a,abc} n_a n_b n_c (2\alpha_4 + 2\alpha_5) + u_{a,abc} n_a n_b n_c (2\alpha_1 + 2\alpha_3),
\]

\[
\tau_\alpha = u_{a,ab} n_a n_b (4\alpha_1 + 2\alpha_2 + 2\alpha_3) + u_{a,bb} n_a n_a (2\alpha_1 + 2\alpha_3) + u_{a,a} n_a n_a + u_{a,ab} n_a n_b (2\alpha_4 + 2\alpha_5) + 2\alpha_3 u_{a,aa} + u_{a,ab} n_a n_b (2\alpha_4 + 6\alpha_5).
\]

We remark that the formulation expressed in (15) and (16) can also be used in the 3-dimensional case. This is the reason why (15) and (16) are expressed in terms of the 5 3-dimensional constitutive coefficients \( \alpha_i \) with \( i = 1, 2, 3, 4, 5 \) and not in terms of the 4 2-dimensional constitutive coefficients \( A, B, C \) and \( D \).

In Fig. 1 we represent the scheme of a rectangle with side-names \( Q, R, S \) and \( T \) and vertex-names \( V_1, V_2, V_3 \) and \( V_4 \).
2.2.2. Characterization of sides

The characterization of side $S$ is done by setting $n_i = \delta_{i1}$. Thus, from (15) with $\alpha = 1, 2$, and from (16) with $\alpha = 1, 2$, we have

\[
t_1 = t_1^S = u_{1,1} (\lambda + 2\mu) + u_{2,2} \lambda - Bu_{1,111} - 2Du_{2,222} - \frac{1}{2} (A + B + 2C) u_{1,122} - (B - A) u_{2,211},
\]
\[
t_2 = t_2^S = \mu (u_{1,2} + u_{2,1}) - (B - A) u_{1,112} - (B - A - 2D) u_{1,222} - Au_{2,111} - \frac{1}{2} (A + B + 2C) u_{2,122},
\]
\[
\tau_1 = \tau_1^S = Bu_{1,11} + \frac{1}{2} (A + B - 2C) u_{1,22} + 2Du_{2,12},
\]
\[
\tau_2 = \tau_2^S = (B - A - 2D) u_{1,12} + Au_{2,11} + \frac{1}{2} (A + B - 2C) u_{2,22}.
\]

The characterization of side $Q$ is done by setting $n_i = -\delta_{i1}$. Thus, from (15) with $\alpha = 1, 2$, and from (16) with $\alpha = 1, 2$, we have

\[
t_1 = t_1^Q = -u_{1,1} (\lambda + 2\mu) - u_{2,2} \lambda + Bu_{1,111} + 2Du_{2,222} + \frac{1}{2} (A + B + 2C) u_{1,122} + (B - A) u_{2,211},
\]
\[
t_2 = t_2^Q = -\mu (u_{1,2} + u_{2,1}) + (B - A) u_{1,112} + (B - A - 2D) u_{1,222} + Au_{2,111} + \frac{1}{2} (A + B + 2C) u_{2,122},
\]
\[
\tau_1 = \tau_1^Q = Bu_{1,11} + \frac{1}{2} (A + B - 2C) u_{1,22} + 2Du_{2,12},
\]
\[
\tau_2 = \tau_2^Q = (B - A - 2D) u_{1,12} + Au_{2,11} + \frac{1}{2} (A + B - 2C) u_{2,22}.
\]

We remark that $t_1^Q$ in (21) and $t_2^Q$ in (22) are the opposite of $t_1^S$ in (17) and of $t_2^S$ in (18), respectively, and that $\tau_1^Q$ in (23) and $\tau_2^Q$ in (24) are the same of $\tau_1^S$ in (19) and of $\tau_2^S$ in (20), respectively.

