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# Higher-order continua derived from discrete media: continualisation aspects and boundary conditions

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**Abstract**

In this paper, the derivation of higher-order continuum models from a discrete medium is addressed, with the following aims: (i) for a given discrete model and a given coupling of discrete and continuum degrees of freedom, the continuum should be defined uniquely, (ii) the continuum is isotropic, and (iii) boundary conditions are derived consistently with the energy functional and the equations of motion of the continuum. Firstly, a comparison is made between two continualisation methods, namely based on the equations of motion and on the energy functional. They are shown to give identical results. Secondly, the issue of isotropy is addressed. A new approach is developed in which two, rather than one, layers of neighbouring particles are considered. Finally, the formulation and interpretation of boundary conditions is treated. By means of the Hamilton–Ostrogradsky principle, boundary conditions are derived that are consistent with the energy functional and the equations of motion. A relation between standard stresses and higher-order stresses is derived and used to make an interpretation of the higher-order stresses. An additional result of this study is the non-uniqueness of the higher-order contributions to the energy.


*Keywords:* Continualisation; Higher-order continuum; Gradient models

## 1. Introduction

In many fields of engineering an interaction between spatial scales exists. Processes on lower scales of observation (e.g. microscale, nanoscale) have an influence on higher scales of observation (e.g. macro-scale) and vice versa. Modelling approaches aim to balance the accuracy and the efficiency of the model, therefore taking into account the full detail of the lower scales is not a feasible option. One of the alternative strategies is to replace the inhomogeneities of the lower scales by an enhanced continuum description on the higher scale. Depending on the model description of the lower scales, use can then be made of homogenisation techniques (translating an inhomogeneous continuum into a homogeneous continuum) or

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continualisation techniques (translating a discrete medium into a homgeneous continuum). In this work, attention is focussed on continualisation of regular discrete media.

The simplest continuum model that can be obtained via continualisation is the so-called classical continuum, in which the constitutive equations relate the standard stresses to the standard strains algebraically. More accurate descriptions of the underlying microstructure or nanostructure can be obtained by enhancing the constitutive relations to differential equations, thereby obtaining so-called higher-order continua. For linear elastic models, the order of the continuum is retrieved by taking the highest order of displacement derivative in the equilibrium equations, minus two. This nomenclature is followed below: a second-order model contains fourth-order displacement derivatives and lower in the equations of motion. Invariably, the higher-order spatial derivatives are accompanied by factors of a certain length scale; it is this length scale that represents the lower scales.

Second-order models have been derived from discrete models and inhomogeneous continua in the literature, see for instance (Rubin et al., 1995; Chang and Gao, 1995; Mühlhaus and Oka, 1996; Suiker et al., 2001; Chen and Fish, 2001; Chang et al., 2002; Andrianov et al., 2003; Triantafyllidis and Bardenhagen, 1993), although their stability is not always guaranteed (Rubin et al., 1995; Mühlhaus and Oka, 1996; Suiker et al., 2001; Chen and Fish, 2001; Chang et al., 2002; Askes et al., 2002; Metrikine and Askes, 2002; Askes and Metrikine, 2002). Other second-order models have been proposed in order to regularise singularities in the solution (Aifantis, 1984; Aifantis, 1987; Schreyer and Chen, 1986; Lasry and Belytschko, 1988; Mühlhaus and Aifantis, 1991; de Borst and Mühlhaus, 1992; Sluys, 1992; Pamin, 1994; Triantafyllidis and Aifantis, 1986; Altan and Aifantis, 1997; Zhu et al., 1997; Fleck and Hutchinson, 2001; Peerlings et al., 1996; Comi and Driemeier, 1998; Askes and Sluys, 2002; Chambon et al., 1998; Gutkin, 2000; Askes and Sluys, 2003). More conditions could be imposed on the format of second-order models, however, below the restriction is made to three issues:

(1) The continuum must be defined uniquely for a given discrete model and for a given link between the degrees of freedom of the discrete model and those of the continuum. Various continualisation strategies exist, but it is required that they yield the same field equations for the continuum, including the same higher-order constitutive coefficients. In Section 2, two approaches will be scrutinised in the context of a one-dimensional system.
(2) Many materials behave isotropically on the higher scales of observation. For these materials, the continuum should be isotropic, even so the underlying discrete model is anisotropic. A new approach to derive an isotropic second-order continuum is presented in Section 3.
(3) Higher-order field equations lead to higher-order boundary conditions. The boundary conditions should be formulated consistently with the energy functional and the equations of motion. This can be accomplished by applying the Hamilton–Ostrogradsky principle, cf. Section 4. Furthermore, the physical meaning of the boundary conditions should be investigated.

Although it is admitted that stability of the derived models is of paramount importance, this issue will only be touched briefly upon in Section 3.3.

## 2. Continualisation procedures

Different strategies can be taken to derive a continuum model from a discrete medium. Below, we distinguish between continualisation procedures that are applied to the equations of motion (Section 2.1) and to the energy functional (Section 2.2). For simplicity, a one-dimensional medium is considered, although the findings can be straightforwardly extended to multiple dimensions (see for instance Section 3).

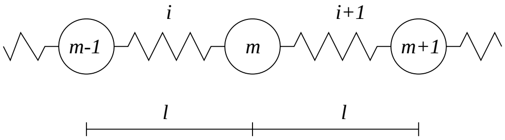


Fig. 1. One-dimensional discrete medium.

The geometry of the discrete medium is depicted in Fig. 1. All particles have mass $M$ and all springs have stiffness $K$. The interparticle distance is denoted as $l$.

## 2.1. Continualisation of the equations of motion

The equation of motion for the discrete particle $m$ is written as

$$Mx_{tt}^{(m)} = F_{i+1} - F_i = K\left(x^{(m+1)} - 2x^{(m)} + x^{(m-1)}\right) \tag{1}$$

In this work, subscripts $x$, $y$ and $t$ denote derivatives. Tensile forces $F$ in the springs are assumed to be positive. To continualise Eq. (1), $x^{(m)}$ is replaced by the displacement of the continuum $u(x)$, whereas the displacements of the neighbouring particles $x^{(m\pm 1)}$ are replaced by $u(x \pm l)$. Taylor series expansions are used for $u(x \pm l)$ according to

$$u(x \pm l) = u(x) \pm lu_x(x) + \frac{1}{2}l^2 u_{xx}(x) \pm \frac{1}{6}l^3 u_{xxx}(x) + \cdots \tag{2}$$

With these substitutions, Eq. (1) is elaborated as

$$\rho u_{tt} = E\left(u_{xx} + \frac{1}{12}l^2 u_{xxxx} + \frac{1}{360}l^4 u_{xxxxxx} + \cdots\right) \tag{3}$$

where the macroscopic material parameters $\rho = M/Al$ and $E = Kl/A$ have been introduced, and $A$ is the cross-sectional area. For notational simplicity, the dependence of $u$ and its derivatives on $x$ and $t$ is not shown explicitly. The classical one-dimensional wave equation is obtained from Eq. (3) by neglecting all terms with powers of $l$ higher than 0.

