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MECHANICS

Nonlinear wave motion and complexity

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Abstract. Contemporary complexity science deals with problems which involve many variables interacting with each other in such a way that a new quality appears. An important cornestone of complex systems is nonlinearity. In this paper nonlinear wave motion in microstructured solids is analysed from the viewpoint of complexity. The basic models are derived by using the concept of internal variables which are related to dissipation inequality. The scale dependence results in wave hierarchies where dispersive effects are important. In such nonlinear models solitary wave structures may emerge – a typical sign of a new quality characteristic of complexity. In addition, examples from biophysics are presented, which demonstrate clearly the similarity to the ideas of complexity shown for waves in solids.

Key words: microstructured solids, Mindlin model, solitary waves, solitons.

1. INTRODUCTION

The history of mechanics is full of remarkable ideas which have shaped the modern understanding of nature and technology. The list of celebrated examples is long: the movement of planets, a three-body system, movements of a pendulum and vibrations of a string, waves on a free surface of fluids, etc. A remarkable physical feature, called nonlinearity (i.e. additivity does not work), is naturally related to many physical phenomena and therefore it is not surprising that mechanics together with thermodynamics is a cornerstone of an interdisciplinary field of knowledge – complexity science. Complex systems, as a rule, are nonlinear. They are far from the equilibrium and exhibit the properties of the emergence of coherent structures. Typically such systems involve many variables (constituents) which interact with each other in such a way that a new quality appears. In terms of mechanics, we may recall that nonequilibrium systems are controlled by thermodynamics, the microstructure of solids (i.e. internal structure of materials) brings in the interaction effects, and constitutive laws or interaction forces are in many cases nonlinear. In terms of complexity science, mechanics has revealed many emergent and qualitatively new phenomena like solitons, attractors, phase transformation, coherent wave fields, etc. The analysis of complexity, however, faces a certain caveat. Said A. Toffler in his preface to the book by Prigogine and Stengers (1984): 'One of the most highly developed skills in contemporary Western civilization is dissection: the split-up of problems into their smallest possible components. We are good at it. So good, we often forget to put the pieces back together again'. However, the idea of putting things back again is not new. Said Aristotle: 'The whole is more than the sum of the parts'. And it is mechanics that has brought this old knowledge to our contemporary understandings. The basic notion which has 'changed the world' is nonlinearity. Although the inverse-square law of gravitation was introduced by Newton, it was much later when H. Poincaré understood its importance when he solved the three-body problem. But only in the mid-twentieth century the concepts like solitons, chaotic attractors, and other members of the nonlinear 'zoo' made clear that a new quality is born when constituents of a whole interact with each other nonlinearly. Nonlinear dynamics has brought many new ideas not only to mechanics but also to many other fields – biology and chemistry, econophysics and social studies, etc., not speaking about many other physical processes. The reason is simple – the world around us is nonlinear and

similar patterns emerge in different processes, similar methods can be used in studies of different fields, and the language of different studies is more understandable to the general community of scientists. Shortly, the world is complex and complexity research, as it is understood now, is an intrinsically transdisciplinary enterprise. The citation above by A. Toffler reflects the general view, but the monograph by Prigogine and Stengers (1984) itself is a proof of the contrary and describes the earlier ideas of complex systems. More recently, Nicolis and Nicolis (2007) summed up the main features of complexity science, but the full and state-of-the-art description of complex systems is presented in the *Encyclopedia of Complexity and System Science* (Mayers, 2009).

