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The Website With O'DEL FOR THE ANALYSIS OF NONSTATIONARY PROCESSES IN MATERIAL SYSTEMS WITH A PERIODIC STRUCTURE

Jowita Rychlewska, Jolanta Szymczyk, Czesław Woźniak

Institute of Mathematics and Computer Science, Technical University of Częstochowa

Abstract. The main aim of this paper is to outline a new approach to the formulation of approximate mathematical models for the analysis of non-stationary thermomechanical processes in micro-periodic solids and structures. The modelling procedure is realized in two steps. First, a system of finite difference equations is formulated by the periodic FEM discretization of the unit cell for a solid under consideration. Second, by applying some smoothness operations we derive continuum model equations directly from the finite difference equations. In contrast to the known homogenization and tolerance averaging methods, the proposed modelling approach can be formulated on different levels of accuracy which depend on the mesh parameter related to the periodic FEM discretization of the unit cell.

Introduction

This paper summarizes and illustrates some from results which have been obtained recently at the Institute of Mathematics and Informatics as a part of researches on the heat transfer and elastodynamics of material systems with a periodic structure. The main attention in this report is given to the formulation of new mathematical models describing behaviour of periodic solids in nonstationary processes. In particular we investigate problems in which the minimum length dimension of a macroscopic deformation and/or temperature pattern is large enough when compared to the maximum period length of the material system under consideration; these situations take place in many engineering problems, e.g. in a study of overall properties of composite materials. At the same time the processes and phenomena related to the periodic structure of a solid medium, in the course of modelling, are described in a certain approximated manner by means of what are called averaged (or macroscopic) models of periodic solids. They are models represented by PDEs with constant (averaged) coefficients. The main motivation for introducing averaged models lies in the fact that the equations of thermomechanics for solids and structures with a micro-periodic inhomogeneity involve, as a rule, functional coefficients which are highly oscillating and noncontinuous. The direct numerical solution to the initial-boundary-value problems related to these equations is an ill-conditioned and complicated computational problem, cf. [4]. This drawback does not take place for the averaged models.

Modelling procedures leading from the well known solid mechanics equations of periodic media to certain macroscopic models can be based on different mathematical assumptions and physical (heuristic) hypotheses. Hence the averaged descriptions of processes and phenomena occurring in micro-periodic solid media can be formulated on different levels of accuracy. Generally speaking, in the existing vast literature on this subject we deal with a variety of mathematical models of material systems with a periodic structure.

The main trend in a formulation of averaged models of micro-periodic solid media (including fluid saturated solids) is based on the fact that the related solid mechanic equations involve lengths of a periodic structure which can be treated as small when compared to a certain macroscopic length dimension. Thus, in the course of modelling we deal at last with two spatial length scales (macroscopic and microscopic) and we can introduce a certain small parameter ε interpreted, from the physical point of view, as a ratio between these scales. This fact is a basis for the application of the asymptotic analysis to most of modelling procedures. The idea of the asymptotic modelling lies in imbedding of the solid mechanics problem under consideration (described by PDEs with periodic coefficients) into a family of similar problems indexed by a small parameter ε . It can be shown that by a limit passage $\varepsilon \to 0$ it is possible to obtain the averaged mathematical model of the problem, i.e. a model which is governed by equations with constant coefficients. These coefficients are referred to as the effective moduli of a periodic medium. The asymptotic modelling procedure outlined above is called homogenization and the resulting equations represent what is called a homogenized model of the periodic solid. From a mathematical point of view homogenization of periodic materials and structures is based on the asymptotic analysis of partial differential equations and integral functionals with periodic coefficients; the bibliography on this subject is very extensive, we mention here the outstanding monographs [2, 4, 10, 12, 21]. The physical idea of homogenization lies in a replacing of a microperiodic nonhomogeneous solid by a certain equivalent homogeneous solid the properties of which are described by the effective moduli. Thus, the main problem of homogenization is to construct these moduli for the periodic solid under consideration. To this end we have to solve a certain periodic BVP on the periodicity cell, which is a standard problem in numerical analysis [4]. From the physical point of view, the homogenization technique can be applied exclusively to situations in which in an arbitrary but fixed periodicity cell situated away from the solid boundaries, the fluctuations of basic unknown fields (like displacements and temperature) can be approximated by periodic functions.

The main drawback of homogenized models for the analysis of non-stationary processes in micro-periodic solids is disregarding in the model equations the effect of microstructure size on the overall solid behaviour. This effect is destroyed in homogenization by the limit passage $\varepsilon \to 0$ which corresponds to the hidden heuristic assumption that the macroscopic material properties of a micro-periodic solid are independent of the period lengths. On the other hand, many physical phenomena, such as the dispersion of waves, the existence of higher-order motions and

higher free vibration frequencies in periodic solids, depend on the microstructure size. That is why the analysis of different phenomena occurring mainly in non-stationary processes requires more general averaged models then those derived by homogenization. This modelling requirement is well known in the literature and resulted in elastodynamics by construction of a series of what are called dispersive macroscopic models of periodic materials and structures. In most cases different dispersive models were formulated independently for different material periodic structures like laminates, fibrous solids, lattice-type structures etc., cf. [1, 3, 5, 6, 8, 9, 13-15, 22]. An overview of some from related models can be found in [14].

