

Thermoelastic wave propagation in inhomogeneous media

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694

Summary A novel approach to the modeling of thermoelastic wave propagation is presented, based on the thermodynamics of discrete systems. The first novelty includes the representation of integral balance laws for thermoelasticity in terms of contact quantities that describe the nonequilibrium state of elements. The next new aspect is a modification of the recently proposed wave-propagation algorithm, which is used as a tool for determining the contact quantities in a finite-volume scheme for the numerical simulation of two-dimensional thermoelastic wave propagation in inhomogeneous media. Such a modification is needed to provide the satisfaction of the thermodynamic consistency conditions between adjacent discrete elements. Results of computations for certain test problems show the efficiency and physical consistency of the algorithm.

Key words Thermoelastic wave, numerical simulation, discrete system

1

Introduction

It is only recently that the question of conceiving an accurate numerical scheme for thermoelasticity has been raised again in conjunction with the problem of the simulation of the propagation of phase-transition fronts in crystalline substances, [1]. With this problem in mind, the authors have developed a numerical scheme starting with the case of materially inhomogeneous thermoelastic conductors with smooth or abrupt property variations, and neglecting phase changes at this stage. The present paper shows that the ideas of (i) the finite-volume method, and (ii) the thermodynamics of discrete systems can be combined in this framework to provide a physically consistent algorithm for the numerical simulation of thermoelastic wave propagation in inhomogeneous media.

It should be noted that the derivation, analysis and implementation of approximate solutions to conservation laws and related problems have been all the major foci of an enormous amount of activities in recent decades [2, 3]. Many algorithms have been developed that achieve high resolution, stability and efficiency of numerical schemes. Nevertheless, it is well known that monotone (or positive) approximations are, at most of first-order accuracy [4]. The lack of monotonicity for higher-order methods is reflected by spurious oscillations in the vicinity of

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jump discontinuities. The usual way to suppress these oscillations is the introduction of certain limiter functions. However, the use of wave limiters can lead to numerical instability in the case of rapidly-varying properties of a medium, [5]. In addition, the limiters may lead to problems of the consistency between adjacent discrete elements in numerical simulation. In particular, the satisfaction of the thermodynamic consistency conditions which follow from the thermodynamics of discrete systems cannot be controlled immediately. These conditions are formulated, however, in terms of the so-called contact quantities that are basic notions in the thermodynamics of discrete systems, [6]. Therefore, in order to provide the satisfaction of these conditions, a certain reformulation of the governing equations of thermoelasticity in terms of parameters related to the discrete elements is needed. In addition, the balance laws for discrete elements should have the integral form, which leads to a finite-volume algorithm in a natural way.

The basic equations of thermoelasticity are described in Sec. 2 of the paper. Next, the concepts of the thermodynamics of discrete systems are briefly presented in Sec. 3. The extension of the concepts of the thermodynamics of discrete systems to the thermoelastic case that allows us to formulate the integral balance laws in terms of contact quantities is described in Sec. 4. Different ways for establishing the connection between bulk and contact quantities are shown in Sec. 5. In the case of heat conduction, such a connection can be deduced directly from the symmetry of the process of heat diffusion. A modification of the wave-propagation algorithm for conservation laws, [7], is successfully used for the connection between bulk and contact quantities in the case of elastic waves. At last, it is possible to eliminate the source terms in the equation of thermoelasticity following the method of balancing source terms, [8], after solving the independent equation of heat conduction. The derived algorithm is used for numerical simulation, and examples are presented illustrating the propagation of a two-dimensional thermoelastic wave in a medium with smoothly varying and piece-wise constant material properties.

2

Basic equations of thermoelasticity

We shall consider here the classical thermoelasticity of heat conductors. Neglecting geometrical nonlinearities, the main two equations of thermoelasticity are the local balance of momentum at each regular material point (in the absence of body force), [9, 10],

$$\rho_0 \frac{\partial v_i}{\partial t} - \frac{\partial \sigma_{ij}}{\partial x_j} = 0 \quad , \quad (1)$$

and the heat conduction equation

$$T \frac{\partial S}{\partial t} + \frac{\partial q_i}{\partial x_i} = 0 \quad , \quad (2)$$

where $\rho_0 = \bar{\rho}_0(\mathbf{x})$ is the density, v_i and σ_{ij} are the components of velocity and Cauchy stress tensor, respectively, t is time, T is the absolute temperature, S is the entropy per unit volume, q_i is the heat flux vector. Here, σ_{ij} , S and q_i are given by

$$\sigma_{ij} = \frac{\partial \bar{W}}{\partial \varepsilon_{ij}}, \quad S = -\frac{\partial \bar{W}}{\partial T}, \quad q_i = \bar{q}_i \left(\frac{\partial T}{\partial x_j}, \varepsilon_{kl}, T; \mathbf{x} \right) \quad ,$$

with a free energy per unit volume given by

$$W = \bar{W}(\varepsilon_{ij}, T; \mathbf{x}), \quad \varepsilon_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \quad , \quad (3)$$

while u_i are the cartesian components of the elastic displacement. In general, the indicated explicit dependence on the point \mathbf{x} means that the body is materially inhomogeneous. For the particular example, we consider linear isotropic thermoelasticity for which

$$W = W^{\text{el}} + W^{\text{th}} + W^{\text{te}} \quad , \quad (4)$$

where the three different contributions that are related to elastic energy, thermal energy and thermoelastic interaction energy, respectively, are given by

$$W^{\text{el}} = \frac{1}{2}[\lambda(\mathbf{x})\varepsilon_{kk}^2 + 2\mu(\mathbf{x})\varepsilon_{ij}\varepsilon_{ij}], \quad W^{\text{th}} = -\frac{C(\mathbf{x})}{2T_0}(T - T_0)^2, \quad W^{\text{te}} = m(\mathbf{x})(T - T_0)\varepsilon_{kk} .$$

Here, $C(\mathbf{x}) = \rho_0 c$, c is the specific heat at constant stress, T_0 is a spatially uniform reference temperature, and only small deviations from it are envisaged. The dilatation coefficient α is related to the thermoelastic coefficient m and to the Lamé coefficients λ and μ by $m = -\alpha(3\lambda + 2\mu)$. Simultaneously, we assume the Fourier law of heat conduction

$$q_i = -k(\mathbf{x})\frac{\partial T}{\partial x_i} , \quad (5)$$

where k is the thermal conductivity.