Besides the main characteristics of complex systems mentioned above, the following should be stressed. First, an important issue in complex systems is their multi-scale structure: a system behaves differently at the macroscopic level than at the microscopic level. This leads to certain hierarchies which are linked physically and should also be reflected by proper mathematical models where scaling is of importance. Second, nonlinearity is also a prerequisite to chaos. But complexity does not mean directly a path to chaos; emergence usually occurs at the edge of chaos (Holland, 1998; Taylor, 2003). In this context it means that both order and chaos must be properly analysed. Mechanics is full of examples of chaotic motion starting from the three-body system and nonlinear pendulums to the celebrated Lorenz attractor which describes the convection in the atmosphere. In this paper the focus is on the analysis of waves in microstructured materials by taking the viewpoint of complexity. Attention is on the proper modelling of microstructure and the effects which follow from scaling and interaction between macro- and microstructure. In addition, some parallels are drawn from biophysics: the modelling of cardiac contraction where mechanics is interwoven with physiology and the ideas of internal variables derived in mechanics are used. In general, the paper reflects the studies of the Centre for Nonlinear Studies, Tallinn, in this field.

2. WAVES IN MICROSTRUCTURED SOLIDS

2.1. General theory

The conventional theories of continua describe the behaviour of homogeneous solids resp. materials. In reality, however, materials are always characterized by a certain microstructure at various scales. The character of a microstructure can be regular (like in laminated composites) or irregular (like in polycrystalline solids or alloys). Even more, regularity and irregularity may be combined like for some FGMs. The characteristic scale l of a microstructure must always be compared with the spatial scale L of an excitation. Intuitively speaking, if $L >> l$, then the excitation 'does not feel' the microstructure; if, however, $L \sim l$, then the excitation 'feels' strongly the microstructure. In general terms, the starting point for describing a microstructure could be either the discrete or the continuum approach. In the discrete approach the volume elements are treated as point masses with interaction forces between them described by using assumptions on energy embedded into the system (Askar, 1985; Maugin, 1999). The system of governing equations is extremely large, creating enormous difficulties in numerical simulation, if it is altogether possible. The discrete approach is often used for laminated composites and then the effective stiffness theory may be useful (Santosa and Symes, 1991). From the viewpoint of continua, the straightforward modelling leads to assigning all physical properties to every volume element dV in a solid, which means introducing the dependence on space coordinates. Thus, the governing equations are so complicated that only numerical simulation is possible. Although the discrete approach seems to be appropriate for modelling the microstructure, the question of how to determine the interaction forces in order to reflect material properties is difficult to answer. This is why generalized continuum theories enter. Generalized continuum theories extend conventional continuum mechanics for incorporating intrinsic microstructural effects into governing equations (Eringen and Suhubi, 1964; Mindlin, 1964; Eringen 1999). A leading concept is to separate the macro- and microstructure in continua and to formulate the balance laws for both structures separately (Eringen and Suhubi, 1964; Mindlin, 1964). However, a more sophisticated way is to introduce the microstructural quantities into one set of balance laws (Maugin, 1993, 2006). It seems that such an approach is useful for two reasons: (i) it reflects clearly the mechanical structure of a solid; (ii) it allows further generalization in order to include internal variables and to cast more light on the thermodynamic character of wave motion. Here we refer to longer papers by Engelbrecht (2009) and Berezovski et al. (2010). First, Maugin (1993, 2006) has shown that on the material manifold $\mathscr{M}^3$, the balance of the canonical (material) momentum reads

$$\left.\frac{\partial \mathbf{P}}{\partial t}\right|_{\mathbf{X}} - \mathrm{Div}_R \mathbf{b} = \mathbf{f}^{\mathrm{int}} + \mathbf{f}^{\mathrm{ext}} + \mathbf{f}^{\mathrm{inh}}, \tag{1}$$

where $\mathbf{P}$ is the material momentum (pseudomomentum), $\mathbf{b}$ is the material Eshelby stress, and $\mathbf{f}^{\mathrm{inh}}, \mathbf{f}^{\mathrm{ext}}, \mathbf{f}^{\mathrm{int}}$ are the material inhomogeneity force, the material external (body) force, and the material internal force, respectively. The energy balance is governed by

$$\left.\frac{\partial (S\theta)}{\partial t}\right|_{\mathbf{X}} + \nabla_R \cdot \mathbf{Q} = h^{\mathrm{int}}, \tag{2}$$

where S is the entropy density per unit reference volume, θ is the absolute temperature, $\mathbf{Q}$ is the material heat flux, and h^{int} is the source term. The dissipation inequality in these terms is

$$S\dot{\theta} + \mathbf{S} \cdot \nabla_R \theta \leq h^{\mathrm{int}} + \nabla_R (\theta \mathbf{K}), \tag{3}$$

where $\mathbf{S}$ is the entropy flux and $\mathbf{K}$ is the extra entropy flux which actually vanishes for most cases.

