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Shell models in the framework of generalized continuum theories: isogeometric implementation and applications

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Micro Abstract
Physico-mathematical models of shells in the framework of couple stress and strain gradient elasticity theories with variational formulations are developed. The models derived are embedded into a commercial finite element software as user subroutines following the isogeometric paradigm. Practical applications such as modelling of microarchitectured materials and materials with microstructure, or problems of fracture mechanics, illustrate the advantages of the non-classical continuum theories.

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Introduction

Commercial software for computational structural engineering and applied mechanics are based on classical theories, such as theory of elasticity, which rely on classical continuum mechanics and does not take into account the material microstructure. However, materials with microstructure are the future direction of material design (cf. architectured materials, micro- and nanoelectromechanical systems MEMS and NEMS, topology optimization, 3D-printing). Generalized continua theories, incorporating length scale parameters related to additional energy terms, have shown to be appropriate for (1) modelling materials with microstructures of different scales [7], or (2) for homogenisation models of structures with substructures [8]; as well as (3) for smoothening unphysical macro-scale singularities in crack tips or sharp corners [2]. With this background, the importance of developing efficient and reliable numerical methods for these models becomes unquestionable.

In the current contribution, we consider one of the most complex representatives from a family of generalized continua theories, namely, gradient elasticity (introduced in [6]). Models and methods for some others, for example, modified couple-stress theory, can be obtained by simplifications and minor changes of the presented derivations.

Numerical methods for gradient-elastic structural models such as bars, beams or plates are well-developed and extensively covered in the literature. However, there are no contributions on numerical methods for gradient-elastic shells.

1 Energy expressions for the gradient-elastic Kirchhoff-Love shell model

The core concept of the strain gradient elasticity theory is the introduction of a new term into the internal energy of elastically deformable continuum:

$$W_{int} = \frac{1}{2}\int\limits_V \boldsymbol{S} : \boldsymbol{E}\,\mathrm{d}V + \frac{1}{2}\int\limits_V \boldsymbol{\tau} \vdots \boldsymbol{\mu}\,\mathrm{d}V, \tag{1.1}$$

where $\boldsymbol{E}$ and $\boldsymbol{S}$ stand for the energy conjugated Green-Lagrange strain and second Piola-Kirchhoff stress tensors respectively, $\boldsymbol{\mu}$ and $\boldsymbol{\tau}$ are the strain and stress tensors of third rank, and body volume is denoted by V. The third-rank strain tensor $\boldsymbol{\mu}$ is defined as the gradient of the Green-Lagrange strain tensor:

$$\boldsymbol{\mu} = \nabla \mathbf{E} = E_{ij;k} \mathbf{G}^k \otimes \mathbf{G}^i \otimes \mathbf{G}^j, \tag{1.2}$$

where indices denoted by Latin letters take values from set $\{1,2,3\}$, $\boldsymbol{G}^i$ are the local contravariant basis vectors of the reference configuration, $E_{ij;k}$ denotes the covariant derivative which in a general case of curvilinear coordinates is expressed as follows [3]:

$$E_{ij;k} = E_{ij,k} - E_{lj}\ \Gamma_{ik}^{\ l} - E_{il}\ \Gamma_{jk}^{\ l} = E_{ij,k} + E_{ij|k}, \tag{1.3}$$

with $\Gamma_{ik}^{\ l}$ standing for the second kind Christoffel symbols, "$_{,k}$" denotes the k-th partial derivative and "$_{|k}$" is just the covariant derivative without the partial derivative. Note that here and below the Einstein summation by repeated indices is applied.

Taking into account the plane stress assumption – one of the basic shell theory assumptions – we can neglect out-of-plane components of stress tensor $\boldsymbol{S} = S^{\alpha\beta} \boldsymbol{G}_\alpha \otimes \boldsymbol{G}_\beta$ (Greek letters are used for indices taking values 1 and 2). By "plane" we mean here the vectors lying in the plane tangential to the middle surface of a shell.

The constitutive laws – generalized Hooke's law and its analogue for the third-rank tensors have the following form:

$$S^{\alpha\beta} = C^{\alpha\beta\gamma\rho} E_{\gamma\rho}; \quad \tau^{i\alpha\beta} = A^{i\alpha\beta j\gamma\rho} \mu_{j\gamma\rho}, \tag{1.4}$$

where $C^{\alpha\beta\gamma\rho}$ and $A^{i\alpha\beta j\gamma\rho}$ denote the components of the tensors of elastic moduli; upper and lower indexes relate to covariant and contravariant local bases accordingly. For the isotropic case, the following expression can be established:

$$C^{\alpha\beta\gamma\rho} = \lambda \delta^{\alpha\beta} \delta^{\gamma\rho} + \mu(\delta^{\alpha\gamma}\delta^{\beta\rho} + \delta^{\alpha\rho}\delta^{\beta\gamma}), \tag{1.5}$$

with λ and μ being the Lame parameters and $\delta^{\alpha\beta}$ denoting the Kronecker delta symbol.