A general approach to the modelling of periodic composite materials, which preserves the effect of the microstructure size on the overall solid behaviour, was proposed in a series of papers summarised in monograph [26], where the list of references can be found. This macro-modelling method was referred to as the tolerance averaging technique (for the concept of tolerance cf. [29]). The underlying heuristic hypothesis of the tolerance averaging technique is similar to that which constitutes the physical foundations of homogenization. In both approaches it is assumed that away from the boundaries of the periodic solid the fluctuations of basic unknown fields (displacements and temperature), caused by nonhomogeneous periodic structure of a solid, are periodic-like, i.e. in every periodicity cell can be independently approximated by certain periodic functions. At the same time the tolerance averaging, in contrast to homogenization, does not treat periods of inhomogeneity as small parameters in the asymptotic meaning of this terms. The main idea of this technique is based on heuristic assumption that the values of every physical field can be measured and calculated only to within a certain negligible quantity. This idea was introduced by G. Fichera in his paper [7] and generalised in [26] by introducing the concept of the tolerance system. It is a mapping which assigns to every physical field, which is unknown in the problem under consideration, a certain tolerance parameter. These parameters determine allowable deviations in calculations and measurements of values of the given physical quantity and correspond to what was called in [7] the upper bounds for negligibles. By combining the notion of the tolerance system with that of the microstructure length (which can be defined as a diameter of a periodicity cell) the tolerance averaging technique introduces the concept of slowly-varying and periodic-like functions and makes it possible to specify certain approximations in calculation of averaged values of products involving slowly-varying and periodic--like functions. The tolerance averaging technique leads to a certain periodic cell problem but, in contrast to homogenization, this problem involves terms depending also on the period lengths. Solutions to these cell problems are obtained by applying the Galerkin approximation. To this end we can introduce certain mode-shape functions and extra unknowns which are referred to as the fluctuation variables. In thermomechanics this procedure leads to a system of PDEs with constant coefficients for the averaged displacement and temperature fields as well as for the fluctuation variables. The tolerance averaging technique has been applied recently to the analysis of many engineering problems, cf. [11, 16, 24-28] and is

used as a mathematical tool for some investigations which now are carried out in Poland.

The scope of applications of both homogenization and tolerance averaging technique is restricted to processes in which fluctuations of basic fields (like temperature and displacement), caused by the periodic heterogeneity of a medium, are periodic-like. As we have stated above it means that the above fluctuations, restricted to an arbitrary but fixed periodicity cell situated away from the solid boundary, can be approximated by periodic functions. More general modelling technique, rejecting this restriction, was proposed recently in [18, 19] by the authors of this report (cf. also [20, 23] and a series of related papers in the course of publication). In the framework of the proposed modelling technique the continuum averaged models are derived not directly from the governing equations of microperiodic solids but from certain discrete models of these solids. The new discrete models proposed by the authors of this report can be formulated on different levels of accuracy and hence are able to describe also non stationary problems with wavelengths of an order of the periods lengths (high-frequency wave propagation problems). However, the passage from discrete to continuum models can be carried on only under condition that the typical macroscopic wavelength is sufficiently large when compared to the period lengths (low-frequency wave propagation problems).

The aim of this contribution is twofold. First, we outline the aforementioned new modelling technique. Second, we illustrate the results on the example of a non-stationary heat transfer process in a composite nonhomogeneous medium with a periodic structure. For the sake of simplicity this illustration is restricted to the linear problem and a rigid conductor. In order to investigate the wave propagation phenomena the Cattaneo-type model of the heat transfer is taken as the physical basis of the analysis, cf. [27]. Obviously, the general procedure outlined below can be also applied to the macroscopic modelling of an arbitrary micro-periodic material system.

Denotations. Throughout the paper super- and subscripts a, b run over 1,2,...,n. Subscripts A, B run over 0,1,2,...,N unless otherwise stated. Superscript e takes the values 1,...,E.

1. Preliminaries

To make this paper self-consistent we recall some preliminary concepts which have been introduced in [18, 19]. Let $(\mathbf{d}_1, \mathbf{d}_2, \mathbf{d}_3)$ be the vector basis in the physical space E^3 and denote by Λ the Bravais lattice in E^3 given by

$$\Lambda := \left\{ \mathbf{z} \in E^3 : \mathbf{z} = \eta_1 \mathbf{d}_1 + \eta_2 \mathbf{d}_2 + \eta_3 \mathbf{d}_3, \ \eta_{\alpha} = 0, \pm 1, \pm 2, ..., \alpha = 1, 2, 3 \right\}$$

Let Δ be a polyhedron with a centre at point $\mathbf{z} = \mathbf{0}$ such that for every $\mathbf{x} \in \partial \Delta$ and some \mathbf{d}_{α} there is either $\mathbf{x} + \mathbf{d}_{\alpha} \in \partial \Delta$ or $\mathbf{x} - \mathbf{d}_{\alpha} \in \partial \Delta$ but not both. Subsequently for

every subset Ξ in E^3 we use the denotation $\Xi(\mathbf{z}) := \mathbf{z} + \Xi$ and for every $\mathbf{p} \in \overline{\Delta}$ we denote $\mathbf{p}(\mathbf{z}) := \mathbf{z} + \mathbf{p}$. Hence $\Xi(\mathbf{0}) = \Xi$, $\mathbf{p}(\mathbf{0}) = \mathbf{p}$.

