Interaction and Multiscale Mechanics, Vol. 3, No. 1 (2010) 1-22
DOI: http://dx.doi.org/10.12989/imm.2010.3.1.001

Collection of dynamical systems with dimensional reduction as a multiscale method of modelling for mechanics of materials

Jarosław Kaczmarek*

Institute of Fluid-Flow Machinery, Polish Academy of Sciences, 80-952 Gdańsk, ul. J.Fiszera 14, Poland

(Received December 1, 2009, Accepted February 19, 2010)

Abstract. In this paper one introduces a method of multiscale modelling called collection of dynamical systems with dimensional reduction. The method is suggested to be an appropriate approach to theoretical modelling of phenomena in mechanics of materials having in mind especially dynamics of processes. Within this method one formalizes scale of averaging of processes during modelling. To this end a collection of dynamical systems is distinguished within an elementary dynamical system. One introduces a dimensional reduction procedure which is designed to be a method of transition between various scales. In order to consider continuum models as obtained by means of the dimensional reduction one introduces continuum with finite-dimensional fields. Owing to geometrical elements associated with the elementary dynamical system we can formalize scale of averaging within continuum mechanics approach. In general presented here approach is viewed as a continuation of the rational mechanics.

Keywords: mechanics of materials; multiscale modelling.

1. Introduction

In last years we observe a tendency in engineering towards decreasing of scale where design of devices is carried out. The most outstanding example of this tendency is promotion of nanotechnology. Frequently, design of nanotechnological devices has to be based on experience of scientists which realize experiments in corresponding field. This is so since quality of design depends on quality of theory which describes behavior of designed objects. In particular experience of scientific workers can be interpreted as a kind of theory.

Above discussion suggests that role of theory in small scale should increase with increasing of activity of engineering sciences in small scale. Moreover, in order to obtain systematical design methods in small scale we should have at our disposal theoretical models and possibility of numerical simulations which are reliable and have well defined range of validity.

In case of mechanics of materials which should be an area of activity for small scale engineering we have many theoretical models. However, they have not usually well defined range of validity. In such a case automatization of design process necessary for engineering is rather impossible. This

* Professor, E-mail: jarekk@imp.gda.pl

induces a necessity of more advanced formalization of descriptions related to smaller scales in order to enable cooperation of models corresponding to various ranges of validity.

First important property of theoretical models which should be formalized is scale of averaging of physical properties applied in modelling. We observe in literature various models related also to small scale. However, usually such a scale is not formalized or even precisely declared. Consequently, one postulates to formalize scale of averaging in order to introduce by this more precise physical interpretation of models.

Physical content of models is of key importance especially for small scale phenomena where complexity of physical processes increases. Frequently, we would like to support our considerations by interpretations related directly to atomic scale. In this area we apply usually molecular dynamics method. At larger scale we use various kinds of continuum descriptions. Consequently, a unification of such theoretical descriptions seems to be a natural need.

The last statement suggests that we should search a multiscale approach in order to discuss in a consistent way various phenomena in materials. Decreasing of scale leads to increasing role of dynamics within material. Consequently, we should introduce a description which is based on dynamical systems with a possibility of transition between various scales.

In this paper we introduce a multiscale method of modelling called here the collection of dynamical systems with dimensional reduction which try to take into account all discussed above needs for theoretical modelling.

Various engineering applications have led to necessity of formalization of continuum mechanics in the past. Let us mention the rational mechanics approach which provided clear system of assumptions for continuum mechanics (Truesdell and Noll 1965, Gurtin and Williams 1967, Truesdell 1972, Williams 1972, Noll 1973). This direction has been developed towards a theory of constitutive equations. Then, necessity of considering smaller scale descriptions becomes important. As a result methods of micromechanics representing a multiscale approach has been intensively developed. Let us mention here (Mura 1982, Nemat-Nasser and Hori 1999, Chen and Mehraeen 2005, Zhang *et al*. 2006) for instance.

Discussed in this paper approach can be viewed as a continuation of formalization of mechanics in general which was introduced by concepts of the rational mechanics. The aim of this continuation is to integrate discrete, especially molecular dynamics simulations with various continuum models, develop constitutive equations theory by better description of dynamical processes, and expand ability for better determination of range of validity of equations. In the last case we tend towards creation of situation when numerical simulations could be more stable in applications by ability to transition between various descriptions. All these ends have relations to formalization of scale of averaging of physical processes in modelling.

At this moment we should perhaps discuss whether this paper is a rigorous mathematical paper or a paper which uses mathematics for attaining some engineering aims. Rigorous formulation is characterized by ability to discuss theorems together with their proofs. They need a precise set of assumptions. On the other hand we can model a reality with the aid of mathematics. Then, we always apply an approximation of reality. Consequently, having in mind this approximation we do not use so precise set of assumptions in order to have at our disposal a flexibility in doing the approximation.

The aim of this paper is to indicate a method of approximation of realty associated with processes in materials accentuating to more degree dynamics of such processes. It is expected that improving of this approximation will rest on introducing gradually more precise assumptions which will be

manifested by development of more rigorous mathematical description and more reliable numerical simulations.

In the first section we distinguish the collection of dynamical systems within an elementary dynamical system. Such a concept creates basis for determination of the dimensional reduction procedure. In the next section one introduces continuum with finite dimensional fields. Then, continuum models can be obtained by means of the dimensional reduction procedure. One discusses premises for postulating forms of skeletal dynamical systems. Role of nanoscale models in mechanics of materials is accentuated.

2. Collection of dynamical systems with dimensional reduction

2.1 Collection of dynamical systems

In order to do a step toward formalization of scale of averaging in modelling we introduce a method of division of a dynamical system into subsystems. We have intention to model a real physical system. Therefore our method is carried out in a way which allows us to consider the most general physical laws such as the energy conservation law and the mass conservation law.

Let us introduce a dynamical system purposed to describe phenomena on the most elementary level. Such a system called here the elementary dynamical system (*EDS*) is given in a general form

$$\dot{\varphi} = L(\varphi, \mathbf{f}) \tag{1}$$

where $\varphi \in \mathcal{M}_\varphi$ is the variable of this system, $\mathcal{M}_\varphi$ is a space of admissible values of this variable, $\mathbf{f} \in \mathcal{F}$ represents external interactions acting on this system and $\mathcal{F}$ stands for space of admissible values of $\mathbf{f}$.

Form of external interactions is not always expressed in relative simple form given by $\mathbf{f}$. Sometimes, they appear as interactions with other dynamical systems. Therefore, let us introduce also an extended dynamical system

$$\dot{\varphi}^r = L(\varphi^r, \mathbf{f}^r) \tag{2}$$

where $\varphi^r = \{\varphi, \varphi^e\} \in \mathcal{M}_{\varphi r}$ and $\mathbf{f}^r = \{\mathbf{f}, \mathbf{f}^e\} \in \mathcal{F}_r$. In other words the dynamical system (1) is a part of that one defined by (2) and can be viewed as a particular case of (2). As a result an external dynamical system with variable φ^e can be additionally distinguished as a model of external interactions acting on *EDS*. This gives a possibility of discussing larger class of interactions of (1) with an external world.

The dynamical system (1) describes more elementary processes and its form is, by assumption, the most complex. We tend towards simplifications of this system. To this end we introduce a partition of (1) onto a collection of P dynamical systems. This is carried out by partition of variable $\varphi = \{\varphi_h\}$, $h \in I_P = \{1, 2, \ldots, P\}$.

In order to use this partition for further simplifications we introduce also additional notations, sets and mappings. Let $\Pi_h \mathcal{M}_h$ be Cartesian product of sets $\mathcal{M}_h$, where $\mathcal{M}_h$ stands for set of admissible values of φ_h. Let us introduce $\mathcal{M}_\Pi \subset \Pi_h \mathcal{M}_h$ as a subset of the Cartesian product. Then, $\mathcal{M}_\Pi$ consists of $\varphi = \{\varphi_h\}$ which are possible solutions of the Eq. (1) or (2). We consider also a general projection π_h of various objects of the whole dynamical system into h-th subsystem.

Let us distinguish also a collection of dynamical systems for the extended system and a set of indexes I_R related to them. Then, $I_R = I_P \cup I_E, I_P \cap I_E = \varnothing$, where I_P is related to (1) and $I_E = I_R - I_P$ is connected with the external system. Furthermore we distinguish a group of dynamical subsystems $I_G \subset I_P$ by selection of corresponding indexes. Then, $I_O = I_R - I_G$ represents indexes defining external with respect to I_G dynamical subsystems within (2).

New simplified equations have to be based on balance of mass and energy equations as the most fundamental physical laws for mechanics of materials. In order to create such equations for the collection of dynamical systems we should have at our disposal a set of additional notions making possible to formulate them. Therefore we introduce the following assumptions which represent general properties of the collection of dynamical systems distinguished within the elementary dynamical system:

1. Subsystems are distinguished by determination of groups of variables $\varphi_h = \{\varphi_{h\alpha}\}$ s, where $\alpha \in I_{Ah}, I_{Ah}$ is a finite set related to separate h-th subsystem and $h \subset I_P$.
2. There exists a function $\overline{m}_h(\varphi_h) = \{m_{h1}, \ldots, m_{h\beta_h}\}$ which assigns a set of masses for h-th subsystem. The total mass of the system is $m_h = \Sigma_i m_{hi}$. We have also that $\Sigma_h \beta_h = N$, where N is the total number of masses. Then, the functions $\tilde{m} : \mathcal{M}_\Pi \to R^P$ with property $\pi_h \circ \tilde{m}(\{\varphi_h\}) = m_h$ and $m : \mathcal{M}_\Pi \to R, m(\{\varphi_h\}) = \Sigma m_h$ determine the total mass related to each subsystem and the total mass related to (1) respectively.
3. There exists a function $\tilde{E} : \mathcal{M}_\Pi \to R^P, \pi_h \circ \tilde{E}(\{\varphi_h\}) = E_h$ which assigns a value of energy to each of subsystems and $E : \mathcal{M}_\Pi \to R, E(\{\varphi_h\}) = \Sigma_h E_h$ determines the total energy related to (1).
4. There exists a family of mappings $J_{ij} : \mathcal{M}_\Pi \to R, i,j \in I_P, J_{ij}(\{\varphi_h\}) = J_{ij}$ called flux of mass from j-th subsystem to i-th subsystem and $J_{ij} + J_{ji} = 0$, $J_{ii} = 0$.
5. There exists a family of mappings $W_{ij} : \mathcal{M}_\Pi \to R, i,j \in I_P, W_{ij}(\{\varphi_h\}) = W_{ij}$ called flux of energy from j-th subsystem to i-th subsystem and $W_{ij} + W_{ji} = 0$, $W_{ii} = 0$.
6. Source of mass is determined by the function $c : \mathcal{M}_\Pi \to R^P, c(\{\varphi_h\}) = \{c_i\}$. Then, $c_i = \pi_i \circ c(\{\varphi_h\})$ can be considered for each subsystem of the whole system and stands for source of mass in i-th subsystem.
7. Source of energy is determined by the function $R : \mathcal{M}_\Pi \to R^P, R(\{\varphi_h\}) = \{R_i\}$. Then, $R_i = \pi_i \circ R(\{\varphi_h\})$ can be considered for each subsystem of the whole system and stands for source of energy in i-th subsystem.
8. Geometrical objects can be assigned to each subsystem. This is carried out with the help of mappings $G_x : \mathcal{M}_\Pi \to E_e^P$, $G_L : \mathcal{M}_\Pi \to (2^{E_e})^P$, $G_S : \mathcal{M}_\Pi \to (2^{E_e})^P$, $G_V : \mathcal{M}_\Pi \to (2^{E_e})^P$, where E_e is the Euclidean space. The map G_x assigns some distinguished points to subsystems, G_L introduces one-dimensional, G_S two-dimensional, G_V three-dimensional geometrical objects considered as subsets of E_e and accompanied by distinguished subsystems.

