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NONLINEAR WAVES

Complexity in engineering and natural sciences

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Abstract. An overview is presented on interdisciplinary studies into complexity of wave processes with the main attention to wave–wave, field–field, wave–internal structure a.o. interactions. The nonlinearity of these processes creates specific physical phenomena as a result of interactions. The basic assumptions of modelling, main hypotheses adopted and resulting governing equations are presented. Due to complexity of processes, numerical methods are mainly used for the analysis. However, in many cases the methods (the finite volume method, the pseudospectral method) must be modified in order to guarantee the accuracy and stability of solutions. The spectrum of problems modelled and analysed is wide including dynamical processes in solids, fluids and tissues.

Key words: wave motion, interactions, complexity.

1. INTRODUCTION

Classical research aims to split up general problems into their simpler components and then to study them as deep as possible. Contemporary understanding, however, takes problems or systems to be composed by simpler components or constituents but pays special attention to the interaction between them which results in emerging properties of the system as a whole. Such systems are called complex and as a rule they are nonlinear. This is the reason why the interactions may lead to new coherent states of systems which display new global properties not predictable from the properties of the constituents. And that is why complex systems are studied not only in physics and chemistry but also in biology, econophysics, social studies etc. Similar patterns may emerge in different processes, similar methods can be used in studies of different fields and language of different studies is more understandable to the general community of scientists. The keywords like hierarchies, emergence, power laws, networks, unpredictability, self-organized criticality, and many others are widely used in many fields of studies [44].

In short, the main issues of complex systems are: (i) complex systems comprise many different constituents which are connected in multiple ways; (ii) complex systems produce global effects including emergent structures generated by local interactions; (iii) complex systems are typically nonlinear; (iv) emergent structures occur far from equilibrium.

There are many excellent overviews on complexity studies. Limiting ourselves to physical systems, the basic understanding is described in [23,45,49]. For wave motion the earlier results, focusing on nonlinearity and accompanying effects, can be found in [14,40,61]. Our interest is on time-dependent processes in continua where different physical fields act and continua themselves may have inner structure which is called microstructure. A field is a physical quantity that has value for each point of a medium at a certain time. A typical moving dynamical entity is a wave – a disturbance which propagates from one point in the medium to another without giving the medium as a whole any permanent displacement. Based on main issues on complex systems, the basic considerations on time-dependent processes including fields and waves are specified in following statements:

- mechanical behaviour (stresses, velocities, deformations, temperature) of continua depends on the interactions of constituents and fields;
- properties of waves as carriers of information and energy reflect the interaction processes;
- physical properties of waves (amplitudes, velocities, spectra, shapes) are measurable; beside the analysis of

a process (direct problem) this information can be used for determining the properties of fields or the internal structures (inverse problem);
– the physical consistency of mathematical models is guaranteed by satisfying thermodynamical conditions;
– the different scales (macro-, meso-, microscales and molecular structures) need to be specified.

From that follows that there are several interactions: wave–wave, wave–field, wave–internal structure and their combinations which must be carefully studied in order to understand the physical mechanisms that govern the behaviour of continua, let them be solids, fluids or tissues. As far as the processes usually are nonlinear, there are few analytical solutions and the asymptotical and numerical methods should be elaborated. Although the wave motion is a large field of studies, the mathematical models are based on the theory of continua, which gives a joint basis and leads to similar basic governing equations. However, classical theories of homogeneous continua are not able to reflect such complicated processes mentioned above and therefore must be modified, especially in the direction of heterogeneous media. The methods for the analysis must also be modified and even tailored to meet the conditions of consistency and accuracy.

In what follows, an overview of complex engineering and physical phenomena is given from the viewpoint of the Centre for Nonlinear Studies. It is certainly not the whole Nonlinear Universe [54] but a part of it. CENS was launched in 1999 in order to create a unit for nonlinear studies with a focus on wave motion, optics, system biology and control. The studies have certainly been embedded into the general framework of nonlinear science because of numerous interactions of ideas and thoughts needed for building a whole. Section 2 is devoted to mathematical models for solids, fluids and tissues leading, if possible, to concrete novel governing equations. Next, in Section 3 the methods used in analysis are described starting from main numerical methods to some specific methods. The main physical results reflecting the interaction of waves, fields and structures are collected in Section 4. Finally, the summary and conclusions are presented.

