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MICROSTRUCTURE DESCRIBED BY HIERARCHICAL INTERNAL VARIABLES

Abstract. In this paper a clear distinction is made between the different scales and the different processes in the microstructure which influence the dynamics at the macrolevel. In the first case the governing equation for wave propagation is represented by a hierarchy of waves. In the second case it has been shown, how useful the concept of internal variables is. The different processes can be best described by a hierarchy of internal variables. An example of cardiac muscle contraction is briefly described, demonstrating the dependence of the active stress on sliding the molecules and ion concentration involving the corresponding internal variables.

1. Introduction

Continuum mechanics is usually based on macroscopic concepts and quantities, such as energy density, stress, strain, etc. However, materials (whatever their origin is) have usually a microstructure because of inhomogeneities, pores, embedded layers, reinforcements, etc.. This list can be prolonged but one is clear - the description of the behaviour of many materials should take into account both the macroscopic and microscopic properties, occuring at different length scales and involving different physical effects. Within the framework of continuum mechanics, such a behaviour is best described by distinguishing macro stresses and microstresses with interactive microforces ([1], [2]). We feel however, that for materials with complicated properties indicated above, one should start distinguishing clearly the observable and internal variables ([10], [13]). Although the formalism of internal variables is well known ([10], [13]), for the clarity sake we repeat here some basic concepts.

The observable variables are the usual macroscopic field quantities such as elastic strain, for example. These variables are governed by conservation laws and possess inertia. The internal structure of the material (body, tissue, composite, etc.) is supposed to be described by internal variables which are not observable and do not possess inertia. They should compensate our lack of knowledge of the precise description of the microstructure. The formalism of internal variables involves constructing of a dissipation potential $\mathcal{D}$ in parallel to the Lagrangian $\mathcal{L}$ for the observable variable. However, the governing equations of internal variables are kinetic equations (not hyperbolic) – see [10], [13].

The idea of using internal variables for describing dynamical processes in microstructured materials has earlier been presented in [12], [4]. The problems become more complicated when either the scales or possible processes in materials are different and form a certain hierarchy. This brings us directly to the idea of hierarchical internal variables that certainly need generalization

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of the existing formalism. An example and main concepts of hierarchical internal variables are given in [6], here a certain systematic approach is presented following by an example.

In Section 2 basic ideas of modelling are briefly described. The description involves continuum mechanics, internal variables and evolution equations - all needed for further presentation. More detailed description can, for example, be found in [3]. Section 3 presents the central ideology of this paper. It makes clear distinction between different scales and different processes in the microstructure. In the first case the result is a wave hierarchy, in the second case - a hierarchy of internal variables. In Section 4 an example is presented, illustrating the hierarchical internal variables. The case study is based on the contraction of the cardiac muscle depending on the cell energetics. Last Section 5 includes conclusions and open problems.

2. Basic modelling

2.1. Continuum mechanics

To be brief, we refer to [1], [2] for basic concepts for microstructured solids. For a body $\mathcal{B} \subset \Re^3$ with microstructure, an added field δ describes the mechanical characteristics of the microstructure. The stress fields can be introduced after the definition of the expended power in arbitrary processes [9], including a macroscopic (gross structure) stress and force, a microscopic (fine structure) stress and force, and an interaction force between the macro- and microstructures. In [2], this approach has been extended to include different microstructures at their characteristic scales. Then for arbitrary region $\mathcal{W}$ in $\Re^3$ with outward unit normal $\mathbf{m}$ we have for the actual power $\Pi_0(\mathcal{W})$:

$$\Pi_0(\mathcal{W}) = \int_{\partial\mathcal{W}} \mathbf{T}_g \mathbf{m} \cdot \mathbf{v} da + \int_{\mathcal{W}} \mathbf{f}_g \cdot \mathbf{v} dv + \Pi_{micro,1}(\mathcal{W}).$$

Here $\mathbf{v}$ is the velocity, $\mathbf{T}_g$ is the macroscopic stress, and $\mathbf{f}_g$ is the macroscopic body force. Note that indexing has here and below been changed compared with [2]. The field $\Pi_{micro,1}(\mathcal{W})$ is the power expended by the microstructure. Further, the difference from the general theory [9] involves a sequence of microscopic processes $\mathbf{d}_k, k = 2, 3, ...$ Now, we can magnify a small region of $\mathcal{W}$ iteratively by magnifications λ^k. At the first stage

$$\Pi_{micro,1}(\mathcal{W}) = \int_{\partial\mathcal{W}_1} \mathbf{T}_1 \mathbf{m} \cdot \mathbf{v_1} da + \int_{\mathcal{W}_1} \mathbf{f}_1 \cdot \mathbf{v}_1 dv + \Pi_{micro,2}(\mathcal{W}).$$

