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Discrete models of coupled dynamic thermoelasticity for stress–temperature formulations

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Abstract

In this article, the author studies the properties of discrete approximations for mathematical models of coupled thermoelasticity in the stress–temperature formulation. Since many applied problems deal with steep gradients of thermal fields, the main emphasis is given to the investigation of non-smooth solutions of non-stationary thermoelasticity. Convergence of operator–difference schemes on weak solutions of thermoelasticity is proved, and the dispersion analysis of models is performed. Error estimates and the results of computational experiments are presented. © 2001 Elsevier Science Inc. All rights reserved.

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1. Mixed modes in dynamics described by mathematical models of coupled field theory

In essence, any mathematical model describes a transformation of different types of *energy*. The recognition of this fact leads to an integral reformulation

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of differential models. On the one hand, such a reformulation is a fundamental step in obtaining effective numerical procedures of projective-variational type. On the other, such a reformulation allows us to relax the theoretical assumptions about a solution's smoothness typically made for differential problems.

In the final analysis, we do not know a priori regularity of the solution when solving a practical problem. Hence it is always necessary to cover a gap between mathematical assumptions on the solution smoothness and the smoothness of the solution in a real problem. Properly organized computational experiments may not only verify the validity of theoretical assumptions and estimates, but also identify new effects and tendencies that may lead to new directions in the development of theory. Of course, a high level of understanding of physical, chemical, biological processes or even properties of the solution of an abstract evolutionary problem may not be achieved by purely theoretical analysis [36]. Human experience will always play a fundamental role in the validation of theoretical results. The acquisition of new information through such experience leads to the *possibility* of the inclusion of additional *information* about the process, system or phenomenon into the mathematical model (for example, by an improved physical parameterization or by additional relations between system parameters). In turn, this ultimately leads to a change of solution regularity. The process of model improvement may continue indefinitely, and hence it is important to find a balance between the energetic and informational parts of the model's complexity [23,39]. Coupling, which is a natural way of reflecting additional information about a process (system, phenomenon) requires the relaxation of traditional regularity assumptions. Otherwise, a priori estimates of solutions may become meaningless [17,21].

Non-smoothness of solutions is a typical feature of many important problems in structural mechanics where a structure may be subjected to extreme mechanical and/or thermal loads. A lack of regularity in the solutions of thermoelasticity problems is also typical in many other areas of application. During recent years increasing attention has been paid to the investigation of processes in crystals under sharp impulse heating of the surface, in particular, through the investigation of physical effects in semiconductors that critically influence the characteristics of electronic devices. Thermal perturbations in the crystal result in elastic waves, and the process of their propagation cannot be considered without taking into account the thermal field. The rate of temperature change for such processes may be quite large. Hence, for the investigation of thermal deformations in crystals it is essential to take into account dynamic effects, induced by the motion of particles of solid under a rapid thermal expansion.

The study of weak solutions in thermoelasticity is especially important when the coupling between thermal and mechanical fields is relatively strong and has to be considered in the dynamics. Coupled problems in computational physics and other sciences is a two-way dynamic interaction between physically distinct components [9]. Such components may be mechanical, thermal, electromagnetic, biological in nature, but at least one component of the system as a whole has the *hyperbolic mode*. This leads to mathematical challenges in the investigation of such problems which have to be addressed. Computationally we also have a challenging problem because the states of all components should be considered when integrating over time. It is often inappropriate to approximate the mathematical models in coupled field theory using the arguments of 'parabolization' [10]. The latter may lead to a distorted picture in the description of real objects by mathematical models. While for coupled mathematical models L^2-type estimates may provide an important characterization of unknown solutions, after the 'parabolic' approximation such estimates may be completely inadequate for grasping changes in the solution behaviour [21]. Since the time of Fourier the heat equation has played a special role in mathematical physics, but despite its wide applicability it does not provide an adequate description of thermal processes since it predicts an infinite velocity of heat propagation. This fact led to different formulations of hyperbolic equations for heat conduction starting from the publication of a well-known paper by Cattaneo that followed on Peshkov's experiments [29].

The key to the nature of heat propagation lies in the understanding of the fact that the thermal field *never* acts on its own. It is always coupled to some other physical fields, such as elastic and/or electromagnetic fields. The effects of such fields may not be negligible. As a result of the interaction with other fields the dynamics of heat propagation acquires mixed hyperbolic–parabolic modes. The competition between these modes is at the heart of the physical process itself. Such a competition is fundamental for many other mathematical models including the convection–diffusion-reaction equation. One realises that the inclusion of additional information into such equations may continue indefinitely subject to the specification of a reaction law, time scale of the processes involved, and coupling with other processes. A side effect of the inclusion of additional information into the mathematical model is a change in the solution regularity. As a result of this effect when the smoothness of the solution decreases methods based on the model parabolization may become inappropriate. Hence, ideally we have to have error estimates that automatically react to the solution smoothness. Since the solution smoothness is a priori unknown we have to balance between a priori and a posteriori information [26]. Such a balance reflects the essence of *the adaptive property* of computational algorithms. In this paper we use Steklov's operator technique combined with the application of the Bramble–Hilbert lemma [25,26] in order to get a priori estimates depending on the solution's smoothness that may be predicted using a posteriori information from computational experiments.

The physical, chemical and biological processes that involve the thermal field are dissipative in their nature. Since mathematical models for such processes can be treated analytically only in exceptional cases, it is important to attain a better correspondence between dispersion properties of discrete and continuous problems. Moreover, it appears that using a dispersion relationship it is possible to obtain stability conditions for the discrete problem.

The remaining part of the paper is organized as follows:

- Section 2 provides the reader with the basic mathematical and numerical models that are investigated in the paper.
- In Section 3 we consider a more general operator–difference scheme, prove its stability and obtain a new estimate for its solution. Convergence results for the classical case follow easily from our consideration.
- Section 4 deals with the case of generalized solutions. Using Steklov's operator technique and the Bramble–Hilbert lemma, we prove the convergence result when the solution of the problem is from the Sobolev class $W_2^2(Q_T)$.
- In Section 5 we perform the dispersion analysis of continuous and discrete models of thermoelasticity and derive stability conditions using the Cayley transform.
- In Section 6 we present results of computational experiments on the investigation of planar nonstationary waves in a thermoelastic layer under instantaneous action of surface forces.
- Future directions of present work are addressed in Section 6.

2. Mathematical models of coupled dynamic thermoelasticity

Thermoelasticity is one of the first areas in coupled field theory that attracted the attention of mathematicians [5]. Nevertheless there are still many problems in this field that have to be addressed. At present, the development of theory is driven by at least two interconnected features: the non-local nature of heat propagation and its non-equilibrium character. Difficulties arise from the need to take into account the dispersive nature of thermoelastic wave propagation [3,4]. One possibility is to use non-Fourier type models with time relaxations for heat fluxes (i.e. to allow time for acceleration of the heat flow in response to an applied temperature gradient). Secondly, if we consider a uniform asymptotic expansion with respect to the inertial constant for linear thermoelasticity, the usual coupled quasi-static approximation of the temperature, displacement, and stress (which sets the inertial constant to zero) *is not* uniformly asymptotically correct even to the lowest order [7]. This result underlines the importance of the role of energy dissipation in thermoelasticity and confirms that adequate models cannot ignore dissipative processes. Such models may be discrete and non-local in principle because of the discrete characteristics of the medium itself (for example, in applications involved phonon dispersion in solids, in fracture mechanics, in electromagnetic solids, etc.). Moreover, there is a strong experimental evidence indicating that thermally-induced transformations due to the relaxation of elastic strain energy proceed through a series of *discrete* steps between metastable equilibrium states [31]. In such cases (for example, when high-rate heat sources such as lasers or microwave devices with short duration and/or high frequency are applied) there is not enough time to reach thermodynamic equilibrium, and hence the transport of heat may be better approximated by a wave propagation process rather than diffusion. Although hyperbolic modes in the dynamics become important (or even dominant), the system of partial differential equations for coupled non-stationary thermoelasticity cannot be treated as strictly hyperbolic (see also [3,40]). The fact of competition between different modes in dynamics causes major difficulties in the construction and investigation of discrete mathematical models.