A simplicial division of E^3 will be called Δ -periodic if it implies a simplicial subdivision of every $\Delta(\mathbf{z})$, $\mathbf{z} \in \Lambda$, into simplexes $T^e(\mathbf{z}) = \mathbf{z} + T^e$, e = 1,...,E. Let

$$P := \left\{ \mathbf{p}_0^a \in \overline{\Delta}, \ a = 1, ..., n \right\}$$

stand for the smallest set of vertexes in $\overline{\Delta}$ so that $\bigcup P(\mathbf{z})$, $\mathbf{z} \in \Lambda$, is a set of all vertexes of the given simplicial division of E^3 . Denoting $\mathbf{d}_0 = \mathbf{0}$ we shall also introduce the system of vectors \mathbf{d}_A , A = 0,1,...,N, where $N \geq 3$, so that every vertex in $\overline{\Delta}$ can be uniquely represented in the form $\mathbf{p}_0^a + \mathbf{d}_A$. Setting

$$I := \{(a, A) \in \{1, ..., n\} \times \{0, 1, ..., N\} : \mathbf{p}_0^a + \mathbf{d}_A \in \overline{\Delta}\}$$

we define $\mathbf{p}_A^a := \mathbf{p}_0^a + \mathbf{d}_A$, for every $(a,A) \in I$. It follows that $\{\mathbf{p}_A^a : (a,A) \in I\}$ is a set of all vertexes in $\overline{\Delta}$ and every simplex T^e in $\overline{\Delta}$ can be given by $T^e = \mathbf{p}_A^a \mathbf{p}_B^b \mathbf{p}_C^c \mathbf{p}_D^d$ for some $(a,A),...,(d,D) \in I$. We shall also denote:

$$I_0 := \{ (a, A) \in I : A \neq 0 \}$$

$$I^e := \left\{ (a, A) \in I : \mathbf{p}_A^a \in \overline{T}^e \right\}$$

It means that \mathbf{p}_A^a is a vertex of \overline{T}^e iff $(a, A) \in I^e$.

For an arbitrary real valued function $f(\cdot)$ defined on Λ we introduce finite differences

$$\Delta_A f(\mathbf{z}) = f(\mathbf{z} + \mathbf{d}_A) - f(\mathbf{z})$$

$$\overline{\Delta}_A f(\mathbf{z}) = f(\mathbf{z}) - f(\mathbf{z} - \mathbf{d}_A)$$
(1)

For A = 0 the above formulae reduce to $\Delta_0 f(\mathbf{z}) = \overline{\Delta}_0 f(\mathbf{z}) = 0$.

In the subsequent analysis the lengths $l_{\alpha} = |\mathbf{d}_{\alpha}|$ will represent the periods of inhomogeneity of a material solid medium and the polyhedron Δ will be interpreted as the periodicity cell. It will be assumed that the periodic medium has piecewise constant properties and every simplex T^e can be treated, with a sufficient accuracy, as homogeneous. We shall also define $h = \max \left\{ diam T^1, ..., diam T^e \right\}$ where $diam T^e$ is a diameter of T^e . It has to be remembered that the Δ -periodic simplicial division of E^3 is uniquely determined by a pertinent simplicial sub-

division of the periodicity cell Δ ; this subdivision also will be referred to as Δ -periodic.

2. Discrete models

Let Ω be a region in E^3 with the smallest characteristic length dimension L satisfying condition $L >> \max\{l_1, l_2, l_3\}$ and let us define the subset Λ_0 of Λ given by

$$\Lambda_0 := \{ \mathbf{z} \in \Lambda : \Delta(\mathbf{z} \pm \mathbf{d}_A) \subset \Omega, A = 0, 1, ..., N \}$$

By $q(\cdot,t)$ we shall denote a physical (scalar, vector or tensor) field which for every time $t \in (t_0,t_1)$ is defined in Ω . Subsequently Ω will be interpreted as a region in the physical space occupied by the Δ -periodic composite solid in its reference configuration and $t \to q(\cdot,t)$ stands for a certain physical process related to this solid. We shall also assume that this process in every $\Delta(\mathbf{z})$, $\mathbf{z} \in \Lambda_0$, is governed by the field equation derived from the principle of stationary action for the functional

$$\mathcal{A}(\mathbf{z}) = \iint_{t} \mathcal{Q}(\mathbf{y}, q(\mathbf{z} + \mathbf{y}, t), \nabla q(\mathbf{z} + \mathbf{y}, t), \dot{q}(\mathbf{z} + \mathbf{y}, t)) d\mathbf{y} dt$$
 (2)

