Rend. Sem. Mat. Univ. Pol. Torino
Vol. 67, 3 (2009), 293 – 325

J. Engelbrecht

COMPLEXITY IN MECHANICS*

Abstract. Contemporary complexity science deals with problems involving many variables which interact with each other (and with the environment) in such a way that new quality appears. Nonlinearity is a cornerstone of complex systems which as a rule are far from equilibrium and exhibit properties of emergence of coherent structures, possibly over many scales. Generalized continuum theories incorporate intrinsic microstructural and nonlinear effects in the mechanical behaviour of solids. The effects like emergence of solitary waves and solitary wave structures, scale-dependence and wave hierarchy clearly demonstrate that contemporary mechanics exhibits many complex effects. In this paper, nonlinear wave propagation in microstructured solids is analysed as a significant example of complexity. The basic models are derived from the canonical (material) momentum equation where the interaction forces are separated. Novel concepts like dual internal variables and wave hierarchy are described. Besides solid mechanics, some insights into fluid dynamics and biophysics are also given and some numerical results presented.

1. Introduction

The long history of mechanics has revealed many brilliant ideas which have shaped the modern understanding of the world. The great scholars like Archimedes, Galilei, Newton and others were later followed by Euler, Lagrange, and Laplace, just to mention a few names among many. One of the characteristic features of scientists in the past was their commitment to many problems of mechanics, mathematics, optics, etc. Solids and fluids were often both treated alike by Newton in his *Principia*. Many problems solved by our predecessors are now classical examples, such as the movement of planets, the three-body system, movement of a pendulum, waves on the free surface of fluid — this list can easily be prolonged. Closer to the present time, specialisation was needed in order to overcome a myriad of specific details and nowadays the communities around one field usually meet at specialised conferences and publish their findings in specialised journals (IUTAM congresses are one exception). Armin Toffler, in his preface to the book by Prigogine and Stengers [42], says: "One of the most highly developed skills in contemporary Western civilization is dissection: the splitting-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". Is this really so? What happens when we put the pieces back together?

The idea of putting things back together is not new. Said Aristotle: "The whole is more than the sum of the parts". And again it is mechanics that has brought this old knowledge to our contemporary understanding. The basic notion that "has changed the world" is nonlinearity. Although the inverse-square law of gravitation was introduced by Newton, it was much later that H. Poincaré understood its importance when he solved the three-body problem. But only in the mid-twentieth century did concepts

*A *Lezione Lagrangiana* given in Turin on 7 May 2009

like solitons, chaotic attractors and other members of the nonlinear "zoo" make clear that new quality is born if 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, not to mention many other physical processes. In this way, the development spiral involves many fields together just like in the past. The reason is simple — the world around us is nonlinear and similar patterns emerge in various processes, similar methods can be used in studies of various fields, and a language uniting different studies is understandable to the general community of scientists. In short, the world is complex and complexity research, as it is now understood, is an intrinsically transdisciplinary enterprise. A complex system is composed of its constituents, small elements that interact with each other resulting in emergent properties of the system as a whole. The citation above by A. Toffler reflected the general understanding, but the monograph by Prigogine and Stengers [42] itself is a proof of the contrary and describes the earlier ideas of complex systems. More recent treatises are, for example, the monographs by Christiansen and Moloney [9], and Nicolis and Nicolis [40].

In what follows, the mechanics of solids is analysed from the viewpoint of complexity. The analysis is mostly based on studies of CENS (Centre for Nonlinear Studies, Institute of Cybernetics at Tallinn University of Technology) during the last decade although the preliminary ideas were already presented earlier [14]. The starting point is a brief overview on general theories of microstructured solids with a special attention to modelling the hidden internal structure. The mathematical models derived according to novel concepts reflect the hierarchical structure of solids at various scales. Nonlinearities are briefly described in order to bring the mathematical models closer to reality. In this presentation, two main questions are actually addressed. The first is: how to model deformation waves in solids with their physical structure, i.e. taking into account constituents. The second refers to the links between the constituents, or closer to mechanics, the forces between the constituents. The result is not surprising — nonlinear mechanics is a typical example of complexity. The last part of this paper is devoted to general problems and/or specific examples drawn from the analysis of waves.

2. Basic theory

2.1. Motivation

The conventional theories of continua describe the behaviour of solids and materials respectively. In reality, however, materials are always characterized by a certain microstructure at various scales (see [23]). The character of a microstructure can be regular (like in laminated composites) or irregular (like in polycrystalline solids or alloys). Furthermore, 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 $L \gg l$ 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 [1, 34, 36]. The crucial point then is to assume the functional dependencies of interactive forces between discrete masses using energetic considerations. The discrete approach is often used for laminated composites and then the effective stiffness theory may usefully occur [45, 50]. As a result, the governing equations describe a certain continuum the properties of which are related to the initial discrete system [36]. From the viewpoint of continua, straightforward modelling leads to the assignment of all the physical properties to every volume element dV in a solid, which means introducing dependence on space coordinates. Thus, the governing equations are so complicated that they can be solved only by numerical methods.

Although the discrete approach seems to be appropriate for modelling the microstructure, the question of how to determine the interactive forces in order to reflect material properties is difficult to answer. That is why the generalized continuum theories seem to be more plausible.

Generalised continuum theories extend conventional continuum mechanics for incorporating intrinsic microstructural effects in the mechanical behaviour of materials [8, 21, 22, 37, 53]. A leading concept is to separate macro- and microstructure in continua and to formulate the conservation laws for both structures separately (see, for example [21, 37]). However, a more sophisticated way is to introduce the microstructural quantities into one set of conservation laws [31, 35]. It seems that such an approach is extremely useful for two reasons: (i) it reflects clearly the mechanical structure of a solid; (ii) it allows further generalisation in order to include internal variables and cast more light on the thermodynamical character of wave motion.

2.2. Balance laws

The local balance laws in the so-called Piola–Kirchhoff formulation are [31] for mass, linear momentum, and energy, respectively:

$$\left.\frac{\partial \rho_0}{\partial t}\right|_{\mathbf{x}} = 0, \tag{1}$$

$$\left.\frac{\partial (\rho_0 \mathbf{v})}{\partial t}\right|_{\mathbf{x}} - \mathrm{Div}_R \mathbf{T} = \mathbf{f_0}, \tag{2}$$

$$\left.\frac{\partial \mathcal{K}}{\partial t}\right|_{\mathbf{x}} - \nabla_R \cdot (\mathbf{T}\cdot\mathbf{v} - \mathbf{Q}) = \mathbf{f_0}\cdot\mathbf{v}, \tag{3}$$

together with the second law of thermodynamics

$$\left.\frac{\partial S}{\partial t}\right|_{\mathbf{x}} + \nabla_R \cdot \mathbf{S} \geq 0, \qquad \mathbf{S} = \frac{\mathbf{Q}}{\theta} + \mathbf{K}. \tag{4}$$

Here ρ_0 is the mass density in the reference configuration, $\mathbf{v}$ is the physical velocity, $\mathbf{x}$ is the position of a material point $\mathbf{X}$ in the reference configuration, $\mathbf{x} = \chi(\mathbf{X}, t)$. $\mathbf{T}$ is the first Piola–Kirchhoff stress tensor, $\mathbf{f_0}$ is the body force per unit reference volume, $\mathcal{K} = K + E$, K is the kinetic energy, E is the internal energy per unit reference volume. $\mathbf{Q}$ is the material heat flux, S is the entropy density per unit reference volume, $\mathbf{S}$ is the extropy flux, θ is the absolute temperature, and $\mathbf{K}$ is the extra entropy flux (which vanishes in most cases). The balance of momentum (2) is the most important governing equation for wave motion. It is possible to reformulate eq. (2) so that the role of material forces exerted on material inhomogeneities is explicity seen. For that the equation of balance must be written on the material manifold $\mathcal{M}^3$ of points X constituting the body. This is done by Maugin [31, 35] and here we follow his ideas (see also [2]). Leaving aside the technical details, the canonical (material) momentum equation reads

$$\left.\frac{\partial \mathbf{P}}{\partial t}\right|_{\mathbf{x}} - \mathrm{Div}_R \mathbf{b} = \mathbf{f}^{int} + \mathbf{f}^{ext} + \mathbf{f}^{inh}, \tag{5}$$

where the material momentum $\mathbf{P}$, the material Eshelby stress $\mathbf{b}$, the material inhomogeneity force $\mathbf{f}^{inh}$, the material external (body) force $\mathbf{f}^{ext}$, and the material internal force $\mathbf{f}^{int}$ are defined by

$$\mathbf{P} := -\rho_0 \mathbf{v} \cdot \mathbf{f}, \tag{6}$$

$$\mathbf{b} = -\left(\mathscr{L}\mathbf{I}_R + \mathbf{T} \cdot \mathbf{f}\right), \tag{7}$$

$$\mathbf{f}^{inh} := \left.\frac{\partial \mathscr{L}}{\partial \mathbf{X}}\right|_{expl} \equiv \left.\frac{\partial \mathscr{L}}{\partial \mathbf{X}}\right|_{fixed\ \ fields} = \left(\frac{1}{2}\mathbf{v}^2\right) \nabla_R \rho_0 - \left.\frac{\partial \overline{W}}{\partial \mathbf{X}}\right|_{expl}, \tag{8}$$

$$\mathbf{f}^{ext} := -\mathbf{f_0} \cdot \mathbf{f}, \tag{9}$$

$$\mathbf{f}^{int} := \mathbf{T} : \left(\nabla_R \mathbf{f}\right)^T - \left.\nabla_R W\right|_{impl}. \tag{10}$$

Here $\mathbf{f} = \left.\partial\chi/\partial\mathbf{X}\right|_t = \nabla_R \chi$, $\mathscr{L} = K - W$, $W = \overline{W}(\mathbf{f}, \ldots, \mathbf{X}, z)$ and the subscripts *expl* and *impl* mean, respectively, the material gradient keeping the fields fixed and taking the material gradient only through the fields present in the function.

The energy conservation is governed by

$$\left.\frac{\partial (S\theta)}{\partial t}\right|_{\mathbf{X}} + \nabla_R \cdot \mathbf{Q} = h^{int}\ ,\ \ h^{int} := \mathbf{T} : \dot{\mathbf{F}} - \left.\frac{\partial W}{\partial t}\right|_{\mathbf{X}}, \tag{11}$$

and the second law by

$$S\dot{\theta} + \mathbf{S} \cdot \nabla_R \theta \le h^{int} + \nabla_R \cdot (\theta \mathbf{K}). \tag{12}$$

2.3. Internal variables

Although the presentation of the balance law in form (5) includes the forces caused by inhomogeneities, i.e. by the constituents, their character needs more explanation. One step forward is to separate variables into observable and internal variables [30, 32]. The observable variables are the usual field quantities like elastic strain or displacement that are observable in the real sense of the word. Internal variables however are supposed to describe the internal structure of the solid (or body, in general) and are not observable. This means that internal variables should compensate for our lack of a precise description of a microstructure. There are several examples [32] 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 also been used for describing the dynamics of microstructured continua [4, 55]. Here we follow these ideas with $\mathbf{K} = 0$.