Exact solutions of initial-boundary value problems in thermoelasticity, obtainable by analytic technique, are known for a quite narrow class of problems, mainly for problems in uncoupled thermoelasticity. In general, the application of analytic procedures to non-stationary thermoelasticity problems and the necessity of taking coupling phenomenon into consideration lead to serious mathematical difficulties. As a result, the development of numerical methods for coupled nonstationary problems of thermoelasticity is a fruitful area of investigation abounding in new mathematical ideas.

A general mathematical model describing the dynamics of a thermoelastic system can be represented in the form of the following non-linear coupled system with non-local non-linearities written with respect to the vector of displacements $\boldsymbol{u}(\boldsymbol{x},t) = (u_1, u_2, u_3)$, where $\boldsymbol{x} = (x_1, x_2, x_3) \in \mathbb{R}^3$, $t \in \mathbb{R}_+$ and the temperature deviation θ [33,35]

$$\begin{aligned} &\frac{\partial^2 \boldsymbol{u}}{\partial t^2} + M(\boldsymbol{u},\theta)A^2\boldsymbol{u} + N(\boldsymbol{u},\theta)A\theta = \boldsymbol{F}_1, \\ &R(\boldsymbol{u},\theta)\frac{\partial \theta}{\partial t} + Q(\boldsymbol{u},\theta)A\theta - N(\boldsymbol{u},\theta)A\frac{\partial \boldsymbol{u}}{\partial t} = F_2, \end{aligned} \tag{2.1}$$

where A is a non-negative, self-adjoint linear operator, $R, M, |N|, Q$ are strictly positive operators in a Hilbert space, and $\boldsymbol{F}_1$, F_2 are given functions.

In this paper we limit ourselves by the framework of the thermodynamics of linear irreversible processes and we focus on linear thermoelasticity for a homogeneous, isotropic medium with bounded reference configuration $\Omega \subset \mathbb{R}^3$, having a smooth boundary $\partial\Omega$. In this case the equations of thermoelasticity consist of three equations of motion and a strain-dependent heat conduction equation. They take the following form [16,18,19,30]:

$$\begin{aligned} &\rho\frac{\partial^2 \boldsymbol{u}}{\partial t^2} = \mu\nabla^2\boldsymbol{u} + (\lambda+\mu)\text{grad div}\boldsymbol{u} - (3\lambda+2\mu)\alpha_{\text{T}}\,\text{grad}T + \boldsymbol{f}_1, \\ &\nabla^2 T - \frac{1}{a}\frac{\partial T}{\partial t} - \frac{(3\lambda+2\mu)T_0\alpha_{\text{T}}}{\lambda_{\text{T}}}\text{div}\frac{\partial \boldsymbol{u}}{\partial t} = -\frac{f_2}{a}, \end{aligned} \tag{2.2}$$

where T is the absolute temperature of the thermoelastic body, ρ is its density, λ and μ are the Lamé constants for isothermal deformation, α_T is the coefficient of thermal expansion, T_0 is the temperature of the body in the unstrained state, λ_T is the coefficient of thermal conductivity, a is the thermal diffusivity ($a = \lambda_T/c_\epsilon$, where c_ϵ is the specific heat at constant strain), $\boldsymbol{f}_1$ is the specific volume force, and f_2 is the heat source. Under appropriate assumptions (such as $|\theta/T_0| \ll 1$, where $\theta = T - T_0$) the stress–strain–temperature relation, known as the Duhamel–Neumann relation, is obtained from the expansion of the free energy function in the vicinity of the natural state $\epsilon_{ij} = 0,\ T = T_0$,

$$\sigma_{ij} = \lambda \epsilon_{kk}\delta_{ij} + 2\mu\epsilon_{ij} - (3\lambda + 2\mu)\alpha_T(T - T_0)\delta_{ij}, \tag{2.3}$$

where σ_{ij} and ϵ_{ij} are the stress and strain tensors, respectively, δ_{ij} is the Kronecker symbol and

$$\epsilon_{kk} = \frac{\sigma_{kk}}{3\lambda + 2\mu} + 3\alpha_T(T - T_0). \tag{2.4}$$

Substituting (2.4) into (2.3) the Duhamel–Neumann relation can be re-written in the form

$$\epsilon_{ij} = \frac{(1 + v)\sigma_{ij}}{E} - \frac{v\sigma_{kk}}{E}\delta_{ij} + \alpha_T(T - T_0)\delta_{ij}, \tag{2.5}$$

where v is Poisson's ratio and E is Young's modulus which are connected with the Lamé constants by the well-known equations

$$\lambda = \frac{vE}{(1 + v)(1 - 2v)}, \qquad \mu = \frac{E}{2(1 + v)}. \tag{2.6}$$

Eq. (2.2) together with relation (2.5) and appropriate initial and boundary conditions are sufficient for the determination of the time-dependent thermomechanical field [16,18,19].

Note that when on the surface of the body the boundary conditions are given for stresses, the problem becomes even more challenging. One has to deal not only with the coupling of Eq. (2.2), but also with the coupling of mechanical and thermal fields on the surface of the body (by means of (2.3)). In classical elasticity the system of partial differential equations re-formulated in terms of the stresses is often referred to as the Beltrami–Mitchell system [18,19]. With the idea of such a reformulation in mind (applied to coupled dynamic thermoelasticity problems), let us now consider a special case of the model (2.2), (2.5) when $u_2 = u_3 = 0$ and all derivatives w.r.t. x_2 and x_3 are zero

$$\epsilon_{22} = \epsilon_{33} = \epsilon_{12} = \epsilon_{13} = \epsilon_{23} = 0.$$

This case arises, for example, when one describes the dynamic behaviour of a thermoelastic rod or a thermoelastic layer. From the Duhamel–Neumann relation (2.5) we have that

$$\sigma_{22} = \sigma_{33} = \frac{v}{1-v}\sigma_{11} - \frac{1}{1-v}\alpha_T E(T - T_0), \tag{2.7}$$

and

$$\epsilon_{11} = \frac{(1+v)(1-2v)}{(1-v)E}\sigma_{11} + \frac{1+v}{1-v}\alpha_T(T - T_0). \tag{2.8}$$

If we now differentiate the equation of motion (since we have only one equation in this case, we set $u_1 \equiv u$, $x_1 \equiv x$)

$$\rho\frac{\partial^2 u}{\partial t^2} = \frac{\partial \sigma_{11}}{\partial x} + f_1 \tag{2.9}$$

w.r.t. x and replace the derivative $\partial u/\partial x$ by expression (2.8), we get the equation of motion in the following form (we set $\sigma_{11} \equiv \sigma$):

$$f_1 + \frac{\partial^2 \sigma}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2 \sigma}{\partial t^2} = \frac{1+v}{1-v}\rho\alpha_T\frac{\partial^2 T}{\partial t^2}, \tag{2.10}$$

where c is the velocity of propagation of thermoelastic longitudinal waves. This velocity is determined by the equation

$$c^2 = \frac{\lambda + 2\mu}{\rho} \equiv \frac{E(1-v)}{(1+v)(1-2v)\rho}. \tag{2.11}$$

Further, we notice that an equivalent (tensor) form of the heat conduction equation is

$$T_{,ii} - \frac{1}{a}\frac{\partial T}{\partial t} - \frac{(3\lambda + 2\mu)T_0\alpha_T}{\lambda_T}\frac{\partial \epsilon_{kk}}{\partial t} = -\frac{f_2}{a}. \tag{2.12}$$

Hence, using (2.5) (or more precisely, its special case (2.8)), it is straightforward to get the stress–temperature form of this equation

$$\frac{\partial^2 T}{\partial x^2} - \frac{1}{a}(1+\varepsilon)\frac{\partial T}{\partial t} = \frac{(1+v)\alpha_T T_0}{(1-v)\lambda_T}\frac{\partial \sigma}{\partial t} - \frac{f_2}{a}, \tag{2.13}$$

where ε is the coupling coefficient between the mechanical and thermal fields which is determined by the equation

$$\varepsilon = \frac{T_0\alpha_T^2 E(1+v)}{c_\epsilon(1-2v)(1-v)}. \tag{2.14}$$

The system of equations (2.10) and (2.13) is the stress–temperature formulation of coupled dynamic thermoelasticity that shall be analysed in the remainder of this paper.

