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NUMERICAL SIMULATION OF WAVES AND FRONTS IN INHOMOGENEOUS SOLIDS

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Abstract: Dynamic response of inhomogeneous materials exhibits new effects, which often do not exist in homogeneous media. It is quite natural that most of studies of wave and front propagation in inhomogeneous materials are associated with numerical simulations. To develop a numerical algorithm and to perform the numerical simulations of moving fronts we need to formulate a kinetic law of progress relating the driving force and the velocity of the discontinuity. The velocity of discontinuity is determined by means of the non-equilibrium jump relations at the front. The obtained numerical method generalizes the wave-propagation algorithm to the case of moving discontinuities in thermoelastic solids.

Keywords: wave and front propagation, inhomogeneous solids, finite-volume methods

1. Introduction

The understanding of the behavior of materials under very high strain rate loading conditions is vital in many areas of civilian and military applications. So far, the most practical structures/materials to absorb impact energy and resist impact damage are designed in the form of layered composites. Other possibilities are provided by functionally graded materials and shape memory alloys. In order to characterize the dynamic behavior of materials under impact loading, diagnostic experiments are usually carried out using a plate impact test configuration under a one-dimensional strain state. The plate impact test serves the exact purpose of characterizing materials under high-pressure dynamic loading, analogous to that of uniaxial tensile tests under quasi-static loading conditions.

Laminated composites. The major past work in studying wave profiles in alternating layered systems using specifically the plate impact test configuration are summarized recently in Chen and Chandra (2004); Chen, Chandra and Rajendran (2004). For almost all the experiments, stress (or velocity) response have shown an oscillatory behavior in the pulse duration segment. This behavior is conspicuously absent in homogeneous systems. The oscillatory behavior about a mean value in the periodically layered systems are consistently exhibited in the systematic experimental work by Zhuang, Ravichandran and Grady (2003). As pointed out in Zhuang, Ravichandran and Grady (2003), stress wave propagation through layered media made of isotropic materials provides an ideal model to investigate the effect of heterogeneous materials under shock loading, because the length scales, e.g., thickness of individual layers, and other measures of heterogeneity, e.g., impedance mismatch, are well defined. The origin of the observed structure of the stress waves was attributed to material heterogeneity at the interfaces. For high velocity impact loading conditions, it was fully realized that material nonlinear effects may play a key role in altering the basic structure of the shock wave.

Shape memory alloys. A polycrystalline shape memory alloy body subjected to external impact loading will experience deformations that will propagate along the SMA body as stress waves. The experimental investigation concerning impact-induced austenite-martensite phase transformations was reported by Escobar and Clifton (1993). In their experiments, Escobar and Clifton used thin plate-like specimens of Cu-14.44Al-4.19Ni shape-memory alloy single crystal. One face of this austenitic specimen was subjected to an oblique impact loading, generating both shear and compression. As Escobar and Clifton noted, measured velocity profiles provide several indications of the existence of a propagating phase boundary, in particular, a difference between the measured particle velocity and the transverse component of the projectile velocity. This velocity difference, in the absence of any evidence of plastic deformation, is indicative of a stress induced phase transformation that propagates into the crystals from the impact face. The determination of this velocity difference is most difficult from the theoretical point of view, because it depends on the velocity of the moving phase boundary.

In this paper, wave and front propagation is simulated numerically in a one-dimensional case. The propagation is modeled by the one-dimensional hyperbolic system of conservation laws

$$\rho \frac{\partial v}{\partial t} = \frac{\partial \sigma}{\partial x}, \qquad \frac{\partial \varepsilon}{\partial t} = \frac{\partial v}{\partial x}, \tag{1}$$

where ρ is the mass density, ε is the strain, and v the particle velocity.

The densities of the materials may be different, and the materials response to compression is characterized by the distinct stress-strain relations $\sigma(\varepsilon)$. To close the system of Eqs. (1), the stress-strain relation for each material can be chosen as linear

$$\sigma = \rho c^2 \varepsilon, \tag{2}$$

or weakly nonlinear

$$\sigma = \rho c^2 \varepsilon (1 + A\varepsilon), \tag{3}$$

where c is the longitudinal wave velocity and A is a parameter of nonlinearity, values and sign of which are supposed to be different for hard and soft materials. Due to rapidly-varying properties, we apply the finite-volume wave-propagation algorithm in its conservative form (Bale et al. (2003)) to solve the system of equations (1)-(2) (or (3)). At the moving phase boundary the algorithm is extended as described in Berezovski and Maugin (2005a).

