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NUMERICAL SIMULATION OF DISCONTINUOUS SOLUTIONS IN NONLINEAR ELASTICITY THEORY

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A mathematical model of a nonlinear elastic medium is considered. Discontinuous solutions of the model are studied numerically for the one-dimensional case.

Key words: *nonlinear elasticity theory, discontinuous solution, numerical solution, Godunov diagram.*

Introduction. Previously, it has been shown [1] that smooth solutions of the nonlinear elasticity equations for an isotropic medium are described by a quasilinear symmetric hyperbolic system. Thermodynamic relations are satisfied on these solutions.

Because theory for discontinuous (generalized) solutions has been developed only for the linear case, the question arises: whether the indicated nonlinear equations and conservation laws (which are compatible on smooth solutions) can be used to study solutions with discontinuities (shock waves) in the same way as was done in gas dynamics in the 1950s.

The present paper describes tentative numerical calculations of the dynamics of discontinuous solutions of the equations constructed in [1] to model continuous media subjected to large deformations (for example, explosive deformations of metals).

1. Formulation of the Problem. The motion of the medium is described using the velocity field of its particles, i.e., it is assumed that, each particle present at a point with Cartesian coordinates x_1, x_2, and x_3 at time t is described by a velocity vector with the components

$$u_1 = u_1(t, x_1, x_2, x_3), \qquad u_2 = u_2(t, x_1, x_2, x_3), \qquad u_3 = u_3(t, x_1, x_2, x_3).$$

The strain of the medium can be described by the strain gradient tensor $C = [c_{ij}]$, where $c_{ij} = \partial x_i/\partial \xi_j$ (x_i are Eulerian coordinates and ξ_j are Lagrangian coordinates, which parametrize the initial position of the medium; $i, j = 1, 2, 3$). In continuum mechanics, it is reasonable to consider mappings C with a positive determinant; therefore, it will be assumed that $\det C > 0$.

The internal-energy density of unit mass will be denoted by E. In elasticity theory, internal energy is a function of the quantities c_{ij}, initial density of the medium ρ_0, and entropy S. In the present work, the dependence $E(\rho_0)$ is not considered; therefore it is assumed that

$$E = E(c_{11}, c_{21}, \ldots, c_{33}, S).$$

In the construction of elasticity theory, along with the internal-energy density E, a function $\Phi = \rho_0 E$ is introduced, which is called the elastic potential and represents the internal energy of unit initial volume. The dependence $\Phi(c_{11}, c_{21}, \ldots, c_{33}, S)$ will be used as the equation of state.

The equation of state specifies the properties of a particular medium and is considered known in solving problems. However, since the internal energy should not depend on the rotations of the medium as a whole, we assume that the function Φ depends on three orthogonal invariants of the tensor C, namely, we use the model equation of state proposed in [1]:

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$$\Phi = \rho_0\Big(\frac{c_0^2\,\mathrm{e}^{(\gamma-1)S}}{\gamma(\gamma-1)}\Big(W^{-(\gamma-1)} + (\gamma-1)\Big(\frac{K}{3}\Big)^3\Big) + c_1^2 D\Big), \qquad \gamma > 1, \quad \beta \ge 1. \tag{1}$$

Here W, K, and D are invariants of the matrix C:

$$W = \det C = \det\sqrt{CC^*}, \qquad K = \operatorname{tr}\sqrt{CC^*},$$

$$D = \operatorname{tr}\,((\sqrt{CC^*} - \operatorname{tr}\sqrt{CC^*}\,I/3)^2) = \operatorname{tr}\,(CC^*) - (\operatorname{tr}\sqrt{CC^*}\,)^2/3.$$

It should be noted that, in linear elasticity theory, the equation of state depends only on two invariants K and D [2], which describe bulk compression and pure shear, respectively. In nonlinear elasticity theory, it is necessary to consider the dependence of the equation of state on all three invariants of the tensor C. We note that, for small strains, the invariants W and K are interpolated by the same formulas, i.e., they coincide. The invariant W also has a physical meaning: W is the material volume, which is equal to unity before deformation and is related to the commonly used specific volume V by the equality $W = \rho_0 V$.