## 2.2. Continualisation of the energy functional

Alternatively, the transition from discrete model to continuum can be made on the level of the energy functionals. The Lagrangian $\mathscr{L}^{(m)}$ associated with particle $m$ is written as the difference of the kinetic energy and potential energy:

$$\mathscr{L}^{(m)} = \mathscr{U}_{\text{kin}}^{(m)} - \mathscr{U}_{\text{pot}}^{(m)} = \frac{1}{2}M\{x_t^{(m)}\}^2 - \frac{1}{2}K\left\{[x^{(m+1)} - x^{(m)}]^2 + [x^{(m)} - x^{(m-1)}]^2\right\} \tag{4}$$

Eq. (4) expresses the kinetic energy of particle $x^{(m)}$ and the potential energy corresponding to the two springs attached to this particle. For a continuous medium, the Lagrangian must be recast as a Lagrangian *density*. However, it must be realised that spring $i$ is attached to two particles, therefore the contribution of the potential energy as given in Eq. (4) must be divided by two to obtain the correct potential energy density. Thus,

$$\lambda = \frac{\mathscr{U}_{\text{kin}}^{(m)} - \frac{1}{2}\mathscr{U}_{\text{pot}}^{(m)}}{Al} \tag{5}$$

where $\lambda$ is the Lagrangian density of the continuum. In the continualisation the discrete degrees of freedom are again replaced by their continuous counterparts, and Taylor series expansions are applied where appropriate. This yields

$$\lambda = \frac{1}{2}\rho\{u_t\}^2 - \frac{1}{4}E\left\{\left(u_x + \frac{1}{2}lu_{xx} + \frac{1}{6}l^2u_{xxx} + \frac{1}{24}l^3u_{xxxx} + \cdots\right)^2 + \left(u_x - \frac{1}{2}lu_{xx} + \frac{1}{6}l^2u_{xxx} - \frac{1}{24}l^3u_{xxxx} + \cdots\right)^2\right\} \tag{6}$$

The equation of motion in its Lagrangian format reads (Metrikine and Askes, 2002)

$$\frac{\partial}{\partial t}\frac{\partial\lambda}{\partial u_t} = -\frac{\partial}{\partial x}\frac{\partial\lambda}{\partial u_x} + \frac{\partial^2}{\partial x^2}\frac{\partial\lambda}{\partial u_{xx}} - \frac{\partial^3}{\partial x^3}\frac{\partial\lambda}{\partial u_{xxx}} + \cdots \tag{7}$$

Substituting Eq. (6) in Eq. (7) and grouping together the various powers of $l$ yields

$$\rho u_{tt} = E\left\{u_{xx} + \left(\frac{1}{6} - \frac{1}{4} + \frac{1}{6}\right)l^2u_{xxxx} + \left(\frac{1}{120} - \frac{1}{48} + \frac{1}{36} - \frac{1}{48} + \frac{1}{120}\right)l^4u_{xxxxxx} + \cdots\right\} \tag{8}$$

which is identical to Eq. (3). Note that the $l^2$-term in Eq. (8) is obtained via three contributions from Eq. (6), corresponding to $u_xu_{xxx}$, $u_{xx}u_{xx}$ and $u_{xxx}u_x$, respectively. Similar observations hold for terms of $l^4$ and higher.

## 3. Derivation of an isotropic second-order continuum

With the conclusion, obtained from Section 2, that continualisation of the equations of motion and of energy are equivalent, either approach could be chosen in the sequel to derive a continuum model from a discrete medium.

### 3.1. Discrete model

Intuitively, discrete media resemble closely the material that they are intended to model, e.g. granular media such as soil or concrete, or metals and ceramics on the atomistic level. Normally, some degree of randomness is present in the structure of these materials, e.g. in terms of particle size distribution and regularity of the interparticle connections. However, taking into account this randomness would complicate the continualisation process significantly, therefore *periodicity* of the discrete medium is often assumed.

Two popular discrete and periodic representations of microstructured materials are depicted in Fig. 2, i.e. a hexagonal lattice and a square lattice (Suiker et al., 2001). In both lattices, the characteristic distance between the different particles is denoted by $l$. In the hexagonal lattice all springs are identical, whereas in the square lattice axial springs of length $l$ and diagonal springs of length $l\sqrt{2}$ are distinguished. In principle, all springs could be of the longitudinal, transversal or rotational type, which corresponds to the normal stiffness, shear stiffness and rotational stiffness of the interparticle contact, respectively.

An inherent anisotropy is present in the two lattices of Fig. 2. In contrast, the materials that are to be modelled with these lattices are nearly isotropic at the macroscale. Thus, in the continualisation process certain restrictions need to be enforced such that isotropy results. For instance, an isotropic classical continuum based on a square lattice with only longitudinal springs is obtained by taking the stiffness of the diagonal springs half the stiffness of the axial springs (Suiker et al., 2001). The classical continuum based on the hexagonal lattice with only longitudinal springs is automatically isotropic; however, this does not imply

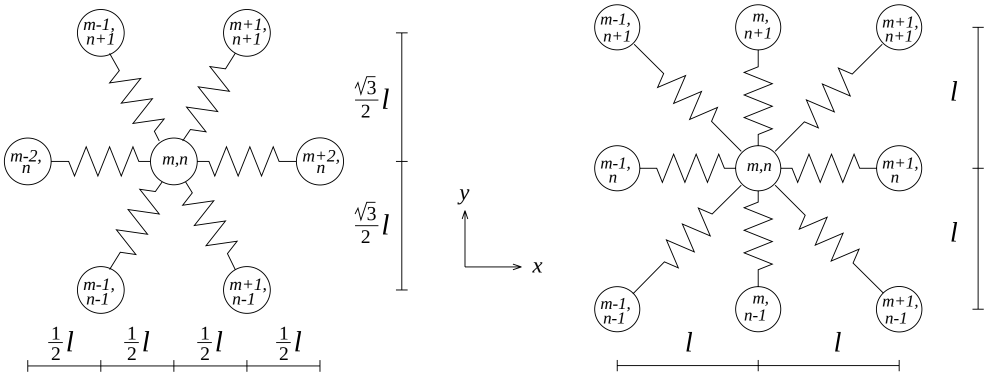


Fig. 2. Two-dimensional discrete lattices—hexagonal lattice (left) and square lattice (right).

that also second-order models based on the hexagonal lattice are automatically isotropic, which will be elucidated in Section 3.2.

Since the classical continuum based on the hexagonal lattice is isotropic without further assumptions, this lattice is used in the remainder of this work and the square lattice is left out of consideration. The kinetic and potential energy corresponding to the central particle, depicted in Fig. 2 (left) and denoted by $(m,n)$, read

$$\mathscr{U}_{\text{kin}}^{(m,n)} = \frac{1}{2}M\left\{\left(x_t^{(m,n)}\right)^2 + \left(y_t^{(m,n)}\right)^2\right\} \tag{9}$$

and

$$\mathscr{U}_{\text{pot}}^{(m,n)} = \frac{1}{2}K\sum_{i=1}^{6}\Delta l_i^2 \tag{10}$$

respectively, where $x^{(m,n)}$ and $y^{(m,n)}$ are the displacement components of particle $(m,n)$ and $\Delta l_i$ is the elongation of spring $i$. These elongations can be elaborated as

$$\Delta l_1 = x^{(m+2,n)} - x^{(m,n)} \tag{11a}$$

$$\Delta l_2 = \frac{1}{2}\left(x^{(m+1,n+1)} - x^{(m,n)} + \sqrt{3}\left(y^{(m+1,n+1)} - y^{(m,n)}\right)\right) \tag{11b}$$

$$\Delta l_3 = \frac{1}{2}\left(x^{(m,n)} - x^{(m-1,n+1)} + \sqrt{3}\left(y^{(m-1,n+1)} - y^{(m,n)}\right)\right) \tag{11c}$$

$$\Delta l_4 = x^{(m,n)} - x^{(m-2,n)} \tag{11d}$$

$$\Delta l_5 = \frac{1}{2}\left(x^{(m,n)} - x^{(m-1,n-1)} + \sqrt{3}\left(y^{(m,n)} - y^{(m-1,n-1)}\right)\right) \tag{11e}$$

$$\Delta l_6 = \frac{1}{2}\left(x^{(m+1,n-1)} - x^{(m,n)} + \sqrt{3}\left(y^{(m,n)} - y^{(m+1,n-1)}\right)\right) \tag{11f}$$

