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A METHOD OF INTEGRATION OF MOLECULAR DYNAMICS AND CONTINUUM MECHANICS FOR SOLIDS

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Abstract: In this paper a formal system called collection of dynamical systems with dimensional reduction is considered. This is a multiscale method of mathematical description which allows to consider molecular dynamics and continuum mechanics within one theoretical framework. Transition between molecular dynamics and continuum mechanics is realized by means of the dimensional reduction procedure. In order to realize such a procedure the formulation of continuum mechanics is modified. This modification consists in incorporation scale of averaging for properties of processes considered during modelling into this formulation. As a result we introduce finite-dimensional fields on continuum only. All fundamental terms of continuum mechanics are now joined with an elementary dynamical system. In such a case continuum mechanics can be obtained by means of the dimensional reduction procedure applied to the elementary dynamical system. A numerical example of vibrating chain of material points is realized in order to show how in practice the dimensional reduction can be carried out. In this example decomposition of processes into slowly and quickly varying parts is accomplished. To this end a finite element representation of averaged fields is applied. Solutions of equations of the elementary dynamical system and the dimensionally reduced dynamical system are compared.

Keywords: continuum mechanics, molecular dynamics, multiscale modelling

Nomenclature

EDS – elementary dynamical system
SDS – skeletal dynamical system
RDS – dimensionally reduced dynamical system
π_T – mapping which transforms processes between scales
π_{fT} – mapping which transforms forces between scales
V_T – space of processes of EDS
$\bar{V}_T$ – space of processes of SDS
$\mathcal{B}$ – continuous body
χ – deformation function
G_x – mapping which assigns zero-dimensional geometrical objects to subsystems
G_L – mapping which assigns one-dimensional geometrical objects to subsystems
G_S – mapping which assigns two-dimensional geometrical objects to subsystems
G_V – mapping which assigns three-dimensional geometrical objects to subsystems

1. Introduction

Modelling behaviour of solids is predominantly based on two approaches. The first one describes evolution of atoms represented by a set of material points. Let us mention molecular dynamics as the most successful method of this kind [1, 2]. The second one is based on continuum description [3], where averaging of properties of processes occurring in materials is considered. Both mentioned approaches enable modelling and simulation of a large variety of phenomena in solids.

Complexity of physical processes in materials forces considerations and modelling of rather some distinguished and separate phenomena only if we take into account present possibilities of numerical calculations. Simulation of the whole complexity of processes seems to be possible when we organize cooperation of various methods.

The problem of cooperation between atomistic models and continuum mechanics has been considered for a long time. Let us note that formulation of statistical mechanics was directed towards explanation where the averaged properties of multiatomic systems, usually described by continuum mechanics, follow from. Nowadays, relations between molecular dynamics and continuum mechanics are of great interest. Let us mention Parrinello Rahman method [4, 5] or smooth particle applied mechanics developed by Hoover and Posch [6–8].

In general, solution of the problem of cooperation between the discussed methods of modelling is rather difficult. Let us discuss several obstacles. The first one is connected with a large number of processes in materials, associated with intermediate scales. The last term means that the scale of averaging necessary for description of these phenomena is placed between the atomic one and that corresponding to continuum modelling. Continuum models are connected usually with a scale larger than one micrometer. Let us mention for instance the crystal plasticity which applies gradient of deformation as a measure of plastic deformation [9] or models of the martensitic transformation based on micromechanics [10, 11]. However, the most elementary mechanisms associated with the slip plasticity or the martensitic transformation are placed below 100 nm. Indeed, this is a distance between single slip surfaces or interfaces between various martensite variants. Furthermore, transformation of a martensite variant into another one changes also slip systems, which additionally complicates the situation when we would like to describe interactions between these phenomena.

Consequently, it is difficult to use atomic models for determination of properties of a material within a representative volume related to scale above 1μm when so complicated processes can appear there. This suggests directly that it would be convenient to develop models of some intermediate scales. Nanoscale seems to be the most convenient to obtain this. Nanoscale models for plasticity and martensitic transformation have been discussed in [12] and [13]. In order to incorporate them into a multiscale approach, methods of transition between various scale descriptions should be elaborated.

Let us mention that molecular dynamics uses a finite number of atoms. Then, simplified, more averaged models have to be characterized by smaller numbers of degrees of freedom. In this case we encounter a new obstacle for cooperation between the discussed methods. Namely, fields of continuum mechanics are infinite-dimensional

in general. Consequently, formulation of the continuum mechanics has to be adapted to cooperation with molecular dynamics.

The continuum mechanics has a bounded range of applications below a scale which is caused by the atomic structure. On the other hand we have suggested above application of continuum description related to various scales. Consequently, introduction of finite-dimensional fields on continuum should be realized together with formalization of scale of averaging. The last aspect is also helpful for determination of methods of transition between various scale models.

Summarizing, the above discussion suggests a general way for integration of molecular dynamics and continuum mechanics. This way is based on the following elements:

- introduction of a concept of multiscale modelling by means of a dimensional reduction procedure which enables transition between models related to various scales,
- adaptation of formulation of continuum mechanics for realization of a dimensional reduction procedure by formalization of scale of averaging,
- distinguishing special status for nanoscale models designed to direct cooperation with molecular dynamics as an intermediate stage between atomic methods of modelling and more averaged continuum models.

This is in fact very large program which cannot be realized within a single paper. However, by this discussion a general motivation governing the approach presented here is characterized.

The aim of this paper is to introduce a collection of dynamical systems with dimensional reduction which is a formal system which represents methods of multiscale modelling. This theoretical approach enables discussion of molecular dynamics and continuum mechanics within one theoretical scheme after discussed above modification of formulation of continuum theory.

2. Collection of dynamical systems with dimensional reduction

2.1. General discussion

In order to integrate various methods of modelling we should consider a formal system in which discussed methods could be immersed. It means that defined notions associated with each method of modelling are also expressible in this more general description.

Suggested formal system designed to integrate molecular dynamics and continuum mechanics is called here the collection of dynamical systems with dimensional reduction and represents multiscale method of modelling. The most elementary processes are described by an elementary dynamical system (EDS) by assumption. Thus the elementary dynamical system is usually very complex. By means of the dimensional reduction we obtain a simplified model based on theoretical foundations provided by the EDS.

Let us consider an elementary dynamical system in the following form:

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

where φ are variables of our dynamical system and $\mathbf{f}$ represents external interactions.

Transition to larger scale of averaging is connected with a simplification of this model and corresponds to reduction of degrees of freedom. Our concept of this simplification consists in division of the elementary dynamical system (1) into subsystems. Division into subsystems is a starting point for introducing new variables, representing reduced number of degrees of freedom, which describe behaviour of each subsystem in a simplified way.

We introduce this by means of mappings $\pi_T : V_T \to \bar{V}_T$, where V_T is a space of processes $\varphi(t)$, $t \in T$ on the time interval T and $\bar{V}_T$ is a space of processes $\mathbf{d}(t)$ realized by new variables. Similar mapping $\pi_{fT} : \mathcal{F}_T \to \bar{\mathcal{F}}_T$ is defined for external interactions considered on both levels of averaging.

The main element of the dimensional reduction procedure (DR) is a skeletal dynamical system $SDS(\mathbf{C})$ depending on new variables. This is a family of dynamical systems parameterized by constants $\mathbf{C}$. Having EDS and SDS we are able to construct two kinds of processes. The first one is based on solution $\varphi(\varphi_0, \mathbf{f})(t)$ of the Equation (1) with initial conditions φ_0 and has the form $\pi_T(\varphi(\varphi_0, \mathbf{f})(t))$. The second one is created by solutions of equations of the skeletal dynamical system with assumed constants $\mathbf{C}$ as $\mathbf{d}(\mathbf{C}, \pi(\varphi_0), \bar{\mathbf{f}})(t)$, where $\bar{\mathbf{f}}(t) = \pi_{fT}(\mathbf{f}(t))$ and the mapping $\pi(\varphi_0)$ transfers initial conditions into the dimensionally reduced level of description.