where $\mathbf{v_1} = \lambda \mathbf{v} + \dot{\mathbf{d}}_1$ and $\mathbf{T}_1$ is the microscopic stress at this level. Further on,

$$\Pi_{micro,2}(\mathcal{W}) = \int_{\partial\mathcal{W}_2} \mathbf{T}_2 \mathbf{m} \cdot \mathbf{v_2} da + \int_{\mathcal{W}_2} \mathbf{f}_2 \cdot \mathbf{v}_2 dv + \Pi_{micro,3}(\mathcal{W}),$$

etc. (for details, see [2]. The general balance laws can now easily be rewritten in the referential form.

2.2. Internal variables

The formalism of internal variables is presented in [10], [13]. Here we need point out just essentials for further analysis in Section 3. The behaviour of a system, i.e. dynamic state of a body involves description of observable state variables χ (e.g. elastic strain and particle velocity) and a certain number of internal variables α. The dependent variable(s) (e.g. the stress) must be simultaneously a function of both

$$\sigma = \sigma(\chi, \alpha)$$

which must be complemented by a governing equation for α:

$$\dot{\alpha} = f(\chi, \alpha) + g(\chi, \alpha)\dot{\chi}. \tag{1}$$

It is assumed that the strain ϵ is split up in an elastic part ϵ^e and an "anelastic" part ϵ^p:

$$\epsilon = \epsilon^e + \epsilon^p.$$

The free energy function ψ is assumed to be

$$\psi = \psi(\epsilon^e, T; \alpha, \nabla\alpha)$$

where T is temperature. The equations of motion are then easily derived. In addition, we need to concretize Eq (1). For that, a dissipation potential $\mathcal{D}$ is postulated

$$\mathcal{D} = \mathcal{D}(\sigma, \dot{\alpha}, \epsilon^e, T, \alpha, \nabla\alpha) > 0$$

possessing certain properties [10]. Then the governing Eq (1) for α is derived as

$$\frac{\delta\psi}{\delta\alpha} + \frac{\partial\mathcal{D}}{\partial\dot{\alpha}} = 0.$$

As a rule, this equation is not hyperbolic.

2.3. Mathematical models

It is clear that mathematical models involving both observable and internal variables are of the mixed (e.g. inertial-diffusive [10]) type. The general ideas for asymptotic analysis of such systems are presented in [4], [5]. To get an idea, the simplest 1D case could be described. Let an n-vector $\mathbf{U}$ be the vector of the observable variables, a scalar w – the internal variable and $X_1 = X$. Then the governing system is of the following form

$$I\frac{\partial\mathbf{U}}{\partial t} + A_1\frac{\partial\mathbf{U}}{\partial X} + \epsilon B_{11}\frac{\partial^2\mathbf{U}}{\partial t\partial X} + h.o.t = \mathbf{H}(\mathbf{U}, w) \tag{2}$$

$$\frac{\partial w}{\partial t} + d_{11}\frac{\partial^2 w}{\partial X^2} + h.o.t = p(\mathbf{U}, w) \tag{3}$$

where I is a unit matrix, $A_1(\mathbf{U}, X)$, $B_{11}(\mathbf{U}, X)$ are the matrices of parameters, $\mathbf{H}(\mathbf{U}, w)$ and $p(\mathbf{U}, w)$ are the coupling vector and function, respectively, d_{11} is a constant and ϵ a small parameter while h.o.t stands for higher order terms (derivatives).

It is proposed [4], [5] to use conventional asymptotic approach for deriving the evolution equation(s) for system (2), (3) (see [3]).

3. Types of models

Depending on the different length and time scales, the asymptotic governing equations derived along the ideas of Section 2, may have different character. Nevertheless, it is possible to distinguish between the two types of governing equations.

The *first type* is based on structural hierarchy of a material (body) and strong dependence on length scales within the material and of the excitation which are the leading factors. The simplest example is just a material where macro- and microstructure are described by their own balance laws [1], [9]. It means that the dynamic behaviour of the constituents is basically similar and differs in parameters.

The *second type* is based on process hierarchy in a material (body) where at various levels various dynamical processes are of importance, all influencing the macrobehaviour. This is an example of the cardiac muscle [6] and characterized best by internal variables that form a hierarchy.

Below both types are briefly characterized.