We consider a *single* internal variables of state $\boldsymbol{\alpha}$ as a second order tensor. Then the free energy per unit volume W is specified as the general sufficiently regular (differentiable) function

$$W = \overline{W}\left(\mathbf{f}, \theta, \boldsymbol{\alpha}, \nabla_R \boldsymbol{\alpha}\right). \tag{13}$$

Then the equations of state are given by

$$\mathbf{T} = \frac{\partial \overline{W}}{\partial \mathbf{f}}, \quad S = -\frac{\partial \overline{W}}{\partial \theta}, \quad \mathbf{A} := -\frac{\partial \overline{W}}{\partial \boldsymbol{\alpha}}, \quad \mathcal{A} := -\frac{\partial \overline{W}}{\partial \nabla_R \boldsymbol{\alpha}}. \tag{14}$$

From (10) and (14) we obtain now

$$\mathbf{f}^{int} = \mathbf{f}^{th} + \mathbf{f}^{intr}, \tag{15}$$

$$\mathbf{f}^{th} = S\nabla_R \theta, \quad \mathbf{f}^{intr} = A : \left(\nabla_R \boldsymbol{\alpha}\right)^T + \mathcal{A} \vdots \nabla_R \left(\nabla_R \boldsymbol{\alpha}\right)^T. \tag{16}$$

From (11) and (14) it follows that

$$h^{int} = h^{th} + h^{intr}, \tag{17}$$

$$h^{th} = S\dot{\theta}, \quad h^{intr} = A : \dot{\alpha} + \mathcal{A} \vdots \left(\nabla_R \dot{\alpha}\right)^T. \tag{18}$$

Now the governing equations (5), (11) read

$$\frac{\partial \mathbf{P}}{\partial t} - \mathrm{Div}_R \widetilde{\mathbf{b}} = \mathbf{f}^{th} + \widetilde{\mathbf{f}}^{intr}, \tag{19}$$

$$\frac{\partial (S\theta)}{\partial t} + \nabla_R \widetilde{\mathbf{Q}} = h^{th} + \widetilde{h}^{intr}. \tag{20}$$

Here we have

$$\widetilde{\mathbf{b}} = -\left(\mathscr{L}\mathbf{I}_R + \mathbf{T}\cdot\mathbf{f} - \mathcal{A} \;:\; \left(\nabla_R\boldsymbol{\alpha}\right)^T\right). \tag{21}$$

$$\widetilde{\mathbf{f}}^{intr} := \widetilde{\mathcal{A}} \;:\; \left(\nabla_R\boldsymbol{\alpha}\right)^T, \quad \widetilde{\mathcal{A}} = \mathbf{A} - \mathrm{Div}_R\mathcal{A}. \tag{22}$$

$$\widetilde{\mathbf{Q}} = \mathbf{Q} - \mathcal{A} : \dot{\boldsymbol{\alpha}}, \tag{23}$$

$$\widetilde{h}^{int} := \widetilde{\mathcal{A}} : \dot{\boldsymbol{\alpha}}. \tag{24}$$

The simplest choice to satisfy the dissipation inequality in an isothermal case is

$$\dot{\boldsymbol{\alpha}} = k\widetilde{\mathcal{A}}, \quad k \geq 0. \tag{25}$$

This is actually a reaction-diffusion type equation

$$\dot{\boldsymbol{\alpha}} = k\left(\mathbf{A} - \mathrm{Div}_R\mathcal{A}\right) \tag{26}$$

which can be found in numerous applications. This straightforward approach can be generalized by introducing the *dual* internal variables $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$, each of which is a second-order tensor [55]. The idea of dual internal variables was originally introduced to explain the links between internal variables and internal degrees of freedom. It is shown later [4] that such a generalization permits one to better interpret the behaviour of microstructured continua.

The free energy should now be taken in the form

$$W = \overline{W}\left(\mathbf{f}, \theta, \boldsymbol{\alpha}, \nabla_R\boldsymbol{\alpha}, \boldsymbol{\beta}, \nabla_R\boldsymbol{\beta}\right). \tag{27}$$

In addition to equations of state (14) we have

$$\mathbf{B} := -\frac{\partial\overline{W}}{\partial\boldsymbol{\beta}}, \quad \mathcal{B} := -\frac{\partial\overline{W}}{\partial\nabla_R\boldsymbol{\beta}}. \tag{28}$$

The canonical equation of momentum keeps its form (19) but now [5]

$$\widetilde{\mathbf{b}} = -\left(\mathscr{L}\mathbf{I}_R + \mathbf{T}\cdot\mathbf{f} - \mathcal{A} \;:\; \left(\nabla_R\boldsymbol{\alpha}\right)^T - \mathcal{B} \;:\; \left(\nabla_R\boldsymbol{\beta}\right)^T\right), \tag{29}$$

$$\widetilde{\mathbf{f}}^{intr} := \widetilde{\mathcal{A}} \;:\; \nabla_R\boldsymbol{\alpha} + \mathcal{B} \;:\; \nabla_R\boldsymbol{\beta}, \tag{30}$$

$$\widetilde{\mathcal{B}} = \mathbf{B} - \mathrm{Div}_R\mathcal{B}. \tag{31}$$

In order to satisfy the dissipation inequality, the simplest form of evolution equations for $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ is

$$\begin{pmatrix} \dot{\boldsymbol{\alpha}} \\ \dot{\boldsymbol{\beta}} \end{pmatrix} = \mathbf{L} \begin{pmatrix} \widetilde{\mathcal{A}} \\ \widetilde{\mathcal{B}} \end{pmatrix} = \begin{pmatrix} \mathbf{L}^{11} & \mathbf{L}^{12} \\ \mathbf{L}^{21} & \mathbf{L}^{22} \end{pmatrix} \begin{pmatrix} \widetilde{\mathcal{A}} \\ \widetilde{\mathcal{B}} \end{pmatrix}, \tag{32}$$

where the components of the linear operator $\mathbf{L}$ are dependent on state variables [24]. It is possible to decompose $\mathbf{L}$ into the sum of symmetric and skew-symmetric components. Based again on dissipation inequality [5], we get

$$\begin{pmatrix} \dot{\boldsymbol{\alpha}} \\ \dot{\boldsymbol{\beta}} \end{pmatrix} = \begin{pmatrix} \mathbf{L}^{11} & 0 \\ 0 & \mathbf{L}^{22} \end{pmatrix} \begin{pmatrix} \widetilde{\mathcal{A}} \\ \widetilde{\mathcal{B}} \end{pmatrix} + \begin{pmatrix} 0 & \mathbf{L}^{12} \\ -\mathbf{L}^{12} & 0 \end{pmatrix} \begin{pmatrix} \widetilde{\mathcal{A}} \\ \widetilde{\mathcal{B}} \end{pmatrix}. \tag{33}$$

In the case of non-dissipative processes the fully coupled evolution equations are simply

$$\dot{\boldsymbol{\alpha}} = \mathbf{L}^{12}\, \widetilde{\mathcal{B}}, \quad \dot{\boldsymbol{\beta}} = -\mathbf{L}^{12}\, \widetilde{\mathcal{A}}. \tag{34}$$

In this case, the evolution of one internal variable is driven by another one that expresses the duality between the internal variables. In the usual context of internal variables the resulting evolution equation is of the reaction-diffusion type (cf. eq. (26)) which demonstrates that the internal variable is not inertial. In case of dual internal variables it is also possible to account for inertial effects. For example, let $\mathcal{B} = 0$. Then the free energy function W (see (27)) is independent of $\nabla_R \boldsymbol{\beta}$ and relations (34) reduce to

$$\dot{\boldsymbol{\alpha}} = \mathbf{L}^{12}\, \mathbf{B}, \quad \dot{\boldsymbol{\beta}} = -\mathbf{L}^{12}\, \widetilde{\mathcal{A}}. \tag{35}$$

Let us assume further a quadratic dependence of the free energy with respect to $\boldsymbol{\beta}$. Then $\mathbf{B} = -\boldsymbol{\beta}$ and instead of (35) we have

$$\dot{\boldsymbol{\alpha}} = -\mathbf{L}^{12}\, \boldsymbol{\beta}, \quad \dot{\boldsymbol{\beta}} = -\mathbf{L}^{12}\, \widetilde{\mathcal{A}}. \tag{36}$$

This system can be written as one equation

$$\ddot{\boldsymbol{\alpha}} = \left(\mathbf{L}^{12} \cdot \mathbf{L}^{12}\right) \cdot\, \widetilde{\mathcal{A}}, \tag{37}$$

which is a hyperbolic evolution equation for the internal variable $\boldsymbol{\alpha}$. In physical terms it means that the inertia of the internal variable is taken into account (cf. eq. (26)).

2.4. Micromorphic elasticity

Mindlin [37] has formulated an elegant theory for describing the microstructured solids. In his presentation the microstructure is "interpreted as a molecule of a polymer, a crystallite of a polycrystal or a grain of a granular material". We know now several modifications of the continuum theory (see for example, [8, 22]) but the Mindlin micromorphic theory is extremely well suited for describing the wave processes in microstructured solids because its clear physical reasoning. Here we follow his presentation [37]

and then show that his model of a microstructure can be easily formulated in terms of internal variables.

The displacement **u** of a material particle in terms of macrostructure is defined by its components $u_i \equiv x_i - X_i$, $i = 1,2,3$, where x_i, X_i are the components of the spatial and material position vectors $\mathbf{x}, \mathbf{X}$, respectively. Within each material volume (particle) there is a microvolume and the microdisplacement $\mathbf{u}'$ is defined by its components $u_i' \equiv x_i' - X_i'$ where the origin of the coordinates x_i' moves with the displacement $\mathbf{u}'$. The basic assumption of Mindlin is that the microdisplacement can be expressed as a sum of products of specified functions of x_i' and arbitrary functions of x_i and t. Then the first approximation of this assumption is $u_i' = x_k' \psi_{kj}(x_i, t)$ and consequently the microdeformation is

$$\frac{\partial u_j'}{\partial x_i'} = \psi_{ij}(x_i, t), \tag{38}$$

and the relative deformation tensor is $\gamma_{ij} \equiv \partial_j u_i - \psi_{ij}$.

A microdeformation gradient is then

$$\kappa_{ijk} \equiv \partial_i \psi_{ik}. \tag{39}$$

From the variational equation of motion, we obtain the following governing equations (no body force):

$$\rho_o \ddot{u}_j = \partial_i(\sigma_{ij} + \tau_{ij}), \tag{40}$$

$$\frac{1}{3}\rho' d_{ji}^2 \ddot{\psi}_{ik} = \partial_i(\mu_{ijk} + \tau_{jk}). \tag{41}$$

Here σ_{ij} is the Cauchy stress, τ_{ij} the relative stress and μ_{ij} the double stress; in addition $\rho' d_{ji}^2$ is a microinertia tensor where ρ' is the density of the microstructure. The balance laws (40) and (41) for macro- and microlevel are introduced independently. The next step will be to introduce the free energy density W and then determine

$$\sigma_{ij} \equiv \frac{\partial W}{\partial \varepsilon_{ij}}, \quad \tau_{ij} = \frac{\partial W}{\partial \gamma_{ij}}, \quad \mu_{ijk} = \frac{\partial W}{\partial \kappa_{ijk}}. \tag{42}$$

Now we apply the internal variable theory described in Section 2.3. We need to represent the constitutive relations in terms of distortion $\partial_j u_i$ and microdeformation tensor ψ_{ji}. Then the stresses are

$$\sigma_{ij}' \equiv \frac{\partial W'}{\partial(\partial_i u_j)} \quad , \quad \tau_{ij}' = \frac{\partial W'}{\partial \psi_{ij}}, \tag{43}$$

where W' is rearranged in terms of $\partial_j u_i$ and ψ_{ij}. The double stress μ_{ijk} remains unchanged. Then eqs. (40), (41) can be rewritten as

$$\rho_o \ddot{u}_j = \partial_i \sigma_{ij}', \tag{44}$$

$$\frac{1}{3}\rho' d_{ij}^2 \ddot{\psi}_{ik} = \partial_i \mu_{ijk} - \tau'_{jk}. \tag{45}$$

We consider now the microdeformations tensor ψ_{ij} as an internal variable α and apply the formalism shown in Section 2.3. Obviously the microdeformation gradient κ_{ijk} plays the role of the gradient of the internal variable $\boldsymbol{\alpha}$ and consequently (this is a non-dissipative case) it must be a dual internal variable $\boldsymbol{\beta}$. Then, following (37) we may write

$$\ddot{\boldsymbol{\alpha}} = \left(\mathbf{L}^{12} \cdot \mathbf{L}^{12}\right) \cdot \tilde{\mathcal{A}} = \left(\mathbf{L}^{12} \cdot \mathbf{L}^{12}\right) \cdot \left(-\frac{\partial \overline{W}}{\partial \boldsymbol{\alpha}} + \mathrm{Div} \frac{\partial \overline{W}}{\partial (\nabla \boldsymbol{\alpha})} \right). \tag{46}$$

In terms of ψ_{ij}, eq. (46) yields

$$\left(L^{12} \cdot L^{12}\right)^{-1}_{ji} \ddot{\psi}_{ik} = \left(-\frac{\partial \overline{W}}{\partial \psi_{jk}} + \mathrm{Div} \frac{\partial \overline{W}}{\partial (\nabla \psi_{jk})} \right) = \partial_i \mu_{ijk} - \tau'_{jk}. \tag{47}$$

This equation coincides with (45) which is derived directly from the Mindlin theory. However, there is an important difference — this equation of motion is not derived from the balance of momentum but it follows from the dissipation inequality (see Section 2.3 and expressions for h^{intr}) for the chosen functional dependence of free energy in the considered nondissipative case.

