Static analysis of Gradient Elastic 3-D solids with surface energy by BEM

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Abstract: A three dimensional (3-D) boundary element methodology (BEM) is presented for the static analysis of three-dimensional solids and structures on the basis of a combination of the gradient elastic theories of Mindlin and Aifantis enhanced with surface energy terms, as described by Vardoulakis and co-workers. The gradient elastic fundamental solution as well as the boundary integral representations for displacements and their normal derivatives are presented. Quadratic quadrilateral boundary elements are employed and the singular integrals are numerically computed using advanced algorithms. A numerical example demonstrates the accuracy of the above methodology.

Key-Words: Boundary Element Method, Gradient elasticity, Surface energy.

1 Introduction

The effect of microstructure on the macroscopic description of the mechanical behavior of a linear elastic material can be adequately taken into account with the aid of higher-order strain gradient theories. Among those who have developed such theories one can mention Mindlin[1, 2], Aifantis[3, 4] and Vardoulakis and Sulem[5]. Although Mindlin's theory can be considered as the most general and comprehensive gradient elastic theory appearing to date in the literature, the simpler theories of Aifantis and Vardoulakis have been successfully used in the past to eliminate singularities or discontinuities of classical elasticity theory and to demonstrate their ability to capture size and edge effects, necking in bars, nano-structured materials behavior and wave dispersion in cases where this was not possible in the classical elasticity framework. However, use of the gradient elastic theory in boundary value problems increases considerably the solution difficulties in comparison with the case of classical elasticity. For this reason, the need of using numerical methods for the treatment of those problems is apparent. Shu et al[6] and Amanatidou and Aravas[7] have used the finite element method (FEM) for solving two-dimensional elastostatic problems in the framework of the general theories of Mindlin, while Polyzos et al[8] employing the boundary element method (BEM) have solved three dimensional elastostatic problems in the context of the simple strain-gradient theory proposed by Aifantis and co-workers. In the present work a direct BEM for solving three-dimensional (3D) elastostatic problems in the framework of the gradient with surface energy theory, described in the book of Vardoulakis and Sulem[5], is addressed. The paper is structured as follows: The constitutive equations and the classical as well as the non-classical boundary conditions of the problem are presented in the next section. The integral representation of the problem, for both cases
of smooth and non-smooth boundaries, is given in section 3. In section 4, the numerical implementation of the method and the BEM solution procedure are illustrated. Finally, in section 5 a numerical example that demonstrates the high accuracy of the method is given.

2 Constitutive Equations-Boundary Conditions

In this section the equation of equilibrium and the corresponding boundary conditions that should be satisfied by any linear elastic material with microstructure described by the gradient elastostatic theory with surface energy [9] are presented in brief. Consider a three dimensional linear elastic body with microstructure of volume \( V \) surrounded by a surface \( S \). The geometry of this body is described with the aid of the unit normal vector \( \mathbf{n} \) on \( S \) and a Cartesian co-ordinate system \( OX_1X_2X_3 \) with its origin located interior to \( V \). For this body, Mindlin [1], considering isotropic materials and a special case of his theory where the macroscopic strain coincides with the micro-deformation, defines the variation of the potential energy-density as follows

\[
\delta W = \mathbf{\tau} : \delta \mathbf{e} + \mathbf{\bar{\mu}} : \nabla \delta \mathbf{e}
\]  

(1)

where \( \mathbf{\tau} \) is the Cauchy stress tensor being in duality with the macroscopic strain tensor \( \mathbf{\varepsilon} \) and \( \mathbf{\bar{\mu}} \) is a third order tensor, called by Mindlin double stress tensor, which is dual to the strain gradient \( \nabla \mathbf{\varepsilon} \). The two and three dots in Eq. (1) indicate inner product between tensors of second and third order, respectively. Considering the variation of the potential energy-density (1) over \( V \) and performing some algebra [8], one obtains the following gradient elastic equation of equilibrium

\[
\nabla \cdot (\mathbf{\tau} - \mu \nabla \mathbf{\varepsilon}) + \mathbf{f} = 0
\]  

