CONTINUOUS CELLULAR AUTOMATA FOR SIMULATION OF THERMOELASTICITY

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Abstract. In the paper a generalization of cellular automata algorithm is proposed to simulate some thermomechanical processes in a continuum. The essential feature of the method is the absence of any partial differential equations commonly used for the description of thermomechanical processes. Therefore, the method is rather a tool for the direct simulation of a process than for the solution of partial differential equations. One-dimensional thermoelasticity in solids is considered as an example. Calculations show that predictions of the proposed model fully coincide with those of the classical theory in the case of homogeneous solids.

Key words: cellular automata, thermodynamics, thermoelasticity.

1. INTRODUCTION

A simple approach is proposed for thermomechanical simulations, which, on the one hand, is based on cellular automata technique and, on the other hand, on thermodynamic laws. The basic ideas are demonstrated on the example of the one-dimensional thermoelasticity. This is a well-known coupled problem in the simplest form.

It is widely known that a cellular automaton is an array of identically programmed automata, or "cells", which interact with one another [1]. An essential feature of a cellular automaton is its state. As a rule, the state of a cell is considered as a set of numbers or properties. The other essential feature is the program, which is the set of rules that define how the state of a cell changes in response to its current state and that of its neighbours.

However, from the thermodynamic point of view, we cannot arbitrarily change the states of elements of a continuum, because these changes should satisfy

the first and the second law of thermodynamics. Thermodynamic concepts are usually introduced into mechanical problems by means of the hypothesis of local equilibrium [2, 3]. Such a hypothesis is needed to assign the entropy and thermodynamic temperature of an accompanying equilibrium state to a non-equilibrium state of an element of a continuum. However, some properties of the thermodynamic parameters expose themselves only in the Gibbsian state space. In particular, each thermodynamic parameter should have the property to be a function of state. Such a feature is often lost by the pure mechanical description. Namely, as shown by Chen and Eu [4], there is no possibility that entropy will become a function of state in the physical space. Therefore, it seems more convenient to have for practical calculations a direct description of the coupled thermodynamic behaviour for the finite amount of interacting elements or cells. The difficulty here, as noted by Truesdell and Bharatha [5], is that "the formal structure of classical thermodynamics describes the effects of changes undergone by some single body. While it allows these effects for one body to be compared with corresponding effects for another body, it does not represent the effects associated with two bodies simultaneously or in any way conjointly."

In this paper an attempt is made to overcome these difficulties and to offer a pure thermodynamic way to describe the simultaneous evolution for a finite count of elements. In the case of a homogeneous medium, such a description should be independent of size, shape, and amount of elements chosen. Therefore, the problem of thermodynamic descriptivity arises: to determine the conditions of the consistency between thermodynamic descriptions for the same medium by means of different partitions. This problem is briefly considered in the 2nd part of the paper. The conditions of thermodynamic descriptivity are deduced from the property of internal energy to be a function of state.

An algorithm for the calculation of thermoelastic processes in a continuum is elaborated on the basis of such a method of description. It is shortly described in the 3rd part of the paper, where the one-dimensional thermoelasticity problem is considered as an example. Results of calculations for thermoelastic wave propagation are presented as well.

Some conclusions concerning the energy redistribution due to interaction are given in the 4th part.

2. THERMODYNAMIC BACKGROUND

We consider a one-dimensional thermoelasticity problem, formulated as follows: What is the character of distributions of stress and temperature in the layer placed between parallel surfaces, each of which has its own specified course of the variation of temperature and stress. As will be shown below, the method of calculation is based on the interaction between neighbouring elements or cells.

In thermodynamic terms, the problem of the interaction between neighbouring elements can be expressed as follows: What can we tell about the state of system 2, placed between systems 1 and 3, if states of systems 1 and 3 are known?