The introduction of dimensionless variables

$$s = \sigma/\sigma_{cr}, \quad \Theta = T/T_{cr}, \quad x' = x/x_{cr} \quad \text{and} \quad t' = t/t_{cr} \tag{2.15}$$

with

$$x_{\mathrm{cr}} = 1/c, \quad t_{\mathrm{cr}} = 1/c^2 \quad \text{and} \quad \frac{1+\nu}{1-\nu}\rho\alpha_{\mathrm{T}}c^2\frac{T_{\mathrm{cr}}}{\sigma_{\mathrm{cr}}} = 1 \tag{2.16}$$

allows us to show that

$$\frac{\sigma_{\mathrm{cr}}}{T_{\mathrm{cr}}}\frac{(1+\nu)\alpha_{\mathrm{T}}T_0}{(1-\nu)\lambda_{\mathrm{T}}} = \varepsilon. \tag{2.17}$$

This reduces the system (2.10), (2.13) to the following form (we use here old notation for space and time variables):

$$\begin{aligned} &\frac{\partial^2 s}{\partial t^2} - \frac{\partial^2 s}{\partial x^2} + \frac{\partial^2 \Theta}{\partial t^2} = f_1(x,t), \\ &(1+\epsilon)\frac{\partial \Theta}{\partial t} - a\frac{\partial^2 \Theta}{\partial x^2} + \epsilon\frac{\partial s}{\partial t} = f_2(x,t). \end{aligned} \tag{2.18}$$

We assume that the system (2.18) holds in the space–time domain $Q_{\mathrm{T}} = \{(x,t)\colon 0 < x < 1;\ 0 < t \leqslant \bar{T}\}$, thus the problem is considered in $\bar{Q}_{\mathrm{T}} = Q_{\mathrm{T}} \cup \Gamma \cup \bar{\Upsilon}$, where $\Gamma = \{(x,t)\colon x = 0,\ x = 1;\ 0 < t \leqslant \bar{T}\}$, $\bar{\Upsilon} = \{(x,t)\colon 0 \leqslant x \leqslant 1, t = 0\}$. The system (2.18) is supplemented by the initial and boundary conditions

$$\Theta(x,0) = \Theta_0(x), \quad s(x,0) = s_0(x), \quad \frac{\partial s(x,0)}{\partial t} = \bar{s}_0(x) \quad \text{for } t = 0, \tag{2.19}$$

$$s(x_i,t) = s_i(t), \quad \frac{\partial \Theta(x_i,t)}{\partial x} = \Theta_i(t) \quad \text{for } x_i \in \Gamma, \tag{2.20}$$

where $i = 0,1,\ x_0 = 0,\ x_1 = 1$.

For many applied problems the values of the stress are the principal unknowns of practical importance, even though mathematically we solve the problem in displacements. But in considering the problem of thermoelasticity in displacements, we have to perform the operation of differentiation (which is ill-posed numerically). This leads to a reduction of the order accuracy [6]. Hence, numerical methods for coupled problems of dynamic thermoelasticity formulated for stress–temperature are preferred in many situations. However, they have not been adequately explored.

The problem in stresses (2.18)–(2.20) is equivalent to the problem in deformations. The former can be reduced to the latter by the change of variables $r = s + \Theta$:

$$\begin{aligned} &\frac{\partial^2 r}{\partial t^2} = \frac{\partial^2 r}{\partial x^2} - \frac{\partial^2 \Theta}{\partial t^2} + f_1(x,t), \\ &\frac{\partial \Theta}{\partial t} + \epsilon\frac{\partial r}{\partial t} - a\frac{\partial^2 \Theta}{\partial x^2} = f_2(x,t), \end{aligned} \tag{2.21}$$

with the corresponding initial and boundary conditions. The variable r in the system (2.21) denotes deformations, which at the initial moment of time will be denoted by r_0. The rate of change of deformations at the initial moment of time will be denoted by $\bar{r}_0$ (defined more precisely below) and other notation will be as for problem (2.18)–(2.20). The main reason for the introduction of the model (2.21) lies in the fact that numerical schemes for this model are more easily realizable algorithmically than numerical schemes for the model (2.18).

We note that the above models of thermoelasticity do not belong to any of the classical type of partial differential equations. Such a situation is typical in coupled field theory. We have mixed equations which contain different modes: hyperbolic, parabolic, elliptic. Such mathematical models are important for both mathematical theory and application [8,26]. In fact, in the case of thermoelasticity we can see that one of the equations of the system contains a hyperbolic type operator, whereas the other contains a parabolic type operator. There is a coupling effect between these equations by the parameter ϵ, which in the case of the formulation in deformations is amplified by non-homogeneous boundary conditions. In the general case coupling effects between thermal and elastic fields may lead to the appearance of boundary layers. Indeed when the material moduli depend both on the temperature and the stretch, their effects can either reinforce or mitigate one another. As a result we may observe the accentuation or annihilation of the boundary layer structure [34]. On the other hand, if we formally set $\epsilon = 0$ one may apply a splitting technique based on the solution of the parabolic equation and substitution the temperature function into the hyperbolic equation. However, in all practical applications the value of ϵ may be small but still positive. Such a coupling between parabolic and hyperbolic modes of thermoelastic waves is an essential prerequisite in an adequate description of underlying processes.

Using the basic principles of the construction of difference schemes (see, for example [37] and references therein), let us approximate the problem in deformations. We introduce the grid $\bar{\omega}_{h\tau} = \bar{\omega}_h \times \bar{\omega}_\tau$ in $\bar{Q}_{\mathrm{T}}$, where

$$\bar{\omega}_h = \{x_i = ih,\ h = 1/N,\ i = 1, \dots, N\},$$

$$\bar{\omega}_\tau = \{t_j = j\tau,\ \tau = T/M,\ j = 1, \dots, M\}.$$

Let $(y, \eta) \equiv (y_i^j, \eta_i^j)$ be the difference approximation on this grid for the solution (r, Θ) of the problem in deformations. Then we construct the following difference scheme with respect to (y, η) (without the loss of generality we assume here that $s_i = \Theta_i = 0,\ i = 1, 2$):

$$\begin{aligned} &y_{\bar{t}t} = \Lambda y - \Lambda\eta + \varphi_1, \qquad (x,t) \in \omega_h \times \omega_\tau, \\ &\eta_t = \bar{\Lambda}\eta^{(\sigma)} - \epsilon y_t + \varphi_2, \quad (x,t) \in \bar{\omega}_h \times \omega_\tau, \end{aligned} \tag{2.22}$$

$$\begin{aligned} &y = \eta, \quad x \in \Gamma; \quad y = r_0(x), \quad \eta = \Theta_0(x), \quad y_t = r_1(x), \\ &x \in \omega_h, \quad t = 0. \end{aligned} \tag{2.23}$$

In schemes (2.22) and (2.23) we use the following notation:
- φ_1 and φ_2 denote approximations to the functions f_1 and f_2, respectively;
- $r_0(x) = s_0(x) + \Theta_0(x)$;
- $r_1(x) = \bar{r}_0(x) + \tau[r_0'' + \Theta_0'' + f_1(x,0)]/2$;
- $\bar{r}_0(x) = [f_2(x,0) + \bar{s}_0(x) + a\Theta_0'']/(1+\epsilon)$.

The operator Λ denotes the second difference derivatives in space, that is $\Lambda y = y_{\bar{x}x}$, and

$$\bar{\Lambda}\eta = \begin{cases} \Lambda\eta & \text{when } x \in \omega_h, \\ 2\eta_x/h & \text{when } x = 0, \\ -2\eta_{\bar{x}/h} & \text{when } x = 1. \end{cases}$$

We use the difference scheme with weights σ ($0 \leqslant \sigma \leqslant 1$) in order to achieve the second-order of approximation in space and time (in the general case we have $\Lambda y^{(\sigma)} = \sigma\Lambda\hat{y} + (1-\sigma)\Lambda y$, where the hat denotes the value of y taken from the upper time-level). The approximations to f_1 and f_2 are chosen by analogous reasoning, for example, $\varphi_1 = f_1(x_i, t_j)$, $\varphi_2 = f_2(x_i, t_{j+0.5})$ (another way to approximate the functions f_1 and f_2 will be given in Section 4).