(2)

accompanied by the classical boundary conditions

\[
\begin{align*}
\mathbf{p}(\mathbf{x}) &= \mathbf{n} \cdot \mathbf{\tau} - (\mathbf{n} \otimes \mathbf{n}) : \frac{\partial \mathbf{\bar{\mu}}}{\partial \mathbf{n}} \\
\mathbf{u}_0 - (\mathbf{\nabla}_{\mathbf{S}} \cdot \mathbf{n}) - \mathbf{n} \cdot [\nabla_{\mathbf{S}} \cdot (\mathbf{\bar{\mu}})^{(213)}] + \\
\mathbf{n} \cdot (\mathbf{\nabla}_{\mathbf{S}} \cdot \mathbf{n}) (\mathbf{n} \otimes \mathbf{n}) : \mathbf{\bar{\mu}} - (\mathbf{\nabla}_{\mathbf{S}} \mathbf{n}) : \mathbf{\bar{\mu}} &= \mathbf{P}_0 \\
\mathbf{u}(\mathbf{x}) &= \mathbf{u}_0
\end{align*}
\]  

(3)

and/or

\[
\mathbf{R}(\mathbf{x}) = \mathbf{n} \cdot \mathbf{\bar{\mu}} = \mathbf{R}_0
\]

and/or

\[
\frac{\partial \mathbf{u}(\mathbf{x})}{\partial \mathbf{n}} = \mathbf{q}_0
\]

(4)

\[
\mathbf{E}(\mathbf{x}) = \| (\mathbf{\bar{\mu}} \otimes \mathbf{n}) : \mathbf{\bar{\mu}} \| = \mathbf{E}_0
\]

where \( \mathbf{P}_0, \mathbf{u}_0, \mathbf{R}_0, \mathbf{q}_0 \) and \( \mathbf{E}_0 \) denote prescribed values. The vector \( \mathbf{f} \) in Eq. (2) represents body forces while The symbols \( \otimes \) and \( \nabla_{\mathbf{S}} \) indicate dyadic product and surface gradient. The double lines \( \| \| \) in Eq. (4) stand for the difference of the values of the function \( \circ \) taken at two surfaces \( S_1 \) and \( S_2 \), which form a corner across a line \( C \). Mindlin relates the double stress tensor \( \mathbf{\bar{\mu}} \) with the strain gradient \( \nabla \mathbf{\varepsilon} \) through the classical Lame’ constants \( \lambda, \mu \) and five more material constants. An alternative and mathematically more tractable theory is that proposed by Vardoulakis and Sulem [5] where the double stresses are correlated to the space derivatives as follows

\[
\mathbf{\tau} = \mathbf{\tau}^{(\circ)} + \ell \cdot \nabla \mathbf{\tau}^{(\circ)}
\]

(5)

\[
\mathbf{\bar{\mu}} = \ell \otimes \mathbf{\tau}^{(\circ)} + g^2 \nabla \mathbf{\tau}^{(\circ)}
\]

(6)

\[
\mathbf{\tau}^{(\circ)} = 2\mu \mathbf{\bar{\varepsilon}} + \lambda \left( \mathbf{tr} \mathbf{\bar{\varepsilon}} \right) \mathbf{I}
\]

(7)

\[
\mathbf{\bar{\varepsilon}} = \frac{1}{2} \left( \nabla \mathbf{u} + \mathbf{u} \nabla \right), \quad \mathbf{tr} \mathbf{\bar{\varepsilon}} = \nabla \cdot \mathbf{u}
\]

(8)

where \( g^2 \) is the volumetric energy strain gradient coefficient, the only constant that relates the microstructure, and \( \ell \) is the surface energy strain gradient vector coefficient. \( \mathbf{\bar{\varepsilon}} \) represents unit tensor and \( \mathbf{u} \) displacements. Adopting the above strain gradient theory with surface energy and inserting the constitutive Eqs (5)-(8) into Eq. (2) one obtains the equation of equilibrium of a gradient elastic continuum with surface energy in terms of the displacement field \( \mathbf{u} \) in the form

\[
\mu \nabla^2 \mathbf{u} + (\lambda + \mu) \nabla \nabla \cdot \mathbf{u} -
\]

\[
g^2 \nabla^2 \left( \mu \nabla^2 \mathbf{u} + (\lambda + \mu) \nabla \nabla \cdot \mathbf{u} \right) + \mathbf{f} = 0
\]

(9)

3 Boundary integral representation of a 3-D Gradient elastic problem with surface energy

As it is proved in [8], the integral representation of the problem described in the previous section is
where the vector $\tilde{p}$ represents the surface traction vector given by Eq. (3), $R$ is the double traction vector given in Eq. (4) and $\tilde{u}^*(x,y)$ is the fundamental solution of Eq. (9) that, as it is shown in [8], has the following form

$$\tilde{u}^*(x,y) = \frac{1}{16\pi\mu(1-\nu)}[\Psi(r)\hat{1} - X(r)\hat{r} \otimes \hat{r}]$$