whereby the springs have been numbered counter-clockwise. The equations of motion are derived via

$$\frac{\partial \mathscr{L}^{(m,n)}}{\partial x^{(m,n)}} = \frac{\partial}{\partial t}\frac{\partial \mathscr{L}^{(m,n)}}{\partial x_t^{(m,n)}} \tag{12a}$$

and

$$\frac{\partial \mathscr{L}^{(m,n)}}{\partial y^{(m,n)}} = \frac{\partial}{\partial t}\frac{\partial \mathscr{L}^{(m,n)}}{\partial y_t^{(m,n)}} \tag{12b}$$

where again the Lagrangian $\mathscr{L}^{(m,n)} = \mathscr{U}_{\rm kin}^{(m,n)} - \mathscr{U}_{\rm pot}^{(m,n)}$. In terms of particle displacements, Eqs. (12a) and (12b) can be elaborated as

$$\begin{aligned} Mx_{tt}^{(m,n)} = \frac{K}{4}\Big\{ & -12x^{(m,n)} + 4x^{(m+2,n)} + 4x^{(m-2,n)} + x^{(m+1,n+1)} + x^{(m-1,n+1)} + x^{(m-1,n-1)} + x^{(m+1,n-1)} \\ & + \sqrt{3}\big(y^{(m+1,n+1)} - y^{(m-1,n+1)} + y^{(m-1,n-1)} - y^{(m+1,n-1)}\big)\Big\} \end{aligned} \tag{13a}$$

and

$$\begin{aligned} My_{tt}^{(m,n)} = \frac{K}{4}\Big\{ & -12y^{(m,n)} + 3\big(y^{(m+1,n+1)} + y^{(m-1,n+1)} + y^{(m-1,n-1)} + y^{(m+1,n-1)}\big) \\ & + \sqrt{3}\big(x^{(m+1,n+1)} - x^{(m-1,n+1)} + x^{(m-1,n-1)} - x^{(m+1,n-1)}\big)\Big\} \end{aligned} \tag{13b}$$

for the $x$ and $y$-direction, respectively. The anisotropic character of the discrete model can be verified from the magnitude of the coefficients in Eqs. (13a) and (13b).

### 3.2. Continualisation of hexagonal lattice

For the central particle $(m,n)$ the continuous displacement components $u$ and $v$ are set equal to the discrete displacement components $x^{(m,n)}$ and $y^{(m,n)}$, respectively. For the neighbouring particles, Taylor series expansions are used, that is

$$x^{(m\pm2,n)} = u(x \pm l, y) = \sum_i (\pm1)^i \frac{l^i}{i!}\frac{\partial^i u(x,y)}{\partial x^i} \tag{14a}$$

$$x^{(m\pm1,n\pm1)} = u\left(x \pm \frac{1}{2}l, y \pm \frac{1}{2}\sqrt{3}l\right) = \sum_i \sum_j (\pm1)^i(\pm1)^j \frac{\left(\frac{1}{2}l\right)^i\left(\frac{1}{2}\sqrt{3}l\right)^j}{i!j!}\frac{\partial^{i+j}u(x,y)}{\partial x^i \partial y^j} \tag{14b}$$

for the $x$-direction, and

$$y^{(m\pm2,n)} = v(x \pm l, y) = \sum_i (\pm1)^i \frac{l^i}{i!}\frac{\partial^i v(x,y)}{\partial x^i} \tag{15a}$$

$$y^{(m\pm1,n\pm1)} = v\left(x \pm \frac{1}{2}l, y \pm \frac{1}{2}\sqrt{3}l\right) = \sum_i \sum_j (\pm1)^i(\pm1)^j \frac{\left(\frac{1}{2}l\right)^i\left(\frac{1}{2}\sqrt{3}l\right)^j}{i!j!}\frac{\partial^{i+j}v(x,y)}{\partial x^i \partial y^j} \tag{15b}$$

for the $y$-direction.

Expressions (14a)–(15b) can be substituted into Eqs. (13a) and (13b) to yield the equations of motion of the continuum, that is

$$\rho u_{tt} = \frac{2}{5}E\big(3u_{xx} + u_{yy} + 2v_{xy}\big) + \frac{1}{120}El^2\big(11u_{xxxx} + 6u_{xxyy} + 3u_{yyyy} + 4v_{xxxy} + 12v_{xyyy}\big) \tag{16a}$$

$$\rho v_{tt} = \frac{2}{5}E\left(v_{xx} + 3v_{yy} + 2u_{xy}\right) + \frac{1}{120}El^2\left(v_{xxxx} + 18v_{xxyy} + 9v_{yyyy} + 4u_{xxxy} + 12u_{xyyy}\right) \tag{16b}$$

whereby all terms of order $l^4$ and higher have been neglected. From the relative magnitude of the classical terms it can be concluded that the Poisson's ratio predicted by the continuum is always equal to $\nu = 1/4$. With this Poisson's ratio, a unique relation between the discrete spring stiffness $K$ and the Young's modulus of the continuum $E$ can be derived fitting the classical Lamé equations as $K = 16Eh/15$, in which $h$ is the dimension in the third direction. For the mass density $\rho$ it is found that $M = \rho l^2 h$. Crosschecking the coefficients in Eqs. (16a) and (16b) reveals that the classical contributions (i.e. the terms of order $l^0$) are isotropic, whereas the second-order terms are anisotropic.

The same results can be obtained by substituting Eqs. (14a)–(15b) into Eqs. (12a) and (12b), in which expressions (9), (10) and the two-dimensional counterpart of (5) must be used. The so-obtained Lagrangian density is written as

$$\begin{aligned}\lambda = {} & \frac{1}{2}\rho\{u_t^2 + v_t^2\} - \frac{1}{5}E\left\{3u_x^2 + u_y^2 + v_x^2 + 3v_y^2 + 2u_x v_y + 2u_y v_x\right\} - \frac{1}{240}El^2\Big\{33u_{xx}^2 + 9u_{yy}^2 + 3v_{xx}^2 \\ & + 27v_{yy}^2 + 12u_{xy}^2 + 36v_{xy}^2 + 6u_{xx}u_{yy} + 18v_{xx}v_{yy} + 12u_{xy}\left(v_{xx} + 3v_{yy}\right) + 12v_{xy}\left(u_{xx} + 3u_{yy}\right) \\ & + 4u_x\left(11u_{xxx} + 3u_{xyy} + 3v_{xxy} + 3v_{yyy}\right) + 4v_y\left(u_{xxx} + 9u_{xyy} + 9v_{xxy} + 9v_{yyy}\right) \\ & + 4(u_y + v_x)\left(3u_{xxy} + 3u_{yyy} + v_{xxx} + 9v_{xyy}\right)\Big\}\end{aligned} \tag{17}$$

from which the equations of motion (16a) and (16b) can be retrieved via

$$\begin{aligned}\frac{\partial}{\partial t}\frac{\partial\lambda}{\partial u_t} = {} & -\frac{\partial}{\partial x}\frac{\partial\lambda}{\partial u_x} - \frac{\partial}{\partial y}\frac{\partial\lambda}{\partial u_y} + \frac{\partial^2}{\partial x^2}\frac{\partial\lambda}{\partial u_{xx}} + \frac{\partial^2}{\partial x\partial y}\frac{\partial\lambda}{\partial u_{xy}} + \frac{\partial^2}{\partial y^2}\frac{\partial\lambda}{\partial u_{yy}} - \frac{\partial^3}{\partial x^3}\frac{\partial\lambda}{\partial u_{xxx}} - \frac{\partial^3}{\partial x^2\partial y}\frac{\partial\lambda}{\partial u_{xxy}} \\ & - \frac{\partial^3}{\partial x\partial y^2}\frac{\partial\lambda}{\partial u_{xyy}} - \frac{\partial^3}{\partial y^3}\frac{\partial\lambda}{\partial u_{yyy}}\end{aligned} \tag{18a}$$