To answer this question, we begin with a simpler thermodynamic situation. Let us consider two interacting homogeneous thermodynamic systems 1 and 2, each of which is characterized by the same equations of state. Let the states of systems 1 and 2 be specified. In addition, we consider the thermodynamic system 1–2, containing both system 1 and system 2. The problem to solve is to determine the values of parameters of the integral system remaining at the thermodynamic level of description.

The most general way to characterize the system is to determine its internal energy

$$dU_{12} = dU_1 + dU_2 - dE_{1-2}, \tag{1}$$

where E_{1-2} is the energy of interaction between subsystems 1 and 2, which is considered as a function of state.

Owing to the additivity of energy, we can divide the interaction energy into two parts which correspond to each subsystem and rewrite the expression for energy variation in the form

$$dU_{12} = dU_1 + dU_2 + dE_1 + dE_2. \tag{2}$$

The obtained condition of energy conservation is too general for direct applications, even if the energies of interaction are specified. To have more convenient conditions, we take the property of energy to be a function of state into account. This property allows us to compare the sum of total differentials of energy for subsystems with an analogous total differential for the system as a whole, expressed by the same variables T, V, M, where T is temperature, V is volume, M is mass. Such a comparison leads to the conditions of thermodynamic descriptivity in the form [6, 7]

$$\left(\frac{\partial U_{12}}{\partial V_{12}}\right)_{T,M} = \left(\frac{\partial (U_1 + E_1)}{\partial V_1}\right)_{T,M} = \left(\frac{\partial (U_2 + E_2)}{\partial V_2}\right)_{T,M}. \tag{3}$$

This condition ensures the equivalence between the thermodynamic description on the level of subsystems and that on the level of the integral system. The state of the integral system is completely determined if the energies of interaction are given. It is natural that the energy of interaction depends on the kind of the process performed. We shall restrict ourselves to the one-dimensional thermoelasticity.

3. ONE-DIMENSIONAL THERMOELASTICITY

In the classical theory of thermoelasticity the governing laws determine stresses by means of two elastic parameters λ, μ (or Young's modulus E, and Poisson's

ratio, ν) and linear expansion coefficient α (all these quantities are supposed to be constant) [8, 9]

$$\sigma_{ij} = [\lambda\varepsilon_{kk} - \alpha(3\lambda + 2\mu)(T - T_0)]\delta_{ij} + 2\mu\varepsilon_{ij}, \tag{4}$$

where σ_{ij} and ε_{ij} are components of stress and strain tensors, respectively. In the one-dimensional case, variations in only one direction, say, z, are considered, and Hooke's law obtains a simpler form

$$\sigma_{zz} = \lambda\varepsilon_{zz} - \alpha(3\lambda + 2\mu)(T - T_0) + 2\mu\varepsilon_{zz}. \tag{5}$$

The expression for free energy ψ per unit volume is commonly used as the equation of state for thermoelastic media [8, 9]

$$\rho\psi = \mu\varepsilon_{ij}\varepsilon_{ij} + \frac{\lambda}{2}\varepsilon_{kk}\varepsilon_{nn} - \alpha(3\lambda + 2\mu)(T - T_0)\varepsilon_{kk} - h(T). \tag{6}$$

Here ρ is the density and $h(T)$ is a certain function depending only on the temperature. The internal energy u per unit volume is more suitable for our algorithm (in its one-dimensional form)

$$\begin{aligned}
\rho u &= \rho(\psi + sT) \\
&= \mu\varepsilon_{zz}^2 + \frac{\lambda}{2}\varepsilon_{zz}^2 + \alpha(3\lambda + 2\mu)T_0\varepsilon_{zz} + Th'(T) - h(T), \tag{7}
\end{aligned}$$

where s is entropy per unit volume. It follows from relations (5) and (7) that

$$\left(\frac{\partial u}{\partial \varepsilon_{zz}}\right)_T = \frac{1}{\rho}\left[\sigma_{zz} - T\left(\frac{\partial \sigma_{zz}}{\partial T}\right)_{\varepsilon_{zz}}\right]. \tag{8}$$

The last expression can be coupled with the derivatives contained in the thermodynamic descriptivity conditions (3), while in the one-dimensional case

$$\left(\frac{\partial U}{\partial V}\right)_{T,M} = \left(\frac{\partial u}{\partial v}\right)_T = \frac{1}{v}\left(\frac{\partial u}{\partial \varepsilon_{zz}}\right)_T, \tag{9}$$

where v is specific volume.