Let us consider the function:

$$H(\varphi_0, \mathbf{f}) = \inf_{\mathbf{C} \in \mathcal{C}_E} \rho(\mathbf{d}(\mathbf{C}, \pi(\varphi_0), \bar{\mathbf{f}})(t), \pi_T(\varphi(\varphi_0, \mathbf{f})(t))), \tag{2}$$

where $\mathcal{C}_E$ is an admissible set of constants and ρ is a metric in the space of processes $\bar{V}_T$.

Let $\mathbf{C}^*(\mathbf{d}_0, \bar{\mathbf{f}})$ stand for constants for which the function H attains an infimum for given $\mathbf{d}_0$ and $\bar{\mathbf{f}}$. Then, a satisfactory approximation should have the property that $\mathbf{C}^*$ exhibits a weak dependence on $\mathbf{d}_0$ and $\bar{\mathbf{f}}$. This is connected with assumed functions π_T, π_{fT} and form of SDS which reflect correctness of averaged modelling. Finally, we have to choose a constant $\bar{\mathbf{C}}$ from the set of $\mathbf{C}^*$ by an averaging method. Then,

$$\bar{\mathbf{C}} = Av\{\mathbf{C}^* : \mathbf{C}^*(\mathbf{d}_0, \bar{\mathbf{f}}), \mathbf{d}_0 \in \bar{\mathcal{M}}, \bar{\mathbf{f}} \in \bar{\mathcal{F}})\}, \tag{3}$$

where Av stands for an averaging operation and $\bar{\mathcal{M}}$ is space of all admissible values of $\mathbf{d}$. Obtained constants $\bar{\mathbf{C}}$ determine a dimensionally reduced dynamical system $RDS = SDS(\bar{\mathbf{C}})$. All methods applied in the procedure of approximation and identification of constants are denoted by *app*.

Summarizing, the dimensional reduction procedure $DR = \{\pi_T, \pi_{fT}, SDS, app\}$ consists of four elements. Application of DR into EDS leads to obtaining the reduced dynamical system.

2.2. Skeletal dynamical system

In order to postulate a form of the skeletal dynamical system we have to introduce a set of assumptions which enable to transfer fundamental physical laws into the reduced level.

Let $\mathcal{M}_\Pi = \{\{\varphi_h\}\}$, $h \in I_P$ stand for space of solutions of the elementary dynamical system (1) with distinguished groups of variables φ_h related to h^{th} subsystem and $I_P = \{1,\ldots,P\}$ is a set of all indexes which number subsystems. We introduce the following set of assumptions:

1. There exists a function $\bar{m}_h(\varphi_h) = \{m_{h1},\ldots,m_{h\beta_h}\}$ which assigns a set of masses for h^{th} subsystem. The total mass of this subsystem is then $m_h = \sum_i m_{hi}$. We have also that $\sum_h \beta_h = N$, where N is the total number of masses in the whole system. The function $\tilde{m}: \mathcal{M}_\Pi \to R^P$ with property $\tilde{m}(\{\varphi_h\}) = \{m_h\}$ determines distribution of masses in subsystems and $m: \mathcal{M}_\Pi \to R$, $m(\{\varphi_h\}) = \sum m_h$ determines the total mass related to dynamical system given by Equation (1).
2. There exists a function $\tilde{E}: \mathcal{M}_\Pi \to R^P$, $\tilde{E}(\{\varphi_h\}) = \{E_h\}$ which determines distribution of energy assigned to subsystems and $E: \mathcal{M}_\Pi \to R$, $E(\{\varphi_h\}) = \sum_h E_h$ determines the total energy related to dynamical system given by Equation (1).
3. 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 $J_{ij} + J_{ji} = 0$, $J_{ii} = 0$.
4. 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 $W_{ij} + W_{ji} = 0$, $W_{ii} = 0$.
5. A source of mass is determined by a function $c: \mathcal{M}_\Pi \to R^P$, $c(\{\varphi_h\}) = \{c_i\}$. $c_i = \pi_i \circ c(\{\varphi_h\})$ can be considered for each subsystem of the whole system and stands for a source of mass in the i^{th} subsystem.
6. A source of energy is determined by a function $R: \mathcal{M}_\Pi \to R^P$, $R(\{\varphi_h\}) = \{R_i\}$. $R_i = \pi_i \circ R(\{\varphi_h\})$ can be considered for each subsystem of the whole system and stands for a source of energy in the i^{th} subsystem.

Taking into account these assumptions we are able to express a general form of balance of mass equation for an arbitrary group of subsystems defined by set of indexes $I_G \subset I_P$:

$$\sum_{i \in I_G} (\dot{m}_i - c_i + \sum_{j \in I_O} J_{ij}) = 0, \quad J_{ij} = \bar{J}_{ij}, \quad j \in I_O, \tag{4}$$

where $I_O = I_P - I_G$. The terms J_{ij} describe interchange of mass with an external system indexed by elements of I_O. As a result the first equation in (4) is not entirely determined. Therefore the second equation in (4) is additionally postulated, where $\bar{J}_{ij}$ describes an assumed form of efflux of mass.

The balance of energy equation has a similar structure to the balance of mass equation and is given by:

$$\sum_{i \in I_G} (\dot{E}_i - R_i + \sum_{j \in I_O} W_{ij}) = 0, \quad W_{ij} = \bar{W}_{ij}, \quad j \in I_O, \tag{5}$$

where $\bar{W}_{ij}$ is an assumed form of efflux of energy. Let us note that E_i and W_{ij} depend, in general, on the state of the whole system in accordance with assumptions 2 and 4.

Equations (4) and (5) are the starting point for postulating the form of the skeletal dynamical system. This is realized by option of representations of quantities which appear in Equations (4) and (5). They are parameterized by a set of constants which should next be identified.

Particular representations of quantities in Equations (4) and (5) have to take into account interactions between subsystems. These interactions are modelled by means of functions of kinematical dependence. Let $H_{dh} = \{\{\mathbf{d}_j : j \in I_h^a\}\}$ be a set of values of variables $\mathbf{d}_j$ determined on a set of subsystems indexed by elements of I_h^a. I_h^a represents all subsystems which interact with the h^{th} one. Let us introduce a function $a_h : H_{dh} \to V_{ah}$, where V_{ah} 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. The function a_h is called the function of kinematical dependence between subsystems. The form of this dependence is embodied in the structure of elements which belong to V_{ah}.

We also introduce an additional concept of taking into account interactions between subsystems. Let us consider a set of variables $\{\mathbf{d}_h\}$. In order to describe interactions between different subsystems, a value of $\mathbf{d}_h$ type in a given point of space $\mathbf{X}$ can be useful. Let us note that our variables are not, in general, connected with any geometrical point. We assume, however, that it is possible to introduce a transmission function $\mathcal{T}_x(\{\mathbf{d}_h\}) = \mathbf{d}_x$ which assigns $\mathbf{d}_x$ in the point $\mathbf{X}$ to the set of values $\{\mathbf{d}_h\}$. Then, interactions can be considered in the chosen point of space. Let us note that such a function does not produce any additional degrees of freedom.

2.3. Continuum skeletal dynamical system

We discuss here continuum mechanics as a theory obtained by means of a dimensional reduction procedure from an elementary dynamical system. *EDS* is usually assumed to be finite-dimensional (molecular dynamics dynamical system for instance). Then, the dimensional reduction leads to a continuum with finite-dimensional fields. Therefore, we have to adapt formulation of continuum mechanics for consistency with this procedure.