(11)

where $\nu$ is the Poisson ratio, $\hat{r}$ the unit vector in the direction $r = y - x$ and $X$, $\Psi$ are scalar functions given by the relations

$$X(r) = -\frac{1}{r} + \frac{6g^2}{r^3} - \left(\frac{6g^2}{r^3} + \frac{6g^2}{r^3} + \frac{2}{r}\right)e^{-rg}$$

$$\Psi(r) = (3 - 4\nu)\frac{1}{r} + 2(1 - 2\nu)\left[-\frac{g^2}{r^2} + \left(\frac{g^2}{r^2} + \frac{g^2}{r^2}\right)e^{-rg}\right]$$

$$+ 4(1 - \nu)\left[\frac{g^2}{r^2} - \left(\frac{g^2}{r^2} + \frac{g^2}{r^2} + \frac{1}{r}\right)e^{-rg}\right]$$

(12)

For the gradient coefficient $g$ being equal to zero, one can easily prove that

$$X(r) = -\frac{1}{r} \quad \Psi(r) = \frac{(3 - 4\nu)}{r}$$

(13)

are the expressions of the 3-D classical elastostatic fundamental solution$^{10}$. Also, utilising the Taylor expansion

$$e^{-rg} = 1 - \frac{r}{g} + \frac{r^2}{2!g^2} - \frac{r^3}{3!g^3} + \frac{r^4}{4!g^4} - \cdots$$

(14)

it is easy to prove one$^{8}$ that both functions $X$ and $\Psi$ given by Eqs (12), are regular with respect to the distance $r \rightarrow 0$ according to the asymptotic relations

$$X(r) = O(1), \quad \Psi(r) = O(r)$$

(15)

The integral representation (10) concerns smooth boundaries. In case where the boundary is non smooth consisting of two smooth surfaces $S_1$ and $S_2$ intersecting across the closed line $C$, then the integral representation (10) is replaced by the following one

$$\tilde{c}(x) \cdot u(x) + \int_S \left\{ \tilde{p}^*(x,y) \cdot u(y) - \tilde{u}^*(x,y) \cdot p(y) \right\} dS_y +$$

$$\int_C \left\{ \frac{\partial\tilde{u}^*(x,y)}{\partial n_y} \cdot R(x,y) - \frac{\partial\tilde{R}^*(x,y)}{\partial n_y} \cdot \frac{\partial u(y)}{\partial n_y} \right\} dC_y$$

(16)

(17)

where $\tilde{c}(x)$ is the well-known jump tensor$^{10}$, and $E$ is the vector defined in Eq. (4). All the kernels appearing in the integral Eqs. (10) and (16) are given explicitly in [11]. Observing Eq. (21), one realizes that this equation contains two unknown vector fields, $u(x)$ and $\tilde{u}(x)$. For example, for the case of the traction field $p(x)$ prescribed on $S$ (classical boundary condition) as well as the fields $R(x)$ and $E(x)$ prescribed on $S$ (non-classical boundary conditions), the unknown vector fields in Eq. (16) are two, $u(x)$ and $\tilde{u}(x)$. Thus, the evaluation of the unknown fields $u(x)$ and $\tilde{u}(x)$ requires the existence of one more integral equation. This integral equation is obtained by applying the operator $\tilde{c}/\tilde{n}$ on Eq. (16) and has the form

$$\tilde{c}(x) \cdot \frac{\partial u(x)}{\partial n_x} + \int_S \left\{ \frac{\partial\tilde{p}^*(x,y)}{\partial n_y} \cdot u(y) - \frac{\partial\tilde{u}^*(x,y)}{\partial n_y} \cdot p(y) \right\} dS_y +$$

$$\int_C \left\{ \frac{\partial\tilde{u}^*(x,y)}{\partial n_y} \cdot R(x,y) - \frac{\partial\tilde{R}^*(x,y)}{\partial n_y} \cdot \frac{\partial u(y)}{\partial n_y} \right\} dC_y$$

(17)

The kernels appearing in Eq. (17) are given explicitly in [11]. The integral Eqs (16) and (17) accompanied by the classical and non-classical boundary conditions form the integral representation of any gradient elastic boundary value problem.