All discussed above assumptions and functions can also be introduced for the extended dynamical system (2).

With the help of above assumptions we are able to carry out analysis of interchange of mass between subsystems as well as to consider possible sources of mass which appear within subsystems. Then, we are able also to express the balance of mass equation for collection of dynamical systems in the following form

$$\sum_{i \in I_G} (\dot{m}_i - c_i) + \sum_{i,j \in I_G} J_{ij} + \sum_{i \in I_G, j \in I_O} (J_{ij} + J_{ji}) + \sum_{i,j \in I_O} J_{ij} + \sum_{i \in I_O} (\dot{m}_i - c_i) = 0 \tag{3}$$

where quantities m_i, c_i and J_{ij} are mass, production of mass, and efflux of mass introduced in accordance with previously discussed assumptions related to subsystems.

Sum of masses interchanged between subsystems within I_G without any interchange with an external subsystems is equal to zero. Thus, we have $\Sigma_{i,j \in I_G} J_{ij} = 0$. As a result we can express the balance of mass equation connected with group of subsystems represented by I_G with the help of formula

$$\sum_{i \in I_G} \left(\dot{m}_i - c_i + \sum_{j \in I_O} J_{ij} \right) = 0 \tag{4}$$

The terms J_{ij} describing interchange of mass with external system I_O appear in the Eq. (4). Then, the Eq. (4) is not entirely determined. Therefore we should introduce additional conditions

$$J_{ij} = \bar{J}_{ij}, j \in I_O \tag{5}$$

Form of $\bar{J}_{ij}$ should be postulated by a kind of constitutive equations.

The balance of energy equation has similar structure as the balance of mass equation and is given by

$$\sum_{i \in I_G} (\dot{E}_i - R_i) + \sum_{i \in I_G, j \in I_O} (W_{ij} + W_{ji}) + \sum_{i \in I_O} (\dot{E}_i - R_i) = 0 \tag{6}$$

The balance of energy equation for group of subsystems I_G interacting with groups of subsystems I_O, is given by

$$\sum_{i \in I_G} \left(\dot{E}_i - R_i + \sum_{j \in I_O} W_{ij} \right) = 0 \tag{7}$$

with additional conditions

$$W_{ij} = \overline{W}_{ij}, j \in I_O \tag{8}$$

Let us note that E_i and W_{ij} depend, in general, on state of the whole system in accordance with assumptions 3 and 5.

Eqs. (4), (5) and (7), (8) represent a general form of balance of mass and energy equations related to arbitrary distinguished group of subsystems within the collection of dynamical systems.

2.2 Dimensional reduction procedure

Transition from elementary dynamical system to the more simple one and describing more averaged physical properties, is realized by means of the dimensional reduction procedure. Consequently, it is assumed that the dimensional reduction is carried out in order to describe a chosen physical characteristics of a physical system and neglect some other ones which are viewed to be less important.

The first step of the dimensional reduction consists in option of new variables. Let $\mathbf{d} = \{\mathbf{d}_h\}$, $h \in I_R$ be a set of new variables which allows to describe, approximately, physical states represented by miscellaneous φ^r. Let $\overline{\mathcal{M}}$ stands for space of admissible values of $\mathbf{d}$. Then, $\mathbf{d}_h$ as component of $\mathbf{d}$ describes behaviour of h-th subsystem in a simplified form. Thereby, we have assumed that $dim\ \overline{\mathcal{M}}$ is considerably smaller than $dim\ \mathcal{M}_\varphi$.

Let $V_T = \{\varphi(t) : t \in T\}$, $V_{Tr} = \{\varphi^r(t) : t \in T\}$ and $\overline{V}_T = \{\mathbf{d}(t) : t \in T\}$. The first element of the dimensional reduction procedure is based on introduction of a mapping $\pi_T : V_{Tr} \to \overline{V}_T$ which assigns dimensionally reduced process $\mathbf{d}(t)$ to $\varphi^r(t)$ on the time interval T.

We introduce also $\mathcal{F}_T = \{\mathbf{f}(t), t \in T\}$ and $\overline{\mathcal{F}}_T = \{\bar{\mathbf{f}}(t), t \in T\}$ with mapping $\pi_{fT} : \mathcal{F}_T \to \overline{\mathcal{F}}_T$ which transform forces between elementary and reduced dynamical system.

We can discriminate parts $\mathbf{d}^p(t)$ and $\mathbf{d}^e(t)$ related to *EDS* and external dynamical system within the process $\mathbf{d}(t)$. Similar partition is possible for $\mathbf{f}(t)$ and $\bar{\mathbf{f}}(t)$ since they are considered here for extended system. Thus, we carry out the dimensional reduction for the extended dynamical system (2). However, our interest is related mainly to *EDS* given by (1). We will use φ instead of φ^r and $\mathbf{f}$ instead of $\mathbf{f}^r$ in what follows if it does not lead to mistake.

Let us introduce an operator $\mathcal{L} : \mathcal{M}_{\varphi r} \to \mathcal{F}_T$ constructed with the help of Eq. (2) as $\mathcal{L}(\varphi) = \tilde{\mathcal{L}}(\varphi, \dot{\varphi})$ where $\tilde{\mathcal{L}}$ is obtained from equivalent to (2) equation in the form $\tilde{\mathcal{L}}(\varphi, \dot{\varphi}) = \mathbf{f}^r$.

Then, the operator acting on processes $\mathcal{L}_T : V_{Tr} \to \overline{\mathcal{F}}_T$ is induced directly by means of $\mathcal{L}$ for each $t \in T$. Let us consider a diagram

$$\begin{array}{ccc} V_{Tr} & \xrightarrow{\mathcal{L}_T} & \mathcal{F}_T \\ \pi_T \downarrow & & \downarrow \pi_{fT} \\ \bar{V}_T & \xrightarrow{\bar{\mathcal{L}}_T} & \bar{\mathcal{F}}_T \end{array} \tag{9}$$

Accordingly, the initially introduced equation $\mathcal{L}_T(\varphi(t)) = \mathbf{f}(t)$ induces, owing to assumed mappings π_T and π_{fT}, a dimensionally reduced equation

$$\overline{\mathcal{L}}_T(\mathbf{d}(t)) = \bar{\mathbf{f}} \tag{10}$$

where $\overline{\mathcal{L}}_T = \pi_{fT} \circ \mathcal{L}_T \circ \pi_T^{-1}$. The operator $\overline{\mathcal{L}}_T$ can be determined with the help of solutions of Eq. (2) and postulated mappings π_T, π_{fT} for each value of $\mathbf{d}(t)$.

Let us note that we are not able to discuss structure of the operator $\overline{\mathcal{L}}_T$ in more details yet since too small number of assumptions is done at this moment.

In order to obtain more information on the operator $\overline{\mathcal{L}}_T$, especially in case of its interactions with the external dynamical system we distinguish groups of subsystems.

Let us discuss a similar diagram as above for a group of subsystems $I_G \subset I_P$. Then, we carry out the following decomposition $V_{Tr} = V_{TG} \times V_{TO} = \{\varphi(t) = \varphi_g(t), \{\varphi_l(t)\}, g \in I_G, l \in I_O\}$. The symbol "×" does not stand for Cartesian product operation but means a kind of relation in which φ_g, φ_l together create a solution of (2). We introduce also decomposition $\mathcal{F}_T = \mathcal{F}_{TG} \times F_{TO}$ in similar way.

Owing to above decompositions of domain and range, the operator $\mathcal{L}_T$ can be expressed as $\mathcal{L}_T = \mathcal{L}_{T(\varphi l)}(\{\varphi_g(t)\}) \times \mathcal{L}_{T(\varphi g)}(\{\varphi_l(t)\})$.

The operator $\mathcal{L}_{T(\varphi l)} : V_{TG} \to \mathcal{F}_{TG}$ depends on φ_l. Usually, not all $\varphi_l \in V_{TO}$ are necessary for determination $\mathcal{L}_{T(\varphi l)}$.

Let I_{GO} stands for a set of indexes which indicate variables necessary for determination of the operator $\mathcal{L}_{TG} := \mathcal{L}_{T(\varphi l)}$. Then, the operator $\mathcal{L}_T$ can be expressed in simplified form as $\mathcal{L}_{TG} \times T_C$, where $T_C = T_C(\varphi_g, \varphi_c)$, $c \in I_{GO}$. With the help of T_C we are able to introduce additional equations necessary for determination of φ_c defining form of $\mathcal{L}_{TG}$ within $\mathcal{L}_T$. The space V_{Tr} is reduced to $V_{TG} \times V_{TC}$ in this case.