In order to define fundamental notions of continuum mechanics we assume that geometrical objects of various dimensions can be assigned to each subsystem by means 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, E_e^P stands for Cartesian product of the space E_e taken P times, 2^{E_e} stands for family of all subsets of E_e and $(2^{E_e})^P$ is corresponding Cartesian product.

Consequently, 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.

Let us consider the mapping $G_V(\{\varphi_h\}) = \{K_h\}$, where K_h is a three-dimensional subset of E_e. Let $\mathcal{K} = \{K_h, h \in I_P\}$ and $\mathcal{M}_K = \{\mathcal{K}\}$ stand for all families of K_h obtained by means of G_V. Then, $G_V : \mathcal{M}_\Pi \to \mathcal{M}_K$. We assume also that internal parts of K_h are disconnected for different h.

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

We introduce the function $G_x : \mathcal{M}_\Pi \to \{\{\chi_h\}\}$ which assigns a distinguished point χ_h to each subsystem. Let $H_{\chi h} = \{\chi_m, m \in I_h^a\}$ and V_{ah} be a linear space. The set I_h^a represents indexes of subsystems K_m which interact with K_h. Then, we introduce the function $a_h : \{H_{\chi h}\} \to V_{ah}$ and $a : \{\{H_{\chi h}\}, h \in I_P\} \to \{\{a_h(\{\chi_m\})\}, h \in I_P\}$ as a function of kinematical dependence between subsystems.

Let $\bar{V}_D = \{\{\chi_h, a_h\},\ h \in I_P\}$. 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 $V_\kappa = \{\chi_\kappa : \chi_\kappa = \lambda \circ \kappa^{-1},\ \lambda, \kappa \in \mathcal{C}\}$ as this is done in classical formulation of continuum mechanics [14]. Let furthermore, $\alpha_\chi : \bar{V}_D \to V_\kappa$ be a function and $\chi_\kappa^{\mathcal{K}} = \alpha_\chi(\{\chi_h, a_h\})$, $\chi_\kappa^{\mathcal{K}}(\mathbf{X}_h) = \chi_h$, where $\mathbf{X}_h$ is the value of χ_h in a reference configuration.

Definition 2: *The deformation function associated with the distinguished family of subbodies $\mathcal{K}$ is a function $\chi_\kappa^{\mathcal{K}}$ which has 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 $\chi_t : [0,T] \to \{\chi_\kappa^{\mathcal{K}}\}$.*

Thus, we have defined the body, deformation function, and motion of the body by using the elementary dynamical system. The mappings G_V, G_x determine connections between EDS and continuum description.

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

Assignation of the value T_h to the point χ_h in $\chi(K_h)$ is not so simple as defining χ_h. The latter quantity has a direct geometrical interpretation. This is not the case for T_h. The discussed problem is connected with precise definition of the mapping π_T.

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

Thus, we have obtained finite-dimensional spaces $\alpha_\chi(\bar{V}_D)$ and $\alpha_T(\bar{V}_{TM})$. Therefore, finite-dimensional fields are considered on continuum only.

First stage of the formulation of the skeletal dynamical system is based on using balance of mass and energy equations for collection of dynamical systems. This is realizable owing to the set of assumptions introduced. They admit the existence of functions $\tilde{m}$, $J_{\varphi ij}$, c_φ, E_φ, $W_{\varphi ij}$, R_φ which introduce masses, efflux of mass between subsystems, source of mass, energy, efflux of energy and source of energy related to subsystems respectively. The index φ is introduced in order to accentuate connections with the EDS. We define similar functions in terms of continuum.

Let us consider the mapping $\tilde{m} : \mathcal{M}_\Pi \to \{\{m_h\}\}$ which determines a set of masses related to a collection of dynamical systems. Let $\mathcal{M}_M = \{\{M_h\}\}$ and $M : \mathcal{M}_K \to \mathcal{M}_M$ be a mapping which assigns masses to each K_h. Masses M_h related to continuum model are defined by means of the relation $M \circ G_V = i \circ \tilde{m}$, where i is identity mapping. 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, $M(\mathcal{B}) = \sum_{h \in I_B} M_h$.

The function $\mathcal{E} : \mathcal{M}_K \to \{\{\mathcal{E}_h\}\}$ determines distribution of energy on the family $\{K_h\}$ and is defined by means of the relation $\mathcal{E} \circ G_V = i \circ E_\varphi$. 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 $C \circ G_V = i \circ c_\varphi$ and $R \circ G_V = i \circ R_\varphi$. These quantities can be defined for subbodies with the help of formulas $\mathcal{E}(\mathcal{B}) = \sum_h \mathcal{E}_h$, $C(\mathcal{B}) = \sum_h C_h$, $R(\mathcal{B}) = \sum_h R_h$. We assume furthermore that $\mathcal{E} = E + \mathcal{T}$ is considered as a sum of internal energy and kinetic energy for continuum.

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 $J_{ij}\circ(G_{Vi}\times G_{Vj})=i\circ J_{\varphi ij}$ and $W_{ij}:K_i\times K_j\to R$, where we obtain W_{ij} from $W_{ij}\circ(G_{Vi}\times G_{Vj})=i\circ W_{\varphi ij}$.

Let $\partial\mathcal{B}=\partial\bigcup_h K_h$. We define $J(\partial\mathcal{B})=\sum_{i\in I_B,m\in I_P-I_B}J_{im}$ and $W(\partial\mathcal{B})=\sum_{i\in I_B,m\in I_P-I_B}W_{im}$ as quantities referred to boundary of the body. We consider also $\partial\mathcal{B}_s\subset\partial\mathcal{B}$ which is defined as $\partial\mathcal{B}_s=\bigcup_{h\in I_s}(\partial K_h\cap\partial\mathcal{B})$, $I_s\subset I_B$. 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, $J(\partial\mathcal{B}_s)=\sum_{i,m}J_{im}$.

The functions introduced above enable reformulating the balance of mass equation (4). Now this equation interpreted in terms of continuum is expressed as

$$\dot{M}(\mathcal{B})+J(\partial\mathcal{B})-C(\mathcal{B})=0,\quad J(\partial\mathcal{B}_s)=\bar{J}(\partial\mathcal{B}_s),\tag{6}$$

where $\bar{J}(\partial\mathcal{B}_s)$ is determined for all $\partial\mathcal{B}_s\subset\partial\mathcal{B}$.

The balance of energy equation (5) expressed in terms of continuum is assumed in the following form:

$$\dot{E}(\mathcal{B})+\dot{\mathcal{T}}(\mathcal{B})+W(\partial\mathcal{B})-R(\mathcal{B})=0,\quad W(\partial\mathcal{B}_s)=\bar{W}(\partial\mathcal{B}_s),\tag{7}$$

where $\bar{W}(\partial\mathcal{B}_s)$ is determined for all $\partial\mathcal{B}_s\subset\partial\mathcal{B}$.

Determination of balance of mass and energy equation is a preliminary stage of defining the skeletal dynamical system. The next step consists in postulating representations of quantities introduced in Equations (6), (7). They are dependent on constants. Then, identification of the constants with the help of EDS enables obtaining a continuum model represented by RDS and associated with the elementary dynamical system.

Discrete fields on continuum enable to introduce continuous fields on the body by a set of mappings. We have already discussed α_χ and α_T ones. All remaining discrete fields which appear on the continuum are transformed into continuous ones by means of similar mappings. They should fulfill the well known integral relations between densities and discrete values of quantities on each subbody.

The continuum mechanics discussed here is characterized by finite-dimensional spaces of fields on continuum. In classical case such spaces are infinite-dimensional. This difference is important. In our approach equations are directly finite-dimensional and no discretization method is applied. Furthermore, formulation of a continuum model with finite-dimensional fields is inherently connected with determination of degree of averaging. This is expressed by option of sets K_h and the skeletal dynamical system.