The main properties of the function Φ in the interpolation formula (1) are given below. The function $\Phi = \rho_0 E$ is a convex function of the variables $c_{11}, c_{21}, \ldots, c_{33}, S$ (but not strictly convex in the variables c_{ij}) and reaches the minimum value for the variables $c_{11}, c_{21}, \ldots, c_{33}$ in the absence of deformation, i.e., for $CC^* = I$ (I is a unit 3×3 matrix). At small loads, Eq. (1) becomes the equation of state of classical linear elasticity theory:

$$\Phi = E_0 + \lambda\varepsilon_{kk}^2/2 + \mu\varepsilon_{ij}\varepsilon_{ji} + \rho_0 T_0(S - S_0) = \lambda(\operatorname{tr}\varepsilon)^2/2 + \mu\operatorname{tr}\varepsilon^2 + \rho_0 T_0(S - S_0) + \ldots\ .$$

Here $\varepsilon = [\varepsilon_{ij}] = \sqrt{CC^*} - I$ is the Cauchy small-strain tensor, and λ and μ are Lamé constants (Young's modulus and shear modulus):

$$\lambda = \rho_0\Big(c_0^2\,\mathrm{e}^{(\gamma-1)S}\Big(\frac{\gamma-1}{\gamma} + \frac{\beta-1}{3\gamma}\Big) - \frac{2c_1^2}{3}\Big), \qquad \mu = \rho_0\Big(c_1^2 + \frac{c_0^2\,\mathrm{e}^{(\gamma-1)S}}{2\gamma}\Big).$$

In this case, the bulk compression modulus is expressed by the formula

$$\varkappa = \frac{c_0^2\,\mathrm{e}^{(\gamma-1)S}}{\gamma}\Big(\gamma - 1 + \frac{\beta}{3}\Big).$$

At large compression ($W \ll 1$), Eq. (1) becomes the equation of state of gas dynamics

$$\Phi = \frac{c_0^2\,\mathrm{e}^{(\gamma-1)S}}{\gamma(\gamma-1)}\,W^{-(\gamma-1)} + \ldots\ .$$

In the above formulas, ellipsis denotes terms which can be neglected under the assumptions made.

We now proceed to formulate a model for a nonlinear elastic medium. In the variables of the strain gradient tensor c_{ij}, velocities u_i, and entropy S, the system of elasticity equations is written as follows [3]:

$$\rho_0\,\frac{\partial u_i}{\partial t} - \frac{\partial \Phi_{c_{ij}}}{\partial \xi_j} = 0, \qquad \frac{\partial c_{ij}}{\partial t} - \frac{\partial u_i}{\partial \xi_j} = 0, \qquad \frac{\partial S}{\partial t} = 0. \tag{2}$$

It has been shown [1] that the hyperbolicity (well-posedness of the Cauchy problem for smooth initial data) of system (2) is due to the convexity of the internal energy Φ in the strain gradient tensor elements c_{ij}. In particular, it is shown that the system of conservation laws (2) is symmetric hyperbolic if an only if Φ is strictly convex in the variables c_{ij}. It has also been shown that a criterion for the convexity of the function $\Phi(c_{11}, \ldots, c_{33})$ which is invariant under rotations is the satisfaction of the inequalities

$$\frac{\Phi_{k_i} + \Phi_{k_j}}{k_i + k_j} > 0, \qquad \frac{\Phi_{k_i} - \Phi_{k_j}}{k_i - k_j} > 0$$

and the positive definiteness of the 3×3 matrices: $[\Phi_{k_i k_j}] > 0$ (k_i are the singular numbers of the tensor C).

We recall that the asymmetrical tensor $[\Phi_{c_{ij}}] = [\pi_{ij}]$ is called the Piola–Kirchhoff stress tensor and the quantities Φ_{k_i} are its principal values, which, in the absence of deformation ($k_1 = k_2 = k_3 = 1$), are equal to zero: $\Phi_{k_i} = 0$. Thus, one of the conditions for the strict convexity of the energy Φ is violated since $(\Phi_{k_i} + \Phi_{k_j})/(k_i + k_j) = 0$.

The indicated difficulties can be overcome using the approach proposed in [1]. Along with the variables c_{ij}, we introduce an additional variable W and assume that they are independent:

$$\Phi(c_{11}, c_{21}, \ldots, c_{33}, S) = \tilde\Phi(W, K(c_{11}, c_{21}, \ldots, c_{33}), D(c_{11}, c_{21}, \ldots, c_{33}), S).$$

In this case, for system (2) to be hyperbolic, it is necessary to require that the function $\tilde{\Phi}$ be convex in the variables W, c_{ij}, and S. This modification was proposed by Godunov and is described in detail in [1]. Below, notation Φ (tilde is omitted) is used for the function of the variables W, c_{ij}, and S on the right side of the last equality.