The free energy function W together with the first Piola–Kirchhoff stress tensor must be known in order to determine the needed variables $\mathbf{P},\mathbf{b}$, and forces and the source. Although the structure of the momentum equation shows explicitly how the forces are accounted for, the question of how to construct the free energy function remains.

One step forward to answer this question is to separate variables into observable and internal (Maugin, 1990; Maugin and Muschik, 1994). The observable variables are the usual field quantities like elastic strain or displacement, which are observable in the real sense of the word. Internal variables, however, are supposed to describe the internal structure of a solid (or a body, in general) and are observable but not controllable. This means that internal variables should compensate for our lack of a precise description of a microstructure. There are several examples (Maugin and Muschik, 1994) which demonstrate how liquid crystals, damage, or dislocation movements can be described easily using the concept of internal variables. Recently the concept of internal variables has been used for describing the dynamics of microstructured continua (Berezovski et al., 2009).

The main idea is to introduce the internal variables into the free energy function. Then we can easily calculate all the needed forces but we need also governing equations for internal variables. This is obtained by satisfying the dissipation inequality. So we have followed the main idea – one balance law and all what is to be added come from the energy considerations. Let us consider first a single internal variable of state α as a second-order tensor. Then the free energy W per unit volume is specified as a general sufficiently regular function

$$W = \overline{W}(\mathbf{F},\theta,\alpha,\nabla_R\alpha), \tag{4}$$

where $\mathbf{F}$ is the deformation gradient. Following Berezovski et al. (2009), it is possible to show that after calculating all the needed forces, the simplest choice for the governing equation for α is

$$\dot{\alpha} = k\left(\mathbf{A} - \mathrm{Div}_R\mathscr{A}\right), \tag{5}$$

where $k \geq 0$ and

$$\mathbf{A} := -\frac{\partial\overline{W}}{\partial\alpha}, \quad \mathscr{A} := -\frac{\partial\overline{W}}{\partial\nabla_R\alpha}. \tag{6}$$

This is actually a reaction-diffusion equation which can be found in numerous applications. It means that the microstructure is not inertial. If we introduce dual internal variables α and β, then the situation is different (Ván et al., 2008). We now assume

$$W = \overline{W}\left(\mathbf{F},\theta,\alpha,\nabla_R\alpha,\beta,\nabla_R\beta\right). \tag{7}$$

In order to satisfy the dissipation inequality, the simplest forms of evolution equations for α and β are

$$\begin{pmatrix} \dot{\alpha} \\ \dot{\beta} \end{pmatrix} = \mathbf{L}\begin{pmatrix} \widetilde{A} \\ \widetilde{B} \end{pmatrix} = \begin{pmatrix} \mathbf{L}^{11} & \mathbf{L}^{12} \\ \mathbf{L}^{21} & \mathbf{L}^{22} \end{pmatrix}\begin{pmatrix} \widetilde{A} \\ \widetilde{B} \end{pmatrix},$$

$$\widetilde{A} = \mathbf{A} - \mathrm{Div}_R\mathscr{A}, \quad \widetilde{B} = \mathbf{B} - \mathrm{Div}_R\mathscr{B},$$

$$\mathbf{A} := -\frac{\partial\overline{W}}{\partial\alpha}, \qquad \mathbf{B} := -\frac{\partial\overline{W}}{\partial\beta}, \tag{8}$$

$$\mathscr{A} := -\frac{\partial\overline{W}}{\partial\nabla_R\alpha}, \qquad \mathscr{B} := -\frac{\partial\overline{W}}{\partial\nabla_R\beta},$$

