Nonlinear continuum models for the dynamic behavior of 1D microstructured solids

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Abstract

In this paper we analyze the free longitudinal vibrations of a kind of nonlinear one dimensional structured solid, modeling it as a discrete chain of masses interacting through nonlinear springs. The motion equations of this discrete system are solved numerically and the size effect associated to the structure of solid arises.

In order to derive continuum models which capture this scale effect, we perform a non-standard continualization of the nonlinear lattice, as well as standard Taylor-based continualization up to different approximation orders. After we propose an axiomatic generalized continuum model, based on a version of the Mindlin general model but extended to finite deformations. Both formulations lead to the same continuous equation, which depends on a scale parameter. Meanwhile in the axiomatic model the scale constant need to be fixed independently, with the continualized one it is possible to obtain its value from the microstructural characteristic of the solid.

The nonlinear equations corresponding to the continuum models are solved and, in contrast to other works, we compare the results obtained from the discrete system with those obtained with the continuum ones. This comparison pointed out the capability of the proposed axiomatic model to capture the size effects present in the structured 1D solid, both in the linear and nonlinear regimes. Moreover, the inability of the classical model to capture the scale features when they play a role has been clearly stated.

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1. Introduction

It is well known that matter is essentially discrete. Therefore, atomistic and molecular dynamic formulations could be used to understand and predict its behavior. Due to the high computational cost of these formulations, continuum approaches are widely used to analyze large scale problems. In particular, classical continuum mechanics theories, which assume materials to be homogeneous at the considered scale, have been widely used to solve fundamental problems in civil, mechanical and materials engineering, as well as in various fields of physics and life sciences. The origin of its success lies on the fact that the scale of observation is significantly larger than the characteristic dimensions of the underlying microstructure.

However, there are engineering problems related to composites, functionally graded materials, polycrystalline solids, granular materials, etc., in which the wavelength of the phonons propagating through them are similar to the size of microstructure. In addition, there are systems in which the considered geometry and the material microstructure are of the same order. A kind of systems whose dimensions clearly become comparable to the size of their material microstructures or molecular distances are the nanostructures used in technological applications such as micro- or nano-electromechanical (MEMS or NEMS) devices (Martin, 1996), nanomachines (Drexler, 1992; Han et al., 1997; Fennimore et al., 2003; Bourlon et al., 2004), as well as in biotechnology and biomedical fields (Saji et al., 2010). Other examples involve granular and particulate media (Pal et al., 2013; 2014), where discreteness and nonlinear interactions give rise to waves whose wavelength is comparable to the particle dimensions. In such cases, unrealistic predictions may be reached using classical continuum models, since they are unable to capture size-dependent structural behavior. The classical continuum approach is a scale-free theory because their constitutive equations lack an internal length.

Since the 19th century (works by Cauchy and Voigt), and in the beginning of the 20th century (works by Cosserat brothers) it is possible to find some attempts to capture the effects of microstruc-

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ture using the continuum equations of elasticity with additional higher-order derivatives. However, the works by Mindlin and Tiersten (1962); Kröner (1963); 1967; Toupin (1963); 1964); Green and Rivlin (1964); Mindlin (1964); 1965); Krumhansl (1968); Mindlin and Es enh (1968); Kunin (1968); Eringen (1972a); 1972b), Eringen and Edelen (1972), dated in the 1960s and 1970s led to a great breakthrough in the topic.

In addition, Eringen derived, from his earlier integral nonlocal theories (Eringen, 1972a; 1972b), a differential approach (stress-gradient formulation) which contains only one additional length scale parameter [21], and it has been widely used to address different kinds of problems, such as wave propagation, dislocation, crack singularities, and nanostructures behavior.

Nevertheless, several authors have pointed out the inconsistent results obtained from the Eringen differential model regarding both the static (Peddision et al., 2003; Wang and Liew, 2007; Wang et al., 2008; Challamel and Wang, 2008; Challamel et al., 2014c) and vibration behavior (Lu et al., 2006) of a cantilever beam when compared to other boundary conditions. For all boundary conditions except the cantilever, the model predicts softening effect as the nonlocal parameter is increased.

Recently, (Fernández-Sáez et al., 2016) gave some insights on the origin of this paradoxical behavior, and (Romano et al., 2017) clearly proved that the fully nonlocal formulation of the Eringen elasticity theory leads to ill-posed problems for the most practical applications. This impediment has been highlighted in a bending problem, but it also applies to other solid mechanics problems when dealing with bounded domains.

It is worth noting that the above works assumed a linear relation between strains and displacements (infinitesimal deformations framework). However, several applications involving both macr oscale metastructures and nanostructures can be found in which geometrical nonlinear effects are present, see (Dai et al., 2014; Karparvarfar et al., 2015; Cholipour et al., 2015; Pal et al., 2016; Rimoli and Pal, 2016; Šimšek, 2015) and Andrianov et al. (2015), among others.

In this paper we study the nonlinear axial vibration of a kind of nonlinear one dimensional structured solid, defined as a discrete chain of masses interacting through nonlinear springs, analogous to the Fermi, Pasta, Ulam (FPU) system (Fermi et al., 1955). The size effect associated with the structure of the solid plays a major role.

In order to achieve a continuous governing equation of the 1D nonlinear lattice, we develop a non-standard continuumization based on the work of Rosenau (2003), as well as standard Taylor- based continuumization up to different approximation orders. Then, we postulate a nonlinear generalized continuum model for the modeling of structured solids subjected to finite deformations, which contains a scale parameter in its formulation. By comparison with the non-standard contin uumized model, its value is obtained from the microstructural characteristic of the solid.

To validate the results of the generalized continuum model postulated herein, they are compared with numerical solutions of the nonlinear lattice model, which is uncommon in the literature.

The main conclusion of the work is that the proposed axiomatic continuum model adequately reproduces the behavior of the 1D nonlinear discrete model.

