

# Numerical Simulations of One-dimensional Microstructure Dynamics

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**Abstract.** Results of numerical simulations of one-dimensional wave propagation in microstructured solids are presented and compared with the corresponding results of wave propagation in given layered media. A linear microstructure model based on Mindlin theory is adopted and represented in the framework of the internal variable theory. Fully coupled systems of equations for macro-motion and microstructure evolution are rewritten in the form of conservation laws. A modification of wave propagation algorithm is used for numerical calculations. It is shown how the initial microstructure model can be improved in order to match the results obtained by both approaches.

**Keywords:** wave propagation, microstructured solids, numerical simulations, microstructure evolution, internal variables.  
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## INTRODUCTION

Wave propagation in the medium with microstructure is dispersive [1], [2]. In order to catch the dispersion effects, the classical wave equation for linear elastic wave propagation should be modified. Usually this modification is made by homogenization or continualization methods [3, 4, 5]. Alternatively a generalized continuum theory can be applied [6]. The resulting microstructure models enhance the classical elastic behavior.

As it is recently shown, the concept of dual internal variables [7] can be successfully used for the physical description of the medium with microstructure [8]. Internal variable is associated with the integral distributed effect of the microstructure [9]. In the framework of the internal variable theory, fully coupled systems of equations for macro-motion and microstructure evolution are represented in the form of conservation laws.

However, solution of these equations is not easy task due to their coupling and the absence of natural boundary conditions for internal variable. In addition, parameters of the microstructure model are needed to be determined in each particular case. This is why we performed numerical experiments to compare results of direct numerical calculations of wave propagation in a laminate with prescribed properties and corresponding results obtained for an effective medium with the microstructure modeling. These numerical experiments allowed us to analyze advantages and weaknesses of the model. As a result, we found that some improvements have to be introduced into the microstructure model.

The numerical simulations are performed by means of a finite-volume numerical scheme modifying the wave-propagation algorithm [10] by the introduction of excess quantities instead of numerical fluxes, which simplifies the solution of Riemann problems at boundaries between computational cells at each time step [11]. Source terms are accounted in the jump relations at boundaries between computational cells. The scheme is applied for both macro- and micro-motion. The advantage of the wave-propagation algorithm is high-resolution [12] and the possibility for a natural extension to higher dimensions. It should be emphasized that there is no need for any artificial boundary conditions for the internal variable: the non-trivial solution is provided by the coupling between the macro- and micro-motions.

## GOVERNING EQUATIONS

The most general model for the one-dimensional wave propagation in solids with microstructure is presented in [2]. This model is derived independently from the Euler-Lagrange equations for a Mindlin-type material model [13] and from internal variable theory [8]. In the framework of the internal variable theory it is assumed that the influence of the microstructure on the overall macroscopic behavior can be taken into account by the introduction of an internal variable which is associated with the integral distributed effect of the microstructure [9]. In the case of quadratic free energy dependence, the system of two coupled second-order hyperbolic equations for macro- and micromotion is derived as follows [2]:

$$\rho u_{tt} = \rho c^2 u_{xx} + A \varphi_x, \quad (1)$$

$$I \varphi_{tt} = C \varphi_{xx} - A u_x, - B \varphi, \quad (2)$$

where  $u$  is the macrodisplacement,  $\varphi$  is the internal variable (microdeformation),  $\rho$  is the matter density,  $c$  is the longitudinal wave velocity at the macrolevel,  $A$ ,  $B$ ,  $C$  and  $I$  are material constants for microstructure, subscripts are used to denote derivatives.

The governing equations (1) and (2) can be represented either as a single fourth-order equation [2] or as a system of four first-order equations. While the former representation is more convenient for theoretical considerations, the latter one is more suitable for numerics. Namely, in terms of strain and velocity, Eq. (1) is rewritten as

$$\rho v_t = \rho c^2 \varepsilon_x + A \varphi_x. \quad (3)$$

The particle velocity  $v = u_t$  and the strain  $\varepsilon = u_x$  are related by the compatibility condition

$$\varepsilon_t = v_x. \quad (4)$$

Similarly, introducing microvelocity  $\omega$  we use the compatibility condition at micro-level as follows:

$$\varphi_t = \omega_x. \quad (5)$$

Accounting for Eq. (5) and integrating Eq. (2) over  $x$ , we arrive at

$$I \omega_t = C \varphi_x - \int (A \varepsilon + B \varphi) dx. \quad (6)$$

Thus, we have two coupled systems of equations (3), (4), (5) and (6) for the determination of four unknowns:  $\varepsilon$ ,  $v$ ,  $\varphi$ , and  $\omega$ . To analyze the capabilities of the model and the role of material constants in the microstructure model, we need to solve these systems of equations simultaneously. It is clear that analytical solutions may be found only in highly simplified asymptotic cases. Therefore, we turn to numerical methods. However, even the numerical solution is not simple and straightforward because of the absence of natural boundary conditions for the internal variable [14] and possible instabilities [15].

