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Modeling the Behavior of Complex Media by Jointly Using Discrete and Continuum Approaches

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Abstract—We propose a new approach to modeling the behavior of heterogeneous media, according to which such objects are represented as composed of regions of two types, one being described within the framework of a discrete, and the other, a continuum approach. This joint approach is promising for the numerical modeling of complex media with strongly different properties of components. Possibilities of the proposed method were verified by studying the propagation of elastic waves in a two-component medium with a discrete component, modeled by the method of movable cellular automata, and a continuum component described by a system of equations of motion of continuum solved by the finite difference method. The results of calculations show that this approach provides adequate description of the propagation of elastic waves in complex media and does not introduce nonphysical distortions at the boundaries where the two models are matched.

Investigation of the laws governing the behavior of complex media under the action of various external factors is necessary for solving many basic, technological, and engineering problems. An important part in such investigations belongs to methods and approaches developed by computational mechanics. For a long time, most numerical methods were based on the approaches developed within the framework of the mechanics of continuum. It should be noted that application of the methods of continuum mechanics to description of the process of deformation encounters considerable difficulties in the presence of local straining, discontinuities, intense vortex deformations, and agitation of masses. These problems are especially significant in the case of highly porous and heterogeneous materials and composites with strongly different properties of components.

Discrete approaches capable of explicitly modeling the processes involving agitation of masses were developed predominantly for the investigation of granulated and friable media [1–4], in which the basic elements can be modeled by particles. For this reason, most of these investigations use the equations of motion in the form typical of the method of particles [4] and the interaction forces are calculated within the framework of the model of hard or soft spheres. However, this formalism does not provide correct description of the behavior of continuous isotropic media.

The numerical method of movable cellular automata (MCA) extensively developed in recent years [5–9] is free of this disadvantage. While using a discrete approach, this method is based on the equations of motion, which are different from classical equations. In particular, it was shown [7] that, when the characteristic automaton size tends to zero, the MCA formalism allows a transition to the relations of continuum mechanics. The main advantage of this method is the possibility of explicitly modeling both the motion of continuous media and the agitation of masses, including the formation of discontinuities of various types (from the generation of individual defects to the main crack propagation). This circumstance for the first time provides prerequisites for jointly using discrete and continuum approaches within the framework of a common computational scheme, thus combining the advantages of both approaches for solving problems related to modeling of complex objects containing explicit zones of intense straining and fracture.

This paper is devoted to the joint use of discrete and continuum approaches, which is important for the development of computational mechanics. The new approach is based on two methods successfully used in recent years. The first method, based on the continuum approach, is the finite difference method of solution of the dynamical problems of elastoplastic deformation of continuous media, and the second is the MCA method based on the discrete description.

Since both methods employed in the proposed approach are well known [5, 6, 10], we will only consider the questions pertaining to their joint use. The model medium (Fig. 1) is considered to be composed of regions of two types—continuous (grid) and discrete (MCA). Each node of the grid, occurring at the boundary (interface) where the two models are matched, is set into correspondence with a certain interfacial automaton (element of the MCA model). In the simplest case,

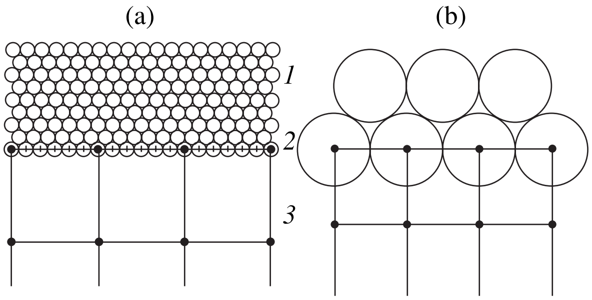

Fig. 1. Matching of the continuous and discrete regions of a model complex medium in the cases when the size of movable cellular automata is (a) smaller than and (b) equal to the grid pitch: (*1*) MCA; (*2*) interface; (*3*) grid.

the automaton size is equal to the grid pitch and there are no additional automata between the interfacial grid nodes.

In order to provide for a correct joint description of consistent behavior of the continuous and discrete regions, it is necessary to ensure continuity of the state parameters on the passage across the interface. In this study, the motion of two models was matched in the step of calculation of the velocities of interfacial nodes. For these nodes, the finite difference equation of motion was written in the form taking into account all forces acting upon the matched interfacial nodes and automata.