We start with the case of pure elasticity. This means that the influence of temperature is neglected, i.e., $T = T_0 = \text{const}$. We divide the layer into n sublayers which represent one-dimensional cells. We identify the state of each cell with the thermodynamic state of the corresponding sublayer.

Returning to the problem of interaction between three neighbouring elements, we should apply the thermodynamic descriptivity conditions to systems 1 and 2, as well as to systems 2 and 3, simultaneously

$$\sigma_1 + \left(\frac{\partial e_{12}}{\partial v_1}\right)_T = \sigma_2 + \left(\frac{\partial e_{21}}{\partial v_2}\right)_T, \quad \sigma_3 + \left(\frac{\partial e_{32}}{\partial v_3}\right)_T = \sigma_2 + \left(\frac{\partial e_{23}}{\partial v_2}\right)_T, \tag{10}$$

where e_{ij} is the interaction energy per unit mass for the system i with respect to the system j.

Let, for definiteness, the elastic signal propagate in the direction from system 1 to system 2. This means, in particular, that $\sigma_1 \neq \sigma_2$, while $\sigma_2 = \sigma_3 = 0$. In the purely elastic case the action of system 1 with respect to system 2 is the same as the action of system 2 with respect to system 1, i.e.,

$$\left(\frac{\partial e_{21}}{\partial v_2}\right)_T = \left(\frac{\partial e_{12}}{\partial v_1}\right)_T, \tag{11}$$

and, therefore, in the next time step the stress in system 2 becomes equal to the stress in system 1

$$\sigma_2^{(k+1)} = \sigma_1^{(k)}. \tag{12}$$

Here superscripts denote the corresponding time step.

We apply this rule of updating cell's states for the layer excited by an impulse on the boundary. We suppose that in the initial situation all sublayers were free from stresses.

In Fig. 1a the propagation of an elastic pulse across a homogeneous copper layer is represented. Since dissipation is absent, the initial form of the impulse is conserved in full correspondence with the classical theory. In the case of a heterogeneous layer, the first half of which is of copper and the second one of aluminium, we obtain a partial reflection of the impulse if stresses and displacements on the interface are equal (Fig. 1b).

In the case of thermoelasticity both stresses and temperatures are significant

$$\left(\frac{\partial u}{\partial v}\right)_T = \rho \left(\frac{\partial u}{\partial \varepsilon_{zz}}\right)_T = \sigma_{zz} - T\left(\frac{\partial \sigma_{zz}}{\partial T}\right)_{\varepsilon_{zz}}. \tag{13}$$

The local thermodynamic descriptivity conditions include the elastic

$$\sigma_1 - T_1 \left(\frac{\partial \sigma_1}{\partial T_1}\right)_{\varepsilon_1} = \sigma_2 - T_2 \left(\frac{\partial \sigma_2}{\partial T_2}\right)_{\varepsilon_2}, \tag{14}$$

and the thermal part [6, 7]

$$T_2 \left(\frac{\partial \sigma_2}{\partial T_2}\right)_{\varepsilon_2} = \frac{1}{2}\left[T_1\left(\frac{\partial \sigma_1}{\partial T_1}\right)_{\varepsilon_1} + T_3\left(\frac{\partial \sigma_3}{\partial T_3}\right)_{\varepsilon_3}\right]. \tag{15}$$