2. Formulation of a nonlinear discrete rod

In order to study the dynamic behavior of a nonlinear microstructured one dimensional system, a FPU kind lattice model is formulated (Fermi et al., 1955). The lattice consists of N particles equally spaced at distance d that have one degree of freedom in the axial direction (Fig. 1). Each particle has the same mass M. Particles are linked to first neighbors by nonlinear interactions given by the following polynomial potential

\[ W_n = \frac{1}{2} G \Delta d_n^2 + \frac{1}{3} A \Delta d_n^3 + \frac{1}{4} B \Delta d_n^4 \] (1)

where \( \Delta d_n \) is the variation of distance between particles from their free equilibrium (\( \Delta d_n = u_{n+1} - u_n \)) and \( u_n \) is the displacement of the \( n \)th particle from its equilibrium position. \( G, A \) and \( B \) are the parameters of the interaction potential.

Consistently with Eq. (1), the interaction force of the springs is

\[ F_n = \frac{\partial W_n}{\partial \Delta d_n} = G(\Delta d_n) + A(\Delta d_n)^2 + B(\Delta d_n)^3 \] (2)

Applying linear momentum balance to each particle, we get

\[ M \ddot{u}_n = G(\Delta d_n-1 + u_n) \]
\[ + A[(u_{n+1} - u_n)^2 - (u_{n} - u_{n-1})^2] \]
\[ + B[(u_{n+1} - u_n)^3 - (u_{n} - u_{n-1})^3] \] (3)

The previous system of equations for \( n = 1 \) to \( N \), with corresponding initial and boundary conditions, permits to analyze the dynamic behavior of the nonlinear lattice. Depending on the constants of the nonlinear springs \( G, A \) and \( B \), different constitutive equation laws can be reproduced. Applying the Verlet algorithm presented in Section 5, the oscillation behavior for a given set of interaction constants \( [G, A, B] \) is encountered.

3. Continualization of the lattice model

Continuous models are inherently efficient since all the information about the system’s behavior is condensed in one or few equations. On the contrary, to solve the discrete model, a (large) system of equations needs to be addressed.

In this section, we develop a non-standard continualization of the lattice model using pseudo-differential operators. This nonstandard approach is based in the works by Rosenau (1987; 2003). As an alternative, we use a Taylor series continualization that leads to a different governing equation. The utility and accuracy of these continuous equations will be discussed in subsequent sections.

3.1. A non-standard continualized equation for the lattice structure

The Lagrangian of the finite discrete model can be written as

\[ L_{\text{d}} = \sum_n \frac{1}{2} M \ddot{u}_n^2 - \sum_n \left[ \frac{1}{2} G (u_{n+1} - u_n)^2 + \frac{1}{3} A (u_{n+1} - u_n)^3 + \frac{1}{4} B (u_{n+1} - u_n)^4 \right] \] (4)

The shift operator

\[ e^{i \theta x} = 1 + \theta \frac{\partial}{d} \right + d^2 \theta^2 + d^4 \theta^4 + \ldots \] (5)

permits to relate displacements at neighbor particles as \( u_{n+1} = e^{i \theta x} u_n \). Now defining a continuum displacement variable \( u \) via

\[ \frac{\partial u}{\partial x} = \frac{u_{n+1} - u_n}{d} \] (6)
Considering that
\[ Q = \frac{d\partial x}{e\partial\dot{x}} \]

\( u_n \) is described in terms of \( u \) as
\[ u_n = Q u = \left( 1 - \frac{d\partial x}{2} + \frac{d^3\partial^2 x}{12} + O(d^4) \right) u \]

Therefore, the kinetic energy in terms of \( u \) is now given by Rosenau (2003)
\[ \ddot{u}_n = (Q\ddot{u}, Q\dot{u}) = \ddot{u}^2 + \frac{d^2}{12} (\ddot{u}'')^2 + O(d^4) \]

Taking advantage of Eqs. (6) and (9), and keeping terms up to order 2 in \( d \) we obtain the approximate continuum Lagrangian
\[ L_{\text{ct}} = \int \frac{1}{2} \frac{M}{d} \left[ u''^2 + \frac{d^2}{12} (u'')^2 \right] dx - \int P(u') dx \]
with \( P(u') \) being the continualized potential energy of the springs
\[ P(u') = \frac{1}{2} G d u'^2 + \frac{1}{3} A d^2 u'^3 + \frac{1}{4} B d^3 u'^4 \]

Applying Hamilton’s Principle and the Fundamental Lemma of Variational Calculus, we get the Euler-Lagrange equation of motion
\[ \ddot{u} = \frac{d^2 G}{M} u'' + \frac{2 d^2 A}{M} u' u'' + \frac{3 d^2 B}{M} (u')^2 u'' + \frac{d^2}{12} \ddot{u}'' \]
and boundary conditions
\[ u = 0 \]
\[ \text{or} \]
\[ G u' + A d (u')^2 + B d^2 (u')^3 + M \frac{d^4}{12} u'' = 0 \]

As mentioned by Rosenau (2003; 1986), this continuous equation is obtained by the non-standard asymptotic expansion up to order 2 in \( d \).

Having a continuous equation of the problem, all the different calculus tools can be applied. The advantage of much computationally efficient numerical methods arise, but the accuracy of the results shall be proven. The continualization process itself will distort the behavior of the model due to truncating after \( O(d^2) \). Adding higher order terms lead to a continuum model with more fidelity respect to the discrete one, but also more complex, which would result in a loss of computational advantage. An effective method for obtaining results from the continuous equation (12) is presented in Section 5. The comparison between both the discrete and continuum models is addressed in Section 6.

3.2. Standard continualization by Taylor series

Another possible way to continualize discrete equations consists in developing a Taylor-based asymptotic expansion of the discrete Lagrangian. We assume that the effects of anharmonicity are no longer secondary and expand the potential energy
\[ P(u') = P(u') - \frac{d^2}{24} u'^2 P''(u') + O(d^4) \]
The series is truncated at the desired order, compromising an equilibrium between the complexity of the obtained equation and the loss of information in the truncation.