We can then rewrite the relevant bulk equations of inhomogeneous linear isotropic thermoelasticity as the following three equations of which the second one is none other than the time derivative of the Duhamel–Neumann thermoelastic constitutive equation:

$$\frac{\partial(\bar{\rho}_0(\mathbf{x})v_i)}{\partial t} - \frac{\partial\sigma_{ij}}{\partial x_j} = 0 , \quad (6)$$

$$\frac{\partial\sigma_{ij}}{\partial t} = \lambda(\mathbf{x})\frac{\partial v_k}{\partial x_k}\delta_{ij} + \mu(\mathbf{x})\left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}\right) + m(\mathbf{x})\frac{\partial T}{\partial t}\delta_{ij} , \quad (7)$$

$$\frac{\partial(C(\mathbf{x})T)}{\partial t} = \frac{\partial}{\partial x_i}\left(k(\mathbf{x})\frac{\partial T}{\partial x_i}\right) + m(\mathbf{x})T_0\frac{\partial v_k}{\partial x_k} . \quad (8)$$

From the mathematical viewpoint, the problem is to find a solution to the system (6)–(8) of equations with corresponding initial and boundary conditions. This is, in general, conceivably difficult so that an efficient numerical method is required. Obviously, numerical schemes deal with discrete elements representing a continuous body. The formulation (6)–(8) paves the way for a reformulation of the governing equations in terms of parameters related to the discrete elements. It happens that the latter can be viewed from both the numerical and thermodynamic viewpoints.

3 Discrete systems

It is salient to remind the reader of the notion of discrete systems in thermodynamics, [11, 6]. In such thermodynamics, the thermodynamic state space is extended by means of so-called contact quantities in order to describe non-equilibrium states. In this perspective, a discrete system is a domain G of \mathbf{R}^3 that is separated from its environment G^* by a partition ∂G . The interaction between G and G^* is described by contact quantities. In a Schottky system per se, this interaction consists of heat, work and mass exchanges. For instance, considering heat exchange \dot{Q} , the so-called contact temperature Θ is defined by the following inequality:

$$\dot{Q}\left(\frac{1}{\Theta} - \frac{1}{T^*}\right) \geq 0 , \quad (9)$$

for vanishing work and mass exchange rates. Here, T^* is the thermostatic temperature of the equilibrium environment. From Eq. (9) it follows that \dot{Q} and the bracket have always the same sign. If we now suppose that there exists exactly one equilibrium environment for each arbitrary discrete system, for which the net heat exchange between them vanishes, then the defining inequality (9) determines the contact temperature Θ of the system, as the thermostatic temperature T^* of the system's environment for which this net exchange vanishes. The dynamic pressure p and the dynamic chemical potential μ are defined by analogy

$$\dot{V}(p - p^*) \geq 0, \quad \dot{M}(\mu^* - \mu) \geq 0 , \quad (10)$$

where p^* and μ^* correspond to the equilibrium environment.

The contact quantities so defined provide a complete thermodynamic description of non-equilibrium states of a separated discrete system, [6]. Note, however, that the values of the defined contact quantities differ from the values of usual bulk parameters in the case of local equilibrium. For interacting elements, which are the case in our study, the values of bulk and contact quantities of adjacent elements are additionally connected by so-called thermodynamic consistency conditions, [12].

4

Integral balance laws

In the required extension of the concepts of the thermodynamics of discrete systems to the thermoelastic case, we divide the body into a finite number of identical elements. This is also the strategy of the numerical method of finite volumes, [2]. The state of each element is then identified by the thermodynamic state of a discrete system associated with that element, each element being assumed in local equilibrium. In thermoelasticity, in addition to the contact temperature Θ and the defining inequality (9) which governs heat exchange, we must define a contact dynamic stress tensor Σ_{ij} since the state space includes the deformation. Analogously to (9) that holds for $\dot{\varepsilon}_{ij} = 0$, we have thus

$$\frac{\partial \varepsilon_{ij}}{\partial t} (\Sigma_{ij} - \sigma_{ij}^*) \geq 0, \quad (\dot{Q} = 0) , \quad (11)$$

an inequality that reminds us of the Hill–Mandel principle of maximal dissipation, [13]. Here, σ_{ij}^* is the Cauchy stress tensor in the environment.