4 BEM Solution procedure

The boundary element methodology presented in this section concerns 3D elastostatics problems of structures with smooth surface $S$. Thus, according to Eqs (16) and (17) the integral representation of the problem takes the form

$$\frac{1}{2} u(x) + \int_S \left\{ \tilde{p}^*(x,y) \cdot u(y) - \tilde{u}^*(x,y) \cdot p(y) \right\} dS_y =$$

$$\int_S \left\{ \frac{\partial\tilde{u}^*(x,y)}{\partial n_y} \cdot R(x,y) - \frac{\partial \tilde{R}^*(x,y)}{\partial n_y} \cdot \frac{\partial u(y)}{\partial n_y} \right\} dS_y$$

(18)
The goal of the Boundary Element methodology is to solve numerically the well-posed boundary value problem constituted by the system of two integral equations (18) and (19) and the boundary conditions (Eqs (3) and (4)). To this end the smooth surface \(S\) is discretised into \(E\) eight-noded quadrilateral and/or six-noded triangular quadratic continuous isoparametric boundary elements. For a nodal point \(k\) the discretized integral equations (18) and (19) have the following form

\[
\frac{1}{2} \mathbf{u}(x) + \sum_{\alpha=1}^{A} \sum_{\beta=1}^{A} \int_{S} \mathbf{p}(x, y) \mathbf{N}^{\alpha} J d\xi_{1} d\xi_{2} \cdot \mathbf{u}_{\beta} + \sum_{\alpha=1}^{A} \sum_{\beta=1}^{A} \int_{S} \mathbf{R}(x, y) \mathbf{N}^{\alpha} J d\xi_{1} d\xi_{2} \cdot \mathbf{q}_{\beta} = \]

\[
\frac{1}{2} \mathbf{q}(x) + \sum_{\alpha=1}^{A} \sum_{\beta=1}^{A} \int_{S} \mathbf{p}(x, y) \mathbf{N}^{\alpha} J d\xi_{1} d\xi_{2} \cdot \mathbf{u}_{\beta} + \sum_{\alpha=1}^{A} \sum_{\beta=1}^{A} \int_{S} \mathbf{R}(x, y) \mathbf{N}^{\alpha} J d\xi_{1} d\xi_{2} \cdot \mathbf{q}_{\beta} =
\]

where \(\mathbf{q} = \frac{\partial \mathbf{u}}{\partial n}\), \(A(e)\) is the number of nodes of the current element \(e\) with \(y^{*}(\xi, \xi)\) \((A = 8 \text{ or } 6 \text{ for quadrilateral or triangular elements, respectively}), \mathbf{N}^{a} \mathbf{N}^{\beta}(\xi, \xi)\) \((a = 1, 2, \ldots, A)\) the shape functions of a typical quadrilateral or triangular quadratic element, \(J(\xi, \xi)\) the corresponding Jacobian magnitude of the transformation from the global to the local co-ordinate system \(\xi, \xi\) and \(\mathbf{u}_{\alpha}, \mathbf{q}_{\beta}, \mathbf{p}_{\alpha}, \mathbf{R}_{\beta}\) are the nodal values of the corresponding field functions. Adopting now a global numbering for the nodes, each pair \((e, a)\) is associated to a number \(\beta\) and the integral equations (20) are written as

\[
\frac{1}{2} \mathbf{u}_{\beta} + \sum_{\beta=1}^{L} \mathbf{H}_{\beta} \mathbf{u}_{\beta} + \sum_{\beta=1}^{L} \mathbf{K}_{\beta} \mathbf{q}_{\beta} = \sum_{\beta=1}^{L} \mathbf{G}_{\beta} \mathbf{p}_{\beta} + \sum_{\beta=1}^{L} \mathbf{L}_{\beta} \mathbf{R}_{\beta}
\]

\[
\frac{1}{2} \mathbf{q}_{\beta} + \sum_{\beta=1}^{L} \mathbf{S}_{\beta} \mathbf{u}_{\beta} + \sum_{\beta=1}^{L} \mathbf{T}_{\beta} \mathbf{q}_{\beta} = \sum_{\beta=1}^{L} \mathbf{V}_{\beta} \mathbf{p}_{\beta} + \sum_{\beta=1}^{L} \mathbf{W}_{\beta} \mathbf{R}_{\beta}
\]

where \(L\) is the total number of nodes. Collocating Eqs (21) at all nodal points \(L\), one obtains the following linear system of algebraic equations

\[
\left[ \begin{array}{c}
\frac{1}{2} \mathbf{I} + \mathbf{H} \\
\mathbf{S}
\end{array} \right] \left[ \begin{array}{c}
\mathbf{u} \\
\frac{1}{2} \mathbf{I} + \mathbf{T}
\end{array} \right] \left[ \begin{array}{c}
\mathbf{q} \\
\mathbf{p}
\end{array} \right] = \left[ \begin{array}{c}
\mathbf{G} \\
\mathbf{L} \\
\mathbf{V} \\
\mathbf{W} \\
\mathbf{R}
\end{array} \right]
\]