$$\begin{aligned}\frac{\partial}{\partial t}\frac{\partial\lambda}{\partial v_t} = {} & -\frac{\partial}{\partial x}\frac{\partial\lambda}{\partial v_x} - \frac{\partial}{\partial y}\frac{\partial\lambda}{\partial v_y} + \frac{\partial^2}{\partial x^2}\frac{\partial\lambda}{\partial v_{xx}} + \frac{\partial^2}{\partial x\partial y}\frac{\partial\lambda}{\partial v_{xy}} + \frac{\partial^2}{\partial y^2}\frac{\partial\lambda}{\partial v_{yy}} - \frac{\partial^3}{\partial x^3}\frac{\partial\lambda}{\partial v_{xxx}} - \frac{\partial^3}{\partial x^2\partial y}\frac{\partial\lambda}{\partial v_{xxy}} \\ & - \frac{\partial^3}{\partial x\partial y^2}\frac{\partial\lambda}{\partial v_{xyy}} - \frac{\partial^3}{\partial y^3}\frac{\partial\lambda}{\partial v_{yyy}}\end{aligned} \tag{18b}$$

### 3.3. Continualisation of extended hexagonal lattice

The hexagonal lattice as described above does not lead to an isotropic second-order model. If isotropy is desired, amendments are needed. In the authors' opinion, these amendments should concern with the discrete medium, such that the continualisation procedure does not require additional assumptions but leads to isotropy *automatically*. To this end, another layer of particles is taken into account, such that an *extended* hexagonal lattice is obtained, see Fig. 3. The two sets of springs (one for the inner layer of neighbouring particles, one for the outer layer) are assumed to have different stiffnesses, denoted by $K_1$ and $K_2$, respectively. Physically, this can be thought of as a representation of inter-particle contact (inner layer) and long-range interaction via a matrix material (outer layer).

The equations of motion of the continuum in terms of the discrete material parameters $M$, $K_1$ and $K_2$ can be elaborated as

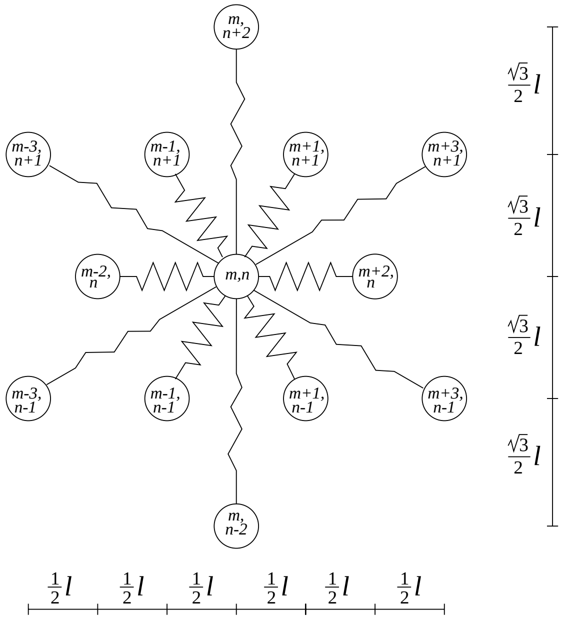


Fig. 3. Extended hexagonal lattice.

$$Mu_{tt} = \frac{3}{8}(K_1 + 3K_2)l^2\{3u_{xx} + u_{yy} + 2v_{xy}\} + \frac{1}{128}l^4\{(11K_1 + 81K_2)u_{xxxx} + (6K_1 + 162K_2)u_{xxyy} + (3K_1 + 9K_2)u_{yyyy} + (4K_1 + 108K_2)v_{xyyy} + (12K_1 + 36K_2)v_{xyyy}\} \tag{19a}$$

and

$$Mv_{tt} = \frac{3}{8}(K_1 + 3K_2)l^2\{3v_{xx} + v_{yy} + 2u_{xy}\} + \frac{1}{128}l^4\{(K_1 + 27K_2)v_{xxxx} + (18K_1 + 54K_2)v_{xxyy} + (9K_1 + 99K_2)v_{yyyy} + (12K_1 + 36K_2)u_{xyyy} + (4K_1 + 108K_2)u_{xyyy}\} \tag{19b}$$

Similar to the continualisation of the hexagonal lattice in Section 3.2, it is found that the classical terms are isotropic. The higher-order terms can be made isotropic by requiring that $K_1 = 9K_2$. Furthermore, fitting the classical Lamé equations yields $K_1 = 4Eh/5$ and $M = \rho l^2 h$. With these substitutions, Eqs. (19a) and (19b) are elaborated as

$$\rho u_{tt} = \frac{2}{5}E(3u_{xx} + u_{yy} + 2v_{xy}) + \frac{1}{40}El^2(5u_{xxxx} + 6u_{xxyy} + u_{yyyy} + 4v_{xxxy} + 4v_{xyyy}) \tag{20a}$$

$$\rho v_{tt} = \frac{2}{5}E(v_{xx} + 3v_{yy} + 2u_{xy}) + \frac{1}{40}El^2(v_{xxxx} + 6v_{xxyy} + 5v_{yyyy} + 4u_{xxxy} + 4u_{xyyy}) \tag{20b}$$

Note that the only changes with respect to Eqs. (16a) and (16b) concern with the higher-order terms.

The Lagrangian density for this model is obtained by continualisation of the Lagrangian function of the extended hexagonal lattice. It is found that

$$\lambda = \frac{1}{2}\rho\{u_t^2 + v_t^2\} - \frac{1}{5}E\Big\{3u_x^2 + u_y^2 + v_x^2 + 3v_y^2 + 2u_xv_y + 2u_yv_x\Big\} - \frac{1}{80}El^2\Big\{15u_{xx}^2 + 3u_{yy}^2 + 3v_{xx}^2 + 15v_{yy}^2 + 12u_{xy}^2 + 12v_{xy}^2 + 6u_{xx}u_{yy} + 6v_{xx}v_{yy} + 12u_{xy}(v_{xx} + v_{yy}) + 12v_{xy}(u_{xx} + u_{yy}) + 4u_x(5u_{xxx} + 3u_{xyy} + 3v_{xxy} + v_{yyy}) + 4v_y(u_{xxx} + 3u_{xyy} + 3v_{xxy} + 5v_{yyy}) + 4(u_y + v_x)(3u_{xxy} + u_{yyy} + v_{xxx} + 3v_{xyy})\Big\} \tag{21}$$

which can be used to derive the equations of motion through Eqs. (18a) and (18b). The Lagrangian density given in Eq. (21) has been derived directly from the energy of the discrete system, and as a result it contains first, second and third derivatives of the displacements. To simplify further manipulations of the Lagrangian density as given below in Section 4, all products of first and third derivatives are replaced by products of second derivatives. Integration by parts of the various products of first and third derivatives, while neglecting boundary terms, yields the following equalities to be understood in a weak sense

$$u_xu_{xxx} = -u_{xx}^2 \tag{22a}$$

$$u_xu_{xyy} = -\frac{1}{3}u_{xx}u_{yy} - \frac{2}{3}u_{xy}^2 \tag{22b}$$

$$u_xv_{xxy} = -\frac{2}{3}u_{xx}v_{xy} - \frac{1}{3}u_{xy}v_{xx} \tag{22c}$$

etc., in which an equal treatment of integration in $x$ and $y$-direction is assumed. By means of the so-obtained identities (22), the Lagrangian density (21) can be elaborated as

$$\lambda = \frac{1}{2}\rho\{u_t^2 + v_t^2\} - \frac{1}{5}E\Big\{3u_x^2 + u_y^2 + v_x^2 + 3v_y^2 + 2u_xv_y + 2u_yv_x\Big\} + \frac{1}{80}El^2\Big\{5(u_{xx}^2 + v_{yy}^2) + u_{yy}^2 + v_{xx}^2 + 4(u_{xy}^2 + v_{xy}^2) + 2(u_{xx}u_{yy} + v_{xx}v_{yy}) + 4(u_{xx}v_{xy} + u_{yy}v_{xy} + u_{xy}v_{xx} + u_{xy}v_{yy})\Big\} \tag{23}$$

such that a functional with at most second derivatives is obtained.