2.5. One-dimensional case

This is the simplest case but demonstrates clearly the physical effects, especially the scale-dependence. First we follow directly the ideas of the Mindlin theory [17, 19]. In the 1D case we drop the indices i, j, k and deal with u and ψ only, the indices t and x denote here differentiation. The balance laws were derived by Mindlin [37] from the Hamilton (variational) principle, here we use Euler–Lagrange equations in term of the Lagrangian $\mathscr{L} = \mathrm{K} - \mathrm{W}$ and u, ψ. The kinetic energy K and the free potential energy W are now

$$\mathrm{K} = \frac{1}{2}\rho u_t^2 + \frac{1}{2} I \psi_t^2, \quad \mathrm{W} = \mathrm{W}(u_x, \psi, \psi_x), \tag{48}$$

where I is microinertia.

The Euler–Lagrange equations have the general form

$$\left(\frac{\partial \mathscr{L}}{\partial u_t}\right)_t + \left(\frac{\partial \mathscr{L}}{\partial u_x}\right)_x - \frac{\partial \mathscr{L}}{\partial u} = 0, \tag{49}$$

$$\left(\frac{\partial \mathscr{L}}{\partial \psi_t}\right)_t + \left(\frac{\partial \mathscr{L}}{\partial \psi_x}\right)_x - \frac{\partial \mathscr{L}}{\partial \psi} = 0. \tag{50}$$

Note that we neglect here the double stress μ_{ijk} but we have two balance laws. Let now the potential energy W be a quadratic function, i.e. we look for a linear case:

$$\mathrm{W} = \frac{1}{2} a u_x^2 + A \psi u_x + \frac{1}{2} B \psi^2 + \frac{1}{2} C \psi_x^2, \tag{51}$$

where a, A, B, C are coefficients, usually $a = \lambda + 2\mu$ with λ, μ being the Lamé parameters. Leaving aside the technical details (see [17]) we arrive to the system of equations of motion

$$\rho_0 u_{tt} = a u_{xx} + A\psi_x, \tag{52}$$

$$I\psi_{tt} = C\psi_{xx} - Au_x - B\psi. \tag{53}$$

This is actually a system of two balance laws that must be solved with proper initial and boundary conditions.

Now we use the concept of dual internal variables. The potential W depends now on u_x and on the internal variables α, β and their derivatives

$$W = W(u_x, \alpha, \alpha_x, \beta, \beta_x), \tag{54}$$

where α and β are scalar quantities. We set

$$\sigma := \frac{\partial W}{\partial u_x} \ , \ \tau := -\frac{\partial W}{\partial \alpha} \ , \ \eta := -\frac{\partial W}{\partial \alpha_x} \ , \ \xi := -\frac{\partial W}{\partial \beta} \ , \ \zeta := -\frac{\partial W}{\partial \beta_x}. \tag{55}$$

Only one balance equation is needed for the macrostructure which in its simplest form is

$$\rho_0 u_{tt} = \sigma_x. \tag{56}$$

Following eqs. (34) for internal variables and calculating $\widetilde{\mathcal{A}}$ and $\widetilde{\mathcal{B}}$, in terms of (55) we obtain

$$\dot{\alpha} = l_{12}(\xi - \zeta_x), \quad \dot{\beta} = -l_{12}(\tau - \eta_x). \tag{57}$$

Following eq. (51) we assume again that the potential is a quadratic function

$$\mathrm{W} = \frac{1}{2} a u_x^2 + A\alpha u_x + \frac{1}{2} B\alpha^2 + \frac{1}{2} C\alpha_x^2 + \frac{1}{2} D\beta^2, \tag{58}$$

where all the coefficients a, A, B, C, D are constants. After calculating the constitutive quantities (55) from (58), we obtain

$$\sigma = a u_x + A\alpha, \quad \eta = -C\alpha_x \ , \ \zeta = 0, \tag{59}$$

$$\tau = -Au_x - B\alpha \ , \ \xi = D\beta. \tag{60}$$

Then we have $\dot{\alpha} = l_{12} D\beta$ and from the evolution equation for β (57_2) it follows that

$$\ddot{\alpha} = -l_{12}^2 D(\tau - \eta_X). \tag{61}$$

As a result, from (56) and (61) we arrive at the equations of motion

$$\rho_0 u_{tt} = a u_{xx} + A\alpha_x \tag{62}$$

$$I\alpha_{tt} = C\alpha_{xx} - Au_x - B\alpha, \tag{63}$$

where $I = 1/\left(l_{12}^2 D\right)$ is the microinertia. It is easily seen that the systems (52), (53) and (62), (63) are identical provided we take ψ as the internal variable α.

2.6. Hierarchy of waves

Waves in microstructured continuum exhibit the hierarchical behaviour in the sense of Whitham [58]. It means that a scale parameter δ plays an important role. Depending on its limit values, $\delta \to \infty$ or $\delta \to 0$, one or another wave operator governs the process asymptotically. In our case the hierarchical behaviour is governed by a parameter which is the ratio of the characteristic scale of a microstructure and the wavelength of the excitation.

There is no such a scale parameter in the governing equations (52), (53) or (62), (63). First we note that the system of two second-order equations can be represented also in the form of one fourth-order equation. In terms of the macrodisplacement u it reads:

$$u_{tt} = \left(c_0^2 - c_A^2\right)\, u_{xx} - p^2 \left(u_{tt} - c_0^2\, u_{xx}\right)_{tt} + p^2\, c_1^2 \left(u_{tt} - c_0^2\, u_{xx}\right)_{xx}, \tag{64}$$

where $c_0^2 = a/\rho_0 = (\lambda + 2\mu)/\rho_0$, $c_1^2 = C/I$, $c_A^2 = A^2 = A^2/\rho_0 B$, and $p^2 = I/B$ is an inherent time constant. It is obvious that this model involves several wave operators. Let us now introduce dimensionless variables and parameters. First, let the scale of the microstructure be l and the excitation characterised by its amplitude U_0 and wavelength L. Then we can introduce

$$U = u/U_0,\;\; X = x/L,\;\; T = c_0 t/L,\;\; \delta_1 = l_1^2/L^2,\;\; \varepsilon = U_0/L. \tag{65}$$

We also suppose that $I = \rho_0 l^2 I^*, C = l^2 C^*$ where I^* is dimensionless and C^* has the dimension of stress. Note that I is scaled against ρ_0, so that any difference of densities is embedded in I^*. By an asymptotic analysis [19] after introducing (65) into (52), (53) we get finally

$$U_{TT} = \left(1 - \frac{c_A^2}{c_0^2}\right) U_{XX} + \frac{c_A^2}{c_B^2}\left(U_{TT} \;-\; \frac{c_1^2}{c_0^2}\, U_{XX}\right)_{XX}, \tag{66}$$

where $c_B^2 \;= B\, L^2/I$. Note that c_B^2 involves the scales L and l and c_A^2 includes the interaction effects between the macro- and microstructure through the parameter A. It means that

$$\frac{c_A^2}{c_B^2} = \delta I^* \frac{A^2}{B^2}. \tag{67}$$

Equation (66) reflects explicitly the hierarchical nature of wave propagation in microstructured solids: 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^2 is large, then waves "feel" more microstructure. In absence of the interaction between macro- and microstructure (i.e. when $A = 0$), the wave operator in terms of U is simply $U_{TT} - U_{XX}$.

For comparison with (64), the dimensions may be restored in eq. (66). It then reads:

$$u_{tt} = \left(c_0^2 - c_A^2\right)\, u_{xx} - p^2 c_A^2 \left(u_{tt} - c_1^2\, u_{xx}\right)_{xx}. \tag{68}$$

It is obvious that the approximated model (68) neglects u_{tttt} completely while the influence of u_{ttxx} is different in (64) and (68). The dispersion analysis [41] permits to establish the ranges of applicability of the derived asymptotic model (66).

It is possible to develop such a hierarchical modelling further by introducing multiple scales. The need is obvious from the general analysis of physical structures of solids [23]. Following the Mindlin model it means in physical terms that every deformable cell of the microstructure includes new deformable cells at a smaller scale. So material is supposed to be composed by the macrostructure including microstructure at a certain scale that includes microstructure at some smaller scale. Then instead of system (52), (53) we obtain a system of three balance laws [19]

$$\rho_0 u_{tt} = a u_{xx} + A_1 \psi_x, \tag{69}$$

$$I_1\ \psi_{tt} = C_1 \psi_{xx} - A_1 u_x - B_1 \psi + A_2 \varphi_x, \tag{70}$$

$$I_2\ \varphi_{tt} = C_2 \varphi_{xx} - A_2 \psi_x - B_2 \varphi, \tag{71}$$

where $I_i, A_i, B_i, C_i, i = 1,2$ are material parameters like previously denoting the parameters for microstructures 1 and 2, respectively. One needs here two scale parameters l_1 and l_2 against the excitation wavelength L. Using the similar asymptotic analysis like above, the two-scale hierarchical equation takes the form [19]:

$$\begin{aligned} u_{tt} \ &= \ \left(c_0^2 - c_{A1}^2\right)\ u_{xx} + p_1^2 c_{A1}^2\ \left[u_{tt} - \left(c_1^2 - c_{A2}^2\right)\ u_{xx}\right]_{xx} \\ &\quad - p_1^2 c_{A1}^2\, p_2^2 c_{A2}^2 \left(u_{tt} - c_2^2\, u_{xx}\right)_{xxxx}, \end{aligned} \tag{72}$$

where $c_1^2 = C_1/I_1,\ c_{A1}^2 = A_1^2/\rho_0 B_1,\ c_2^2 = C_2^2/I_2,\ c_{A2}^2 = A_2^2/I_1 B_2$, and $p_1^2 = I_1/B_1,\ p_2^2 = I_2/B_2$. Parameters c_i, c_{Ai} are velocities while p_i are time constants. This equation must be compared to eq. (64). It is obvious that the result is a step closer to crystal structures of materials [34] and includes more dispersive effects for smaller wavelengths.

2.7. Nonlinearities

In very general terms nonlinearity means an imprint of nature forbidding additivity in many aspects. In this sense, linear models are just a first approximation where the assumption of proportionality dominates. As said before (see the Introduction), nonlinearity is a cornerstone of complexity. Indeed, if the interaction of constituents or parts of a complex system is nonadditive, then the behaviour of a whole is different from a simple sum. There are many sources of nonlinearities influencing wave motion in continua [14]:

– material (physical) nonlinearities, i.e. constitutive law(s) is/are nonlinear; in terms of stress-strain relations it means that the potential energy W has terms of higher order than quadratic;

– geometrical nonlinearities; i.e. deformation (cf. strain tensor in its full form);

– kinematical nonlinearities, i.e. convectivity, compound motion, etc.;

– structural nonlinearities; for example, due to constraints limiting the motion of structural elements;

– combined nonlinearities; i.e. coupling of fields.