The characterization of side $R$ is done by setting $n_i = \delta_{i2}$. Thus, from (15) with $\alpha = 1, 2$, and from (16) with $\alpha = 1, 2$, we have

\[
t_1 = t_1^R = \mu (u_{1,2} + u_{2,1}) - (B - A) u_{2,122} - (B - A - 2D) u_{2,111} - Au_{1,222} - \frac{1}{2} (A + B + 2C) u_{1,112},
\]
\[
t_2 = t_2^R = u_{2,2} (\lambda + 2\mu) + u_{1,1} \lambda - Bu_{2,222} - 2Du_{1,111} - \frac{1}{2} (A + B + 2C) u_{2,112} - (B - A) u_{1,122},
\]
\[
\tau_1 = \tau_1^R = (B - A - 2D) u_{2,12} + Au_{1,22} + \frac{1}{2} (A + B - 2C) u_{1,11},
\]
\[
\tau_2 = \tau_2^R = Bu_{2,22} + \frac{1}{2} (A + B - 2C) u_{2,11} + 2Du_{1,12}.
\]
We remark that, because of isotropy, \( t_1^R \) in (25) and \( t_2^R \) in (26) are the same of \( t_2^S \) in (18) and of \( t_1^S \) in (17), respectively, by changing the indexes 1 and 2. Besides, because of isotropy, \( \tau_1^R \) in (27) and \( \tau_2^R \) in (28) are the same of \( \tau_2^S \) in (19) and of \( \tau_1^S \) in (20), respectively, by changing the indexes 1 and 2.

Finally, the characterization of side \( T \) is done by setting \( n_i = -\delta_{i2} \). Thus, from (15) with \( \alpha = 1, 2 \), and from (16) with \( \alpha = 1, 2 \), we have

\[
t_1 = t_1^T = -\mu (u_{1,2} + u_{2,1}) + (B - A) u_{2,122} + (B - A - 2D) u_{2,111} + Au_{1,222} + \frac{1}{2} (A + B + 2C) u_{1,112},
\]

\[
t_2 = t_2^T = -u_{2,2} (\lambda + 2\mu) - u_{1,1} \lambda + Bu_{2,222} + 2Du_{1,111} + \frac{1}{2} (A + B + 2C) u_{2,112} + (B - A) u_{1,122},
\]

\[
\tau_1 = \tau_1^T = (B - A - 2D) u_{2,12} + Au_{1,22} + \frac{1}{2} (A + B - 2C) u_{1,11},
\]

\[
\tau_2 = \tau_2^T = Bu_{2,22} + \frac{1}{2} (A + B - 2C) u_{2,11} + 2Du_{1,12}.
\]

We remark that \( t_1^T \) in (29) and \( t_2^T \) in (30) are the opposite of \( t_1^R \) in (25) and of \( t_2^R \) in (26), respectively, and that \( \tau_1^T \) in (31) and \( \tau_2^T \) in (32) are the same of \( \tau_1^R \) in (27) and of \( \tau_2^R \) in (28), respectively.

### 2.2.3 Characterization of vertices

The last equation of (8) is reduced, because of (9)2 to

\[
\int_{\partial 328} \delta u_\alpha (f_\alpha - f_\alpha^{ext}) = \\
= \left[ \delta u_\alpha (T_{\alpha ij} V_{ij} - f_\alpha^{ext}) \right]_{V_1} + \left[ \delta u_\alpha (T_{\alpha ij} V_{ij} - f_\alpha^{ext}) \right]_{V_2} \\
+ \left[ \delta u_\alpha (T_{\alpha ij} V_{ij} - f_\alpha^{ext}) \right]_{V_3} + \left[ \delta u_\alpha (T_{\alpha ij} V_{ij} - f_\alpha^{ext}) \right]_{V_4},
\]

For vertex \( V_1 \) the side \( A \) has \( n_j = -\delta_{1j} \) and \( \nu_i = \delta_{i2} \) and the side \( B \) has \( n_j = \delta_{2j} \) and \( \nu_i = -\delta_{i1} \) so that

\[
[V_{ij}]_{V_1} = \left[ \nu_i n_j^1 + \nu_i n_j^2 \right]_{V_1} = -\delta_{i2} \delta_{1j} - \delta_{i1} \delta_{2j}.
\]
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For vertex $V_2$ the side $B$ has $n_j = \delta_{2j}$ and $\nu_i = \delta_{i1}$ and the side $C$ has $n_j = \delta_{1j}$ and $\nu_i = \delta_{i2}$ so that

$$[V_{ij}]_{V_2} = [\nu_i n_j^t + \nu_j n_i^t]_{V_2} = \delta_{11}\delta_{2j} + \delta_{12}\delta_{i1}.$$ 

For vertex $V_3$ the side $C$ has $n_j = \delta_{1j}$ and $\nu_i = -\delta_{i2}$ and the side $D$ has $n_j = -\delta_{2j}$ and $\nu_i = \delta_{i1}$ so that

$$[V_{ij}]_{V_3} = [\nu_i n_j^t + \nu_j n_i^t]_{V_3} = -\delta_{i2}\delta_{1j} - \delta_{i1}\delta_{2j}.$$ 