where $d\mathbf{y} = dy_1 dy_2 dy_3$ and $\mathcal{L}(\mathbf{x}, q, \nabla q, \dot{q})$ is the known lagrangian function which is a Δ -periodic function of argument $\mathbf{x} \in E^3$; hence $\mathcal{L}(\mathbf{z} + \mathbf{y}, \cdot) = \mathcal{L}(\mathbf{y}, \cdot)$ for every $\mathbf{z} \in \Lambda$. It follows that the governing equations of the problem under consideration are assumed to have the well known form

$$\nabla \cdot \frac{\partial \mathcal{L}}{\partial \nabla q} + \frac{\partial}{\partial t} \frac{\partial \mathcal{L}}{\partial \dot{q}} - \frac{\partial \mathcal{L}}{\partial q} = 0$$

In periodic composite structures met in physical problems $\mathcal L$ is piecewise constant but highly oscillating and hence non-continuous function of argument $\mathbf x$. That is why the direct application of the aforementioned equation (together with the jump conditions on the interfaces between composite components) to the investigation of special problems is not advisable mainly from the computational viewpoint. The problem we are to solve is how to formulate approximate mathematical models for the analysis of these problems. To this end we begin with the formation of what will be called a discrete model i.e., a model governed by a system of ordinary differential equations for certain time dependent functions as the basic unknowns. The first step in the formation of discrete models of a periodic composite medium consists of the choice of the basic cell Δ and a Δ -periodic simplicial subdivision of Δ into simplexes T^e . Every simplex $T^e(\mathbf z)$, $\mathbf z \in \Lambda_0$, $e = 1, \dots, E$, will be treated

as a certain C^0 -finite element of the medium. Hence unknown field $q(\cdot,t)$, which is continuous and piecewise smooth for every t, will be approximated by a function $q_h(\cdot,t)$ which is continuous and linear in every $T^e(\mathbf{z})$, $\mathbf{z} \in \Lambda_0$. Following the line of FEM discretization, cf. [17], we shall introduce the Δ -periodic interpolation functions $\phi_a(\mathbf{x})$ which are continuous, linear in every \overline{T}^e , and satisfy conditions

$$\phi_a(\mathbf{p}_A^b) = \delta_a^b$$

for every a=1,...,n and every $(b,A)\in I$. Setting $q^a(\mathbf{z},t):=q(\mathbf{p}_0^a(\mathbf{z}),t)$, $\mathbf{z}\in\Lambda$, we conclude that the approximation $q_h(\cdot,t)$ of $q(\cdot,t)$ in every simplex $T^e(\mathbf{z})$, $\mathbf{z}\in\Lambda_0$, can be written in the form

$$q_h(\mathbf{z} + \mathbf{y}, t) = \sum \phi_a(\mathbf{y}) q^a(\mathbf{z} + \mathbf{d}_A, t), \quad \mathbf{y} \in \overline{T}^e, \quad e = 1, ..., E$$
(3)

where the summation holds with respect to all $(a, A) \in I^e$. By means of the first from formulae (1) we can substitute

$$q^{a}(\mathbf{z} + \mathbf{d}_{A}, t) = q^{a}(\mathbf{z}, t) + \Delta_{A}q^{a}(\mathbf{z}, t)$$
(4)

into (3). It follows that the field $q(\cdot,t)$ in every cell $\overline{\Delta}(\mathbf{z})$, $\mathbf{z} \in \Lambda_0$, can be approximated by a continuous piecewise linear function $q_h(\cdot,t)$ (linear in every $T^e(\mathbf{z})$, $e=1,\ldots,E$) which in every vertex $\mathbf{p}_A^a(\mathbf{z})$, $(a,A)\in I$ attains the value $q^a(\mathbf{z},t)+$ $+\Delta_A q^a(\mathbf{z},t)$. Applying to lagrangian \mathcal{L} the approximation $q(\mathbf{z}+\mathbf{y},t)\approx$ $\approx q_h(\mathbf{z}+\mathbf{y},t)$, for every $\mathbf{z}\in\Lambda_0$ we define

$$\mathcal{L}_{h}(q^{a}, \Delta_{A}q^{a}, \dot{q}^{a}) := \frac{1}{|\Delta|} \int_{\Delta} \mathcal{L}(y, q_{h}(z + y, t), \nabla q_{h}(z + y, t), \dot{q}_{h}(z + y, t),) dy$$

where $|\Delta| = mes\Delta$ and $q_h(\mathbf{z} + \mathbf{y}, t)$ is given by formulae (3) and (4). In this way for every $\mathbf{z} \in \Lambda_0$ we obtain from (2) the new action functional

$$\mathcal{A}_{h} = \int_{t_{0}}^{t} \mathcal{L}_{h}(q^{a}(\mathbf{z},t), \Delta_{A}q^{a}(\mathbf{z},t), \dot{q}^{a}(\mathbf{z},t), \Delta_{A}\dot{q}^{a}(\mathbf{z},t))dt$$
 (5)