Two important observations can be made:

(1) Inspection of Eqs. (21) and (23) shows that the higher-order contribution to the potential energy cannot be expressed uniquely. In particular, the various terms can be written either as products of first and third derivatives or as products of second derivatives. It can be verified that the equations of motion (20a) and (20b) are retrieved from each of the energy functionals, making use of Eqs. (18a) and (18b).

(2) Taking for instance $u_y = v_x = 0$ it is seen that the higher-order part of the potential energy becomes negative. Thus, unconditional positive definiteness of the potential energy is not fulfilled and instabilities may occur (Askes et al., 2002; Metrikine and Askes, 2002; Askes and Metrikine, 2002). This is indeed a severe drawback of this model, which is caused by the truncation of the Taylor series. It can be overcome by a relaxed kinematic coupling of discrete model and continuum, see for instance (Metrikine and Askes, 2002; Askes and Metrikine, 2002) or by using Padé approximations, see (Rubin et al., 1995; Chen and Fish, 2001; Andrianov et al., 2003).

It is noted that the above procedure can be used to derive an isotropic second-order model. Taking into account infinitely many terms in the continualisation procedure will yield the equations of the discrete lattice, which are anisotropic. Thus, additional measures are needed to guarantee that models of order four are isotropic, e.g. considering also the third layer of neighbouring particles.

## 4. Formulation and interpretation of boundary conditions

Above, the equations of motion have been derived that are consistent with the underlying energy functional. To complete the model description, boundary conditions must be derived that are consistent with the equations of motion. To this end, the Hamilton–Ostrogradsky principle is applied to the Lagrangian density derived above. In particular, use is made of Eq. (23) rather than of (21), such that $\lambda$ only depends on the first and second spatial derivatives of $u$ and $v$ and on the first time derivatives. However, employing the original Lagrangian density given through Eq. (21) would give identical results.

### *4.1. Hamilton–Ostrogradsky principle*

A perturbation of the displacements is considered according to

$$\tilde{u} = u + \epsilon\xi \tag{24a}$$

$$\tilde{v} = v + \epsilon\eta \tag{24b}$$

whereby $\xi$ and $\eta$ are normalised perturbations and $\epsilon$ is the amplitude of the perturbation. It is assumed that both $(u, v)$ and $(\tilde{u}, \tilde{v})$ describe the motion of the considered body from time $t_1$ to time $t_2$, therefore $\xi(t_1) = \xi(t_2) = \eta(t_1) = \eta(t_2) = 0$. The body is assumed to be extended over $[(x_a, y_a), (x_b, y_b)]$. The Hamilton–Ostrogradsky principle states that (Goldstein, 1964; Washizu, 1975; Lurie, 2002)

$$\left.\frac{\mathrm{d}}{\mathrm{d}\epsilon}\right|_{\epsilon=0}\left(\int_{t_1}^{t_2}\int_{x_a}^{x_b}\int_{y_a}^{y_b}\lambda\,\mathrm{d}y\,\mathrm{d}x\,\mathrm{d}t\right) = 0 \tag{25}$$

whereby $\lambda$ is evaluated at the perturbed configuration. Thus,

$$\int_{t_1}^{t_2}\int_{x_a}^{x_b}\int_{y_a}^{y_b}\left(\frac{\partial\lambda}{\partial u_t}\xi_t + \frac{\partial\lambda}{\partial u_x}\xi_x + \frac{\partial\lambda}{\partial u_y}\xi_y + \frac{\partial\lambda}{\partial u_{xx}}\xi_{xx} + \frac{\partial\lambda}{\partial u_{xy}}\xi_{xy} + \frac{\partial\lambda}{\partial u_{yy}}\xi_{yy}\right)\mathrm{d}y\,\mathrm{d}x\,\mathrm{d}t = 0 \tag{26a}$$

and

$$\int_{t_1}^{t_2}\int_{x_a}^{x_b}\int_{y_a}^{y_b}\left(\frac{\partial\lambda}{\partial v_t}\eta_t + \frac{\partial\lambda}{\partial v_x}\eta_x + \frac{\partial\lambda}{\partial v_y}\eta_y + \frac{\partial\lambda}{\partial v_{xx}}\eta_{xx} + \frac{\partial\lambda}{\partial v_{xy}}\eta_{xy} + \frac{\partial\lambda}{\partial v_{yy}}\eta_{yy}\right)\mathrm{d}y\,\mathrm{d}x\,\mathrm{d}t = 0 \tag{26b}$$

Since the elaboration of Eq. (26b) follows similar lines as that of Eq. (26a), only Eq. (26a) is considered in the sequel. The terms in Eq. (26a) are rewritten via

$$\frac{\partial\lambda}{\partial u_t}\xi_t = \frac{\partial}{\partial t}\left(\xi\frac{\partial\lambda}{\partial u_t}\right) - \xi\frac{\partial}{\partial t}\frac{\partial\lambda}{\partial u_t} \tag{27a}$$

$$\frac{\partial\lambda}{\partial u_x}\xi_x = \frac{\partial}{\partial x}\left(\xi\frac{\partial\lambda}{\partial u_x}\right) - \xi\frac{\partial}{\partial x}\frac{\partial\lambda}{\partial u_x} \tag{27b}$$

$$\frac{\partial\lambda}{\partial u_y}\xi_y = \frac{\partial}{\partial y}\left(\xi\frac{\partial\lambda}{\partial u_y}\right) - \xi\frac{\partial}{\partial y}\frac{\partial\lambda}{\partial u_y} \tag{27c}$$

$$\frac{\partial\lambda}{\partial u_{xx}}\xi_{xx} = \frac{\partial}{\partial x}\left(\xi_x\frac{\partial\lambda}{\partial u_{xx}}\right) - \frac{\partial}{\partial x}\left(\xi\frac{\partial}{\partial x}\frac{\partial\lambda}{\partial u_{xx}}\right) + \xi\frac{\partial^2}{\partial x^2}\frac{\partial\lambda}{\partial u_{xx}} \tag{27d}$$

$$\frac{\partial\lambda}{\partial u_{yy}}\xi_{yy} = \frac{\partial}{\partial y}\left(\xi_y\frac{\partial\lambda}{\partial u_{yy}}\right) - \frac{\partial}{\partial y}\left(\xi\frac{\partial}{\partial y}\frac{\partial\lambda}{\partial u_{yy}}\right) + \xi\frac{\partial^2}{\partial y^2}\frac{\partial\lambda}{\partial u_{yy}} \tag{27e}$$

For the cross-derivative term, the $x$ and $y$-directions are treated on an equal basis, hence a factor $\frac{1}{2}$:

$$\frac{\partial\lambda}{\partial u_{xy}}\xi_{xy} = \frac{1}{2}\left\{\frac{\partial}{\partial x}\left(\xi_y\frac{\partial\lambda}{\partial u_{xy}}\right) - \frac{\partial}{\partial y}\left(\xi\frac{\partial}{\partial x}\frac{\partial\lambda}{\partial u_{xy}}\right) + \xi\frac{\partial^2}{\partial x\partial y}\frac{\partial\lambda}{\partial u_{xy}}\right\} + \frac{1}{2}\left\{\frac{\partial}{\partial y}\left(\xi_x\frac{\partial\lambda}{\partial u_{xy}}\right) - \frac{\partial}{\partial x}\left(\xi\frac{\partial}{\partial y}\frac{\partial\lambda}{\partial u_{xy}}\right) + \xi\frac{\partial^2}{\partial x\partial y}\frac{\partial\lambda}{\partial u_{xy}}\right\} \tag{27f}$$