The modified diagram (9) can be expressed now in the following form

$$\begin{array}{ccc} V_{TG} \times V_{TC} & \xrightarrow{\mathcal{L}_{TG} \times T_C} & \mathcal{F}_{TG} \times \mathcal{F}_{TC} \\ \pi_T \downarrow & & \downarrow \pi_{fT} \quad \downarrow \pi_{fTC} \\ \bar{V}_{TG} \times \bar{V}_{TC} & \xrightarrow{\bar{\mathcal{L}}_{TG} \times \bar{T}_C} & \bar{\mathcal{F}}_{TG} \times \bar{\mathcal{F}}_{TC} \end{array} \tag{11}$$

Accordingly, the dimensionally reduced equation describing evolution of group of subsystems is given by

$$\bar{\mathcal{L}}_{TG(\mathbf{d}_c)}(\{\mathbf{d}_g(t)\}) = \{\dot{\mathbf{f}}_g\} \tag{12}$$

$$\bar{T}_{Cc}(\mathbf{d}_g(t), \mathbf{d}_c(t)) = \{\mathcal{B}_c\} \tag{13}$$

Diagram (11) allows to solve Eqs. (12), (13) by means of solutions of Eq. (2) and postulated form of π_T, π_{fT}, π_{fTc}.

The first conclusion on form of the reduced dimensionally operator $\mathcal{L}_T$ is related to its part corresponding to external interactions. We can assume simplifications to T_C having by this a kind of boundary conditions.

Let us discuss other possibilities for determination of form of the operator $\mathcal{L}_T$. We can approximate this operator by predicting its general form. We can do this by means of postulating of the skeletal dynamical system *SDS*(**C**) which depends on family of constants **C**.

The role of *SDS* is to represent a larger class of systems which encompass approximately Eqs. (12), (13). Accordingly, the general form of *SDS* in case of (12), (13) can be expressed as $\{\bar{\mathcal{L}}_{TG}, \bar{T}_C\}(\mathbf{C})(d_g, d_c) = \{\dot{\mathbf{f}}, \mathcal{B}\}$. Then, with the help of an identification method, we determine $\mathbf{C} = \bar{\mathbf{C}}$ and as a result a reduced dynamical system $RDS = SDS(\bar{\mathbf{C}})$. Finally, *RDS* represents an approximation of Eqs. (12) and (13).

General structure of SDS should take into account fundamental laws in the first stage of formulation. In case of mechanics of materials such laws are expressed by balance of energy and balance of mass equations. They have been previously formulated for collection of dynamical systems.

We should devote some attention to discussion of kind of variables of the skeletal dynamical system. They need sometimes quite new ways of their application in order to approximate correctly processes at the elementary level.

Let $H_{dh} = \{\mathbf{d}_j : j \in I_h^a\}$ be a set of values of the variable $\mathbf{d}_j$ determined on a set of subsystems indexed by elements of a set I_h^a. I_h^a represents all subsystems which interact with the h-th one.

Let us introduce a function $a_h : H_{dh} \rightarrow V_{ah}$, where Vah is a linear space. Accordingly, the function a_h assigns an element of the linear space connected with h-th subsystem to a set of values of variables $\mathbf{d}_j$ related to interacting subsystems.

It is assumed furthermore that the function a_h can apply geometrical elements obtained by functions G_x, G_L, G_S and G_V assigned to subsystems. Therefore the function a_h can be called the function of kinematical dependence between subsystems.

We introduce also an additional concept of taking into account interactions between subsystems with the aid of geometrical elements. Let us consider a discrete set of variables $\{g_h\}$ related to

dimensionally reduced system. In order to describe interactions between different systems, a value of g_h type in a given point **X** can be useful. Consequently, we admit possibility of introducing this kind of quantity.

We assume that it is possible to introduce a transmission function $\mathcal{T}_x(\{g_h\}) = g_x$ which assigns a value of g_x in the point X to the set of values $\{g_h\}$. We assume also that by means of the transmission function no additional degrees of freedom is produced. Sometimes such a transformation allows to model interactions in more convenient way. This will be discussed also in next sections.

Masses related to dynamical system also undergo dimensional reduction. This is introduced by $\pi_M(\{m_{hi}\}) = \{M_{hp}\}$. Thus, M_{hp} are inertia coefficients related to h-th subsystem and can be present in the form of *SDS*.

Summing up these considerations we have obtained some general tools which can be applied in determination of the skeletal dynamical system. We have discussed possibility of application of geometrical elements assigned to subsystems in order to obtain better approximation of the elementary dynamical system and corresponding interactions. However, further premises, especially related to physical laws, should follow from more detailed specification also of the mappings π_T and π_{fT}. This will be discussed in the next section.

Let us discuss now a concept of an identification method of constants defining *RDS* from *SDS*(**C**). Let $C = \{\psi(t) : \psi \in \overline{\mathcal{M}}, t \in T\}$ be a space of continuous time processes in $\overline{\mathcal{M}}$ with a metric $\rho : C \times C \to \mathrm{R}_+ \cup \{0\}$. We can construct two kinds of processes. The first one is based on solution $\varphi(\varphi_0, \mathbf{f})(t)$ of Eq. (2) and have the form $\pi_T(\varphi(\varphi_0, \mathbf{f})(t))$. The second one is created by the skeletal dynamical system with assumed constants **C**. Thus, we have a solution of equations of *SDS* as $\mathbf{d}(\mathbf{C}, \pi(\varphi_0), \bar{\mathbf{f}})(t)$, where $\bar{\mathbf{f}}(t) = \pi_{fT}(\mathbf{f}(t))$. Let us consider the function

$$h(\varphi_0, \mathbf{f}) = \inf_{\mathbf{C} \in C_E} \rho(\mathbf{d}(\mathbf{C}, \pi(\varphi_0), \bar{\mathbf{f}})(t), \pi_T(\varphi(\varphi_0, \mathbf{f})(t))) \tag{14}$$

where C_E is an admissible set of constants for which energy of the system is well approximated. It means that for each $\mathbf{C} \in C_E$, $E(\varphi)(t) \approx E(\mathbf{d})(t)$.

Let $\mathbf{C}^*$ stands for constants for which the function h attains a minimum. Then, a satisfactory approximation should have the property that $\mathbf{C}^*$ exhibits a weak dependence on $\mathbf{d}_0$ and **f**. This, in turn, is connected with assumed functions π_T and *SDS* which reflect correctness of averaged modelling. Finally, we have to choose a constant $\overline{\mathbf{C}}$ from the set of $\mathbf{C}^*$ by an averaging method. Then

$$\overline{\mathbf{C}} = Av\{\mathbf{C}^* : \mathbf{C}^*(\mathbf{d}_0, \bar{\mathbf{f}}), \mathbf{d}_0 \in \overline{\mathcal{M}}, \bar{\mathbf{f}} \in \overline{\mathcal{F}})\} \tag{15}$$

where *Av* means the averaging operation. Obtained constants $\overline{\mathbf{C}}$ determine a dimensionally reduced dynamical system *RDS*($\overline{\mathbf{C}}$). By means of formulas (14), (15) an approximation and identification procedure denoted generally by *app* is established.

Summing up these considerations let us notice that the following general procedure is established: $\{EDS; DR\} \to RDS(\overline{\mathbf{C}})$. It means that the dimensional reduction procedure $DR = \{\pi_T, \pi_{fT}, SDS, app\}$ acting on an elementary dynamical system (2) leads to obtaining the reduced dynamical system *RDS*. Consequently, *RDS* is considered as describing approximately, evolution of our initially introduced physical system.

3. Dimensional reduction of SQ-type

3.1 Decomposition of variables of SQ-type

Considerable number of physical systems can be characterized by variables of two types. The first one is related to slowly varying and the second one to quickly varying processes. The most known example is a system with deformation and temperature.

Consequently, further premises for more precise method of determination of the skeletal dynamical system consists in specification of the mapping π_T taking into account mentioned above property. Consequently, let us introduce a special case of $\pi_T = \{\pi_{ST}, \pi_{QT}\}$ in which two parts related to slowly and quickly varying variables are discriminated. As a result $\mathbf{d}(t) = \pi_T(\varphi(t))$ can be expressed as $\mathbf{d} = \{\mathbf{d}_S, \mathbf{d}_Q\} = \{\pi_{ST}(\varphi), \pi_{QT}(\varphi)\}$.

Let us assume also that the elementary dynamical system describes evolution of classical point-like particles by the equations

$$\frac{d\mathbf{q}_i}{dt} = \mathbf{v}_i \tag{16}$$

$$m_i \frac{d\mathbf{v}_i}{dt} = -\frac{\partial V}{d\mathbf{q}_i} + \mathbf{f}_i \tag{17}$$

where $i \in I_N = \{1, 2, \cdots, N\}$, V is a potential energy and $\mathbf{f}_i$ is a force acting on i-th material point. Let $\mathbf{q} = \{\mathbf{q}_i\}$, $\mathbf{v} = \{\mathbf{v}_i\}$.

Let us take a set of time instants $t_0 < t_1 < \cdots < t_K$ which belong to the time interval $T = [t_0, t_0 + T]$, $t_K = t_0 + T$. By means of these instants we divide the time interval into the sum $T = \cup_k T_k$, $T_k = [t_{k-1}, t_K]$, $k = 1, \cdots, K$. Then, for each k we can calculate the value of $\tilde{\mathbf{q}}_k$ as

$$\tilde{\mathbf{q}}_k = \frac{1}{T_k} \int_{T_k} \mathbf{q}(t)\, dt \tag{18}$$

A value $\tilde{\mathbf{q}}_0 = \mathbf{q}(t_0)$ is assigned to $k = 0$. With the aid of sequence of values $\{\tilde{\mathbf{q}}_k\}$, $k \in I_K$ we can generate a function $\tilde{\mathbf{q}}(t) = I_q(\{\tilde{\mathbf{q}}_k\})$, where I_q is an approximation procedure. Now, we are able to decompose the variable $\mathbf{q}(t)$ into two summands

$$\mathbf{q}(t) = \tilde{\mathbf{q}}(t) + \delta\mathbf{q}(t) \tag{19}$$

Thus, $\tilde{\mathbf{q}}(t)$ represents the slowly varying part of $\mathbf{q}(t)$ and $\delta\mathbf{q}(t)$ its rapidly varying part.

The decomposition expressed by (19) and carried out with the aid of finite elements approximation corresponding to variable $\tilde{\mathbf{q}}(t)$ is given in the paper (Kaczmarek 2002).