Functions $q^a(\mathbf{z}, \cdot)$, a = 1,...,n, $\mathbf{z} \in \Lambda_0$, will be called the local variables because they determine the values of $q_h(\cdot,t)$ only at points $\mathbf{p}^a(\mathbf{z})$, $\mathbf{z} \in \Lambda_0$. Taking into account the results given in [19], from the principle of stationary action for \mathcal{A}_h we obtain the following system of equations for local variables $q^a(\mathbf{z},t)$, $\mathbf{z} \in \Lambda_0$

$$\overline{\Delta}_{A} \frac{\partial \mathcal{L}_{h}}{\partial \Delta_{A} q^{a}} - \frac{\partial \mathcal{L}_{h}}{\partial q^{a}} = -\frac{d}{dt} \left(\frac{\partial \mathcal{L}_{h}}{\partial \Delta_{A} \dot{q}^{a}} - \overline{\Delta}_{A} \frac{\partial \mathcal{L}_{h}}{\partial \Delta_{A} \dot{q}^{a}} \right), \quad a = 1, ..., n$$
 (6)

which holds for every $\mathbf{z} \in \Lambda_0$ and every time t.

The system of equations (6) represents what will be called *the discrete local variable model* of a periodic material system under consideration. The characteristic feature of this model is the finite difference form of the governing equations (6) with respect to the Bravais lattice Λ . Notice, that this system of equations is overdeterminated because it also containts functions $q^a(\mathbf{z},t)$ for $\mathbf{z} \in \partial \Lambda$, where $\partial \Lambda := (\Omega \cap \Lambda) \setminus \Lambda_0$. To obtain equations for the above extra unknowns we have to apply finite element approximation also in the near boundary layer $\overline{\Omega} \setminus \overline{\Omega}_0$ where $\overline{\Omega}_0 := \{\mathbf{x} \in \overline{\Delta(\mathbf{z})} : \mathbf{z} \in \Lambda_0\}$; this problem will be not discussed here.

Let us observe that if $\mathbf{p}_0^a \in \Delta$ for some $a \in \{1,...,n\}$ then (a,A) does not belong to I_0 and hence \mathcal{L}_h is independent on $\Delta_A q^a$ and $\Delta_A \dot{q}^a$. In this case the local variable q^a will be referred to as the internal local variable and equation (6) for this variable reduces to the form which does not involve finite differences.

It has to be remembered that the introduced Δ -periodic simplicial division of space (generated by the pertinent simplicial subdivision of cell Δ) has to lead to a certain accetable scheme of simplexes $T^e, e = 1, ..., E$, representing finite elements, cf. [17]. The maximum diameter h of simplexes $T^1, ..., T^E$ is a mesh parameter and $q_h(\cdot,t)$ is a finite element interpolant of $q(\cdot,t)$.

In order to obtain a discrete model of the heat transfer in a rigid composite conductor we shall apply results given in Appendix. For the sake of simplicity we shall assume that the composite medium is unbounded, the relaxation time τ is constant for all components of the composite and the heat generation can be neglected. We shall also assume that components of the medium are isotropic and we denote

$$W(\mathbf{x}, \boldsymbol{\vartheta}) = \frac{1}{2}c(\mathbf{x})(\boldsymbol{\vartheta})^2$$

$$V(\mathbf{x}, \nabla \mathcal{S}) = \frac{1}{2} k(\mathbf{x}) \nabla \mathcal{S} \cdot \nabla \mathcal{S}$$

where $\mathcal{G}(\cdot,t)$ is a modified temperature field and $c(\cdot)$, $k(\cdot)$ are Δ -periodic functions representing the specific heat and thermal conductivity, respectively. Hence formula (A4) given in Appendix yields

$$\mathcal{L} = \frac{1}{4\tau} W(\mathbf{x}, \boldsymbol{\vartheta}) + \tau W(\mathbf{x}, \dot{\boldsymbol{\vartheta}}) - V(\mathbf{x}, \nabla \boldsymbol{\vartheta})$$

The Δ -periodic simplicial division of E^3 leads to an approximation \mathcal{G}_h of \mathcal{G} in the form (3), where symbol q has to be replaced by \mathcal{G} . Let \mathcal{G}^0 be an arbitrary but fixed linear combination of $\mathcal{G}^1, \dots, \mathcal{G}^2$. Then

$$\mathcal{L}_{h} = \frac{1}{4\tau} W_{h} \left(\mathcal{G}^{b}, \Delta_{A} \mathcal{G}^{a} \right) + \tau W_{h} \left(\dot{\mathcal{G}}^{b}, \Delta_{A} \dot{\mathcal{G}}^{a} \right) - V_{h} \left(\mathcal{G}^{b} - \mathcal{G}^{0}, \Delta_{A} \mathcal{G}^{a} \right) \tag{7}$$

where V_h is the positive - definite symmetric quadratic form in arguments $\mathcal{G}^b,...,\mathcal{G}^0$, b=1,...,n-1 and $\Delta_A\mathcal{G}^a$, $(a,A)\in I_0$. Moreover, W_h is also the positive definite symmetric quadratic form given by

$$W_h \Big(\mathcal{G}^b, \Delta_A \mathcal{G}^a \Big) = \frac{1}{2} C_{ab} \mathcal{G}^a \mathcal{G}^b + C_{ab}^A \mathcal{G}^b \Delta_A \mathcal{G}^a + \frac{1}{2} C_{ab}^{AB} \Delta_A \mathcal{G}^a \Delta_B \mathcal{G}^b$$

