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Continuous Model of 2D Discrete Media Based on Composite Equations[1]

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This article is dedicated to the memory of prof. A.I. Potapov

Abstract—The paper focuses on the development of 2D continuous models for a theoretical prediction of dynamic properties of discrete microstructures. A new continualization procedure, which refers to nonlocal interactions between variables of the discrete media, is proposed and the corresponding continuous model is obtained. The performed study is based on the application of composite equations. The developed approach is suitable for the dynamic analysis of 2D lattices of micro- and nanoparticles oscillating with arbitrary frequencies.

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INTRODUCTION

In recent years new classes of ultra dispersive and nanocrystalline heterogeneous materials are proposed [1]. Theoretical investigation of such structures requires new modern approaches that have to be principally different from the classical continuous medium theory. This challenge is also characteristic for various problems of nanomechanics [2, 3]. Models established on a continuous medium approximation cannot govern high frequency oscillations, behaviour of the materials in the vicinity of cracks and on the fronts of destruction waves [4, 5], and during phase transitions [6]. Wave dispersion in granular materials [7, 8] represents an important example of microstructural effects, which are also essential in damage mechanics [9] and in the theory of plasticity [10, 11].

The mentioned effects may be analyzed within the frame of discrete models, using molecular dynamics, quasicontinuum analysis or others numerical approaches. However, evaluation of numerical results is very time-consuming. For example, modern practical problems are still intractable for molecular dynamics based analysis, even if the highest computing facility is at disposal.

Hence, refinement of the existing continuum theory for the purpose of more realistic predictions seems to be the only viable alternative. In connection with this, one of the most challenging problems in multiscale analysis is that of finding continuum models for discrete, atomistic models. Although in statistical physics these questions were already addressed 100 years ago, many problems remain open even today. Most prominent is the question of how to obtain irreversible thermodynamics as a macroscopic limit from microscopic models that are reversible. In this paper we consider another part of this field that is far from thermodynamic fluctuation. We are interested in reversible, macroscopic limits of atomic models. Debye approach is the simplest model of this type, but it does not take into account spatial dispersion. More suitable is the Born-von Kármán model of lattice dynamics, which is analogous to the case of a chain with only nearest-neighbour interactions.

Therefore, continuous modeling of micro- and nanoeffects plays a crucial role in mechanics [12, 13]. It seems that the simplest approach to realize this idea relies on a modification of the classical modelling incorporating both the hypothesis of continuity and the main characteristic properties of a discrete structure. Continualization procedures are based on various approximations of a local (discrete) operator by a nonlocal (continuous) one. One can treat the governing difference operator as a pseudo-differential one and then split it in Taylor series. Keeping only the first term of the expansion, the classical continuous approximation is obtained. Taking into account more terms, the so-called intermediate continuous model, which includes a differential operator of the higher order, can be found. Using of one- and two-point Padé approximants gives a possibility to improve accuracy of the approximation with saving the lower order of the differential operator. Results for the 1D case were

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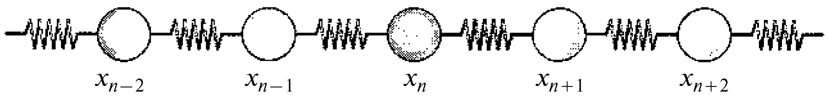

Fig. 1. Chain of particles.

obtained in [14–18]. The technique proposed can be easily generalized to those 2D problems that are still scalar in nature, i.e., that are reducible to a problem for a combination of uncoupled scalar potentials [19, 20], Difficulties arising in the non-scalar case are discussed in [17]. In particular, it is shown that Padé approximants can not be applied; that is why in many papers [7, 8, 17] intermediate continuous models of higher orders were used.

In the present work, the technique of composite equations that was originally developed for a 1D case [21] is extended to 2D problems. As the result, this allows to derive new accurate continuous approximations of the lower order.