Similar *SQ*-decomposition as above can be carried out for forces $\mathbf{f}$. To this end we calculate the following time averaged quantities

$$\tilde{\mathbf{f}}_k = \frac{1}{T_k} \int_{T_k} \mathbf{f}(t)\, dt \tag{20}$$

Then, we have $\tilde{\mathbf{f}}(t) = I_f(\tilde{\mathbf{f}}_k)$ with the help of an approximation procedure I_f. Finally, we obtain the decomposition

$$\mathbf{f}(t) = \tilde{\mathbf{f}}(t) + \delta\mathbf{f}(t) \tag{21}$$

Let us consider the balance of energy equation for our *EDS* given by (16), (17) for further discussion of premises on form of the skeletal dynamical system. We postulate this equation in the following form

$$\dot{E}_{HT} \equiv \sum_g \left[m_g \frac{d^2 \mathbf{q}_g}{dt^2} \dot{\mathbf{q}}_g + \frac{\partial V}{\partial \mathbf{q}_g}(\mathbf{q}_G, \mathbf{q}_C) \dot{\mathbf{q}}_g \right] + \sum_c \frac{\partial V}{\partial \mathbf{q}_c} \dot{\mathbf{q}}_c$$
$$= P_{TG}(\mathbf{f}_G) + P_{TC}(\mathbf{f}_C) \equiv P_T \tag{22}$$

Let us apply the decomposition (19) to the Eq. (22). We carry out summation with the aid of sets of indexes I_d and I_f. They are indexes of variables φ and $\mathbf{f}$ which are transformed into $\mathbf{d}$ and $\tilde{\mathbf{f}}$ correspondingly. Then, the balance of energy (22) can be rewritten as follows

$$\sum_{\mathbf{d}} \left[\sum_{g \in I_d} \left\{ m_g \frac{d^2(\tilde{\mathbf{q}}_g + \delta \mathbf{q}_g)}{dt^2} \ddot{\tilde{\mathbf{q}}}_g + \frac{\partial V}{\partial \tilde{\mathbf{q}}_g}(\mathbf{q}_G, \mathbf{q}_C) \dot{\tilde{\mathbf{q}}}_g \right.\right.$$
$$\left. + m_g \frac{d^2(\tilde{\mathbf{q}}_g + \delta \mathbf{q}_g)}{dt^2} \delta \dot{\mathbf{q}}_g + \frac{\partial V}{\partial \delta \mathbf{q}_g}(\mathbf{q}_G, \mathbf{q}_C) \delta \dot{\mathbf{q}}_g \right\} + \sum_{c(g) \in I_d} \left\{ \frac{\partial V}{\partial \tilde{\mathbf{q}}_c} \dot{\tilde{\mathbf{q}}}_c + \frac{\partial V}{\partial \delta \tilde{\mathbf{q}}_c} \delta \dot{\mathbf{q}}_c \right\} \Bigg]$$
$$- \sum_{\tilde{\mathbf{f}}} \sum_{g \in I_f} (\tilde{\mathbf{f}}_g + \delta \mathbf{f}_g) \dot{\tilde{\mathbf{q}}}_g - \sum_{\tilde{\mathbf{f}}} \sum_{g \in I_f} (\tilde{\mathbf{f}}_g + \delta \mathbf{f}_g) \delta \dot{\mathbf{q}}_g - P_{TC}(\mathbf{f}_C) = 0 \tag{23}$$

We would like to obtain some premises on a general form of the balance of energy equation for *SQ* decomposition. To this end let us consider some parts of the Eq. (23) in detail in order to separate segments corresponding to *SQ*-decomposition. Terms related to external interactions suggest distinguishing the following parts

$$\sum_{\tilde{\mathbf{f}}} \sum_{g \in I_f} (\tilde{\mathbf{f}}_g + \delta \mathbf{f}_g) \dot{\tilde{\mathbf{q}}}_g + \sum_{\tilde{\mathbf{f}}} \sum_{g \in I_f} (\tilde{\mathbf{f}}_g + \delta \mathbf{f}_g) \delta \dot{\mathbf{q}}_g \equiv R_S + R_Q \tag{24}$$

where R_S is equal to the first term on the left side of (24) and R_Q is equal to the second term on the left side of this equation. Let us note that such simple decomposition on R_S and R_Q suggests necessity of plotting these quantities with all variables subsequently considered since both are dependent on $\tilde{\mathbf{f}}_g$ and $\delta \mathbf{f}_g$.

The terms dependent on $\dot{\mathbf{q}}_c$ can be expressed as

$$\sum_c \left\{ \frac{\partial V}{\partial \tilde{\mathbf{q}}_c} \dot{\tilde{\mathbf{q}}}_c + \frac{\partial V}{\partial \delta \mathbf{q}_c} \delta \dot{\mathbf{q}}_c \right\} = W_{SGO} + W_{QGO} = W_{GO} \tag{25}$$

Then, W_{GO} represents interactions between G and O systems. W_{SGO} and W_{QGO} are related to slowly and quickly varying processes respectively.

Summing up concisely above discussion we notice that the first four terms in the Eq. (23) can be interpreted as time derivative of energy $\dot{E} = \dot{E}_S + \dot{E}_Q$ and could be also decomposed on S and Q parts. Furthermore, we have $R = R_S + R_Q$ and $W_{GO} = W_{SGO} + W_{QGO}$.

These considerations allow to postulate the general form of the balance of energy equation for group of dynamical subsystems (7) related to SQ decomposition in a modified form as

$$\sum_{h \in I_G} \left(\dot{E}_h - R_{Sh} - R_{Qh} + \sum_{m \in I_O} (W_{Shm} + W_{Qhm}) \right) = 0 \tag{26}$$

having also premises for postulating $\dot{E}_h$ from (23).

At this moment we have at our disposal the general form of balance of energy represented by (26) as an approximation of (22).

With the aid of previous discussion of variables for the reduced system we can assume their general form $\mathbf{d} = \{\mathbf{d}_S, \mathbf{d}_Q\} = \{\mathbf{d}_{SC}, \mathbf{d}_{S\xi}, \mathbf{d}_{SV}, \mathbf{d}_{QC}, \mathbf{d}_{Q\theta}, \mathbf{d}_{QV}\}$, where $\mathbf{d}_{SC}$ and $\mathbf{d}_{QC}$ have configurational character, $\mathbf{d}_{SV}$ and $\mathbf{d}_{QV}$ are related to generalized velocities and the remaining ones are rather viewed as a kind of internal state variables. We introduce furthermore additional notations $\mathbf{d}_{SC} = \alpha$, $\mathbf{d}_{S\xi} = \xi$, $\mathbf{d}_{SV} = \beta$, $\mathbf{d}_{QC} = \gamma$, $\mathbf{d}_{Q\theta} = \theta$, $\mathbf{d}_{QV} = \delta$ in what follows.

We introduce a convention in using of indexes. Thus, g, h are related to a considered subsystem and do not undergo summation convention, i, j, k, m, n are applied usually for subsystems interacting with g, h ones, p, q, r are connected with components of α, β, $\cdots$ variables.

Let us introduce the following general form of energy of the h-th subsystem $E_h = M_h e_h + \mathcal{T}_h$. We introduce furthermore the property $\dot{m}_h = 0$ or equivalently $\dot{M}_h = 0$. It means that $c_h = 0$ and $J_{hm} = 0$ are also assumed. Consequently, owing to this assumption $\dot{E}_h = \dot{M}_h e_h + M_h \dot{e}_h + \dot{\mathcal{T}}_h = M_h \dot{e}_h + \dot{\mathcal{T}}_h$ undergoes simplification.

Let us discuss e_h in the following form

$$e_h = V_{Sh} + V_{Qh} \tag{27}$$

where

$$V_{Sh} = C_{Sh\mu}\, \Phi_{Sh\mu}(\alpha_h, a_h) \tag{28}$$

$$V_{Qh} = C_{Qh\nu}\, \Phi_{Qh\nu}(\gamma_h, b_h) \tag{29}$$

Furthermore

$$\mathcal{T}_h = \mathcal{T}_h(\beta_h, \dot{a}_h) \tag{30}$$

where $\Phi_{Sh\mu}(0\ 0) = 0$, $\Phi_{Qh\nu}(0\ 0) = 0$, $\mathcal{T}_h(0\ 0) = 0$. These assumptions bring about energy equal to zero for such values of variables. $\mathcal{T}_h$ represents a kinetic energy term. $C_{Sh\mu}$ and $C_{Qh\nu}$ are considered to be constants at this moment. In the next stage of considerations they will depend on introduced variables.

Let us calculate $\dot{\mathcal{T}}_h$. To this end we assume that $\dfrac{\partial \mathcal{T}_h}{\partial \beta_{hp}} \approx \dfrac{\partial^2 \mathcal{T}_h}{\partial \beta_{hp} \partial \beta_{hq}}(0)\beta_{hq}$, $\dfrac{\partial \mathcal{T}_h}{\partial \dot{a}_h} \approx \dfrac{\partial^2 \mathcal{T}_h}{\partial \dot{a}_h^2}(0)\dot{a}_h$ using Taylor expansion of $\mathcal{T}_h$. Then we have

$$\dot{\mathcal{T}}_h = \frac{\partial^2 \mathcal{T}_h}{\partial \beta_{hp} \partial \beta_{hq}}(0)\beta_{hq}\dot{\beta}_{hp} + \frac{\partial^2 \mathcal{T}_h}{\partial \dot{a}_h}(0)\frac{\partial \dot{a}_h}{\partial \dot{\alpha}_{jp}}\frac{\partial \ddot{a}_h}{\partial \ddot{\alpha}_{kq}}\dot{\alpha}_{jp}\ddot{\alpha}_{kq}$$

$$= M_{hpq}\beta_{hq}\dot{\beta}_{hp} + I_{hjqkr}\dot{\alpha}_{jq}\ddot{\alpha}_{kr} = (M_{hpq}\dot{\beta}_{hq})\dot{\alpha}_{hp} + (I_{hjqkr}\ddot{\alpha}_{kr})\dot{\alpha}_{jq} \tag{31}$$

Let us postulate particular forms of $R_{Sh} = \bar{f}_{Shq}\dot{\alpha}_{hq}$ and $\overline{W}_{Shm} = -\bar{f}_{Shmq}\dot{\alpha}_{mq}$. Then, the balance of energy (26) can be expressed as

$$\sum_{h\in I_G}\Bigg\{M_h\Big[C_{Sh\mu}\frac{\partial\Phi_{Sh\mu}}{\partial\alpha_{hq}}\dot{\alpha}_{hq}+C_{Sh\mu}\frac{\partial\Phi_{Sh\mu}}{\partial a_h}\frac{\partial a_h}{\partial\alpha_{js}}\dot{\alpha}_{js}+C_{Qh\nu}\frac{\partial\Phi_{Qh\nu}}{\partial\gamma_h}\dot{\gamma}_h+C_{Qh\nu}\frac{\partial\Phi_{Qh\nu}}{\partial b_h}\frac{\partial b_h}{\partial\gamma_j}\dot{\gamma}_j\Big]+$$

$$+(M_{hpq}\dot{\beta}_{hp})\dot{\alpha}_{hq}+(I_{hjskr}\ddot{\alpha}_{kr})\dot{\alpha}_{js}-\bar{f}_{Shq}\dot{\alpha}_{hq}-R_{Qh}+\sum_{m\in I_O}(W_{Shm}+W_{Qhm})\Big\}=0 \tag{32}$$

and

$$W_{Shm}=\overline{W}_{Shm}\equiv-\bar{f}_{Shmq}\dot{\alpha}_{mq},\ W_{Qhm}=\overline{W}_{Qhm},h\in I_G,m\in I_O \tag{33}$$

We admit dependence of $C_{Sh\mu}, C_{Qh\nu}$ on all variables $\mathbf{d}_S$, $\mathbf{d}_Q$ considered in what follows.

