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Unified finite element methodology for gradient elasticity

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ABSTRACT

In this paper a unified finite element methodology based on gradient-elasticity is proposed for both two- and three-dimensional problems, along with some considerations about the best integration rules to be used and a comprehensive convergence study. From the convergence study it has emerged that for both two and three-dimensional problems, the implemented elements show a convergence rate virtually equal to the corresponding theoretical values. Recommendations on optimal element size are also provided. Furthermore, the ability of the proposed methodology to remove singularities in statics has been demonstrated through a couple of examples, in both two and three dimensions.

1. Introduction

Classical continuum theories are used to solve various fundamental engineering problems and applications. Even if these theories are capable of solving problems in which the scale of the unknowns is appreciable by the human eye, they have been used to characterise phenomena at a very small (atomistic) as well as extremely big (astronomic) scale. Furthermore, classical elasticity has also been recently applied to describe deformation problems at the micron and nano-scale.

Experimental observations have suggested that, at these two last scales of observation, classical continuum theories fail in the accurate description of deformation phenomena. In particular, classical theories produce singularities in the strain and stress fields, for example in correspondence of crack tips and dislocation lines. Furthermore, they are not able to capture size effects, even if the influence of size effects increases with the decrease of the component size.

The failure of classical continuum theories in the description of the above problems is linked to the absence of an internal length in the constitutive equations, representative of the underlying microstructure. To overcome the previously described deficiencies, it has been proposed to enrich the constitutive equations, through the introduction of high-order gradients of particular state variable (e.g. strains or stresses), accompanied by internal length parameters (see [1] for an overview).

The idea of using gradient elasticity to describe the mechanical behaviour of materials and structures dates back to the second half of the 19th century; however, the purpose of these theories has changed significantly over the years (a comprehensive overview of the history of gradient elasticity can be found in [1]).

Despite its ability to overcome the deficiencies of classical elasticity in the solution of different problems, gradient elasticity has not found a significant diffusion in practical applications yet. One of the principal reasons is its non-trivial finite element implementation, mainly related to the continuity requirements imposed on the discretisation. In fact, while the standard equations of solid mechanics are usually second order partial differential equations (p.d.e.), the governing equations of gradient elasticity are typically fourth-order p.d.e.; this means that the discretisation of the gradient elasticity equations requires at least $\mathcal{C}^1$-continuous shape functions, instead of the usual $\mathcal{C}^0$-continuous shape functions, which cannot be straightforwardly defined and implemented in a finite element methodology.

There are two main approaches followed to implement gradient elasticity into a finite element methodology (for a more detailed overview see [1,2]). The first one comprehends approaches that leave the continuum mechanics equations intact, by using Meshless methods [3–11], Penalty methods [12–14], Hermitian finite elements [15–18], next nearest neighbour interaction (instead of the simpler nearest neighbour interaction used in the standard finite element software) [19], etc. The second one includes approaches that transform the governing equations, in order to obtain less demanding continuity requirements; among these is the Ru-Aifantis theorem [20] which splits the original fourth-order p.d.e. in two uncoupled sets of second-order p.d.e.

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In this paper, we build on the finite element technology developed by [2,21] in that we use the aforementioned Ru-Aifantis theorem as a starting point to develop a straightforward C^0-continuous implementation. The work of these earlier papers is extended from 2D to 3D and higher-order elements, whilst also a comprehensive study of optimal numerical integration rules is provided and in-depth convergence studies have been carried out. Thus, recommendations on element types and sizes can now be made.

While in Section 2 the Ru-Aifants theory, implemented in the proposed methodology, is briefly reviewed, in Section 3 an effective C^0 finite element implementation of this theory is described. Section 4 provides details about the best integration rules to use for each of the different implemented finite elements, whilst in Section 5 the convergence behaviours of the different implemented elements are compared and analysed for problems without singularities and in Section 6 the same has been done for a problem characterised by the presence of a singularity. Recommendations on optimal element size are also provided. In Section 7 original results, obtained by applying the proposed methodology to two different problems, are presented in order to demonstrate the ability of the methodology to remove singularities from the stress field for both two- and three-dimensional problems.

2. Ru-Aifantis theory of gradient elasticity

At the beginning of the 1990s, Aifantis and coworkers proposed to enrich the constitutive relations of classical elasticity by means of the Laplacian of the strain as [20,22,23]

$$\sigma_{ij} = C_{ijkl}(\varepsilon_{kl} - \ell^2 \varepsilon_{kl,mm}) \tag{1}$$

where σ_{ij} and ε_{kl} are, respectively, the stress and strain tensor, C_{ijkl} is the constitutive tensor and ℓ is a length scale parameter. The related equilibrium equations are

$$C_{ijkl}(u_{k,jl} - \ell^2 u_{k,jlmm}) + b_i = 0 \tag{2}$$

where u_k is the displacement field and b_i are the body forces.

In a later work [20], Ru and Aifantis proposed an *operator split*, which allows the solution of the fourth-order equilibrium Eq. (2) as a decoupled sequence of two sets of second-order p.d.e., that is

$$C_{ijkl}u^c_{k,jl} + b_i = 0 \tag{3}$$

followed by the following reaction–diffusion equation

$$u^g_k - \ell^2 u^g_{k,mm} = u^c_k \tag{4}$$

that represents the relation between the local displacements u^c_i, obtained by solving the equations of classical elasticity Eq. (3) (carrying for this reason the superscript c), and the non-local displacements u^g_i, affected by the gradient activity (superscript g), which are the same displacements appearing in Eq. (2).