The range of validity of continuum description depends on the ability of selection of similar kind of subsystems and the same type of variables on each subsystem. In such a case fields can be determined only. This means also that transmission functions exist for each point of the body and for each kind of variables. Furthermore, then there has to exist a mapping G_V which introduces three-dimensional sets which can be interpreted as subbodies.

Summarizing, the method of integration of molecular dynamics and continuum mechanics consists in using a dynamical system defined by equations of molecular dynamics as an elementary dynamical system and next introducing a continuum skeletal dynamical system into the dimensional reduction procedure.

3. An example of the dimensional reduction procedure

We discuss here an example which illustrates realization of a dimensional reduction procedure. In order to do this we should determine an elementary dynamical system, a skeletal dynamical system and connections between them represented by mappings π_T, π_{fT}. Furthermore, we should decide what kind of approximation and identification procedures should be applied in order to obtain the final form of the dimensionally reduced dynamical system. We will follow here in accordance with the general outline of this procedure which is shown in Figure 1.

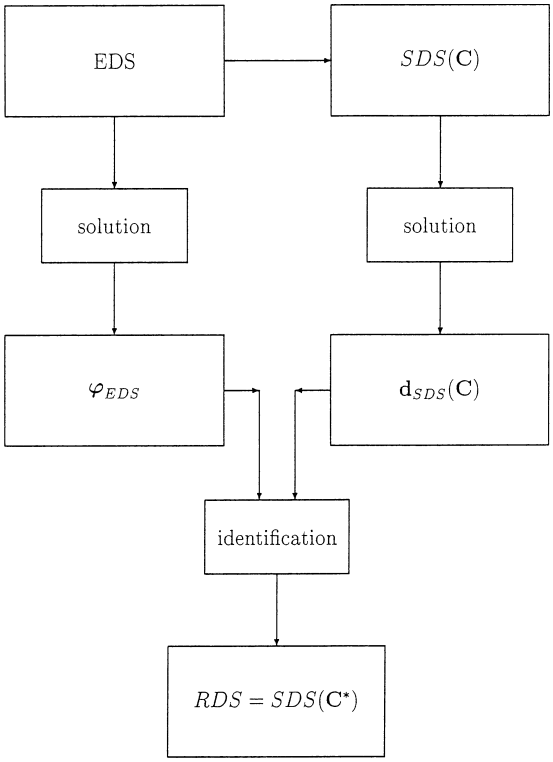

Figure 1. General outline of the dimensional reduction procedure

We discuss first an elementary dynamical system. Let us consider a chain of N particles $\{\mathcal{P}_i, i \in I_N\}$, $I_N = \{1,\ldots,N\}$, with the same mass and distance between them. The particles are distributed along the axis X and have positions X_i, $i \in I_N$ in a reference configuration. Evolution of particles is described by displacement vectors $u_i = x_i - X_i$, where x_i is the current position of i^{th} particle on the axis X. Distance between particles is described by $r_i = x_{i+1} - x_i = u_{i+1} - u_i + \Delta = z_i + \Delta$, where $\Delta = X_{i+1} - X_i$.

The potential energy is given by the expression $V_P = \sum_i \Phi_i\big(r_i(z_i)\big)$. We have applied here the Lennard-Jones potential [15]:

$$\Phi_i = \epsilon\left(\left(\frac{\sigma}{r_i}\right)^{12} - 2\left(\frac{\sigma}{r_i}\right)^{6}\right). \tag{8}$$

Let f_i be a force acting on i^{th} particle. Then, equations describing evolution of our system of particles are given by:

$$\dot{u}_i = v_i, \tag{9}$$

$$m_i \dot{v}_i = \frac{\partial \Phi_i}{\partial z_i} - \frac{\partial \Phi_{i-1}}{\partial z_{i-1}} + f_i. \tag{10}$$

We consider the Equations (9), (10) as equations of the elementary dynamical system.

We use notations $\varphi = \{\mathbf{u}, \mathbf{v}\}$, $\mathbf{u} = \{u_i\}, \mathbf{v} = \{v_i\}$ and space of processes $\varphi(t)$ be denoted by V_T in what follows.

In order to realize the dimensional reduction procedure we have to postulate the skeletal dynamical system in accordance with the scheme shown in Figure 1. Then, we have to determine variables of SDS as well as its form parameterized by some constants $\mathbf{C}$. Let us discuss first the problem of variables related to the dimensionally reduced level of description.

Determination of new variables is associated with determination of the mapping π_T in general. Postulating particular forms of such a mapping has to be motivated by additional assumptions which are connected with physical properties of the system. In the case considered here we assume that evolution of particles determined by the elementary dynamical system Equations (9), (10) can be decomposed into both quickly and slowly varying processes.

The starting point for determination above discussed mappings is the division of EDS into subsystems. Consequently, the set of N particles is divided into subsystems which consist of $N_h = N/N_P$ particles, where N_P is number of subsystems. Thereby, we identify our subsystems with sets of particles $\mathcal{S}_h = \{\mathcal{P}_i : i \in I_h\}\}$, $I_N = \bigcup I_h$, I_h is a set of indexes corresponding h^{th} to subsystem.

We assign geometrical objects to each subsystem by means of mappings G_L and G_x. Consequently, the interval $K_h = [X_{h1}, X_{h2}]$ is assigned to $\mathcal{S}_h$ by the mapping G_L. We have then $X_i \in K_h$, $i \in I_h$ in reference configuration. Furthermore, a distinguished point X_h is assigned to $\mathcal{S}_h$ by means of G_x. This point is a center of K_h.

By means of K_h we define one dimensional body $\mathcal{B} = \bigcup_h K_h$. We introduce also notations $D_X = \mathcal{B}$ and $\Delta X_h = K_h$ in the reference configuration.

Additionally, we determine a domain for time as $D_T = \bigcup_q \Delta T_q$, where ΔT_q are time intervals on which a time averaging is realized.

Solving Equations (9), (10) of the elementary dynamical system we obtain solutions $u_i(t), t \in D_T, i \in I_N$. We would like to describe evolution of $\{u_i(t)\}$ in a simplified way. We have assumed that such a process can be decomposed into slowly and quickly varying parts. In order to realize such a decomposition we introduce a set of values $\bar{u}_h(t_q)$ corresponding to processes $\mathbf{u}(t)$. They represent averaged displacements of the h^{th} subsystem with respect to the reference configuration defined by $\{X_h\}$, for chosen time instants $t_q \in \Delta T_q$.

Let $u(X,t)$ be a function defined on $D_X \times D_T$ with properties $u(X_i,t) = u_i(t)$. Values $u(X,t)$ for $X \neq X_i$ are determined by means of broken lines which join the values determined previously. Considering such a function is a technical step for

realization integration in what follows. We introduce $\bar{u}_h(t_q)$ with the aid of the formula:

$$\bar{u}_h(t_q) = \frac{1}{|\Delta X_h|\,|\Delta T_q|}\int_{\Delta X_h}\int_{\Delta T_q} u(X,t)dXdt, \tag{11}$$

where $|\Delta X_h|$ and $|\Delta T_q|$ stand for lengths of corresponding intervals. Transformation which realizes (11) is denoted by $A_{TX}(\{u_i(t)\}) = \{\bar{u}_h(t_q)\}$.

In the next step we introduce mappings I_{uT} and I_{uX} which assign continuous fields $\bar{u}(X,t)$ determined on the domain $D_X \times D_T$ to the set $\{\bar{u}_h(t_q)\}$. This is realized in two stages by:

$$I_{uT}(\{\bar{u}_h(t_q), h = const\}) = \bar{u}_h(t), \quad t \in D_T \tag{12}$$

and

$$I_{uX}(\{\bar{u}_h(t), t = const\}) = \bar{u}(X,t), \quad X \in D_X. \tag{13}$$

Thereby, the mapping I_{uT} introduces continuous fields on the domain D_T and I_{uX} does the same for each $t \in D_T$ on the domain D_X.