where the components of the linear operator $\mathbf{L}$ are dependent on state variables. Let us consider a non-dissipative process and assume a quadratic dependence of the free energy with respect to β. Then from

$$\dot{\alpha} = L^{12}\,\widetilde{B}, \quad \dot{\beta} = -L^{12}\,\widetilde{A} \tag{9}$$

that provides the vanishing dissipation, we obtain

$$\ddot{\alpha} = \left(\mathbf{L}^{12}\cdot\mathbf{L}^{12}\right)\cdot\widetilde{A}, \tag{10}$$

which is a hyperbolic evolution equation for the internal variable α. In physical terms it means that the inertia of the internal variable is taken into account.

2.2. Mathematical models

Based on arguments in Subsection 2.1, we present here the mathematical models for longitudinal waves in the 1D setting. It has been shown by Engelbrecht et al. (2005) that the Mindlin model can also be represented by the approach using the material momentum (cf. Eq. (1)). Recently Berezovski et al. (2009, 2010) have shown that, by using the concept of dual internal variables again, the same result can be obtained. Therefore, here we shall omit the details of derivation and focus on the analysis of models. The governing system is then the following:

$$\rho_0 u_{tt} = a u_{xx} + N u_x u_{xx} + A\psi_x, \tag{11}$$

$$I\psi_{tt} = C\psi_{xx} + M\psi_x\psi_{xx} - Au_x - B\psi. \tag{12}$$

Here u denotes the longitudinal (macro)displacement and ψ – the microdeformation (according to the Mindlin model) or the internal variable (according to the concept of internal variables). Further, ρ_0 is the density and I inertia of the microstructure, while a,A,B,C,N,M are the material parameters specifying the free energy function (see Engelbrecht et al., 2005). We need to introduce a scale parameter $\delta \ll 1$ which characterizes the smallness of the microstructure and another parameter $\varepsilon \ll 1$ which emphasizes that the displacement u is small compared to the reference length. After introducing the dimensionless variables U,X,T and applying the 'slaving principle'

(see for details Engelbrecht et al., 2005), system (11), (12) is reduced to one equation

$$U_{TT} = \left(1 - \frac{c_A^2}{c_0^2}\right) U_{XX} + \frac{1}{2} k_N \left(U_X^2\right)_X + \frac{c_A^2}{c_B^2}\left(U_{TT} - \frac{c_1^2}{c_0^2} U_{XX}\right)_{XX} + \frac{1}{2} k_M \left(U_{XX}^2\right)_{XX}, \tag{13}$$

where c_0, c_1, c_A, c_B are velocities and k_N, k_M are the parameters expressing the strengths of physical nonlinearities on macro- and microscale, respectively. The small parameters are embedded into the coefficients of Eq. (13). The linear approximation

$$U_{TT} = \left(1 - \frac{c_A^2}{c_0^2}\right) U_{XX} + \frac{c_A^2}{c_B^2}\left(U_{TT} - \frac{c_1^2}{c_0^2} U_{XX}\right)_{XX}, \tag{14}$$

demonstrates clearly the hierarchical nature of the process: if c_A^2/c_B^2 is small, then waves are governed by the properties of macrostructure; if, however, c_A^2/c_B is large, then waves 'feel' more microstructure. In the absence of interaction between macro- and microstructure (i.e. when $A = 0$), the wave operator in terms of U is simply $U_{TT} - U_{XX}$. It is possible to develop such a hierarchical modelling further by introducing multiple scales. Following the Mindlin ideas, it means that every deformable cell of the microstructure includes new deformable cells at a smaller scale (Engelbrecht et al., 2007a). The nonlinear effects in the models above include also dispersive effects caused by the microstructure. This means that soliton emergence is possible when there is a balance between nonlinear and dispersive effects. Indeed, it has been shown (Janno and Engelbrecht, 2005a; Engelbrecht et al., 2007b) that the models like Eq. (13) lead to the emergence of solitary waves. As Eq. (13) is a two-wave equation, it is possible to show that left- and right-going soliton trains emerge from a single initial excitation. The influence of nonlinearity on the microlevel affects the emergent waves, making them asymmetric (Janno and Engelbrecht (2005a).