Therefore, we also modify the Eq. (32). We assume that terms $C_{Sh\mu}\Phi_{Sh\mu}\neq 0$ and $\dot{C}_{Qh\nu}\Phi_{Qh\nu}\neq 0$. We take into account these terms in the balance of energy equation. Consequently, next transformed version of (32) is given by

$$\sum_{h\in I_G}\Bigg\{\Big[M_h(C_{Sh\mu}\frac{\partial\Phi_{Sh\mu}}{\partial\alpha_{hq}}+\sum_{h'}C_{Sh'\mu}\frac{\partial\Phi_{Sh'\mu}}{\partial a_{h'}}\frac{\partial a_{h'}}{\partial\alpha_{hq}}+M_{hpq}\dot{\beta}_{hp}+\sum_{h'}I_{h'hqkr}\ddot{\alpha}_{kr}-\bar{f}_{Shq}\Big]\dot{\alpha}_{hq}$$

$$+M_h\Big(C_{Qh\nu}\frac{\partial\Phi_{Qh\nu}}{\partial\gamma_h}\dot{\gamma}_h+C_{Qh\nu}\frac{\partial\Phi_{Qh\nu}}{\partial b_h}\frac{\partial b_h}{\partial\gamma_j}\dot{\gamma}_j+\dot{C}_{Sh\mu}\Phi_{Sh\mu}+\dot{C}_{Qh\nu}\Phi_{Qh\nu}\Big)-R_{Qh}+\sum_{m=I_O}W_{Qhm}\Big\}$$

$$+\sum_m\sum_{h'}I_{h'mqkr}\ddot{\alpha}_{kr}\dot{\alpha}_{mq}+\sum_{h\in I_G}\sum_{m\in I_O}\Big(\frac{\partial V_{Sh}}{\partial\alpha_{mq}}-\bar{f}_{Shmq}\Big)\dot{\alpha}_{mq}=0 \tag{34}$$

Let us assume that time processes are independent. Then we obtain the equations describing slowly varying processes

$$M_h\Big(C_{Sh\mu}\frac{\partial\Phi_{Sh\mu}}{\partial\alpha_{hq}}+\sum_{h'}C_{Sh'\mu}\frac{\partial\Phi_{Sh'\mu}}{\partial a_{h'}}\frac{\partial a_{h'}}{\partial\alpha_{hq}}\Big)-\bar{f}_{Shq}+M_{hpq}\dot{\beta}_{hp}+\sum_{h'}I_{h'hqkr}\ddot{\alpha}_{kr}=0 \tag{35}$$

with the additional condition

$$\sum_h\frac{\partial V_{Sh}}{\partial\alpha_{mq}}+\sum_h I_{hmkqr}\ddot{\alpha}_{kr}=\sum_h\bar{f}_{Shmq}=\bar{f}_{Smq},h\in I_G,m\in I_O \tag{36}$$

We introduce also the equation which expresses previously introduced notations in the form

$$\dot{\alpha}_{hq}=\beta_{hq},h\in I_G \tag{37}$$

The second time derivative of α_{kr} is present in the last term in (35). In particular indexes k can be found in I_O. This induces necessity of determination of evolution of such variables. As a result we consider also the following condition

$$\dot{\alpha}_{mq}=\bar{\beta}_{mq},m\in I_O \tag{38}$$

Eqs. (35) and (34) leads to the equation describing averaged evolution of quickly varying processes

$$M_h\Big(C_{Qh\nu}\frac{\partial\Phi_{Qh\nu}}{\partial\gamma_h}\dot{\gamma}_h+C_{Qh\nu}\frac{\partial\Phi_{Qh\nu}}{\partial b_h}\frac{\partial b_h}{\partial\gamma_j}\dot{\gamma}_j\Big)$$

$$+ \dot{C}_{Sh\mu}\Phi_{Sh\mu} + \dot{C}_{Qh\nu}\Phi_{Qh\nu}) - R_{Qh} + \sum_{m \in I_O} W_{Qhm} = 0 \tag{39}$$

with the additional condition

$$W_{Qhm} = \overline{W}_{Qhm}, h \in I_G, m \in I_O \tag{40}$$

motivated by considerations related to (8).

Let $\mathcal{H}_h = \{\alpha_h, a_h, \gamma_h, b_h\}$. Above introduced equations have an excessive number of variables. Therefore, additional constitutive equations must be introduced. They are assumed in the following form

$$V_{Sh} = C_{Sh\mu}(\mathbf{C}_{Sh\mu}, \mathcal{H}_h, \xi_h, \theta_h)\, \mathbf{\Phi}_{Sh\mu}(\alpha_h, a_h) \tag{41}$$

$$V_{Qh} = C_{Qh\nu}(\mathbf{C}_{Qh\nu}, \mathcal{H}_h, \xi_h, \theta_h)\, \mathbf{\Phi}_{Qh\nu}(\gamma_h, b_h) \tag{42}$$

$$W_{Qhm} = \overline{W}_{Qhm}(\mathbf{C}_{Wh}, \mathcal{H}_h, \xi_h, \theta_h) \tag{43}$$

$$\dot{\xi}_h = A_\xi(\mathbf{C}_{\xi h}, \mathcal{H}_h, \xi_h, \theta_h) \tag{44}$$

$$\dot{\theta}_h = A_\theta(\mathbf{C}_{\theta h}, \mathcal{H}_h, \xi_h, \theta_h) \tag{45}$$

where the last two equations are evolution equations for internal state variables.

We have obtained a form of the skeletal dynamical system corresponding to SQ-decomposition with the help of Eqs. (35)-(45). In this system we have introduced a set of constants $\mathbf{C} = \{\mathbf{C}_{Sh\mu}, \mathbf{C}_{Qh\nu}, \mathbf{C}_{Wh}, \mathbf{C}_{\xi h}, \mathbf{C}_{\theta h}\}$, $\mathbf{C} \in \mathcal{C}_E$. This kind of the elementary dynamical system can be considered when we apply molecular dynamics method for instance.

Averaged descriptions obtained by considered here *SDS* can be related to models directly based on molecular dynamics and having a kind of temperature as variable. Consequently, we can introduce on this way nanoscale continuum models of mechanics of materials when we add to this kind of modelling quantities representing continuum.

However, discussed above *SDS* need not to be considered as a kind of continuum. It can describe, for instance, behavior of a large molecule divided into subsystems, where a deformation and averaged fluctuations related to vibration are taken into account. Then, the deformation corresponds rather to conformational changes of the molecule. Such models can open possibility of simplified modelling of large molecular systems in biology for instance (Kaczmarek 2002).

4. Continuum mechanics as a special case of the dimensional reduction

4.1 Continuum with finite-dimensional fields

Multiscale modelling in mechanics of materials leads to possibility of considering physical foundations of processes in materials. Atomic models represents the best physical description. However, they have very large number of degree of freedom and therefore should be simplified. We have postulated here that dimensional reduction is appropriate method for such a simplification.

On the other hand continuum description is the most frequently applied in mechanics of materials. It is natural to expect that such models could be considered as skeletal dynamical systems in order to be obtained as a result of dimensional reduction procedures.

Number of degree of freedom for atomic systems described by molecular dynamics is finite. Consequently, simpler systems obtained by means of the dimensional reduction should have less number of degree of freedom. However, fields on continuum create infinite-dimensional spaces. This follows that continuum theories considered here as simpler systems should have finite-dimensional fields. In this section we formulate continuum theory having such a property.

The continuum mechanics is widely applied in material sciences for many years. This is a general theory which has well established mathematical foundations, see for instance (Truesdell and Noll 1965, Gurtin and Williams 1967, Truesdell 1972, Williams 1972, Noll 1973, Kosiński 1985). In this section we modify assumptions of the continuum mechanics in order to obtain continuum with finite-dimensional fields.

The idea of introducing finite dimensional fields consists in assumption on validity of balance equations not for all subbodies of the body $\mathcal{B}$ but only for their determined family $\mathcal{K}$. It is in fact a generalization of classical formulation since all subbodies create a particular case of $\mathcal{K}$.

The notions of the classical continuum should be modified with respect to a finite family of subbodies $\mathcal{K}$ in order to obtain spaces of finite dimensional fields. We would like also to connect notions related to continuum with an elementary dynamical system. To this end mappings defining geometrical objects related to dynamical subsystems will be used. They have been introduced in general assumptions characterizing collection of dynamical systems.

Consequently, we can consider mappings G_x, G_L, G_S, G_V which assign zero, one, two and three dimensional geometrical objects to each subsystem correspondingly.

Let us apply the special case of the map $G_V : \mathcal{M}_\Pi \to (2^{Ee})^P$ as $G_V = G_K$. Let $\mathcal{M}_K = \{\mathcal{K}\}$ be a set of possible families of $\mathcal{K} = \{K_h\}$, where $K_h \subset E_e$ and $intK_g \cap intK_h = \emptyset$, $g, h \in I_P$. Then, $G_K : \mathcal{M}_\Pi \to \mathcal{M}_K$, $G_K(\{\varphi_h\}) = \mathcal{K}$. We introduce also the mapping $G_{Kh}(\varphi_h) = K_h$.