In view of the modified formulation of the problem, the system of elasticity equations in Lagrangian coordinates for the unknowns u_i, W, S, and c_{ij} $(i, j = 1, 2, 3)$ is written as

$$\frac{\partial \rho_0 u_i}{\partial t} - \frac{\partial}{\partial \xi_j}(W a_{ji} \Phi_W + \Phi_{c_{ij}}) = 0, \qquad \frac{\partial W}{\partial t} - W a_{ji} \frac{\partial u_i}{\partial \xi_j} = 0,$$
$$\frac{\partial c_{ij}}{\partial t} - \frac{\partial u_i}{\partial \xi_j} = 0, \qquad \frac{\partial S}{\partial t} = 0. \tag{3}$$

System (3) should be supplemented by the energy conservation law

$$\frac{\partial}{\partial t}\Big(\rho_0 \frac{u_i u_i}{2} + \Phi\Big) - \frac{\partial}{\partial \xi_j}(u_i \rho_0 (W a_{ji} \Phi_W + \Phi_{c_{ij}})) = 0.$$

Here a_{ji} are the elements of the inverse matrix C^{-1}.

It should be noted that, along the trajectories, the equality

$$\frac{d}{dt}(W^{-1} \det C) = 0 \tag{4}$$

holds if it held at the initial time. In the calculation of the derivatives $\Phi_{c_{ij}}$, it is also necessary to take into account that W is independent of the elements of the matrix C.

In the first three equations (momentum conservation law) of system (3), the expressions in parentheses are the components π_{ij} of the Piola–Kirchhoff stress tensor:

$$\pi_{ij} = W \Phi_W a_{ji} + \Phi_{c_{ij}}.$$

The Piola–Kirchhoff stress tensor is related to the usual stress tensor σ by the Murnaghan formula [4], which, after the modification of the problem formulation, becomes

$$\sigma_{ij} = W^{-1} c_{ik} \pi_{kj} = W^{-1} c_{ik} (W \Phi_W a_{kj} + \Phi_{c_{kj}}). \tag{5}$$

We consider the one-dimensional elasticity problem in which all functions u_i, W, c_{ij}, and S in system (3) depend only on one the space variable and time. As such a space variable we use ξ_1 (below, the subscript is omitted); this direction will be called longitudinal, and the other two directions will be called transverse.

In the case of a one-dimensional process, the equations for c_{ij} of system (3) imply that the quantities c_{ik}, $i = 1, 2, 3$ and $k = 2, 3$ (the second and third columns of the matrix C) do not vary with time, i.e., they are only functions of ξ. These quantities are not included in the number of unknown functions.

In the present paper, we consider only solutions for which $W = \det C$ (other solutions have no physical meaning); therefore, denoting the minors $W a_{ji}$ of the matrix C by A_{ji}, we obtain

$$A_{11} = c_{22} c_{33} - c_{23} c_{32}, \qquad A_{12} = c_{32} c_{13} - c_{12} c_{33}, \qquad A_{13} = c_{12} c_{23} - c_{22} c_{13}.$$

Hence, the minors A_{1i}, just as the quantities on the right sides of these equalities, do not depend on time t and are functions only of the variable ξ.

Let us write the equations for the one-dimensional model. For brevity, we omit the subscript j in the quantities c_{ij} and A_{ji}, denoting by c_i the elements of the first column of the matrix C and by A_i the elements of the first row of the matrix of minors $(\det C) C^{-1} = W C^{-1}$. Then, in view of the aforesaid, the one-dimensional system of elasticity equations for the vector of unknowns $\boldsymbol{v} = (u_1, u_2, u_3, W, c_1, c_2, c_3, S)$ can be written as follows [1]:

$$\rho_0 \frac{\partial u_i}{\partial t} - \frac{\partial}{\partial \xi}(A_i \Phi_W + \Phi_{c_i}) = 0, \qquad \frac{\partial W}{\partial t} - A_i \frac{\partial u_i}{\partial \xi} = 0, \qquad \frac{\partial c_i}{\partial t} - \frac{\partial u_i}{\partial \xi} = 0, \qquad \frac{\partial S}{\partial t} = 0.$$