Why are nonlinearities important in modelling the wave motion? Nonlinear models (see [6, 12, 14, 28, 34, 58]) are able to describe distortion of wave profiles (spectral changes), amplitude-dependent velocities, interaction of waves, spatio-temporal chaos, and other important physical effects, going also beyond the elastic limit.

But nonlinearities are not the only sources of complexity, often there are other effects influencing (in this context) wave motion. This is also the case of waves in solids. The other effects could be dispersion, dissipation, forcing, coupling with other fields, etc. Especially interesting are cases in which nonlinearity is balanced by other effects. So solitons and solitonic structures may emerge if nonlinearity/ies and dispersive effects are balanced, shock waves and dissipative structures may emerge if dissipation and nonlinearity are balanced, and forcing in nonlinear systems may lead to chaotic regimes.

This paper is focused on microstructured solids. The models described above have introduced dispersive effects to macromotion due to microstructure. If we introduce now physical nonlinearities into the models then the results are following [17]. First, the potential energy W is assumed in the form (cf. eq. (51)).

$$W = \frac{1}{2}\, a u_x^2 \,+\, A\psi u_x + \frac{1}{2} B\psi^2 + \frac{1}{2} C\psi_x^2 + \frac{1}{6} N u_x^3 + \frac{1}{6} M\psi_x^3, \tag{73}$$

where M and N denote the parameters of nonlinearities for macro- and microstructure, respectively. This is the first step of generalisation while it is possible to assume also more cubic terms. However, this approximation reveals interesting effects into the analysis.

Following the ideas of Section 2.5, we get the governing system of equations

$$\rho_0 u_{tt} = \alpha u_{xx} + N u_x u_{xx} + A\psi_x, \tag{74}$$

$$I\,\psi_{tt} = C\psi_{xx} + M\psi_x\psi_{xx} - A u_x - B\psi. \tag{75}$$

Again we introduce the dimensionless variables (65) and scaling as in Section 2.6, assuming in addition, $M = M^* l^3$. Then we obtain the hierarchical equation (cf. eq. (66)):

$$\begin{aligned} U_{TT} = {} & \left(1 - \frac{c_A^2}{c_0^2}\right) U_{XX} + \frac{1}{2} k_1 \left(U_X^2\right)_X \\ & + \frac{c_A^2}{c_B^2} \left(U_{TT} - \frac{c_1^2}{c_0^2} U_{XX}\right)_{XX} + \frac{1}{2} k_2 \left(U_{XX}^2\right)_{XX}, \end{aligned} \tag{76}$$

where $k_1 = N\varepsilon/a = N\varepsilon/(\lambda+2\mu)$ and $k_2 = \delta^{3/2}\left(A^3M^*\varepsilon\right)/\left(aB^3\right)$ are the parameters expressing the strengths of physical nonlinearities on macro- and microscale, respectively. The leading wave operators in the equations of motion (66) or (76) are of the second order and describe in the 1D setting both left- and right-travelling waves. The higher order terms in this non-dissipative case are responsible for dispersion. In many fields of physics, the notion of evolution equations is introduced which govern just one wave. Physically it means the separation (if possible) of a multi-wave situation into separate waves along properly chosen characteristics. This approach needs stretched coordinates, for example

$$\xi = c_i t - X, \quad \tau = \varepsilon X, \tag{77}$$

where c_i is the velocity from the main operator and ε is a small parameter. For details, see [12], [51], etc. The resulting evolution equation in terms of $\partial U/\partial X \equiv v$ consists usually just the wave operator $\partial v/\partial\tau$.

Historically, however, the celebrated Korteweg–de Vries (KdV) equation derived for describing waves in shallow water must be noted. It reads

$$u_\tau + muu_\xi + du_{\xi\xi\xi} = 0, \tag{78}$$

where m is a nonlinear parameter and d is a dispersion parameter. As shown by Zabusky and Kruskal [59], this nonlinear equation has solutions in a form of a stable solitary wave, called soliton. The KdV equation and solitons have paradigmatic value, such stable solutions have been discovered in many neighbouring fields: in fluid dynamics, in plasma dynamics, and also in dynamics of solids.

From eq. (76) it is possible to derive the following evolution equation [41]:

$$v_\tau + q(v^2)_\xi + dv_{\xi\xi\xi} + r(v_\xi^2)_{\xi\xi} = 0, \tag{79}$$

where

$$q = \frac{N}{4\rho c^2}, \quad d = \frac{c^2 - c_1^2}{2c^2}, \quad r = \varepsilon\frac{c_M^2}{4c^2}, \quad c^2 = \frac{1}{\rho}\left(a - \frac{A^2}{B}\right). \tag{80}$$

If $A = 0$ (no microstructure exists), then eq. (79) yields a KdV equation. In eq. (79), however, the macro- and micro-nonlinearities both are of importance.

A standardized (normalized) KdV equation has an elegant form

$$w_\tau + 6ww_\xi + w_{\xi\xi\xi} = 0, \tag{81}$$

which is obtained from eq. (78) by setting $u = w/m$ and $\xi \to d^{1/3}\xi$, $w \to 6z^{1/3}w$, $\tau \to \tau$. In these terms eq. (79) reads [44]

$$w_\tau + 6ww_\xi + w_{\xi\xi\xi} + 3\frac{r}{qd}(w_\xi^2)_{\xi\xi} = 0. \tag{82}$$

The last coefficient on the left of (82) shows that in a normalized form micro-nonlinearity is weighted in relation to the macro-nonlinearity and dispersion.

3. Complexity

3.1. General ideas

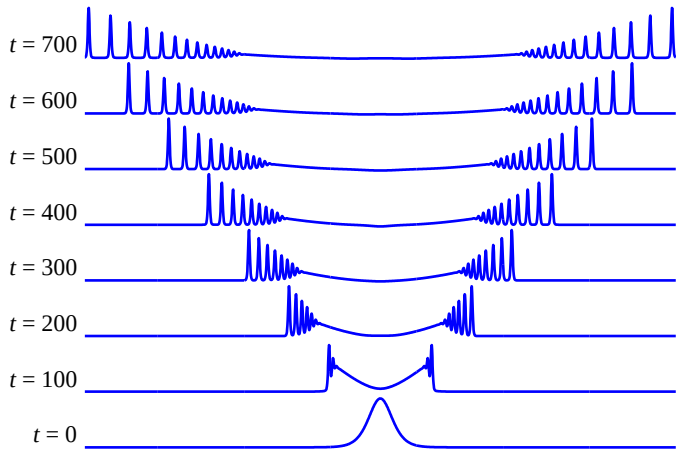
Complexity science was briefly described in the Introduction. Here, after analysing the basic models of microstructured solids with notions of interacting constituents, internal variables, hierarchy of waves and nonlinearity, we return to basic principles of complexity. Taylor [52] has identified the following characteristics of complex systems: complex systems are comprised of many different parts, which are connected in multiple ways; complex systems produce global emergent structures, generated by local interactions; emergence occurs far from equilibrium; complex systems are typically nonlinear. But complexity does not mean chaos in its physical sense, emergence usually occurs at the edge of chaos [26, 52]. If something is at an edge, then certainly both sides must be carefully studied — in context it means that both order and chaos [42] 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 describing convection in the atmosphere [38]. Prigogine [42] said: "One widely-studied example was the three-body system, perhaps the most important problem in the history of dynamics".

Another important issue in complex systems is their multiscale structure. The system behaves differently on a macroscopic level than on the microscopic level. That leads to certain hierarchies which are linked physically and should also be reflected by proper mathematical models. Modern developments in complexity studies are coupled with nonlinearities and scaling. Certain universal arguments help us to make progress within a wide range of problems not only in solids, fluids and soft matter but also in biology, chemistry and social sciences.

In Section 2 a brief description of generalized continua was presented which is extremely important for contemporary advanced technology, including materials science and high intensity or high frequency dynamic processes in solids. Although fluids were not touched, many processes, especially nonlinear waves in fluids are governed by similar models. But turbulence, vortex dynamics, and so forth, form special chapters in fluid dynamics and without any doubt represent excellent examples of complexity.

Let us now collect the essential features from theories presented briefly in Section 2. Hierarchy is clearly evident from the model equations (66), (68), (72). This is the manifestation of multiscale structures of the matter [23]. The internal structure in this context is modelled by internal variables which are connected to thermodynamic conditions. The second law of thermodynamics [42] is therefore one of the governing equations in modelling of waves in microstructured solids. We have also shown that physical nonlinearities can easily be taken into account resulting in a nonlinear hierarchical equation like eq. (76).

The hierarchical models describe dispersive effects dependent on scale factor. The dispersive and nonlinear effects together may lead to the emergence of solitary waves. This demonstrates the universality of main ideas of complexity because solitary waves may emerge in fluids and in solids.



$0 \leq x < 1200\pi$

Figure 1. Soliton trains emerge from pulse-type initial conditions according to (76) [20]

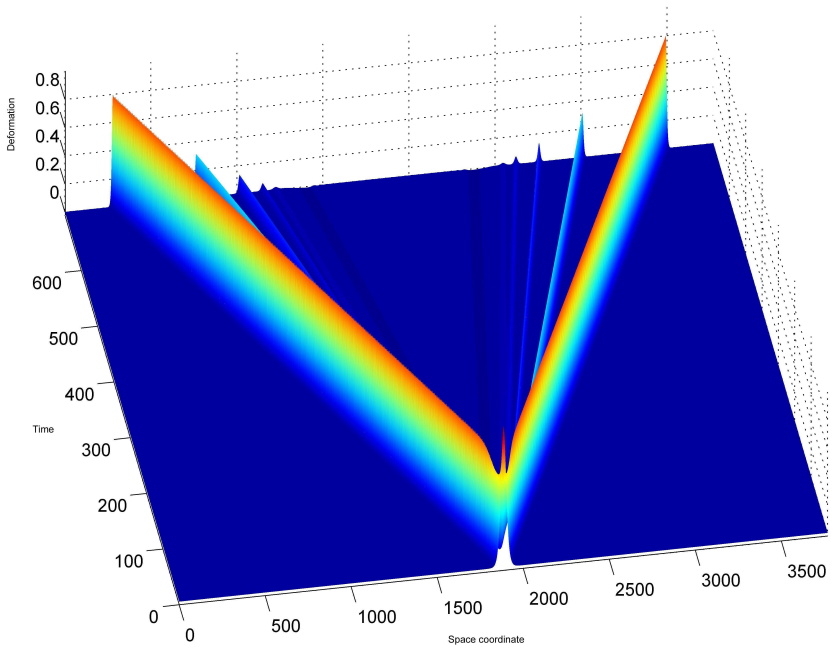


Figure 2. The emergence of solitons shown in the space-time plane, according to (76) [20]

Besides structural hierarchies as described above, functional hierarchies may also be of importance. This is evident, for example, in biophysics where processes at various levels of scale can influence each other (more in Section 3.3).

3.2. Examples from mechanics

One of the celebrated nonlinear phenomena is the emergence of solitons. This is possible when nonlinear effects are balanced by dispersive effects. It all started with the KdV equation [59] but eq. (76), which describes waves in microstructured solids, displays a similar phenomenon. Contrary to the evolution equations, this is a two-wave equation. The emergence of solitons actually means the emergence of strain (a sequence) of solitons which all propagate with different velocities. The process of emergence of two soliton trains from a single pulse-type initial condition is shown in Fig. 1 [20] for discrete time moments. Fig. 2 demonstrates the similar process in the space-time plot. The results are obtained by using the pseudospectral method.