By means of Eqs. (27), Eq. (26a) can be elaborated as

$$\begin{aligned}
&\int_{t_1}^{t_2}\int_{x_a}^{x_b}\int_{y_a}^{y_b}\xi\left(\frac{\partial}{\partial t}\frac{\partial\lambda}{\partial u_t} + \frac{\partial}{\partial x}\frac{\partial\lambda}{\partial u_x} + \frac{\partial}{\partial y}\frac{\partial\lambda}{\partial u_y} - \frac{\partial^2}{\partial x^2}\frac{\partial\lambda}{\partial u_{xx}} - \frac{\partial^2}{\partial x\partial y}\frac{\partial\lambda}{\partial u_{xy}} - \frac{\partial^2}{\partial y^2}\frac{\partial\lambda}{\partial u_{yy}}\right)\mathrm{d}y\,\mathrm{d}x\,\mathrm{d}t \\
&\quad + \int_{x_a}^{x_b}\int_{y_a}^{y_b}\left\{-\xi\frac{\partial\lambda}{\partial u_t}\right\}\Big|_{t_1}^{t_2}\mathrm{d}y\,\mathrm{d}x + \int_{t_1}^{t_2}\int_{y_a}^{y_b}\left\{\xi\left(-\frac{\partial\lambda}{\partial u_x} + \frac{\partial}{\partial x}\frac{\partial\lambda}{\partial u_{xx}} + \frac{1}{2}\frac{\partial}{\partial y}\frac{\partial\lambda}{\partial u_{xy}}\right)\right. \\
&\quad \left. + -\xi_x\frac{\partial\lambda}{\partial u_{xx}} - \frac{1}{2}\xi_y\frac{\partial\lambda}{\partial u_{xy}}\right\}\Big|_{x_a}^{x_b}\mathrm{d}y\,\mathrm{d}t + \int_{t_1}^{t_2}\int_{x_a}^{x_b}\left\{\xi\left(-\frac{\partial\lambda}{\partial u_y} + \frac{\partial}{\partial y}\frac{\partial\lambda}{\partial u_{yy}} + \frac{1}{2}\frac{\partial}{\partial x}\frac{\partial\lambda}{\partial u_{xy}}\right)\right. \\
&\quad \left. + -\frac{1}{2}\xi_x\frac{\partial\lambda}{\partial u_{xy}} - \xi_y\frac{\partial\lambda}{\partial u_{yy}}\right\}\Big|_{y_a}^{y_b}\mathrm{d}x\,\mathrm{d}t = 0
\end{aligned} \tag{28}$$

Eq. (28) should hold for arbitrary $\xi$, therefore each integral is required to vanish separately. Since $\xi(t_1) = \xi(t_2) = 0$, the second integral in Eq. (28) cancels automatically. From the first integral the equation of motion in $x$-direction can be retrieved, i.e.

$$\frac{\partial}{\partial t}\frac{\partial\lambda}{\partial u_t} + \frac{\partial}{\partial x}\frac{\partial\lambda}{\partial u_x} + \frac{\partial}{\partial y}\frac{\partial\lambda}{\partial u_y} - \frac{\partial^2}{\partial x^2}\frac{\partial\lambda}{\partial u_{xx}} - \frac{\partial^2}{\partial x\partial y}\frac{\partial\lambda}{\partial u_{xy}} - \frac{\partial^2}{\partial y^2}\frac{\partial\lambda}{\partial u_{yy}} = 0 \tag{29}$$

which is in agreement with Eq. (18a). The third and fourth integral correspond to boundary integrals, which vanish by prescribing $\xi$ and/or its derivatives (kinematic or essential boundary conditions) or by prescribing the corresponding factors in terms of $\lambda$ (dynamic or natural boundary conditions). Hence, the following stress quantities can be identified:

$$\sigma_{11} = -\frac{\partial\lambda}{\partial u_x} + \frac{\partial}{\partial x}\frac{\partial\lambda}{\partial u_{xx}} + \frac{1}{2}\frac{\partial}{\partial y}\frac{\partial\lambda}{\partial u_{xy}} \tag{30a}$$

$$\sigma_{21} = -\frac{\partial\lambda}{\partial u_y} + \frac{1}{2}\frac{\partial}{\partial x}\frac{\partial\lambda}{\partial u_{xy}} + \frac{\partial}{\partial y}\frac{\partial\lambda}{\partial u_{yy}} \tag{30b}$$

$$\tau_{111} = -\frac{\partial\lambda}{\partial u_{xx}} \tag{30c}$$

$$\tau_{112} = -\frac{1}{2}\frac{\partial\lambda}{\partial u_{xy}} \tag{30d}$$

$$\tau_{211} = -\frac{1}{2}\frac{\partial\lambda}{\partial u_{xy}} \tag{30e}$$

$$\tau_{212} = -\frac{\partial\lambda}{\partial u_{yy}} \tag{30f}$$

where indices 1 and 2 refer to the $x$ and $y$-direction, respectively. The first index denotes the normal of the plane on which the stress acts and the second index denotes the direction of the stress (which equals the $x$-direction in the above equations, since only the variation of $\lambda$ with respect to $\xi$ is discussed in detail). The third index in Eqs. (30c)–(30f) refers to whether the variation of $\xi$ with respect to $x$ or $y$ is taken.

The same procedure can be followed to derive the variation of the energy $\lambda$ with respect to $\eta$, by which the remaining stress components are found. In terms of the displacement derivatives, the standard stresses $\sigma_{ij}$ are expressed as

$$\sigma_{11} = \sigma_{11}^{(0)} + \sigma_{11}^{(1)} = \frac{2}{5}E(3u_x + v_y) + \frac{1}{40}El^2\left(5u_{xxx} + 3v_{xxy} + 3u_{xyy} + v_{yyy}\right) \tag{31a}$$

$$\sigma_{12} = \sigma_{12}^{(0)} + \sigma_{12}^{(1)} = \frac{2}{5}E(u_y + v_x) + \frac{1}{40}El^2\left(v_{xxx} + 3u_{xxy} + 3v_{xyy} + u_{yyy}\right) = \sigma_{21} \tag{31b}$$

$$\sigma_{22} = \sigma_{22}^{(0)} + \sigma_{22}^{(1)} = \frac{2}{5}E\left(u_x + 3v_y\right) + \frac{1}{40}El^2\left(u_{xxx} + 3v_{xxy} + 3u_{xyy} + 5v_{yyy}\right) \tag{31c}$$

whereby the superscripts (0) and (1) refer to the classical part and the higher-order part of the standard stresses. The standard stresses obey the usual symmetry $\sigma_{12} = \sigma_{21}$. For the higher-order stresses $\tau_{ijk}$ it is found that

$$\tau_{111} = -\frac{1}{40}El^2\left(5u_{xx} + 2v_{xy} + u_{yy}\right) \tag{32a}$$

$$\tau_{112} = -\frac{1}{40}El^2\left(v_{xx} + 2u_{xy} + v_{yy}\right) = \tau_{211} = \tau_{121} \tag{32b}$$

$$\tau_{122} = -\frac{1}{40}El^2\left(u_{xx} + 2v_{xy} + u_{yy}\right) = \tau_{221} = \tau_{212} \tag{32c}$$

$$\tau_{222} = -\frac{1}{40}El^2\left(v_{xx} + 2u_{xy} + 5v_{yy}\right) \tag{32d}$$

The symmetry $\tau_{112} = \tau_{211}$ follows directly from Eqs. (30d) and (30e); a similar symmetry holds for $\tau_{221} = \tau_{122}$. The other symmetries $\tau_{121} = \tau_{112}$ and $\tau_{212} = \tau_{221}$ do not follow from the Hamilton–Ostrogradsky principle, and should be considered as specific to this model.