For vertex $V_4$ the side $D$ has $n_j = -\delta_{2j}$ and $\nu_i = -\delta_{i1}$ and the side $A$ has $n_j = -\delta_{1j}$ and $\nu_i = -\delta_{i2}$ so that

$$[V_{ij}]_{V_4} = [\nu_i n_j^t + \nu_j n_i^t]_{V_4} = \delta_{i1}\delta_{2j} + \delta_{i2}\delta_{1j}.$$ 

Thus, finally, the (33) yields

$$\int_{[\partial B]} \delta u_{\alpha} (f_\alpha - f_{\alpha}^{ext}) = [\delta u_{\alpha} (-T_{\alpha 21} - T_{\alpha 12} - f_{\alpha}^{ext})]_{V_1} + [\delta u_{\alpha} (T_{\alpha 12} + T_{\alpha 21} - f_{\alpha}^{ext})]_{V_2} + [\delta u_{\alpha} (-T_{\alpha 21} - T_{\alpha 12} - f_{\alpha}^{ext})]_{V_3} + [\delta u_{\alpha} (T_{\alpha 12} + T_{\alpha 21} - f_{\alpha}^{ext})]_{V_4},$$

where $T_{\alpha 12} + T_{\alpha 21}$, in terms of the displacement field, it is for $\alpha = 1$

$$T_{112} + T_{121} = 2Cu_{1,12} + (B - A - 2D)u_{2,11} + 2Du_{2,22},$$

and for $\alpha = 2$,

$$T_{212} + T_{221} = 2Cu_{2,12} + (B - A - 2D)u_{1,22} + 2Du_{1,11}.$$
3. Numerical simulations

Numerical data for the simulations that will be presented in this paper are here shown (see Fig. 1)

\[ L = 2 \text{m}, \quad l = 1 \text{m}, \quad \mu = 10 \text{MPa m}, \quad \lambda = 15 \text{MPa m}, \quad \rho = 10^5 \text{Kg/m}^2 \quad E = \frac{\mu (3\lambda + 2\mu)}{\lambda + \mu} = 26 \text{MPa m}, \]  
\( \alpha_1 = E l_m^2, \quad \alpha_2 = E l_m^2, \quad \alpha_3 = 2E l_m^2, \quad \alpha_4 = E l_m^2, \quad \alpha_5 = \frac{1}{2} E l_m^2, \quad l_m = 10 \text{cm}, \) 
and therefore

\[ A = 7E l_m^2, \quad B = 34E l_m^2, \quad C = \frac{21}{2} E l_m^2, \quad D = 8E l_m^2. \]

With these data the positive definiteness of the strain energy functional is guaranteed.

3.1. The heavy sheet problem

We consider an heavy sheet appended at the top side \( R \) and constrained at sides \( Q \) and \( S \) to have null horizontal displacement. Thus, the kinematical restrictions are

\[ (\delta u_2)_R = 0, \quad (\delta u_1)_Q = 0, \quad (\delta u_1)_S = 0. \]  
and also represented in Fig. 2. Let the two partial differential equations (6) and (7) be satisfied with the following external forces per unit area,

\[ b_1^{ext} = 0, \quad b_2^{ext} = -\rho g, \]  
and let the edge boundary conditions be as follows,

\[ u_1 = 0, \quad t_2^Q = 0, \quad \tau_1^Q = 0, \quad \tau_2^Q = \tau_2^{ext,Q}, \quad \forall X \in Q, \]  
\[ t_1^R = 0, \quad u_2 = 0, \quad \tau_1^R = 0, \quad \tau_2^R = \tau_2^{ext,R}, \quad \forall X \in R, \]  
\[ u_1 = 0, \quad t_2^S = 0, \quad \tau_1^S = 0, \quad \tau_2^S = \tau_2^{ext,S}, \quad \forall X \in S, \]  
\[ t_1^T = 0, \quad t_2^T = 0, \quad \tau_1^T = 0, \quad \tau_2^T = \tau_2^{ext,T}, \quad \forall X \in T, \]
3.2 The bending problem

Figure 2: Graphical representation of the kinematic restrictions for the heavy sheet problem.