Substituting (7) into (6) and bearing in mind that now $q^a = \mathcal{S}^a$, after some manipulations and introducing the finite difference operator

$$D_{ab}^{h} := C_{ab} + C_{ba}^{A} \Delta_{A} - C_{ab}^{A} \overline{\Delta}_{A} - C_{ab}^{AB} \overline{\Delta}_{A} \Delta_{B}$$

we obtain the system of equations

$$\overline{\Delta}_{A} \frac{\partial V_{h}}{\partial \Delta_{A} \mathcal{G}^{a}} - \frac{\partial V_{h}}{\partial \mathcal{G}^{a}} + D_{ab}^{h} \left(\frac{1}{4\tau} \mathcal{G}^{b} - \tau \ddot{\mathcal{G}}^{b} \right) = 0, \quad a = 1, ..., n$$
 (8)

for the local modified temperatures $\mathcal{G}^a(\mathbf{z},t)$ which approximate the are values of the modified temperature field $\mathcal{G}(\cdot,t)$ at the points $\mathbf{p}^a(\mathbf{z})$, $\mathbf{z} \in \Lambda$, a = 1,...,n. These points are vertexes in the Δ -periodic simplicial division of the space E^3 . Taking into account (A2) we derive from (8) the following discrete local variable model equations for the heat transfer in a periodic rigid conductor

$$\overline{\Delta}_{A} \frac{\partial V_{h}}{\partial \Delta_{A} \theta^{a}} - \frac{\partial V_{h}}{\partial \theta^{a}} - D_{ab}^{h} \left(\dot{\theta}^{b} + \tau \ddot{\theta}^{b} \right) = 0, \quad a = 1, ..., n$$

$$(9)$$

where $V_h = V_h (\theta^b - \theta^0, \Delta_A \theta^a)$, $(a, A) \in I_0$ is the known quadratic form, and θ^0 has the same meaning as θ^0 . The model equations (9) hold for every $\mathbf{z} \in \Lambda$ and represent the infinite system of finite difference equations for local temperatures $\theta^a(\mathbf{z},t)$, a=1,...,n, $\mathbf{z} \in \Lambda$, at nodal points $\mathbf{p}^a(\mathbf{z})$ which are vertexes of the simplicial Δ -periodic division of E^3 . Setting $\tau=0$ in (9) we obtain a discrete local variable model for the Fourier law of heat transfer. The accuracy of the obtained

discrete model depends on the mesh parameter h related to the simplicial Δ -periodic division of Δ into finite elements T^e [17].

3. Continuum models

Let $q^a(\cdot,t)$, a=1,...,n, be sufficiently smooth functions defined on Ω for every time t and assume that these functions, after restriction their domains to $\Lambda \cap \Omega$, coincide with the local variables $q^a(z,t)$, a=1,...,n, $z\in \Lambda$, of the discrete model. The passage from a discrete to a continuum model will be based on assumption that for every $\mathbf{x}\in \Omega$ and for an arbitrary vector \mathbf{d} , such that $|\mathbf{d}| \leq l$ where $l=\operatorname{diam} \Delta$, functions $q^a(\cdot,t)$ in every ball $B(\mathbf{x},l) \subset \Omega$ can be approximated by linear functions. Hence for every vector \mathbf{d} , $|\mathbf{d}| < l$, we obtain an approximation

$$q^{a}(x+d,t) = q^{a}(x,t) + d \cdot \nabla q^{a}(x,t) + O(l^{2})$$

where terms $O(l^2)$ in the subsequent analysis will be neglected. Hence the finite difference operators (1) will be approximated by differential operators

$$\Delta_A \cong \mathbf{d}_A \cdot \nabla, \qquad \overline{\Delta}_A \cong \mathbf{d}_A \cdot \nabla \tag{10}$$

For more general form of approximation see [20]. After rather lengthy calculations we can prove that setting

$$\widetilde{\mathcal{L}}\left(q^{a}, \nabla q^{a}, \dot{q}^{a}, \nabla \dot{q}^{a}\right) := \mathcal{L}_{h}\left(q^{a}, \mathbf{d}_{A} \cdot \nabla q^{a}, \dot{q}^{a}, \mathbf{d}_{A} \cdot \nabla \dot{q}^{a}\right)$$

where $(a, A) \in I_0$, from the finite difference model equations (6) we obtain

$$\nabla \cdot \frac{\partial \widetilde{\mathcal{L}}}{\partial \nabla q^{a}} - \frac{\partial \widetilde{\mathcal{L}}}{\partial q^{a}} = -\frac{\partial}{\partial t} \left(\frac{\partial \widetilde{\mathcal{L}}}{\partial \dot{q}^{a}} - \nabla \cdot \frac{\partial \widetilde{\mathcal{L}}}{\partial \nabla \dot{q}^{a}} \right), \quad a = 1, ..., n$$
(11)