### *4.2. Relation between standard stresses and higher-order stresses*

When the expressions of the standard stresses (31a)–(31c) and those of the higher-order stresses (32a)–(32d) are compared to the Lagrangian density, Eq. (23), it is seen that the higher-order part of the standard stresses $\sigma_{ij}^{(1)}$ and the higher-order stresses $\tau_{ijk}$ both derive from the same contributions to the potential energy. Hence, if the potential energy is to be retrieved from the various stress tensors, it should hold that

$$\int_{x_a}^{x_b}\int_{y_a}^{y_b}\int_{\varepsilon}\sigma_{ij}^{(1)}\,\mathrm{d}\varepsilon_{ij}\,\mathrm{d}y\,\mathrm{d}x = \int_{x_a}^{x_b}\int_{y_a}^{y_b}\int_{\chi}\tau_{ijk}\,\mathrm{d}\chi_{ijk}\,\mathrm{d}y\,\mathrm{d}x \tag{33}$$

where index notation is used, $\varepsilon_{ij}$ are the usual (infinitesimal) strains work-conjugate to the standard stresses $\sigma_{ij}$, and $\chi_{ijk} = \partial\varepsilon_{ij}/\partial x_k$ are the strain gradients work-conjugate to the higher-order stresses $\tau_{ijk}$. Integrating Eq. (33) by parts yields

$$\int_{x_a}^{x_b}\int_{y_a}^{y_b}\int_{\varepsilon}\left(\sigma_{ij}^{(1)} + \frac{\partial\tau_{ijk}}{\partial x_k}\right)\mathrm{d}\varepsilon_{ij}\,\mathrm{d}y\,\mathrm{d}x = 0 \tag{34}$$

whereby boundary terms have been neglected. For arbitrary strain fields it thus follows that

$$\sigma_{ij}^{(1)} = -\frac{\partial \tau_{ijk}}{\partial x_k} \tag{35}$$

which is satisfied by the generic stress definitions (30a)–(30f) as well as by the model-specific stress definitions (31a)–(31c), (32a)–(32d).

### 4.3. Interpretation of natural boundary conditions

The format of the non-standard boundary conditions in a gradient-enhanced continuum has been subject of ongoing debate, see e.g. (Metrikine and Askes, 2002; Mühlhaus and Aifantis, 1991; de Borst and Mühlhaus, 1992; Pamin, 1994; Fleck and Hutchinson, 2001; Peerlings et al., 1996; Toupin, 1962; Mindlin, 1964; Ru and Aifantis, 1993; Polizzotto, 2003). Below, an interpretation is offered that is based on observations found earlier in this work:

(1) From Eq. (28) it follows that the higher-order stresses are work-conjugate to variations with respect to $x$ and $y$ of the perturbations $\xi$ and $\eta$ on the boundaries, e.g. $\tau_{111}$ is work-conjugate to $\xi_x$ on the boundary with $x$ as normal vector, etc. Taking *variations* of $\xi$ and $\eta$ on the boundaries indicates that a lower scale of observation must be chosen.

(2) In Eq. (35) a relation was found between the higher-order part of the standard stresses on the one hand and the higher-order stresses on the other hand. This equation takes the format of an equilibrium equation, in which the divergence of a stress tensor equals minus a body force.

On the higher scale of observation a distinction is made between boundaries with $x$ and $y$ as normal vector, cf. the first index of the stress quantities. These planes will be referred to as the *primary planes*; a primary $x$-plane denotes that the $x$-direction is the normal vector on the higher level of observation, and vice

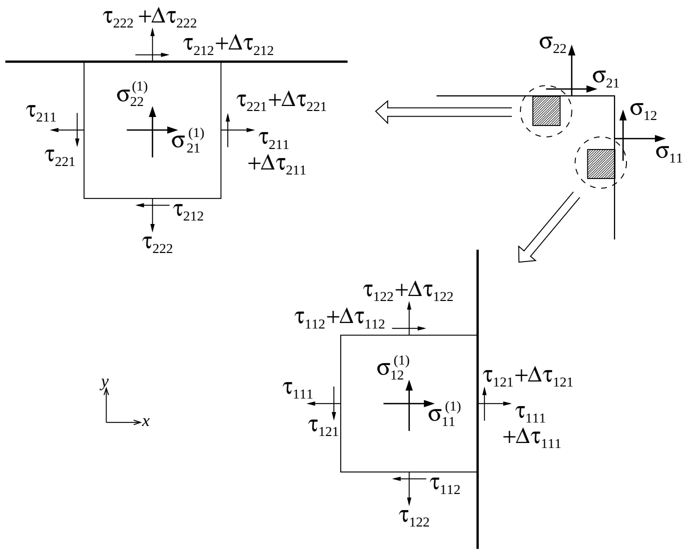


Fig. 4. Physical interpretation of higher-order stresses—higher-scale of observation (top right) and lower scales of observation with primary $x$-plane (bottom) and primary $y$-plane (top left).

versa for the primary $y$-plane. These primary planes are depicted in Fig. 4 together with all stress components (standard and higher-order) that are relevant for each primary plane.

Whereas the classical equations of motion in terms of divergence of (standard) stress hold on the higher scale of observation, on the lower scale of observation fluctuations of the macroscopic stress fields are considered, which are driven by Eq. (35): taking the dimensions of the considered volume on the lower scale as $\Delta x$ and $\Delta y$, Eq. (35) is retrieved by taking the limits $\Delta x \to 0$ and $\Delta y \to 0$.

On the lower level of observation the concept of a secondary plane is introduced, which refers to the normal vectors of the considered lower-level volumes: a secondary $x$-plane has the $x$-direction as normal vector on the lower level of observation. The secondary plane is indicated by the third index of the higher-order stress components. Thus, the symmetry of the higher-order stresses $\tau_{ijk} = \tau_{kji}$ implies that the primary and secondary planes can be interchanged, which occurs at the corners of a considered volume on the higher scale of observation. The model-specific symmetry $\tau_{ijk} = \tau_{ikj}$ refers to the equilibrium of moments on the lower scale of observation.

For the higher-order natural boundary conditions it must be determined which of the higher-order stress components are prescribed. Two cases can be distinguished: the primary plane can be equal to or different from the secondary plane. If they are different, the corresponding stress is balanced by its reaction force on the neighbouring secondary volume, and it cannot be prescribed. In contrast, if the primary plane and secondary plane are the same, the corresponding stress should be equilibrated by externally applied tractions. Thus, the higher-order boundary conditions should be expressed in terms of $\tau_{111}$ and $\tau_{121}$ on the primary $x$-plane and in terms of $\tau_{212}$ and $\tau_{222}$ on the primary $y$-plane.

## 5. Conclusions

Continuum models can be linked to discrete models via continualisation strategies. It is not necessary to restrict to classical continua—also higher-order continua can be derived. In this paper, several aspects concerning the derivation of higher-order continuum models from the corresponding discrete media have been addressed.

Firstly, it has been shown in 1D and 2D that continualisation of the equations of motion and continualisation of the energy yield identical results.

Secondly, an intrinsic element of the continualisation strategy should be the isotropy of the resulting continuum via a suitable selection of parameters. While this is relatively straightforward for classical continua, more sophisticated measures are needed for second-order continua. Here a novel approach is presented in which not one, but two layers of neighbouring particles are accounted for in the continualisation procedure. For a specific stiffness ratio of the two types of interaction, the second-order continuum becomes isotropic. The corresponding energy functional has been derived, and it was found that the higher order part of this functional cannot be expressed uniquely: products of first and third displacement derivatives may be rewritten as products of two second derivatives, and vice versa.