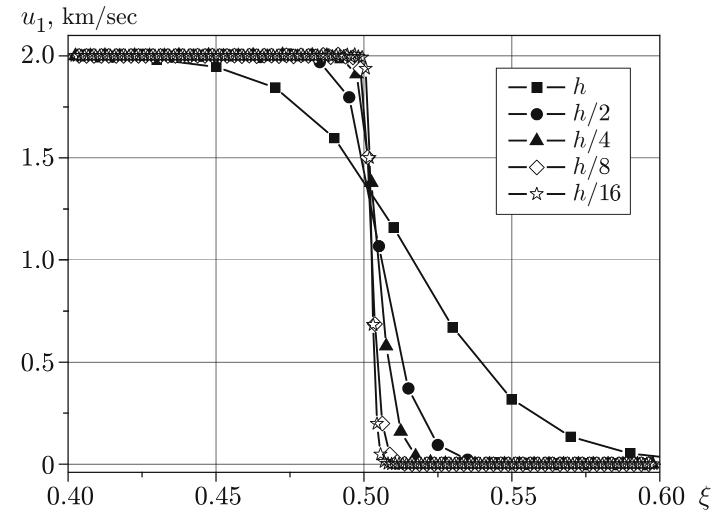

Fig. 1. Longitudinal velocity component u_1 versus longitudinal coordinate ξ ($t = 0.6 \cdot 10^{-6}$ sec).

It should be noted that, under the assumption that the minors A_i are constant in a certain region of the space, both this one-dimensional system and three-dimensional systems are symmetric t-hyperbolic systems, i.e., in the indicated region, system (3) can be written in equivalent form

$$A(\boldsymbol{p})\,\frac{\partial \boldsymbol{p}}{\partial t} + B_j(\boldsymbol{p})\,\frac{\partial \boldsymbol{p}}{\partial \xi_j} = 0,$$

where $\boldsymbol{p}$ is the vector of the new variables which is related to the vector of the former unknowns $\boldsymbol{v}$ by a certain system of nonlinear algebraic equations; $A^* = A > 0$ and $B_j^* = B_j$ are symmetric matrices. In implementing the difference scheme, we assume that the minors A_i are constant (freezing of the coefficients within one computation mesh).

2. Results of Numerical Experiments. To construct a numerical solution, we use the Godunov finite-volume scheme [5] in an acoustic approximation of the solution of the arbitrary discontinuity decay problem (Riemann problem). In the Godunov scheme, the solution of the Riemann problem is the main procedure. In this stage, we use the symmetric hyperbolic form of the equations, which allows the use of the effective modern algorithms of linear algebra for symmetric matrixes.

For the numerical calculations, we chose the equation of state (1) with the parameters $\gamma = 4$, $c_0 = 5.1$ km/sec, $c_1 = 2.54$ km/sec, and $\rho_0 = 2.7$ g/cm^3, which correspond to the parameters of aluminum. In all examples, the examined domain is a plate which is infinite in the transverse directions (ξ_2 and ξ_3) and finite in the longitudinal direction (plate thickness 10 mm). The results of the numerical study of the discontinuous solutions of the examined model are given.

2.1. *Discontinuity of the Longitudinal Velocity Component. Convergence of the Difference Solution.* In the interval $\xi \in [0, 1]$, we consider the problem of a piston moving in the longitudinal direction from left to right at a constant velocity 2 km/sec. At the point $\xi = 1$, the material is assumed to be motionless. In this case, the boundary conditions are written as

$$u_1(t,0) = 2, \qquad u_2(t,0) = u_3(t,0) = 0, \qquad u_1(t,1) = u_2(t,1) = u_3(t,1) = 0.$$

The initial conditions are taken to be

$$u_1(0,\xi) = u_2(0,\xi) = u_3(0,\xi) = 0, \qquad C = I, \qquad W = \det C.$$

The mismatch between the boundary and initial conditions on the left boundary of the plate ($\xi = 0$) specifies a discontinuity of the longitudinal velocity components u_1.

Figure 1 gives the longitudinal velocity component u_1 versus the coordinate ξ for various mesh sizes. The calculations show that, as mesh size is reduced, the numerical solution has the convergence property. Figure 1 shows the solutions for mesh sizes h, $h/2$, $h/4$, $h/8$, and $h/16$ ($h = 0.02$). The limiting solution is a step — a shock wave. Upon the completion of the relaxation process, the initial discontinuity u_1 spreads over approximately seven

