

A MULTI-SCALE GRADIENT ELASTICITY MODEL WITH DISPERSION CORRECTION

*Harm Askes¹ and Dario De Domenico²

¹Department of Civil and Structural Engineering, University of Sheffield, Mappin Street, Sheffield S1 3JD, UK

²Department of PAU, Università Mediterranea Reggio Calabria, Via Melissari, Reggio Calabria 89124, Italy

*h.askses@sheffield.ac.uk

ABSTRACT

We postulate a new gradient elasticity formulation with three higher-order terms and, thus, three independent length scale constants. The formulation has one higher-order stiffness term and two higher-order inertia terms. It is shown that this formulation is better able to capture the wave dispersion characteristics as seen in nano-scale experiments or layered composites. We derive a C^0 finite element implementation based on a newly developed operator split, which allows the governing fourth-order partial differential equations to be rewritten in a set of fully coupled second-order partial differential equations. The fundamental unknowns of these coupled equations are the micro-scale and macro-scale displacement; thus, this is intrinsically a fully coupled multi-scale formulation. With the reduction of the order of the equations, finite element implementation becomes straightforward.

Key Words: *gradient elasticity; wave propagation; length scale; wave dispersion; multi-scale*

1. Introduction

Wave propagation through heterogeneous media is characterised by the occurrence of dispersion, meaning that the different harmonic wave components travel with different velocities. If this is to be captured with computer simulations, classical elasticity theory is only effective if every individual micro-structural constituent is modelled separately — but such an approach is usually deemed prohibitive in terms of associated computer costs. As an alternative, gradient elasticity theory can be used. Compared to classical elasticity theory, additional spatial derivatives of relevant state variables (such as stresses, strains and/or accelerations) are included in the field equations. These additional terms are accompanied by material length scales that represent the micro-structure of the material. An overview of various gradient elasticity formulations is given in [1].

A popular gradient elasticity theory was formulated by Aifantis in the 1990s and can be written, using index notation, as

$$C_{ijkl} (u_{k,jl} - \ell^2 u_{k,jlmm}) + b_i = 0 \quad (1)$$

where u_i are the displacements and b_i are the body forces. Furthermore, C_{ijkl} contains the usual elastic constants and ℓ is a micro-structural length parameter. The Aifantis model has been shown to be effective in removing singularities from stress and strain fields such as occur at the tips of sharp cracks or dislocation cores. However, its use in dynamics is not recommended due to the appearance of unbounded phase velocities [1]. Instead, in [3] it was argued that in a dynamics context gradient enrichment should be applied simultaneously to the stiffness terms and the inertia terms. Thus, a model is obtained according to

$$\rho (\ddot{u}_i - \alpha \ell^2 \ddot{u}_{i,mm}) = C_{ijkl} (u_{k,jl} - \gamma \ell^2 u_{k,jlmm}) + b_i \quad (2)$$

where ρ is the mass density of the material. Dimensionless constants α and γ have been added so that different weights can be assigned to the two higher-order terms. It was shown that the latter model provides a reasonable approximation of the dispersive behaviour of discrete lattice model [3], however further improvement is possible as will be explored below.

2. A gradient elasticity model with two acceleration gradient terms

An effective and simple improvement of the dispersive behaviour of gradient elasticity models can be achieved by adding one more acceleration gradient term. We postulate

$$\rho (\ddot{u}_i - \alpha \ell^2 \ddot{u}_{i,mm} + \beta \ell^4 \ddot{u}_{i,mmmm}) = C_{ijkl} (u_{k,jl} - \gamma \ell^2 u_{k,jlmm}) + b_i \quad (3)$$

where β is yet another dimensionless weighting constant.

To assess the behaviour of the above models in dynamics, a dispersion analysis is carried out by substituting a trial solution $u(x, t) = U \exp(i(kx + \omega t))$ into the one-dimensional equation of motion. Here, k and ω are the wave number and angular frequency, respectively, whereas U is the amplitude. After some straightforward algebra, we obtain the following dimensionless expression:

$$\left(\frac{\omega \ell}{c_e}\right)^2 = \frac{\chi^2 (1 + \gamma \chi^2)}{1 + \alpha \chi^2 + \beta \chi^4} \quad (4)$$

where $c_e \equiv \sqrt{E/\rho}$ is the one-dimensional wave velocity of classical elasticity and $\chi \equiv k\ell$ is the wave number normalised with respect to the material length scale.

In Figure 1 we have plotted the dispersion curves for a range of parameter values. Firstly, the case $\alpha \neq 0$ with $\beta = \gamma = 0$ corresponds to a model with only one higher-order inertia term and leads to a horizontal asymptote for the dimensionless frequency. Next, the case $\alpha \neq 0$ and $\gamma \neq 0$ but $\beta = 0$ leads to a model with one higher-order stiffness term and one higher-order inertia term; in case $\alpha \neq \gamma$ the model is dispersive with a slant asymptote. Taking $\beta \neq 0$ alongside $\alpha \neq 0$ and $\gamma \neq 0$ leads again a horizontal asymptote, but there may also be an inflection point in case $\beta > \alpha\gamma$. Figure 1 includes the case where $\beta < \alpha\gamma$ which leads to a monotonically increasing curve, as well as the case $\beta > \alpha\gamma$ which predicts a curve that is concave for lower wave numbers and convex for larger wave numbers — the latter is in line with certain experimental results [4].

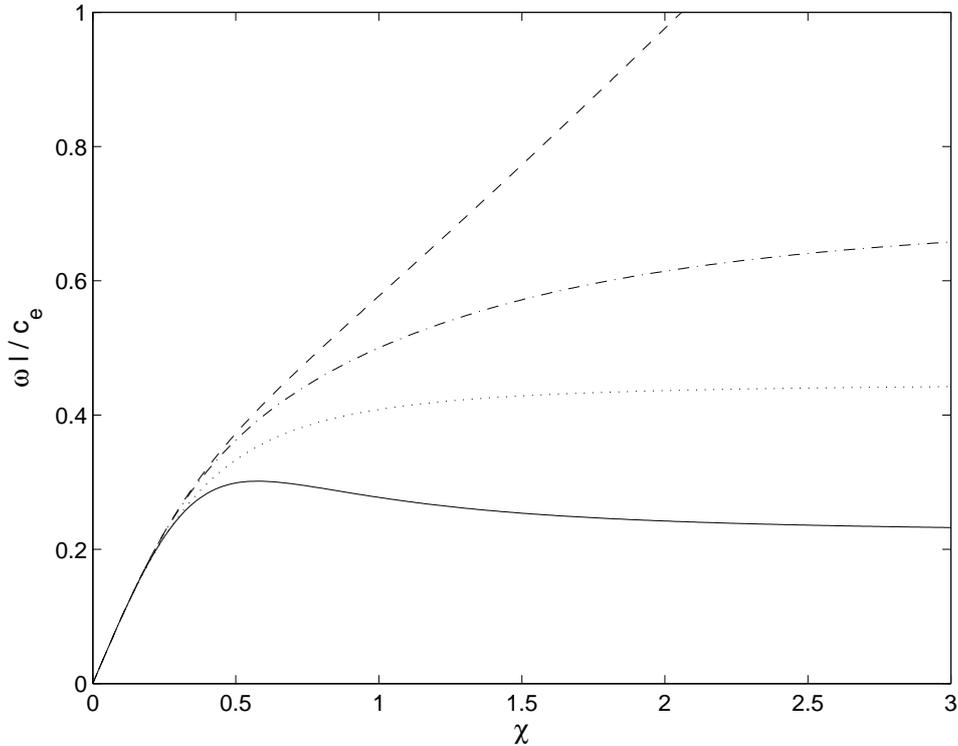


Figure 1: Dispersion curves — normalised frequency against normalised wave number for $\alpha = 5$, $\beta = 0$ and $\gamma = 0$ (dotted); $\alpha = 5$, $\beta = 0$ and $\gamma = 1$ (dashed); $\alpha = 5$, $\beta = 2$ and $\gamma = 1$ (dash-dotted); $\alpha = 5$, $\beta = 20$ and $\gamma = 1$ (solid)

3. Symmetric multi-scale formulation

The equations of motion given in expression (3) contain fourth-order spatial derivatives. This can be problematic for subsequent finite element implementations, which are usually based on C^0 -continuous interpolations. Whilst it is certainly possible to formulate C^1 finite elements for gradient elasticity [5], here we will follow another approach. An operator split has been developed by which the fourth-order spatial derivatives are rewritten in terms of second-order spatial derivatives; this leads to auxiliary equations which, as we will show, can be symmetrised.

First, the right-hand-side of Eq. (3) is rewritten according to

$$\rho \left(\ddot{u}_i^M - \alpha \ell^2 \ddot{u}_{i,mm}^M + \beta \ell^4 \ddot{u}_{i,mmmm}^M \right) = C_{ijkl} u_{k,jl}^m + b_i \quad (5a)$$

$$u_k^M - \gamma \ell^2 u_{k,mm}^M = u_k^m \quad (5b)$$

Superscripts M and m have been used to indicate macro-scale and micro-scale displacements, respectively; this nomenclature is motivated in [2]. Substituting Eq. (5b) back into Eq. (5a) would of course lead to Eq. (3), but instead we will take the double time derivative of Eq. (5b):

$$\ddot{u}_k^M - \gamma \ell^2 \ddot{u}_{k,mm}^M = \ddot{u}_k^m \quad (6)$$

This acceleration format can then be used to rewrite various terms in Eq. (5a), namely

$$\alpha \ell^2 \ddot{u}_{i,mm}^M = \frac{\alpha}{\gamma} \left(\ddot{u}_i^M - \ddot{u}_i^m \right) \quad (7)$$

and, in multiple stages,

$$\beta \ell^4 \ddot{u}_{i,mmmm}^M = \frac{\beta \ell^2}{\gamma} \left(\ddot{u}_{i,mm}^M - \ddot{u}_{i,mm}^m \right) = \frac{\beta}{\gamma^2} \left(\ddot{u}_i^M - \ddot{u}_i^m \right) - \frac{\beta \ell^2}{\gamma} \ddot{u}_{i,mm}^m \quad (8)$$

Substituting Eqns. (7) and (8) into Eq. (5a) and multiplying Eq. (6) with $\rho \left(\alpha/\gamma - \beta/\gamma^2 - 1 \right)$ leads to

$$\rho \left(\frac{\alpha\gamma - \beta}{\gamma^2} \ddot{u}_i^m - \frac{\beta \ell^2}{\gamma} \ddot{u}_{i,mm}^m - \frac{\alpha\gamma - \beta - \gamma^2}{\gamma^2} \ddot{u}_i^M \right) = C_{ijkl} u_{k,jl}^m + b_i \quad (9a)$$

$$\rho \left(-\frac{\alpha\gamma - \beta - \gamma^2}{\gamma^2} \ddot{u}_i^m + \frac{\alpha\gamma - \beta - \gamma^2}{\gamma^2} \ddot{u}_i^M - \frac{(\alpha\gamma - \beta - \gamma^2) \ell^2}{\gamma} \ddot{u}_{i,mm}^M \right) = 0 \quad (9b)$$

4. Spatial and temporal discretisation

The advantages of Eqns. (9) are that they contain at most second-order spatial derivatives (so that C^0 finite element interpolations can be used) and that they are symmetric: the coefficient of \ddot{u}_i^M in Eq. (9a) is equal to the coefficient of \ddot{u}_i^m in Eq. (9b). The latter means that symmetric system matrices can be formulated, which facilitates computer storage.

On the other hand, with the various mathematical manipulations explained above, it is no longer possible to retrieve Eq. (3) because the displacement format of Eq. (5b) has been replaced by the acceleration format of Eq. (6). However, this also means that the inf-sup condition does not apply to Eqns. (9) since the equations are no longer “reducible”. This implies that there are no constraints on the shape functions used for the two displacement fields.

Using the same shape functions \mathbf{N} for u_i^M as well as u_i^m leads to a system of semi-discretised equations as

$$\begin{bmatrix} \frac{\alpha\gamma - \beta}{\gamma^2} \mathbf{M} + \beta \ell^2 \mathbf{D} & -\frac{\alpha\gamma - \beta - \gamma^2}{\gamma^2} \mathbf{M} \\ -\frac{\alpha\gamma - \beta - \gamma^2}{\gamma^2} \mathbf{M}^T & \frac{\alpha\gamma - \beta - \gamma^2}{\gamma^2} \mathbf{M} + \frac{(\alpha\gamma - \beta - \gamma^2) \ell^2}{\gamma} \mathbf{D} \end{bmatrix} \begin{bmatrix} \ddot{\mathbf{d}}^m \\ \ddot{\mathbf{d}}^M \end{bmatrix} + \begin{bmatrix} \mathbf{K} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{d}^m \\ \mathbf{d}^M \end{bmatrix} = \begin{bmatrix} \mathbf{f} \\ \mathbf{0} \end{bmatrix} \quad (10)$$

with the usual definitions of the mass matrix \mathbf{M} and stiffness matrix \mathbf{K} , i.e.

$$\mathbf{M} = \int_{\Omega} \mathbf{N}^T \rho \mathbf{N} \, dV \quad (11)$$

and

$$\mathbf{K} = \int_{\Omega} \mathbf{B}^T \mathbf{C} \mathbf{B} \, dV \quad (12)$$

where \mathbf{B} is the usual strain-displacement matrix containing shape function derivatives and \mathbf{C} is the matrix equivalent of the tensor C_{ijkl} . Furthermore, matrix \mathbf{D} has the structure of a diffusivity matrix and is defined by

$$\mathbf{D} = \int_{\Omega} \sum_{i=1}^3 \frac{\partial \mathbf{N}^T}{\partial x_i} \rho \frac{\partial \mathbf{N}}{\partial x_i} \, dV \quad (13)$$

Finally, the force vector \mathbf{f} contains the effects of all externally applied forces.

Inspection of Eq. (10) shows that lumping of the mass matrix leads to cancellation of all gradient effects. As a consequence, lumping is not an option and there is therefore little value in using an explicit time integrator that is only conditionally stable. Instead, the use of an implicit time integrator is recommended.

5. Conclusions

In this short paper we have reported the formulation of an enhanced gradient elasticity model with one higher-order stiffness term and two higher-order inertia terms. The model is capable of capturing a range of dispersion characteristics. Despite the presence of two terms that contain fourth-order spatial derivatives, it is possible to reformulate the model such that no higher than second-order spatial derivatives are included. This turns out to be a multi-scale formulation whereby micro and macro-scale displacements are the primary unknowns.

We have also carried out a number of parameter identification studies to relate the new constitutive parameters to the properties of a discrete lattice and those of a laminate. Furthermore, variationally consistent boundary conditions have been derived, and numerical results for a number of initial-boundary value problems have been obtained. These results will be presented in a forthcoming journal publication.

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