In the discussed here example I_{uT} and I_{uX} are determined by application of one-dimensional finite element representation of order two with division into finite elements given by points t_q for I_{uT} and X_h for I_{uX}. Illustration of results of acting I_{uX} is shown in Figure 2.

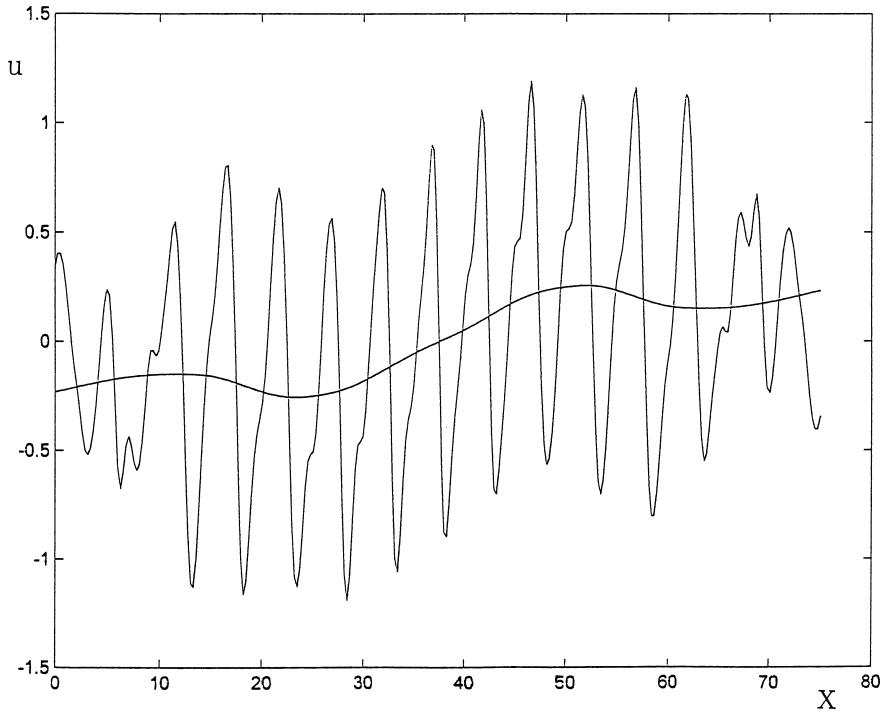

Figure 2. Averaged displacements obtained by means of the mapping I_{uX}

Summarizing, we have realized a procedure which leads from solutions of EDS by averaged set of discrete values to a continuum field defined on the body.

The field $\bar{u}(X,t)$ enables realization of decomposition of the displacements related to the elementary dynamical system by means of the formula:

$$u_i(t) = \bar{u}_i(t) + \delta u_i(t), \quad \bar{u}_i(t) = \bar{u}(X_i,t). \tag{14}$$

Then, we call the process $\bar{u}_i(t)$ as slowly varying and $\delta u_i(t)$ as quickly varying one that defines SQ-decomposition.

Let $D(\bar{u}(X,t)) = \{\bar{u}_i, \delta u_i, \dot{\bar{u}}_i, \delta \dot{u}_i\} = u_{SQ}$ assign components of SQ-decomposition to our averaged continuous configuration. Let $\pi_{uv\theta} = \{\pi_u, \pi_v, \pi_\theta\}$, $\pi_u(u_{SQ}(t)) = \{\bar{u}(X_h,t)\} = \{\bar{u}_h(t)\}$, $\pi_v(u_{SQ}(t)) = \{\dot{\bar{u}}(X_h,t)\} = \{\bar{v}_h(t)\}$ and $\pi_\theta(u_{SQ}) = \theta = \{\theta_h(t)\}$ for each t.

The first two mappings are defined by means of previously introduced field $\bar{u}(X,t)$. The mapping π_θ is aimed at determining averaged effects related to evolution of quickly varying part $\delta u_i(t)$ of EDS solution. In order to obtain a possibly simple description we postulate the variable as proportional to energy associated with the quickly varying process. Consequently, we define $\theta_h = \frac{1}{C_\theta} E_{Qh}$, where E_{Qh} is energy associated with quickly varying processes assigned to h^{th} subsystem. Then, $\frac{1}{C_\theta}$ stands for constant of proportionality. The method of determination of E_{Qh} will be discussed in what follows.

Finally, we have obtained new variables $\mathbf{d} = \{\bar{u}_h, \bar{v}_h, \theta_h\}$ of the dimensionally reduced dynamical system. Space of processes $\mathbf{d}(t), t \in T$ is denoted by $\bar{V}_T$ in the sequel.

Using the above introduced mappings we define $\pi_T : V_T \to \bar{V}_T$ as:

$$\pi_T = \pi_{uv\theta} \circ D \circ I_{uX} \circ I_{uT} \circ A_{TX}. \tag{15}$$

Summarizing, we have defined the mapping π_T which introduces new variables on the dimensionally reduced level of description.

The second problem is connected with postulating the form of the skeletal dynamical system having at our disposal new variables. The starting point for doing this is a balance of energy equation. Consequently, we should discuss a general form of such an equation in relation to SQ-decomposition. To this end let us carry out some general considerations.

Let us consider evolution of a system of material points described by an elementary dynamical system with variables $\varphi = \{\mathbf{q}, \mathbf{v}\}$, where $\mathbf{q} = \{\mathbf{q}_G, \mathbf{q}_C\} \in V_{TG} \times V_{TC}$. Variables $\mathbf{q}_G = \{\mathbf{q}_g\}$ represent a subsystem, called further G, which interacts with another minimal subsystem represented by $\mathbf{q}_C = \{\mathbf{q}_c\}$ and called further C, in such a way that the potential energy $V(\mathbf{q}_G, \mathbf{q}_C)$ is entirely determined. In other words, the set of variables $\{\mathbf{q}_c\}$ is minimal for determination of the potential energy for the subsystem G. We introduce also forces $\mathbf{f}_G = \{\mathbf{f}_g\}$.

Let us consider the balance of energy related to the elementary dynamical system:

$$\sum_g \left[m_g \frac{d^2 \mathbf{q}_g}{dt^2} \dot{\mathbf{q}}_g + \frac{\partial V}{\partial \mathbf{q}_g}(\mathbf{q}_G, \mathbf{q}_C) \dot{\mathbf{q}}_g \right] + \sum_c \frac{\partial V}{\partial \mathbf{q}_c} \dot{\mathbf{q}}_c = \sum_g \mathbf{f}_g \dot{\mathbf{q}}_g. \tag{16}$$

Assuming that we have variables decomposed into the form $\mathbf{q}_g = \bar{\mathbf{q}}_g + \delta\mathbf{q}_g$ and $\mathbf{q}_c = \bar{\mathbf{q}}_c + \delta\mathbf{q}_c$ in accordance with SQ-decomposition and similar decomposition for forces we rewrite the Equation (16) into the new form:

$$\sum_h \Bigg[\sum_{g\in I_h} \Big\{ m_g \frac{d^2(\bar{\mathbf{q}}_g + \delta\mathbf{q}_g)}{dt^2} \dot{\bar{\mathbf{q}}}_g + \frac{\partial V}{\partial \bar{\mathbf{q}}_g}(\mathbf{q}_G, \mathbf{q}_C)\dot{\bar{\mathbf{q}}}_g +$$

$$+ m_g \frac{d^2(\bar{\mathbf{q}}_g + \delta\mathbf{q}_g)}{dt^2} \delta\dot{\mathbf{q}}_g + \frac{\partial V}{\partial \delta\mathbf{q}_g}(\mathbf{q}_G, \mathbf{q}_C)\dot{\delta\mathbf{q}}_g \Big\} \Bigg] + \sum_m \sum_{c\in I_m} \left\{ \frac{\partial V}{\partial \bar{\mathbf{q}}_c}\dot{\bar{\mathbf{q}}}_c + \frac{\partial V}{\partial \delta\mathbf{q}_c}\delta\dot{\mathbf{q}}_c \right\} - \quad (17)$$

$$- \sum_h \sum_{g\in I_h} (\bar{\mathbf{f}}_g + \delta\mathbf{f}_g)\dot{\bar{\mathbf{q}}}_g - \sum_h \sum_{g\in I_h} (\bar{\mathbf{f}}_g + \delta\mathbf{f}_g)\delta\dot{\mathbf{q}}_g = 0,$$

where summation using h and m is interpreted as summation in relation to averaged description.