3.1. Structural hierarchy and hierarchy of waves.

Many materials possess microstructure at various scales. On the other hand, it is widely known that dissipation and dispersion is different for various frequency scales. Hence, given the initial excitation with a fixed frequency (wavelength), the response of the material depends actually on a certain underlying microstructure which is responsible for the governing physical effects. Actually, this could be just a case of macro- and microstructure, or then a case of several microstructures. The outcome, i.e. the governing equation should certainly reflect this possible choice emphasized by certain input-dependent parameters. One could intuitively address the problem asking a question, which material properties are more important: those characteristic to the macrostructure or those characteristic to the microstructure of a certain level. It is clear that a single governing equation should have a certain hierarchy embedded into it.

Wave hierarchies are analysed by Whitham [15], showing the hierarchy of just two orders. A case, demonstrating the wave hierarchy in dissipative solids, is analysed in [4]. For a dissipative microstructured solids where dissipation rates are different for macro- and microstructure, the final linearized governing equation in the dimensionless form is the following:

$$\frac{\partial}{\partial \xi}\left(\frac{\partial u}{\partial \tau} - K_1 \frac{\partial^2 u}{\partial \xi^2}\right) + \lambda^2 \left(L\frac{\partial u}{\partial \tau} + M\frac{\partial u}{\partial \xi} - K_2 \frac{\partial^2 u}{\partial \xi^2}\right) = 0. \tag{4}$$

where u stands for the displacement gradient, τ and ξ are the moving coordinates, K_1, K_2, L, N are the constants and λ is the input-depending scale parameter. Equation (4) is derived from the conventional equations of motion in the reference form by using the asymptotic (reductive perturbative) method (see, for example [3]). For λ small, the influence of the microstructure may be neglected and dissipation is governed by the constant K_1, for λ large, the dissipation is governed by microstructural properties, i.e. by K_2, while $K_1 \neq K_2$.

Waves in dispersive solids (granular materials) where dissipation is neglected are analysed in [7]. In this case for scaled density fluctuation w the governing equation is

$$\frac{\partial^2}{\partial \xi^2}\left(\frac{\partial w}{\partial \tau} + w\frac{\partial w}{\partial \xi} + N_1 \frac{\partial^3 w}{\partial \xi^3}\right) + \mu \left(\frac{\partial w}{\partial \tau} + w\frac{\partial w}{\partial \xi} + N_2 \frac{\partial^3 w}{\partial \xi^3}\right) = 0. \tag{5}$$

where N_1, N_2, μ are the coefficients. Contrary to the case (3.1), here dispersion is important and (5) represents actually a hierarchy of the Korteweg-de Vries equations. Intuitively, denoting by π an operator for the Burger's-type (dissipative) materials, Korteweg-de Vries-type (dispersive) materials, or both, the hierarchy of waves could be represented by

$$\sum_m \epsilon_m \frac{\partial^n}{\partial \xi^n} \pi_m = 0$$

where π_m denotes the operator for m-th scale and ϵ_m – a corresponding small parameter, if any. Hence, π_0 denotes the wave operator in the highest, i.e. in the macrolevel (c.f. Section 2.1). The order of derivatives $n(m)$ represents the order of coupling between various effects. As a conjecture, one could propose that dispersive effects are characterized by n = 2,4,... and dissipative effects – by n = 1,3,... (c.f. Eqs (4) and (5)).

3.2. Process hierarchy and hierarchical internal variables.

Beside the different scales, the embedded microstructures are sometimes characterized by completely different physical processes going on simultaneously. As said before, such processes are internal and governed by internal variables [10], [13]. If now these processes are linked to the macrobehaviour by a certain hierarchy then the corresponding internal variables form also a hierarchy. We use then notion of hierarchical internal variables [6].

In general terms, the idea of building up the mathematical model is the following [6]:
1) a constitutive equation for a dependent variable, say σ (i.e. stress, for example), depends on observable variable χ and the *first-level* internal variable α

$$\sigma = \sigma(\chi, \alpha);$$

2) the evolution law for α is

$$\dot{\alpha} = f(\chi, \alpha, \beta), \tag{6}$$

where β is the next, *second-level* internal variable influencing σ only through dynamics of the first-level internal variable α;
3) the evolution law for β is

$$\dot{\beta} = g(\chi, \alpha, \beta, \gamma), \tag{7}$$

where γ is again the next, now the *third-level* internal variable, influencing σ only through dynamics of the second level internal variable β;
4) the evolution law for γ is

$$\dot{\gamma} = h(\chi, \alpha, \beta, \gamma, ...), \tag{8}$$

etc.

Internal variables $\alpha, \beta, \gamma, ...$ form a hierarchy reflecting the hierarchical processes in the material.

Consequently, the mathematical model of the macrobehaviour is governed by a system including several equations that can be of the various types. Note, however, that Eqs. (6), (7), (8) could also include gradients and then at least the governing system is composed by partial differential equation.