The paper is organized as follows. In Section 2, the main idea of the proposed approach is introduced on the basis of a discrete 1D dynamical model. Continuous models for the 2D case are obtained in Section 3. Section 4 presents brief concluding remarks.

DISCRETE 1D DYNAMICAL MODEL

Let us consider free oscillations of a chain of particles displayed at Fig. 1. Input equations of motion can be written as follows

$$M\ddot{u}_n(t) = K_1(u_{n+1} - 2u_n + u_{n-1}), \tag{1}$$

where u_n is the displacement vector for a particle situated at point x_n, $x_n = nh$; M is the particle mass; K_1 is the stiffness of the springs.

For large number of particles, a continuous approximation to the discrete problem (1) is usually applied:

$$Mu_{tt}(x, t) = K_1h^2u_{xx}(x, t). \tag{2}$$

The "saw-tooth" oscillations ($u_n = -u_{n-1}$) are described by the equation

$$M\frac{\partial^2 u}{\partial t^2} + 4K_1u = 0. \tag{3}$$

Knowing the continuous approximations (1) and (2), it can be possible to construct a composite equation [21], which is uniformly suitable for all frequencies and oscillation modes of the chain. Van Dyke emphasized that composite equations can be obtained by the synthesis of the limiting cases. The key idea of the method is [22, p. 195]:

"(i) Identify the terms in the differential equations whose neglect in the straightforward approximation is responsible for the nonuniformity.

(ii) Approximate those terms insofar as possible while retaining their essential character in the region of nonuniformity."

The composite equation determined on the basis of Eqs. (2), (3) reads:

$$M\left(1 - \alpha^2h^2\frac{\partial^2}{\partial x^2}\right)\frac{\partial^2 u}{\partial t^2} - K_1h^2\frac{\partial^2 u}{\partial x^2} = 0, \tag{4}$$

where $\alpha^2 = 0.25 - \pi^{-2} \approx 0.1487$.

Let us note that the same equation can be obtained using two-point Padé approximants [23]. Term with mixed derivative can be treated as the inertia of normal motion in equation of longitudinal vibrations of rod.

Equation (4) allows calculating the frequencies of discrete chain α_k:

$$\alpha_k = \pi\sqrt{\frac{c}{m}}\frac{k}{\sqrt{(n+1)^2 + \alpha^2\pi^2k^2}}, \quad k = 1, 2, \ldots, n. \tag{5}$$

The largest error in determination of α_k is about 3%; it is achieved at $k = [0.5(n+1)]$, where $[x]$ is the integer part of x. Let us note that Eq. (4) is of the second order with respect to the spatial coordinate, i.e., the essential improvement of accuracy is obtained without the increase in the order of the differential operator.

Eringen [24] showed that the dispersion relation closely matches with the Born-von Kármán model dispersion when $\alpha^2 = 0.1521$. This value is very close to that proposed by Metrikine and Askes [25] on the basis of a certain physical interpretation; they also refer Eq. (4) as the "dynamically consistent model."

The dispersion curve obtained from Eq. (4) does not satisfy the condition $d\alpha_k/dk = 0$ at the end of first Brillouin zone. On order to overcome this contradiction, Eringen [26] (see also [27]) proposed so-called bi-Helmholtz type equation:

$$m\left(1 - \alpha^2h^2\frac{\partial^2}{\partial x^2} + \beta^2h^4\frac{\partial^4}{\partial x^4}\right)u_{tt} - K_1h^2u_{xx} = 0,$$

where $\alpha = 1/\pi$.

