

Numerical Simulation of Thermoelastic Wave and Phase-Transition Front Propagation

Arkadi Berezovski¹, Jüri Engelbrecht¹, and Gerard A. Maugin²

¹ Department of Mechanics and Applied Mathematics, Institute of Cybernetics at Tallinn Technical University, Akadeemia tee 21, 12618 Tallinn, Estonia

² Laboratoire de Modélisation en Mécanique, Université Pierre et Marie Curie, UMR 7607, Tour 66, 4 Place Jussieu, Case 162, 75252, Paris Cédex 05, France

Abstract. A thermodynamically consistent form for the finite-volume numerical algorithm for thermoelastic wave and front propagation is proposed in the paper. Such reformulation provides applicability of the Godunov type numerical schemes based on averages of field variables to the description of non-equilibrium situations. The non-equilibrium description uses contact quantities instead of numerical fluxes. These quantities satisfy the thermodynamic consistency conditions which generalize the classical equilibrium conditions.

1 Introduction

The propagation of waves and phase-transition fronts in thermoelastic solids is governed by the same field equations and equations of state (at least in the integral formulation). In linear thermoelastic media these equations can be reduced to the classical hyperbolic wave equation and to the parabolic heat equation. Problems arise in the propagation of thermoelastic waves and fronts in *inhomogeneous* media. From a practical point of view, these problems are reduced to the construction of relevant numerical algorithms. Possible rapid variations in the properties of considered materials and the simultaneous presence of compression and shear waves require at least a second-order accuracy of the algorithms. Among successful methods with high accuracy and efficiency are the finite-volume schemes.

Finite-volume numerical methods (cf. [1], [2]) are based on the integration of governing equations over a control volume which includes a grid element and a time step. This means that the resulting numerical scheme is expressed in terms of averaged field variables and averaged fluxes at boundaries of the grid elements. The equations of state determining the properties of a medium are also assumed to be valid for the averaged quantities. In fact, this is an assumption of the local equilibrium inside the grid element, where the local equilibrium state is determined by the averaged values of field variables.

To obtain a high-order accuracy, the step-wise distribution of the field variables is changed to a piece-wise linear (or even nonlinear) distribution over the grid (cf. [3]). Such a reconstruction leads to a better approximation from the mathematical point of view and provides a high-order accuracy together with a certain procedure for suppressing spurious oscillations during computation. However, from the thermodynamic point of view, the reconstruction destroys the local equilibrium inside grid cells. This means that the equations of state are not valid in this case and even the meaning of thermodynamic variables (e.g. temperature and entropy) is questionable.

A possible solution of this problem is the description of the non-equilibrium states inside the grid elements in the framework of the thermodynamics of discrete systems [4]. The thermodynamic state space is extended in this theory by accounting for so-called *contact quantities* in addition to the usual local equilibrium variables. The crucial hypothesis then is the connection between the excess energy and contact quantities which describe the non-equilibrium states of discrete systems. The next step is the extension of the classical equilibrium conditions to the non-equilibrium case. In the paper, the corresponding procedure is described on the simple example of a uniaxial motion of a slab.

2 Wave-propagation algorithm

In order to explain some of the key ideas with a minimal mathematical complexity, it is convenient to work in an essentially one-dimensional setting. The system of equations for one-dimensional elastic waves can be represented in the conservative form [6], [7]

$$\frac{\partial q}{\partial t} + \frac{\partial f(q, x)}{\partial x} = 0. \quad (1)$$

The indicated explicit dependence on the point x means that the body is materially inhomogeneous in general. In the standard wave-propagation algorithm [1], a computational grid with interfaces $x_{n-1/2} = (n-1)/2\Delta x$, time levels $t_k = k\Delta t$ and cells $C_n = [x_{n-1/2}, x_{n+1/2}]$ is defined. For simplicity, the grid size Δx and time step Δt are assumed to be constant. Then the cell average

$$Q_n^k \approx \frac{1}{\Delta x} \int_{x_{n-1/2}}^{x_{n+1/2}} q(x, t_k) dx, \quad (2)$$

is updated in each time step as follows

$$Q_n^{k+1} = Q_n^k - \frac{\Delta t}{\Delta x} (F_{n+1}^k - F_n^k), \quad (3)$$

where F_n^k approximates the time average of the exact flux taken at the interface between the cells, i.e.

$$F_n^k \approx \frac{1}{\Delta t} \int_{t_k}^{t_{k+1}} f(q(x_{n-1/2}, t)) dt. \quad (4)$$

The main difficulty here is to determine the appropriate values of numerical fluxes F_n^k . The corresponding procedure was established by LeVeque [1] on the basis of the solution of the Riemann problems at each interface between cells. It was shown in [5] that the characteristic property of the conservative wave-propagation algorithm is the following

$$F_{n-1}^+(Q_{n-1}^k) - F_n^-(Q_n^k) = f_n(Q_n^k) - f_{n-1}(Q_{n-1}^k), \quad (5)$$

where superscripts "+" and "-" denote numerical fluxes from the left and right sides of the cell edge, respectively.