In addition to the consistency of difference scheme (2.22) and (2.23) we need a stability result for our discrete approximation to ensure that the error of such an approximation is small. However, due to non-homogeneity of the Dirichlet boundary conditions for difference approximations of deformations (which are computed using approximate values of temperature!) analysis of the stability of difference scheme (2.22) and (2.23) is hampered. To overcome this difficulty we propose to return to the formulation in stresses for *the discrete rather than for the continuous problem*. This idea is intrinsic in the analysis of stability and in obtaining a new a priori estimate in Section 3. The accuracy of a posteriori error estimates will depend on the accuracy of the recovered stresses which are computed directly from a difference scheme that we propose in Section 3. The implicit balance between a priori and a posteriori estimates provide a foundation for effective adaptive computational procedures [17].

3. Stable operator–difference scheme for problems of thermoelasticity

So far we put into correspondence to the continuous mathematical model of thermoelasticity its discrete analogue. Now let us introduce a *discrete* function $v = y - \eta$ that gives an approximation to the function of stresses. Then the system of difference equations (2.22) and (2.23) may be rewritten in terms of (v, η) as follows:

$$\begin{aligned} &v_{\bar{t}t} = \Lambda v - \eta_{\bar{t}t} + \varphi_1, \\ &(1+\epsilon)\eta_t = \bar{\Lambda}\eta^{(\sigma)} - \epsilon v_t + \varphi_2, \end{aligned} \tag{3.1}$$

$$v = 0, \quad x \in \Gamma; \quad v = s_0(x), \quad v_t = s_1(x), \quad \eta = \Theta_0(x), \quad t = 0, \tag{3.2}$$

where

$$s_1(x) = (1-\epsilon)r_1(x) + \bar{\Lambda}\eta^{(\sigma)}\Big|_{t=0} + \varphi_2(x,0).$$

We introduce two sets of discrete functions

$$H_1 = \{v(x) \colon x \in \bar{\omega}_h\}, \qquad H_2 = \{\eta(x) \colon x \in \bar{\omega}_h\}$$

with the scalar product

$$(y,z) = \sum_{x \in \bar{\omega}_h} \hbar y(x) z(x)$$

($y \in H_i$, and $z \in H_i$ for $i = 1,2$, respectively), where

$$\hbar = \begin{cases} h & \text{when } x \in \omega_h, \\ h/2 & \text{when } x \in \bar{\omega}_h/\omega_h. \end{cases}$$

Instead of the difference schemes (3.1) and (3.2) we shall investigate a more general operator–difference scheme. All results for schemes (3.1) and (3.2) will follow as a special case of our construction.

Let us define operators from

$$\overset{0}{H}_1 = v(x): \quad x \in \bar{\omega}_h; \;\; v = 0, \;\; x = 0, 1$$

into H_1 as follows:

$$D_1 = I - \frac{\sigma_1 + \sigma_2}{2}\tau^2 \Lambda, \quad B_1 = -(\sigma_1 - \sigma_2)\tau\Lambda, \quad A_1 = -\Lambda, \quad C_1 = I, \tag{3.3}$$

and the operators from H_2 into H_2 by the equations

$$B_2 = (1+\epsilon)I + (1-\sigma_3)\tau\bar{\Lambda}, \quad A_2 = -\bar{\Lambda}, \quad C_2 = \epsilon I, \tag{3.4}$$

where $\sigma_i, \; i = 1,2,3$, are weights taking values between zero and one, and I is the identity operator. Let us further assume that

$$\sigma_3 \geqslant \frac{1+\alpha}{2} - \frac{h^2(1-\beta)}{4a\tau}, \qquad \frac{\sigma_1+\sigma_2}{2} \geqslant \frac{1+\gamma}{4} - \frac{h^2}{4\tau^2}, \tag{3.5}$$

where

$$\alpha, \gamma > 0, \quad 0 < \beta < 1, \quad 0 \leqslant \sigma_i \leqslant 1, \quad i = 1,2,3.$$

We note that if conditions (3.5) are satisfied, then the operators defined by the Eqs. (3.3) and (3.4) exist, they are positive definite and self-adjoint. Now we are in the position to consider the following operator–difference generalization of schemes (3.1) and (3.2)

$$\begin{aligned} &D_1 v_{\bar{t}t} + B_1 v_{\overset{\circ}{t}} + A_1 v + C_1 \eta_{\bar{t}t} = \varphi_1, \\ &B_2 \eta_t + A_2 \hat{\eta} + C_2 v_t = \varphi_2, \end{aligned} \tag{3.6}$$

where $v_{\overset{\circ}{t}}$ denotes the central difference derivative (that is $v_{\overset{\circ}{t}} = (v_i^{j+1} - v_i^{j-1})/(2\tau)$). For norms of our discrete functions we introduce the following notation:

$$\|y(t)\|^2 = (y(t), y(t)), \qquad \|y(t)\|_{A_1}^2 = (A_1 y(t), y(t)),$$

$$\|y(t)\|_{(1)}^2 = \|y(t)\|^2, \qquad \|y(t)\|_{(2)}^2 = \| \sum_{t'=0}^{t} A_2 y(t') \|^2.$$

We formulate the main result of this section as follows:

Theorem 3.1. *The operator–difference scheme* (3.6), (3.2) *is stable with respect to initial data and right-hand side if the conditions* (3.5) *are satisfied. For the discrete approximation of problem* (2.18)–(2.20) *by schemes* (3.6), (3.2) *the following estimate*:

$$\begin{aligned} ||v(t_1)||_{(1)} + ||\eta(t_1)||_{(2)} \leqslant M \Big\{ &||v(0)||_{\bar{D}_1} + ||A_2 v_t(0)|| + ||A_2 \eta(0)|| \\ &+ \sum_{t'=0}^{T} \tau ||A_2(\kappa_1 + \kappa_2)|| + \sum_{t'=0}^{T} \tau ||\xi_1 + \xi_2|| + \sum_{t'=\tau}^{T} \tau ||(\kappa_1 + \kappa_2)_{\bar{t}})|| \Big\}, \end{aligned} \tag{3.7}$$

holds, where

$$\bar{D}_1 = \Big(B_2 + \frac{\tau}{2} A_2 \Big) D_1 - C_2, \quad \varphi_1 = (\xi_1)_{\bar{t}} + (\xi_2)_{\bar{x}}, \quad \varphi_2 = (\kappa_1)_{\bar{t}} + (\kappa_2)_{\bar{x}}.$$

Proof. First, we apply the operator $\bar{B}_2 = B_2 + \tau A_2/2$ to both parts of the first equation of the system (3.6). Then, using the expression for the second difference derivative $\eta_{\bar{t}t}$ from the second equation of the system (3.6), and substituting its value into the resulting first equation, we have

$$\bar{D}_1 v_{\bar{t}t} + \bar{B}_2 B_1 v_{\overset{\circ}{t}} + \bar{B}_2 A_1 v - A_2 \eta_{\overset{\circ}{t}} = \bar{B}_2 \varphi_1 - (\varphi_2)_{\bar{t}}, \tag{3.8}$$

where $\bar{D}_1 = \bar{B}_2 D_1 - C_2$.