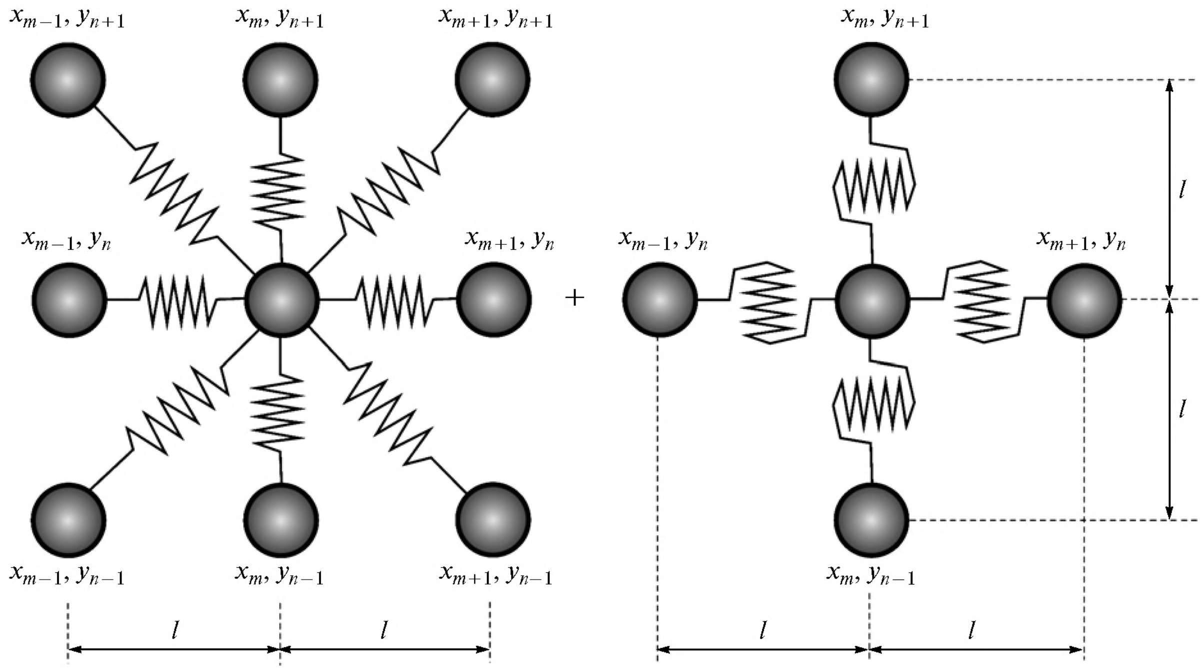

Fig. 2. Square lattice of particles [17].

DISCRETE 2D DYNAMICAL MODEL

Let us consider a square lattice of particles shown in Fig. 2. The input equations of motions are:

$$\begin{aligned} M\ddot{u}_{m,n} &= K_1(u_{m,n-1} - 2u_{m,n} + u_{m,n+1}) \\ &+ K_2(u_{m-1,n} - 2u_{m,n} + u_{m+1,n}) \\ &+ \frac{1}{2}K_0(u_{m-1,n-1} + u_{m+1,n-1} + u_{m-1,n+1} + u_{m+1,n+1} \\ &+ v_{m-1,n-1} - v_{m+1,n-1} - v_{m-1,n+1} \\ &+ v_{m+1,n+1} - 4u_{m,n}), \\ M\ddot{v}_{m,n} &= K_1(v_{m,n-1} - 2v_{m,n} + v_{m,n+1}) \\ &+ K_2(v_{m-1,n} - 2v_{m,n} + v_{m+1,n}) \\ &+ \frac{1}{2}K_0(v_{m-1,n-1} + v_{m+1,n-1} + v_{m-1,n+1} + v_{m+1,n+1} \\ &+ u_{m-1,n-1} - u_{m+1,n-1} - u_{m-1,n+1} \\ &+ u_{m+1,n+1} - 4v_{m,n}), \end{aligned} \tag{6}$$

where $u_{m,n}$, $v_{m,n}$ are the components of the displacement vector for a particle situated at the point (x_m, y_n), $x_m = mh$, $y_n = nh$; M is the particle mass; K_0, K_1 and K_2 are the stiffness factors of the diagonal longitudinal, the axial longitudinal and the axial shear springs, respectively.