What we need is to extend this well developed numerical method to the simulation of moving phase boundaries in solids. It should be noted that a stress-induced phase transformation in a single crystal of a thermoelastic solid is a strongly non-equilibrium process, because of a fast propagation of sharp interfaces through the material. Therefore, we need to reformulate the algorithm in a consistent form for non-equilibrium situations.

3 Thermodynamic representation

The most convenient non-equilibrium thermodynamic theory for such a description is the thermodynamics of discrete systems [4]. In this theory, the state space of any discrete system is extended by means of *contact quantities* in order to describe non-equilibrium states. In the simplest case of a fluid-like system, they are contact temperature, dynamic pressure, and dynamic chemical potential. The contact quantities provide a complete thermodynamic description of non-equilibrium states of a separated discrete system. Note, however, that the values of the defined contact quantities differ from the values of usual bulk parameters of the case of local equilibrium.

In the required extension of the concepts of the thermodynamics of discrete systems to the *thermoelastic case*, we must define a *contact dynamic stress tensor* Σ_{ij} [6], [7] since the state space includes the deformation. Now it remains to establish the connection between the *bulk* quantities and the *contact* quantities.

3.1 Thermodynamic consistency conditions

Classical equilibrium conditions for any two single component simple systems consist in the equality of temperatures, pressures and chemical potentials in both systems

$$T^{(1)} = T^{(2)}, \quad p^{(1)} = p^{(2)}, \quad \mu^{(1)} = \mu^{(2)}. \quad (6)$$

Here superscripts denote distinct systems, and temperature, T , pressure, p , and chemical potential, μ , are given by

$$\left(\frac{\partial U}{\partial S}\right)_{V,N} = T, \quad \left(\frac{\partial U}{\partial V}\right)_{S,N} = -p, \quad \left(\frac{\partial U}{\partial N}\right)_{S,V} = \mu. \quad (7)$$

Here U is the internal energy, S is the entropy, V is volume, and N is mass. In general, the internal energy of a discrete system, U , that is not in equilibrium differs from the local equilibrium value, U_{eq} , by an excess energy, U_{ex} :

$$U(S, V, N) - U_{eq}(S_{eq}, V_{eq}, N_{eq}) = U_{ex}. \quad (8)$$

Assuming that the local equilibrium variables are defined as usual (7), the contact quantities can be associated with the excess energy:

$$\left(\frac{\partial U_{ex}}{\partial S}\right)_{V,N} = \Theta, \quad \left(\frac{\partial U_{ex}}{\partial V}\right)_{S,N} = -\pi, \quad \left(\frac{\partial U_{ex}}{\partial N}\right)_{S,V} = \nu. \quad (9)$$

Therefore, the equilibrium conditions (6) can be generalized to non-equilibrium case as follows

$$T^{(1)} + \Theta^{(1)} = T^{(2)} + \Theta^{(2)}, \quad p^{(1)} + \pi^{(1)} = p^{(2)} + \pi^{(2)}, \quad \mu^{(1)} + \nu^{(1)} = \mu^{(2)} + \nu^{(2)}. \quad (10)$$

In the considered elastic case, only the condition (10)₂ is relevant. It should be applied in a tensorial form

$$\sigma_{ij}^{(1)} + \Sigma_{ij}^{(1)} = \sigma_{ij}^{(2)} + \Sigma_{ij}^{(2)}, \quad (11)$$

where σ_{ij} is the Cauchy stress tensor. We will apply the consistency condition (11) to determine the values of the contact quantities.

3.2 Contact quantities

The finite-volume algorithm (3) can also be represented in terms of contact quantities [6]-[7]:

$$Q_i^{n+1} = Q_i^n - \frac{\Delta t}{\Delta x} (C_i^+(Q_i^n) - C_i^-(Q_i^n)), \quad (12)$$

where C^\pm denote corresponding contact quantities,

$$C^\pm(Q_i) = \begin{pmatrix} \Sigma^\pm(Q_i) \\ \mathcal{V}^\pm(Q_i) \end{pmatrix}. \quad (13)$$

Here \mathcal{V} denotes, by duality, the contact deformation velocity. The consistency condition