As it is mentioned, numerical simulations are performed by means of a finite-volume numerical scheme modifying the wave-propagation algorithm [11]

$$(\rho \bar{v})_n^{k+1} - (\rho \bar{v})_n^k = \frac{\Delta t}{\Delta x} (\Sigma_n^+ - \Sigma_n^-) + A \frac{\Delta t}{\Delta x} (\Phi_n^+ - \Phi_n^-), \quad (7)$$

$$\bar{\varepsilon}_n^{k+1} - \bar{\varepsilon}_n^k = \frac{\Delta t}{\Delta x} (V_n^+ - V_n^-), \quad (8)$$

$$\bar{\varphi}_n^{k+1} - \bar{\varphi}_n^k = \frac{\Delta t}{\Delta x} (\Omega_n^+ - \Omega_n^-), \quad (9)$$

$$(I\bar{\omega})_n^{k+1} - (I\bar{\omega})_n^k = \frac{C\Delta t}{\Delta x} (\Phi_n^+ - \Phi_n^-), \quad (10)$$

where  $n$  and  $k$  denote space and time steps, respectively, overbars denote averaged quantities which are introduced together with excess quantities both for macro- and microfields as follows:

$$\sigma = \bar{\sigma} + \Sigma, \quad v = \bar{v} + V, \quad \varphi = \bar{\varphi} + \Phi, \quad \omega = \bar{\omega} + \Omega, \quad (\sigma = \rho c^2 \varepsilon). \quad (11)$$

The source terms in Eqs. (3) and (6) are accounted by including them into jump conditions at the boundaries between computational cells which are used for the solution of Riemann problems at each time step, namely,

$$\rho c^2 \varepsilon_{n-1} + A\varphi_{n-1} = \rho c^2 \varepsilon_n + A\varphi_n, \quad (12)$$

$$C\varphi_{n-1} - (A\varepsilon_{n-1} + B\varphi_{n-1}) \Delta x^2 = C\varphi_n - (A\varepsilon_n + B\varphi_n) \Delta x^2. \quad (13)$$

We do not apply any boundary conditions for the internal variable due to the coupling between micro- and macromotions.

## NUMERICAL SIMULATIONS

To have a reference solution, the propagation of a pulse in a one-dimensional medium which can be represented as an elastic bar is considered first. This bar is assumed homogeneous except of a region of length  $l$ , where periodically alternating layers of size  $d$  are inserted (Fig. 1).

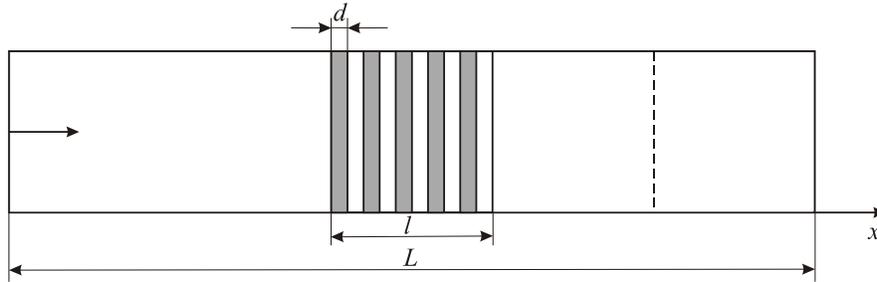
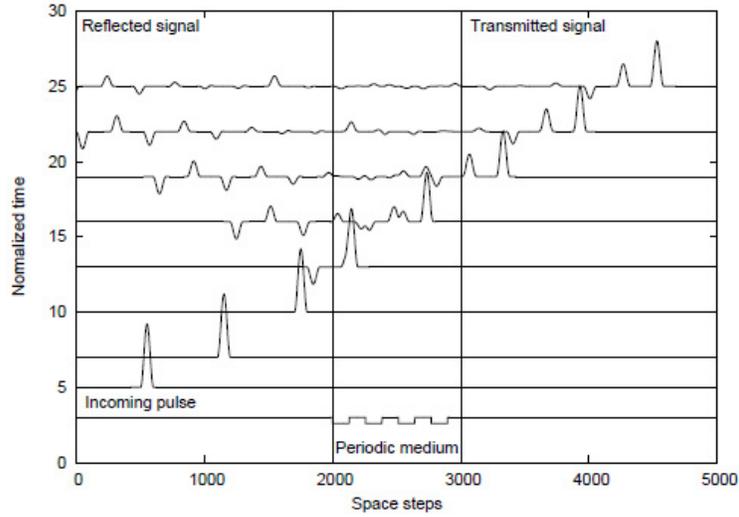


