Simulation of Wave and Front Propagation in Elastic and Thermoelastic Heterogeneous Materials

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Abstract

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

Key words: thermoelastic waves, phase transition fronts, finite-volume methods, thermodynamics of discrete systems

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, such as laminated composites, functionally graded

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materials, mesoscopic granular media, two-phase media, in other words, in medium with a microstructure. 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. LeVeque (1997, 1998)) 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 (Barth and Larson, 2002). 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 nonequilibrium states inside the grid elements in the framework of the thermodynamics of discrete systems (Muschik, 1993). The thermodynamic state space is extended in this theory by accounting for so-called contact quantities in addition to the usual local equilibrium variables. These quantities can be introduced into the finite-volume schemes in a natural way. 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 Uniaxial motion of a slab

Consider a slab, which in an unstressed reference configuration occupies the region $0 < x_1 < L, -\infty < x_2, x_3 < \infty$. Uniaxial motion means that all the displacements depend on only one spatial coordinate, say, $x_1$:

$$u_i = u_i(x, t), \quad v_i(x, t) = \frac{\partial u_i}{\partial t}, \quad x = x_1,$$  \hspace{1cm} (1)
where \( t \) is time, \( x_i \) are spatial coordinates, \( u_i \) are components of the displacement vector, \( v_j \) are particle velocities. In this case, we have only three non-vanishing components of the strain tensor, namely, \( \varepsilon_{11}, \varepsilon_{12}, \) and \( \varepsilon_{13} \). Without loss of generality, we can set \( \varepsilon_{13} = 0, v_3 = 0 \) because of zero initial and boundary conditions for these components. Then we obtain uncoupled systems of equations for longitudinal and shear components which express the balance of linear momentum and the time derivative of the Duhamel-Neumann thermoelastic constitutive equation, respectively (Berezovski, Engelbrecht and Maugin, 2001; Berezovski and Maugin, 2000):

\[
\rho_0(x) \frac{\partial v_1}{\partial t} = \frac{\partial \sigma_{11}}{\partial x}, \quad \frac{\partial \sigma_{11}}{\partial t} = (\lambda(x) + 2\mu(x)) \frac{\partial v_1}{\partial x} + m(x) \frac{\partial \theta}{\partial t},
\]

and

\[
\rho_0(x) \frac{\partial v_2}{\partial t} = \frac{\partial \sigma_{12}}{\partial x}, \quad \frac{\partial \sigma_{12}}{\partial t} = \mu(x) \frac{\partial v_2}{\partial x},
\]

which are complemented by the heat conduction equation

\[
C(x) \frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x} \left( k(x) \frac{\partial \theta}{\partial x} \right).
\]

Here \( \sigma_{ij} \) is the Cauchy stress tensor, \( \rho_0 \) is the density, \( \theta \) is temperature, \( C(x) \) is the heat capacity per unit volume for a fixed deformation. The dilatation coefficient \( \alpha \) is related to the thermoelastic coefficient \( m \), and the Lamé coefficients \( \lambda \) and \( \mu \) by \( m = -\alpha(3\lambda + 2\mu) \). The indicated explicit dependence on the point \( x \) means that the body is materially inhomogeneous in general. These systems of equations, (2) and (3), can be solved separately. For the simplicity, we focus our attention on the system of equations (3) for shear components.

2.1 Dynamic loading

In a dynamic problem we shall look for piecewise smooth velocity and stress fields \( v_2(x, t), \sigma_{12}(x, t) \) for inhomogeneous thermoelastic materials, which obey the following initial and boundary conditions:

\[
\sigma_{12}(x, 0) = v_2(x, 0) = 0, \quad \text{for} \quad x > 0,
\]

\[
\sigma_{12}(0, t) = \sigma_0(t), \quad \sigma_{12}(L, t) = 0 \quad \text{for} \quad t > 0,
\]
and satisfy the field equations
\[
\frac{\partial(\rho_0(x)v_2)}{\partial t} - \frac{\partial \sigma_{12}}{\partial x} = 0, \quad \frac{\partial}{\partial t} \left( \frac{\sigma_{12}}{\mu(x)} \right) - \frac{\partial v_2}{\partial x} = 0.
\] (7)

The formulated problem looks like a very simple one, because no information about the placement and the velocity of a phase boundary is included, yet.