2. MATHEMATICAL MODELS

The mathematical analysis of physical effects can be based only on properly derived models, which are physically consistent and satisfy thermodynamical requirements. This concerns solids and fluids, as well as biological tissues. The aims of modelling may be different but clearly the homogeneity of a medium is a simplifying assumption. For solids, for example, there is an urgent need to account for microstructures in order to understand mechanisms responsible for physical phenomena starting from wave motion to phase changes and fracture. One of the possibilities to model internal structures in solids is to use the concept of internal variables [7,21,39,60]. Internal variables are not observable and replace the constituents by corresponding internal fields in the solid. The main idea is to use the material momentum equation where the forces are explicitly shown [41] for deriving the wave equation and the Clausius–Duhem inequality for determining the governing evolution equations for internal variables.

The material momentum equation [41] is

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

where $\mathbf{P}$ is the material momentum (pseudomomentum), $\mathbf{b}$ is the material Eshelby stress and $\mathbf{f}^{inh}, \mathbf{f}^{ext}, \mathbf{f}^{int}$ are material inhomogeneity force, the material external (body) force, and the material internal force, respectively, (for details, see [7]). The Classius–Duhem inequality derived from the second law of thermodynamics is [41]:

$$-\left.\left(\frac{\partial W}{\partial t} + S\frac{\partial \theta}{\partial t}\right)\right|_X + \mathbf{T} : \dot{\mathbf{F}} + \nabla_R(\theta \mathbf{J}) - \mathbf{S} \cdot \nabla_R \theta \geq 0, \tag{2}$$

where W is the Helmholtz free energy, θ is the absolute temperature, S is the entropy density per unit reference volume, $\mathbf{S}$ is the entropy flux, $\mathbf{J}$ is the extra entropy flux, $\mathbf{F}$ is the deformation gradient, $\mathbf{T}$ is the first Piola-Kirchhoff stress tensor and colon denotes the tensor contraction.

These equations are also suitable to describe wave processes in heterogeneous solids. The introduction of microdeformations into the consideration means that the corresponding theory is a multi-field one [43]. One of the possibilities to derive governing equations for such solids is to use the concept of internal variable. As shown in [7,21,58], the formalism of dual internal variables permits to use Eq. (1) for describing macroeffects and Eq. (2) for deriving governing equations for describing effects on the microlevel. In principle, it means that the microstructure is described by additional internal fields [21]. This approach permits to replace interactions between waves and internal structures by interactions between waves and fields. In physical terms it brings in thermodynamical considerations for deriving the governing equations and in mathematical terms leads to more simple models preserving at the same time physical consistency.

2.1. Waves

Based on Eqs (1)–(2) and the concept of internal variables many mathematical models are derived: for waves in elastic solids with microstructure [8,10,16]; in thermoelastic solids [7,9,59] and in thermoelastic solids with microstructure and microtemperature [11].

We present here the 1D governing wave equations in terms of the macrodisplacement $u_1 = u$. For a microstructured solid, composed by macro- and microstructure, the linear equation of motion is the following [10]:

$$u_{tt} = (c^2 - c_A^2)u_{xx} + a_1(u_{tt} - c^2 u_{xx})_{xx} - a_2(u_{tt} - c^2 u_{xx})_{tt} + a_3 u_{xxxx}, \quad (3)$$

where c is the velocity in the macrostructure, c_A is the velocity related to the microstructure, a_1, a_2, a_3 are constants which describe the elasticity and inertia of the microstructure. The asymptotic analysis permits to derive a simplified form [10]

$$u_{tt} = \left(c^2 - c_A^2\right) u_{xx} + p^2 c_A^2 \left(u_{tt} - c_1^2 u_{xx}\right)_{xx}, \quad (4)$$

where c_1 is the modified velocity and p characterizes the inertia of the microstructure. The modifications of these models involve the influence of nonlinearities, the influence of several microstructures (hierarchical and concurrent), and the influence of thermal effects. For example, the waves in hierarchically microstructured solids composed by a macrostructure and microstructures (the second one embedded into the first) are asymptotically described by

$$u_{tt} = \left(c^2 - c_{A1}^2\right) u_{xx} + \delta_1 b_1 \left(u_{tt} - c_1^2 u_{xx}\right)_{xx} + \delta_2^2 b_2 \left(u_{tt} - c_2 u_{xx}\right)_{xxxx}, \quad (5)$$

where δ_1 and δ_2 are the scaling parameters, b_1, b_2 describe coupling effects and c_1, c_2 are velocities related to microstructures [17]. In the nonlinear case, the governing equation of motion involving the macro- and microstructure is [20]

$$u_{tt} = \left(c^2 - c_A^2\right) u_{xx} + \frac{1}{2} q_1 \left(u_x^2\right)_x + p^2 c_A^2 \left(u_{tt} - c_1^2 u_{xx}\right)_{xx} - \frac{1}{2} \delta^{1/2} q_2 \left(u_{xx}^2\right)_{xx}, \quad (6)$$

where q_1, q_2 are coefficients of nonlinearities on macro- and microscale, respectively and δ is a scaling parameter.