For the isotropic strain gradient elasticity theory, the introduction of five new material parameters for strain-stress relations is required. In a simplification by Aifantis and his co-authors (see [1], for example), the number of constants for the static case is reduced to one, denoted by g with dimension of length. With this, the components of the six-order tensor of material constants for the isotropic case can be written :

$$A^{i\alpha\beta j\gamma\rho} = g^2 \delta^{ij} \left[\lambda \delta^{\alpha\beta} \delta^{\gamma\rho} + \mu(\delta^{\alpha\gamma}\delta^{\beta\rho} + \delta^{\alpha\rho}\delta^{\beta\gamma}) \right] = g^2 \delta^{ij} C^{\alpha\beta\gamma\rho}. \tag{1.6}$$

Let us recall some expressions of the classical shell theory derived with the aid of differential geometry (see [5] for explanations). Thus, strain tensor can be decomposed into the membrane and bending parts $\varepsilon_{\alpha\beta}$ and $\kappa_{\alpha\beta}$ with the use of a straight cross section assumption:

$$E_{\alpha\beta} = \varepsilon_{\alpha\beta} + \theta^3 \kappa_{\alpha\beta}, \tag{1.7}$$

where θ^3 is the coordinate along the thickness direction of a shell.

Similarly, stress resultants can be divided by two parts, namely, normal forces $n^{\alpha\beta}$ and bending moments $m^{\alpha\beta}$ (with an assumption about a linear stress distribution along thickness t):

$$n^{\alpha\beta} = \int_{-t/2}^{t/2} S^{\alpha\beta}\, \mathrm{d}\theta^3 = t\ C^{\alpha\beta\gamma\rho} \varepsilon_{\gamma\rho}; \qquad m^{\alpha\beta} = \int_{-t/2}^{t/2} S^{\alpha\beta} \theta^3\, \mathrm{d}\theta^3 = \frac{t^3}{12}\ C^{\alpha\beta\gamma\rho} \kappa_{\gamma\rho}. \tag{1.8}$$

In view of the above, the variation of the internal strain energy can be written in the following form:

$$
\begin{aligned}
\delta W_{int} = & \int\limits_A (\boldsymbol{n} : \delta\boldsymbol{\varepsilon} + \boldsymbol{m} : \delta\boldsymbol{\kappa})\, \mathrm{d}A + g^2 \int\limits_A (\nabla_S \boldsymbol{n} \,\vdots\, \delta\nabla_S\boldsymbol{\varepsilon} + \nabla_S \boldsymbol{m} \,\vdots\, \delta\nabla_S \boldsymbol{\kappa})\, \mathrm{d}A \\
& + g^2 \int\limits_A (\frac{12}{t^2}\boldsymbol{m} + \boldsymbol{n}_{|3}) : \delta(\boldsymbol{\kappa} + \boldsymbol{\varepsilon}_{|3})\, \mathrm{d}A + g^2 \int\limits_A \boldsymbol{m}_{|3} : \boldsymbol{\kappa}_{|3}\, \mathrm{d}A,
\end{aligned}
\tag{1.9}
$$

where ∇_S stands for the surface gradient: $\nabla_S \boldsymbol{\varepsilon} = \varepsilon_{\alpha\beta;\gamma} \boldsymbol{G}^\gamma \otimes \boldsymbol{G}^\alpha \otimes \boldsymbol{G}^\beta$, and bold letters stand for tensor notations of the strains and stress resultants.

By substitution of expression (1.9) into the variational principle

$$
\delta(W_{ext} - W_{int}) = 0 \tag{1.10}
$$

and adoption of the appropriate form for the variation of work done by external forces W_{ext}, one can obtain the governing differential equations of the gradient-elastic shell model.

2 Numerical solution

All the expressions presented in the previous section are valid in the framework of non-linear theory of elasticity. For simplicity, in the following section we restrict ourself to linear formulations.