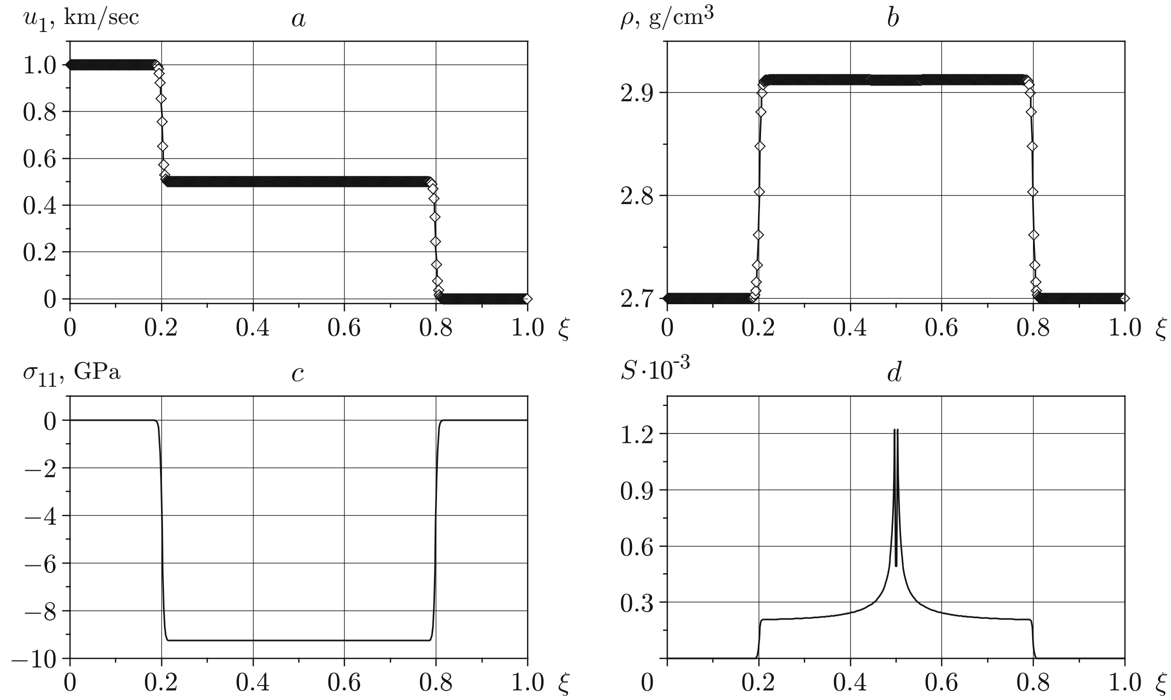

Fig. 2. Longitudinal velocity component (a), density (b), longitudinal stress (c), and entropy (d) versus longitudinal coordinate in the discontinuity decay problem (discontinuity at the point $\xi = 0.5$ cm) of the longitudinal velocity component ($t = 0.15 \cdot 10^{-6}$ sec).

computational meshes and its shape remains unchanged with time. From an analysis of the curves presented in Fig. 1, it follows that the numerical solution converges to a discontinuous solution as the mesh size is reduced.

2.2. *Discontinuity of the Longitudinal Velocity Component. Discontinuity Decay Problem.* At the point $\xi = 0.5$ mm, we specify a discontinuity of the longitudinal velocity component equal to 1 km/sec, so that the medium on the left of the discontinuity (impactor) moves to the right with a velocity $u_1 = 1$ km/sec and the medium on the right of the discontinuity (target) is at rest: $u_1 = 0$. The remaining parameters the medium are the same as in the example considered in Sec. 2.1. The calculation results are given in Fig. 2.

The initial discontinuity disintegrates into two compression shock waves which propagate to the left and right. The entropy trace, which is clearly seen at the location of the initial discontinuity in Fig. 2d is a nonphysical manifestation of the numerical method. Usually, such a trace appears in the zones of formation of the wave profile, such as the region of the initial discontinuity or near rigid impenetrable boundaries of the calculation domain. Taking into account the physical requirements of the problem, it is common to employ entropy correction procedures [6]. In the present work, such procedures are not used: from a point of view of the generalized solution, this trace is of no significance because its width is equal to a fixed number of computation meshes and tends to zero as the mesh size is reduced.

2.3. *Discontinuity of the Transverse Velocity Component.* We consider the discontinuity decay problem for the transverse velocity component u_2 using as an example the case of plane oblique collision of two plates with ideal friction (the collision angle is equal to zero). The left plate ($\xi \in [0; 0.5]$) moves in the transverse direction with a velocity $u_2 = 1$ km/sec, and the right plate ($\xi \in [0.5; 1]$) is at rest ($u_2 = 0$). The other initial data are given by the following conditions:

$$u_1(0, \xi) = u_3(0, \xi) = 0, \qquad C = I, \qquad W = \det C.$$

From the results of the numerical experiments presented in Fig. 3, it follows that, with time, the initial discontinuity of the transverse velocity component becomes a wave which extends to an increasing number of computation meshes. In Fig. 3a, it is evident that, unlike the waves propagating in the longitudinal direction, the transverse waves also produce a perturbation of the material in the longitudinal direction and are rarefaction