Beside the wave equations, which model two-wave processes, the evolution equations (one-wave equations) are widely used. In this case one should use the moving coordinates $\big(\xi = c_0 t - x$ and $\tau = \varepsilon x$, for example$\big)$ and certain asymptotic procedures in order to derive them from wave equations. For 1D processes, the wave-equation (6) yields to the evolution equation [50]

$$\frac{\partial \alpha}{\partial \tau} + k\alpha \frac{\partial \alpha}{\partial \xi} + d\frac{\partial^3 \alpha}{\partial \xi^3} + \varepsilon p \frac{\partial^2}{\partial \xi^2} \left(\frac{\partial \alpha}{\partial \xi}\right)^2 = 0, \quad (7)$$

where k, d and p are constants. This is of the Korteweg–de Vries (KdV) equation type but the last term describes the nonlinearity on the microlevel. For 2D unidirectional processes, Eq. (7) is modified to [55]

$$\frac{\partial}{\partial \xi} = \left[\frac{\partial \alpha}{\partial \tau} + k\alpha \frac{\partial \alpha}{\partial \xi} + d\frac{\partial^3 \alpha}{\partial \xi^3} + \varepsilon p \frac{\partial^2}{\partial \xi^2} \left(\frac{\partial \alpha}{\partial \xi}\right)^2\right] = q\frac{\partial^2 \alpha}{\partial \eta^2}, \quad (8)$$

where $\xi = c_0 t - x_1, \tau = \varepsilon x_1, \eta = \varepsilon^{1/2} x_2$ and q is the constant reflecting diffractional expansion in the transverse direction. Equation (8) is the modified Kadomtsev–Petviashvili (KP) equation. For waves in shallow water it is usually presented in the dimensionless form [29,47]:

$$(v_t + 6vv_x + v_{xxx})_x + 3v_{yy} = 0, \quad (9)$$

where t, x, y correspond to τ, ξ, η in Eq. (8).

In models above, the parameters, which describe the material properties, are taken as constants. Nevertheless in many cases these parameters are space-dependent. Bearing in mind nondestructive testing (NDT) for determining the prestress or material inhomogeneous properties, several mathematical models are derived in [12,52].

For example, the one-dimensional waves in the material, subjected to two-dimensional prestressed state, are described by [51]

$$\left[1 + k_1 U_{1,1}^0 + k_2 U_{2,2}^0\right] U_{1,11} + \left[k_1 U_{1,22}^0 + k_3 U_{1,22}^0 + k_4 U_{2,12}^0\right] U_{1,1} + k_1 U_{1,1} U_{1,11} - c^2 U_{1,tt} = 0. \quad (10)$$

Here the wave and the prestress are characterized by displacements $U_1(X_1, t)$ and $U_{I,J}^0(X_1, X_2)$, respectively. Indices $I; J (= 1, 2)$ and t after comma denote differentiation, and k_1, k_2, k_3, k_4 and c are related to material parameters including also the Murnaghan third order elastic constants.

The variety of microstructures in materials is reflected in wave equations (evolution equations) presented above: Mindlin-type models $\big($Eqs (3)–(6); (7)–(8)$\big)$ and models with prestress $\big($Eq. (10)$\big)$. If, however, the microstructure has more complicated mechanical properties, then it might be physically expedient to start with stress–strain relations and to use the Cauchy method for deriving the wave equations. For example, in case of felt materials the behaviour of the material is hereditary [56,57]. For such a case, the corresponding wave equation is [36]

$$\left[(u_x)^p\right]_x - u_{tt} + \left[(u_x)^p\right]_{xt} - \delta u_{ttt} = 0, \quad (11)$$

where p is the nonlinearity exponent, $\delta = 1 - \gamma$, γ is the hereditary amplitude.