4. Example: cardiac muscle contraction

Here we refer to the fundamental treatises on cardiac performance [8], [16]. In terms of continuum mechanics, ventricles are thick-walled shells made of anisotropic fibres. These fibres have complicated microstructure and act as following. The muscle fibres are made up by the bunches of smaller elements called myofibrils with a surrounding sarcotubular system. The main task of myofibrils is to convert metabolic energy into mechanical energy while the surrounding sarcotubular system governs the behaviour of Ca^{2+} ions needed for activation. In sense of continuum mechanics, these processes include the internal variables compared to the observable macrovariables like strain. The stress in the muscle is the dependent variable and its constitutive law is linked to the observable variable and then the hierarchy of internal variables. Leaving aside the details of this extremely fascinating mechanism (the reader is referred to [6], [14]), we concentrate here on the description of the mathematical model.

We assume, that the total (Cauchy) stress in the muscle can be split up into two parts

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}_p + \boldsymbol{\sigma}_a,$$

where $\boldsymbol{\sigma}_p$ and $\boldsymbol{\sigma}_a$ denote passive and active stress, respectively. The passive stress results from the elastic deformation of the tissue and can be calculated traditionally like

$$\boldsymbol{\sigma}_p = \frac{\partial \psi}{\partial \boldsymbol{\epsilon}^e},$$

where ψ is the free energy and $\boldsymbol{\epsilon}^e$ is the strain. Given ψ, the passive stress is easily calculated. The active stress σ_a is generated in myofibrils by activation and is directed parallel to the fibre orientation. Hence

$$\boldsymbol{\sigma}_a = \sigma_a \boldsymbol{\epsilon}_1 \boldsymbol{\epsilon}_1,$$

where ϵ_1 is the unit vector showing the orientation. Now the complicated mechanism producing active stress needs the more detailed description of the sequence of internal variables, which are the main actors. At this structural level, myofibrils are the starting point. A myofibril is composed of repeating units of myosin and actin filaments, called sarcomeres. The actin filament 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 releases Ca^{2+} ions in the sarcotubular system which then activate the troponin molecules so that they will be able to attach the heads of myosin molecules. This attaching means swivelling of myosin molecules that cause sliding the actin and myosin filaments against each other. As a result, active stress is created.

The mechanism briefly described above (for details see [6], [14] and the references therein) needs to be cast into a mathematical model.

We start here 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

$$F_A = K_A\, z, \qquad F_B = K_B\, z$$

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 crossbridges between z and $z - dz$ in both states. We take the uniform distribution of crossbridges in z over an internal d. The active stress is then found by

$$\sigma_a = \frac{ml_s K}{2d}\left(\int_{-d/2}^{d/2} n_A(z)dz + \int_{-d/2}^{d/2} n_B(z)dz\right)$$

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 (c.f. Section 3.2) are governed by the following kinetic equations

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

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

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

$$A = n_A + n_B + n_C.$$

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 kinetic equation

$$\frac{dA}{dt} = c_1(l_s)[Ca^{2+}](1 - A) - c_2(l_s)A, \tag{9}$$

with $c_1(l_s), c_2(l_s)$ as certain parameters. Equation (9) involves the *third-level internal variable* $[Ca^{2+}]$ which must be governed by its own kinetic equation

$$\frac{d[Ca^{2+}]}{dt} = f([Ca^{2+}]).$$

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 and will be published elsewhere.

5. Discussion

As explained in Section 3 and demonstrated in Section 4, hierarchies of the internal structure of a material (body, tissue) lead to certain hierarchies in mathematical models. These hierarchies can be either the hierarchy of waves in the Whitham's sense [15] or the hierarchy of internal variables. Both cases need actually more detailed analysis. The models are complicated that is why in order to get practical results, numerical simulation must be used. However, there are many open questions also from the theoretical viewpoint.

For example, the question on dispersive properties embedded into the hierarchy of waves must be analysed. It is known that higher-order dispersion terms are the same in the wave hierarchy ((3.2) in [7]) and in the governing equation obtained by a direct asymptotic derivation [11].

This certainly shows the correctness in leading terms but the properties of the wave hierarchy are not clear.

For hierarchical internal variables the line of questions seems to be longer. The extra entropy flux **k** in the formalism of internal variables [10], [13] depends then also on internal variables in a certain sequence that must be analysed. Open is the question, how to construct dissipative potentials $\mathcal{D}_\alpha, \mathcal{D}_\beta, \mathcal{D}_\gamma, \ldots$ corresponding to the each level of internal variables. It seems, that a more detailed formalism of internal variables might cast light over the formation of dissipative structures.

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