PHASE TRANSITIONS AND OSCILLATION WAVES IN AN ELASTIC BAR

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Abstract

In this note we present the results of a study of numerical solutions for a system representing a rate-type viscoelastic model describing the evolution of a material point in a bar of a material capable of phase transition. The appearance of the so-called oscillation waves is investigated and its mathematical meaning is understood, regarding the viscoelastic system and the passage to the limit when the relaxation time goes to zero. We call attention to the resemblance between the pattern associated with the oscillation waves and the experimentally observed laminated microstucture of alternating phases in single crystal samples of shape memory alloy. A number of numerical experiments concerning the asymptotic behavior of many important physical quantities, such as stress, strain and phase fractions, is shown and the results are seen to be consistent with the expected ones, resulting from physical considerations.

Resumo

Neste artigo apresentamos os resultados de um estudo sobre a solução numérica de um sistema representando um modelo viscoelástico "rate-type" para o movimento de pontos materiais em uma barra elástica capaz de realizar mudança de fase. Quando o parâmetro de relaxação vai para infinito o sistema se reduz a um sistema 2×2 modelando elasticidade não-linear com função de tensão não-monótona. Ao perturbar um estado na região das misturas de fase observa-se a ocorrência de oscilações persistentes, denominadas ondas de oscilação. Mostra-se que tais ondas estão associadas a soluções no sentido de funções a valores-medidas do sistema limite 2×2. Para a obtenção dos valores esperados de funções de estado de interesse, como tensão, energia, fração de fase, etc., correspondentes às soluções a valores-medidas associadas às ondas de oscilação, um método numérico baseado nos resultados teóricos mencionados é fornecido, e os resultados analisados, obtendo-se plena coerência com os fatos físicos conhecidos.

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1. Introduction

We give a numerical treatment of phase transition in elasticity with a non-monotone stress-strain relation [1]. It is obtained from a sequence of solutions for a rate-type viscoelastic problem, for which in the limit as the relaxation parameter tends to zero the viscoelastic problem reduces to the rate-independent elastic problem. It is interesting to note that numerical solutions may present an evolution marked by the appearance of a progressive chain of stationary jump discontinuities, which we call oscillation waves. Jump discontinuities in strain, between two values representing two different phases, resemble the experimentally observed interface patterns of phase mixtures in single crystals of shape memory alloys during martensitic transformation [2].

For one dimensional motion of a solid body in the absence of external forces, we have

$$\begin{aligned} &\rho\,\partial_t v - \partial_x \sigma_e(\varepsilon) = 0, \\ &\partial_t \varepsilon - \partial_x v = 0, \end{aligned} \tag{1}$$

where ρ is a constant representing the reference mass density, v the velocity, ε the Lagrangian strain, and $\sigma = \sigma_e(\varepsilon)$ the stress-strain relation for an elastic body. The system (1) is hyperbolic if $d\sigma_e/d\varepsilon$ is positive, and elliptic if $d\sigma_e/d\varepsilon$ is negative. It is well-known from stability analysis that the states with negative $d\sigma_e/d\varepsilon$ are not stable equilibrium states.

We shall consider the initial value problems for (1) with initial data

$$v(x,0) = v_0(x), \quad \varepsilon(x,0) = \varepsilon_0(x), \quad x \in \mathbb{R}. \tag{2}$$

In order to describe phase transitions and for simplicity in our numerical experiments, we shall take a non-monotone piecewise linear stress-strain relation:

$$\sigma_e(\varepsilon) = \begin{cases} E_1\varepsilon, & \varepsilon \le \varepsilon_A, \\ E_1\varepsilon_A - M(\varepsilon - \varepsilon_A), & \varepsilon_A < \varepsilon < \varepsilon_M, \\ E_1\varepsilon_A - M(\varepsilon_M - \varepsilon_A) + E_2(\varepsilon - \varepsilon_M), & \varepsilon \ge \varepsilon_M, \end{cases} \tag{3}$$

where $0 < \varepsilon_A < \varepsilon_M$, and E_1, E_2, and M are positive material constants.