Now we apply

- the operator C_2 to both parts of the Eq. (3.8), and
- the operator A_2 to the following consequence of the second equation in (3.6)

$$B_2 \eta_{\overset{\circ}{t}} + A_2(\hat{\eta} + \eta)/2 + C_2 v_{\overset{\circ}{t}} = \varphi_2 + \check{\varphi}_2,$$

where the above-check denotes values taken from the previous time layer. As a result we obtain the following system of operator–difference equations:

$$\begin{aligned} &C_2 \bar{D}_1 v_{\bar{t}t} + C_2 \bar{B}_2 B_1 v_{\overset{\circ}{t}} + C_2 \bar{B}_2 A_1 v - C_2 A_2 \eta_{\overset{\circ}{t}} = C_2 \bar{B}_2 \varphi_1 - C_2 (\varphi_2)_{\bar{t}}, \\ &A_2 B_2 \eta_{\overset{\circ}{t}} + (A_2)^2 (\hat{\eta} + \eta)/2 + A_2 C_2 v_{\overset{\circ}{t}} = A_2(\varphi_2 + \check{\varphi}_2). \end{aligned} \tag{3.9}$$

We note that the operators A_2 and C_2 are commutative. Then we perform the following two operations:

- we multiply both parts of the first equation in Eq. (3.9) by the function of the discrete argument $t \in \omega_\tau$

  $$w(t) = \sum_{t'=t+\tau}^{t_1} \tau[v(t') + v(t' - \tau)],$$

  which has the following properties [28]

  $$w_{\bar{t}} = -(v + \check{v})/2, \quad w(t) = 0, \quad t \geqslant t_1,$$

  and
- multiply both parts of the second equation in Eq. (3.9) by the function of the discrete argument $t \in \omega_\tau$

  $$\zeta(t) = \sum_{t'=t+\tau}^{t_1} \tau[\eta(t') + \eta(t' - \tau)].$$

Then the resulting equalities are added together, the result is multiplied by 2τ, and is summed up in t from τ to t_1. Using a technique developed for hyperbolic equations (see [28]) we can get an energy identity. Assuming that

$$\varphi_1 = (\xi_1)_{\bar{t}} + (\xi_2)_{\bar{x}}, \qquad \varphi_2 = (\kappa_1)_{\bar{t}} + (\kappa_2)_{\bar{x}},$$

we use conditions (3.5) and apply Cauchy–Schwarz inequality and the discrete analogue of the Gronwall lemma [11] to ensure the validity of the estimate (3.7). □

Convergence results under classical assumptions on solution smoothness follow easily from Theorem 3.1. For example, from the analysis of approximation error using the Taylor equation and the a priori estimate (3.7) we can readily come to the following conclusion:

Corollary 3.1. *If conditions* (3.5) *are satisfied, then the solution* (v, η) *of schemes* (3.6), (3.2) *converges to the solution of problem* (2.18)–(2.20) $(s, \Theta) \in C^{4,4}(\bar{Q}_T) \times C^{4,3}(\bar{Q}_T)$, *and the error of the scheme is characterized by the following estimate*:

$$||v^j - s^j||_{(1)} \leqslant M_1 \Phi_1(h, \tau), \qquad ||\eta^j - \Theta^j||_{(1)} \leqslant M_2 \Phi_1(h, \tau),$$

where j is the index of the current time layer, M_1 and M_2 are constants that do not depend on h and τ, and $\Phi_1(h, \tau) = h^2 + \tau^2 + (\sigma_1 - \sigma_2)\tau + (\sigma_3 - 0.5)\tau$.

In the next section Theorem 3.1 enables us to prove convergence of difference approximations under relaxed smoothness assumptions that are typical in many applications of thermoelasticity.

4. Convergence of the operator–difference scheme on weak solutions of thermoelasticity problems

It is well known that the analysis of error approximation using the technique of the classical Taylor equation leads to *excessive requirements* on the smoothness of the sought-for solution [26,32]. Below we shall show how such requirements can be relaxed using the Steklov operators.

Let us assume that conditions under which the solution of problem (2.18)–(2.20) belongs to the class $W_2^2(Q_\mathrm{T})$ are satisfied (see [14,15,20] and references therein). That is, we assume that $(s, \Theta) \in W_2^2(Q_\mathrm{T}) \times W_2^2(Q_\mathrm{T})$.

We consider the operator–difference scheme (3.6), (3.2) with the following source terms:

$$\varphi_1 = S^x \otimes S^{t_1} f_1(x,t), \qquad \varphi_2 = S^x \otimes S^{t_2} f_2(x,t),$$

where $S^x \otimes S^{t_i},\ i = 1,2$ denote the composition of averaging Steklov's operator acting in space and time. The operators S^x and S^{t_i} acting on a function $u(x,t)$ are introduced as follows:

$$S^x u(x,t) = \begin{cases} 2\int_0^{h/2} u(\xi,t)\,\mathrm{d}\xi/h & \text{when } x = 0, \\ \int_{x-h/2}^{x+h/2} u(\xi,t)\,\mathrm{d}\xi/h & \text{when } 0 < x < 1, \\ 2\int_{1-h/2}^{1} u(\xi,t)\,\mathrm{d}\xi/h & \text{when } x = 1, \end{cases}$$

$$S^{t_1} u(x,t) = \begin{cases} \int_{t-\tau/2}^{t+\tau/2} u(x,\mu)\,\mathrm{d}\mu/\tau & \text{when } t > 0, \\ 2\int_0^{\tau/2} u(x,\mu)\,\mathrm{d}\mu/\tau & \text{when } t = 0, \end{cases}$$

$$S^{t_2} u(x,t) = \begin{cases} \int_{t}^{t+\tau} u(x,\mu)\,\mathrm{d}\mu/\tau & \text{when } t > 0, \\ 2\int_0^{\tau/2} u(x,\mu)\,\mathrm{d}\mu/\tau & \text{when } t = 0. \end{cases}$$

Then the scheme error

$$z_1 = v - s, \qquad z_2 = \eta - \Theta$$

is the solution of the following problem:

$$\begin{aligned} &D_1(z_1)_{\bar{t}t} + B_1(z_1)_{\overset{\circ}{t}} + A_1 z_1 + C_1(z_2)_{\bar{t}t} = \psi_1, \\ &\bar{B}_2(z_2)_t + A_2(\hat{z}_2 + z_2)/2 + C_2(z_1)_t = \psi_2, \end{aligned}$$

$$z_1 = 0 \quad \text{when } x = 0,1; \qquad z_1 = 0, \quad (z_1)_t = \psi_1 \quad \text{when } t = 0, \tag{4.1}$$

where

$$\psi_1 = \varphi_1 - [D_1 s_{\bar{t}t} + B_1 s_{\overset{\circ}{t}} + A_1 s + C_1 \Theta_{\bar{t}t}] \qquad \text{if } t \in \omega_\tau,$$

$$\psi_2 = \varphi_2 - [\bar{B}_2 \Theta_t + A_2(\hat{\Theta} + \Theta)/2 + C_2 s_t] \qquad \text{if } t \in \omega_\tau,$$

$$\psi_1 = \bar{r}_0 + \tau[r_0'' - \Theta_0'' + \varphi_1(x,0)]/2 - s_t(x,0) \quad \text{if } t = 0.$$

We apply the composition of the operators $S^x \otimes S^{t_1}$ and $S^x \otimes S^{t_2}$ to the first and the second equations of the system (2.18), respectively. Then we use the basic properties of Steklov's operators as follows:

$$S^x \frac{\partial u}{\partial x} = \frac{1}{h}[u(x+h/2,t) - u(x-h/2,t)] = (u^{(-0.5)})_x,$$
$$S^{t_1} \frac{\partial u}{\partial t} = (\breve{u})_t, \qquad S^{t_2} \frac{\partial u}{\partial t} = u_t,$$

where $\bar{u} = u(x, t + \tau/2)$. In words, the above equations allow us to transform derivatives that may not exist in the classical sense into difference derivatives. As a result, such a transformation naturally leads to a discrete problem which is constructed with respect to the smoothness requirements on the unknown solution.

It is straightforward to deduce a representation for the scheme error, for example, for internal nodes we have

$$\psi_1 = (\eta_1)_t + \frac{\sigma_1 + \sigma_2}{2} \tau^2 (\eta_2)_t + (\eta_3)_x + (\sigma_1 - \sigma_2)\tau(\eta_5)_t,$$

where the functionals η_i, $i = 1, \ldots, 5$, are defined as follows:

$$\eta_1 = S^x \left(\frac{\partial \breve{s}}{\partial t} \right), \qquad \eta_2 = \Lambda s_{\bar{t}}, \qquad \eta_3 = s_{\bar{x}} - S^{t_1} \left(\left(\frac{\partial s}{\partial x} \right)^{(-0.5)} \right),$$

$$\eta_4 = S^x \left(\frac{\partial \breve{\Theta}}{\partial t} \right) - \Theta_{\bar{t}}, \qquad \eta_5 = \Lambda(s - \tau s_{\bar{t}}/2),$$

and similarly

$$\psi_2 = (1 + \epsilon)(\eta_6)_t + \epsilon(\eta_7)_t - (\sigma_3 - 0.5)\tau(\eta_8)_t + a(\eta_9)_x,$$

where the functionals η_i, $i = 6, 7, 8, 9$ are defined by the equations:

$$\eta_6 = S^x \Theta - \Theta, \qquad \eta_7 = S^x s - s, \qquad \eta_8 = A_2 \Theta,$$

$$\eta_9 = \left(\frac{\hat{\Theta} + \Theta}{2} \right)_{\bar{x}} - S^{t_2} \left(\left(\frac{\partial \Theta}{\partial x} \right)^{(-0.5)} \right).$$

Analogous functions are present in the representations of error approximation of

- boundary conditions for temperature, and
- initial conditions of the problem.