3 Jump relations

To consider the possible irreversible transformation of a phase into another one, the separation between the two phases is idealized as a sharp, discontinuity surface \( S \) across which most of the fields suffer finite discontinuity jumps. Let \([A]\) and \(< A >\) denote the jump and mean value of a discontinuous field \( A \) across \( S \), the unit normal to \( S \) being oriented from the “minus” to the “plus” side: \([A] := A^+ - A^-\), \(< A > := 1/2(A^+ + A^-)\).

3.1 Quasi-static conditions

Classical equilibrium conditions for heterogeneous media consist, for fluid-like systems, in the equality of temperatures, pressures and chemical potentials in the two phases:
\[
[\theta] = 0, \quad [p] = 0, \quad [\mu] = 0.
\] (8)

Remembering the definitions of temperature, \( \theta \), pressure, \( p \), and chemical potential, \( \mu \), in the energy representation, \( U = U(S, V, M) \)
\[
\left( \frac{\partial U}{\partial S} \right)_{V,M} = \theta, \quad \left( \frac{\partial U}{\partial V} \right)_{S,M} = -p, \quad \left( \frac{\partial U}{\partial M} \right)_{S,V} = \mu,
\] (9)
we can represent the equilibrium conditions (8) in the form
\[
\left[ \left( \frac{\partial U}{\partial S} \right)_{V,M} \right] = 0, \quad \left[ \left( \frac{\partial U}{\partial V} \right)_{S,M} \right] = 0, \quad \left[ \left( \frac{\partial U}{\partial M} \right)_{S,V} \right] = 0.
\] (10)

Here \( U \) is the internal energy, \( S \) is the entropy, \( V \) is the volume, and \( M \) is mass. In the quasi-static uniaxial case in a solid we will have for shear components:
\[
[\theta] = 0, \quad [\sigma_{12}] = 0, \quad [\mu_{12}] = 0,
\] (11)
where the chemical potential tensor is introduced (Grinfeld, 1991)

\[
\mu_{ij} = W \delta_{ij} - \varepsilon_{ik} \sigma_{kj}.
\] (12)

Here \( W \) is the free energy per unit volume. The formulated equilibrium conditions have no difference for the processes with and without entropy production. More general conditions can be obtained if we consider the following stability conditions.

3.2 Stability conditions

The intrinsic stability of single-component simple fluid-like systems may be expressed by the following two conditions (Callen, 1960), ch.8

\[
\left(\frac{\partial T}{\partial S}\right)_{V,M} > 0, \quad -\left(\frac{\partial p}{\partial V}\right)_{\theta,M} > 0.
\] (13)

If the criteria of stability (13) are not satisfied, then a system breaks up into two or more phases. The critical point that forms the boundary between full stability and instability is determined by several conditions, the first of them (necessary, but not sufficient) being the following one (Callen, 1960), ch.9

\[
\left(\frac{\partial p}{\partial V}\right)_{\theta,M} = 0 \quad \text{or} \quad \left(\frac{\partial U}{\partial V}\right)_{\theta,M} = \left(\frac{\partial U}{\partial V}\right)_{p,M}.
\] (14)

Therefore, the critical point of stability is controlled by other thermodynamic derivatives than those in the equilibrium condition (10). It is natural to express the conditions of the equilibrium between phases in those terms which are used in the condition (14). This leads to another choice of independent variables in the fundamental equation, namely, \( \theta, V, M \) or \( p, V, M \). Choosing the set of independent variables \( \theta, V, M \), or \( p, V, M \), we obtain instead of (10), respectively,

\[
\left[\left(\frac{\partial U}{\partial V}\right)_{\theta,M}\right] = 0, \quad \text{or} \quad \left[\left(\frac{\partial U}{\partial V}\right)_{p,M}\right] = 0.
\] (15)

The equilibrium condition (15)_1 can be associated with the equilibrium of any heterogeneous fluid phases or materials without phase transformation and the second one (15)_2 with the presence of a phase transformation process accompanied by entropy production at the phase boundary. At the critical point of instability we have a continuous change of the equilibrium conditions.
from \((15)_1\) to \((15)_2\). Therefore, the two conditions \((15)_1\) and \((15)_2\) should be satisfied at this point simultaneously.