Even the 1D models described above, are rather complicated. If we take into account the rotation of microstructural elements like in Cosserats model then the mathematical models become systems of coupled equations with many interactions involved. In addition, the microstructure can have an orientation like in short fibre reinforced materials [24–26]. In this case, the constitutive equation is written in the form

$$T^{ij} = T^{ij}\left(T_{matrix}^{kl}, \mu, a^{kl}, a^{klmn}, T_{fibres}^{kl}\right), \quad (12)$$

where T^{ij} is the total stress tensor, T^{kl}_{matrix} – the stress tensor for the matrix (concrete, composite), μ – the volume factor, T^{kl}_{fibres} – stress tensor of an isotropic fibre orientation distribution and a^{kl}, a^{klmn} are alignment tensors. The theoretical and experimental analysis of the behaviour of the steel fibre reinforced concrete opens a way to many practical applications [13].

Finally, let us turn to modelling of stress states in living tissues, which are certainly much more complicated by their structure and accompanying chemical processes than man-made microstructured materials. The muscle contraction is modelled by the sliding filament theory, which explains the shortening of the basic elements in a muscle, i.e. sarcomeres by thick and thin filaments sliding along each other [27]. The corresponding Huxley-type crossbridge model is derived [35,60] together with the formalism of internal variables [15].

2.2. Fields

The interaction of fields considerably widens the area of physical phenomena which could be described as complexity. The proper modelling gives insight to the formation of patterns and/or the possibility to solve inverse problems using data from interaction.

The interaction of stress and light fields is the basic idea for the theory of photoelasticity. The photoelastic phenomena and technology have been studied in the Institute Cybernetics for a long time [2]. The main attention nowadays is the integrated photoelasticity for the measurement of 3D stress fields. It is based on the measurement of the transformation of the polarization of light when it passes a 3D test object. The transformation of the polarization is described by the following system [2]

$$\frac{dE_1^p}{dz} = -\frac{1}{2} iC_0(\sigma_1 - \sigma_2)E_1^p + \frac{d\varphi}{dz}E_2^p, \tag{13}$$

$$\frac{dE_2^p}{dz} = -\frac{d\varphi}{dz}E_1^p + \frac{1}{2} iC_0(\sigma_1 - \sigma_2)E_2^p, \tag{14}$$

where E_1^p and E_2^p are the components of the electric vector along the principal stress axes in the plane (x_1, x_2), σ_1 and σ_2 are the principal stresses in this plane and $d\varphi/dz$ describes the rotation of the principal stress axes along the light ray. The photoelastic constant is denoted by C_0.

Based on these fundamental models, the theory of photoelastic tomography is developed [5], a new physical phenomenon – interference blots – discovered [3] and many practical problems solved [4]. New polariscopes have been constructed which are effectively used worldwide. Magnetophotoelasticity [1] has been applied by Pilkington Ltd for measuring tempering stress in windshields.

The complexity of fields in turbulent mixing is modelled in [30,32,34] and models for coupling the fields of microdeformation and microtemperature are derived in [11].

In the mesoscopic scale, the situation is even more complicated. For example, in the context of liquid crystals the balance of spin must be taken into account [24]. Here the mesoscopic space may be non-contiguous despite the macroscopic material being contiguous. In this case "virtual" boundaries appear and special boundary conditions have to be introduced [26].

3. METHODS

Mathematical models described in Section 2 govern dynamical processes which, as a rule, reflect interactions between waves, fields and structures. Only in few cases direct analytical solutions to governed equations are known like for example the solutions to the KdV-like equations. In most cases numerical and/or asymptotical methods must be used. It is not always straightforward to use numerics because one should be aware of all the limitations of numerical schemes, the convergence of calculations must be understood and thermodynamical consistency, if needed, must be evident. Some methods used for the analysis of problems indicated above are briefly listed.

First, the finite volume wave-propagation algorithm [38] is modified and widely used [6]. Second, the pseudo-spectral method for solving the nonlinear evolution equation is used in [53] and for Boussinesq-type equations – in [20]. Special attention is devoted to deriving the various ODE solvers [28,48].