2.1 Finite-element formulation, stiffness matrix and force vector

The discretization of the displacement vector is the starting point for any finite-element formulation:

$$
\boldsymbol{u} = \sum_i^n N^i \hat{\boldsymbol{u}}^i, \tag{2.11}
$$

where n is the number of nodes, N^i are basis functions, vector $\hat{\boldsymbol{u}}^i$ contains 3 components of the displacement at each node. Therefore there are 3n degrees of freedom $u_r,\ r = 1, ..., 3n$. Equilibrium equation (1.10) must be fulfilled for any arbitrary variation of the displacement variable (degree of freedom) δu_r:

$$
\delta(W_{ext} - W_{int}) = \frac{\partial(W_{ext} - W_{int})}{\partial u_r} \delta u_r = 0, \tag{2.12}
$$

which means that

$$
\frac{\partial(W_{ext} - W_{int})}{\partial u_r} = (W_{ext} - W_{int})_{,r} = 0 \tag{2.13}
$$

and leads to the following standard finite element matrix equation:

$$
\boldsymbol{K}\hat{\boldsymbol{u}} = \boldsymbol{F}, \tag{2.14}
$$

where the components of stiffness matrix $\boldsymbol{K}$ are written as

$$
\begin{aligned}
K_{rs} = (W_{int})_{,rs} = & \int_A (\boldsymbol{n}_{,s} : \boldsymbol{\varepsilon}_{,r} + \boldsymbol{m}_{,s} : \boldsymbol{\kappa}_{,r})\, \mathrm{d}A + g^2 \int\limits_A (\nabla_S \boldsymbol{n}_{,s} \,\vdots\, \delta\nabla_S \boldsymbol{\varepsilon}_{,r} + \nabla_S \boldsymbol{m}_{,s} \,\vdots\, \delta\nabla_S \boldsymbol{\kappa}_{,r})\, \mathrm{d}A \\
& + g^2 \int\limits_A (\frac{12}{t^2}\boldsymbol{m} + \boldsymbol{n}_{|3})_{,s} : \delta(\boldsymbol{\kappa} + \boldsymbol{\varepsilon}_{|3})_{,r}\, \mathrm{d}A + g^2 \int\limits_A \boldsymbol{\mu}_{|3,s} : \boldsymbol{\kappa}_{|3,r}\, \mathrm{d}A,
\end{aligned}
\tag{2.15}
$$

and the the components of force vector $\boldsymbol{F}$ are written as

$$F_r = (W_{ext})_{,r}. \tag{2.16}$$

Equation (2.15) contains the partial derivatives of the stress and strain tensor components. In order to calculate them, it is necessary to know how the stresses and strains depend on displacements. Interested readers are advised to see section 3 of [5].

The derivations above are not specific to any certain type of basis functions N^i. However, we prioritize the isogeometric paradigm (IGA) [4] with NURBS basis functions. There are two main reasons for this choice. First, the main idea of IGA is the use of the exact CAD geometry directly for analysis, and for obvious reasons this is exceptionally beneficial for curved shells with complex geometries. Second, NURBS basis functions of order p provide C^{p-1} continuity across the element boundaries and this is especially crucial in the context of gradient elasticity for Kirchhove-Love shells requiring third-order derivatives of basis functions and, accordingly, at least C^2 continuity.

2.2 Benchmark problem: bending of a cantilever strip

For the verification of the method and its implementation accomplished as Abaqus User Element subroutines, let us consider a bending problem of a cantilever slab. The problem setting is depicted tn Figure 1.

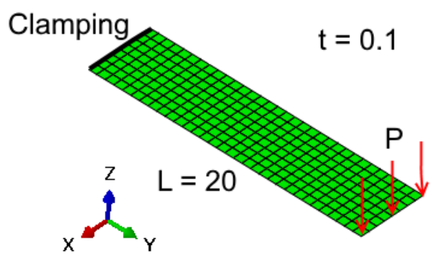

Figure 1. Problem setting.

For small strip width, the Bernoulli-Euler gradient-elastic beam model can be used as reference, giving the normalized bending rigidity expression for $g = t$ in the following form [7]:

$$\frac{D^{\nabla}}{D^{\text{class}}} \approx 1 + 12\frac{g^2}{t^2} = 13. \tag{2.17}$$

The result obtained in Abaqus for the implemented gradient-elastic user shell element show a good correlation with the analytical estimation of (2.17). Thus, the ratio of the calculated maximal deflections of the shell slab for the gradient and classical theories is (almost equal to (2.17))

$$\frac{D^{\nabla}}{D^{\text{class}}} = \frac{w^{\nabla}(L)}{w^{\text{class}}(L)} = \frac{12.8}{0.984} = 12.998. \tag{2.18}$$

Conclusions

An isogeometric Galerkin method for gradient-elastic linear Kirchhoff-Love shells is implemented as Abaqus User Element subroutines. First tests show that the implementation performs correctly but further verifications such as comparison with full-scale 3D modelling need to be accomplished as well. The realized method can be easily extended to solving problems with geometrical non-linearities and can be used for some other generalized continua models without major changes.

The theoretical background and examples in literature allows conclude that the developed method can be used in many industrial applications for more reliable modelling the mechanical behaviour of micro- and nano- objects as well as macro-objects with complex micro-architecture.

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