In the classical KdV case (eq. (78)), the emergence follows a similar pattern resulting in one train of solitons. Zabusky and Kruskal [59] studied the emergence of solitons from a harmonic initial conditions. They identified an emerging soliton train with a certain number of solitons and the process of recurrence — after several interactions of emergent solitons, the initial situation is restored. Their calculations were carried out until the first recurrence time τ_R. The calculations up to $100 \ldots 200\,\tau_R$ have revealed a remarkable regular pattern of trajectories of single solitons in the space-time plane [18]. These patterns are shown in Fig. 3 while in time units shown there the recurrence time $\tau_R = \sim 30$. The striking periodicity is easily seen from the rhombus-like patterns (here $m = 1$, $d_l = 2,3209$, $d_l = -\log d$), initial condition $u(\xi,0) = -\sin\xi$, boundary conditions are periodic.

Periodicity is usually related to certain periodic initial conditions or to periodic external forces. In this case some resonance may occur. Here we present results when the process is modelled by a standard KdV equation with a right-hand side term:

$$u_t + muu_x + du_{xxx} = f(u), \tag{83}$$

where we take $f(u) = \alpha_1 \sin\beta_1 u$ with $\alpha_1\beta_1$ being constants [18]. Here x and t are the moving coordinates like (77). The dependence on forcing parameters is observed. For example, the wave profiles in space-time plane for moderate and strong forcing are shown in Fig. 4 and Fig. 5, respectively $(m = 1)$. The amplitudes of emerging solitons are amplified and instead of a train of solitons with different amplitudes, some special soliton groups will emerge. Clear periodicity of pattern of trajectories is seen.

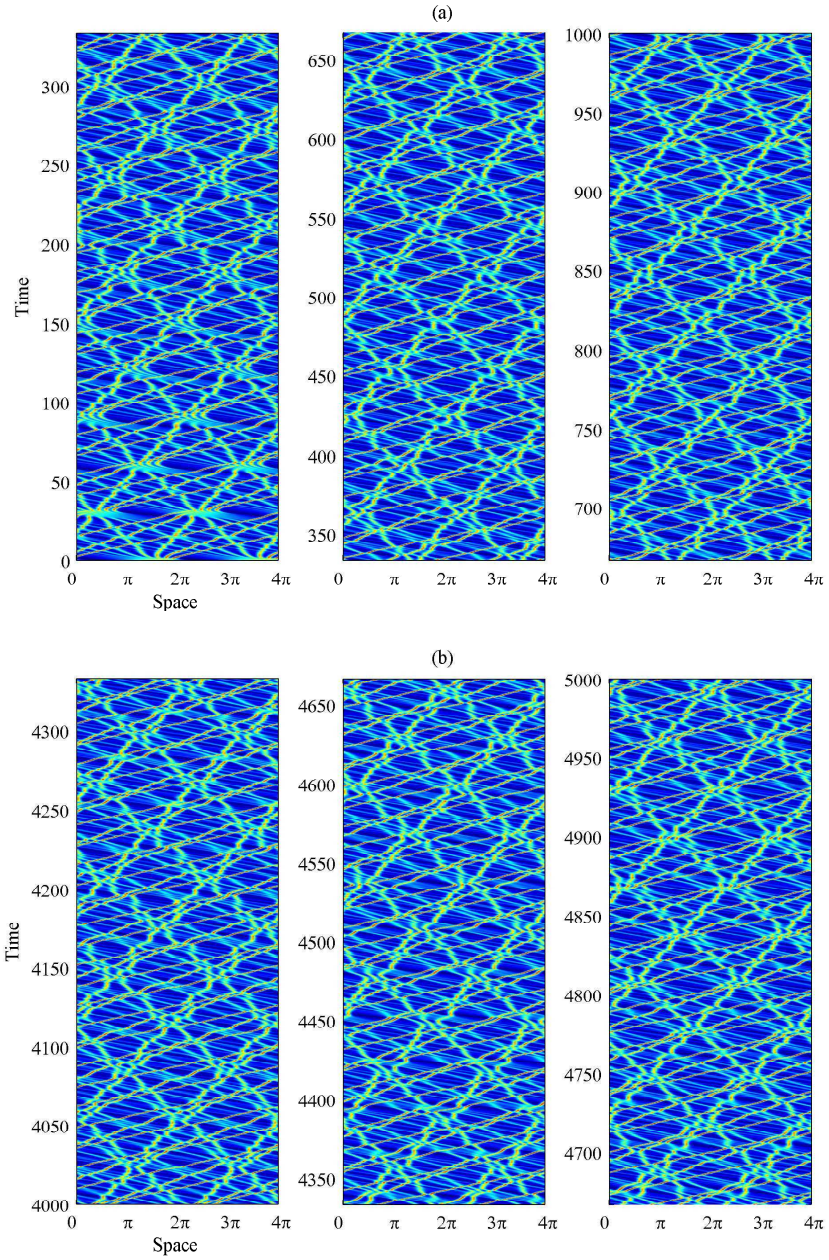


Figure 3. Rhombus-like pattern of trajectories in the space-time plane, model is (78): (a) $\tau = (0 \ldots 1000)$, (b) $\tau = (4000 \ldots 5000)$ [18]

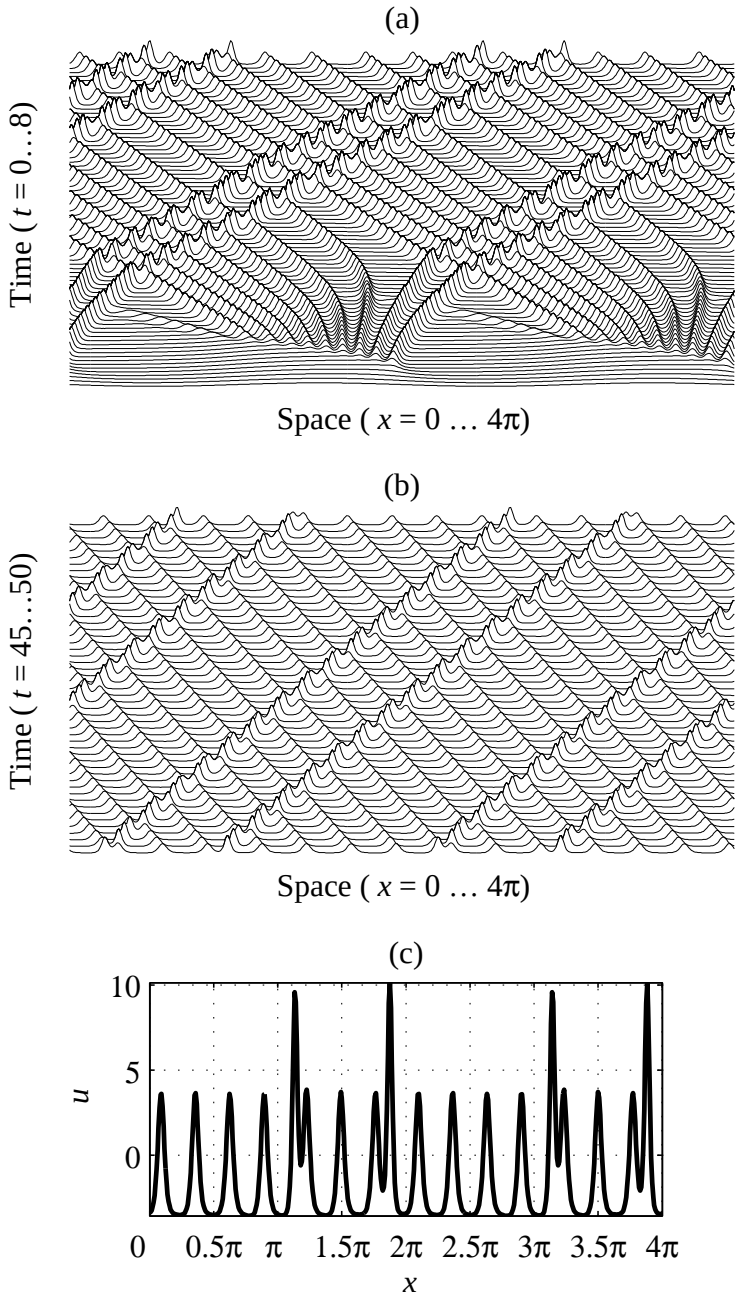


Figure 4. Solitonic structures with forcing, eq. (83). Moderate field $(d_l = 2.2, \alpha = 3, \beta = 1)$; time-slice plots for: (a) $0 \leq t \leq 8$, (b) $45 \leq t \leq 50$, (c) single profile at $t = 46,9$ [18]

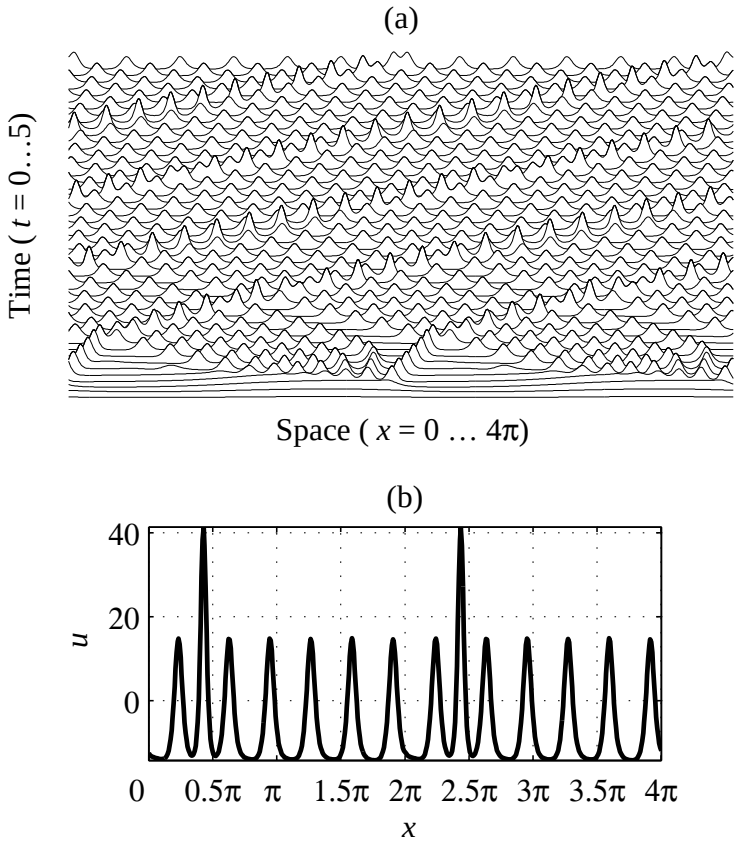


Figure 5. Solitonic structures with forcing, (94). Strong field ($d_l = 1.4, \alpha = 50, \beta = 0.25$): (a) time-slice plots, (b) single profile at $t = 47,0$ [18]

The example above are all governed by quadratic nonlinearity and cubic dispersion which is characteristic to classical KdV equation. For martensitic alloys, for example, the situation can be different [27]. Then the dispersion is quadratic-quartic and dispersion cubic-quintic. The governing evolution equation is then

$$u_t + [P(u)]_x + du_{3x} + bu_{5x} = 0, \tag{84}$$

$$P(u) = -\frac{1}{2}u^2 + \frac{1}{4}u^4, \tag{85}$$

where d and b are constants. This model leads to many types of solitary waves including one interesting case of "plaited " solitons. Such a stable soliton structure is shown in Fig. 6, generated by a single initial pulse.

The waves in hyperelastic rods are governed by even a more complicated evolution equation. For example, in a Mooney–Rivlin rod the evolution equation takes a form [10]

$$u_t + \sigma_1 u u_x + \sigma_2 u_{xxt} + \sigma_3 (2u_x u_{xx} + u u_{xxx}) = 0, \tag{86}$$

where $\sigma_1, \sigma_2, \sigma_3$ are constants. Again, beside other solitonic structures, a special "plaited"-type solitonic structure may emerge, as shown in Fig. 7.