The above equations are assumed to hold for every $\mathbf{x} \in \Omega$ and every time t and represent the system of differential equations for the fields $q^a(\cdot,t)$ defined in E^3 for every t. Similarly to the case of a discrete model, the fields q^a will be also referred to as the local variables. If $q^a(\mathbf{z},t)$ is an internal local variable then $\widetilde{\mathcal{L}}$ is independent of ∇q^a , $\nabla \dot{q}^a$ and equation (11) for an internal local variable q^a becomes an ordinary differential equation. Equations (11) for the local variables have constant coefficients and hence they represent a certain continuum averaged model of the periodic medium. This model will be referred to as the continuum local variable model of a periodic material system.

In order to apply the aforementioned model to the heat transfer in a periodic unbounded composite medium, instead of functions V_h and W_h we have to introduce functions

$$\begin{split} \widetilde{V} \Big(\mathcal{G}^b - \mathcal{G}^0, \nabla \, \mathcal{G}^a \Big) &:= V_h \Big(\mathcal{G}^b - \mathcal{G}^0, \mathbf{d}_A \cdot \nabla \, \mathcal{G}^a \Big) \\ \\ \widetilde{W} \Big(\mathcal{G}^b, \nabla \, \mathcal{G}^a \Big) &:= \frac{1}{2} \, C_{ab} \mathcal{G}^a \mathcal{G}^b + C_{ab}^A \mathcal{G}^b \mathbf{d}_A \cdot \nabla \, \mathcal{G}^a + \frac{1}{2} \, C_{ab}^{AB} \mathbf{d}_A \cdot \nabla \, \mathcal{G}^a \, \mathbf{d}_B \cdot \nabla \, \mathcal{G}^b \end{split}$$

and assume that

$$\widetilde{\mathcal{L}} = \frac{1}{4\tau} \widetilde{W} + \tau \widetilde{W} - \widetilde{V}$$

In this case, after defining the differential operator

$$\widetilde{D}_{ab} := C_{ab} + \left(C_{ba}^A - C_{ab}^A\right)\mathbf{d}_A \cdot \nabla - C_{ab}^{AB}\left(\mathbf{d}_A \otimes \mathbf{d}_B\right) : \left(\nabla \otimes \nabla\right)$$

we shall obtain from (11) the system of equations

$$\nabla \cdot \frac{\partial \widetilde{V}}{\partial \nabla \mathcal{G}^{a}} - \frac{\partial \widetilde{V}}{\partial \mathcal{G}^{a}} - \widetilde{D}_{ab} \left(\frac{1}{4\tau} \mathcal{G}^{b} - \tau \ddot{\mathcal{G}}^{b} \right) = 0, \quad a = 1, ..., n$$
 (12)

for the modified temperature fields $\theta^a(\cdot,t)$ as local variables. Taking into account (A2) and setting $\widetilde{V} = \widetilde{V}(\theta^b - \theta^0, \nabla \theta^a)$, we derive from (12) the following system of equations for fields $\theta^a(\cdot)$, which will be called local temperatures

$$\nabla \cdot \frac{\partial \widetilde{V}}{\partial \theta^{a}} - \frac{\partial \widetilde{V}}{\partial \nabla \theta^{a}} - \widetilde{D}_{ab} \left(\dot{\theta}^{b} + \tau \ddot{\theta}^{b} \right) = 0, \quad a = 1, ..., n$$
 (13)

The above equations represent a continuum local variable model for the heat transfer in a periodic rigid conductor. For $\tau = 0$ we obtain from (13) the averaged continuum model of the heat transfer in the framework of the Fourier constitutive law.

It has to be emphasized that the proposed continuum averaged model has a physical sense only if there exist sufficiently smooth functions $q^a(\cdot,t)$, a=1,...,n, such that the finite differences $\Delta_A q^a(\mathbf{z},t)$, $\overline{\Delta}_A q^a(\mathbf{z},t)$, $\mathbf{z} \in \Lambda_0$, $(a,A) \in I_0$, can be approximated, with a sufficient accuracies, by the derivatives $\mathbf{d}_A \cdot \nabla q^a(\mathbf{z},t)$. This condition restricts the scope of physical applications of continuum models to problems in which the local variables representing the basic physical fields (like temperature or displacement field) and their derivatives in every ball in Ω with a radius $l = max|\mathbf{d}_A|$, A = 1,...,N, can be approximated by linear functions (cf. also [20] for more general form of approximation).

4. Concluding remarks

At the end of the paper we summarize some new results and informations on the mathematical modelling of non stationary processes in micro periodic material system. The proposed line of modelling is based on the concept of what was called the local variable and hence the resulting models are referred to as the local variable models.

- 1º In order to investigate non-stationary processes in thermomechanics of microperiodic material systems (composite solids and lattice structures) two new mathematical models of these systems have been proposed. The discrete local variable model, represented by the finite difference equations (6), makes it possible to describe wave propagation phenomena in which a typical wavelength of temperature-deformation pattern is of an order of the periods of inhomogeneity (high-frequency wave propagation). The scope of applications of the local variable model, with governing equations (11), is restricted to the analysis of low-frequency wave propagation problems in which the typical wavelength of a macroscopic deformation-temperature pattern is large when compared to the periods of inhomogeneity.
- 20 The discrete local variable models can be formulated on different levels of accuracy which depends on the mesh parameter h. So far, the direct applications of these models have been confined to the analysis of some simple special problems related to the wave propagation in periodic lattice-type structures and composite materials [19, 20, 23]. However, the main role of the discrete local variable models is that they constitute the background for the formulation of new continuum models. The formal passage from discrete to continuum models takes into account the fact that the discrete models, away from the solid boundaries, are represented by the finite difference equations.
- 3º The local variable continuum models can be used only to the analysis of low frequency wave propagation problems. These models have been successfully applied to investigations of some special problems of heat conduction and elastodynamic behaviour of periodic materials and structures [20, 23].
- 4° It was shown by the direct analysis of some special wave propagation problems that for a sufficiently small wave number the solutions derived on the basis of the continuum local variable models nearly coincide with those resulting from the discrete local variable models [23].
- 5^0 In contrast to homogenization, the proposed local variable continuum models describe the effect of the microstructure size on the overall behaviour of a periodic medium. Hence these models can be successfully applied to the dispersion analysis in micro-periodic elastic media. The main difference between the local variable continuum models and models based on tolerance averaging is that the former can be formulated on different levels of accuracy determined by the mesh parameter h.
- 6° So far, the applications of both discrete and continuum models have been restricted to the linear problems. However, equations (6) and (11) representing

the above models also describe non linear problems provided that these problems can be derived from the principle of stationary action.

7º The main drawback of the proposed approach to the modelling of micro-periodic material systems lies in a large number of local variables which may be necessary in order to obtain the proper description of the problem under consideration. This situation takes place in many problems met in engineering and solid state physics. Thus, the crucial problem in applying local variables lies in the development of computational methods which may reduce the number of unknowns. This can be done, for example, by taking into account the presence of the small parameter (microstructure length) in the local variable model equations, cf. [15].

For particulars related to the application of the local variable models the reader is referred to [18-20, 23] and to forthcoming papers on this subject. So far, the obtained results in formulation and applications of local variable models, outlined in this report, constitute only the first step in investigations of periodic media, which has to be verified, confirmed and supplemented by subsequent researches on this field.

Appendix

The heat transfer in a rigid conductor is described by the energy balance law and heat transfer constitutive equation. Denoting by \mathbf{q} the heat flux vector, by k and c the modulus of thermal conductivity (for an isotropic material) and the specific heat (per unit volume), respectively, by f the heat generation and by τ the relaxation time (in the Cattaneo sense), the aforementioned equations have the well known form:

$$\nabla \cdot \mathbf{q} + c \dot{\theta} = f$$
$$\mathbf{q} + \tau \dot{\mathbf{q}} = -k \nabla \theta$$

which leads to the Cattaneo-type heat transfer equation

$$\nabla \cdot (k\nabla \theta) - c(\dot{\theta} + \tau \dot{\theta}) = -(f + \tau \dot{f}) \tag{A1}$$

For $\tau = 0$ equation (A1) reduces to the well known Fourier heat transfer equation. In this Appendix we are going to show that the above equation (as well as the Fourier heat transfer equation) can be obtained from the principle of stationary action. To this end we introduce a modified temperature field

$$\theta = \theta \exp \frac{t}{2\tau} \tag{A2}$$

and introduce the action functional

$$A = \int_{t_1}^{t_1} \int_{\Omega} \mathcal{L}(\theta, \dot{\theta}, \nabla \theta) d\mathbf{x} dt$$
 (A3)

with

$$\mathcal{L} = \frac{1}{8} \frac{c}{\tau} (\vartheta)^2 + \frac{1}{2} \pi c (\dot{\vartheta})^2 - \frac{1}{2} k \nabla \vartheta \cdot \nabla \vartheta - (f + \dot{\tau}) \vartheta \exp \frac{t}{2\tau}$$
 (A4)

In this case the Euler-Lagrange equation has the form

$$\frac{1}{4}\frac{c}{\tau}\vartheta - \tau c\,\ddot{\vartheta} + k\nabla \cdot \nabla\vartheta = \left(f + \tau \dot{f}\right)\exp\frac{t}{2\tau} \tag{A5}$$

Substituting the right-hand side of (A2) into (A5) we obtain (A1). The finial conclusions is that the action functional for the linearized heat transfer problems can be assumed in the form given by (A3) and (A4) where ϑ is defined by (A2). It has to be emphasised that this line of approach can be also applied to the heat-transfer problems governed by the Fourier constitutive heat transfer law leading to the parabolic-type equation. In this case the relaxation time τ has to be interpreted as a formal small parameter which in the final form of model equations is assumed as equal to zero.

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