It remains now to introduce the link between the bulk quantities that appear in Eqs. (6)–(8) and the contact quantities. This is achieved as follows. The contact stress tensor Σ_{ij} being defined at the boundary ∂V of the volume element V , and V_i denoting, by duality, the contact deformation velocity at that boundary of unit outward normal n_i , integration over the finite volume element of Eqs. (6)–(8) and the definition of the strain rate yield the following set of integral forms:

$$\frac{\partial}{\partial t} \int_V \rho_0 v_i dV = \int_{\partial V} \Sigma_{ij} n_j dA , \quad (12)$$

$$\frac{\partial}{\partial t} \int_V \varepsilon_{ij} dV = \int_{\partial V} H_{ijk} n_k dA , \quad (13)$$

$$\frac{\partial}{\partial t} \int_V \sigma_{ij} dV = \int_{\partial V} (2\mu H_{ijk} n_k + \lambda \delta_{ij} V_k n_k) dA + \varphi_{ij} , \quad (14)$$

$$\frac{\partial}{\partial t} \int_V CT dV = \int_{\partial V} (k n_i \frac{\partial T}{\partial x_i} + m V_k n_k) dA + \varphi^{\text{inh}} , \quad (15)$$

where

$$H_{ijk} = \frac{1}{2} (\delta_{ik} V_j + \delta_{jk} V_i) ,$$

and source terms due to material inhomogeneities (labelled “inh”) and thermoelastic couplings (labelled “te”) are given by

$$\varphi_{ij} = \varphi_{ij}^{\text{te}} + \varphi_{ij}^{\text{inh}}, \quad \varphi_{ij}^{\text{te}} = \int_V m \delta_{ij} \frac{\partial T}{\partial t} dV,$$

$$\varphi_{ij}^{\text{inh}} = - \int_V \left(v_k \frac{\partial \lambda}{\partial x_k} \delta_{ij} + v_i \frac{\partial \mu}{\partial x_j} + v_j \frac{\partial \mu}{\partial x_i} \right) dV, \quad \varphi^{\text{inh}} = - \int_V v_k T_0 \frac{\partial m}{\partial x_k} dV .$$

As m here does not depend on time, the contribution ϕ_{ij}^{te} could possibly be rewritten as a time derivative, and grouped with the left-hand side of Eq. (14), leaving only terms originating from material inhomogeneities as source terms. However, we keep the above formalism, in order to distinguish between the purely elastic and thermoelastic cases. The reason for this is that in “classical” thermoelasticity, the thermoelastic coupling in Eq. (8) is usually considered small and, hence, negligible, leaving from (8) an equation determining temperature independently of other fields, even in inhomogeneous materials. In that thermal stress approximation, Eq. (15) is reduced to

$$\frac{\partial}{\partial t} \int_V CT \, dV = \int_{\partial V} kn_i \frac{\partial T}{\partial x_i} \, dA . \quad (16)$$

Equations (12)–(15) or (16) are in a form suitable for a numerical approach by the method of finite volumes. It remains, however, to determine contact quantities.

5 Links between bulk and contact quantities

5.1 Heat conduction

In the case of heat conduction, the relation between bulk temperatures in neighbouring cells can be obtained directly. Considering the one-dimensional case, we should apply the thermodynamic consistency conditions, [12], to each pair of adjacent elements

$$\frac{\partial(U_1 + E_1)}{\partial V} = \frac{\partial(U_2 + E_2)}{\partial V} , \quad (17)$$

where U is the internal energy, V is volume and E is the energy of interaction. These conditions should be satisfied for systems $n - 1$ and n as well as for systems n and $n + 1$

$$\left(\frac{\partial U_{n-1}}{\partial V_{n-1}} \right)_T + \left(\frac{\partial E_{n-1n}}{\partial V_{n-1}} \right)_T = \left(\frac{\partial U_n}{\partial V_n} \right)_T + \left(\frac{\partial E_{nn-1}}{\partial V_n} \right)_T , \quad (18)$$

$$\left(\frac{\partial U_{n+1}}{\partial V_{n+1}} \right)_T + \left(\frac{\partial E_{n+1n}}{\partial V_{n+1}} \right)_T = \left(\frac{\partial U_n}{\partial V_n} \right)_T + \left(\frac{\partial E_{nn+1}}{\partial V_n} \right)_T , \quad (19)$$

where E_{nm} is the interaction energy per unit mass for the system n with respect to the system m .

It must be noted that even if the explicit expressions for the interaction energies are unknown, we can determine the state of the system n in the case of the heat conduction. In fact, due to the symmetry of the process of heat conduction, we have no preferences between systems $n - 1$ and $n + 1$ with respect to system n . Consequently, their actions relative to the system n should be equal, i.e.

$$\left(\frac{\partial E_{nn-1}}{\partial V_n} \right)_T - \left(\frac{\partial E_{n-1n}}{\partial V_{n-1}} \right)_T = - \left(\frac{\partial E_{nn+1}}{\partial V_n} \right)_T + \left(\frac{\partial E_{n+1n}}{\partial V_{n+1}} \right)_T . \quad (20)$$

Then we can represent the thermodynamic consistency conditions in terms of the states of neighbouring systems only. It must be noted that initial values of all thermodynamic quantities could be arbitrary. Therefore, to satisfy the obtained condition, we should prescribe the value for the central system only in the next time step

$$\left(\frac{\partial U_n^{k+1}}{\partial V_n^{k+1}} \right)_T = \frac{1}{2} \left[\left(\frac{\partial U_{n-1}^k}{\partial V_{n-1}^k} \right)_T + \left(\frac{\partial U_{n+1}^k}{\partial V_{n+1}^k} \right)_T \right] , \quad (21)$$

where superscript k denotes the time step. Thus, now we have the method for calculation of the state of a cell, if states of its neighbouring cells at the previous time step are known.