Our approach to find the numerical solution of the elastic problem (1), (2) will proceed by means of a numerical scheme which is primarily intended to approximate the solution which describes the one dimensional motion of a viscoelastic body by replacing the elastic stress-strain relation with a rate type viscoelastic relation (see [3]):

$$\begin{aligned} &\rho\, \partial_t v - \partial_x \sigma_e(\varepsilon) = 0, \\ &\partial_t \varepsilon - \partial_x v = 0, \\ &\partial_t \sigma - E\partial_x v = -\kappa\,(\sigma - \sigma_e(\varepsilon)), \end{aligned} \tag{4}$$

where $\kappa > 0$ is a Maxwell-type viscosity constant, or $1/\kappa$ is referred to as the relaxation time parameter. We shall refer to $\sigma_e(\varepsilon)$ as the equilibrium stress-strain relation. Note that the system (4) is strictly hyperbolic, and we shall consider the following initial data corresponding to (2):

$$v(x,0) = v_0(x), \quad \varepsilon(x,0) = \varepsilon_0(x), \quad \sigma(x,0) = \sigma_e(\varepsilon_0(x)), \quad x \in I\!R. \tag{5}$$

Intuitively, if one can obtain a sequence of solutions, $(v^\kappa, \varepsilon^\kappa, \sigma^\kappa)$, for the viscoelastic problem (4), (5), as parameter $\kappa \to \infty$, one would expect that the sequence $(v^\kappa, \varepsilon^\kappa)$ might converge to a solution of the elastic problem (1), (2).

2. Approximate Solutions of Riemann Problems

We shall consider Riemann problems for (1), which can be written as a 2×2 system of conservation laws in the form,

$$\partial_t \boldsymbol{u} + \partial_x \boldsymbol{F}(\boldsymbol{u}) = 0, \qquad \boldsymbol{u} \in I\!R^2, \tag{6}$$

with initial data,

$$\mathbf{u}(x,0) = \begin{cases} \mathbf{u}_L, & \text{for } x < 0, \\ \mathbf{u}_R & \text{for } x > 0, \end{cases} \tag{7}$$

where $\boldsymbol{u} = (v, \varepsilon)$ and $\boldsymbol{F}(\boldsymbol{u}) = (-\sigma_e(\varepsilon), -v)$. Such a problem has the property that if $\boldsymbol{u}(x,t)$ is a solution then so is $\boldsymbol{u}(ax, at)$ for any $a \in I\!R$. We shall refer to this as the scaling property. Numerically, this property implies that approximate solutions for successive refinements of grid spacings can be obtained simply by scaling from a solution based on a fixed grid spacing at successive time steps.

Following the idea stated in the previous section, we shall consider successive approximate solutions of the corresponding Riemann problem for the hyperbolic viscoelastic system (4), (5) as the Maxwell viscosity $\kappa \to \infty$ in such a way that the grid spacing is inversely proportional to κ. In this manner, owing to the scaling property mentioned above, one can construct a sequence of approximate solutions for successive refinements of grid spacing and increasing κ simultaneously from a fixed one at successive time steps, for certain given κ and grid spacing.

Let Δx, Δt be grid spacings and $\alpha = \kappa \Delta t$. For some given α, the approximate solution at the grid points, $x = i\Delta x$ and $t = j\Delta t$, is defined as

$$v_\alpha(x,t) = v_i^j, \quad \varepsilon_\alpha(x,t) = \varepsilon_i^j, \quad \sigma_\alpha(x,t) = \sigma_i^j. \tag{8}$$