Turning now the attention to interaction process it is clear that direct numerics needs additional methods for explaining the specific features of interaction and special tools for obtaining information about fields and/or structures. First, wave–wave interaction in prestressed or inhomogeneous solids permits to solve the inverse NDT problems. Such algorithms, based on perturbation method and Laplace transform technique, have been elaborated for acoustodiagnostics [51,52]. Second, for field–field interaction in solids, spectral methods in photoelasticity have been proposed based on the tensor tomography and on the hybrid method which combines experimental results with analytics [4,5]. Third, for field interaction in fluids the combination of analytics and numerics is used. The triplet-map-model is elaborated for describing the small-scale anisotropy of passive scalar in nonsmooth flows [33]. As far as turbulent mixing has close connection with statistical topography, some specific methods have been proposed: the 4-vertex model of random surfaces [31] and the method for efficient extraction of scaling exponents from Monte-Carlo simulation data [42].

In addition, a stereoscopic 3D visualization system has been designed and built [46]. This system played a decisive role in calculating orientation distributions of short fibres in concrete [13].

Finally, one should note the importance of software for scientific computation and for control of laboratory equipment. Most of such software is developed under open source model available in Python library [28,48].

4. RESULTS AND DISCUSSION

The analysis of mathematical models described above has greatly benefitted from interdisciplinarity studies by using various concepts of complexity of nonlinear systems. In such systems, the whole after interactions is not only "bigger" (like Aristotle said) but also different. The models of dynamical processes in solids, fluids and tissues analysed intensively in CENS over recent years have proved that. In what follows, the main results from these studies are summarized.

As said in Introduction, the main attention is paid to wave–wave, field–field, and wave–field nonlinear interactions. An important problem for heterogeneous media is related to the modelling of their internal structures. In many cases, it is possible to use the concept of internal variables which helps to model the influence of internal structures to macrobehaviour of a medium [21].

Leaving aside the details, the selected essential results are now briefly presented.

Waves in solids:

- mathematical modelling and analysis of wave motion in microstructured solids (Mindlin-type, functionally graded materials, felts, etc.), phase-transformation, propagation of fronts, etc;
- determining physical effects characteristic to wave motion in microstructured solids: negative group velocity, microtemperature effects, dimensionless parameters governing dispersive effects, mesoscopic effects, etc;
- describing the soliton interaction and emergence of soliton trains modelled by KdV-type and Boussinesq-type systems;
- explaining the concept of hidden solitons and mechanisms of amplification of solitons.

Inverse problems:

- elaborating the theory of integrated photoelasticity with many practical applications (stress determination in cylindrical objects, glass panels, automotive glazing, etc);
- describing physical effects in photoelasticity like appearance of interference plots and mechanisms of magnetophotoelasticity;
- elaborating algorithms for the NDT of materials based profile changes (spectral distortions).

Fluid dynamics:

- establishing mechanisms for turbulent mixing in many cases (chaotic velocity fields, non-smooth compressible flows, etc);
- determining scaling exponents for turbulent mixing and percolation;
- analysis of fractal effects like diffusion on fractal structures, intersection of moving fractals, emergence of coastlines and landscapes, cracking of films, etc.

For tissues (combining modelling and experiments):

- elaborating a cross-bridge model for mechano-energetics of actomyosin interactions;
- proposing an integrated method to quantify calcium fluxes in cardiac excitation-contraction coupling;
- analysis of lattice-like obstructions to diffusion in heart muscle cells.

Even this brief overview demonstrates clearly how useful the interdisciplinary approach is – complexity studies are characterized by interactions and similarity of methods and concepts permit more effectively to analyse various dynamical processes [18,19]. It is not only the physical processes, similar methods can be used also for the analysis of financial markets [37]. A more detailed overview on nonlinear wave motion is presented in [22].

We live in a nonlinear universe [54] and the success of generating new knowledge depends not only on the progress of physics, chemistry, biology, etc but definitely depends very much on the progress of nonlinear mathematics like pointed out already by W. Heisenberg. Indeed, mathematics is sometimes called intellectual machine and nonlinear science benefits largely upon the wisdom to use this machine [44]. Nonlinear interactions in their turn bring in new qualities, characteristic to complexity.

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Komplekssüsteemid tehnika- ja loodusteadustes

Jüri Engelbrecht

On esitatud kokkuvõte interdistsiplinaarsetest uuringutest TTÜ Küberneetika Instituudi mittelineaarsete protsesside analüüsi keskuses (CENS). Põhitähelepanu on mittelineaarsete vastasmõjude matemaatilisel modelleerimisel, mis haarab laine-laine, laine-välja ja laine-sisestruktuuri tüüpi interaktsioone ning nendest tulenevaid muutusi. On kirjeldatud ka kasutatud numbrilisi meetodeid.