We are aimed to obtain some premises for discussion of a general form of the balance of energy equation for SQ decomposition. To do so let us distinguish some parts of the Equation (17) in order to separate segments corresponding to SQ-decomposition. Terms related to external interactions suggest distinguishing the following parts:

$$\sum_h \sum_{g\in I_h} (\bar{\mathbf{f}}_g + \delta\mathbf{f}_g)\dot{\bar{\mathbf{q}}}_g + \sum_h \sum_{g\in I_h} (\bar{\mathbf{f}}_g + \delta\mathbf{f}_g)\delta\dot{\mathbf{q}}_g \equiv R_S + R_Q. \quad (18)$$

The component R_S is equal to the first term on the left side of Equation (18) and R_Q is equal to the second term on the left side of this equation.

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

$$\sum_m \sum_{c\in I_m} \left\{ \frac{\partial V}{\partial \bar{\mathbf{q}}_c}\dot{\bar{\mathbf{q}}}_c + \frac{\partial V}{\partial \delta\mathbf{q}_c}\delta\dot{\mathbf{q}}_c \right\} = W_{SGC} + W_{QGC} = W_{GC}. \quad (19)$$

Then, W_{GC} represents interactions between G and C subsystems. W_{SGC} and W_{QGC} are related to slowly and quickly varying processes, respectively.

Summing up this discussion we notice that the first four terms in the Equation (17) can be interpreted as time derivative of energy $\dot{E} = \dot{E}_S + \dot{E}_Q$ and could also be decomposed into S and Q parts. Furthermore, we have $R = R_S + R_Q$ and $W_{GC} = W_{SGC} + W_{QGC}$.

The above considerations allow to modify the general form of balance of energy equation (5) for group of subsystems $I_G \subset I_P$ discussed in Subsection 2.2, to the case related to the SQ-decomposition in the following way:

$$\sum_{h\in I_G} (\dot{E}_h - R_{Sh} - R_{Qh} + \sum_{m\in I_O} (W_{Shm} + W_{Qhm})) = 0 \ , \quad (20)$$

having also premises for postulating $\dot{E}_h$ from Eqution (17). In particular we can take into account the decomposition $\dot{E}_h = \dot{E}_{Sh} + \dot{E}_{Qh}$ in the first approximation and next postulate conjugations between these terms by plotting introduced constants with the whole set of variables considered for SDS.

Let us return to our example. Now we have at our disposal a general form of balance of energy equation (20). In order to define the skeletal dynamical system we postulate the form of quantities which appear in this equation as follows:

$$E_h = M_h e_h + \mathcal{T}_h, \tag{21}$$

where M_h is the total mass assigned to h^{th} subsystem. We assume furthermore that the balance of mass equation takes the form $\dot{M}_h = 0$. This leads to simplification in calculation of time derivative of energy. We have then $\dot{E}_h = \dot{M}_h e_h + M_h \dot{e}_h + \dot{\mathcal{T}}_h = M_h \dot{e}_h + \dot{\mathcal{T}}_h = \dot{E}_{Mh} + \dot{\mathcal{T}}_h$.

Variables of our dimensionally reduced dynamical system take the form $\mathbf{d} = \{\{\bar{u}_h, \bar{v}_h, \theta_h\} : h \in I_G\}$. We also define $a_h = \bar{u}_{h+1} - \bar{u}_h$, $b_h = \theta_{h+1} - \theta_h$ and $\theta_{Ah} = \frac{1}{2}(\theta_h + \theta_{h+1})$.

We postulate further that

$$E_{Mh} = C_1(\theta_{Ah}) a_h^2 + C_2 \theta_{Ah} a_h + C_3(\theta_{Ah}) \theta_h, \tag{22}$$

$$\mathcal{T}_h = \frac{1}{2} M_h \dot{u}_h^2. \tag{23}$$

With the aid of Equations (22) and (23) the balance of energy equation (20) can be expressed by:

$$\begin{aligned} &\sum_h \Big(\frac{\partial C_1}{\partial \theta_{Ah}} a_h^2 \dot{\theta}_{Ah} + 2C_1 a_h \frac{\partial a_h}{\partial \bar{u}_p} \dot{\bar{u}}_p + C_2 a_h \dot{\theta}_{Ah} + C_2 \theta_{Ah} \frac{\partial a_h}{\partial \bar{u}_p} \dot{\bar{u}}_p + \frac{\partial C_3}{\partial \theta_{Ah}} \theta_h \dot{\theta}_{Ah} + \\ &+ C_3 \dot{\theta}_h + \sum_h (M_h \ddot{\bar{u}}_h - \bar{f}_h) \dot{\bar{u}}_h) + \sum_h \left(\sum_m W_{Qhm} - R_{Qh} \right) + \sum_{h,m} W_{Shm} = 0, \end{aligned} \tag{24}$$

where $R_{Sh} = \bar{f}_h \dot{\bar{u}}_h$ is additionally postulated and the summation convention is applied for the index p.

The Equation (24) can be transformed into the next, more convenient form:

$$\begin{aligned} &\sum_{h \in I_G} \left(\frac{\partial C_1}{\partial \theta_{Ah}} a_h^2 + C_2 a_h + \frac{\partial C_3}{\partial \theta_{Ah}} \theta_h \right) \dot{\theta}_{Ah} + \\ &+ \sum_{h \in I_G} \left[\sum_{l \in I_G} \left(2C_1 a_l \frac{\partial a_l}{\partial \bar{u}_h} + C_2 \theta_{Al} \frac{\partial a_l}{\partial \bar{u}_h} \right) - \bar{f}_h + M_h \ddot{\bar{u}}_h \right] \dot{\bar{u}}_h + \\ &+ \sum_{h \in I_G} \left[C_3 \dot{\theta}_h + \sum_m (W_{Qhm}) - R_{Qh} \right] + \sum_{l \in I_G} \sum_{m \in I_O} (H_{lm} - \bar{f}_{Slm}) \dot{\bar{u}}_m = 0, \end{aligned} \tag{25}$$

where $W_{Slm} = -\bar{f}_{Slm} \dot{\bar{u}}_m$ is postulated and $H_{lm} = 2C_1 a_l \frac{\partial a_l}{\partial \bar{u}_m} + C_2 \theta_{Al} \frac{\partial a_l}{\partial \bar{u}_m}$.

We assume that processes $\dot{\bar{u}}_h$ and $\dot{\theta}_{Ah}$ are independent. Then, from Equation (25) we obtain

$$\frac{\partial C_1}{\partial \theta_{Ah}} a_h^2 + C_2 a_h + \frac{\partial C_3}{\partial \theta_{Ah}} \theta_h = 0. \tag{26}$$

Taking into account that $\frac{\partial a_l}{\partial \bar{u}_h} = -1$ for $l = h$ and $\frac{\partial a_l}{\partial \bar{u}_h} = 1$ for $l = h-1$ we obtain also the equations:

$$\dot{\bar{u}}_h = \bar{v}_h, \tag{27}$$

$$M_h \dot{\bar{v}}_h = C_S(a_h - a_{h-1}) + \frac{\beta}{2}(b_h + b_{h-1}) + \bar{f}_h, \tag{28}$$

where $C_S = 2C_1$ and $\beta = C_2$.