where the non-null external edge double forces are as follows,

\[
\tau_{2,ext,S} = \tau_{2,ext,Q} = (A + B - 2C) \frac{\rho g}{2(\lambda + 2\mu)}, \quad \tau_2^{R,ext} = \tau_2^{T,ext} = \frac{\rho g B}{(\lambda + 2\mu)},
\]  \hspace{1cm} (45)

and let the only wedge conditions that are not implied by (41-44) be as follows,

\[
(f_2^{ext})_{V_3} = 0, \quad (f_2^{ext})_{V_4} = 0.
\]  \hspace{1cm} (46)

The analytical solution of this problem is achieved in [61] and here represented in terms of the displacement field,

\[
u_1 = 0, \quad u_2 = \frac{\rho g (X_2 - l)(3l + X_2)}{2(\lambda + 2\mu)}.
\]  \hspace{1cm} (47)

The numerical simulations of this problem is shown in Fig. 3a and have shown remarkable identification between exact analytical solution and the respective numerical simulation (Fig. 3b)

3.2. The bending problem

We consider the bending problem and constrain the whole side \(A\) to not displace in the horizontal direction and one of its point, the origin \(O\), to have also null vertical displacement. Thus, the kinematical restrictions are

\[
(\delta u_1)_A = 0, \quad (\delta u_2)_O = 0.
\]  \hspace{1cm} (48)
Figure 3: Vertical displacement of the heavy sheet problem. (a) Graphical representation of the numerical simulation and (b) comparison between the exact analytical solution and the respective numerical one through a given vertical cut.

and they are represented in Fig. 4. It has to be remarked that such kinematical constrains are not of a general type. In fact, the (48)\( _2 \) is referred to a single point that is not a vertex of the domain. This means that the results will be reasonable only in the case of vertical null force at point \( O \). Let the two partial differential equations (6) and (7) be satisfied with the null external forces per unit area,

\[
b_1^{\text{ext}} = 0, \quad b_2^{\text{ext}} = 0, \quad (49)
\]

and the edge boundary conditions be as follows,

\[
\begin{align*}
&u_1 = 0, \quad t_2^Q = 0, \quad \tau_1^Q = 0, \quad \tau_2^Q = \tau_2^{\text{ext},Q}, \quad \forall X \in Q, \\
&t_1^R = 0, \quad t_2^R = 0, \quad \tau_1^R = 0, \quad \tau_2^R = \tau_2^{\text{ext},R}, \quad \forall X \in R, \\
&t_1 = t_1^{\text{ext},S}, \quad t_2^S = 0, \quad \tau_1^S = 0, \quad \tau_2^S = \tau_2^{\text{ext},S}, \quad \forall X \in S, \\
&t_1^T = 0, \quad t_2^T = 0, \quad \tau_1^T = 0, \quad \tau_2^T = \tau_2^{\text{ext},T}, \quad \forall X \in T,
\end{align*}
\]

(50) to (53)

where the non-null external edge force and double forces are as follows,

\[
\tau_2^{\text{ext},Q} = \tau_2^{\text{ext},S} = \frac{3M^{\text{ext}}}{2l^3} \left[ -(5\lambda + 8\mu)A + (\lambda + 4\mu)B + 2\lambda C - (4\lambda + 8\mu)D \right] \frac{1}{16l^3 \mu (\lambda + \mu)},
\]

and

\[
t_1^{\text{ext},S} = \frac{3M^{\text{ext}} X_2}{2l^3},
\]
3.2 The bending problem

The analytical solution of this problem is achieved in [61] and here represented in terms of the displacement field,

\[ u_1 = \frac{3M_{ext}(\lambda + 2\mu)X_1X_2}{8l^3\mu(\lambda + \mu)}, \quad u_2 = -\frac{3M_{ext}[\lambda X_2^2 + (\lambda + 2\mu)X_1^2]}{16l^3\mu(\lambda + \mu)}, \tag{57} \]

The numerical simulations of this problem are shown in Figs. 5.
3.3 The bending problem without double forces

We consider the same bending problem of the previous subsection, with the same kinematical restrictions (48), the same external forces per unit area (49), the same edge boundary conditions (50-53) with the same edge force (54) but with null edge double forces

\[ \tau_{2,ext}^Q = \tau_{2,ext}^S = 0, \quad \tau_{2,ext}^{R,ext} = \tau_{2,ext}^{T,ext} = 0, \]
3.4 The flexure problem