The paper is organized as follows. In the next Section we repeat the classical results for linear wave propagation in periodic media. Then we examine the effect of weak nonlinearity on the material response. The introduction of the nonlinearity allows us to reproduce the shock response in laminated composites observed experimentally. Linear and nonlinear wave propagation in functionally graded materials is considered in the Section 5. Another type of nonlinearity affects the front propagation in shape memory alloys under impact. This nonlinearity is connected to the motion of the phase front.

2. One-dimensional linear waves in periodic media

As the first example, we consider the propagation of a pulse in a periodic medium composed by alternating layers of dissimilar materials. The initial pulse shape is presented in Figure 1 where the periodic variation in density (normalized by its maximal value) is also schematically shown by dashed lines. Clearly, the wavelength is much larger than the periodicity scale. For the test problem, materials are chosen as polycarbonate (ρ = 1190 kg/m^3, c = 4000 m/s) and Al 6061 (ρ = 2703 kg/m^3, c = 6149 m/s). Calculations are performed with Courant-Friedrichs-Levy number equal to 1. The result of simulation for 4000 time steps is shown in Figure 2. We observe a distortion of the pulse shape and a decrease in the velocity of the pulse propagation in comparison of the maximal longitudinal wave velocity in the materials. These results correspond to the prediction of the effective media theory by Santosa and Symes (1991) both qualitatively and quantitatively (Fogarthy and LeVeque (1999)).

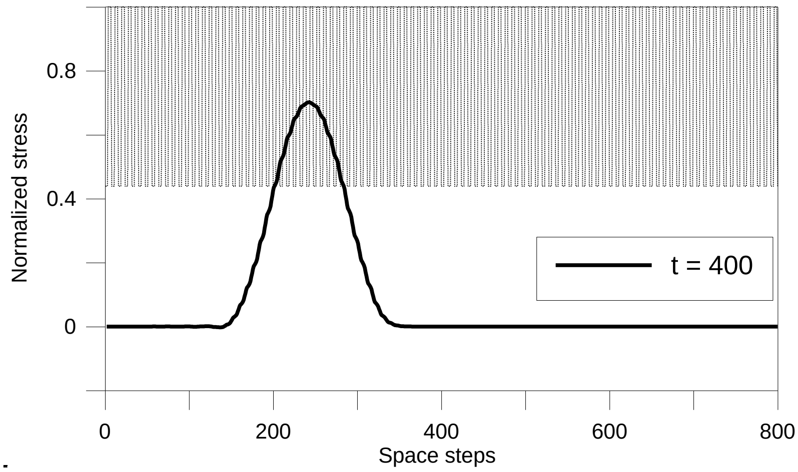

Figure 1. Initial pulse shape

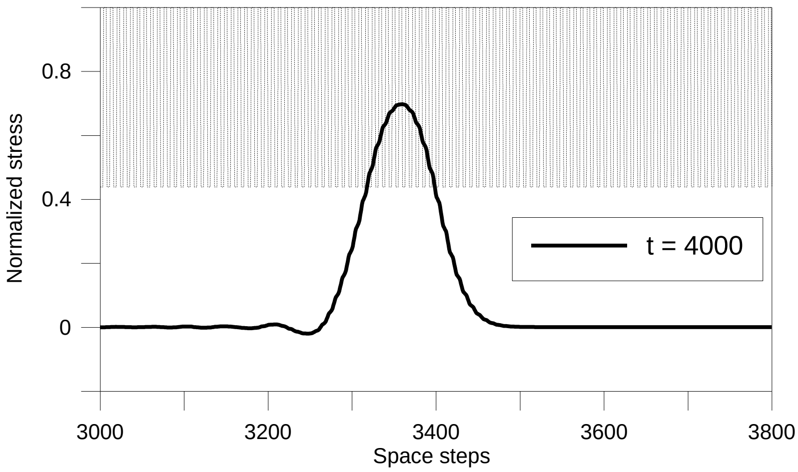

Figure 2. Pulse shape at 4700 time step. Linear case

3. One-dimensional weakly nonlinear waves in periodic media

In the next example, we will see the influence of material nonlinearity on the wave propagation. The approximate Riemann solver for the nonlinear elastic media (Eq. 3) is similar to that used in LeVeque (2002). This means that a modified longitudinal wave velocity, c_1, following the nonlinear stress-strain relation (3) is applied at each time step