Functionals η_i, $i = 1, \ldots, 9$, are estimated using the Bramble–Hilbert lemma (see [26] and references therein). For example, it is easy to see that the linear functional η_3 is bounded in the space $W_2^2(Q_{\mathrm{T}})$, therewith

$$|\eta_3| \leqslant Mh^{(-1)} ||s||_{W_2^2(e)},$$

where

$$e = \{(x', t'):\ x - h < x' < x,\ t - \tau/2 < t' < t + \tau/2\}.$$

By a standard linear change of variables we can pass from the domain e to the domain

$$E = \{(u_1, u_2):\ -1 < u_1 < 0,\ -0.5 < u_2 < 0.5\}.$$

Since a linear change of variables does not change the class of functions, we have

$$|\eta_3| \leqslant Mh^{(-1)} ||s||_{W_2^2(E)}.$$

Now it is easy to verify that the functional

$$\eta_3 = \frac{1}{2h} \left\{ \tilde{s}(0,0) - \tilde{s}(-1,0) - \int_{-0.5}^{0.5} \frac{\partial \tilde{s}(-0.5, u_2)}{\partial u_1} \mathrm{d}u_2 \right\}$$

(where $\tilde{s}(u) = s(x(\xi_1), t(\xi_2)))$ is zero for polynomials up to first degree inclusive. Therefore, from the Bramble–Hilbert lemma we have

$$|\eta_3| \leqslant Mh^{-1} |\tilde{s}|_{W_2^2(E)},$$

and passing to the variables (x, t) we finally get

$$|\eta_3| \leqslant M \frac{h^2 + \tau^2}{h} (h\tau)^{(-1/2)} |s|_{W_2^2(E)}.$$

Using the technique of the Bramble–Hilbert lemma for other functionals, and applying the estimate (3.7), we come to the following result:

Theorem 4.1. *The solution of the operator–difference scheme* (3.6), (3.2) with $\varphi_i = S^x \otimes S^{t_i} f_i$, $i = 1, 2$ *converges to the generalized solution of problem* (2.18)–(2.20) $(s, \Theta) \in W_2^2(Q_{\mathrm{T}}) \times W_2^2(Q_{\mathrm{T}})$ *if the stability conditions* (3.5) *are satisfied. Therewith the following accuracy estimate holds*:

$$||v^j - s^j||_{(1)} \leqslant M_1 \Phi_2(h, \tau), \qquad ||\eta^j - \Theta^j||_{(1)} \leqslant M_2 \Phi_2(h, \tau), \tag{4.2}$$

where j is the index of the current time layer, M_1 *and* M_2 *are constants that do not depend on h and* τ, *and* $\Phi_2(h, \tau) = h + \tau$.

Remark 4.1. In the case of uncoupled thermoelasticity (when $\epsilon = 0$) and homogeneous boundary conditions for deformations the accuracy estimate (4.2) can be improved using the result of Theorem 3.1.

Remark 4.2. In the coupled case the second-order accuracy estimate may be obtained in some special cases if we use a weaker than L^2 metric for the thermoelastic field (see [25] and references therein).

5. Dispersion analysis

Impulses of arbitrary shape may be decomposed in a Fourier integral or a Fourier series as a superposition of harmonic waves of the form [38]

$$u(x,t) = \exp[(\kappa x - \omega t)\mathrm{i}],$$

where ω is the wave frequency, $\kappa = 2\pi/\lambda$ the wave number, and λ the wave length. Due to the dependence of the phase velocity of wave propagation on the wave length (i.e. due to the presence of dispersion) harmonic components of the signal are shifted with respect to each other. As a result, we observe a distortion of the impulse profile [38]. In order to find such a dependency for a thermoelastic media we substitute the harmonics of the differential problems (2.21),

$$r = R\exp[\mathrm{i}(\kappa x - \omega t)] \quad \text{and} \quad \theta = T\exp[\mathrm{i}(\kappa x - \omega t)], \tag{5.1}$$

into the differential system of thermoelasticity. In (5.1) R and T denote amplitudes of the corresponding harmonics. Expanding the system determinant and equating it to zero, we get the following dispersion relationship for the differential problem:

$$(\omega^2 - \kappa^2)(\mathrm{i}\omega - \kappa^2) - \mathrm{i}\epsilon\kappa^2\omega = 0. \tag{5.2}$$

To find the phase velocity from Eq. (5.2) we may use arguments based on the method of a small parameter. Such an approach may be often justified from the physical point of view, since the coupling parameter ϵ is small for a wide range of known materials. From the mathematical point of view such an approach requires $\epsilon \to 0$, that may not be true in practice. Indeed, the value of ϵ may be very small, but is nevertheless always positive. If we formally substitute the series

$$\omega = \sum_{k=0}^{\infty} \epsilon^k \omega_k$$

into the dispersion relationship (5.2) and neglect terms of the order $\mathrm{O}(\epsilon^2)$, we get two equations that have to be satisfied simultaneously:

$$\begin{aligned}&(\omega_0^2-\kappa^2)(\mathrm{i}\omega_0-\kappa^2)=0,\\&\mathrm{i}\omega_1(\omega_0^2-\kappa^2)+2\omega_0\omega_1(\mathrm{i}\omega_0-\kappa^2)-\mathrm{i}\kappa^2\omega_0=0.\end{aligned}\tag{5.3}$$

From (5.3) we find three distinct modes, that are approximate roots of the dispersion relationship (5.2), $\omega_{1,\mathrm{app}}$, $\omega_{2,\mathrm{app}}$, $\omega_{3,\mathrm{app}}$. They give us the dependencies of the frequency on the wave number, namely

$$\begin{aligned}\omega_{1,\mathrm{app}}&=\kappa\left(1+\frac{\epsilon}{2(1+\kappa^2)}\right)-\mathrm{i}\frac{\epsilon\kappa^2}{2(1+\kappa^2)},\\\omega_{2,\mathrm{app}}&=-\kappa\left(1+\frac{\epsilon}{2(1+\kappa^2)}\right)-\mathrm{i}\frac{\epsilon\kappa^2}{2(1+\kappa^2)},\\\omega_{3,\mathrm{app}}&=-\mathrm{i}\kappa^2\left(1-\frac{\epsilon}{1+\kappa^2}\right).\end{aligned}\tag{5.4}$$

It is well known that the quantity $\mathrm{Re}\,\omega$ is responsible for the phase velocity of the harmonics, whereas $\mathrm{Im}\,\omega$ is for the increase or damping of harmonics. Since the phase velocity of propagation of harmonics is defined as

$$v=\mathrm{Re}\,\omega/\kappa,$$

we can easily define from (5.4) approximate phase velocities of harmonic propagation for the differential problem (2.21). They are

$$v_1=1+\epsilon/[2(1+\kappa^2)],\qquad v_2=-v_1,\qquad v_3=0.\tag{5.5}$$

Furthermore, we know that when approximate solutions of differential problems are sought (for example, using difference schemes), it is important to take into account the dispersion properties of numerical methods used for such approximations. Such properties may be crucial when problems contain a hyperbolic type operator. Indeed, in this case numerical solutions of such problems are typically accompanied by parasitic oscillations that are connected with the dispersion of harmonics of the applied numerical scheme. In other words such oscillations have purely numerical origin [22]. Therefore it is important to achieve a better correspondence of dispersion properties of differential and discrete problems. Ultimately it is this correspondence that determines the quality of the problem solution because in coupled field theory it is rarely the case that a differential problem may be solved analytically.