3. MECHANICS TO BIOPHYSICS

Mathematical modelling of biological processes and biomechanics means describing the physiological phenomena and structural behaviour of living tissues, organs, cells, neuronal networks, etc. There are many specific features which must be taken into account (Vendelin et al., 2007):

- biological systems need energy exchange with the surrounding environment and represent the systems far from the thermodynamic equilibrium;
- the processes operate over different time scales, are spatially extended, and include many hierarchies;
- in physical terms, the models should account for nonlinearities, dissipation, activity/excitability, spatiotemporal coupling, etc.

These features are characteristic of complex systems and biophysics, nowadays clearly a part of complexity science under the chapter 'systems biology' (Kitano, 2001). The existence of scales and, consequently, hierarchies must, however, be explained in more detail (Vendelin et al., 2007). Namely, in biological tissues one should distinguish two possible types of hierarchies: (i) a *structural hierarchy* which involves strong dependence on length scales like in mechanics (see Section 2) and (ii) a *functional hierarchy* meaning that at various levels of scale, various dynamical processes are of importance, all of which influence the behaviour on the macroscale. *Structural hierarchies* actually reflect the enormously rich architecture of biological tissues. The fundamental structural hierarchy is *atom* → *molecule* → *cell* → *tissue* → *organ* → *human*. But tissues have themselves a complicated structure which should be taken into account when stresses and strains in tissues are calculated. In this sense living tissues resemble microstructured man-made materials. For example, for heart contraction the structural elements in the hierarchy are: *sarcomeres* → *myofibrils* → *fibres* → *myocardium* → *heart*. *Functional hierarchies* reflect the complexity of functioning biosystems. The same example of heart contraction has the following functional hierarchy: *oxygen consumption* → *energy transfer* → Ca^{2+} *signals* → *cross-bridge motion* → *contraction*. The concept of internal variables, explained briefly above and used for microstructured materials, can effectively be generalized for description of hierarchies in biotissues. A structural hierarchy can be easily described by the theory presented in Section 2; a functional hierarchy needs a generalization (Engelbrecht et al., 2000). The idea is the following (Engelbrecht and Vendelin, 2000; Vendelin et al., 2007). In addition to an observable variable χ, there is a set of internal variables $\alpha, \beta, \gamma, \ldots$. Any dependent variable, say σ, is then calculated by an expression

$$\sigma = \sigma(\chi, \alpha). \tag{15}$$

The internal variable α is governed by an evolution equation

$$\dot{\alpha} = f_1(\chi, \alpha, \beta), \tag{16}$$

the variable β by

$$\dot{\beta} = f_2(\chi, \alpha, \beta, \gamma, \ldots), \tag{17}$$

and γ by

$$\dot{\gamma} = f_3(\chi, \alpha, \beta, \gamma, \ldots). \tag{18}$$

Clearly the internal variables α, β, γ form a hierarchy which corresponds to the physical/chemical processes in the functional hierarchy. Such an approach is used for modelling cardiac contraction (Engelbrecht et al., 2000; Engelbrecht and Vendelin, 2000). Here the *structural hierarchy* starts from myofibrils which are composed of repeating units of myosin and actin filaments,

called sarcomeres. The actin filaments are made of a double helix of actin molecules with troponin molecules localized in certain intervals. The myosin filament consists of myosin proteins with certain spatially localized meromyosin molecules with heads resembling 'golf-clubs'. These heads are called cross-bridges. The excitation of a muscle is triggered by an action potential from the conducting system. This potential in its turn releases Ca^{2+} ions in the sarcotubular system, which then activate the troponin molecules so that they will be able to attach the heads of myosin molecules. This attaching means swivelling of myosin molecules that cause sliding the actin and myosin filaments against each other, and as a result stress is created. An ingenious mechanism, indeed.