Consequently, the mapping G_K introduces three-dimensional disjoint subsets of E_e which will be further interpreted as partition of the body $\mathcal{B}$ on the set of subbodies K_h and $\bigcup K_h$.

Let us note that $G_K(\{\varphi_h\}(t)) = \{K_h\}(t)$ describes evolution of $\mathcal{B}(t) = \bigcup_h K_h(t)$ in time. $K_h(t)$ will be also denoted by $\chi_t(K_h)$ in what follows, where K_h corresponds to a reference configuration.

Definition 1: The body associated with the dynamical system $\dot{\boldsymbol{\varphi}} = L(\boldsymbol{\varphi}, \mathbf{f})$ is defined with the help of mapping G_K as $\mathcal{B}_\varphi = \bigcup_{h \in I_P} K_h$.

Let us apply also the function $G_x = G_\chi$ which assigns a point χ_h as a distinguished point of $\chi(K_h)$ to each subsystem. Thereby, $G_\chi : \mathcal{M}_\Pi \to \{\{\chi_h\}\}$. We introduce also a mapping $\bar{\chi} : \mathcal{M}_K \to \{\{\chi_h\}\}$. Consequently, $G_\chi = \bar{\chi} \circ G_K$. In particular $G_\chi = G_I$ defines $\mathbf{X}_h$ as a distinguished point of K_h in reference configuration.

Let us consider the set $H_{\chi h} = \{\chi_m, m \in I_h^a\}$. Then, we introduce the function $a_h : H_{\chi h} \to V_{ah}$, where V_{ah} is a linear space, and $a : \{\{H_{\chi h}\}\} \to \{\{a_h(\{\chi_m\})\}\}$ as a function of kinematical dependence between subsystems defined here with the help of family $\mathcal{K}$.

The function $\bar{\chi}$ assigns a set of discrete values of the field χ_h, $h \in I_P$ to the body $\mathcal{B}$ with the help of the family $\mathcal{K}$. Similarly, the function a assigns a set of discrete values of the field a_h, $h \in I$ to the body. Indexes from the set I_h^a will be related usually to some neighboring sets K_i of K_h. Let $\bar{V}_D = \{\{\bar{\chi}, a\} : \{\bar{\chi}, a\} = \{\chi_h, a_h\}, h \in I_P\}$. Let us define the space V_κ of deformation functions χ_κ of the body $\mathcal{B}$ with respect to a given configuration κ as $V_\kappa = \{\chi_\kappa : \chi_\kappa = \lambda \circ \kappa^{-1}, \lambda, \kappa \in \mathcal{C}\}$. In this case $\mathcal{C}$ is the set of configurations considered within classical continuum mechanics formulation.

Let furthermore, $\alpha_\chi : \bar{V}_D \rightarrow V_\kappa$ be a function and $\chi_\kappa^{\mathcal{K}} = \alpha_\chi(\{\chi_h, a_h\})$, $\chi_\kappa^{\mathcal{K}}(\mathbf{X}_h) = \chi_h$.

Definition 2: The deformation function associated with the distinguished family of subbodies $\mathcal{K}$ is a function $\chi_\kappa^{\mathcal{K}}$ of the form $\chi_\kappa^{\mathcal{K}} = \alpha_\chi(\{\chi_h\ a_h\})$.

Definition 3: The motion of the body $\mathcal{B}$ associated with the family of sets $\mathcal{K}$ is a continuous map $\chi_t : [0, T] \rightarrow \{\chi_\kappa^{\mathcal{K}}\}$.

With the help of above definitions we have obtained deformation function and motion of the body in relation to the elementary dynamical system.

Considering fields on continuum we need frequently also temperature field. Let us note that assignation of the value of temperature T_h to the point χ_h in $\chi(K_h)$ is not so simple as defining χ_h which has direct geometrical interpretation. We do this here formally only. However, deeper understanding of such a variable can be obtained when we consider SQ decomposition and corresponding projection mappings.

Consequently let us introduce a function $\bar{T}$ on $\mathcal{K}$, which represents temperature, as $\bar{T} : \mathcal{K} \rightarrow R^P$, $\bar{T}(\{K_h\}) = \{T_h\}$. Let $I_h^b \subset I_P$ and $H_{Th} = \{T_n, n \in I_h^b\}$. Then, wy introduce function b_h by analogy to a_h as $b_h : H_{Th} \rightarrow V_{bh}$ and $b : \{\{H_{Th}\}\} \rightarrow \{\{b_h(T_n)\}\}$.

Let $\bar{V}_{TM} = \{\{\bar{T},\ b\} : \{\bar{T},\ b\} = \{T_h,\ b_h\},\ h \in I_P\}$, $V_{TM} = \{T(\mathbf{x}) : \mathbf{x} \in \chi(\mathcal{B})\}$. Let us consider a function $\bar{V}_{TM} \rightarrow V_{TM}$ and $T^{\mathcal{K}} = \alpha_T(\{T_h, b_h\})$.

Definition 4: The temperature field $T^{\mathcal{K}}$ associated with the distinguished family of subbodies $\mathcal{K}$ is the field obtained with the help of the function α_T as $T^{\mathcal{K}} = \alpha_T(\{T_h, b_h\})$.

The function α_χ assigns a deformation function field $\chi_\kappa^{\mathcal{K}}$ to the set of its discrete values. The aim of this function is to introduce a continuous field χ on the body $\mathcal{B}$. Similar role plays the function α_T for T. Thus, the spaces of such fields $Im\,\alpha_\chi \subset V_\kappa$ and $Im\,\alpha_T \subset V_{TM}$ are finitedimensional, where $Im\,\phi$ means the image of a function ϕ.

4.2 Balance of mass and energy equations for continuum with finite-dimensional fields

Previously we have introduced assumptions related to collection of dynamical systems. They admit existence of functions $\tilde{m}$, $J_{\varphi ij}$, c_φ, E_φ, $W_{\varphi ij}$, R_φ which introduce masses m_i, efflux of mass J_{ij}, source of mass c_i, efflux of energy W_{ij} and source of energy R_i accompanied by subsystems. Consequently, mentioned functions indexed here by φ are referred directly to the elementary dynamical system.

We use these functions to reformulation of general form of balance of mass and energy equations defined for collection of dynamical system to the case of continuum.

Let $\tilde{m} : \mathcal{M}_\Pi \rightarrow \{\{m_h\}\}$ be mapping which determines a set of mass related to collection of dynamical systems. Let $\mathcal{M}_M = \{\{M_h\}\}$ and $M : \mathcal{M}_K \rightarrow \mathcal{M}_M$ be a function which determines masses assigned to K_h. We have also that $\pi_h \circ M(K) = M_h$, where M_h is the total mass related to K_h. M_h are defined by means of the relation $M \circ G_K = i \circ \tilde{m}$, where i is a mapping which identify mass of h-th subsystem with mass assigned to K_h. Consequently, a system of mass related to continuum is introduced by means of mapping $\tilde{m}$ defined on elementary dynamical system.

Let $\mathcal{B} = \bigcup_h K_h$, $h \in I_B$, where $I_B \subset I_P$ is a set of indexes defining an arbitrary subbody $\mathcal{B}$ of the body also denoted by $\mathcal{B}$. Then, $M(\mathcal{B}) = \Sigma_{h \in I_B} M_h$. Using this definition we obtain mass related to subbodies as a kind of measure defined on the body.

Energy accompanied by the elementary dynamical system is introduced by means of the function $E_\varphi : \mathcal{M}_\Pi \rightarrow R^P$. Then, energy $\mathcal{E} : \mathcal{M}_K \rightarrow \{\mathcal{E}_h\}$, $\mathcal{E}_h = \pi_h \circ \mathcal{E}\ (\{K_h\})$ assigned to each K_h, is defined by means of the relation $\mathcal{E} \circ G_K = i \circ E_\varphi$. As a result, we are able to define energy related to subbody as

$\mathcal{E}(\mathcal{B}) = \Sigma_h\, \mathcal{E}_h$. We assume further that $\mathcal{E} = E + \mathcal{T}$ is sum of internal energy and kinetic energy.

Source of mass $c_\varphi : \mathcal{M}_\Pi \to R^P$ and source of energy $R_\varphi : \mathcal{M}_\Pi \to R^P$ are defined now as $C : \mathcal{M}_K \to R^P$, $R : \mathcal{M}_K \to R^P$ by means of relations $C \circ G_K = i \circ c_\varphi$ and $R \circ G_K = i \circ R_\varphi$. These quantities are defined for subbodies by means of expressions $C(\mathcal{B}) = \Sigma_h\, C_h$, $R(\mathcal{B}) = \Sigma_h\, R_h$.

Efflux of mass $J_{\varphi ij} : \mathcal{M}_\Pi \to R$ and efflux of energy $W_{\varphi ij} : \mathcal{M}_\Pi \to R$ are defined as $J_{ij} : K_i \times K_j \to R$, where J_{ij} is determined by means of $J_{ij} \circ (G_{Ki} \times G_{Kj}) = i \circ J_{\varphi ij}$ and $W_{ij} : K_i \times K_j \to R$, where we obtain W_{ij} from $W_{ij} \circ (G_{Ki} \times G_{Kj}) = i \circ W_{\varphi ij}$.

Let us consider the boundary of the body $\partial \mathcal{B} = \partial \bigcup_h K_h$. Then, $J(\partial \mathcal{B}) = \Sigma_{i \in I_B,\, m \in I_P - I_B}\, J_{im}$ and $W(\partial \mathcal{B}) = \Sigma_{i \in I_B,\, m \in I_P - I_B}\, W_{im}$.

We consider also $\partial \mathcal{B}_s \subset \partial \mathcal{B}$ which is defined as $\partial \mathcal{B}_s = \bigcup_{h \in I_S} (\partial K_h \cap \partial \mathcal{B})$, $I_s \subset I_B$. There exists relation between $\partial \mathcal{B}_s$ and set of J_{im}. We assume that pair of indexes $\{i, m\}$ is associated with $\partial \mathcal{B}_s$ if $\partial \mathcal{B}_s$ is a border between subsystems i and m. Then, $J(\partial \mathcal{B}_s) = \Sigma_{i \in I_s,\, m \in I_{si}}\, J_{im}$.