Substituting Eq. (4) into Eq. (3), the original Eq. (2) are recovered and imposing suitable boundary conditions the solution of Eqs. (3) and (4) coincides with that of the original Eq. (2). Nevertheless, the most interesting aspect of Eqs. (3) and (4) is their uncoupled format, which significantly simplifies both the analytical and numerical solution of the system of equations.

The first Ru-Aifantis approach introduces the gradient-enrichment in terms of displacements, as given in Eq. (4), but through a simple differentiation it is also possible to express the gradient-enrichment in terms of strains [2,24,25], that is

$$\varepsilon^g_{kl} - \ell^2 \varepsilon^g_{kl,mm} = \varepsilon^c_{kl} = \frac{1}{2}(u^c_{k,l} + u^c_{l,k}) \tag{5}$$

or stresses as [2,26]

$$\sigma^g_{ij} - \ell^2 \sigma^g_{ij,mm} = C_{ijkl}u^c_{k,l} \tag{6}$$

3. Finite element implementation

As briefly explained in Section 2 and in more details in [1], the Ru-Aifantis theorem consists in solving two uncoupled sets of second-order p.d.e. instead of the original fourth-order p.d.e., which significantly simplifies the solution of the problem. From now on matrix–vector notation is adopted, instead of the index notation used in Section 2.

The first step of the Ru-Aifantis theory consists in determining the local displacements $\mathbf{u}^c$ by solving the second-order p.d.e. of classical elasticity:

$$\mathbf{L}^T\mathbf{C}\mathbf{L}\mathbf{u}^c + \mathbf{b} = 0 \tag{7}$$

where $\mathbf{b}$ are the body forces, $\mathbf{C}$ is the constitutive matrix, while the derivative operator $\mathbf{L}$ is defined as

$$\mathbf{L} = \begin{bmatrix} \frac{\partial}{\partial x} & 0 & 0 & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} & 0 \\ 0 & \frac{\partial}{\partial y} & 0 & \frac{\partial}{\partial x} & 0 & \frac{\partial}{\partial z} \\ 0 & 0 & \frac{\partial}{\partial z} & 0 & \frac{\partial}{\partial x} & \frac{\partial}{\partial y} \end{bmatrix}^T \tag{8}$$

The continuum local displacements $\mathbf{u}^c = \left[u^c_x, u^c_y, u^c_z\right]^T$ are expressed in terms of the nodal local displacements $\mathbf{d}^c = \left[d^c_{1x}, d^c_{1y}, d^c_{1z}, d^c_{2x}, d^c_{2y}, d^c_{2z}, \ldots\right]^T$ through the relation $\mathbf{u}^c = \mathbf{N_u}\mathbf{d}^c$, where $\mathbf{N_u}$ is the matrix which collects the traditional shape functions N_i and can be written as:

$$\mathbf{N_u} = \begin{bmatrix} N_1 & 0 & 0 & N_2 & 0 & 0 & \ldots \\ 0 & N_1 & 0 & 0 & N_2 & 0 & \ldots \\ 0 & 0 & N_1 & 0 & 0 & N_2 & \ldots \end{bmatrix} \tag{9}$$

Considering the finite element discretisation just described and integrating by parts, the weak form of Eq. (7) reads

$$\int_\Omega \mathbf{B}^T_u\mathbf{C}\mathbf{B}_u d\Omega\, \mathbf{d}^c \equiv \mathbf{K}\mathbf{d}^c = \mathbf{f} \tag{10}$$

where $\mathbf{K}$ is the stiffness matrix, $\mathbf{B}_u = \mathbf{L}\mathbf{N}_u$ is the strain–displacement matrix and $\mathbf{f}$ is the force vector, where the contributions of both the body forces and the external tractions are included.

At this point, knowing the local displacements $\mathbf{u}^c$ from the previous step, it is possible to evaluate the stress field by solving the second set of equations (second step):

$$(\boldsymbol{\sigma}^g - \ell^2\nabla^2\boldsymbol{\sigma}^g) = \mathbf{C}\mathbf{L}\mathbf{u}^c \tag{11}$$

where $\boldsymbol{\sigma}^g$ is the non-local stress tensor and the derivative operator ∇ is defined as

$$\nabla = \begin{bmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{bmatrix} \quad \text{with} \quad \nabla^2 \equiv \nabla^T\nabla \tag{12}$$

Considering the weak form of Eq. (11) and integrating by parts, we obtain

$$\int_\Omega \left[\mathbf{w}^T\boldsymbol{\sigma}^g + \ell^2\left(\frac{\partial \mathbf{w}^T}{\partial x}\frac{\partial \boldsymbol{\sigma}^g}{\partial x} + \frac{\partial \mathbf{w}^T}{\partial y}\frac{\partial \boldsymbol{\sigma}^g}{\partial y} + \frac{\partial \mathbf{w}^T}{\partial z}\frac{\partial \boldsymbol{\sigma}^g}{\partial z}\right)\right] d\Omega - \oint_\Gamma \mathbf{w}^T\ell^2(\mathbf{n}\cdot\nabla\boldsymbol{\sigma}^g)d\Gamma = \int_\Omega \mathbf{w}^T\mathbf{C}\mathbf{L}\mathbf{u}^c d\Omega \tag{13}$$