As already stated, the KdV equation was originally derived for waves in shallow water. The KdV soliton is constant in the direction transversal to propagation. A soliton along a channel of finite width is clearly modelled by the KdV equation. On an infinite plane, the solitons may propagate in any direction and the interaction process of solitons propagating in different directions needs more accurate modelling. In this case the influence of transversal direction must be taken into account. In this case instead of a standard KdV equation, the Kadomtsev–Petviashvili (KP) equation is used [46]. The standard KP equation in normalized variables (x, y, t, u) reads [47]

$$(u_t + 6uu_x + u_{xxx})_x + 3u_{yy} = 0, \tag{87}$$

where u has the meaning of elevation of the water surface. The 1D KdV operator is easily recognized between the parentheses of eq. (87). A remarkable nonlinear effect occurs in the interaction process of two solitons modelled by eq. (87) [48, 49]. The interaction process may result in a particularly high and steep wave hump. For example, interactions of equal amplitude solitons may lead to water surface elevations up to four times as high as the amplitude of the counterparts and the slope of the wave front may encounter eightfold increase. This is a very clear manifestation of the character of nonlinear processes — the whole is more than the sum of its parts! This process is illustrated in Fig. 8 [49] for four cases with different angles of propagation. The interaction soliton (hump) is clearly detected, for details see [49]. Fig. 9 shows a photograph from a real situation. Actually it can be said that the soliton interaction may serve as a possible mechanism for freak waves.

3.3. Examples from 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 [56]:

– biological systems need energy exchange with the surrounding environment and represent the systems far from thermodynamic equilibrium;

– the processes operate over different time scales, are spatially extended, and include many hierarchies;

– in physical terms, one should account for nonlinearities, dissipation, activity/excitability, spatiotemporal coupling, etc.

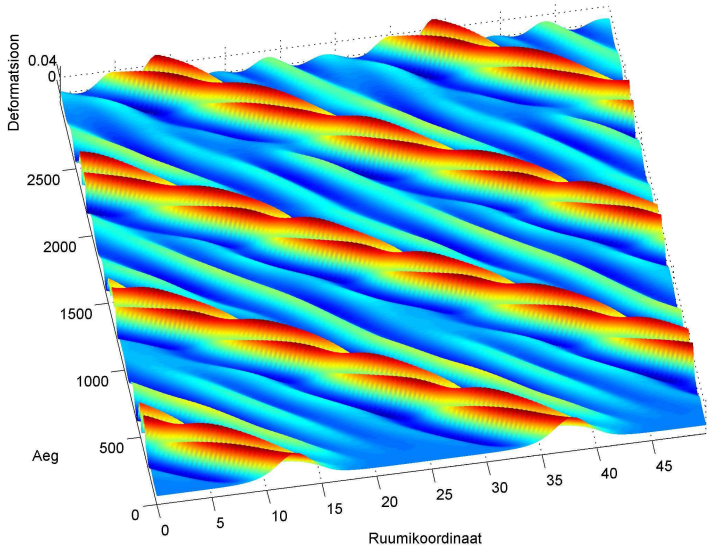


Figure 6. Plaited solitons according to (84) and (85), $d_l = 1.6,\ b_l = 2.0$ [27]

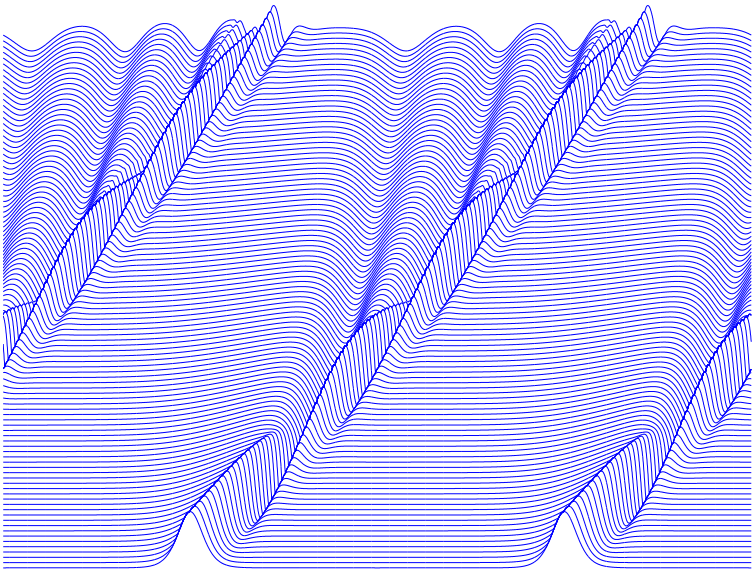


Figure 7. Solitonic structure for (86), time-slice plot [54]

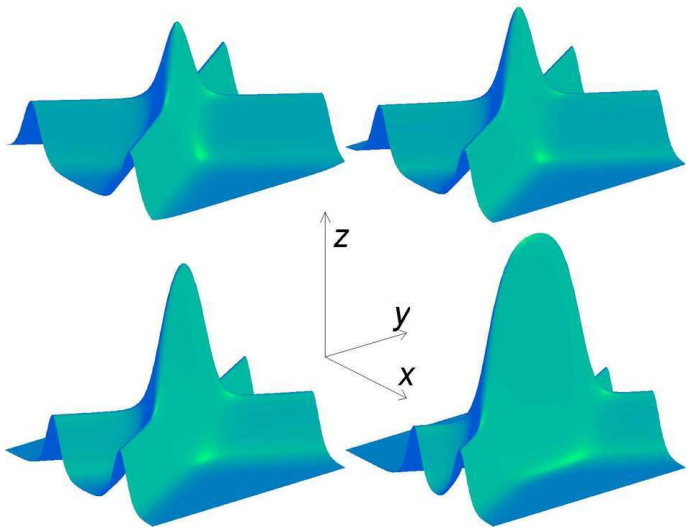


Figure 8. Interaction of two solitons according to (87), panels differ by the interaction angle. The highest interaction soliton is shown in the lower right panel [49]

Figure 9. A real interaction soliton in the Baltic Sea, near Saaremaa island, Estonia (photograph courtesy of T. Soomere)

These features are characteristic of complex systems, and biophysics is nowadays clearly a part of complexity science under the chapter "systems biology" [29]. The existence of scales and, consequently, hierarchies must however be explained in more detail [56]. Namely, in biological tissues one should distinguish two possible types of hierarchies: (i) a structural hierarchy, involving strong dependence on length scales, 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 $\rightarrow$ molecule $\rightarrow$ cell $\rightarrow$ tissue $\rightarrow$ organ $\rightarrow$ human. But tissues have themselves a complicated structure which should be taken into account when the stresses and strains in tissues are calculated. In this sense, living tissues resemble microstructured materials. For example, for the heart contraction the structural elements are: sarcomeres $\rightarrow$ myofibrils $\rightarrow$ fibres $\rightarrow$ myocardium $\rightarrow$ heart. Functional hierarchies reflect the complexity of functioning biosystems. The same example of the heart contraction has the following functional hierarchy: oxygen consumption $\rightarrow$ energy transfer $\rightarrow$ Ca^{2+}signals $\rightarrow$ cross-bridge motion $\rightarrow$ contraction.

The concept of internal variables, explained and used above for microstructured materials, can effectively be generalized for description of hierarchies in living tissues. Structural hierarchy can easily be described by the theory presented in Section 2.3, functional hierarchy needs a generalization [15]. Let the observable variable be denoted by χ and the internal variable by α. The evolution law for α is above given by (26), but here we follow a simplified presentation [16, 56].

We introduce the hierarchy of internal variables $\alpha, \beta, \gamma, \ldots$. The constitutive equation for a dependent variable (stress, for example) σ depends on the observable variable χ and the first-level internal variable α

$$\sigma = \sigma(\chi, \alpha). \tag{88}$$

The evolution law for α is (cf. (26))

$$\dot{\alpha} = f_1(\chi, \alpha, \beta), \tag{89}$$

where β is the next, second-level internal variable influencing σ only through dynamics of α. The evolution law for β is

$$\dot{\beta} = f_2(\chi, \alpha, \beta, \gamma, \ldots), \tag{90}$$

where γ is the third-level internal variable. The evolution law for γ is

$$\dot{\gamma} = f_3(\chi, \alpha, \beta, \gamma, \ldots), \tag{91}$$

etc.

Such an approach is used modelling the cardiac contraction [15, 16]. The stress in myocardium can be split into active $\boldsymbol{\sigma}_a$ and passive $\boldsymbol{\sigma}_p$ stresses. The passive stress is calculated from the elastic deformation of the tissue, i.e. the free energy must be known.

Active stress $\boldsymbol{\sigma}_a$ needs more sophisticated approach. It is generated in myofibrils by activation and is directed parallel to fibres

$$\boldsymbol{\sigma}_a = \sigma_a \boldsymbol{\varepsilon}_1 \boldsymbol{\varepsilon}_1, \tag{92}$$

where $\boldsymbol{\varepsilon}_1$ is the unit vector showing orientation. At the structural level, myofibrils are the starting point. A myofibril is composed of repeating units of myosin and actin filaments, called sarcomeres. The actin filaments is 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 released 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. As a result, active stress is created.

We start from the macrolevel down. The force on actin molecules (along the actin filament) depends on the distance z between an attached cross-bridge and the nearest actin site. There are two states through the cycle, producing force. Denoting them by A and B, we may calculate the corresponding forces by

$$F_A = K_A\, z, \quad F_B = K_B\, z, \tag{93}$$

where K_A, K_B are elastic constants. Further we take $K_A = K_B = K$. The total force over a sarcomere of the length l_s depends on the number of cross-bridges between z and $z - dz$ in both states. We take the uniform distribution of cross-bridges in z over an interval d. The active stress is then found by

$$\sigma_a = \frac{m\, l_s\, K}{2d} \left(\int_{-d/2}^{d/2} n_A(z)\, dz + \int_{-d/2}^{d/2} n_B(z)\, dz \right), \tag{94}$$

where m is the number of cross-bridges per unit volume and $n_A(z), n_B(z)$ are relative amounts of cross-bridges producing force (i.e. being in states A and B). These variables, n_A and n_B are nothing else than the *first-level* internal variables. They (cf. Section 2.3) are governed by the following evolution equations

$$\frac{\partial\, n_A}{\partial\, t} + w\, \frac{\partial\, n_A}{\partial\, z} = f_1\, n_C + g_2\, n_B - (g_1 + f_2)\, n_A, \tag{95}$$

$$\frac{\partial\, n_B}{\partial\, t} + w\, \frac{\partial\, n_B}{\partial\, z} = f_1\, n_A - (g_2 + f_3)\, n_B, \tag{96}$$

where w is the velocity of lengthening, f_1, f_2, f_3, g_1, g_2 are kinetic constants between the states and n_C is the amount of cross-bridges that does not produce force. Clearly the summation of all activated cross-bridges gives

$$A = n_A + n_B + n_C. \tag{97}$$

Now, A is the next, i.e. the *second-level* internal variable, the changes of which affects the variable σ_a only over n_A, n_B. The internal variable A (the activation parameter) has its own evolution equation

$$\frac{d\,A}{d\,t} = c_1\,(l_s)\,[Ca^{2+}]\,(1-A) - c_2\,(l_s)\,A, \tag{98}$$

with $c_1(l_s), c_2(l_s)$ as certain parameters. Equation (98) involves the *third-level* internal variable $[Ca^{2+}]$ which must be governed by its own evolution equation

$$\frac{d\,[Ca^{2+}]}{d\,t} = f\,\left([Ca^{2+}]\right). \tag{99}$$

In practice, the last equation is usually replaced by the approximation of experimental curves.