With the help of introduced functions, the balance of mass Eq. (4) interpreted in terms of continuum is given by

$$\dot{M}(\mathcal{B}) + J(\partial \mathcal{B}) - C(\mathcal{B}) = 0 \tag{46}$$

with the additional condition satisfied for arbitrary $\partial \mathcal{B}_s \subset \partial \mathcal{B}$

$$J(\partial \mathcal{B}_s) = \bar{J}\ (\partial \mathcal{B}_s) \tag{47}$$

The balance of energy Eq. (7) expressed in terms of continuum is assumed in the following form

$$\dot{E}\ (\mathcal{B}) + \dot{\mathcal{T}}(\mathcal{B}) + W(\partial \mathcal{B}) - R(\mathcal{B}) = 0 \tag{48}$$

with the additional condition satisfied for arbitrary $\partial \mathcal{B}_s \subset \partial \mathcal{B}$

$$W(\partial \mathcal{B}_s) = \overline{W}\ (\partial \mathcal{B}_s) \tag{49}$$

Neglecting at the moment detailed representations of introduced below quantities, we formulate also the second law of thermodynamics as a supplementary postulate. This is given with the help of the balance entropy expressed as

$$P(\mathcal{B}) = \dot{S}\,(\mathcal{B}) + H(\partial \mathcal{B}) - N(\mathcal{B}) \geq 0 \tag{50}$$

where S is entropy, H is efflux of entropy and N stands for source of entropy. P represents production of this quantity.

We accept SQ decomposition in this version of continuum theory. Therefore, the skeletal dynamical system for continuum description can be expressed in similar form as Eqs. (35)-(45). In order to do it we should interpret in details particular representations of quantities which occur in balance of energy and mass equations as well as entropy balance Eqs. (46)-(50).

Having such representations we can compare them with corresponding quantities in (35)-(45). We can introduce and interpret in these equations geometrical structure of objects K_h assigned to subsystems and also other geometrical properties. In particular we can introduce gradient of deformation by means of functions a_h and b_h, Div operation interpreting summation with respect to distribution of K_h and corresponding boundary conditions.

4.3 A comparison with the finite elements method

Discussed in this paper approach to continuum by finite subsets suggests connections with finite

elements. Indeed we consider a finite family of subsets K_h. We have at our disposal mappings G_x. Consequently, such mappings can indicate vertexes of simplexes $\{x_{hp}\}$ for each K_h.

Let us introduce assumption that $x_{hp} = x_{h'q}$ for every coinciding vertexes of adjacent K_h and $K_{h'}$. We can construct various functions a_{hm} which could determine derivatives of arbitrary rank for each vertex of K_h. Then, we can introduce the deformation function $\chi^{\mathcal{K}} = \alpha_\chi(\{x_{hp}\}, \{a_{hm}\})$ interpreted as a finite-element representation of the deformation function (Oden and Reddy 1976).

Let us notice that we do not consider any discretization when we postulate continuum equations. Introduced equations are directly finite-dimensional. However, variational approach can be useful for postulating forms of skeletal dynamical systems.

Summarizing, finite elements can be interpreted as subsystems which can generate continuum with finite-dimensional fields. However, subsystems are not finite-elements in general since continuum fields can be introduced on various ways.

5. Continuum with a discontinuity surface

Discontinuity surface occurs frequently when we apply a small scale for averaging of material properties. In particular discriminating of separate slip surfaces needs nanoscale approach for instance. Similarly strong discontinuity appears when we consider separate cracks. Thereby, the discontinuity surface can be associated with important mechanisms responsible for inelastic deformation.

Above remarks suggest necessity of discussion on premisses for constructing of the skeletal dynamical system also in the case when the discontinuity surface appears. We discuss here the

situation where the discontinuity surface is related to the deformation function χ introduced for the body $\mathcal{B}$. Then, the body undergoes separation into parts. In case of multiscale description presented in this work, appearing of such a discontinuity surface induces change of the dimensional reduction during evolution.

Let us introduce a surface $\mathcal{S}$ in the body $\mathcal{B}$. Then, many of $K_h \in \mathcal{K}$ is intersected by this surface. As a result we have to consider a new family $\mathcal{K}_\mathcal{S}$ of subsets of $\mathcal{B}$ which consists of $K_h \in \mathcal{K}$ and additionally $K_{h'l}$ instead of $K_{h'}$, $h' \neq h$, $l = 1, 2$, where $K_{h'} = K_{h'1} \cup K_{h'2}$ and $\partial K_{h'1} \cap \partial K_{h'2} = \mathcal{S} \cap K_{h'}$. We assume also that $I_S = \{h'\}$. Consequently, the surface $\mathcal{S}$ intersects some $K_{h'}$ and divide them into two parts. Let us introduce a common index for all sets from $\mathcal{K}_\mathcal{S}$. Let $a \in \{h, h'1\ h'2\}$, $h \neq h'$. Then, $\mathcal{K}_\mathcal{S} = \{K_a\}$.

The surface $\mathcal{S}$ is not introduced consistently with the above discussed theory of continuum with finite-dimensional fields. In case of the material surface, for instance, we have that $\mathcal{S} = \chi(\mathcal{S}_0)$. It means that $\mathcal{S}$ is an image of the deformation function χ. On the other hand χ is introduced with the help of $\{\chi_h\}$ and $\alpha(\chi_h, a_h)$. The last remark suggests that the surfaces, $\mathcal{S}$ should be introduced by means of discrete set of values.

Let $\mathcal{S}_{h1} = \mathcal{S} \cap \chi^-(K_{h1})$ and $\mathcal{S}_{h2} = \mathcal{S} \cap \chi^+(K_{h2})$, $h \in I_S$. We assign values of deformation functions χ^-_{Sh1} and χ^+_{Sh2} to distinguished points on $\mathcal{S}_{h1}$ and $\mathcal{S}_{h2}$ respectively. These points can be applied to generation of continuous surface $\mathcal{S}$.

Interaction through the surface should be introduced at the same point of the surface of both $\mathcal{B}^-$ and $\mathcal{B}^+$ systems. However, χ^-_{Sh1} and χ^+_{Sh2} do not coincide in general during evolution. Therefore, we will use transmission functions discussed previously in Subsection 2.2, for quantities depending on χ, which express interactions at the same point of both sides of the surface.

Let us distinguish $\mathcal{B}^- = \bigcup_{h \in I_{B-}} K_h \cup \bigcup_{h \in I_S} K_{h1}$ and $\mathcal{B}^+ = \bigcup_{m \in I_{B+}} K_m \cup \bigcup_{m \in I_S} K_{m2}$. Then, $I_{B-} = I_{BI-} \cup \{h1\}$, $I_{B+} = I_{BI+} \cup \{h2\}$ are sets of indexes related to parts of the body on both sides of the surface.

Let $\mathcal{P}_{hn}$ stands for quantity defined for continuum description and analogous to the left side of the Eq. (35). Furthermore let Q_h stands for quantity defined for continuum description and analogous to the left side of Eq. (39).

Using the balance of energy Eq. (34) we postulate the balance of energy equation for continuum with the discontinuity surface $\mathcal{S}$ in the following form

$$\sum_{h \in I_{B-}} \left(\mathcal{P}_{hr} \dot{\chi}_{hr} + \sum_{g2} W_{\mathcal{S}(h1)(g2)}(\mathcal{S}) + Q_h + \sum_{g2} W_{Q(h1)(g2)}(\mathcal{S}) \right)$$

$$+ \sum_{mI_{B+}} \left(\mathcal{P}_{mp} \dot{\chi}_{mp} + \sum_{p1} W_{\mathcal{S}(m2)(p1)}(\mathcal{S}) + Q_m + \sum_{p1} W_{Q(m2)(p1)}(\mathcal{S}) \right) = 0 \tag{51}$$

where indexes $h1$ and $m2$ corresponds to indexes h' of subsystems divided by the discontinuity surface. In case when $h \neq h'$ then sumation over indexes $g2$ and $p1$ is not active.

Role of indexes $g2$ and $p1$ can be explained by means of particular representation of the quantity $W_{\mathcal{S}\,(h1)(g2)}(\mathcal{S})$ which can be defined as follows

$$W_{\mathcal{S}(h1)(g2)}(\mathcal{S}) = \frac{\partial V_{h1}}{\partial \chi^-_{(g2)r}} \dot{\chi}^-_{(g2)r} \tag{52}$$

We have to do here with variables $\chi^-_{(g2)r}$ having indexes $g2$ which do not belong to I_{B-}. Thereby equations describing evolution of part $\mathcal{B}^-$ of the body $\mathcal{B}$ have an axcessive number of variables. We should determine them by some boundary conditions. Similar situation happens in case of excessive variables for part of $\mathcal{B}^+$ and related to the term $W_{\mathcal{S}\,(m2)(p1)}(\mathcal{S})$.

Dependence of V_{h1} on variables which do not belong to $\mathcal{B}^-$ is associated with dependence of V_{h1} on the function of $a_h(\chi)$ type. With the aid of such a function various forms of gradients of deformation can be introduced. The function V_h can be identified with the free energy.

When the parts $\mathcal{B}^-$ and $\mathcal{B}^+$ are joined then $\chi^-_{(g2)r}$ can be assigned to subsystem represented by K_{g2}. However, in case when we discuss separately $\mathcal{B}^-$ we can consider $\chi^-_{(g2)r}$ as a surface quantity.

The balance of energy Eq. (51) should be prepared to derivation of balance of momentum equation for corresponding parts of the body and on the discontinuity surface. In case when we consider the two parts of the body in a contact then we should have at our disposal possibility of efective comparison of quantities on the surface. Thereby let us consider the following transmission functions

$$-\frac{\partial \tilde{V}_{h1}}{\partial \chi^+_{(g2)r}} \dot{\chi}^-_{(g2)r} = \tilde{\mathcal{T}}_{(h1)(g2)r} \left(\left\{ \frac{\partial V_{m2}}{\partial \chi^+_{(p1)r}} \dot{\chi}^+_{(p1)r} \right\} \right) \tag{53}$$

which assign values on the left side of the relation (53) having form corresponding to the body $\mathcal{B}^-$. Negative sign appears as a result of taking into account orientation of the surface.

Let us note that the transmission function $\mathcal{T}$ can be introduced with the aid of the mapping α_S which assigns continuous form of the surface $\mathcal{S}$ for a discrete set of position vectors defining the surface. All discrete fields should be distributed on the surface by densities of such fields. Then,

transition to various points of the surface is possible.