$$c_1 = c\sqrt{1+2A\varepsilon} \qquad (4)$$

instead of the piece-wise constant one corresponding to the linear case. We consider the same pulse shape and the same materials (polycarbonate and Al 6061) as in the case of the linear periodic medium. However, the nonlinear effects appear only for a sufficiently high magnitude of loading. The values of the parameter of nonlinearity A were chosen as 0.24 for Al 6061 and 0.8 for polycarbonate. The results of simulations corresponding to 5200 time steps are shown in Figure 3.

We observe that an initial bell-shaped pulse is transformed in a train of soliton-like pulses propagating with amplitude-dependent speeds. Such kind of behavior was first reported in LeVeque (2002), who called these pulses as "stegotons" because their shape is influenced by the periodicity.

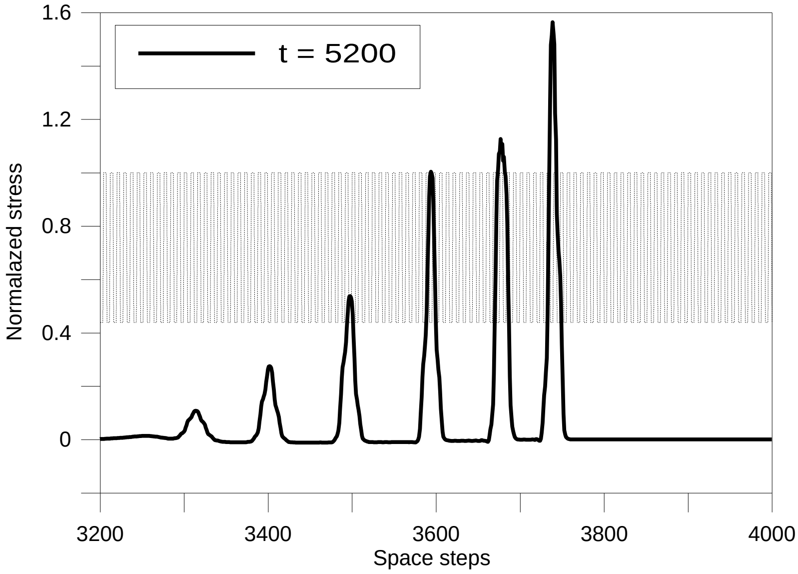

Figure 3. Pulse shape at 5200 time step. Nonlinear case

4. Nonlinear elastic wave in laminates under impact loading

To analyze the influence of multiple reflections of internal interfaces on shock wave propagation in the layered composites, we consider the initial-boundary value problem of impact loading of a heterogeneous medium composed of alternating layers of two different materials (Berezovski et al. (2006)). The impact is provided by a planar flyer which has an initial velocity v_0. A buffer of the same material as the soft component of the specimen is used to eliminate the effect of wave reflection at the stress-free surface. Both left and right boundaries are stress-free. As previously, we apply a nonlinear stress-strain relation $\sigma(\varepsilon, x)$ for each material (3) (cf. Meurer, Qu and Jacobs (2002)). Results of numerical calculations depend crucially on the choice of the parameter of nonlinearity A. We choose this parameter from the conditions to match the numerical simulations to experimental results (see discussion in Berezovski et al. (2006)).