In the case of solids, thermal properties can be described in terms of thermal expansion coefficient α and the bulk modulus B . The product of the bulk modulus and the thermal expansion coefficient determines another thermodynamic derivative

$$\alpha B = -v \left(\frac{\partial p}{\partial v} \right)_T \frac{1}{v} \left(\frac{\partial v}{\partial T} \right)_p = \left(\frac{\partial p}{\partial T} \right)_v, \quad (22)$$

p is the pressure and v is the specific volume, that is directly related to the thermodynamic consistency condition (17). In fact, due to the differential relations of thermodynamics, we get

$$\left(\frac{\partial U}{\partial V} \right)_T = T \left(\frac{\partial S}{\partial V} \right)_T - p = T \left(\frac{\partial p}{\partial T} \right)_v - p.$$

Therefore, at a uniform pressure, we have from (21)

$$\alpha_n B_n T_n^{k+1} = \frac{1}{2} (\alpha_{n-1} B_{n-1} T_{n-1}^k + \alpha_{n+1} B_{n+1} T_{n+1}^k). \quad (23)$$

In the case of homogeneous media, all the cells have the same thermomechanical properties, and the temperature in each cell is determined as the arithmetical mean of its neighbour's temperatures at the previous time step

$$T_n^{k+1} = \frac{1}{2} (T_{n-1}^k + T_{n+1}^k). \quad (24)$$

It is easy to see that such a rule is equivalent to the finite-difference algorithm for the heat conduction equation. In fact, we can rewrite this relation in the form

$$T_n^{k+1} - T_n^k = \frac{1}{2} (T_{n-1}^k - 2T_n^k + T_{n+1}^k). \quad (25)$$

Introducing the usual dependence between space and time steps h and τ , namely,

$$\frac{k}{\rho c} = \frac{h^2}{2\tau},$$

we obtain, after dividing both parts of the relation (25) by the same value of the time step τ

$$\frac{T_n^{k+1} - T_n^k}{\tau} = \frac{k}{\rho c} \frac{T_{n-1}^k - 2T_n^k + T_{n+1}^k}{h^2}. \quad (26)$$

The latter equation is nothing more than the well-known finite-difference approximation of the heat conduction equation, [14]. Thus, the proposed algorithm in this simple case can be reduced to the usual one.

The same result can be obtained from the Eq. (16), if the contact temperatures at the left and right sides of the cell n are determined by

$$\Theta^+ = \frac{1}{2} (T_{n+1}^k - T_n^k), \quad \Theta^- = \frac{1}{2} (T_n^k - T_{n-1}^k). \quad (27)$$

Figure 1 shows the result of numerical calculation for two-dimensional heat conduction in a rectangular solid domain with point sources. In the initial situation, all elements had the same temperature 300 K. Heating elements at the boundary and inside the plate have temperature 400 K. Left boundary is supposed to be thermally insulated. All other boundaries hold their initial temperature. Isotherms are given at every 2 K. More examples of heat conduction calculations are given in, [15]–[16].

5.2

Elastic waves

The connection between bulk and contact quantities in the elastic case will be established by means of the wave-propagation algorithm, [7]. The general form for the integral Eqs. (12)–(15) in the considered case is

$$\frac{\partial}{\partial t} \int_V q \, dV = \int_{\partial V} Q \cdot n \, dA. \quad (28)$$

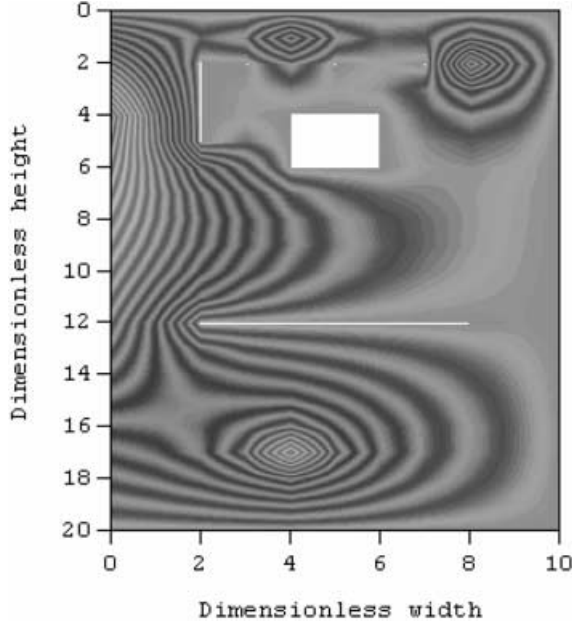


Fig. 1. Steady-state isotherms in a plate with point sources of heating

A finite-volume scheme corresponding to these equations in two space dimensions can be represented in the form

$$q_{nm}^{k+1} = q_{nm}^k - \frac{\Delta t}{\Delta x} (AQ_{nm}^+ - AQ_{nm}^-) - \frac{\Delta t}{\Delta y} (BQ_{nm}^+ - BQ_{nm}^-) , \quad (29)$$

where subscripts n and m indicate the placement of a discrete element in a two-dimensional grid, AQ^\pm and BQ^\pm are the contact quantities in the horizontal and vertical directions, respectively. At the same time, the first step in the construction of the wave-propagation algorithm for the system of equations of linear elasticity in an inhomogeneous medium

$$\frac{\partial q}{\partial t} + A(x, y) \frac{\partial q}{\partial x} + B(x, y) \frac{\partial q}{\partial y} = 0 , \quad (30)$$

is the first-order Godunov scheme, [7],

$$q_{nm}^{k+1} = q_{nm}^k - \frac{\Delta t}{\Delta x} (\mathcal{A}^+ \Delta q_{nm} + \mathcal{A}^- \Delta q_{n+1m}) - \frac{\Delta t}{\Delta y} (\mathcal{B}^+ \Delta q_{nm} + \mathcal{B}^- \Delta q_{nm+1}) . \quad (31)$$

Here, the fluctuations arising from Riemann problems at the interface between grid cells in the x - and y -directions, respectively, are determined exactly

$$\begin{aligned} \mathcal{A}^- \Delta q_{nm} &= \sum_{p=1} \alpha_{nm}^{(p-)} W^{(p-)} , & \mathcal{A}^+ \Delta q_{nm} &= \sum_{p=1} \alpha_{nm}^{(p+)} W^{(p+)} , \\ \mathcal{B}^- \Delta q_{nm} &= \sum_{p=1} \beta_{nm}^{(p-)} w^{(p-)} , & \mathcal{B}^+ \Delta q_{nm} &= \sum_{p=1} \beta_{nm}^{(p+)} w^{(p+)} , \end{aligned} \quad (32)$$

where $\alpha_{nm}^{(p)}$ and $\beta_{nm}^{(p)}$ are eigenvalues of matrices A_{nm} and B_{nm} , with coefficients dependent on the state of the cell (nm); $W^{(p)}$ and $w^{(p)}$ are horizontal and vertical waves corresponding to the local Riemann problem, superscripts “+” and “-” denote positive and negative eigenvalues.

The simplest way to link fluctuations and contact quantities is the following:

$$\begin{aligned} AQ_{nm}^+ &= \mathcal{A}^- \Delta q_{n+1m} , & AQ_{nm}^- &= -\mathcal{A}^+ \Delta q_{nm} , \\ BQ_{nm}^+ &= \mathcal{B}^- \Delta q_{nm+1} , & BQ_{nm}^- &= -\mathcal{B}^+ \Delta q_{nm} . \end{aligned} \quad (33)$$

The thermodynamic consistency conditions (17) express the continuity of derivatives of the internal energy at constant temperature. For instance, for two cells numbered 1 and 2 and separated by a coordinate line, we have in the thermoelastic case

$$\sigma_{ij}^{(1)} + \Sigma_{ij}^{(1)} - T^{(1)} \left(\frac{\partial \sigma_{ij}^{(1)}}{\partial T} \right)_{\varepsilon} - \Theta^{(1)} \left(\frac{\partial \Sigma_{ij}^{(1)}}{\partial T} \right)_{\varepsilon} = \sigma_{ij}^{(2)} + \Sigma_{ij}^{(2)} - T^{(2)} \left(\frac{\partial \sigma_{ij}^{(2)}}{\partial T} \right)_{\varepsilon} - \Theta^{(2)} \left(\frac{\partial \Sigma_{ij}^{(2)}}{\partial T} \right)_{\varepsilon} . \quad (34)$$

It should be noted that the definitions of the contact stresses (33) satisfy the thermodynamic consistency conditions (34) in their isothermal form.

The Godunov's method is extended to a higher resolution method by adding correction terms. The form of the extended method is

$$q_{nm}^{k+1} = q_{nm}^k + \Delta_{nm}^{\text{up}} - \frac{\Delta t}{\Delta x} (\bar{F}_{n+1m}^k - \bar{F}_{nm}^k) - \frac{\Delta t}{\Delta y} (\bar{G}_{nm+1}^k - \bar{G}_{nm}^k) , \quad (35)$$

where Δ_{nm}^{up} is the update for a first-order upwind Godunov method. The second-order correction terms take the form, [7],

$$\bar{F}_{nm}^k = \frac{1}{2} \sum_{p=1}^4 |\alpha_{nm}^{(p)}| \left(1 - \frac{\Delta t}{\Delta x} |\alpha_{nm}^{(p)}| \right) W^{(p)} , \quad (36)$$

$$\bar{G}_{nm}^k = \frac{1}{2} \sum_{p=1}^4 |\beta_{nm}^{(p)}| \left(1 - \frac{\Delta t}{\Delta x} |\beta_{nm}^{(p)}| \right) w^{(p)} , \quad (37)$$

and provide second-order accuracy. The obtained algorithm is a variant of the well-known Lax-Wendroff method, [2]. In this case the thermodynamic consistency conditions (34) remain satisfied.

The multidimensional motion is accomplished by splitting each fluctuation $\mathcal{A}^* \Delta q_{nm}$ and $\mathcal{B}^* \Delta q_{nm}$ into two transverse fluctuations, which will be called $\mathcal{B}^+ \mathcal{A}^* \Delta q_{nm}$ (the up-going transverse fluctuation), $\mathcal{B}^- \mathcal{A}^* \Delta q_{nm}$ (the down-going transverse fluctuation), $\mathcal{A}^+ \mathcal{B}^* \Delta q_{nm}$ (the right-going transverse fluctuation), and $\mathcal{A}^- \mathcal{B}^* \Delta q_{nm}$ (the left-going transverse fluctuation). The total effect of vertical transverse propagation at the interface between cells $(n-1m)$ and (nm) is determined as follows:

$$G_{nm}^k = \frac{\Delta t}{2\Delta x} (\mathcal{B}^- \mathcal{A}^+ \Delta q_{nm}^k + \mathcal{B}^+ \mathcal{A}^+ \Delta q_{nm-1}^k + \mathcal{B}^+ \mathcal{A}^- \Delta q_{n+1m-1}^k + \mathcal{B}^- \mathcal{A}^- \Delta q_{n+1m}^k) . \quad (38)$$

Analogously, the total effect of horizontal transverse propagation at the interface between cells $(nm-1)$ and (nm) is

$$F_{nm}^k = \frac{\Delta t}{2\Delta y} (\mathcal{A}^- \mathcal{B}^- \Delta q_{nm+1}^k + \mathcal{A}^+ \mathcal{B}^- \Delta q_{n-1m+1}^k + \mathcal{A}^- \mathcal{B}^+ \Delta q_{nm}^k + \mathcal{A}^+ \mathcal{B}^+ \Delta q_{n-1m}^k) . \quad (39)$$

The introduction of the transverse fluctuations improves the stability limit up to Courant number 1, and conserves the fulfilling of the thermodynamic consistency conditions. The whole algorithm is implemented in the form

$$q_{nm}^{k+1} = q_{nm}^k + \Delta_{nm}^{\text{up}} + \Delta_{nm}^{\text{trans}} - \frac{\Delta t}{\Delta x} (\bar{F}_{n+1m}^k - \bar{F}_{nm}^k) - \frac{\Delta t}{\Delta y} (\bar{G}_{nm+1}^k - \bar{G}_{nm}^k) , \quad (40)$$

where Δ_{nm}^{up} is the update for the first-order upwind Godunov method, and $\Delta_{nm}^{\text{trans}}$ represents the effect of transverse fluctuations

$$\Delta_{nm}^{\text{trans}} = -\frac{\Delta t}{\Delta x} (F_{n+1m}^k - F_{nm}^k) - \frac{\Delta t}{\Delta y} (G_{nm+1}^k - G_{nm}^k) . \quad (41)$$

It is well known that the Lax–Wendroff scheme produces oscillations behind discontinuities, [17]. The usual way to reduce spurious oscillations involves introducing limiter functions to modify the second-order corrections near discontinuities. However, the application of limiters still seems to be more of an art than a science. Moreover, in this case, the fulfilling of the thermodynamic consistency conditions cannot be directly controlled. It seems that the recently proposed composite schemes, [17], are more reliable, because of using filters that are consistent with differential equations. Here, the composite scheme is obtained by application of the Godunov step after each three second-order Lax–Wendroff steps. Obviously, the thermodynamic consistency conditions remain satisfied at each step.

As the first example, a short-time symmetrical excitation of a part of the boundary of a rectangular domain by nonzero normal stress is considered. All other boundaries are stress-free. Physical parameters for aluminium were used in the calculation: $c_p = 6420$ m/s, $c_s = 3040$ m/s, $\rho_0 = 2700$ kg/m³. Figure 2 represents a situation close to the initial one in terms of the normal stress. Results of the simulation of the wave propagation by means of the composite Lax–Wendroff–Godunov scheme are given in Figs. 3–4. The corresponding Courant number was 0.9. More complete description of the numerical simulation is given in [18].

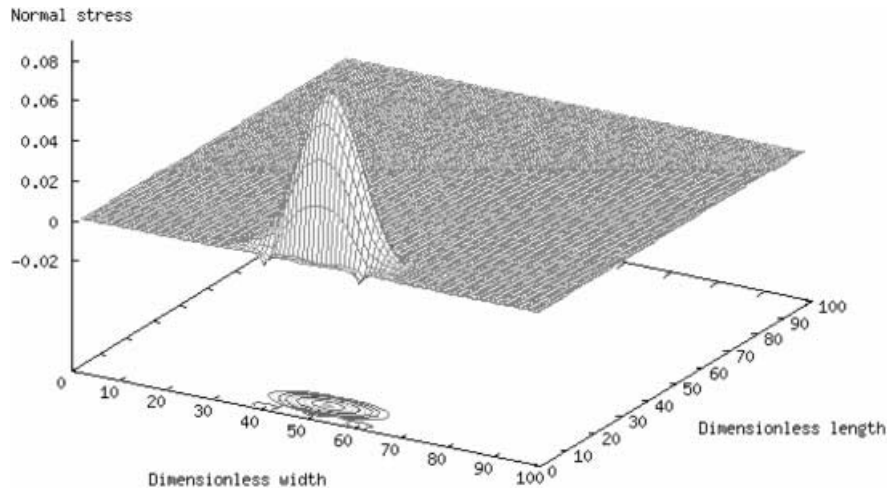


Fig. 2. Elastic wave formation, symmetrical loading, eight time steps

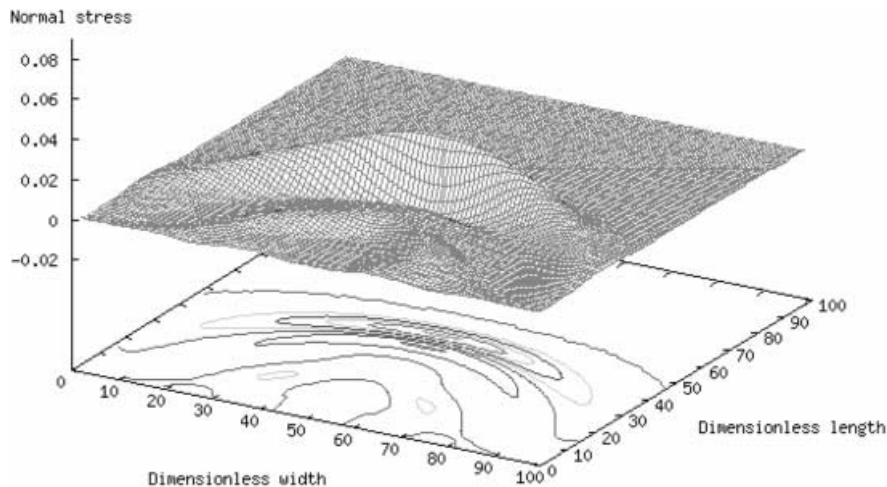


Fig. 3. Surface plot of elastic wave propagation, composite Lax–Wendroff–Godunov scheme, 90 time steps, Courant number 0.9

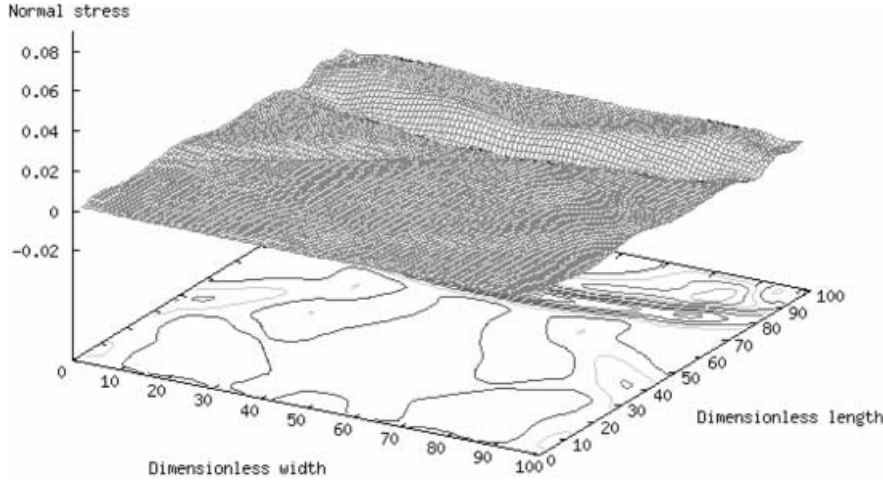


Fig. 4. Surface plot of elastic wave propagation, composite Lax–Wendroff–Godunov scheme, 150 time steps, Courant number 0.9

5.3

Thermoelastic waves

In the thermoelastic case, the equation for the temperature in two dimensions

$$\frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left(a(x, y) \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(a(x, y) \frac{\partial T}{\partial y} \right), \quad (42)$$

is solved by means of the algorithm for the heat conductivity equation in an inhomogeneous medium

$$T_{nm}^{k+1} = \frac{a_{nm} \Delta t}{4(\Delta x)^2} \frac{\alpha_{n+1m} B_{n+1m} T_{n+1m}^k + \alpha_{n-1m} B_{n-1m} T_{n-1m}^k - 2\alpha_{nm} B_{nm} T_{nm}^k}{\alpha_{nm} B_{nm}} + \frac{a_{nm} \Delta t}{4(\Delta y)^2} \frac{\alpha_{nm+1} B_{nm+1} T_{nm+1}^k + \alpha_{nm-1} B_{nm-1} T_{nm-1}^k - 2\alpha_{nm} B_{nm} T_{nm}^k}{\alpha_{nm} B_{nm}}, \quad (43)$$

where $B = \lambda + 2/3\mu$ is the bulk modulus.

According to the method of balancing source terms, [8], the modified bulk velocities both in x - and y -directions

$$(v_1)_{nm}^{\pm} = (v_1)_{nm} \pm \frac{\alpha_{nm}(3\lambda_{nm} + 2\mu_{nm})}{2(\lambda_{nm} + 2\mu_{nm})} \left(\frac{\partial T}{\partial t} \right)_{nm} \Delta x, \quad (44)$$

$$(v_2)_{nm}^{\pm} = (v_2)_{nm} \pm \frac{\alpha_{nm}(3\lambda_{nm} + 2\mu_{nm})}{2(\lambda_{nm} + 2\mu_{nm})} \left(\frac{\partial T}{\partial t} \right)_{nm} \Delta y, \quad (45)$$

are used for the calculation of normal dynamic stresses and corresponding contact velocities, which allows to eliminate the source terms.

The computational derivative for the temperature is calculated as follows:

$$\left(\frac{\partial T}{\partial t} \right)_{nm}^k = \frac{T_{nm}^{k+1} - T_{nm}^k}{\Delta t}. \quad (46)$$

Defining the contact temperatures as

$$(\Theta^r)_{nm}^k = \frac{\alpha_{n+1m}(3\lambda_{n+1m} + 2\mu_{n+1m})T_{n+1m}^k - \alpha_{nm}(3\lambda_{nm} + 2\mu_{nm})T_{nm}^k}{2\alpha_{nm}(3\lambda_{nm} + 2\mu_{nm})}, \quad (47)$$

$$(\Theta^l)_{nm}^k = -\frac{\alpha_{nm}(3\lambda_{nm} + 2\mu_{nm})T_{ij}^k - \alpha_{n-1m}(3\lambda_{n-1m} + 2\mu_{n-1m})T_{n-1m}^k}{2\alpha_{nm}(3\lambda_{nm} + 2\mu_{nm})}, \quad (48)$$

$$(\Theta^u)_{nm}^k = \frac{\alpha_{nm+1}(3\lambda_{nm+1} + 2\mu_{nm+1})T_{nm+1}^k - \alpha_{nm}(3\lambda_{nm} + 2\mu_{nm})T_{nm}^k}{2\alpha_{nm}(3\lambda_{nm} + 2\mu_{nm})}, \quad (49)$$

$$(\Theta^b)_{nm}^k = -\frac{\alpha_{nm}(3\lambda_{nm} + 2\mu_{nm})T_{nm}^k - \alpha_{nm-1}(3\lambda_{nm-1} + 2\mu_{nm-1})T_{nm-1}^k}{2\alpha_{nm}(3\lambda_{nm} + 2\mu_{nm})}, \quad (50)$$

where superscripts l, r, u, b denote left, right, upper and bottom boundaries, respectively, we satisfy directly the thermodynamic consistency conditions (34). The first-order Godunov method as well as transverse propagation, second-order correction, and composition are utilized then as above.