If we apply these conditions as the rules of updating cell's states by thermal shock, when the temperature of one of the boundaries is impulsively shifted to a fixed temperature $2T_0$, then an elastic wave is generated and will propagate across the layer. As we can see in Fig. 2a, the influence of temperature is significant only in the neighbourhood of the heated boundary, since the corresponding temperature distribution is far from equilibrium (Fig. 2b).
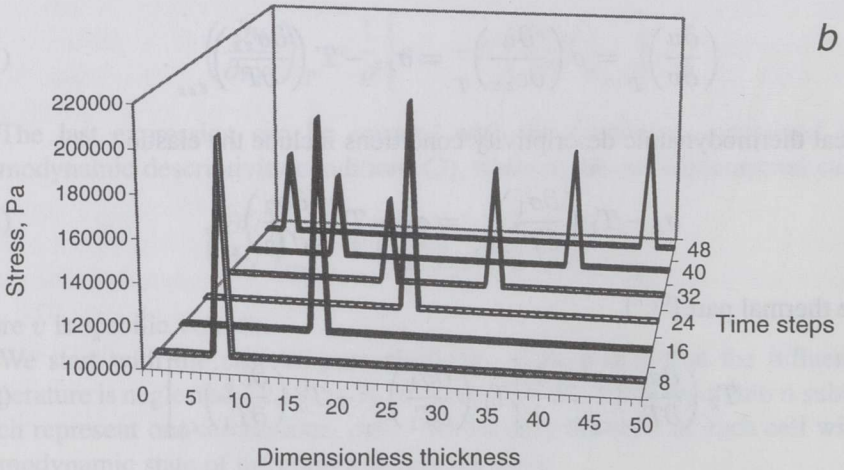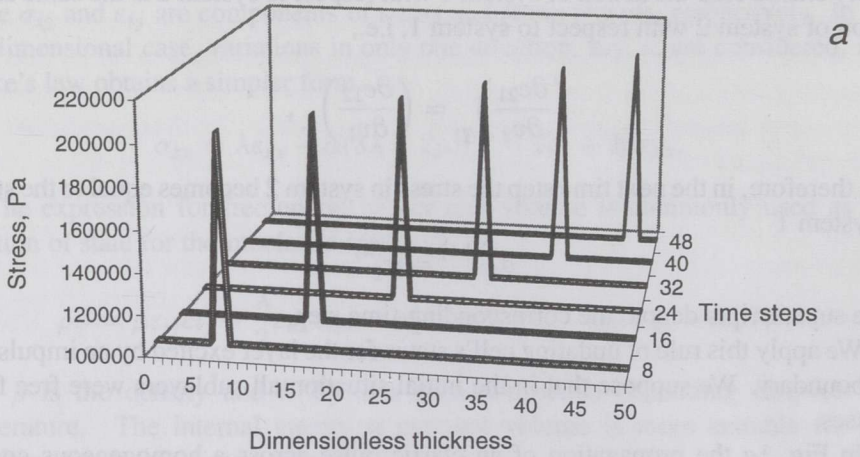
Fig. 1. Elastic wave propagation across a solid layer: *a,* homogeneous; *b,* heterogeneous.