Using the characteristic variables,

$$p = \sigma + cv, \qquad q = \sigma - cv, \qquad r = \sigma - E\varepsilon,$$

where $c = \sqrt{E}$, the system (4) becomes

$$\begin{aligned} &\partial_t p - c\,\partial_x p = -\kappa\, G(p,q,r), \\ &\partial_t q + c\,\partial_x q = -\kappa\, G(p,q,r), \\ &\partial_t r = -\kappa\, G(p,q,r), \end{aligned} \tag{9}$$

where $G(p,q,r) = (p+q)/2 - \sigma_e(1/E((p+q)/2 - r))$. Given fixed Δt, $\Delta x = c\Delta t$, and κ, we obtain an approximate solution for (4), with the method of characteristics using (9) [3], by setting

$$\begin{aligned} p_i^{j+1} &= p_i^j - \kappa \Delta t\, G_{i+1}^j \\ q_i^{j+1} &= q_i^j - \kappa \Delta t\, G_{i-1}^j \\ r_i^{j+1} &= r_i^j - \kappa \Delta t\, G_i^j, \end{aligned} \tag{10}$$

where $G_i^j = G(p_i^j, q_i^j, r_i^j)$. It is easy to see that such a scheme has the scaling property.

Now, let $\alpha = \kappa' \Delta t'$ be fixed for some given κ' and $\Delta t'$. By the scaling property, we can construct a sequence of approximate solutions with $\kappa = n\kappa'$

and $\Delta t = \Delta t'/n$, from the approximate solution (8) (or equivalently (10)) with fixed α by defining

$$\boldsymbol{u}^n(x,t) = \boldsymbol{u}_\alpha(nx, nt). \tag{11}$$

Successive refinements of grid spacing and increasing κ are thus effected simultaneously from a fixed one, with given κ and grid spacing, as the time step n increases.

This scheme allows an energy estimate (see [4, 5]) and hence ensures the uniform local boundedness of the total energy if α is small enough. Such a scheme is absolutely stable and can be proceeded to arbitrary number of time steps.

Indeed, we recall that the viscoelastic system admits a free energy function $\psi(\varepsilon,\sigma)$, given by [5]

$$\psi(\varepsilon,\sigma) = \frac{\sigma^2}{2E} + \varphi(\sigma - E\varepsilon),$$

where φ is defined by

$$\varphi'(\tau) = \frac{-1}{E}\sigma_e(h^{-1}(\tau)), \quad \phi(0) = 0, \quad \tau \in I\!R,$$

with $h(\varepsilon) = \sigma_e(\varepsilon) - E\varepsilon$, $\varepsilon \in I\!R$. This function satisfies

$$\frac{\partial\psi}{\partial v} + E\frac{\partial\psi}{\partial\sigma} = \sigma, \quad \frac{\partial\psi}{\partial\sigma}(\sigma - \sigma_e(\varepsilon)) \geq 0, \quad \psi(0,0) = 0.$$

For smooth solutions, the total energy e^* defined by

$$e^*(v,\varepsilon,\sigma) = \frac{v^2}{2} + \psi(\varepsilon,\sigma)$$

satisfies

$$\frac{\partial e^*}{\partial t} - \frac{\partial(\sigma v)}{\partial x} = -\kappa\,\frac{\partial\psi}{\partial\sigma}(\varepsilon,\sigma)(\sigma - \sigma_e(\varepsilon)).$$

We define the total energy for the body at $0 \leq t \leq T$ by

$$e(t;\Delta t,\kappa) = \int_{-R-c(T-t)}^{R+c(T-t)} e^*((v,\varepsilon,\sigma)(x,t;\Delta t,\kappa))\,dx,$$

which have the following property:

Proposition 1. *Assume that*

$$\kappa\Delta t \le 2\,\frac{E-E_1}{E+M}.$$

Then, for any $T>0$, $0\le t\le T$, *we have*

$$e(t;\Delta t,\kappa)\le e(0;\Delta t,\kappa).$$

This result allows us to obtain local uniform bounds in L^2 for the sequence of approximate solutions $\boldsymbol{u}^n$. Indeed, for any compact domain $K\subset I\!R\times[0,\infty)$, we have

$$\|\boldsymbol{u}^n\|_{L^p(K)}\le M(K), \tag{12}$$

for $p=2$ and for some positive constant $M(K)$ independent of n.