3.3 Dynamic conditions at phase-transition fronts

In the case of phase transition fronts, the material condition

\[
[V] = 0 \quad \text{at} \quad S
\]  \hspace{1cm} (16)

is referred to as the condition of coherency, for it implies in discrete terms (on the lattice structure) that material points of \(S\) belong simultaneously to both phases at \(S\) at all times (Maugin, 1999). The material velocity \(V\) is defined by means of the inverse mapping \(X = \chi^{-1}(x,t)\), where \(X\) denotes the material points (Maugin, 1993). We consider that the transition across \(S\) is homothermal, so that

\[
[\theta] = 0 \quad \text{at} \quad S.
\]  \hspace{1cm} (17)

Jump relations associated with the conservation laws in the bulk are formulated according to the theory of weak solutions of hyperbolic systems. Thus the jump relations associated with the balance of linear momentum and balance of entropy read (Maugin, 1997, 1998):

\[
\tilde{V}_N[\rho_0 v_2] + [\sigma_{12}] = 0, \quad \tilde{V}_N[S] + \left[\frac{k}{\theta} \frac{\partial \theta}{\partial x}\right] = \sigma_S \geq 0,
\]  \hspace{1cm} (18)

where \(\tilde{V}_N\) is the normal component of the material velocity of the points of \(S\), and \(\sigma_S\) is the entropy production at the interface. In the dynamic case, the condition \((11)_3\) is replaced by

\[
[\mu_{12}] = -f_S \neq 0,
\]  \hspace{1cm} (19)

where \(f_S\) is the scalar value of the driving force applied along the normal to \(S\)

\[
f_S = -[W - \sigma_{ij} \varepsilon_{ij}].
\]  \hspace{1cm} (20)

As shown in (Maugin, 1997, 1998), the entropy production can be expressed in terms of the driving force \(f_S\) such that the dissipation at the interface reads

\[
f_S \tilde{V}_N = \theta_S \sigma_S \geq 0,
\]  \hspace{1cm} (21)
where $\theta_S$ is the temperature at $S$. Formulated dynamic conditions look like completely non-equilibrium ones. However, it is implicitly supposed that all the field variables (including temperature and entropy) are correctly defined. This means that the hypothesis of local state is quietly assumed. At the same time, martensitic phase transformations are strongly non-equilibrium processes. That is why we need to establish true non-equilibrium conditions at the phase boundary.

### 3.4 Non-equilibrium thermodynamic conditions at the phase boundary

It is commonly assumed that there exists a constitutive relation for a two-phase material (e.g., double-well potential). This means that a two-phase body as a whole has a local accompanying state. Definitely, there exists a constitutive relation for each phase. Therefore, each phase can be separately considered as a thermodynamic system having a local accompanying state. The problem is to describe the non-equilibrium thermodynamic states of each subsystem and the whole two-phase system in a consistent way. The most convenient non-equilibrium thermodynamic theory for such a description is the thermodynamics of discrete systems (Muschik, 1993). In this theory, the state space of any discrete system is extended by means of so-called contact quantities. In the simplest case of a fluid-like system, they are contact temperature, dynamic pressure, and dynamic chemical potential. In general, the internal energy of a discrete system that is not in equilibrium, differs from the local equilibrium value in such a way that

$$
U(S, V, M) - U^{eq}(S^{eq}, V^{eq}, M^{eq}) = U^{ex}.
$$

Assuming that the local equilibrium variables are defined as usual (9), we can associate the contact quantities with the excess energy, $U^{ex}$.

In the required extension of the concepts of the thermodynamics of discrete systems to the thermoelastic case, in addition to the contact temperature $\Theta$ (Muschik, 1993), which governs heat exchange, we must define a contact dynamic stress tensor $\Sigma$ since the state space includes the deformation. We have thus

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

Here $\sigma^*$ is the Cauchy stress tensor in the environment.
In the thermoelastic case, the thermodynamic derivatives which we should exploit instead of \( \left( \frac{\partial U}{\partial V} \right)_p \) and \( \left( \frac{\partial U}{\partial V} \right)_\theta \) are the following ones:

\[
\left( \frac{\partial E^{eq}}{\partial \varepsilon_{ij}} \right)_\theta = -\theta \left( \frac{\partial \sigma^{eq}_{ij}}{\partial \theta} \right) + \sigma^{eq}_{ij}, \quad \left( \frac{\partial E^{eq}}{\partial \varepsilon_{ij}} \right)_\sigma = \theta \left( \frac{\partial S^{eq}}{\partial \varepsilon_{ij}} \right) + \sigma^{eq}_{ij},
\]

(24)

where \( E \) is the internal energy per unit volume.