The *functional hierarchy* starts from the cross-bridges producing force. Two states produce force and the relative amounts of those cross-bridges, α_1 and α_2, are the internal variables of the first level. The next level is the number of all activated cross-bridges β, which is the second-order internal variable. This internal variable in its turn depends on the Ca^{2+} signal, which is the third-order internal variable. The calculations start from the bottom, i.e. from the third level and work step by step up to dependent variable, which in this case is the active stress.

The calculations for contraction of the left ventricle by such an approach have shown good matching with measured results (Vendelin et al., 2000). Another good example of how the notions of mechanics can put biophysical studies into a wider context is the nerve pulse transmission. A nerve pulse is actually an action potential which is transmitted down the axoplasm core of a nerve fibre. The process is accompanied by ion currents through the membrane between the core and the surroundings. These currents actually 'feed' the process with energy and as a result, a stable asymmetric solitary nerve pulse propagates along the fibre. The celebrated Hodgkin–Huxley model has specified the ion currents by introducing three variables called 'phenomenological' (Hodgkin and Huxley, 1952). These variables govern: n – the potassium conductance (turning on), and m, h – the sodium conductance (turning on and off, respectively). A very useful simplification of the model is called after FitzHugh–Nagumo, which includes only one ion current called 'recovery' variable. These phenomenological and/or recovery variables are actually internal variables in terms of continua. Maugin and Engelbrecht (1994) have shown how to use the formalism of internal variables for the Hodgkin–Huxley and FitzHugh–Nagumo equations.

4. FINAL REMARKS

Nonlinearities in wave motion are important because nonlinear models are able to describe important physical effects like distortion of wave profiles (spectral changes), amplitude-dependent velocities, interaction of waves, etc. going also beyond the elastic limit. However, nonlinear effects are usually combined with other effects – dispersion, dissipation, forcing, and coupling with other fields (Engelbrecht, 1997). These combinations will in many cases bring in even more effects and the signatures of complexity are clearly seen. So, for example, nonlinearities combined with dispersive effects lead to coherent wave structures, scale dependence, hierarchies, etc. Characteristically to complexity science, the different fields are related by phenomena, methods, and language. The concepts elaborated in mechanics can be generalized, as shown above, to biophysics. The waves in solids and fluids are similar in many respects, as explicitly demonstrated by solitonics. Besides general analysis of complexity of waves in solids, the applications are important. For example, the knowledge of the influence of the microstructure on phase velocities or asymmetry of solitary pulses opens new ways for solving the inverse problems (Janno and Engelbrecht, 2005b, 2005c, 2008). Certainly there many challenges for further studies. A great challenge is to build multiscale models which relate mesoscopic physics to continuum mechanics reflecting the existence of nonlinearities over the scales, dispersive/dissipative effects, and thermodynamical consistency.

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Mittelineaarsed lained ja komplekssüsteemid

Jüri Engelbrecht

Komplekssüsteemid koosnevad paljudest seostatud ja üksteisega interakteeruvatest komponentidest ning interaktsiooni tulemusena võib tekkida uus kvaliteet. Taolises protsessis on oluline koht mittelineaarsusel. Käesolevas artiklis on analüüsitud lainelevi mikrostruktuursetes materjalides komplekssüsteemide vaatenurgast. Põhivõrrandid on tuletatud sisemuutujate kontseptsiooni kasutades, mis on otseselt seotud termodünaamika tingimustega. Sisemised mastaabitegurid viivad lainehierarhiate moodustumisele, kus on oluline ka dispersiooni arvestamine. Mittelineaarsuse ja dispersiooni koosmõjul võivad tekkida solitonstruktuurid, mis on selgeks märgiks uue kvaliteedi tekkimisest. Paar probleemi on lisatud biofüüsikast, mis näitavad, et põhimõtteliselt on sisemuutujate kontseptsioon samuti rakendatav ja lainelevi aspektist on mittelineaarsusel tähtis osa.