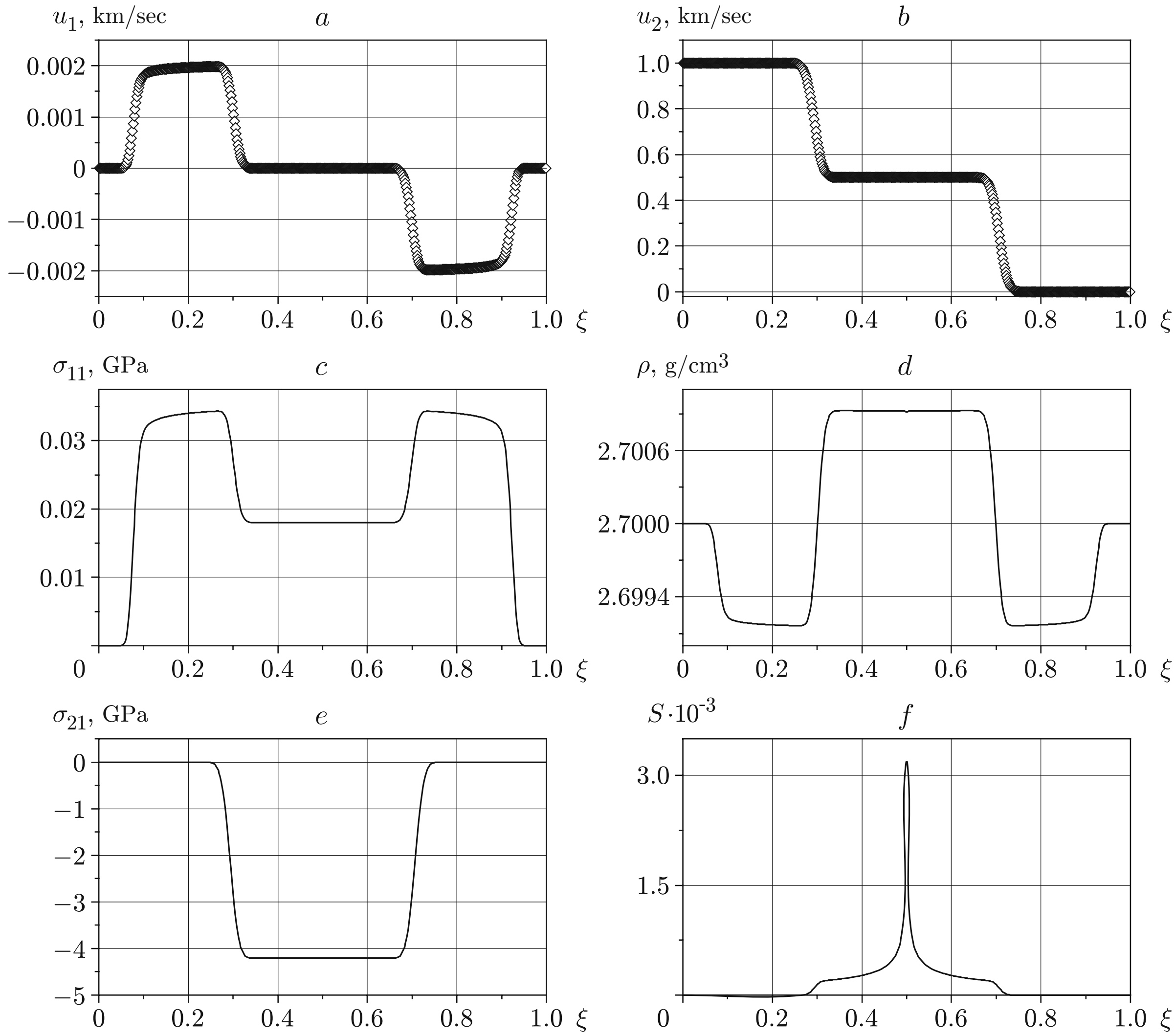

Fig. 3. Longitudinal (a) and transverse (b) velocity components, longitudinal stress (c), density (d), shear stress (e), and entropy (f) versus longitudinal coordinate in the discontinuity decay problem (discontinuity at the point $\xi = 0.5$ cm) of the transverse velocity components ($t = 0.66 \cdot 10^{-6}$ sec).

gas-dynamic waves regardless of the sign of the quantity u_2. We note that the leading edge of the perturbation of the longitudinal velocity u_1 moves at the longitudinal sound velocity, and the trailing edge at the transverse sound velocity.