We postulate furthermore the constitutive equation $W_{Qhm} = -C_\theta b_{h-1}$ for $m = h-1$ and $W_{Qhm} = C_\theta b_h$ for $m = h+1$. Then, assuming that the Equations (26) and (28) are satisfied and $I_G = \{h\}$ contains one element only, we obtain from Equation (25) additionally that

$$C_3\dot{\theta}_h = -C_\theta(b_h - b_{h-1}) + R_{Qh}. \tag{29}$$

Equations (27)–(29) are postulated equations of the skeletal dynamical system in our example. We assume that $C_3 = 1$ and $R_{Qh} = 0$ in the sequel.

Having the skeletal dynamical system we tend towards obtaining the reduced dynamical system in accordance with scheme presented in Figure 1. Constants C_S, β and C_θ which appear in Equations (27)–(29) are determined by comparison of solutions of the elementary dynamical system with those obtained by means of SDS for some given constants. Then, option of the best constants is accomplished with the help of a functional which is a measure of a distance between discussed solutions in the space $\bar{V}_T$.

In order to compare such solutions we have first to transform processes of EDS into $\bar{V}_T$ by means of $\pi_T = \{\pi_{Tu}, \pi_{Tv}, \pi_{T\theta}\}$. This decomposition is defined by means of mappings π_u, π_v, π_θ which appear in definition of π_T given by (15).

The mapping π_{Tu} is realized in the way described by expressions (11)–(13). The same procedure is applied for π_{Tv}. Thereby, we have independently realized averaging for $\bar{v}_h$ and for $\bar{u}_h$. The mapping $\pi_{T\theta}$ is based on previously introduced SQ-decomposition. Then we are able to calculate total energy E_{Th} related to each subsystem and using slowly varying parts of $\mathbf{u}$ and $\mathbf{v}$ we can calculate corresponding energy E_{Sh} assigned to each subsystem. Then, $\theta_h = E_{Qh}/C_\theta$, where $E_{Qh} = E_{Th} - E_{Sh}$ and $C_\theta = 1$ for simplicity.

We define the following functional:

$$\begin{aligned} H = \sum_h \sum_q [&(\bar{u}_h(t_q) - \pi_h \circ \pi_{Tu}(\{\mathbf{u},\mathbf{v}\})(t_q))^2 + \\ &+ (\bar{v}_h(t_q) - \pi_h \circ \pi_{Tv}(\{\mathbf{u},\mathbf{v}\})(t_q))^2 + (\theta_h(t_q) - \pi_h \circ \pi_{T\theta}(\{\mathbf{u},\mathbf{v}\})(t_q))^2], \end{aligned} \tag{30}$$

where π_h is projection into h^{th} subsystem.

Solutions of the elementary dynamical system are obtained for larger system of material points than that corresponding to SDS. A number of subsystems has been applied for realization of SQ-decomposition for calculation of second order derivatives in order to use finite element basis of second order. Some subsystems are also lost during calculation $\bar{u}_h(t_q)$ in accordance with (11). Consequently, the range of summation in (30) is smaller than the total number of subsystems. Evolution of SDS has been calculated with initial conditions defined by the mapping π_T and solutions of EDS using a number of neighbouring subsystems. Boundary conditions for solution of SDS have been maintained in accordance with solutions of EDS also with the help of some external subsystems.

The number of masses for the elementary dynamical system in our example is $N = 800$. The number of subsystems $N_P = 20$. Furthermore, we have considered the number of time steps $N_T = 380$ for solution of EDS and the number of time intervals for averaging with respect to time, $N_{TP} = 19$.

The minimum of the functional (30) has been obtained for $C_S = 0.034$, $\beta = -1.285$ and $C_\theta = -2.88$. Solutions of the elementary dynamical system and the reduced dynamical system are shown in Figure 3 for displacements and in Figure 4 for velocities at a time instant. Similar solutions are shown for another time instant in Figures 5 and 6. In these figures we can observe parallel evolution of the elementary dynamical system and the reduced dynamical system. Thereby, we can estimate how a reduced dynamical system represents averaged properties of EDS.

Let us notice that we have not introduced continuous fields on discussed continuum in fact. The skeletal dynamical system is considered rather as a discrete system. We are able to introduce continuous fields in a similar way as for SQ decomposition using finite element representations for instance. However, this is not necessary since we do not need such fields at this moment. This induces a discussion whether such continuous fields are necessary at all. Continuous fields can be useful in case of modelling interactions between subsystems when values of fields should be determined in points of interactions changing with time. Furthermore, distribution of fields by their densities can improve precision of calculations. By means of mass density we can model more precisely inertia effects for instance. Summarizing, continuous fields can be applied if we choose the way of improving precision of modelling by using such fields or when we must have at our disposal values of fields at intermediate distinguished points different than those initially introduced.

4. Final remarks

Various aspects of continuum mechanics and molecular dynamics are considered in literature. Let us mention calculation of thermodynamic quantities using statistical mechanics supported by molecular dynamics [2]. More direct application of molecular dynamics for creation of continuous fields is accomplished in smooth particle applied mechanics [6–8].

The method of cooperation of molecular dynamics and continuum mechanics presented in this paper is based on the dimensional reduction procedure. Consequently, we suggest multiscale modelling for integration of both methods.

The dimensional reduction procedure discussed here is at an initial stage of development. Various problems related to realization of such a procedure should be discussed for the future. Let us mention for instance methods of division of the elementary dynamical system into subsystems, premises for postulating the skeletal dynamical system, connections between dimensionally reduced variables and corresponding forces. The range of validity of applied dimensional reduction procedure seems to be the most important problem.

Complexity of processes in materials necessitates perhaps using various dimensional reduction procedures in a sequence, in order to describe their evolution. Indeed, complicated evolution can necessitate changes of models in order to obtain a satisfactory approximation. Therefore, methods of changing of dimensional reduction procedures during calculations have to be elaborated. To obtain this we just need a range of validity for such a procedure.

A possible solution of the problems mentioned above relies perhaps on introducing nanoscale continuum models as designed to direct cooperation with molecular

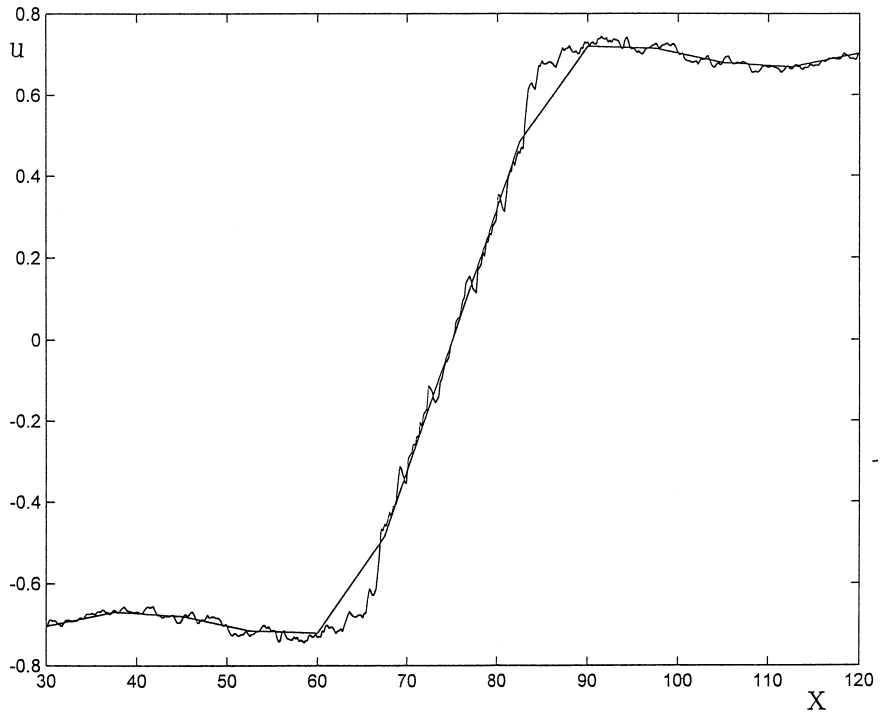

Figure 3. Comparison of solutions of EDS and SDS for displacemnts at an initial instant