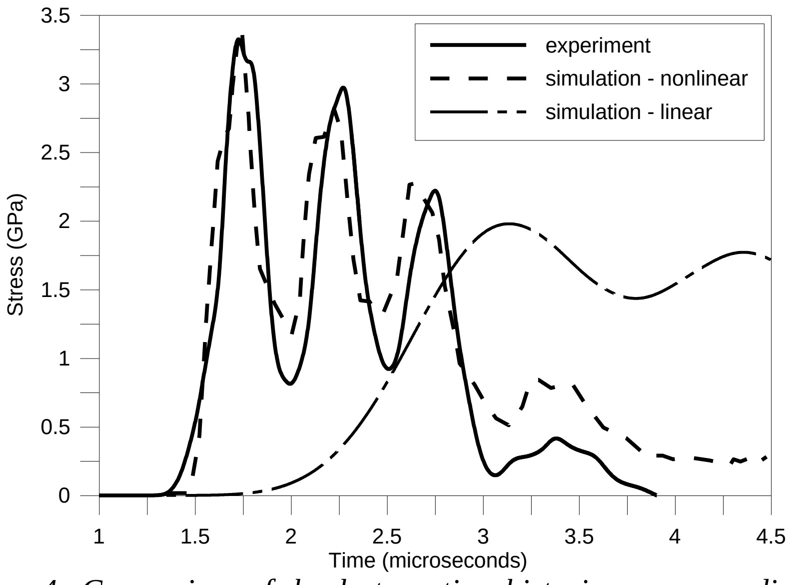

Figure 4. Comparison of shock stress time histories corresponding to the experiment 110501 by Zhuang, Ravichandran and Grady (2003)

Figure 4 shows the stress time histories in the composite, which consists of 16 units of polycarbonate, each 0.37 mm thick, and of 16 units of stainless steel, each 0.19 mm thick. The stress time histories correspond to the distance 3.44 mm from the impact face. Calculations are performed for the flyer velocity 1043 m/s and the flyer thickness 2.87 mm.

The nonlinear parameter *A* is chosen here to be 2.80 for polycarbonate and zero for stainless steel. Additionally, the stress time history corresponding to the linear elastic solution (i.e., nonlinear parameter *A* is zero for both components) is shown. One can see that the stress time history computed by means of the considered nonlinear model is very close to the experimental one. It reproduces three main peaks and decreases with distortion, as it is observed in the experiment by Zhuang, Ravichandran and Grady (2003). As one can see, the agreement between results of calculations and experiments is achieved by the adjustment of the nonlinear parameter *A*.

5. Waves in functionally graded materials

Studies of the evolution of stresses and displacements in FGMs subjected to quasistatic loading (Suresh and Mortensen (1998)) show that the utilization of structures and geometry of a graded interface between two dissimilar layers can reduce stresses significantly. Such an effect is also important in the case of dynamical loading where energy-absorbing applications are of special interest. Following Chiu and Erdogan (1999), we consider the one-dimensional problem in elastodynamics for an FGM slab in which material properties vary only in the thickness direction.

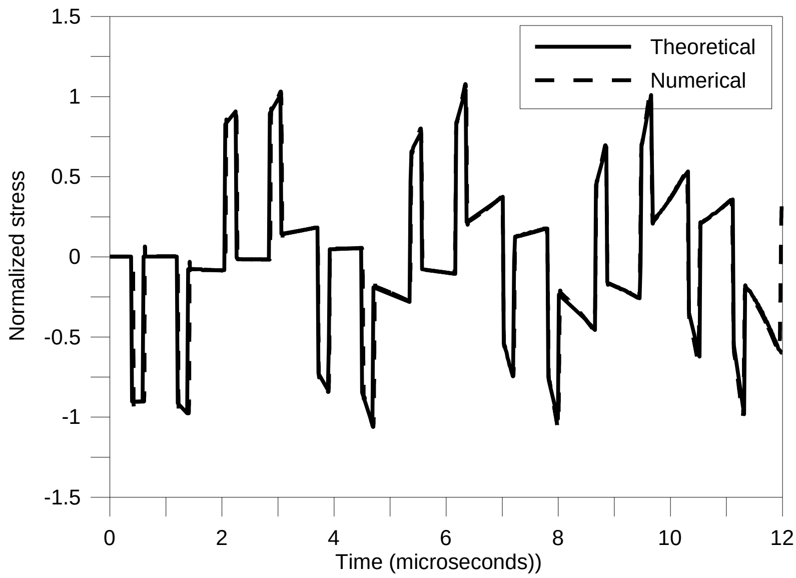

Figure 5. Variation of stress with time in the middle of the slab

It is assumed that the slab is isotropic and inhomogeneous with the following fairly general properties:

$$E(x) = E_0\left(a\frac{x}{l}+1\right)^m, \qquad \rho(x) = \rho_0\left(a\frac{x}{l}+1\right)^n, \qquad (5)$$

where *l* is the thickness, *a, m,* and *n* are arbitrary real constants with $a > -1$, E_0 and ρ_0 are the elastic constant and density at $x = 0$. It is assumed that the slab is at rest for $t < 0$. Following Chiu and Erdogan (1999), we consider an FGM slab that consists of nickel and zirconia. The thickness of the slab is $l = 5$ mm, on one surface the medium is pure nickel, on the other surface pure zirconia, and the material properties *E(x)* and *ρ(x)* vary smoothly in thickness direction. A pressure pulse defined by

$$\sigma(l,t) = \sigma_0(H(t) - H(t - t_0)) \qquad (6)$$

is applied to the surface $x = l$ and the boundary $x = 0$ is "fixed". Here H is the Heavyside function. The pulse duration is assumed to be $t_0 = 0.2$ μs. The properties of the constituent materials used are given in Table 1 (Chiu and Erdogan (1999)). The material parameters for the FGMs used are (Chiu and Erdogan (1999)): a = - 0.12354, m = - 1.8866, and n = - 3.8866. The stress is calculated up to 12 μs (the propagation time of the plane wave through the thickness $l = 5$ mm is approximately 0.77 μs in pure ZrO_2 and 0.88 μs in Ni).

Table 1. *Properties of materials*

Property	Value	Unit	Material
Density	5331 8900	kg/m^3	ZrO_2 Ni
Young modulus	151 207	GPa	ZrO_2 Ni
Poisson's ratio	0.33 0.31		ZrO_2 Ni

Numerical simulations were performed by means of the same algorithm as above. Comparison of the results of the numerical simulation and the analytical solution Chiu and Erdogan (1999) for the time dependence of the normalized stress σ/σ_0 at the location $x/l = 1/2$ is shown in Figure 5. As one can see, it is difficult to make a distinction between analytical and numerical results.

Variation of stress in nonlinear case for same materials with the nonlinearity parameter $A = 0.19$ is shown in Figure 6. The amplitude amplification and pulse shape distortion in comparison with linear case is clearly observed. In addition, velocity of a pulse in nonlinear material is increased.

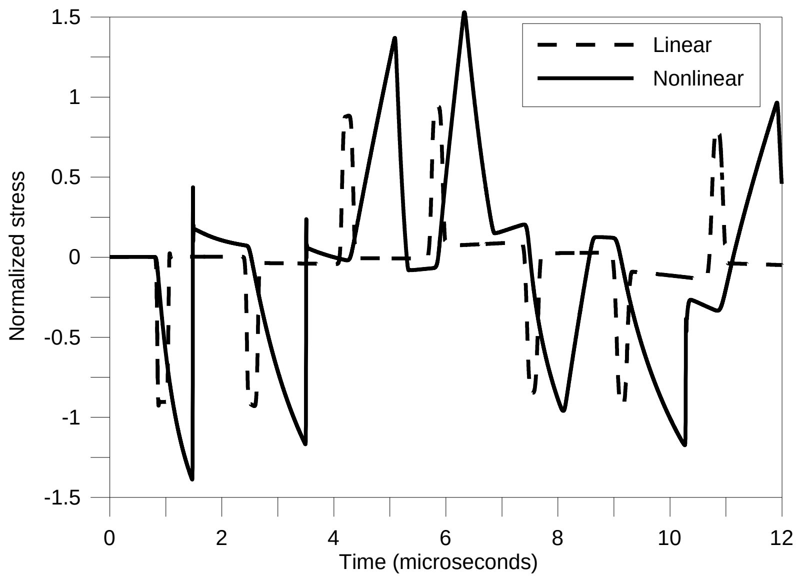

Figure 6. Variation of stress with time in the middle of the slab

6. Phase-transition fronts

In the case of phase-transition front propagation, we consider the boundary value problem of the tensile loading of a 1-D shape memory alloy bar that has uniform cross-sectional area and temperature. The bar occupies the interval $0 < x < L$ in a reference configuration and the boundary $x = 0$ is subjected to the tensile loading. The bar is assumed to be long compared to its diameter so it is under a uniaxial stress state and the stress $\sigma(x,t)$ depends only on the axial position and time. The density of the material ρ is assumed constant. All field variables are averaged over the cross-section of the bar.