Thus, keeping terms up to the order 2 in \( d \), the following continuum Lagrangian is obtained (Rosenau, 2003; Triantafyllidis and Bardenhagen, 1993)
\[ L_{\text{ct}} = \int \left[ \frac{1}{2} \frac{M}{d} \ddot{u}^2 - P(u') + \frac{d^2}{24} u'^2 P''(u') \right] dx \]

Applying Hamilton’s Principle and the Fundamental Lemma of Variational Calculus, we get the subsequent equation of motion for the Taylor-based \( O(d^2) \) model
\[ \ddot{u} = \frac{G d^2}{M} \left( u'' + \frac{d^2}{12} u''^2 \right) + A d^2 \left( 2 u' u'' + \frac{d^2}{3} u''^2 + \frac{d^2}{6} u''' \right) + B d^4 \left( 3 u'^2 u'' + \frac{d^2}{4} u''^3 + d^2 u'^2 u''' + \frac{d^2}{4} u''^2 u'' \right) \]
and two boundary conditions apply at each end
\[ u = 0 \]
\[ \text{or} \]
\[ G \left( u' + \frac{d^2}{12} u'' \right) + A d^2 \left( u'' + \frac{d^2}{12} u''^2 + 2 u' u'' \right) + B d^4 \left( 3 u'^2 u'' + 3 u''^2 u''' \right) = 0 \]

The continuous equation of motion of a quadratic nonlinear chain may be recovered by making \( B = 0 \). Then, Eq. (17) will be reduced to
\[ \ddot{u} = \frac{G d^2}{M} \left( u'' + \frac{d^2}{12} u''^2 \right) + A d^2 \left( 2 u' u'' + \frac{d^2}{3} u''^2 + \frac{d^2}{6} u''' \right) \]
which has been previously obtained by Kruskal and Zabusky (1964).

If the same procedure is applied by considering terms only up to order 0 in \( d \), the following nonlinear Lagrangian is obtained
\[ L_{\text{ct}} = \int \left[ \frac{1}{2} \frac{M}{d} \ddot{u}^2 - P(u') \right] dx \]
The Taylor-based \( O(d^0) \) nonlinear wave equation reads
\[ \ddot{u} = \frac{d^2 G}{M} u'' + \frac{2 d^2 A}{M} u' u'' + \frac{3 d^2 B}{M} (u')^2 u'' \]
with boundary conditions
\[ u = 0 \]
\[ \text{or} \]
\[ G u' + A d (u')^2 + B d^2 (u')^3 = 0 \]

Despite the fact that the distance between particles \( d \) appears in the previous equation, it will be demonstrated how the behavior of a system described by this equation of motion does not depend on the lattice spacing \( d \), and therefore this equation is unable to capture the discrete effects in an structured system.

4. Axiomatic continuum models

In this section, a nonlinear generalized continuum model is postulated. This model is inspired by the linear Mindlin strain gradient model in its Form I, see (Mindlin, 1964; Askes and Aifantis, 2011).

Afterwards, the classical nonlinear St. Venant-Kirchhoff model is recovered by discarding microstructural effects.
4.1. An inertia gradient nonlinear generalized continuum model for a rod

To reproduce the behavior of the aforementioned 1D structured solid, we propose an axiomatic generalized continuum theory formulated from the energetic point of view. This model is based in the existence of two mechanical energies:

- A strain energy density that takes into account the nonlinearity of the material. We use here the strain energy density corresponding to the St. Venant-Kirchhoff constitutive equation.

\[ W(X, t) = \frac{1}{2} \mu (\mathbf{e}^1(X, t))^2 + \frac{1}{2} K(X, t) \mathbf{e}^2(X, t) \]

(27)

where \( \mu \) and \( K \) are the Lamé constants, \( \mathbf{e}^1(X, t) \) is the Green-Lagrange strain tensor and \( \mathbf{e}^2(X, t) \) is the displacement vector. Other nonlinear hyperelastic models may be used to represent the desired behavior.

- A kinetic energy density stated by Mindlin to account for the underlying micro-inertia in structured elements. In this work we keep the classical expression for the strain energy function, and include gradients of the velocities in the kinetic energy density function

\[ T(X, t) = \frac{1}{2} \rho_0 \left( \frac{\partial u}{\partial t} \right)^2 + \frac{1}{2} \rho_0 \left( \frac{\partial u}{\partial t} \right)^2 + \frac{1}{2} \rho_0 \left( \frac{\partial u}{\partial t} \right)^2 \]

(28)

where \( \chi \) is the scale parameter that accounts for the micro-inertia and \( \rho_0 \) represents the material time derivative.

This generalized continuum theory leads to the following energy densities in a rod

\[ W = \frac{1}{2} E \left( u^2 + \frac{1}{2} (u')^2 \right)^2 \]

(29)

In behalf of notation simplicity, from now on spatial derivatives \( \frac{\partial u}{\partial x} \) will be expressed by \( (\cdot)' \) and material time derivatives \( \frac{\partial u}{\partial t} \) will be expressed by \( (\cdot) \). Applying Hamilton’s principle, the governing equation of a finite nonlinear continuous microstructured rod is derived. In absence of external loads, \n
\[ -\left( \frac{\partial L}{\partial (\dot{u})} \right)' - \frac{\partial L}{\partial (\dot{u})} + \frac{\partial L}{\partial (\dot{u})} = 0 \]

(30)

and either one of the following boundary conditions (at \( X = 0 \) and \( X = L \)) must be satisfied

\[ u = 0 \]

(31)

\[ \frac{\partial L}{\partial (\dot{u})} = 0 \]

(32)

The governing equation is then expressed by

\[ \ddot{u} = c_0^2 \left( \frac{3}{2} (u)^2 + \frac{1}{2} (u')^2 \right) + c_0^2 u'' + \chi^2 (\dot{u})'' \]

(33)

where \( c_0 = \sqrt{\frac{E}{\rho_0}} \) is the classical sound velocity.