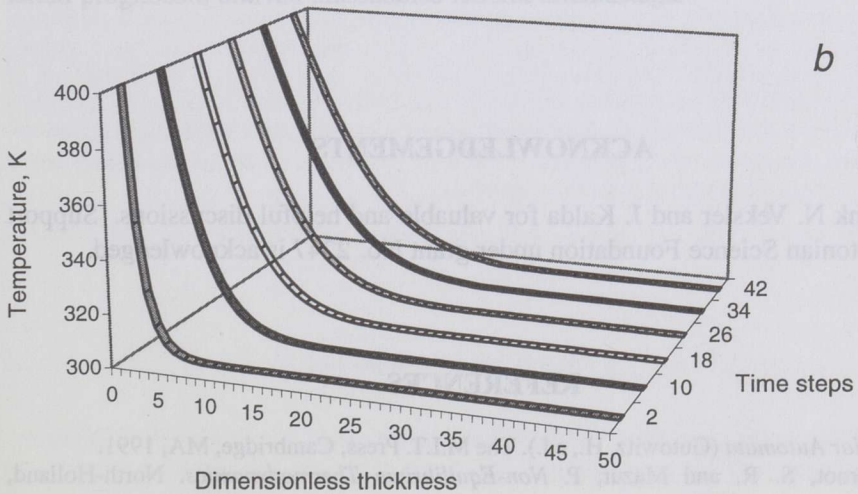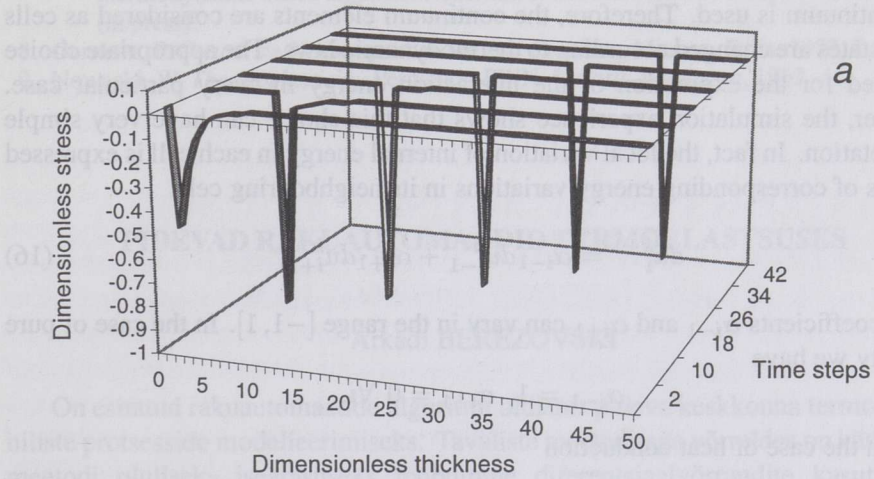Fig. 2. Thermoelastic wave propagation across a solid layer: *a*, wave profiles; *b*, temperature evolution.

4. CONCLUSIONS

The proposed method is a tool for the direct simulation of mechanical processes rather than for the solution of partial differential equations. In this method, the correspondence between points in the Gibbsian phase space and states of elements in a continuum is used. Therefore, the continuum elements are considered as cells whose states are changed according to thermodynamic laws. The appropriate choice is needed for the expression of the interaction energy in every particular case. However, the simulation experience shows that this choice can have very simple interpretation. In fact, the local variation of internal energy in each cell is expressed in terms of corresponding energy variations in its neighbouring cells

$$du_i^{k+1} = \alpha_{i-1} du_{i-1}^k + \alpha_{i+1} du_{i+1}^k, \tag{16}$$

where coefficients α_{i-1} and α_{i+1} can vary in the range $[-1, 1]$. In the case of pure elasticity we have

$$\alpha_{i-1} = 1, \ \alpha_{i+1} = 0 \ \forall i,$$

while in the case of heat conduction

$$\alpha_{i-1} = \alpha_{i+1} = \frac{1}{2} \ \forall i.$$

Therefore, the local interaction between cells can be characterized by means of two parameters, which should be chosen from physical considerations.

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PIDEVAD RAKUAUTOMAADID TERMOELASTSUSES

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On esitatud rakuautomaatide algoritmi üldistus pideva keskkonna termomehaaniliste protsesside modelleerimiseks. Tavaliste meetoditega võrreldes on käsitletava meetodi oluliseks iseärasuseks loobumine diferentsiaalvõrrandite kasutamisest termomehaaniliste protsesside kirjeldamisel. Meetod on seega protsesside modelleerimise vahend, aga mitte diferentsiaalvõrrandite lahendusmeetod.

Rakendusnäitena on vaadeldud tahke keha ühemõõtmelist termoelastsust. Homogeensete tahkete kehade puhul näitavad arvutused, et esitatud mudeli kohaselt leitud prognoosid ühtivad klassikalise teooria tulemustega.