It is supposed that the introduced contact quantities are connected with the excess energy in a similar way

\[
\left( \frac{\partial E^{ex}}{\partial \varepsilon_{ij}} \right)_\theta = -\Theta \left( \frac{\partial \Sigma^{eq}_{ij}}{\partial \theta} \right) + \Sigma_{ij}, \quad \left( \frac{\partial E^{ex}}{\partial \varepsilon_{ij}} \right)_\sigma = \Theta \left( \frac{\partial S^{ex}}{\partial \varepsilon_{ij}} \right) + \Sigma_{ij}.
\]

(25)

In fact, the latter two equations are relations of the constitutive type for the introduced contact quantities. The thermodynamic equilibrium conditions (15) are generalized to non-equilibrium situations as follows (square brackets still denote jumps):

\[
\left[ -\theta \left( \frac{\partial \sigma^{eq}_{ij}}{\partial \theta} \right) + \sigma^{eq}_{ij} - \Theta \left( \frac{\partial \Sigma^{eq}_{ij}}{\partial \theta} \right) + \Sigma_{ij} \right] = 0,
\]

(26)

\[
\left[ \theta \left( \frac{\partial S^{eq}_{ij}}{\partial \varepsilon_{ij}} \right) + \sigma^{eq}_{ij} + \Theta \left( \frac{\partial S^{eq}_{ij}}{\partial \varepsilon_{ij}} \right) + \Sigma_{ij} \right] = 0.
\]

(27)

We refer to the obtained relations (26) and (27) as thermodynamic consistency conditions. The first kind of consistency (26) is valid for all processes with no entropy production, while the second kind (27) corresponds to any inhomogeneity accompanied by entropy production. We do not need to derive the consistency condition for the chemical potential, because the previously mentioned nonequilibrium condition (19)

\[
[\mu_{12}] = -f_S \neq 0,
\]

(28)

can be interpreted in terms of the dynamic chemical potential tensor \( \nu_{ij} \)

\[
[\mu^{eq}_{12}] = -f_S = [\nu_{12}].
\]

(29)

4 Finite-volume approximation

Now we can return to the solution of the system of equations for one-dimensional shear elastic wave propagation (5). This system of equations can be repre-
sented in the form of a conservation law
\[ \frac{\partial q}{\partial t} + \frac{\partial f(q, x)}{\partial x} = 0 \] (30)

where
\[ q(x, t) = \begin{pmatrix} \rho(x) v(x, t) \\ \sigma(x, t) / \mu(x) \end{pmatrix}, \quad f(q, x) = \begin{pmatrix} -\sigma(\varepsilon, x) \\ -v(x) \end{pmatrix} \] (31)

In the standard wave-propagation algorithm (LeVeque, 1997), a computational grid with interfaces \( x_{n-1/2} = (n - 1)/2\Delta x \), time levels \( t_k = k\Delta t \) and cells \( C_n = [x_{n-1/2}, x_{n+1/2}] \) are defined. For simplicity, the grid size \( \Delta x \) and time step \( \Delta t \) are assumed to be constant. Then the cell average
\[ Q_k^k \approx \frac{1}{\Delta x} \int_{x_{n-1/2}}^{x_{n+1/2}} q(x, t_k) \, dx \] (32)

is updated in each time step as follows
\[ Q_k^{k+1} = Q_k^k - \frac{\Delta t}{\Delta x} (F_{n+1}^k - F_n^k) \] (33)

where \( F_n^k \) approximates the time average of the exact flux taken at the interface between the cells, i.e.
\[ F_n^k \approx \frac{1}{\Delta t} \int_{t_k}^{t_{k+1}} f(q(x_{n-1/2}, t)) \, dt. \] (34)

The main difficulty here is to determine the appropriate values of numerical fluxes \( F_n^k \). The corresponding procedure was established by LeVeque (1997) on the basis of the solution of the Riemann problems at each interface between cells. It was shown (Bale et al., 2002) that the characteristic property of the conservative wave-propagation algorithm is the following
\[ F_{n-1}^+(Q_{n-1}^k) - F_n^-(Q_n^k) = f_n(Q_n^k) - f_{n-1}(Q_{n-1}^k), \] (35)

where superscripts ”+” and ”−” denote numerical fluxes from the left and right sides of the cell edge, respectively. The advantages of the wave-propagation algorithm are high-resolution and the possibility for a natural extension to higher dimensions.
5 Thermodynamically consistent algorithm