Boundary condition of Eq. (31) remains the same and the Eq. (32) reads

\[ \frac{c_0^2}{2} (2u'' + 3(u')^2 + (u')^2) + \chi^2 (\dot{u})'' = 0 \]

(34)

This relation constitutes the movement equation for this Mindlin-type one-dimensional solids subjected to finite deformations, which must be solved for appropriate initial and boundary conditions.

To have a better understanding of the governing equations of motion, Eq. (33) shall be non-dimensionalized in space and time variables using

\[ \ddot{u} = \frac{u}{\dot{u}}; \quad \frac{X}{\dot{u}}; \quad \tau = t \omega_0; \quad \omega_0 = \frac{c_0}{\dot{u}}; \quad h = \frac{X}{\dot{u}} \]

(35)

where \( \omega_0 \) is the characteristic frequency of the problem under study. Then, the following equation is reached

\[ \ddot{u} = \left( \frac{3}{2} (\ddot{u})^2 + \frac{1}{2} (\dot{u})^2 \right) + \ddot{u}'' + h^2 \dot{u}'' = 0 \]

(36)

From Eqs. (31) and (32), either one of the subsequent boundary conditions must be satisfied at each end

\[ \ddot{u} = 0 \]

(37)

\[ \frac{1}{2} \left( 2 \ddot{u} + 3 (\dot{u})^2 + (\dot{u})^2 \right) + h^2 \dot{u}'' = 0 \]

(38)

Note that, in non-dimensional equations, partial derivatives are done respect to dimensionless space \( s \) and time \( \tau \), \( \ddot{u} = \frac{\ddot{u}}{\dot{u}} \) and \( \dot{u} = \frac{\dot{u}}{\dot{u}} \), meanwhile in dimensional equations derivatives are still done respect to \( X \) and \( t \), \( u' = \frac{u'}{\dot{u}} \) and \( \ddot{u} = \frac{\ddot{u}}{\dot{u}} \).

4.2. Recovery of the classical nonlinear St.Venant-Kirchhoff rod

If the total length is much greater than the microstructural one, the length-scale parameter \( h \) becomes negligible (\( \chi \ll L \)), then \( h \to 0 \). Thus, the classical nonlinear rod formulation is recovered (Abedinnasab and Hussein, 2013; Zhifang and Shanyuan, 2006).

\[ \ddot{u} = \left( \frac{3}{2} (\ddot{u})^2 + \frac{1}{2} (\dot{u})^2 \right) + \ddot{u}'' \]

(39)

This governing equation was found in the past by making use of the axiomatic scale-free St. Venant-Kirchhoff continuum model. The application of that model to a one-dimensional element vibrating axially reduces to

\[ W = \frac{1}{2} E \left( u' + \frac{1}{2} (u')^2 \right)^2 \]

(40)

\[ T = \frac{1}{2} \rho_0 (u)^2 \]

(41)

Applying Hamilton’s principle, Eq. (39) is found. The St. Venant-Kirchhoff axiomatic constitutive relation is known to have a non-polyconvex energy density function, which may lead to instabilities. Nevertheless, the instability occurs for \( u' = -1 \), which has no physical meaning, as it implies superposition of different sections. In addition, the results exhibited in Section 6 are for oscillations under finite but moderate deformations, ensuring that no section of the rod goes beyond the stability region. Despite the inherent instability of the St. Venant-Kirchhoff continuum model, we chose it to illustrate the performance of the non-linear generalized continuum one because it is a well known and widely used model.

4.3. Comparison between proposed axiomatic and discrete-based continuum models

Let us compare the generalized and classical continuum models to the non-standard and Taylor series continualized discrete ones. We can notice that the scale-free nonlinear classical continuum model in 1D, Eq. (39), is formally equivalent to the Taylor-based 0(d0) continualization, Eq. (41). In fact, both equations are identical when the force interaction parameters of the nonlinear chain are adjusted to the following values

\[ G = \frac{E}{\rho_0 d^2}; \quad A = \frac{3}{2} G d; \quad B = \frac{G}{2} d^2 \]

(42)
The following values of the continuum model constants $E$ and $\rho_0$ are compatible with the relations given in Eq. (42)

$$E = \frac{G}{2(1-\nu)}; \quad \rho_0 = \frac{M}{d^2} \quad (43)$$

In addition, the nonlinear generalized continuum 1D model postulated herein is equivalent to the non-standard continualization formulation. It can be seen that using the relation (42), together with the dimensionless value of the scale parameter

$$h = \frac{d}{\sqrt{12L}} \quad (44)$$

the equations corresponding to the proposed axiomatic continuum model, Eq. (36), and the discrete-based non-standard continualized model, Eq. (12), are identical.

We found, in a novel way, the dimensionless micro-inertia parameter $h$ by an analytic procedure, comparing the formulations of the proposed axiomatic and the non-standard continualized models. For the linear formulation of generalized continuum models, other authors in the field (Challamel et al., 2014a; 2014b; Eringen, 1983; Aydogdu, 2012) encountered the exact same value of $h$ after a phenomenological calibration comparing with the results of linear discrete models for different problems. It is noteworthy how the value of the a priori analytical comparison performed in this work predicts the a posteriori calibration from the solutions.

For the case of the Taylor-based $O(d^2)$ continualization in Eq. (17), the application of the obtained relations between the parameters of discrete and continuum models leads to the following dimensionless equation of motion

$$\ddot{u} - \left(\bar{u}^2 + h^2\bar{u}^{IV} - 3\bar{u}\bar{u}'' + 3h^2\bar{u}\bar{u}'' + 6h^2\bar{u}\bar{u}''\right)$$

$$- \left(\frac{3}{2} \bar{u}^2 \bar{u}'' + \frac{3}{2} h^2\bar{u}\bar{u}'' + 6h^2\bar{u}\bar{u}'' + \frac{3}{2} h^2\bar{u}\bar{u}''\right) = 0 \quad (45)$$

Last equation is also investigated as a candidate to predict the dynamic behavior of structured 1-D elements. The basic equations of the different nonlinear continuum models are quoted in Table 1.