As in the example considered in Sec. 2.2, in Fig. 3f one can clearly see a peak at the location of the initial discontinuity, whose width is equal to a definite number of computation meshes.

2.4. *Discontinuity of the Longitudinal Velocity Component in Prestressed Material.* We consider an example of wave propagation in a prestrained material for which linear elasticity theory is inapplicable. Problems in this formulation can be encountered in many applications. Let, at the initial time, the matrix C have the form

$$C = \begin{pmatrix} 1 & -0.7 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{6}$$

and let the longitudinal velocity component have a discontinuity: $u_1(0,\xi) = 2$ km/sec on the left of the point $\xi = 0.5$ cm and $u_1(0,\xi) = 0$ on the right of it. The remaining initial data are as follows: $u_2(0,\xi) = u_3(0,\xi) = 0$ and $W = \det C$. We recall that, in the one-dimensional problem, the second and third columns of the matrix C in the coordinate $\xi = \xi_1$ remain constant in time.

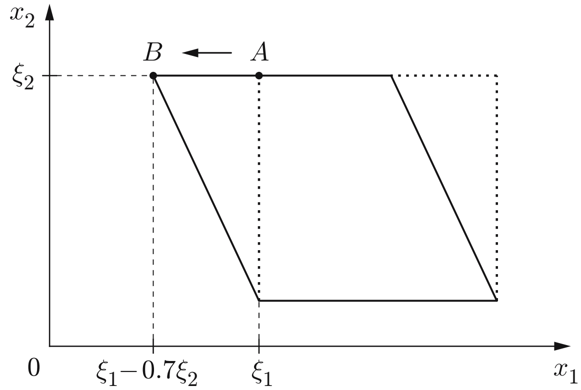

Fig. 4. Deformation of the crystal lattice corresponding to the matrix C of the form (5): square shows the initial position of the crystal lattice, and parallelogram shows the position of the crystal lattice resulted from the action of the tensor (5).