Results of simulation for thermoelastic wave propagation in inhomogeneous media are presented in Figs. 5–8. First, the interaction of a thermoelastic wave with an interface between two distinct, but otherwise spatially homogeneous, thermoelastic materials (copper and aluminium) has been simulated. The step-wise distribution of material properties is shown in Fig. 5. In the inhomogeneous case, we need to prescribe additionally the physical parameters for copper: $c_p = 4560$ m/s, $c_s = 2600$ m/s, $\rho_0 = 8960$ kg/m³. The wave was excited by a purely thermal shock at a part of the bottom boundary, as it is shown by narrow black rectangle in Fig. 5, all other boundaries being stress free. Figure 6 corresponds to the wave hitting first time the interface. For a medium with laterally continuously varying properties, as in Figs. 7, 8 shows a snapshot of the mechanical trace (normal stress) of a thermoelastic wave inside it. The

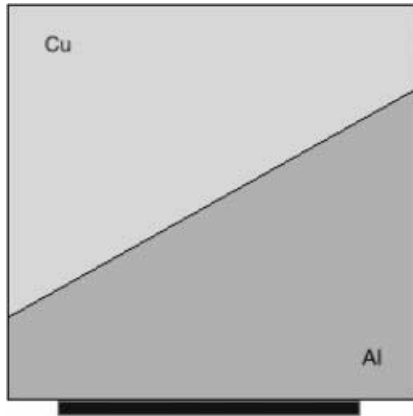


Fig. 5. Step-wise distribution of material properties inside the computational domain

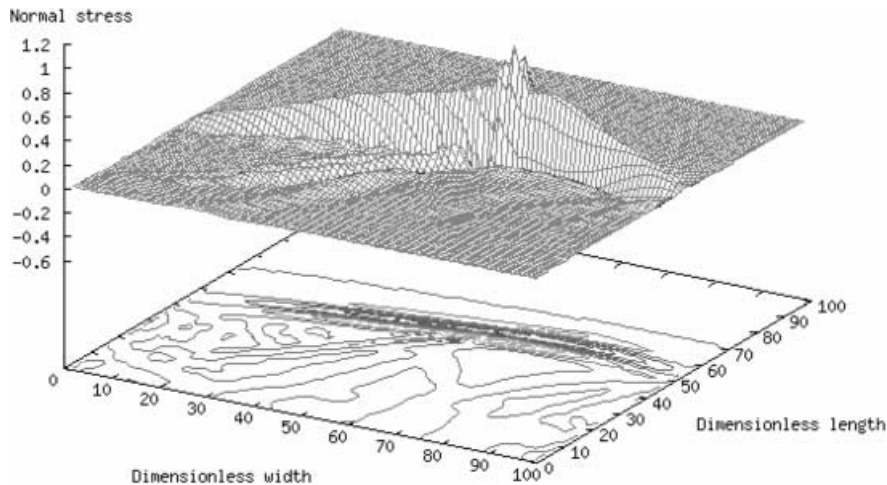


Fig. 6. Interaction of a thermoelastic wave with an interface between two distinct media, 70 time steps, the Courant number 0.9

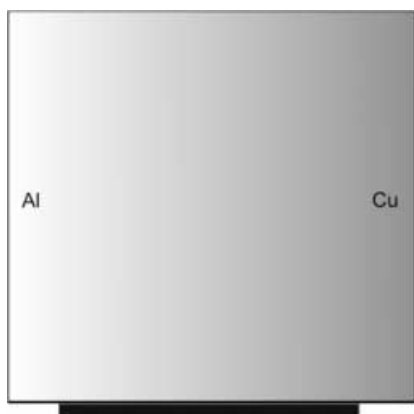


Fig. 7. Continuous variation of material properties inside the computational domain

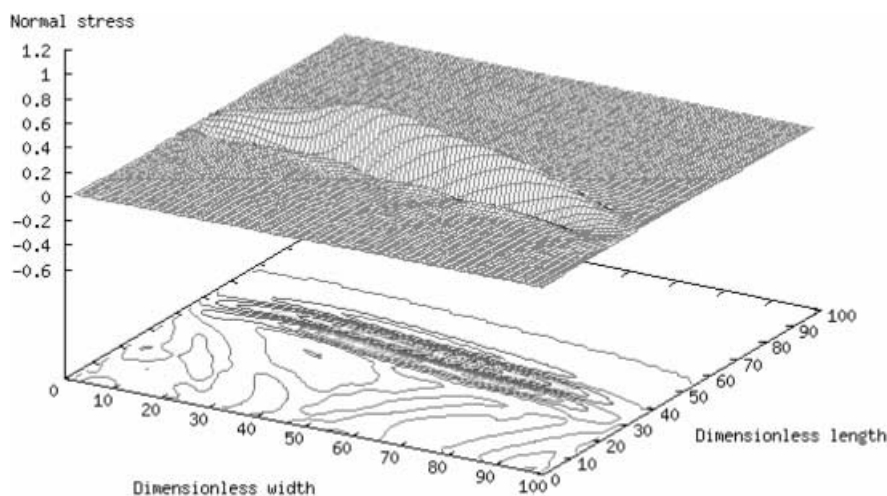


Fig. 8. Thermoelastic wave propagation inside a medium with laterally varying properties, 70 time steps, Courant number 0.9

initial excitation is the same as in the previous case. The wave front curves as it propagates, due to lateral inhomogeneity. (Animated pictures can be obtained via e-mail by request.)

6

Conclusions

The thermodynamic description of interacting discrete elements leads to the formulation of integral balance laws for thermoelasticity in terms of contact quantities and to the thermodynamic consistency conditions, which should be fulfilled for each pair of adjacent elements. The corresponding finite-volume numerical scheme consists of two steps, because the values of the contact quantities are needed for the updating of the state for each element. Fortunately, the contact quantities can be determined by means of the recently proposed wave-propagation technique in the inhomogeneous thermoelastic case. Moreover, the satisfaction of the thermodynamic consistency conditions is provided by using a composite scheme, where each three Lax–Wendroff steps are followed by one Godunov step. The combination keeps the advantage of the wave-propagation algorithm, which is stable up to the Courant number equal one, and allows us to avoid the application of limiter functions that may be not compatible with the thermodynamic consistency conditions. The proposed algorithm has a clear physical background, and is successfully applied for the simulation of thermoelastic wave propagation in inhomogeneous media.

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