FIGURE 1. Geometry of the bar.

The density and the longitudinal velocity in the bar are chosen as  $\rho = 4510 \text{ kg/m}^3$  and  $c = 5240 \text{ m/s}$ , respectively. The corresponding parameters for the material of the inhomogeneity layers are  $\rho_1 = 2703 \text{ kg/m}^3$  and  $c_1 = 5020 \text{ m/s}$ , respectively. The shape of the pulse before the crossing of the inhomogeneity region is formed by an excitation of the strain at the boundary for a limited time period ( $0 < t < 100\Delta t$ )

$$u_x(0, t) = (1 + \cos(\pi(t - 50\Delta t)/50)). \quad (14)$$

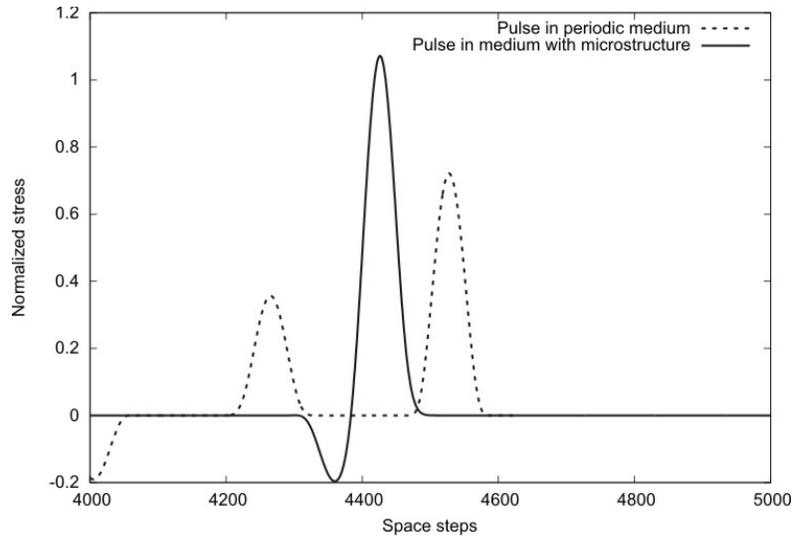
The length of the pulse ( $\lambda = 100\Delta x$ ) is comparable with the size of inhomogeneity ( $d = 128\Delta x$ ). The pulse holds its shape up to the entering into the inhomogeneity region. The problem is solved directly, i.e., without application of the microstructure model, since the location and properties of substructure are prescribed. The solution shows that after the interaction with the periodic multilayer, the single pulse is separated into many reflected and transmitted parts as it can be seen in Fig. 2.



**FIGURE 2.** Scattering of a pulse by a periodic multilayer.

The dispersion occurs because of the successive reflections at each interface between the alternating layers.

The same pulse propagation was simulated by the microstructure model (3) - (6) with  $A = 550\rho c^2$ ,  $I = \rho_1$ ,  $C = Ic_1^2$ ,  $B = 6.7 A^2/\rho c^2$ . In this case, there is no assumption of periodicity, however, in calculations of the pulse propagation, the internal length  $d$  for the microstructure is kept the same as in the case of periodic multilayer. The ratio of scales  $d$  and  $\lambda$  together with the value of the parameter  $A$  determines the contribution of the microstructure to macromotion. The result of the numerical simulation is presented in Fig. 3, where the corresponding transmitted pulses from the solution of the problem with periodic multilayer are also shown.