Analogues of the harmonics (5.1) on the discrete grid $\bar{\omega}_{h\tau}$ have the following form:

$$y=Rq^n\xi^j,\qquad \eta=Tq^n\xi^j,\tag{5.6}$$

where $\xi=\exp(\mathrm{i}\kappa h)$, and q is the transfer factor of the difference scheme. It is straightforward to get the dispersion relationship for the difference scheme (2.22), namely

$$p^2/(\tau^2 - \zeta p - \zeta)([(1/\tau - \sigma\zeta) - \zeta]\epsilon\zeta p(p+1)/\tau = 0, \tag{5.7}$$

where

$$p = \sum_{k=0}^{\infty} \epsilon^k p_k, \qquad \zeta = (\xi - 2 + \xi^{-1})/h^2 = 4\sin^2(\kappa h/2)/h^2.$$

Using the method of a small parameter we can derive the analogue of (5.3) for the discrete problem (2.22) (see details in [22]). Standard requirements for the proper representation of dispersion effects are the conditions of superiority of the dispersion of the original differential problem compared to the numerical dispersion. Such conditions, which were derived in [22], have to be satisfied together with the stability conditions for the difference scheme. Here we sketch an alternative approach to the investigation of stability of difference schemes.

Let us represent the dispersion relationship (5.7) for the discrete problem through a polynomial of the third degree $Q_3(p) = 0$. Under quite general assumptions the question on system stability can be reduced to the question of whether the roots of the characteristic equation of the linearized system are to the left from the imaginary axis. If such a condition is satisfied then such polynomials are called stable.

We consider a stable polynomial given by the equation $Q_3(z) = 0$ (i.e. the stability domain of $Q_3(z)$ is assumed to be the whole left semi-plane). By the Cayley transform

$$q = (z+1)/(z-1) \tag{5.8}$$

the domain $\operatorname{Im} z \leqslant 0$ is mapped into the unit circle in the complex q plane. This domain is the stability domain of a transformed polynomial $\bar{Q}_3(q) = 0$. Now the transformation

$$p = q - 1 = 2/(z-1) \tag{5.9}$$

will lead us to the polynomial $Q_3(p)$, the stability domain of which is a circle of unit radius with the center in $(-1, 0)$. The described transformations are sketched in Fig. 1. Now we can substitute into the dispersion equation (5.7) instead of p its expression in terms of z. As a result, we get

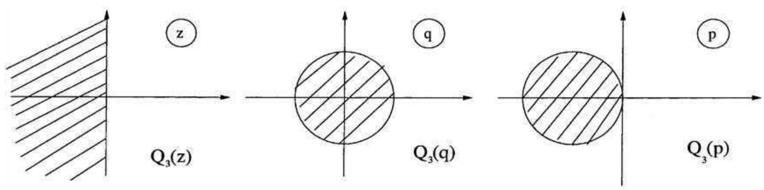

Fig. 1.

$$[-\zeta\tau^2 z^3 + 4\zeta\tau^2][-\zeta\tau z + 2(1-\sigma\zeta\tau) + \zeta\tau] - 2\epsilon\zeta\tau^2(z^2-1) = 0. \tag{5.10}$$

It is easy to see that Eq. (5.10) may be rewritten in the form

$$a_0 z^3 + a_1 z^2 + a_2 z + a_3 = 0, \tag{5.11}$$

where

$$a_0 = \zeta^2\tau^3, \qquad a_1 - \zeta\tau^2[2(1-\sigma\zeta\tau) + \zeta\tau + 2\epsilon],$$
$$a_2 = -\zeta\tau(4+\zeta\tau^2), \qquad a_3 = (4+\zeta\tau^2)[2(1-\sigma\zeta\tau) + \zeta\tau] + 2\epsilon\zeta\tau^2.$$

A special case of the Routh–Hurwitz theorem on stability of polynomials is the Vyshegradsky criterion that gives necessary and sufficient conditions for stability of third degree polynomials, namely

$$a_i > 0, \quad i = 0,1,2,3, \quad a_1 a_2 > a_0 a_3. \tag{5.12}$$

In our case the conditions $a_0 > 0$ and $a_1 a_2 > a_0 a_3$ will be satisfied for all values of σ, τ, h. The condition $a_2 > 0$ will be satisfied whenever the following inequality:

$$\frac{\tau^2}{h^2}\sin^2(\kappa h/2) < 1 \tag{5.13}$$

holds. The conditions $a_1 > 0$ and $a_3 > 0$ will be satisfied if

$$\tau(1-2\sigma) < (1+\epsilon)h^2/[2\sin^2(\kappa h/2)]. \tag{5.14}$$

We note that the conditions (5.13), (5.14) are equivalent to the stability conditions (3.5) for the difference schemes (2.22) and (2.23).

In conclusion we recall that the main property of the Cayley transform is the preservation of the main global properties of the system. Indeed, the transform (5.8) is a special case of a more general operator Cayley transform

$$T_\gamma = (\gamma I + A)(\gamma I - A)^{-1}, \tag{5.15}$$

where A is a linear operator acting in Banach spaces, $\gamma > 0$. The Cayley transform (5.15) allows us to transform conservative dissipative systems evolving in continuous time into discrete systems with the same global properties [1]. Under quite general assumptions the Cayley transform technique provides a general way for the construction of effective numerical approximations for differential equations in Banach spaces [13]. We will discuss these questions in details elsewhere.

6. Computational experiments

In this section we consider an application of the constructed and rigorously justified discrete models to the investigation of planar non-stationary waves in a thermoelastic layer under instantaneous action of surface forces of intensity p_0. Assuming that surfaces of the layer are thermo-isolated, the subject of investigation is reducible to the following initial-boundary value problem:

$$\begin{aligned} &\frac{\partial^2 \bar{\sigma}}{\partial \xi^2} - \frac{1}{c^2}\frac{\partial^2 \bar{\sigma}}{\partial \zeta^2} = \frac{1+v}{1-v}\rho\alpha_{\mathrm{T}}\frac{\partial^2 (T-T_0)}{\partial \zeta^2},\\ &\frac{\partial^2 T}{\partial \xi^2} - \frac{1}{a}(1+\epsilon)\frac{\partial T}{\partial \zeta} = \frac{(1+v)\alpha_{\mathrm{T}} T_0}{(1-v)\Lambda_q}\frac{\partial \bar{\sigma}}{\partial \zeta}, \end{aligned} \tag{6.1}$$

$$T = T_0, \quad \bar{\sigma} = 0, \quad \frac{\partial \bar{\sigma}}{\partial \zeta} = 0 \quad \text{for } \zeta = 0, \tag{6.2}$$

$$\bar{\sigma} = -p_0 H(\xi), \quad \frac{\partial T}{\partial \xi} = 0 \quad \text{for } \xi = 0, L, \tag{6.3}$$

where $\bar{\sigma}$ denotes the stress in the layer, $H(\zeta)$ is the unit Heaviside function. Other notation is standard (see Section 2).

After rescaling problem (6.1)–(6.3) may be cast in the form of the model (2.18)–(2.20) with

$$f_1 = f_2 = 0, \quad \Theta_0 = s_0 = \bar{s}_0 = 0, \quad \Theta_i(t) = 0, \quad s_i = -H(t).$$

Then the discrete model (2.22), (2.23) allows us to compute deformations explicitly. The algorithm goes as follows. Assuming that we have computed

- the values of deformations on the ith and $(i+1)$st time layers (except at the two ends of the layer), and
- the values of temperature on the ith time layer (for $i = 0$ they are known from the initial conditions),

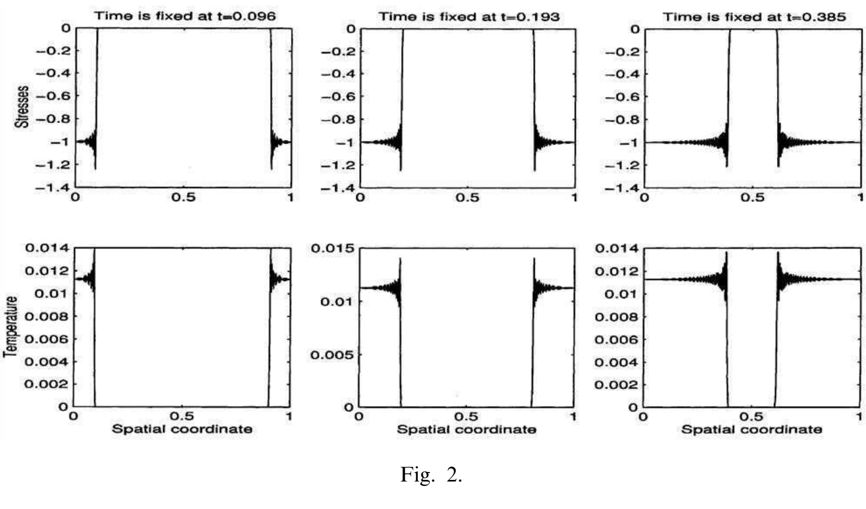

Fig. 2.