So, in this case the variable σ_a is influenced by three levels of internal variables that form a hierarchy.

The calculations of contraction are performed by using this model and FEM for the idealized spheroidal left ventricle [15, 56].

Another important problem in biophysics is the pulse transmission in nerve fibres. A nerve pulse is actually an action potential which is transmitted down the axoplasm core of a nerve fibre. The process is accompanied by the ion currents through the membrane. 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 phenomenological variables *n, m, h* [25]. Variable *n* governs the potassium conductance (turning on), and m, h govern the sodium conductance (turning on and off, respectively). Together with parabolic (inductance neglected) telegraph equations and expressions for ion currents, this Hodgkin–Huxley model is carved on a stone tablet. A very useful simplification of the model is called after FitzHugh–Nagumo [39] which includes only one ion current called recovery variable. Engelbrecht [11] has derived an evolution equation for a nerve pulse based on full, i.e. hyperbolic telegraph equations and FitzHugh–Nagumo type ion current (see also [13]).

The evolution equation is certainly an one-wave equation. In suitably chosen variables it reads for the action potential z

$$z_{\xi x} + f(z) z_\xi + g(z) = 0, \tag{100}$$

with $f(z) = k_0 + k_1 z + k_2 z^2$ and $g(z) = g_0 z$. Here k_0, k_1, k_2, g_0 are constants and the roots of $f(z) = 0$ are $z_1 > 0, z_1 > 0, z_1 \neq z_2$. The independent variable $\xi = c_0 t - x$ where c_0 is the velocity of pulse. This equation must be solved under initial excitation $z(0, \xi)$ and the proper boundary conditions. Equation (100) is able to describe (i) the asymptotic solitary with an overshoot; (ii) the all-or-none phenomenon, i.e. the existence of a threshold; (iii) refractoriness, i.e. a second action potential cannot be generated if the second stimulus is applied too soon after the first one. As an one-wave equation, if cannot be used for the description of the head-on collision of pulses. A stationary wave

in terms of $\eta = x + \lambda\xi, \lambda = const$ is described by a Liénard type equation

$$z'' + f(z)z' + \lambda^{-1}g(z) = 0, \tag{101}$$

where $' = \partial/\partial\eta$. In contrast to the celebrated van der Pol equations, the roots of $f(z)$ are both positive. For a more detailed analysis of (100) and (101) see [13]. The phenomenological (recovery) variables related to ion current are actually internal variables in terms of continua [32]; Maugin and Engelbrecht [33] have shown how to use the formalism of internal variables for the FitzHugh–Nagumo and Hodgkin–Huxley models.

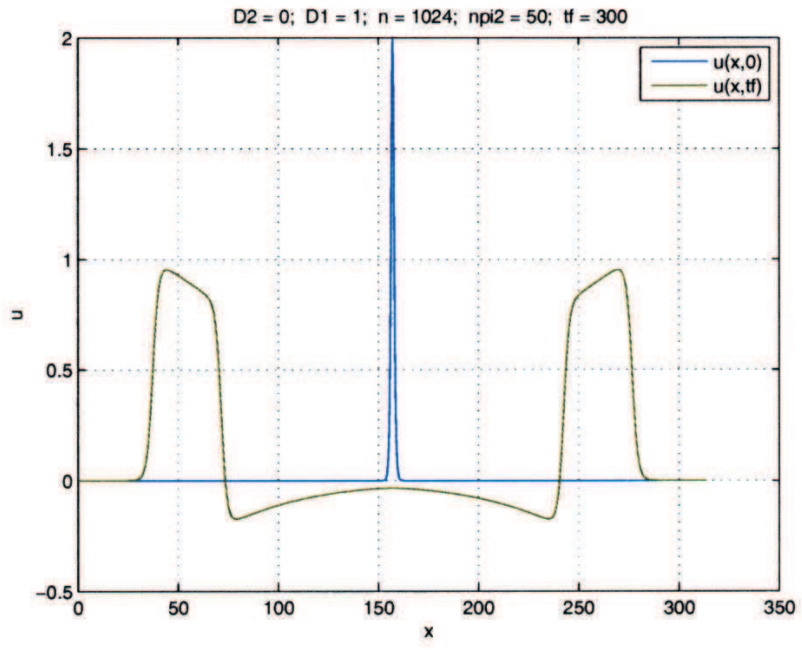


Figure 10. Emergence of single nerve pulses from a single excitation according to (102) and (103) [57]

Compared to solitons in conservative media, nerve pulses also propagate without changing their profile but have more interesting features. The nerve pulses are separated by a refraction length, and at head-on collision process pulses annihilate each other. Here we demonstrate some solutions to the FitzHugh–Nagumo type model [7]

$$u_t = u(1-u)(u-a) - v + D_1 u_{xx} \tag{102}$$

$$v_t = \varepsilon(-v + bu) + D_2 v_{xx}, \tag{103}$$

where u is the action potential and v is the recovery variable — comparable to the potassium ion current in the Hodgkin–Huxley model and to the internal variable in continuum theory. In addition ε is the difference of time scales of u and v, a is related to velocity and D_1, D_2 are the diffusion coefficients. Here $D_1 \gg D_2$ and in calculations we may take $D_1 \neq 0, D_2 = 0$.

The profiles were calculated by the pseudospectral method [57]. Fig. 10 shows the generation of typical pulses propagating to right and left from the initial excitation.

Fig. 11 shows the generation of periodic pulses from repeated excitations that should be separated in time more than the refraction time. At the head-on collision, the pulses annihilate each other as shown in Fig. 12.

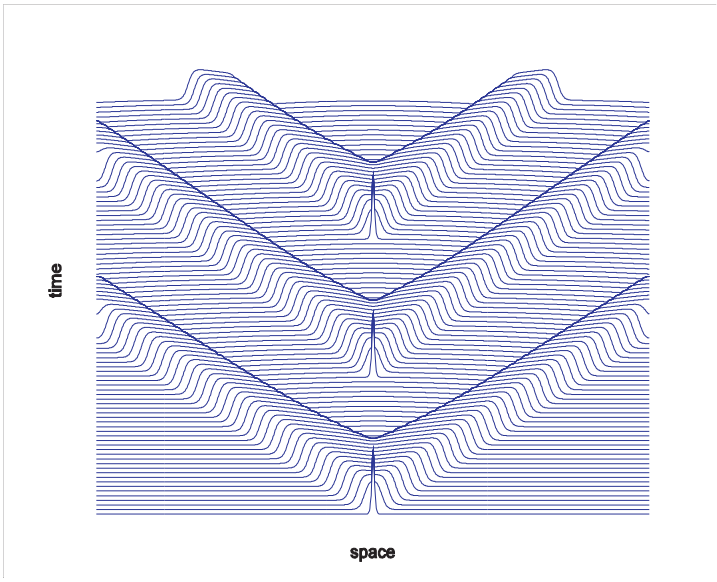
The examples above on cardiac contraction and nerve pulse transmission demonstrate clearly that the concept of internal variables is applicable also in biophysics.

4. Final remarks

Nonlinear wave motion in solids and fluids accompanied by dispersive effects exhibits many characteristics of complexity: coherent structures, scale-dependence, hierarchies, etc. The concepts elaborated in mechanics can easily be generalized to other fields, for example, biophysics. The examples given above demonstrate the rich world of complexity in physical and biological systems. More could be found in longer treatises on that topic [3, 43]. There are many challenges for further studies. A great challenge, for example, is to build multiscale models relating mesoscopic physics to continuum mechanics reflecting the existence of nonlinearities over the scales, dispersive/dissipative effects and thermodynamical consistency. In studies on surface waves, a breakthrough is feasible through systematic investigation of nonlinear interactions of directionally spread or crossing highly nonlinear shallow water waves, combined with studies of the run up of various incident waves. Clearly of importance are the problems of turbulent mixing where several methods can be used for establishing anomalous scaling exponents. But nonlinearities also have an essential influence on neighbouring fields of mechanics. Due to the nonlinearity of optical phenomena in anisotropic and inhomogeneous media, the inverse problem of photoelastic tomography used for determining the stress fields is nonlinear and needs special methods to be developed in order to get solutions with required accuracy. The studies on diffusion restrictions in the cardiac muscle cells and the regulative processes of oxidative phosphorylation permit one to estimate intracellular energy fluxes. These studies, together with proper hierarchical modelling of myocardium fibres, pave the road to a better understanding of the complex mechanisms of cardiac contraction.

It is a fascinating era in mechanics for which classical knowledge is enriched with new concepts — for better understanding nature and the man-made world.

(a)



(b)

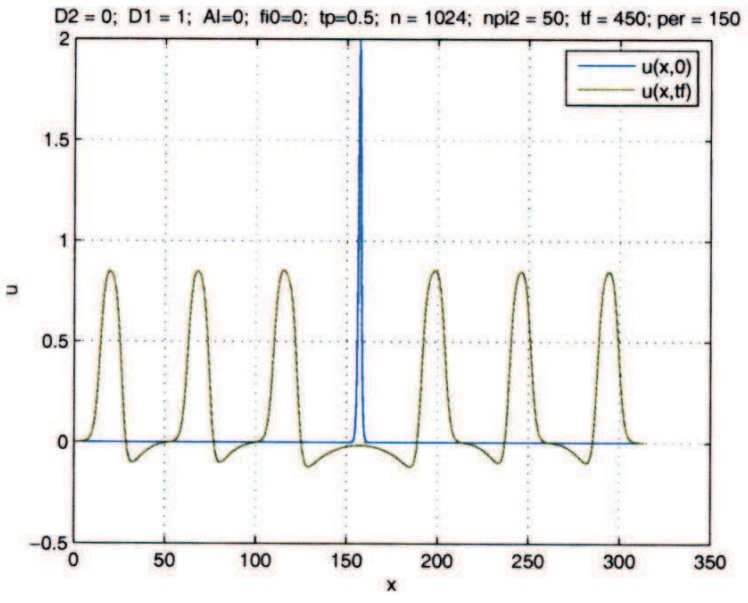
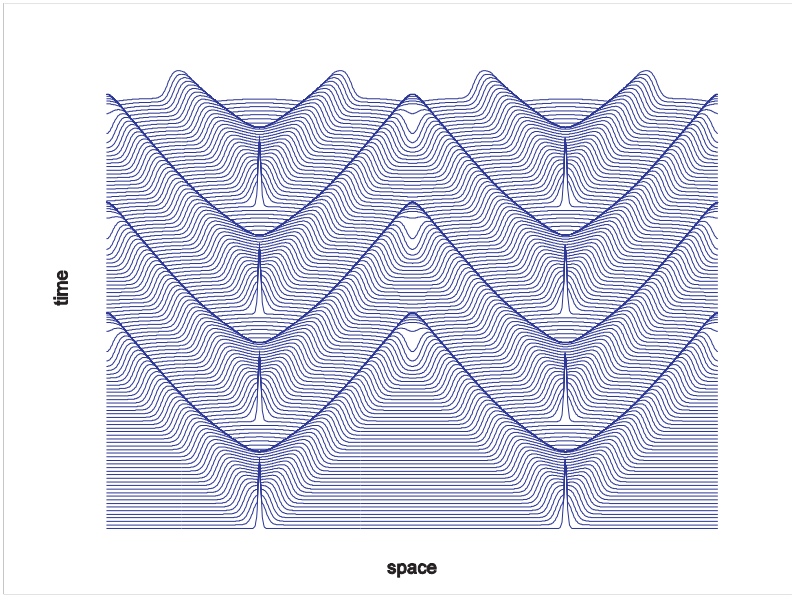


Figure 11. Emergence of periodic trains of nerve pulses according to (102), (103): (a) space-time plot, (b) profiles [57]

(a)



(b)

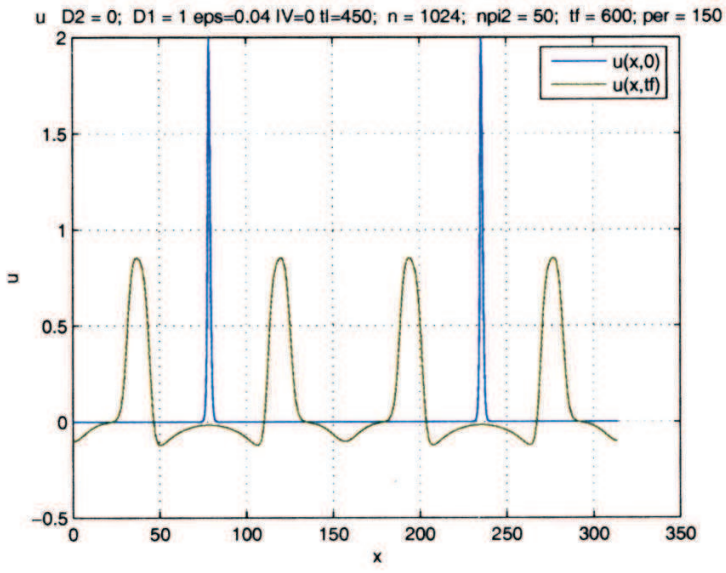


Figure 12. Annihilation process of pulses at head-on collision according to (102), (103): (a) space-time plot, (b) profiles [57]

Acknowledgments

The author is grateful to all his co-authors with whom many ideas presented above were developed over the course of years of fruitful collaboration.