We consider the flexure problem and constrain the whole side $C$ to displace in the vertical direction and one of the point of side $A$, the origin $O$, to have null horizontal and vertical displacements.

and null wedge conditions

$$ (f_{2}^{ext})_{V_1} = 0, \quad (f_{2}^{ext})_{V_2} = 0, \quad (f_{2}^{ext})_{V_3} = 0, \quad (f_{2}^{ext})_{V_4} = 0, \quad (f_{1}^{ext})_{V_2} = - (f_{1}^{ext})_{V_3} = 0. $$

In this case we do not have an analytical solution but we make numerical simulations, that are shown in Figs 9 and 10. It can be remarked that the presence of double forces has a relatively strong influence on the numerical results.

3.4. The flexure problem

We consider the flexure problem and constrain the whole side $C$ to displace in the vertical direction and one of the point of side $A$, the origin $O$, to have null horizontal and vertical displacements.
Thus, the kinematical restrictions are

\[(\delta u_1)_S = 0, \quad (\delta u_1)_O = 0 \quad (\delta u_2)_O = 0.\]  \hspace{1cm} (58)

and they are represented in Fig. 11. It has to be remarked that such kinematical constrain are not of a general type. In fact, the $(58)_{2,3}$ is referred to a single point that is not a vertex of the domain. This means that the results will be reasonable only in the case of null force at point $O$. Let the two partial differential equations (6) and (7) be satisfied with null external forces per unit area (49), let the edge boundary conditions be as follows,

\begin{align*}
t_1 &= t_1^{ext,Q}, \quad t_2^Q = t_2^{ext,Q}, \quad \tau_1^Q = \tau_1^{ext,Q}, \quad \tau_2^Q = \tau_2^{ext,Q}, \quad \forall X \in Q, \hspace{1cm} (59) \\
t_1 &= t_1^{ext,R}, \quad t_2^R = 0, \quad \tau_1^R = \tau_1^{ext,R}, \quad \tau_2^R = \tau_2^{ext,R}, \quad \forall X \in R, \hspace{1cm} (60) \\
t_1 &= 0, \quad u_2 = -\delta, \quad \tau_1^S = \tau_1^{ext,S}, \quad \tau_2^S = 0, \quad \forall X \in S, \hspace{1cm} (61) \\
t_1 &= t_1^{ext,T}, \quad t_2^T = 0, \quad \tau_1^T = \tau_1^{ext,T}, \quad \tau_2^T = \tau_2^{ext,T}, \quad \forall X \in T, \hspace{1cm} (62)
\end{align*}

where the non-null external edge force and double forces are as follows,

\[t_1^{ext,Q} = -\frac{3LQX_2}{2l^3}.\]  \hspace{1cm} (63)
3.4 The flexure problem

\[ t_{2_{\text{ext},Q}} = \frac{3Q \left[ -A\lambda + B (5\lambda + 4\mu) + 2C\lambda + 4D (3\lambda + 4\mu) + 4\mu\lambda (l^2 - X_2^2) + 4\mu^2 (l^2 - X_2^2) \right]}{16l^3\mu (\lambda + \mu)} \]  

\[ t_{1_{\text{ext},T}} = -t_{1_{\text{ext},T}} = -\frac{3Q}{16l^3\mu (\lambda + \mu)} [ (\lambda + 2\mu) (A - 2C - 4D) + B (3\lambda + 2\mu) ] \]  

\[ t_{1_{\text{ext},S}} = \frac{3M_{\text{ext}} X_2}{2l^3} \]  

\[ A_{\lambda} - 2C - 4D + B (3\lambda + 2\mu) \]  

\[ t_{2_{\text{ext},Q}} = t_{2_{\text{ext},S}} = \frac{3Q X_2 [(3\lambda + 4\mu) (A - 2C) + \lambda (B + 4D)]}{16l^3\mu (\lambda + \mu)} \]  

\[ t_{1_{\text{ext},T}} = -t_{1_{\text{ext},T}} = \frac{3QL [(5\lambda + 8\mu) A - (\lambda + 4\mu) B - 2\lambda C + (\lambda + 2\mu) 4D]}{16l^3\mu (\lambda + \mu)} \]  

\[ t_{2_{\text{ext},R}} = t_{2_{\text{ext},T}} = \frac{-3Q (L - X_1) [(\lambda + 2\mu) (A - 2C - 4D) + (3\lambda + 2\mu) B]}{16l^3\mu (\lambda + \mu)} \]  