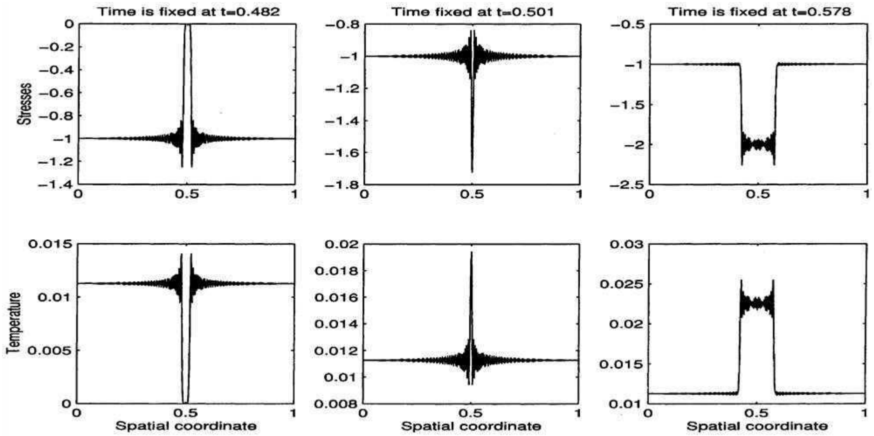

Fig. 3.

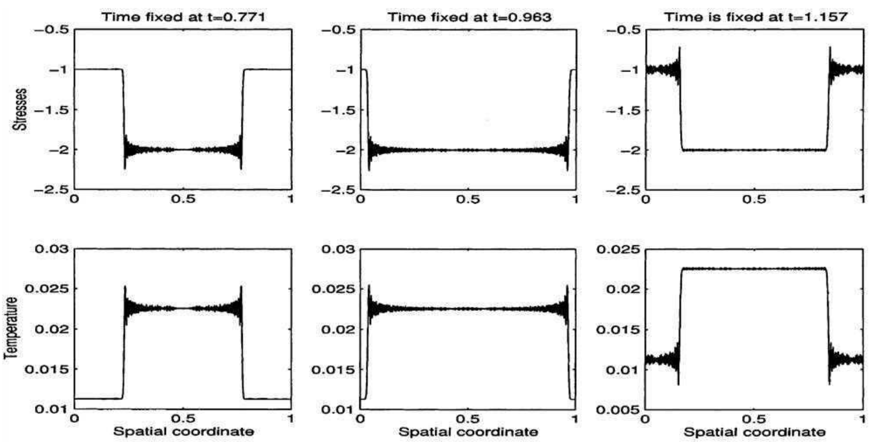

Fig. 4.

we obtain a system of linear algebraic equation for the determination of the values of temperature in all spatial points of the $(i+1)$st time layer. Then we compute the values of deformations at both ends of the layer. This allows us to determine explicitly the values of deformations on the $(i+2)$nd time layer (again, except for the ends of the layer), etc.

Figs. 2–5 show the distribution of stress and temperature in a steel layer ($\epsilon = 0.0114, a = 0.2 \times 10^{-8}$). A jump at the beginning of the observation is due to the action of inertia after surface forces were applied. Two thermoelastic waves, propagating from the layer boundaries, have not met yet. As a result,

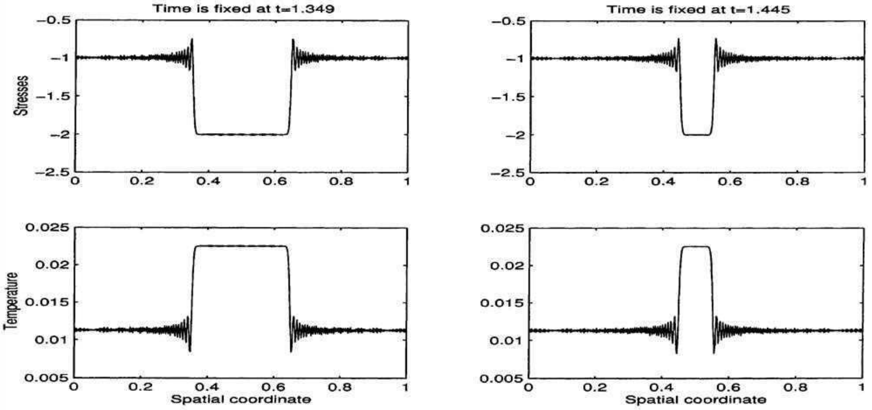

Fig. 5.

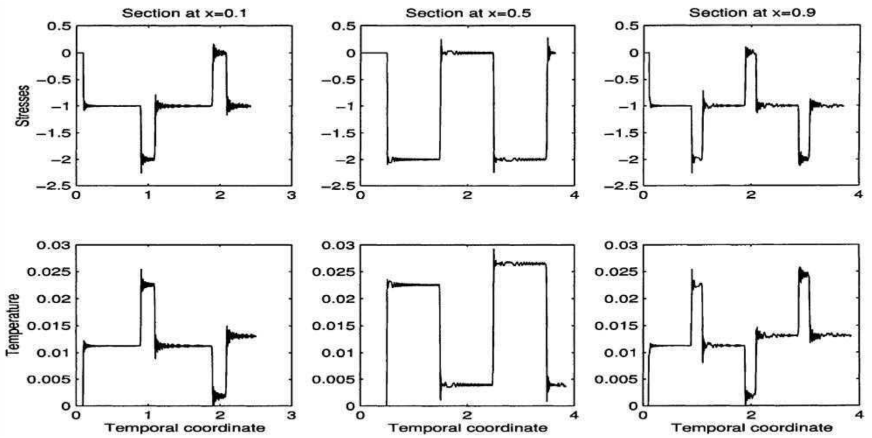

Fig. 6.

we observe a contractive stress that appears in the layer. As time goes on, waves meet and we observe the 'concentration' of stresses of magnitude $-2p_0$. Such a concentration is expanding with time from the middle to the layer boundaries. This reflects the physical essence of the process. Finally, Fig. 5 shows the distribution of stress and temperature with respect to time in different sections of the layer. The problem provides an example where neither spatial (see Figs. 2–5) nor temporal (see Fig. 6) derivatives exist in the classical sense. However, the developed computational procedures based on discrete models for thermoelasticity allowed us to correctly convey both qualitative and quantitative features of the process under investigation.

7. Future directions

The effective computational procedures developed for problems in coupled thermoelasticity can be used as building blocks for the development of refined models in other areas of coupled field theory, for example, in coupled thermo-electroelasticity. Interest in piezoelectrics has been revitalized [2] by its significance for smart materials [27] and the importance of piezoelectricity in biopolymers [12]. Mathematical models of dynamic electroelasticity have been extensively studied in the literature (see [26] and references therein). However, notwithstanding the coupled treatment of electro-mechanical fields in such models, for many practical applications it is important to take into consideration thermal effects as temperature has a profound influence on the properties of piezoelectrics.

To be competitive numerical codes in coupled field theory have to be adaptive. One of the major goals of adaptive computational schemes is to control the computational process. The success of this process often hinges on how well the numerical error can be estimated. This implies that in the general case we need a combination of a priori and a posteriori estimates [17]. The major difficulty in obtaining such a combination stems from the fact that the error needs to be integrated *with respect to time* which complicates numerical analysis in the nonstationary case. Computationally we are inevitably led to an optimization problem and the whole computational process can be seen as a problem of *optimal error control* (see [24] and references therein).

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