2.1. Measure-valued solutions

We recall here an adaptation of TARTAR's result about the existence of Young measures [6]. We denote by $C_p(I\!R^N)$ the space of the functions $h\in C(I\!R^N)$ such that

$$\sup_{\boldsymbol{u}\in I\!R^N}\frac{|h(\boldsymbol{u})|}{1+|\boldsymbol{u}|^q}<\infty,$$

for some $q\in[0,p)$.

Lemma 2. *Let* K *be a compact domain of* $I\!R\times[0,\infty)$, $\boldsymbol{u}^n$ *be a sequence satisfying (12) and let* F *be a closed subset of* $I\!R^N$ *such that* $\boldsymbol{u}^n(x,t)\in F$ *for a.e.* $(x,t)\in K$. *Then, there exist a subsequence* $\boldsymbol{u}^{n_k}$ *and a parametrized family of probability measures* $\nu_{x,t}$, *called Young measures, satisfying the following:*

1. $\operatorname{supp}\nu_{x,t}\subseteq F$, *for a.e.* $(x,t)\in K$;
2. *for each* $h\in C_p(I\!R^N)$ *we have* $h(\boldsymbol{u}^{n_k})\rightharpoonup\bar h$, *in the sense of the distributions, where* $\bar h$ *is given by*

$$\bar h(x,t)=\langle\nu_{x,t},h\rangle:=\int h(\boldsymbol{u})\,d\nu_{x,t}(\boldsymbol{u}). \tag{13}$$

In dealing with our numerical experiments, we use the following result [4]:

Theorem 3. *Assume that $\boldsymbol{u}^n$, $n \in I\!N$, have the scaling property and satisfy (12) for any compact domain $K \subset I\!R^N$. Suppose that for some $h \in C_p(I\!R^N)$ the sequence of functions in $L^1_{\text{loc}}(I\!R)$, the mean value of h up to the instant $t = T$,*

$$\langle h(\boldsymbol{u})\rangle_T(\xi) = \frac{2}{T^2}\int_0^T h(\boldsymbol{u}_\alpha(\xi t, t))t\,dt, \tag{14}$$

converges weakly, as Radon measures, to a certain function $\langle h\rangle(\xi) \in L^1_{\text{loc}}(I\!R)$. Then, for a.e. $\xi = x/t$, we have

$$\langle \nu_{x,t}, h(\boldsymbol{u})\rangle = \langle h\rangle(x/t), \tag{15}$$

and hence $\bar{h}(x,t)$, is a function of x/t only. Furthermore, assume that

$$\langle \boldsymbol{u}\rangle_T \rightharpoonup \langle \boldsymbol{u}\rangle, \qquad \langle |\boldsymbol{u}|^q\rangle_T \rightharpoonup |\langle \boldsymbol{u}\rangle|^q,$$

in the above sense, where $\langle \boldsymbol{u}\rangle(\xi)$ is a vector function in $L^1_{\text{loc}}(I\!R)$, and $1 < q < p$. Then $\boldsymbol{u}^n$ converges strongly in $L^1_{\text{loc}}(I\!R \times [0,\infty))$ to a vector function $\boldsymbol{u}(x,t)$ with the scaling property.

In [4], by the use of Proposition 1, we have proved that when $n \to \infty$, hence $\kappa \to \infty$ too, a subsequence of the approximate solutions (11) converges weakly and generate a measure-valued solution of the original elastic problem (1), (2).

Theorem 4. *If*

$$\kappa\Delta t < 2\,\frac{E - E_1}{E + M},$$

then the Young measure $\nu_{x,t}$ obtained applying Lemma 2 to the sequence (u^n, v^n) is a measure-valued solution of the Riemann problem for (6), (7).

The notion of measure-valued solution, after DiPerna [7], is given in the following definition.

Definition 5. *Let $P(I\!R^n)$ denote the set of all probability measures over $I\!R^n$. A measure-valued solution to (6), (7) is a mapping $\nu : I\!R \times [0,\infty) \to P(I\!R^n)$, denoted by $\nu_{x,t}$, such that $\nu_{x,t}$ are Young measures and satisfy*

$$\iint_{I\!R\times[0,\infty)} \{\langle \nu_{x,t}, \boldsymbol{u}\rangle\phi_t + \langle \nu_{x,t}, \boldsymbol{F}(\boldsymbol{u})\rangle\phi_x\}\,dx dt + \int_{-\infty}^{\infty} \boldsymbol{u}(x,0)\phi(x,0)\,dx = 0$$

for all $\phi \in C_0^\infty(\mathbb{R} \times [0,\infty))$.