At each instant t during a process, the strain $\varepsilon(x,t)$ varies smoothly within the bar except at phase boundaries; across a phase boundary, it suffers jump discontinuity. Away from a phase boundary, balance of linear momentum and kinematic compatibility require the satisfaction of equations (1). Suppose that at time t there is a moving discontinuity in strain or particle velocity at $x = \Sigma(t)$. Then one also has the corresponding jump conditions (cf. Abeyaratne et al. (2001))

$$\rho V_\Sigma[v] + [\sigma] = 0, \qquad V_\Sigma[\varepsilon] + [\mathrm{v}] = 0, \qquad (7)$$

where V_Σ is the velocity of the phase-transition front and square brackets denote jumps.

The entropy inequality and the corresponding jump relation read

$$\theta \frac{\partial S}{\partial t} + \frac{\partial q}{\partial x} \geq 0, \qquad V_\Sigma \theta [S] = V_\Sigma f_\Sigma, \qquad (8)$$

where the driving traction $f_\Sigma(t)$ at the discontinuity is defined by (cf. Truskinovsky (1987); Abeyaratne and Knowles (1990))

$$f_\Sigma = -[W] + \langle \sigma \rangle [\varepsilon], \qquad (9)$$

W is the free energy per unit volume, θ is temperature, S is entropy, and q is heat flux. If f_Σ is not zero, the sign of V_Σ, and hence the direction of motion of discontinuity, is determined by the sign of f_Σ.

Applying the satisfaction of the non-equilibrium jump relation at the phase boundary we obtain the value of the stress jump at the phase boundary (Berezovski and Maugin (2005b)). Having the value of the stress jump, we can determine the material velocity at the moving phase boundary by means of the jump relation for linear momentum (7) rewritten in terms of averaged quantities because of the continuity of excess quantities at the phase boundary (Berezovski and Maugin (2005a)).

To compare the results of modeling with experimental data by Escobar and Clifton (1993), the calculations of the particle velocity were performed for different impact velocities. The results of the comparison are given in Figure 7. As a result, we can see that the computed particle velocity is practically independent of the impact velocity.

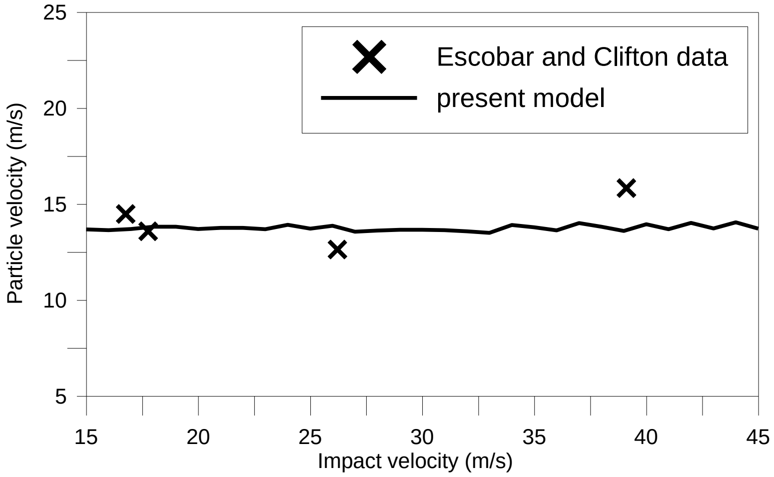

Figure 7. Particle velocity versus impact velocity

7. Conclusions

As we have seen, linear and non-linear wave propagation in media with rapidly-varying properties as well as in functionally graded materials can be successfully simulated by means of the modified wave-propagation algorithm (Berezovski and Maugin (2001)). The applied algorithm is conservative, stable up to Courant number equal to 1, high-order accurate, and thermodynamically consistent. To apply the algorithm to moving singularities, we simply should change the non-equilibrium jump relation for true inhomogeneities to another non-equilibrium jump relation valid for quasi-inhomogeneities.

Acknowledgements

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