where matrices \(\mathbf{H}, \mathbf{K}, \mathbf{S}, \mathbf{T}, \mathbf{G}, \mathbf{L}, \mathbf{V}\) and \(\mathbf{W}\) contain all the submatrices given by Eqs. (20), respectively. Applying the boundary conditions (Eqs (3) and (4)) and rearranging Eq. (22) one produces the final linear system of algebraic equations of the form

\[
\mathbf{A} \cdot \mathbf{X} = \mathbf{B}
\]

where the vectors \(\mathbf{X}\) and \(\mathbf{B}\) contain all the unknown and known nodal components of the boundary fields. In the present work the singular and hypersingular integrals appeared in Eqs (20) are evaluated with high accuracy applying a methodology for direct treatment in unified manner of CPV and hypersingular integrals proposed by [12] and [13].

5 Numerical examples

In this section two characteristic problems with known analytical solutions are presented to illustrate the accuracy of the proposed 3-D BEM.

5.1 Radial deformation of a sphere

Consider a gradient elastic with surface energy solid sphere with radius \(a\) subjected to an external uniform radial deformation and assume that the double surface traction vanishes at the boundary, i.e.,

\[
u_{r}(r = a) = u_{0}
\]

\[
R|_{r=a} = 0
\]

where \(u_{r}\) is the radial displacement, \(R\) is the double surface traction and \(r\) the distance from the center of the sphere. This problem can be easily solved analytically and its solution is presented in [11], i.e.,

\[
u_{r}(r) = c_{1} r + c_{2} F(r)
\]

where

\[
F(r) = -g \frac{\sinh(r/g)}{r} + g \frac{\cosh(r/g)}{r}
\]
and $c_1$, $c_2$ known constants depicted by applying the boundary conditions (24), (25) in Eq. (26). The problem has also been solved numerically by the BEM presented in the previous section for $\alpha = 1$ and $u_0 = 1$. Due to the symmetry of the problem, only one octant of the sphere needs to be discretized. In the present work, a mesh of thirty-eight quadrilateral quadratic elements was used. The radial displacement and its first derivative (radial strain) as functions of the distance $r$ for a value of the material characteristic length $g^2$ and different values of the surface energy parameter $\ell$ have been evaluated. The results, as it is evident in Figs 1.a & b, are in a very good agreement with those obtained analytically by using Eq. (26). In the same figures the classical elasticity solution is also displayed for reasons of comparison.

Consider now, the problem of a spherical cavity of radius $\alpha$ embedded into an infinite gradient elastic with surface energy 3D space and subjected to an external pressure $P_0$ radially applied at infinity, while the double stresses $R$ vanish at the boundary. Thus, the boundary conditions of the problem read

$$P(r)\bigg|_{r=a} = P_0 \hat{r}$$

(28)

$$R(r)\bigg|_{r=a} = 0$$

(29)

This problem can be easily solved analytically and its solution has the form

$$u = \left\{ \frac{1}{r} + D \frac{G(r)}{r^2} \right\} \hat{r},$$

(30)

with $G(r) = \sqrt{\frac{\pi}{2(r/g)^2}} K_0 \left( \frac{r}{g} \right)$ and $B$ and $D$ known constants depicted applying the boundary conditions (28) and (29) into Eq. (30). The radial displacement and strain fields as well as the radial double stress of this boundary value problem obtained numerically via the proposed BEM for $\alpha = 1$, $P_0 / E$, $\nu = 0$, $g = 0.5$ and various values of the surface energy parameter $\ell$ are presented in Fig.2 (a)-(c), respectively. Again, the agreement between numerical and analytical results is very good.

### 5.2 Radial deformation of a spherical cavity
Fig. 2 (a): Radial strain versus distance $r$ for $g^2=0.25$ and various values of $\ell$.

Fig. 2 (a): Double stresses $\mu_{rr}$ versus distance $r$ for $g^2=0.25$ and various values of $\ell$.

6 Conclusions
A boundary element method has been developed for the static analysis of three-dimensional bodies characterized by a linear elastic material behavior taking into account microstructural effects with the aid of a simple strain gradient theory with surface energy. The boundary integral equations of the problem consist of one equation for the displacement and another one for its normal derivative. Their numerical implementation is accomplished with the aid of quadratic quadrilateral elements and advanced integration algorithms for the highly accurate evaluation of singular integrals. A representative numerical example has been used to illustrate the application of the method and demonstrate its advantages, which are the surface-only discretization character of the method and its accuracy.

References: