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NUMERICAL MODELLING OF MICRO-STRUCTURE USING THE CONCEPT OF ENHANCED CONTINUUM

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Abstract

This paper considers the peculiarities arising in numerical implementations of theories for enhanced continua. Firstly, governing equations of such theories are often not strongly elliptic. We propose a technique for reformulating the governing equations that does not affect their truncation error. Secondly, we discuss non-physical boundary layers that correspond to extraneous integrals and are characteristic to higher-order governing equations. It is established that the effect of these boundary layers may be minimised by formulating appropriate boundary conditions. To this end, a new asymptotic procedure for deriving such boundary conditions is proposed and illustrated by a simple one-dimensional example.

Introduction

Nowadays, effective continuum theories for micro-structure are well understood and routinely used for numerical modelling. These theories are, essentially, leading order terms long-wave approximations of the associated multi-scale formulations (either discrete or continuum). The use of effective continua remains justified as long as the separation between macro- and micro-scales is well-pronounced. The numerical accuracy of these models may be further improved by taking into account higher-order refinements; this results in a variety of enhanced continuum ("strain gradient") theories. Unfortunately, the presence of higher-order terms in governing equations also results in certain unwanted features that complicate the associated computational schemes.

Consider linear harmonic vibrations of a crystalline solid, governed by the equations

$$\sigma_{mi,m} = \rho\omega^2 u_i \,, \tag{1}$$

$$\sigma_{mi} = c_{milk}\varepsilon_{lk} = c_{milk}u_{l,k} \,, \tag{2}$$

where $\boldsymbol{\sigma}$ is the stress, $\boldsymbol{\varepsilon}$ the strain, $\boldsymbol{u}$ the displacement, and c_{milk} the tensor of effective elastic constants. Commas denotes differentiation with respect to the implied spatial variable and summation over repeated indices is assumed. Equations (1)–(2) may be obtained as long-wave limits for lattice structures describing arrangements of atoms within crystals. As frequency increases, the assumptions implied in (1)–(2) become less accurate and higher-order corrections may be taken into the account. For a centro-symmetric solid they may be given by

$$\sigma_{mi} = c_{milk}\varepsilon_{lk} + \ell^2 d_{milker}\varepsilon_{lk,er} \,, \tag{3}$$

with tensor d_{milker} describing weak dispersion produced by micro-structure with a characteristic length scale ℓ^2. When constitutive equations (3) are suitably non-dimensionalised, parameter ℓ^2 may be interpreted as the ratio between a typical grain size and the wavelength.

Local stability of enhanced continua

Constitutive equations (3) are derived within the context of a perturbation procedure and only meaningful when $\ell^2 \ll 1$. It is, therefore, not surprising that (1)–(3) with $\ell^2 \gg 1$ may violate positive-definiteness of the energy functional and result in a non-uniqueness, see [1]. In elastodynamics this is usually referred to as the loss of strong ellipticity. A traditional phenomenological solution to this problem involves replacing the plus sign in (3) with a minus. However, the resulting models feature unrealistic dispersion and cannot be easily linked to explicit descriptions of micro-structure.

In scalar problems it is always possible to use equations of motion (1) to replace strain gradients in (3) with inertia corrections. In application to formally identical higher-order asymptotics for plates and shells, the authors of [2] term such models as *the theories with modified inertia.* Theories with constitutive equations similar to (3) imply non-local response and require formulating additional boundary conditions. In contrast, theories with modified inertia can be used for modelling harmonic vibrations on bounded domains using the original boundary conditions for underlying effective continuum.

The described procedure works only for scalar problems or vector problems that may be reformulated in terms of scalar potentials, see [3]. However, this approach may be generalised by noticing that since (3) implies $\sigma_{mi,m} \sim \rho\omega^2 u_i$, an arbitrary superposition of

$$c_{milk}u_{k,lm} + \ell^2 d_{milker}u_{l,kerm} = \rho\omega^2 u_i + O(\ell^4) \,, \tag{4}$$

$$\ell^2 c_{milk}u_{k,lm} = \ell^2\rho\omega^2 u_i + O(\ell^4) \,, \tag{5}$$

results in a theory with the same truncation error $O(\ell^4)$. While it is not known at present whether this procedure would enable one to ensure strong ellipticity for a three-dimensional solid with general anisotropy, paper [4] demonstrates that strong ellipticity is achievable at least in two-dimensional materials with cubic symmetry.

Boundary conditions: a model example

Since the equation obtained by superimposing (4)–(5) are singularly perturbed, they feature extraneous integrals corresponding to short-wave boundary layers. The situation is best described by considering a simple model problem for an enhanced continuum governed by

$$\frac{\partial^2 u}{\partial x^2} + \omega^2 u - \alpha^2 \ell^2 \frac{\partial^4 u}{\partial x^4} = 0\,, \tag{6}$$

in the semi-infinite domain $\Gamma = \{x | x \geqslant 0\}$. Equation (6) has two particular integrals. The first of them, $\bar{u}$, is given to the leading order by

$$\frac{\partial^2 \bar{u}}{\partial x^2} + \omega^2 \bar{u} \sim 0\,, \tag{7}$$

and is, essentially, a thought for homogenised solution that is physically relevant. The second integral u_* is described to the leading order by

$$\frac{\partial^2 u_*}{\partial x^2} - \alpha^2 \ell^2 \frac{\partial^4 u_*}{\partial x^4} \sim 0\,, \tag{8}$$

and describes a spurious non-long-wave boundary layer

$$u_* = C e^{-x/\alpha\ell}\,. \tag{9}$$

Suppose that we want to solve a Dirichlet problem on Γ and pose a boundary condition of the form

$$u|_{x=0} = f\,. \tag{10}$$

Every solution of (6) $u = \bar{u} + u_*$ and, therefore, solutions of boundary value problem (6), (10) would implicitly assume the distorted boundary condition given by $\bar{u}|_{x=0} = f - u_*|_{x=0}$. Thus, in order to solve Dirichlet problem for the governing equation (6) we need to find a way of ensuring that $\bar{u}|_{x=0} = f$.

Fourth-order differential equation (6), certainly, requires a second boundary condition that cannot be extrapolated by considering the effective continuum. We can use this opportunity to fix the boundary layer and ensure the physicality of the solution. Let us, for example, consider the second boundary condition

$$\left.\frac{\partial u}{\partial x}\right|_{x=0} = \left.\frac{\partial \bar{u}}{\partial x}\right|_{x=0} + \left.\frac{\partial u_*}{\partial x}\right|_{x=0} = F_1\,, \tag{11}$$

with the function F_1 to be chosen later. By referring to (9) it is possible to conclude that $u_*|_{x=0} = 0$ when

$$F_1 = \left.\frac{\partial \bar{u}}{\partial x}\right|_{x=0}\,. \tag{12}$$

This implies that the numerical scheme for solving the boundary value problem (6), (10) may be implemented in two steps. Firstly, the leading order problem (7) must be solved subject to (10) to find the leading order of $\bar{u}$. Secondly, the resulting leading order solution must be differentiated to define F_1 in the additional boundary condition (11). This technique may be iterated to obtain higher-order corrections and generalised to work for the vector problems and with more complex boundary layers.

For some problems it may also be possible to find purely analytic solutions. For example, if we introduce another second boundary condition

$$\left.\frac{\partial^2 u}{\partial x^2}\right|_{x=0} = \left.\frac{\partial^2 \bar{u}}{\partial x^2}\right|_{x=0} + \left.\frac{\partial^2 u_*}{\partial x^2}\right|_{x=0} = F_2\,, \tag{13}$$

straightforward application of (7) and (9) yields

$$\frac{1}{\alpha^2 \ell^2} u_*|_{x=0} = -\omega^2 \bar{u}|_{x=0} - F_2\,. \tag{14}$$

Thus, in order to satisfy the required boundary condition $\bar{u}|_{x=0} = f$ we have to select

$$F_2 = -\omega^2 f\,. \tag{15}$$

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