In other words, a measure-valued solution satisfies the conservation laws with the mean values of the state vector and its flux,

$$\partial_t \langle \boldsymbol{u} \rangle(x,t) + \partial_x \langle \boldsymbol{F}(\boldsymbol{u}) \rangle(x,t) = 0, \tag{16}$$

in the sense of distribution. Numerically, according to (14), we can calculate those mean values up to the instant T from the following approximate formulas:

$$\langle \boldsymbol{u} \rangle_T(\xi) \approx \frac{2}{n(n+1)} \sum_{k=1}^{n} k\, \boldsymbol{u}_{j_k}^k, \tag{17}$$

and

$$\langle \boldsymbol{F}(\boldsymbol{u}) \rangle_T(\xi) \approx \frac{2}{n(n+1)} \sum_{k=1}^{n} k\, \boldsymbol{F}(\boldsymbol{u}_{j_k}^k), \tag{18}$$

where $T = n\Delta t$, $j_k = [kc^{-1}\xi]$. Similarly, we can also calculate

$$\langle |\boldsymbol{u}|^2 \rangle_T(\xi) \approx \frac{2}{n(n+1)} \sum_{k=1}^{n} k\, |\boldsymbol{u}_{j_k}^k|^2, \tag{19}$$

and hence compute the numerical quadratic error by

$$e_T^2(\xi) = \langle |\boldsymbol{u}|^2 \rangle_T(\xi) - |\langle \boldsymbol{u} \rangle_T|^2(\xi). \tag{20}$$

We have, by Theorem 3, that if $\langle \boldsymbol{u} \rangle_T$ converges, and e_T^2 converges to zero, then $\langle \boldsymbol{u} \rangle_T(x/t)$ converges strongly to $\bar{\boldsymbol{u}}(x,t)$ giving by (13).

Remark. A more thorough discussion of measure-valued solutions would have to include some sort of admissibility criteria to rule out physically irrelevant solutions. For hyperbolic systems this can be done by means of an entropy inequality, as in [7]. In the case of systems that change type as the one considered here, no such criteria are readily available. One way around for this problem is to resort to the reliability of the approximation sequence that generates the measure-valued solution. We then remark that the admissibility of the measure-valued solutions considered here is clearly assured by the fact that they are obtained from a reliable numerical scheme. We avoid here further discussions on this subject and we refer to [4] for a numerical experiment concerning entropy-rate criterion and the oscillation waves.

3. Numerical Results for Phase Mixtures

We take a typical set of material parameters from a shape memory alloy, a CuZnAl single crystal with its experimental data [2]: $\rho = 7740\,\mathrm{Kg/m^3}$, $\varepsilon_A = 0.92\,\%$, $\varepsilon_M = 7.60\,\%$, $E_1 = E_2 = 12.31\,\mathrm{GPa}$, $M = 0.272\,\mathrm{GPa}$. We also take $E = 20.00\,\mathrm{GPa}$ and $\alpha = \kappa\Delta t = 0.755$.

Figure 1: Strain oscillation for $\varepsilon_0 = 2\,\%$ at time step 500000

We restrict our attention to the instability of the states in the unstable region. Therefore we consider Riemann problems with the same left and right initial data: $v_i^0 = v_0$, $\varepsilon_i^0 = \varepsilon_0$, $\sigma_i^0 = \sigma_e(\varepsilon_0)$, for $i = \pm 1, \pm 2, \cdots$, together with a small disturbance, say, at a single grid point, $i = 0$. We remark that, at large number of time steps, the mean values of state functions associated with the numerical solution does not depend upon the particular choice of disturbance.