References

[1] ASKAR A., *Lattice Dynamical Foundations of Continuum*, World Scientific, Singapore 1985.

[2] BEREZOVSKI A., ENGELBRECHT J. AND MAUGIN G.A., *Internal variables and microstructured materials*, ICTAM 2008, CD-ROM Proc., Adelaide (2008), 11079.

[3] BEREZOVSKI A., ENGELBRECHT J. AND MAUGIN G.A., *Numerical Simulation of Waves and Fronts in Inhomogeneous Solids*, World Scientific, New Jersey 2008.

[4] BEREZOVSKI A., ENGELBRECHT J. AND MAUGIN G.A., *Internal variables and generalized continuum theories*, In: Borodich F.M. (ed.) IUTAM Symp. on Scaling in Solid Mechanics. Springer. Heidelberg, 2009, 69–80.

[5] BEREZOVSKI A. AND ENGELBRECHT J., *Generalized thermomechanics with internal variables*, In: Maugin G.A. and Metrikine A.V. (eds.) Mechanics of Generalized Continua (submitted).

[6] BLAND D.R., *Nonlinear Dynamics Elasticity*, Blaisdell, Waltham (Mass) 1969.

[7] BOUNTIS T., STARMER C.F. AND BEZERIANOS A., *Stationary pulses and wave front formation in an excitable medium*, Progr. Theor. Phys. Suppl. **139** (2000), 12–33.

[8] CAPRIZ G., *Continua with Microstructure*, Springer, Heidelberg 1989.

[9] CHRISTIANSEN K. AND MOLONEY N.R., *Complexity and Criticality*, Imperial College Press, London 2005.

[10] DAI H.-H., *Model equations for nonlinear dispersive waves in a compressible Mooney–Rivlin rod*, Acta Mechanica **127** (1998), 193–2072.

[11] ENGELBRECHT J., *On theory of pulse transmission in a nerve fibre*, Proc. R. Soc. London **A375** (1981), 195–209.

[12] ENGELBRECHT J., *Nonlinear Wave Processes of Deformation in Solids*, Pitman, London 1983.

[13] ENGELBRECHT J., *An Introduction to Asymmetric Solitary Waves*, Longman, Harlow 1991.

[14] ENGELBRECHT J., *Nonlinear Wave Dynamics: Complexity and Simplicity*, Kluwer, Dordrecht 1997.

[15] ENGELBRECHT J., VENDELIN M. AND MAUGIN M., *Hierarchical internal variables reflecting microstructural properties: application to cardiac muscle contraction*, Rend. Sem. Mat. Univ. Pol. Torino **58** (2000), 83–90.

[16] ENGELBRECHT J. AND VENDELIN M., *Microstructure described by hierarchical internal variables*, J. Non-Equilib. Thermodyn. **25** (2000), 119–130.

[17] ENGELBRECHT J., BEREZOVSKI A., PASTRONE F. AND BRAUN M., *Waves in microstructured materials and dispersion*, Phil. Mag. **85** (2005), 4127–4141.

[18] ENGELBRECHT J. AND SALUPERE A., *On the problem of periodicity and hidden solitons for the KdV model*, Chaos **15** (2005), 015114.

[19] ENGELBRECHT J., PASTRONE F, BRAUN M. AND BEREZOVSKI A., *Hierarchies of waves in nonclassical materials*, In: Delsanto P.P. (ed.), Universality in Nonclassical Nonlinearity: Applications to nondestructive evaluations and ultrasonics, Springer, New York, 2007, 29–47.

[20] ENGELBRECHT J., BEREZOVSKI A. AND SALUPERE A., *Nonlinear deformation waves in solids and dispersion*, Wave Motion **44** (2007), 493–500.

[21] ERINGEN A.C. AND SUHUBI E.S., *Nonlinear theory of simple microelastic solids I & II*, Int. J. Eng. Sci. **2** (1964), 189–203, 389–404.

[22] ERINGEN A.C., *Microcontinuum Field Theories*, Springer, New York, 1999.

[23] GATES T.S. ODEGARD G.M., FRANKLAND S.J.V. AND CLANCY T.C., *Computational materials: multiscale modeling and simulation of nanostructured materials*, Composites Science and Technology **65** (2005), 2416–2434.

[24] GURTIN M.E., *Generalized Ginsburg–Landau and Cahn–Hilliard equations based on a microforce balance*, Physica D **92** (1996), 178–192.

[25] HODGKIN A.L. AND HUXLEY A.F., *Quantitative description of membrane current and its application to conduction and excitation in nerve*, J. Physiol. **117** (1952), 500–544.

[26] HOLLAND J.H., *Emergence. From Chaos to Order*, Oxford University Press, Oxford 1998.

[27] ILISON O. AND SALUPERE A., *On the propagation of solitary pulses in microstructured materials*, Chaos, Solitons & Fractals **29** (2006), 202–214.

[28] JEFFREY A. AND ENGELBRECHT J. (EDS.), *Nonlinear Wave in Solids*, Springer, Vienna 1994.

[29] KITANO H., *Foundation of Systems Biology*, MIT Press, Boston 2001.

[30] MAUGIN G.A., *Internal variables and dissipative structures*, J. Non-Equilib. Thermodyn. **15** (1990), 173–192.

[31] MAUGIN G.A., *Material Inhomogeneities in Elasticity*, Chapman and Hall, London 1993.

[32] MAUGIN G.A. AND MUSCHIK W., *Thermodynamics with internal variables I & II*, J. Non-Equilib. Thermodyn. **19** (1994), 217–249, 250–289.

[33] MAUGIN G.A. AND ENGELBRECHT J., *A thermodynamical viewpoint on nerve pulse dynamics*, J. Non-Equilib. Thermodyn. **19** (1994), 9–23.

[34] MAUGIN G.A., *Nonlinear Waves in Elastic Crystals*, Oxford University Press, Oxford 1999.

[35] MAUGIN G.A., *On canonical equations of continuum thermomechanics*, Mech. Res. Comm. **33** (2006), 705–710.

[36] METRIKINE A.V. AND ASKES H., *One-dimensional dynamically consistent gradient elasticity models derived from a discrete microstructure. Part I: Genetic formulation*, Eur. J. Mech. A/Solids **21** (2002), 555–572.

[37] MINDLIN R.D., *Micro-structure in linear elasticity*, Arch, Rat. Mech. Anal. **16** (1964), 51–78.

[38] MOON F.C., *Chaotic Vibrations*, J. Wiley, New York 1987.

[39] NAGUMO J., ARIMOTO S. AND YOSHIZAWA S., *On active pulse transmission line simulating nerve axon*, Proc. IRE **50** (1962), 2061–2070.

[40] NICOLIS C. AND NICOLIS G., *Foundations of Complex Systems*, World Scientific, New Jersey 2007.

[41] PEETS T., RANDRÜÜT M. AND ENGELBRECHT J., *On modelling dispersion in microstructured solids*, Wave Motion **45** (2008), 471–480.

[42] PRIGOGINE I. AND STENGERS I., *Order out of Chaos*, Heinemann, London 1984.

[43] QUAK E. AND SOOMERE T. (EDS.), *Applied Wave Mathematics*, Springer, Heidelberg 2009.

[44] RANDRÜÜT M. AND BRAUN M., *On one-dimensional solitary waves in microstructured solids* (submitted, 2009).

[45] SANTOSA F. AND SYMES W.W., *A dispersive effective medium for wave propagation in periodic composites*, SIAM J. Appl. Math. **51** (1991), 984–1005.

[46] SATSUMA J., *N-soliton solution of the two-dimensional Korteweg-de Vries equation*, J. Phys. Soc. Japan **40** (1976), 286–290.

[47] SEGUR H. AND FINKELS A., *An analytical model of periodic waves in shallow water*, Stud. Appl. Math. **73** (1985), 183–220.

[48] SOOMERE T. AND ENGELBRECHT J., *Extreme elevations and slopes of interacting solitons in shallow water*, Wave Motion **41** 2 (2005), 179–192.

[49] SOOMERE T. AND ENGELBRECHT J., *Weakly two-dimensional interaction of solitons in shallow water*, European J. Mech. B/Fluids, **25** 5 (2006), 636–648.

[50] SUN C.T., ACHENBACH J.D. AND HERRMANN G., *Continuum theory for a laminated medium*, J. Appl. Mech. **35** (1968), 467–475.

[51] TANIUTI T. AND NISHIHARA K., *Nonlinear Waves*, World Scientific, Singapore 1983 (in Japanese 1977).

[52] TAYLOR M.C., *The Moment of Complexity*, Chicago University Press, Chicago 2003.

[53] TOUPIN R.A., *Elastic materials with couple stresses*, Arch. Rat. Mech. Anal. **11** (1962), 385–414.

[54] VALLIKIVI M., SALUPERE A. AND DAI. H.-H., *Numerical simulation of solitary deformation waves in a compressible hyperelastic rod*, CENS Report Mech., 2008.

[55] VÁN P., BEREZOVSKI A. AND ENGELBRECHT J., *Internal variables and dynamic degrees of freedom*, J. Non-Equilib. Thermodynamics, **33** (2008), 235–254.

[56] VENDELIN M., SAKS V. AND ENGELBRECHT J., *Principles of mathematical modeling and in silico studies of integrated cellular energetics*, In: V.Saks (ed.), Molecular System Bioenergetics: Energy for Life, Wiley VCH, Weinheim 2007, 407–433.

[57] VESKI K., *Influence of parameters in forming the action potential*, MSc Thesis, Tallinn Univ. of Techn., 2007.

[58] WHITHAM G.B., *Linear and Nonlinear Waves*, J. Wiley, New York 1974.

[59] ZABUSKY N.J. AND KRUSKAL M.D., *Interaction of "solitons" in a collisionless plasma and the recurrence of initial states*, Phys. Rev. Lett. **15** (1965), 240–243.

AMS Subject Classification: 35Q51, 74A60, 74J05, 74J30, 92C05

Jüri ENGELBRECHT,
Centre for Nonlinear Studies (CENS), Institute of Cybernetics at Tallinn University of Technology,
Akadeemia tee 21 Tallinn, 12618, EESTI
e-mail: je@ioc.ee

Lavoro pervenuto in redazione il 07.05.2009 e, in forma definitiva, il 25.09.2009