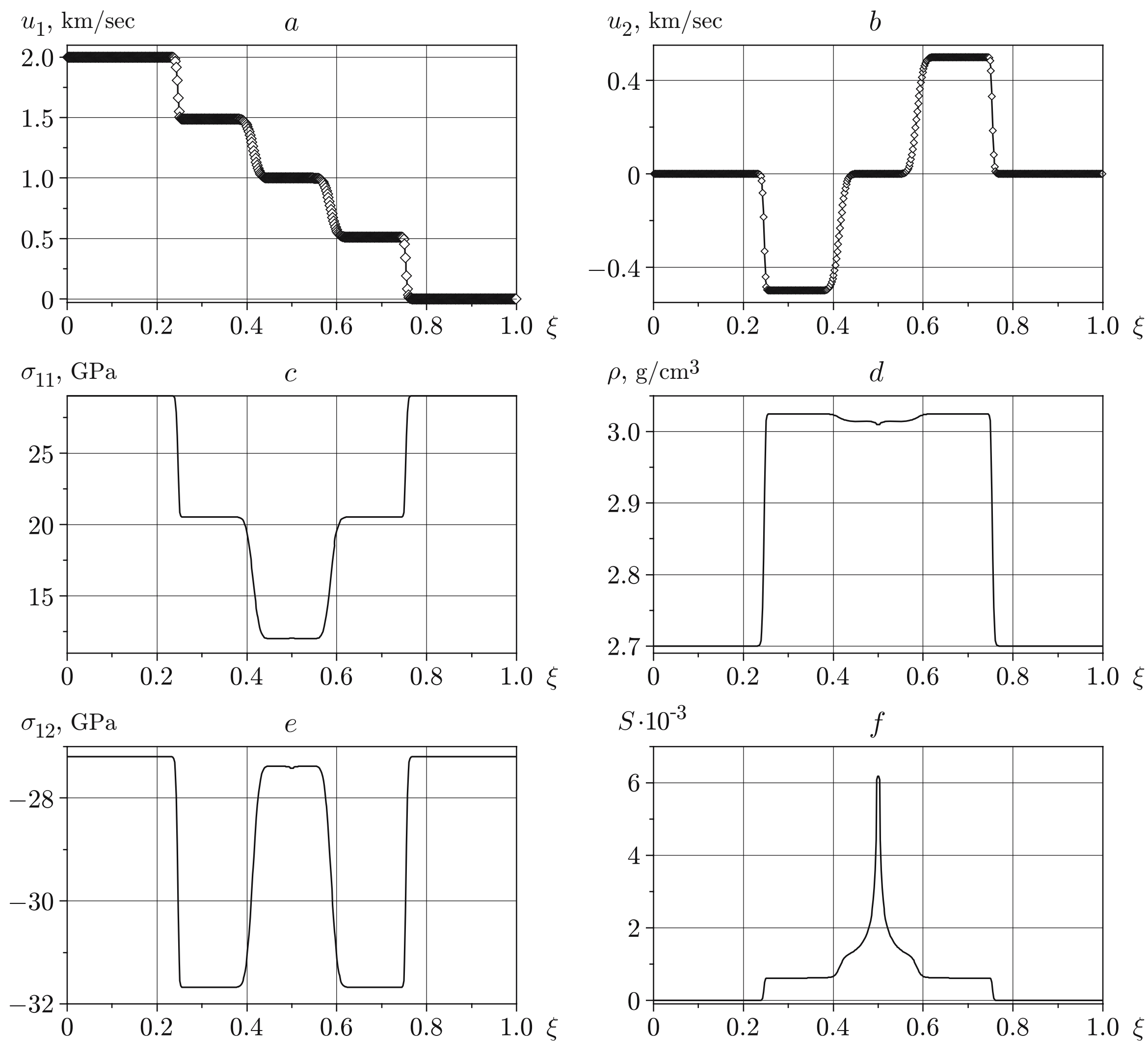

Fig. 5. Longitudinal (a) and transverse (b) velocity components, longitudinal stress (c), density (d), shear stress (e), and entropy (f) versus longitudinal coordinate in the discontinuity decay problem for the longitudinal velocity component in a prestressed material ($t = 0.27 \cdot 10^{-6}$ sec).

The prestrain of the medium given by tensor (6) is responsible for the initial stress. In this case, the stress tensor calculated by the Murnaghan formula (5) has the form

$$\sigma = \begin{pmatrix} 14.1 & -18.7 & 0 \\ -18.7 & 1 & 0 \\ 0 & 0 & 0.04 \end{pmatrix}.$$

Notwithstanding the fact that the solid is modeled by a continuous medium, it can be assumed that the tensor C in the form of (6) models the distortion of a conditional crystal lattice (Fig. 4). If, at $t = 0$, a point of the isotropic medium A had the coordinates $(\xi_1; \xi_2)$ in the plane x_1x_2, in the anisotropic material, it becomes a point B with the coordinates $(\xi_1 - 0.7\xi_2; \xi_2)$.

The solution profiles are given in Fig. 5. It is evident that, in the longitudinal direction, two waves propagate from the discontinuity opposite to each other, one of which is a shock (leading) wave and the other is a transverse wave. The second wave is caused by the distortion of the crystal lattice, i.e., the faces of the lattice which were initially perpendicular to the longitudinal direction rotate so as to make at a certain acute angle with this direction. As a result, a planar impact in the longitudinal direction induces longitudinal and transverse perturbations of each crystal cell.

From the results of the numerical experiments, it follows that the system of equations of nonlinear elasticity theory derived in [1] assuming smooth variation in the parameters of the medium is suitable for describing discontinuous solutions. However, in the near future, a rigorous theoretical justification of this model for the case of media exhibiting discontinuous behavior is hardly possible: complete theory for this case does not exist, just as it does not exist for the gas-dynamics equations and other nonlinear equations of mathematical physics.

Conclusions. The calculations are tentative. There still remain many questions to be investigated, one of which — the control of the accuracy of the calculated material parameters — seems to be especially important and nontrivial. The nontriviality of this question is due to the fact that the model proposed in the present work is an overdetermined system of equations. The formulation of the problem was modified (the variable W was isolated) to ensure the well-posedness of system (3); as a result, the system became even more overdetermined: in addition to the fact that, before the modification, the number of conservation laws exceeded the number of unknowns, new relations on the characteristics of the system appeared. For example, Eqs. (3) implies relation (4), which holds along the particle trajectories $dx_i/dt = u_i$ if it held at the initial time. Naturally, the problem has many other solutions on which relation (4) does not hold. These solutions are of no interest because they have no physical meaning. However, in numerical calculations, mathematically rigorous relations may not hold due to approximation errors resulting from discretization, especially in the cases where derivatives of discontinuous functions are calculated. Such facts known in magnetic hydrodynamics (nonconservation of magnetic charge) [6] are apparently inherent in all overdetermined systems of mathematical physics.

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