Figure 2: Mean strain for $\varepsilon_0 = 2\,\%$ at time step 500000

Note that for $v_0 = 0$, the initial state is an equilibrium state, however, if $\varepsilon_A < \varepsilon_0 < \varepsilon_M$, it is not a stable state. Indeed, we have found that a small disturbance at $x = 0$ at the initial time does not die out and, instead, it may evolve into a non-trivial solution with persistent oscillations. In Fig. 1 the approximate solution $\varepsilon(x,t)$ at time step 500000 for $(v_0, \varepsilon_0) = (0, 0.02)$ is shown as a function of x/t, more convenient in view of the scaling property. It shows an oscillation between two values of ε, around ε_A and ε_M. We can also determine the mean values by (18) for the state variables v, ε and the stress σ in order to verify that the mean values satisfy (1). In Fig. 2 we show, as an example, the mean value $\bar{\varepsilon}(x,t)$ also as a function of x/t. From this graph, it is easy to see that $\bar{\varepsilon}$ converges to the initial value almost everywhere. The same is true for the mean values of v and σ. Therefore, the mean values $(\bar{v}, \bar{\varepsilon})$ coincides in the limit with the equilibrium solution $(v, \varepsilon) = (0, 0.02)$.

Figure 3: Patterns of phase mixtures

Comparison of the oscillation patterns in the approximate solutions at different time steps reveals an interesting fact that the oscillation patterns tend to become stationary at the grid points. In Fig. 3 we amplify the graphs of $\varepsilon(x,t)$ in an interval of 2000 grid points, for the initial equilibrium strains $\varepsilon_0 = 3\,\%$ and $\varepsilon_0 = 1.75\,\%$. It shows an oscillation between two states ε_A and ε_M, corresponding to the two different phases. These patterns can be interpreted as the microscopic structure of the phase mixture with stationary interfaces, resembling the experimentally observed band-like structure of single crystal samples of shape memory alloy during martensitic transformation [2].

Physically, we can associate the phase fractions with each strain ε_0 in the interval $(\varepsilon_A, \varepsilon_M)$ as the coefficients in the convex combination of the corresponding strains, $\varepsilon_1 \le \varepsilon_A$ and $\varepsilon_2 \ge \varepsilon_M$, in the two pure phases at the same stress level, namely, $\sigma_e(\varepsilon_0) = \sigma_e(\varepsilon_1) = \sigma_e(\varepsilon_2)$,

$$\varepsilon_0 = (1 - z)\,\varepsilon_1 + z\,\varepsilon_2, \tag{21}$$

where z is the phase fraction of the martensitic phase. From the numerical point of view, at each time step from the above oscillation pattern, we can determine the phase fraction over a fixed interval of grid points as the fraction of the length of the intervals of that phase to the total length of the interval and we have found an almost perfect agreement between the phase fractions determined numerically in this manner and that calculated from (21) for $1.5\,\% < \varepsilon_0 < 7.0\,\%$ at large number of time steps in our experiments: As examples, we obtain $z = 0.312$ for $\varepsilon_0 = 3\,\%$ and $z = 0.124$ for $\varepsilon_0 = 1.75\,\%$.

On the other hand, from the approximate solution, we can also define phase fraction as a state function given by

$$f_1(\varepsilon) = \begin{cases} 1, & \text{if } \varepsilon \leq \varepsilon_A, \\ 0, & \text{otherwise,} \end{cases} \qquad f_2(\varepsilon) = \begin{cases} 1, & \text{if } \varepsilon \geq \varepsilon_M, \\ 0, & \text{otherwise.} \end{cases}$$

In our numerical experiments, we have also determined the mean values of these functions, with respect to the measure-valued solutions associated with the states $(0, \varepsilon)$ for $\varepsilon \in (\varepsilon_A, \varepsilon_M)$. The experiments show that these mean values also agree with the coefficients $(1 - z)$ and z in (21) respectively, and more interestingly, the mean phase fraction is constant almost everywhere in the limit, which means that the phase mixture is macroscopically homogeneous. For more discussions on phase fractions and the interface patterns see [8].

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