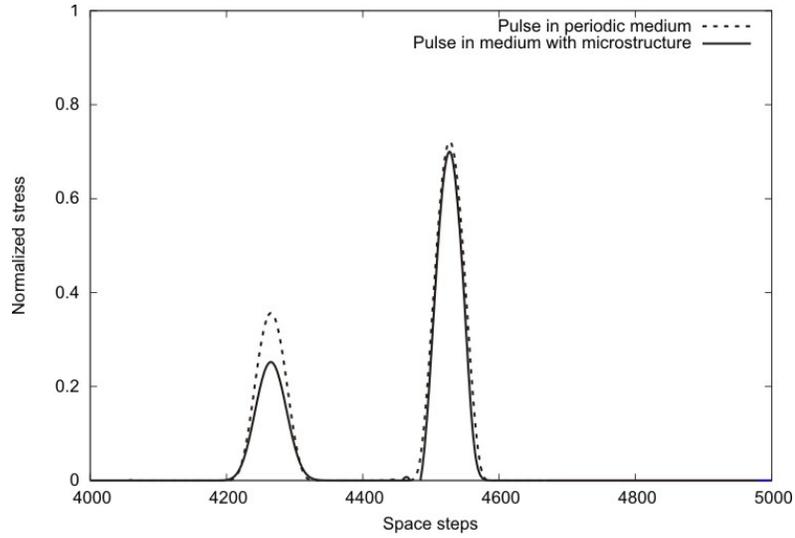


**FIGURE 3.** Leading transmitted pulses.

The obtained result is rather disappointing. Moreover, as numerous numerical experiments show, it cannot be improved by the varying of the values of microstructure parameters. Therefore, we have to reconsider the microstructure model. It turns out that the change of the sign in source term in Eq. (6) (corresponding to the internal interaction force)

$$I\omega_t = C\varphi_x + \int (A\varepsilon + B\varphi)dx, \quad (15)$$

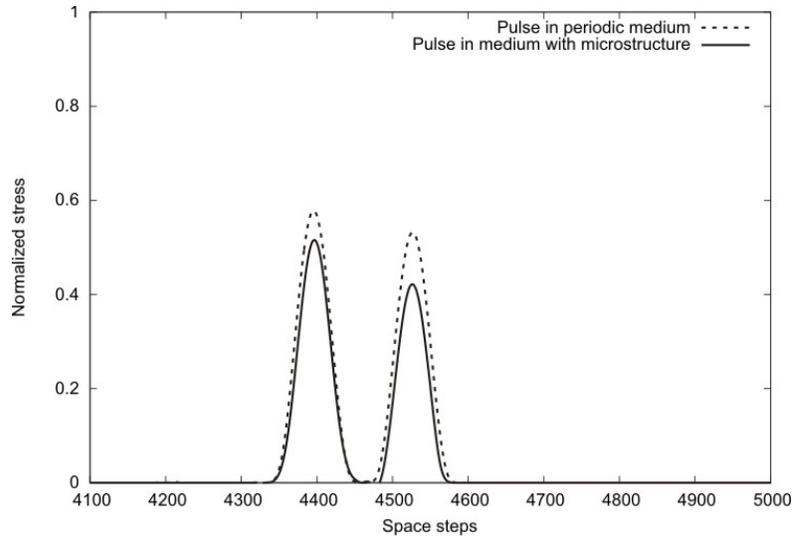
leads to a more appropriate result. The corresponding results of computations by using Eq. (15) instead of Eq. (6) are shown in Fig. 4.



**FIGURE 4.** Leading transmitted pulses: improved model.

As one can see, the improved microstructure model is capable to reproduce the two leading transmitted pulses in a consistent way. The second pulse is smaller than the reference one because of the absence of a reflected trail in the case of the microstructure model.

The improved model can also reproduce the change in the pulse behavior due to the variation of the size of inhomogeneity ( $d = 64\Delta x$  in Fig. 5). The size effect manifests itself in the change of the mutual location of small and big pulses.



**FIGURE 5.** Leading transmitted pulses for  $d = 64\Delta x$ .

## CONCLUSIONS

If we know all the details of given microstructure, namely, size, shape, composition, location and properties of inclusions as well as properties of carrier medium, the classical wave equation is sufficient for the description of wave propagation. The less we know concerning the microstructure, the more complicated equation is needed for the equivalent description of waves in the carrier medium which may be considered as simple as possible. In the paper, we have compared results of direct numerical calculations of wave propagation in laminates with the corresponding numerical simulations by using a microstructure model. As it is shown, numerical experiments demonstrate the need for a modification of the applied microstructure model. Nevertheless, the problem of parameters identification remains: some fitting is required to obtain the desirable behavior. At the same time, it is clear that the improved microstructure model qualitatively reproduce the microstructure influence on the macroscopic dynamics.

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