With the aid of expressions (52) and (53) we can rewrite the balance energy Eq. (51) in the form

$$\sum_{h\in I_{B-}}\left\{\mathcal{P}_{mp}\dot{\chi}_{hr}+\sum_{g2}\left(\frac{\partial V_{h1}}{\partial \chi^{-}_{(g2)r}}+f_{\mathcal{S}(h1)(g2)r}\right)\dot{\chi}^{-}_{(g2)r}\right.$$
$$\left.+Q_h+\sum_{g2}W_{Q(h1)(g2)}(\mathcal{S})+E_{h1}(\mathcal{S})\right\}+\sum_{h\in I_{B-}}\sum_{g2}\tilde{\mathcal{T}}_{(h1)(g2)r}\left(\left\{\frac{\partial V_{m2}}{\partial \chi^{+}_{(p1)r}}\dot{\chi}^{+}_{(p1)r}\right\}\right)$$
$$+\sum_{m\in I_{B+}}\left\{\mathcal{P}_{mp}\dot{\chi}^{+}_{mp}+Q_m+\sum_{p1}W_{Q(m2)(p1)}(\mathcal{S})\right\}=0 \tag{54}$$

where we have added the term $E_{h1}(\mathcal{S})+f_{\mathcal{S}\,(h1)(g2)r}\dot{\chi}_{(g2)r}=0$. The force $f_{\mathcal{S}\,(h1)(g2)r}$ is responsible for dissipation of energy on the surface. We do not discuss of this aspect in details at this moment.

Consequently, taking into account independence of time processes $\dot{\chi}^{-}_{(g2)r}$ we obtain from (54) and (53) among others the following equation

$$\frac{\partial V_{h1}}{\partial \chi^{-}_{(g2)r}}-\frac{\partial \tilde{V}_{h1}}{\partial \chi^{+}_{(g2)r}}-f_{\mathcal{S}(h1)(g2)r}=0 \tag{55}$$

corresponding to local form of balance of momentum on the surface $\mathcal{S}$.

We can obtain also other equations related to the surface starting from the balance of energy Eq. (54). The aim of this discussion is to show how discontinuities can appear in the skeletal dynamical system describing material having strong discontinuities. We see that the equation of type (55) should be a part of such a skeletal dynamical system together with all necessary constants associated with this equation.

Propagation of the discontinuity surface changes incessantly dimensional reduction procedure due to varying number of variables associated with interction of new subsystems. Conditions for initiation of particular discontinuity surfaces needs more detailed models, taking for instance particular forms of the free energy represented here by the functions V_h.

Skeletal dynamical systems with discontinuity surface can be applied in cooperation with smaller scale models. Let us mention for instance molecular dynamics which could support models of crack propagation.

On the other hand, we can apply an elementary dynamical system with the disontinuity surface describing crack propagation for instance to determine more averaged models. Then, more averaged models have to average effects following from particular cracks and introduce to this end new variables. Let us mention for instance damage tensor as representing such variables. Discussion of this kind of description is done in (Kaczmarek and Ostachowicz 2005).

6. Conclusions

Application of multiscale descriptions and corresponding numerical simulations of phenomena in materials are more widespread in last years. Development of computational methods in mechanics has considerable influence on methods applied in this area. We can consider large systems and

apply various grids for simulation and modelling at various scales. However, it seems that complexity of phenomena in materials in relation to small scales needs also development of a set of theoretical notions which allow to describe such phenomena.

In general, it seems that dynamics of processes in smaller scales is not sufficiently modelled yet. Therefore, in this paper an approach based on dynamical systems is suggested. Furthermore, we should distinguish between multiscale discretization and multiscale modelling. In the first case we have to do rather with known models. In the second case we should construct such models.

In the present multiscale approach models related to various scales are clearly separated. Thereby, we carry out modelling of physical processes for each scale separately. This is done by assuming form of the skeletal dynamical system. During option of scales for modelling we should be aware which levels are appropriate for distinguishing mechanisms responsible for modelled processes.

Let us note that within the concept of multiscale modelling presented in this paper we accentuate role of molecular dynamics corresponding to atomic scale, nanoscale continuum models and more averaged continuum models.

Role of nanoscale models seems to be very important. Let us note that nanoscale models are rather not developed. This is so since they are too complex for direct engineering applications and by this their status is not well justified. On the other hand various mechanisms responsible for inelastic deformation happen just in relation to nanoscale. Let us mention slip plasticity where we would like to distinguish separate slip surfaces. Such a model has been discussed in (Kaczmarek 2003). Another example is related to martensitic transformation where moving interfaces appear. Then, dynamics of such a system needs more careful investigations by distinguishing separate interfaces. Models of this kind has been discussed in (Kaczmarek 1994, Kaczmarek 1998, Kaczmarek 2001). Phenomena at the tip of the crack are also associated with various types of inelastic deformation and have complex dynamics. Therefore nanoscale approach to fracture mechanics (Kaczmarek and Ostachowicz 2005) is also justified.

Let us note that small elementary volume for nanoscale models makes more easy cooperation of such models with molecular dynamics. In such a case we have smaller number of atoms in the elementary volume. Then, by means of the dimensional reduction procedure, we could create nanoscale models from molecular dynamics simulations. This is also a proposition for application of molecular dynamics. We could remember complex calculations of molecular dynamics in form of nanoscale models.

As it was mentioned above modelling for each scale applied is manifested by postulated form of the skeletal dynamical system. Introduction of the skeletal dynamical system can be direct and arbitrary in fact. However, then approximation of phenomena can be not correct. On the other hand we can try to obtain some premises on form of such a dynamical system by analysis of form of the elementary dynamical system as it was discussed in Section 3 for instance. We can support our knowledge by experimental observations corresponding to the chosen scale. We can also try to maximize our efforts towards theoretical derivation of form of *SDS* from *EDS*.

Form of the free energy seems to be important in relation to modelling of various phenomena and using it for determination of the skeletal dynamical system. Having such a motivation complex forms of the free energy is applied in the martensitic transformation model (Kaczmarek 1994, Kaczmarek 1998) and slip plasticity (Kaczmarek 2003). In both cases form of the free energy and their variables correspond to phenomena at the nanoscale. Furthermore such a function is convenient for unification in modelling of various phenomena. In particular the slip plasticity and martensitic transformation can be unified on this way (Kaczmarek 2001).

Nanoscale models can have independent status as phenomenological theories. However, large number of constants, appearing in the free energy for instance, needs determination. At the nanoscale it is difficult to carry out experiments related to separate phenomena. Then, cooperation with molecular dynamics seems to be inevitable in a longer perspective. This is possible just within presented here multiscale approach.

Determination of range of validity of particular elaborated models is important. We see that many phenomena and corresponding to them processes have to be described by application of a varying number of variables. This is especially frequent when the scale is smaller. Let us mention the slip plasticity. When we exceed a critical condition and the slip appears a set of new variables is activated. Then, we apply also a new dimensional reduction procedure. Thereby, cooperation of models having different sets of variables has to be permanent. Range of validity of models has to be determined by a set of critical conditions corresponding to each model.

Summarizing, by above discussion we accentuate role of nanoscale models in order to give them a separate status in mechanics of materials. They are convenient for joining atomic simulations with more averaged continuum models which are more applicable in engineering. Furthermore, development of nanotechnology can give them additionally a separate status as models which have direct engineering applications.

Discussed in this paper multiscale method of modelling is aimed at giving a theoretical context and justification for development of nanoscale models. Furthermore, it is accentuated that unification of theoretical approach to molecular dynamics and continuum description for solids is very important with respect to physical aspects of mechanics of materials.

References

Truesdell, C. (1972), *A first course in rational mechanics*, Baltimore, Maryland.

Truesdell, C. and Noll, W. (1965), *The nonlinear field theories of mechanics*, (Ed. Flüugge, S.), Handbuch der Physik, III/3, Springer, Berlin.

Gurtin, M.E. and Williams, W.O. (1967), "An axiomatic foundations for continuum thermodynamics", *Arch. Ration. Mech. An.*, **26**, 83-117.

Williams, W.O. (1971), "Axioms for work and energy in general continua I", *Arch. Ration. Mech. An.*, **42**(2), 93-114.

Williams, W.O. (1971), "Axioms for work and energy in general continua II", *Arch. Ration. Mech. An.*, **49**(3), 225-240.

Noll, W. (1973), "Lectures on the foundations of continuum mechanics and thermodynamics", *Arch. Ration. Mech. An.*, **52**(1), 62-69.

Mura, T. (1982), *Micromechanics of defects in solids*, Martinus Nijhoff Publishers.

Nemat-Nasser, S. and Hori, M. (1999), *Micromechanics: overall properties of heterogeneous materials*, Elsevier.

Chen, J.S. and Mehraeen, S. (2005), "Multi-scale modelling of heterogeneous materials with fixed and evolving microstructures", *Model. Simul. Mater. Sc.*, **13**, 95-121.

Zhang, X., Mehraeen, S., Chen, J.S. and Ghoniem, N. (2006), "Multiscale total lagrangian formulation for modelling dislocation-induced plastic deformation in polycrystalline materials", *Int. J. Multiscale Com.*, **4**(1), 1-17.

Kosiński, W. (1985), *Field singularities and waves analysis in continuum mechanics*, Ellis Horwood Limited and PWN-Polish Scientific Publishers, Warsaw.

Oden, J.T. and Reddy, J.N. (1976), *An introduction to the mathematical theory of finite elements*, John Wiley & Sons.

Kaczmarek, J. (2002), "Concept of a formal system aimed at modelling biological processes in cell", *Comput.*

Method. Sci. Technol., **8**(1), 31-62.
Kaczmarek, J. (2003), "A nanoscale model of crystal plasticity", *Int. J. Plasticity*, **19**, 1585-1603.
Kaczmarek, J. (1994), "A model of the free energy for materials which undergo martensitic phase transformations with shuffles", *Int. J. Eng. Sci*., **32**(2), 369-384.
Kaczmarek, J. (1998), "A thermodynamical description of the martensitic transformation. A model with small volume of averaging", *Arch. Mech*., **50**(1), 53-81.
Kaczmarek, J. (2001), "A nanoscale model of the transformation-induced plasticity", *Tran. Institute F-Flow Machin.*, **108**, 5-32.
Kaczmarek, J. and Ostachowicz, W. (2005), "A description of damage based on nanoscale modelling of fracture", *Key Eng. Mater.*, Vols. 293-294, 235-244.
Kaczmarek, J. (2002), "A method of integration of molecular dynamics and continuum mechanics for solids", *TASK Quaterly,* **6**(2), 253-271.