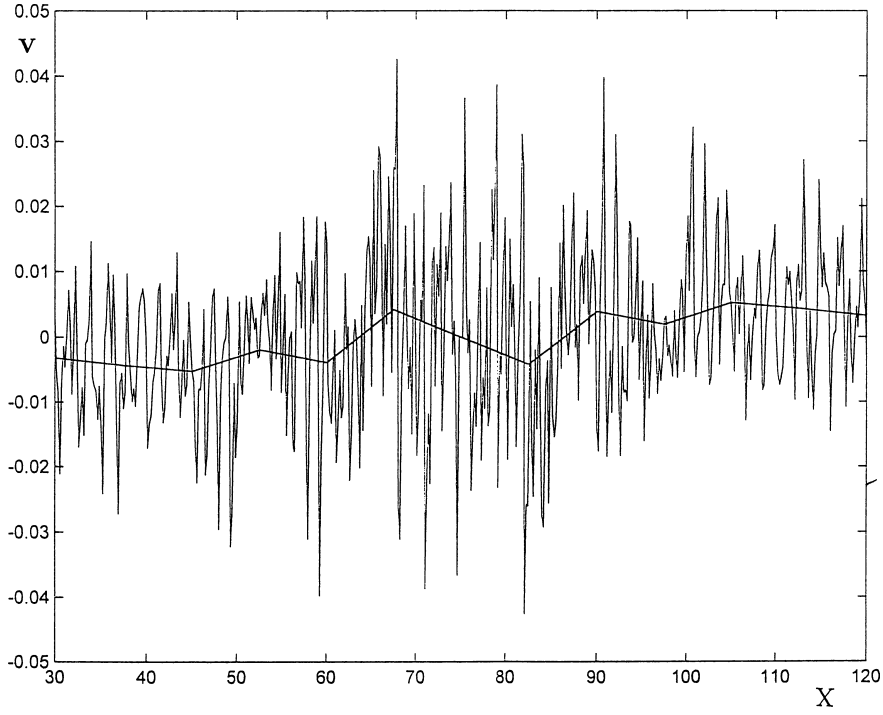

Figure 4. Comparison of solutions of EDS and SDS for velocities at an initial instant

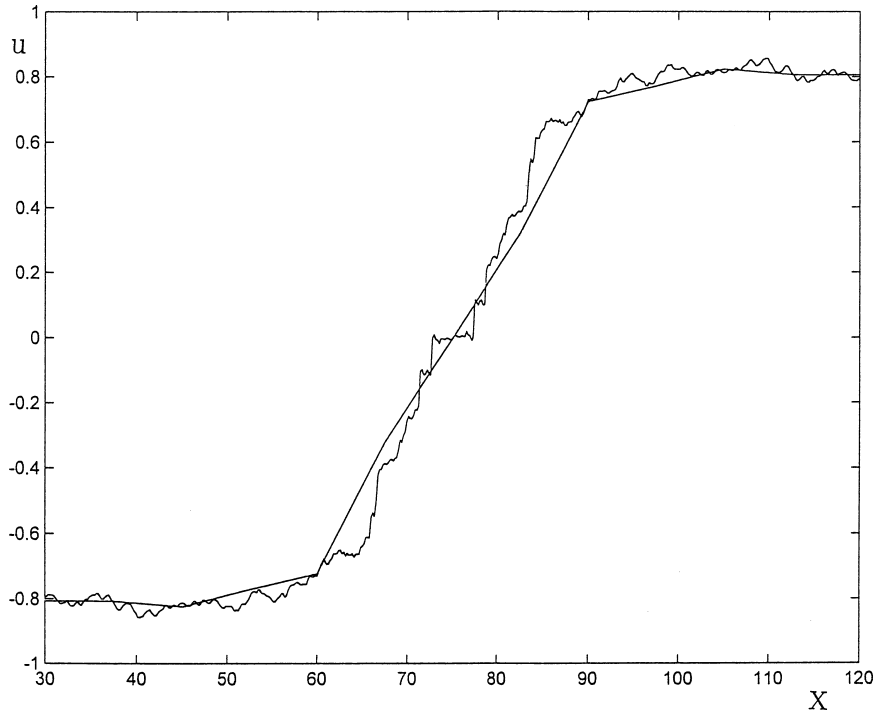

Figure 5. Comparison of solutions of EDS and SDS for displacemnts at a final instant

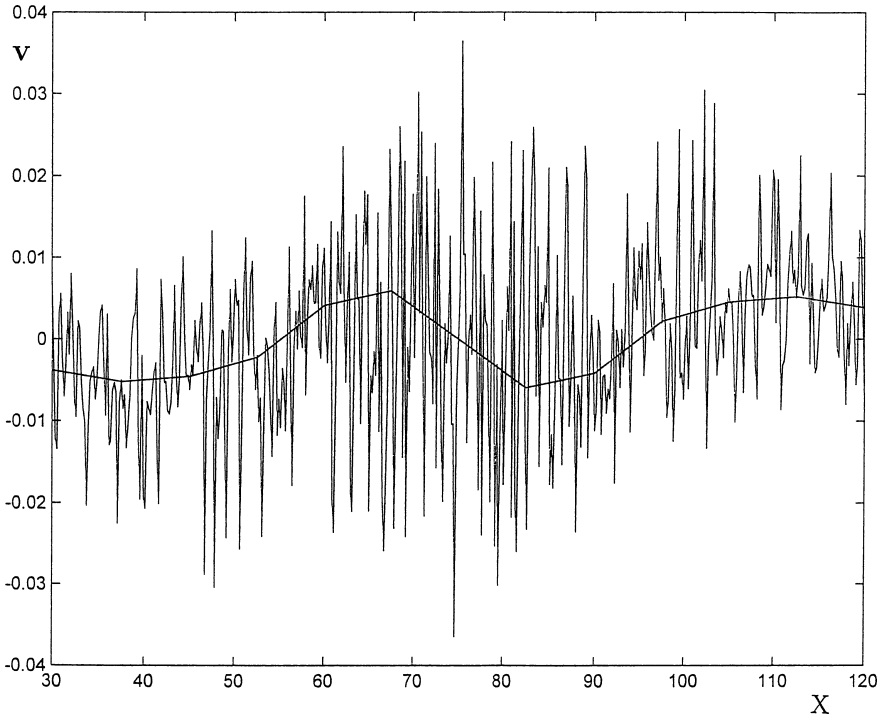

Figure 6. Comparison of solutions of EDS and SDS for velocities at a final instant

dynamics. Then, small representative volume for such models, as well as possibility of description of processes in small scale, could make the dimensional reduction procedure more simple and clear for interpretation. In the next stage, the nanoscale models considered as EDS could be averaged towards obtaining more simple continuum descriptions. Such a discussion suggests that integration of continuum mechanics and molecular dynamics needs development of continuum models related to scale close to the atomic one in order to make the transition between scales more gradual.

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