Thirdly, boundary conditions have been derived that are consistent with the energy functional and with the equations of motion. Due to the higher order of the field equations, also higher-order boundary conditions are obtained. Two types of stresses can be distinguished: standard stresses work-conjugate to the classical strain, and higher-order stresses work-conjugate to the strain gradients. The standard stresses consist of a classical part and a higher-order part; the higher-order part of the standard stresses have been linked to the higher-order stresses, and the physical interpretation of this relation is identified as a state of equilibrium on a lower scale of observation.

Finally, let us briefly address the fundamental issue of whether continuous (and homogeneous) models derived from discrete models to be preferred over the underlying discrete models themselves. Obviously, continualisation leads to a loss of accuracy. On the other hand, in many situations the continuous models are much more efficient for numerical evaluation. The reason is that in discrete models the number of degrees of freedom is univocally set by the number of particles in the considered volume, whereas in continuous models the number of degrees of freedom can be chosen in relation to the specific loading conditions. This means that for continuous models the number of degrees of freedom to be considered can be lowered dramatically, for instance in zones of slowly varying deformations.

## References


Aifantis, E.C., 1984. On the microstructural origin of certain inelastic models. ASME Journal of Engineering Materials and Technology 106, 326–330.

Aifantis, E.C., 1987. The physics of plastic deformation. International Journal of Plasticity 3, 211–247.

Altan, B.S., Aifantis, E.C., 1997. On some aspects in the special theory of gradient elasticity. Journal of the Mechanical Behavior of Materials 8, 231–282.

Andrianov, I.V., Awrejcewicz, J., Barantsev, R.G., 2003. Asymptotic approaches in mechanics: new parameters and procedures. ASME Applied Mechanics Reviews 56, 87–110.

Askes, H., Metrikine, A., 2002. One-dimensional dynamically consistent gradient elasticity models derived from a discrete microstructure. Part 2: Static and dynamic response. European Journal of Mechanics A/Solids 21, 573–588.

Askes, H., Sluys, L.J., 2002. Explicit and implicit gradient series in damage mechanics. European Journal of Mechanics A/Solids 21, 379–390.

Askes, H., Sluys, L.J., 2003. A classification of higher-order strain gradient models in damage mechanics. Archive of Applied Mechanics 73, 448–465.

Askes, H., Suiker, A.S.J., Sluys, L.J., 2002. A classification of higher-order strain gradient models—linear analysis. Archive of Applied Mechanics 72, 171–188.

Chambon, R., Caillerie, D., El Hassan, N., 1998. One-dimensional localisation studied with a second grade model. European Journal of Mechanics A/Solids 17, 637–656.

Chang, C.S., Gao, J., 1995. Second-gradient constitutive theory for granular material with random packing structure. International Journal of Solids and Structures 32, 2279–2293.

Chang, C.S., Askes, H., Sluys, L.J., 2002. Higher-order strain/higher-order stress gradient models derived from a discrete microstructure, with application to fracture. Engineering Fracture Mechanics 69, 1907–1924, see also subsequent discussion in Engineering Fracture Mechanics 70, 1219–1221 and 1223–1224.

Chen, W., Fish, J., 2001. A dispersive model for wave propagation in periodic heterogeneous media based on homogenization with multiple spatial and temporal scales. ASME Journal of Applied Mechanics 68, 153–161.

Comi, C., Driemeier, L., 1998. On gradient regularization for numerical analysis in the presence of damage. In: de Borst, R., van der Giessen, E. (Eds.), Material Instabilities in Solids. Wiley, pp. 425–440. Chapter 26.

de Borst, R., Mühlhaus, H.-B., 1992. Gradient-dependent plasticity: formulation and algorithmic aspects. International Journal for Numerical Methods in Engineering 35, 521–539.

Fleck, N.A., Hutchinson, J.W., 2001. A reformulation of strain gradient plasticity. Journal of the Mechanics and Physics of Solids 49, 2245–2271.

Goldstein, H., 1964. Classical Mechanics. Addison-Wesly, Reading.

Gutkin, M.Y., 2000. Nanoscopics of dislocations and disclinations in gradient elasticity. Reviews on Advanced Materials Science 1, 27–60, Available from <http://www.ipme.ru>.

Lasry, D., Belytschko, T., 1988. Localization limiters in transient problems. International Journal of Solids and Structures 24, 581–597.

Lurie, A.I., 2002. Analytical Mechanics. Springer, Berlin.

Mühlhaus, H.-B., Aifantis, E.C., 1991. A variational principle for gradient plasticity. International Journal of Solids and Structures 28, 845–857.

Mühlhaus, H.-B., Oka, F., 1996. Dispersion and wave propagation in discrete and continuous models for granular materials. International Journal of Solids and Structures 33, 271–283.

Metrikine, A., Askes, H., 2002. One-dimensional dynamically consistent gradient elasticity models derived from a discrete microstructure. Part 1: Generic formulation. European Journal of Mechanics A/Solids 21, 555–572.

Mindlin, R.D., 1964. Micro-structure in linear elasticity. Archive for Rational Mechanics and Analysis 16, 51–78.

Pamin, J., 1994. Gradient-Dependent Plasticity in Numerical Simulation of Localization Phenomena, Dissertation. Delft University of Technology.

Peerlings, R.H.J., de Borst, R., Brekelmans, W.A.M., de Vree, J.H.P., 1996. Gradient enhanced damage for quasi-brittle materials. International Journal for Numerical Methods in Engineering 39, 3391–3403.

Polizzotto, C., 2003. Gradient elasticity and nonstandard boundary conditions. International Journal of Solids and Structures 40, 7399–7423.
Ru, C.Q., Aifantis, E.C., 1993. A simple approach to solve boundary-value problems in gradient elasticity. Acta Mechanica 101, 59–68.
Rubin, M.B., Rosenau, P., Gottlieb, O., 1995. Continuum model of dispersion caused by an inherent material characteristic length. Journal of Applied Physics 77, 4054–4063.
Schreyer, H.L., Chen, Z., 1986. One-dimensional softening with localization. ASME Journal of Applied Mechanics 53, 791–797.
Sluys, L.J., 1992. Wave Propagation, Localisation and Dispersion in Softening Solids, Dissertation. Delft University of Technology.
Suiker, A.S.J., Metrikine, A.V., de Borst, R., 2001. Comparison of wave propagation characteristics of the Cosserat continuum and corresponding discrete lattice models. International Journal of Solids and Structures 38, 1563–1583.
Suiker, A.S.J., de Borst, R., Chang, C.S., 2001. Micro-mechanical modelling of granular material. Part 1: Derivation of a second-gradient micro-polar constitutive theory. Acta Mechanica 149, 161–180.
Toupin, R.A., 1962. Elastic materials with couple-stresses. Archive for Rational Mechanics and Analysis 11, 385–414.
Triantafyllidis, N., Aifantis, E.C., 1986. A gradient approach to localization of deformation. I. Hyperelastic materials. Journal of Elasticity 16, 225–237.
Triantafyllidis, N., Bardenhagen, S., 1993. On higher gradient continuum theories in 1-D nonlinear elasticity. Derivation from and comparison to corresponding discrete models. Journal of Elasticity 33, 259–293.
Washizu, K., 1975. Variational Methods in Elasticity and Plasticity. Pergamon, Oxford.
Zhu, H.T., Zbib, H.M., Aifantis, E.C., 1997. Strain gradients and continuum modeling of size effect in metal matrix composites. Acta Mechanica 121, 165–176.