and the only wedge conditions that are not implied by (59-62) are as follows,

\[ (f_{1_{\text{ext}}}^c)_{V_1} = -(f_{1_{\text{ext}}}^c)_{V_4} = -\frac{3QL [(\lambda + 2\mu) (A - B + 2C) + 4\mu D]}{8l^3\mu (\lambda + \mu)} \]  

\[ (f_{2_{\text{ext}}}^c)_{V_1} = (f_{2_{\text{ext}}}^c)_{V_4} = \frac{3Q [(3\lambda + 4\mu) (A - B) - 2\lambda C + 4 (2\lambda + 3\mu) D]}{8l^2\mu (\lambda + \mu)} \]  

\[ (f_{1_{\text{ext}}}^c)_{V_2} = 0, \quad (f_{1_{\text{ext}}}^c)_{V_3} = 0. \]

The analytical solution of this problem is achieved in [61] and here represented in terms of the
3.4 The flexure problem

Figure 12: Numerical simulation for the flexure problem. In particular, (a) horizontal and (b) vertical displacements are represented.

Figure 13: Comparison between the exact analytical solution and numerical simulation through the horizontal cuts of Fig. 6a. In particular, (a) horizontal and (b) vertical displacements are represented.

displacement field,

\[
\begin{align*}
    u_1 &= -\frac{Q X_2 \left[ (\lambda + 2\mu) \left( 3X_1^2 - X_2^2 - 6LX_1 \right) + 2 (\lambda + \mu) \left( 6l^2 - X_2^2 \right) \right]}{16l^3 \mu (\lambda + \mu)}, \\
    u_2 &= -\frac{Q \left[ (3L - X_1) (\lambda + 2\mu) X_1^2 + 3 (L - X_1) \lambda X_2^2 \right]}{16l^3 \mu (\lambda + \mu)},
\end{align*}
\]

(71)  

(72)

The numerical simulations of this problem are shown in Figs. 12.

The comparisons between the exact analytical solution and the numerical simulation have been done through the horizontal and vertical cuts of Figs. 6 and the respective numerical simulation is shown in Figs. 13 and 14.
3.5 Convergence analysis for the wedge force problem

We consider again the bending problem with the same kinematical restrictions (48) (see also Fig. 4), the same external forces per unit area (49), the same edge boundary conditions (50-53) but with null edge forces and double forces at side $C$ as follows,

$$t_1^{ext,S} = 0, \quad \tau_2^{ext,Q} = \tau_2^{ext,S} = 0, \quad \tau_2^{R,ext} = \tau_2^{T,ext} = 0,$$

and with the following system of wedge conditions

$$(f_2^{ext})_V^1 = 0, \quad (f_2^{ext})_V^2 = 0, \quad (f_2^{ext})_V^3 = -F, \quad (f_2^{ext})_V^4 = 0, \quad (f_1^{ext})_V^2 = - (f_1^{ext})_V^3 = 0.$$

Even in this modified bending case we do not have an analytical solution but we make numerical simulations, that are shown in Figs 15. On the left-hand side we show the results of a numerical simulation of the analogous problem in the classical first gradient model and on the right-hand side the results of a numerical simulation with the present second gradient model.

It is immediately visible from Fig. 15 that the first gradient model is not adequate for wedge concentrated external forces. In Fig. 16 a convergence analysis is performed. From such a convergence analysis we deduce that first gradient models are not adequate to model concentrated external forces.
4. Experimental evidence of elastic second gradient contribution to the deformation energy

In [31] it is shown that second-gradient energy terms allow the onset of internal shear boundary layers. These boundary layers are transition zones between two different shear deformation modes. In the same paper, on the one hand it is claimed that their existence cannot be described by a simple first-gradient model, and on the other hand that they are related to second-gradient material coefficients. In this section we show a result, on the pantographic structure of Fig. 17, that makes explicit the experimental evidence of such a boundary layer. Besides, by using the second gradient model of [25], we show that it is possible to characterize the largeness of the boundary layer in terms of the second gradient coefficient (i.e., $K_{II}$) of that model, that means that a simple first gradient model (i.e., a model with $K_{II} = 0$) is not sufficient to predict the correct experimental evidence.