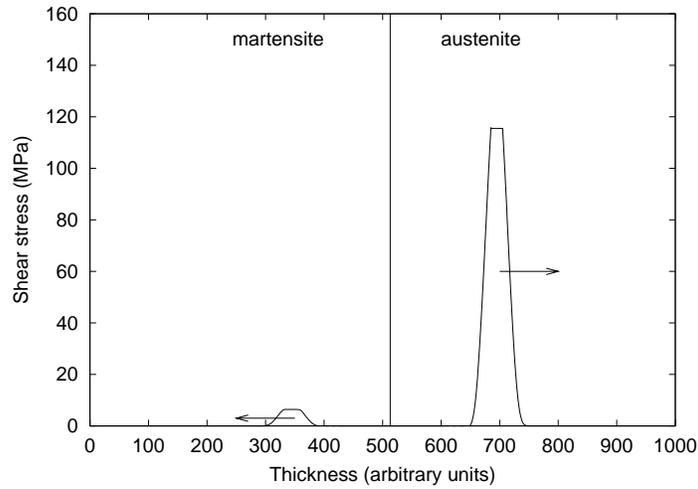


Fig. 1. Shear wave after interaction with phase boundary.

(11) in the uniaxial case

$$(\Sigma_{11}^+)_{i-1} - (\Sigma_{11}^-)_i = (\sigma_{11})_i - (\sigma_{11})_{i-1}, \quad (14)$$

should be complemented by the kinematic condition [8] which can be rewritten in the small-strain approximation as follows (v is the particle velocity)

$$(\mathcal{V}_1^+)_{i-1} - (\mathcal{V}_1^-)_i = (v_1)_i - (v_1)_{i-1}. \quad (15)$$

The two relations (14) and (15) can be expressed in vectorial form as follows:

$$C_{i-1}^+(Q_{i-1}^n) - C_i^-(Q_i^n) = f_i(Q_i) - f_{i-1}(Q_{i-1}). \quad (16)$$

It is easy to see that the last expression is nothing else but the characteristic property (5) for the conservative wave-propagation algorithm. Thus, the thermodynamic consistency conditions and kinematic conditions at the cell edge automatically lead to the conservative wave-propagation algorithm. From another point of view, this means that *the wave-propagation algorithm is thermodynamically consistent*.

4 Numerical results

Examples of numerical simulations of thermoelastic wave propagation are presented in [6], [7]. The most significant generalization of the wave-propagation algorithm consists in the possibility of numerical modeling of phase-transition front propagation [9], [10]. In the latter case we apply another consistency condition at the phase boundary. Details can be found in above cited papers. To show the capability of the algorithm, we present here the results of numerical simulation of the interaction of a shear stress wave with a phase boundary. We simulate the wave propagation induced by an impulsive loading of a slab by a shear stress. After interaction with the phase boundary initially set at abscissa 500, we obtain transmitted and reflected waves, amplitudes of which are cut due to the martensitic phase transformation (Fig.1). In addition, we observe a slight displacement of the phase boundary into the previous austenitic region.

Acknowledgment

Support of the Estonian Science Foundation under contract No.4504 (A.B.) and of the European Network TMR. 98-0229 on "Phase transitions in crystalline substances" (G.A.M.) is gratefully acknowledged.

References

1. R.J.LeVeque: J. Comp. Physics **131**, 327 (1997).
2. R.J.LeVeque: J. Comp. Physics **148**, 346 (1998).
3. T.J.Barth, M.G.Larson: 'A *Posteriori* Error Estimates for Higher Order Godunov Finite Volume Methods on Unstructured Meshes'. In: *Finite Volumes for Complex Applications III*. ed. by R.Herbin, D.Kröner (Hermes, London 2002) pp.41-63.
4. W.Muschik: 'Fundamentals of Non-Equilibrium Thermodynamics'. In: *Non-Equilibrium Thermodynamics with Application to Solids*. ed. by W.Muschik (Springer, Wien 1993) pp. 1-63.
5. D.S.Bale, R.J.LeVeque, S.Mitran, J.A.Rossmanith: (to appear in SIAM J. Sci. Comp.)
6. A.Berezovski, J.Engelbrecht, G. A.Maugin: Arch. Appl. Mech. **70**, 694 (2000).
7. A.Berezovski, G.A.Maugin: J. Comp. Physics **168**, 249 (2001).
8. G.A.Maugin: *Material Inhomogeneities in Elasticity* (Chapman and Hall, London 1993).
9. A.Berezovski, J.Engelbrecht, G.A.Maugin: 'A Thermodynamic Approach to Modeling of Stress-Induced Phase-Transition Front Propagation in Solids'. In: *Mechanics of Martensitic Phase Transformation in Solids* ed. by Q.P.Sun (Kluwer, Dordrecht 2002) pp. 19-26.
10. A.Berezovski, G.A.Maugin: Technische Mechanik **22**, 118 (2002).