### 4.4. Recovery of linear continuum models

From Eq. (36), the Form I of linear Mindlin generalized continuum model formulation can be recovered

$$\ddot{u} = \ddot{u} + h^2 \ddot{u}'' \quad (46)$$

It suffices neglecting the powers of elongation ($u^2$ and $u^3$), as they are insignificant compared to $u''$ when the deformations are infinitesimal. Following a bottom-up approach, (Fish et al., 2002) and (Wang and Sun, 2002) also derived the Eq. (46) by applying homogenization for a periodically inhomogeneous solid.

Moreover, the classical linear continuum model can be recovered from Eq. (39). Applying the classical linear continuum mechanics hypothesis ($u'' \ll 1$), nonlinear terms are dismissed. Finally, neglecting nonlinear terms in (45), the linear version of the Taylor-based $O(d^2)$ continualized model is recovered (Mühlhaus and Oka, 1996; Suiker et al., 2001).

Table 2 shows a resume of the governing equations for the different linearized models.

### 5. Methodologies for the solution of continuum and discrete models

The problem to be solved consists in a finite microstructured rod oscillating freely and subjected to large deformations. This rod may be formulated as a discrete 1D lattice of length $L$, particles of mass $M$, springs with interaction constants $G$, $A$, $B$ and distance $d$ between particles. However, the problem of the continuum rod is formulated as a uniform elastic finite one dimensional element with length $L$ and density $\rho_0$, vibrating longitudinally undergoing large deformations. The relations between all the parameters of the models playing a role in the governing equations are stated in Eqs. (42), (44) and (43).

For validation of the generalized continuum model, solutions will be obtained by making use of both discrete and continuum models in a problem with specific initial and boundary conditions. In this example, free ends are considered as boundary conditions. As initial condition, the rod is at rest and deformed following a sinusoidal shape. In the discrete system this means

$$\tau = 0 \quad \ddot{u}_0 = \ddot{A}_0 \cos \left(\pi \left(n - \frac{1}{2}\right) \frac{d}{L}\right); \quad \tau = 0 \quad \ddot{u}_0 = 0 \quad (47)$$

as the position of particles in equilibrium is

$$X(n) = \left(n - \frac{1}{2}\right) d \quad (48)$$

Initial conditions in the continuum model are expressed by

$$\ddot{u}(X, 0) = \ddot{A}_0 \cos \left(\pi \frac{X}{L}\right); \quad \ddot{u}(X, 0) = 0 \quad (49)$$

where $A_0$ is a free parameter of the problem that will be used to control the amplitude of deformations in the rod, thus enabling to study the induced vibrations under different regimes.

#### 5.1. Numerical solution of the nonlinear lattice problem

The discrete system consists in a finite lattice of equally spaced particles at equilibrium positions stated by Eq. (48). Recall that this system is governed by Eq. (3).

The Verlet algorithm has been used to solve the problem numerically. This algorithm integrates movement equations step by step at each particle, based on time series expansion of displacement $u_n$

$$\ddot{u} + \Delta t u_n = \frac{1}{2} \dddot{u} - \frac{1}{2} \Delta t^2 + \dddot{u} + \Delta t^3 \quad (50)$$

where $1/F_n$ is total force over $n^{th}$ particle at instant $t$, $\Delta t$ is the time increment of numerical integration and $\varepsilon$ is the numerical error, which is of order $(\Delta t)^3$. The forces are evaluated from particle distances using Eq. (2).

Due to the free boundary conditions, particles at left and right ends are only attached to their right and left spring respectively. Given the initial condition in Eq. (47), the temporal evolution of the particles in the lattice is obtained.
5.2. Solution of the continuum model by Galerkin method

According to Galerkin method, an approximate solution $\hat{U}$ is assumed as

$$\hat{u}(s, \tau) \approx \hat{U}(s, \tau) = \Phi(s)q(\tau)$$

(51)

where $\Phi(s)$ is the shape function that must satisfy at least essential boundary conditions and $q(\tau)$ is the unknown time-dependent function to be determined. In this case, initial condition is stated by Eq. (49) and boundary conditions are free ends, stated in Eq. (38).

The function $\hat{U}$ is introduced in Eqs. (39), (36) or (45), in order to obtain the approximate solution of the classical, the axiomatic generalized or the Taylor-based continuous models

$$\mathbb{L}(\hat{U}) = r(s, \tau) \neq 0$$

(52)

where $\mathbb{L}$ is the differential operator associated to each nonlinear governing equation, that can be obtained from the expressions in Table 1, and $r(s, \tau)$ is the residual term.

Applying the Galerkin method

$$\int_0^1 \Phi \mathbb{L}(\hat{U}) ds = 0$$

(53)

Then, $q(\tau)$ and its derivatives are extracted to get

$$\hat{q}(\tau) + D_1q(\tau) + D_2\dot{q}(\tau) + D_3\ddot{q}(\tau) = 0$$

(54)

where the expressions of $D_1$, $D_2$ and $D_3$ are different for each model. See the Appendix for details.

Let us condense Eq. (54) in

$$\hat{q}(\tau) = -g(q(\tau))$$

(55)

with

$$g(q(\tau)) = D_1q(\tau) + D_2\dot{q}(\tau) + D_3\ddot{q}(\tau)$$

(56)

Using the following transformation of Eq. (55)

$$\frac{1}{2} \frac{d}{dq} \dot{q}^2 = -f(q)$$

(57)

Eq. (57) is then solved by quadrature

$$\dot{q}^2 - \dot{q}_0^2 = -2 \int_{\hat{A}_0}^q g(\xi) d\xi$$

(58)

To meet boundary conditions stated in Eq. (38), shape function $\Phi = \cos(\pi s)$ is chosen, which impose a longitudinal deformation with wavelength $\lambda = 2L$. In order to meet initial conditions, Eq. (49), following values of time-dependent function have been set: $\dot{q}_0 = \dot{q}(0) = 0$ and $q(0) = \hat{A}_0$, where $\hat{A}_0 = \frac{A_0}{2}$.

Then, $\dot{q}(\tau)$ and $q(\tau)$ can be obtained as follows

$$\dot{q} = \pm \sqrt{-2 \int_{\hat{A}_0}^q g(\xi) d\xi}$$

(59)

$$\tau = \pm \frac{1}{\sqrt{2}} \int_{\hat{A}_0}^q \sqrt{-\int_{\hat{A}_0}^q g(\xi) d\xi}$$

(60)

6. Discrete and continuum approaches. comparison of results and discussion

Taking the discrete description of the solid as a reference, the results of the developed generalized continuum model will be contrasted paying attention to the specific features resulting from the nonlinear behavior.

Since the parameters $E$ and $\rho_0$ of the continuum model have been related to the parameters $G$, $A$, $B$ and $M$ of the discrete counterpart through Eqs. (42) and (43), by stating the equivalence between the governing equations of nonlinear continuum and continualized discrete models, the comparison of results is feasible. Regarding the third parameter present in the generalized continuum formulation, $h$, we will see how its value, determined from the non-standard continualization of the discrete system equation, permits the continuum model to properly capture the size effects in both linear and nonlinear regimes.

6.1. Results from the discrete models

A first insight into the influence of nonlinear effects in the vibrational behavior of the solid can be provided by comparing the deformation shapes and frequencies corresponding to two different initial amplitudes, one of them of small value $A_0 = 0.01$ and the other $A_0 = 0.1$, one order of magnitude greater. The variables are presented in non-dimensional form, following the same procedure used for the continuum model, see Eq. (35). Notice that the discrete model behavior is highly dependent on the spring constants values $G$, $A$ and $B$. These constants have been adjusted to reproduce St. Venant-Kirchhoff constitutive law. As this model present
instabilities, the lattice may have instable points too. Nevertheless, the deformations reached in the performed simulations never go beyond the stability limit.

Fig. 2 shows the deformation profiles of a lattice with \( N = 20 \), for the case of small vibration amplitude \( A_0 = 0.01 \). It is noteworthy that the dimensionless elongation is calculated from the positions at two adjacent particles as \( \bar{A} = \frac{A}{d} \). It can be seen that the deformed shape follows the sine function, both in tension and in compression phases. Likewise, the trajectory of the particles is harmonic as shown in Fig. 3, implying equal amplitudes and semiperiods in tension and compression phases.

However, the nonlinear effect emerges as the amplitude increases. For \( A_0 = 0.1 \), the deformed shape diverges from the initial sine function as time increases, as can be seen in Fig. 4. Contrary to the features observed in the small amplitude regime, the trajectory of the particles is no longer harmonic and the compression semi-period becomes longer than the tensile one (see Fig. 3). Likewise, the amplitudes corresponding to each regime reach different values. Due to the nonlinear constitutive relation, the material softens under compression and hardens under tension. Peak values of deformation are therefore lower when the rod is elongated. Both effects are related to the spring constitutive function \( F(\Delta d) \), that can be deduced from Eqs. (2) and (42).

With the aim to extend the previous analysis, the relation between amplitude and frequency has been determined in greater detail. This relation will subsequently be used to validate the suitability of the developed continuum model in the nonlinear regime, and also to assess the potential advantage of the generalized continuum approach to capture the size effect found in the discrete approach. The Fast Fourier Transform permitted to identify the excited frequencies of oscillation \( \bar{\omega} \) and their amplitudes. As the initial shape is not exactly the shape of the normal mode of oscillation, some other normal modes are also excited. Thus, the frequency domain function exhibits a clear peak corresponding to the main excited mode and a number of much smaller peaks for the additional modes. The frequency \( \bar{\omega} \) corresponding to the main peak of amplitude is the frequency of oscillation of the first mode, this frequency being independent of the particle selected to sample the time-displacement function.

Fig. 5 shows the influence of the initial amplitude \( A_0 \) in \( \bar{\omega} \) for several ratios of \( \frac{T}{d} \) in the discrete model: the frequency decreases with increasing amplitude independently of the \( \frac{T}{d} \) ratio. The reason for such a behavior is linked to the fact that the compression semi-period notably increases with \( A_0 \), whereas tension semi-period decreases moderately. Fig. 5 also shows how the frequency decreases with increasing microstructural ratio \( \frac{T}{d} \). This outcome clearly illustrates the size effect present in a microstructured solid.

Several comments arise from the results of the discrete model which, for the sake of clarity, are summarized as follows:

- If the displacement amplitude is small enough, the vibratory behaviour approaches that of a linear system, described by both harmonic shape and displacement time-history.
- As the displacement amplitude increases, the vibratory behaviour starts to show nonlinear features and the trajectory of the particles is no longer harmonic. Furthermore, the specific characteristics of the interaction force selected in this work causes a shorter semi-period and a smaller amplitude in tension. 
- The size effect emerges as the distance between particles changes, leading to smaller frequencies when \( d \) increases approaching the wavelength 2L.

6.2. Predictions of the nonlinear continuous models

Next, the results of the proposed axiomatic and Taylor-based \( O(d^2) \) nonlinear models, obtained through approximate solutions
in the form of Eq. (51), will be shown. It should be noted that, according to the strain profile imposed by the shape function $\Phi(s)$, a positive value of the time dependent function $q$ corresponds to a compressive state.