The elastic non-linear anisotropic internal energy density of the model that is used in [25] to numerically evaluate the shear angles that are shown in Fig. 18 is the following,

$$U(F, \nabla F) = \sum_{\alpha=1}^{2} \left\{ \frac{K_\alpha}{2} (F_{ab}D_{b}^{\alpha} - 1)(F_{ac}D_{c}^{\alpha} - 1) + \frac{K_{II}}{2} \left[ \frac{F_{ab,c}F_{ad,e}D_{b}^{\alpha}D_{c}^{\alpha}D_{d}^{\alpha}D_{e}^{\alpha}}{F_{fg}F_{fh}D_{g}^{\alpha}D_{h}^{\alpha}} - \left( \frac{F_{ab,c}F_{ad,e}D_{b}^{\alpha}D_{c}^{\alpha}D_{d}^{\alpha}D_{e}^{\alpha}}{F_{fg}F_{fh}D_{g}^{\alpha}D_{h}^{\alpha}} \right)^2 \right] \right\}$$

(73)
Figure 16: Comparison between the vertical displacement at the center of side S in the (a) first and (b) second gradient models in the case of an external vertical wedge force at $V_3$.

\[ + \frac{K_b}{2} \left[ \arccos \frac{F_{ab}F_{ac}D_1^1 D_2^2}{\sqrt{F_{de}F_{df}D_1^1 D_2^2}} \sqrt{F_{gh}F_{gi}D_1^1 D_2^2} - \frac{\pi}{2} \right]^\gamma \]

where the two families of fibers are initially directed along the two orthogonal unit vectors $\mathbf{D}^1$ and $\mathbf{D}^2$ and where the material coefficients that have been used are $K_e = 0.134 \, MN/m$, $K_p = 159 \, N/m$ and $\gamma = 1.36$. We also remark that the bias test that is shown in Fig. 17 is accomplished by imposing a displacement, towards the direction parallel to the long side of the rectangle, of the short-side of the rectangle, that in turn is directed at $\pi/4$ with respect to the two orthogonal unit vectors $\mathbf{D}^1$ and $\mathbf{D}^2$. In the deformed configuration the angle $\varphi$ between the two families of fibers is not anymore at $\pi/2$. It is

\[ \varphi = \arccos \frac{F_{ab}F_{ac}D_1^1 D_2^2}{\sqrt{F_{de}F_{df}D_1^1 D_j^2}} \sqrt{F_{gh}F_{gi}D_1^1 D_j^2} \]

and the shear angle $\phi$ (or shear deformation in Fig. 18) is simply

\[ \phi = \varphi - \frac{\pi}{2}. \]
If we evaluate the shear angle $\phi$ along the arc-length that is shown in Fig. 17, it is almost zero near short side of the rectangle and reach a finite value by passing through a boundary layer. The largeness of such a boundary layer is related to the second gradient parameter $K_{II}$.

In Fig. 18 we show that the optimal value for the second gradient constitutive parameter $K_{II}$ is $K_{II} = 0.0192\, Nm$. However, we also shown that different values of this parameter give a wrong largeness of the boundary layer. In particular we observe that a reduction $1/4$ of the second gradient constitutive parameter $K_{II}$ give a smaller boundary layer and a magnification of $4$ give a larger boundary layer. Finally, a numerical simulation in which the second gradient contribution of the strain energy (73) is assumed to vanish, i.e. $K_{II} = 0$, produce no-boundary layer. Besides, numerically instability is observed in this last case.

5. Conclusions

A perfect overlap of numerical simulations obtained with a commercial code and closed form solution of selected classical benchmark boundary value problems have bee found and reported in this paper. The role of external double and wedge forces has also been presented. Besides, we show a mesh-independent behaviour of second gradient numerical solution with respect to the correspond-
Figure 18: The boundary layer of the case related to the experiment that is shown in Fig. 17 is shown. The angles across the two families of fibers in the deformed configuration are evaluated by image analysis of the experimental result of Fig. 17 and by numerical simulations with different values of second gradient coefficients $K_{II}$.

ing first gradient counterpart. Finally, we show an experimental bias test on a specific pantographic structure and extrapolate an internal boundary layer in terms of the shear angles across initially orthogonal fibers. A non-linear anisotropic model is also presented aimed to reproduce the shown experimental results. In particular, we exhibit comparisons between the numerical simulation of the proposed theoretical model and the experimental results in terms of the internal boundary layer. Such a comparison has permitted to identify the second gradient coefficient of this model.

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