The commonly used continualization procedure for Eqs. (6) is based on the introduction of a continuous displacement field $u(x_m, y_n) = u_{m,n}$, $v(x_m, y_n) = v_{m,n}$ and expanding the components $u_{m\pm1,n\pm1}$, $v_{m\pm1,n\pm1}$, into Taylor series around $u_{m,n}$, $v_{m,n}$. The second-order continuous theory in respect to the small parameter h implies:

$$\begin{aligned} M\frac{\partial^2 u}{\partial t^2} &= K_1h^2\frac{\partial^2 u}{\partial x^2} + K_2h^2\frac{\partial^2 u}{\partial y^2} + 2K_0h^2\frac{\partial^2 v}{\partial x\partial y}, \\ M\frac{\partial^2 v}{\partial t^2} &= K_1h^2\frac{\partial^2 v}{\partial x^2} + K_2h^2\frac{\partial^2 v}{\partial y^2} + 2K_0h^2\frac{\partial^2 u}{\partial x\partial y}. \end{aligned} \tag{7}$$

One can construct equations of the higher-order in special variables, however, as it was shown in [17], it is not possible to create asymptotic theories that do not possess extraneous solutions in the non-scalar context.

The "saw-tooth" oscillations of the 2D discrete lattice can be described by the following equations:

$$\begin{aligned} M\frac{\partial^2 u}{\partial t^2} &= 4\left(K_1\frac{\partial^2 u}{\partial x^2} + K_2\frac{\partial^2 u}{\partial y^2}\right), \\ M\frac{\partial^2 v}{\partial t^2} &= 4\left(K_1\frac{\partial^2 v}{\partial x^2} + K_2\frac{\partial^2 v}{\partial y^2}\right). \end{aligned} \tag{8}$$

The composite equation determined from the limiting models (7), (8) is:

$$M\left(1 - \alpha^2h^2\frac{\partial^2}{\partial x^2} - \alpha^2h^2\frac{\partial^2}{\partial y^2}\right)\frac{\partial^2 u}{\partial t^2}$$

$$= K_1 h^2 \frac{\partial^2 u}{\partial x^2} + K2h^2 \frac{\partial^2 u}{\partial y^2} - (K_1 + K_2)h^4\gamma^2 \frac{\partial^4 u}{\partial x^2 \partial y^2}$$

$$+ 2K_0 h^2 \left[1 + \frac{1}{4(K_1 + K_2)} \frac{\partial^2}{\partial t^2}\right] \frac{\partial^2 v}{\partial x \partial y},$$

$$M\left(1 - \alpha^2 h^2 \frac{\partial^2}{\partial x^2} - \alpha^2 h^2 \frac{\partial^2}{\partial y^2}\right) \frac{\partial^2 v}{\partial t^2} \quad (9)$$

$$= K_1 h^2 \frac{\partial^2 v}{\partial x^2} + K2h^2 \frac{\partial^2 v}{\partial y^2} - (K_1 + K_2)h^4\gamma^2 \frac{\partial^4 v}{\partial x^2 \partial y^2}$$

$$+ 2K_0 h^2 \left[1 + \frac{1}{4(K_1 + K_2)} \frac{\partial^2}{\partial t^2}\right] \frac{\partial^2 u}{\partial x \partial y},$$

where $\gamma^2 = (4 - \pi^2 + 8\pi^2\alpha^2)/(4\pi^2)$.

Term with mixed spatial-time derivatives can be treated as the inertia of normal motion. In 1D cases, expressions (9) are reduced to Eq. (4) for u and the same for v. In a case of small variability by spatial and time co-ordinates, Eqs. (9) can be approximated by Eqs. (7); in a case of large variability—by Eqs. (8).

CONCLUSIONS

Free oscillations of 1D and 2D discrete structures are considered. New lower-order continuous models are obtained by the method of composite equations. Derived analytical solutions for the eigenfrequencies exhibit a high numerical accuracy. The results of the paper can be used for a theoretical prediction of dynamic properties of heterogeneous media with micro-and nanostructures. Generalization of the developed procedure to equations of bi-Helmholtz type [27] is a subject to further research.

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