Fig. 6 depicts the phase diagram, $q$ versus $q$, for an initial amplitude $A_0 = 0.1$ and different values of the length scale parameter $h$, for both proposed axiomatic, Eq. (36), and Taylor-based $O(d^2)$, Eq. (45), formulations. Closed trajectories indicate periodic movement. The results of the axiomatic continuum model (Fig. 6a) suggest two different conclusions, both of them fully consistent with the outcomes of the discrete model listed above. First, the amplitude of the compression semi-period is larger. This results from the relation between stress and elongation in St. Venant-Kirchhoff materials subjected to large deformations. Second, the velocity of the oscillation, $q$, decreases for increasing values of the length scale parameter $h$. This confirms the ability of the proposed axiomatic model to capture the size effect observed in the discrete model. However, the Taylor-based $O(d^2)$ model (Fig. 6b), becomes unstable in tension for high values of $h$, and the motion is no longer periodic. As shown by different authors (Rubin et al., 1995; Chen and Fish, 2001; Metrikine and Askes, 2002; Rosenau, 2003), the linear version of this model given by Eq. (46) is also unstable to short wavelength perturbations ($kL > 1/h$). Given the wavenumber $\kappa = \pi/L$ imposed by the shape function $\Phi(s)$, the linear problem is unstable when $h > 1/\pi$. In the nonlinear problem, the instability appears even for lower values of $h$ as $A_0$ increases. This behavior is not consistent with the results of the discrete model.

Fig. 7 shows the time-history of function $q$ derived with the proposed axiomatic continuum model for different values of $A_0$ and $h$. It is worth highlighting that the solution predicted by the nonlinear classical model is recovered (Abedinhasab and Hussein, 2013; Zhifang and Shanyuan, 2006) for $h = 0$, as the influence of the micro-inertia is neglected. The classical model is, however, unable to capture the size effects. Nevertheless, the proposed axiomatic model shows larger periods as the length scale parameter $h$, related to the microstructural effect, increases. In addition, it is also able to capture the transient from linear to nonlinear behavior of the solid as the amplitude of the oscillation increases. When the initial amplitude is small ($A_0 = 0.01$), the continuum model recovers the harmonic trajectory of the particles. However, at higher amplitudes ($A_0 = 0.1$, $A_0 = 0.2$) the oscillation becomes nonlinear with shorter semiperiod and smaller amplitude in tension, in full accordance with the results of the discrete model.

Fig. 8 shows the results of the Taylor-based $O(d^2)$ model. In linear regime ($A_0 \ll 1$, Fig. 8a), the oscillations are harmonic, and increasing values of $h$ lead to longer periods, in agreement with the discrete model results (Fig. 4). In nonlinear regime, it is shown that this model predicts asymmetric periodic behavior for small values of the scale parameter $h$, with longer periods and smaller values in tension than compression, also in agreement with the discrete model. However, this behavior changes for increasing values of the scale parameter $h$, and the asymmetry gets inverted for oscillations with amplitude $A_0$ and scale parameter $h$ above certain values, see Figs. 8(b) and 8(c). For values beyond higher limits of $A_0$ or $h$, the model becomes unstable in tension. For these cases, e.g. $A_0 = 0.1$, $h = 0.3$ in Figs. 6(b) and 8(b), the model predicts unbounded growth of the stretch. These results prevent the use of the Taylor-based $O(d^2)$ model for the analysis of the considered 1D nonlinear structured solid.

So far, the comparison between discrete and continuum models has been strictly qualitative. The trends predicted by both models are all consistent, but a quantitative validation is still required. To that aim, the relation between amplitude and frequency has been further developed, as it was done with the discrete model. The

![Fig. 5. Discrete model. Non-dimensional frequency of oscillation $\tilde{\omega}$ for different $\hat{\xi}$ ratios and different initial amplitudes $\tilde{A}_0$.](image)

![Fig. 6. Continuous models. Phase diagram of the nonlinear oscillation with $\tilde{A}_0 = 0.1$ and different values of length scale parameter $h$. (a) Proposed axiomatic continuum model. (b) Taylor-based $O(d^2)$ model.](image)
non-dimensional angular frequency has been determined with the aid of Eq. (60), where the period \(T\) has been calculated as twice the difference between the time instants corresponding to two consecutive extrema of the function \(q\)

\[
T = \frac{1}{\omega_0} 2|\tau_{q,\text{min}} - \tau_{q,\text{max}}| 
\]

thus leading to

\[
\hat{\omega} = \frac{\pi}{|\tau_{q,\text{min}} - \tau_{q,\text{max}}|} 
\]

The main outcomes of the quantitative comparative analysis are discussed below.

6.3. Quantitative comparison. The accuracy of the proposed axiomatic model

The results of the discrete model highlighted the nonlinear and scale effects present in the vibratory behavior of this 1D media. The first is triggered by increasing values of \(\bar{A}_0\), while the second is related to changes in the microstructural ratio \(\bar{q}\).

Fig. 9 shows the dimensionless angular frequency \(\hat{\omega}\) obtained with the considered models, for different values of the initial amplitude \(\bar{A}_0\) and of the length scale parameter \(h\). The curves are replicated in each of these sub-figures in order to compare them with the results of the discrete model for \(N = \{20, 15, 8, 4\}\) particles, corresponding to \(\bar{q} = \{\frac{1}{20}, \frac{1}{15}, \frac{1}{8}, \frac{1}{4}\}\).

The curve corresponding to \(h = 0\), which represents the classical case, is obviously the same for all subfigures. As shown in Fig. 9(a), the results obtained with the classical nonlinear model are close to those of the discrete model if the number of particles is large, i.e., \(d \ll L\). In such a case, the wave number is small compared to the limit of first Brillouin zone, and the hypotheses of the classical continuum are still valid.

On the contrary, as \(L\) and \(d\) become comparable in a discrete media with a lower \(\frac{d}{L}\) ratio, the oscillation frequencies predicted by the classical continuum differ significantly from those predicted by the discrete model. Since the classical continuum is independent of the ratio \(\frac{d}{L}\), it is unable to properly capture size effects.