We propose to apply the thermodynamic consistency conditions to determine the values of field quantities at the phase boundary. However, we can develop a general procedure for the calculation of numerical fluxes at each interface between discrete elements. For this purpose, we represent the finite-volume algorithm (33) in terms of contact quantities (Berezovski, Engelbrecht and Maugin, 2000, Maugin and Berezovski, 2000, Berezovski and Maugin, 2001):

\[
Q_{n}^{k+1} = Q_{n}^{k} - \frac{\Delta t}{\Delta x} \left( C_{n}^{+}(Q_{n}^{k}) - C_{n}^{-}(Q_{n}^{k}) \right),
\]

(36)

where \( C^{\pm} \) denote contact quantities corresponding to the right and left interfaces of the element, respectively,

\[
C^{\pm}(Q_{n}) = \begin{pmatrix} \Sigma^{\pm}(Q_{n}) \\ V^{\pm}(Q_{n}) \end{pmatrix}.
\]

(37)

Here \( V \) denotes, by duality, the contact deformation velocity.

We distinguish "dynamic" and "thermal" parts of the condition (26) as follows

\[
[\bar{\sigma}_{ij} + \Sigma_{ij}] = 0,
\]

\[
\left[ -\bar{\theta} \left( \frac{\partial \bar{\sigma}_{ij}}{\partial \theta} \right)_{\varepsilon} - \Theta \left( \frac{\partial \Sigma_{ij}}{\partial \theta} \right)_{\varepsilon} \right] = 0,
\]

(38)

and treat them separately. For each computational cell, the dynamic part of the consistency condition (38)\(_{1}\) in the uniaxial case

\[
(\Sigma_{12})_{i-1} - (\Sigma_{12})_{i} = (\bar{\sigma}_{12})_{i} - (\bar{\sigma}_{12})_{i-1},
\]

(39)

should be complemented by the kinematic condition (Maugin, 1993) which can be rewritten in the small-strain approximation as follows

\[
[\bar{v} + V] = 0.
\]

(40)

Assuming that the jump of contact velocity is such that

\[
[V] = [\bar{V}],
\]

(41)

we obtain for each computational cell in the uniaxial case

\[
(V_{2}^{+})_{i-1} - (V_{2}^{-})_{i} = (\bar{v}_{2})_{i} - (\bar{v}_{2})_{i-1}.
\]

(42)
The two relations (39) and (42) can be expressed in vectorial form as follows:

\[ C_{i-1}^+(Q_{i-1}^n) - C_i^-(Q_i^n) = f_i(Q_i) - f_{i-1}(Q_{i-1}) \]  

(43)

It is easy to see that the last expression is nothing else but the characteristic property (35) 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.

Examples of numerical simulations of thermoelastic wave propagation are presented in (Berezovski and Maugin, 2000; Berezovski, Engelbrecht and Maugin, 2001; Berezovski and Maugin, 2002a). The most significant generalization of the wave-propagation algorithm consists in the possibility of numerical modeling of phase-transition front propagation (Berezovski, Engelbrecht and Maugin, 2002; Berezovski and Maugin, 2002b). In the latter case we apply another consistency condition (27) at the phase boundary. Details can be found in above cited papers. To show the capability of the algorithm, we compare the results of computation for the stress-strain relation at the phase boundary with the experimental data by Goo and Lexcellent (1997). The properties of austenite phase of the Cu-25.63Zn-4.2Al shape-memory alloy are extracted from the paper of Goo and Lexcellent (1997): the density \( \rho = 8228 \text{ kg/m}^3 \), the elastic modulus \( E = 67 \text{ GPa} \). For the martensitic phase we choose, respectively, \( E = 31 \text{ GPa} \), with the same density value. It should be noted that the best correspondence is achieved by the value of the dilatation coefficient.
Fig. 2. Stress-strain relation at the phase boundary: comparison with experimental data from (Goo and Lexcellent, 1997).

\[ \alpha = 2.125 \times 10^{-6} \, \text{1/K} \]

To compare the results of dynamic computations with the quasi-static experimental data with the loading rate 1 MPa/s, the shape of the initial pulse was chosen as shown in Fig. 1. The results of comparison of the stress-strain relation in the case of the full recovering of austenite after unloading are shown in Fig. 2. Here the solid line corresponds to computations, and crosses denote the experimental data.

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