According to the results shown in Fig. 9, the Taylor-based O(\(d^2\)) model provides more accurate predictions for the behavior of the discrete chain than the classical continuum one. Nonetheless, it is seen that the proposed axiomatic continuum model leads to slightly better results. In addition, the Taylor-based O(\(d^3\)) model is unstable in linear regime for short wavelength perturbations.
model 7. nanostructures predict structured model of vibration trends able conflict the (Fig. 8. Continuous Taylor-based $O(d^2)$ model. Time-dependent function $q$ versus non-dimensional time $\tau$ for different values of length scale parameter $h$ and initial amplitude (a) $A_0 = 0.001$ (b) $A_0 = 0.1$ (c) $A_0 = 0.2$.

$(kL > 1/h)$, and the instability appears for lower wavenumber $k$ in the nonlinear regime as the amplitude $A_0$ is increased, which is in conflict with the discrete model behavior.

On the other side, the continuum model presented herein is able to appropriately capture both nonlinear and scale effects. The trends observed with the discrete model in the angular frequencies $\hat{\omega}$, as well as the features related with the distinctive behavior in tension and compression, are properly captured. In addition, calibration of micro-inertia parameter was not needed, since the value of $h$ was naturally determined by a non-standard continualization of the discrete model formulation.

The comparison shows that the proposed axiomatic nonlinear model provides a continuum tool for the study of nonlinear 1D structured solids. This generalized continuum model is able to predict scale effects that occur in microstructured materials and nanostructures undergoing finite deformations.

7. Conclusions

The main objective of this work was to develop a continuum model able to accurately reproduce the essential features of the dynamical behavior of a kind of 1D structured solids undergoing finite deformations.

To that aim, the axial vibration problem of a chain of masses interacting through nonlinear springs has been formulated and solved. The equations of this problem were later continualized using both standard (Taylor-based up to different approximations orders) and non-standard (pseudo-differential operators) methods in order to derive continuum equations corresponding to the discrete problem. Alternatively, two axiomatic continuum models were formulated. The first one is a specialization of the classical St. Venant-Kirchoff hyperelastic model to a 1D axial vibrations problem, which coincides with the standard Taylor-based $O(d^2)$ continualized model. The second -and original- one consists in an extension of the former model, including a velocity gradient term in the kinetic energy density, to capture scale effects. The continuum equation corresponding to this axiomatic model is formally equivalent to that derived as an asymptotic expansion of the discrete model Lagrangian, using Padé approximants, and keeping terms up to the order $2$ in $d$.

The parameters of the continuum models were determined by stating the equivalence between their governing equations and those of the continualized discrete models. This permitted a suit-
The continuum model of the Lagrangian variation leads to the Kirchhoff constitutive equation and the Taylor-based $O(d^2)$ continualization. From this observation, we have derived an original axiomatic generalized continuum model for capturing scale parameters derived from the non-standard continualization, which shows the utmost performance in capturing scale and nonlinear effects.

In the discrete model, and for the adjustment to the St. Venant-Kirchhoff constitutive model, higher amplitudes of vibration lead to lower frequencies.

The higher the characteristic size in the underlying structure of the chain, the lower the frequencies of oscillation. This observation stresses the scale effects present in the discrete solid.

The standard Taylor-based $O(d^2)$ continualization of the discrete Lagrangian leads to an equation that is formally equivalent to the nonlinear classical model resulting from the specialization of the St. Venant-Kirchhoff hyperelastic model. This continuum model has proven to be unable to capture the size effect, although it is valid for the long wave regime.

The Taylor-based $O(d^2)$ model produces more accurate predictions for the behavior of the discrete chain than the classical continuum model regarding the variation in the frequencies with the oscillation amplitude and the scale parameter. However, this model is unstable to short wavelength perturbations, and the critical wavelength at which the instability occurs increases as the amplitude of oscillation increases.

- The governing equation of the proposed axiomatic continuum model and of the non-standard continualized one are identical, but the latter permits to obtain the scale parameter from the characteristics of the solid.
- The proposed axiomatic model leads to the nonlinear classical one if the length-scale parameter vanishes. Similarly, it leads to the linear classical model if both nonlinear and length-scale terms are dismissed.
- The proposed axiomatic model, with the scale parameters derived from the non-standard continualization, shows the best performance in capturing scale and nonlinear effects.
- The original axiomatic generalized continuum model proposed in this work captures both scale and nonlinear effects of the chain, both qualitatively and quantitatively (transient from linear to nonlinear behavior as the amplitude of the oscillation increases, and sensitivity to variations in the structural length).

All in all, in this paper we have derived an original continuum equation to predict the dynamic behavior of nonlinear one-dimensional lattices and we compared the predictions with sim-
ulations of a reference discrete system. The formulation of the model proposed herein is axiomatic and applicable to higher di-
dimensions elements. Its application to predict the axial dynamic be-
havior of a nonlinear 1D element produces satisfactory results.

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Appendix A. Coefficients $D_i$ in the differential Eq. (56)

<table>
<thead>
<tr>
<th>Table A1</th>
<th>Expressions for the coefficients $D_i$ in the time-dependent Eq. (56).</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Model</td>
<td>$D_1$</td>
<td>$D_2$</td>
</tr>
<tr>
<td>---------</td>
<td>---------------------------------------------------------------------</td>
<td>-------</td>
</tr>
<tr>
<td>Classical continuum</td>
<td>$\pi^2$</td>
<td>$-4\pi^2$</td>
</tr>
<tr>
<td>Generalized continuum</td>
<td>$\pi^2/(1 + h^2\pi^2)$</td>
<td>$-4\pi^2/(1 + h^2\pi^2)$</td>
</tr>
<tr>
<td>Taylor based</td>
<td>$\pi^2 - h^2\pi^2$</td>
<td>$-4\pi^2 + 12h^2\pi^2$</td>
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</tbody>
</table>


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