The five-step computational algorithm is as follows:

1. Calculate the stress-strained state in the continuous region, including the velocities and coordinates of nodes.

2. Calculate the velocities of interfacial nodes, in contrast to those of the internal nodes, using the equations of motion involving forces acting from the discrete region.

3. Call a subroutine realizing the MCA method, introduce the coordinates and velocities of matched interfacial nodes and automata, and set the integration step.

4. Perform the MCA integration step (for smaller automata, several steps) to calculate the new positions and velocities of all automata, including those matched with interfacial nodes.

5. Introduce new data on the matched interfacial automata into the grid model and set a new time step for the integration.

In order to check for the possibility of jointly using the discrete and continuum approaches within the framework of a common computational scheme and verify the algorithm, we studied the propagation of elastic waves in a two-component medium with a free surface, involving only one linear boundary where the two models have to be matched (Fig. 2). The mechanical characteristics of continuous and discrete media were taken to be identical, so that the medium was formally homogeneous and the interface should not be manifested. It should be noted that numerical methods used in this study were previously successfully applied to description of dynamical processes, including the propagation of elastic waves [8, 9, 11–13].

In the first stage, we considered the propagation of a plane elastic wave with a front parallel to the line of matching. The results of calculations showed that the wave crossing the boundary in both possible directions did not give rise to a reflected wave and the pulse shape was not distorted. This was evidence that the algorithm of joint use of the two methods ensured complete momentum transfer in the absence of shear strain.

In the second stage, we studied a more complicated problem involving the generation and propagation of waves of all types in the medium with a free surface. For this purpose, a region on the surface of an elastic medium occupying a half-space was subjected to a short pulse of a local vertical load. The pulse source was either arranged symmetrically on the line of matching the grid and MCA regions (case 1) or displaced into one of these regions (case 2). We analyzed the detailed

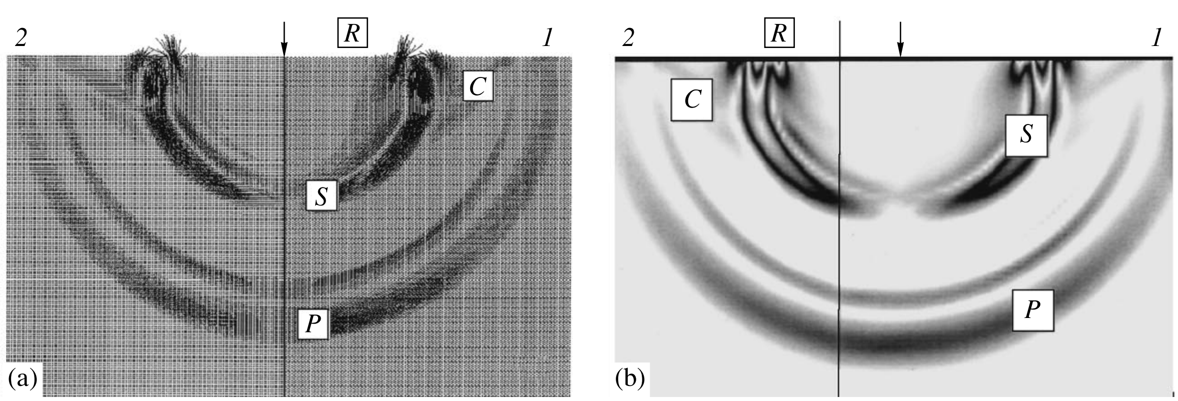

Fig. 2. Wave field patterns observed when the pulse source is (a) arranged symmetrically relative to the interface (indicated by the arrow) and (b) shifted toward the discrete region: (*1*) MCA; (*2*) grid. See the text for explanation.

pattern of propagation of waves of all types and the symmetry of the displacement velocity field. The tests were performed for both square and close (hexagonal) packing of automata in the discrete region.

In both cases, the pulsed action resulted in the formation of longitudinal (*P*) and transverse (*S*) waves at a certain distance from the pulse source, which propagated with different velocities (Fig. 2). The presence of the free surface leads to the formation of so-called conical and surface waves. As can be seen in Fig. 2, the conical (*C*) wave is manifested only in the region where the longitudinal wave interacts with the free surface. The *C*-wave front extends from the point where the *P* wave emerges on the surface to the tangency point on the *S*-wave front. The surface Rayleigh (*R*) wave propagates at the free surface, lagging slightly behind the *S* wave. The *R* wave has an elliptical polarization and rapidly decays with depth.

As is known, the passage of a wave across the interface of two media possessing different mechanical properties or across the surface of discontinuity of displacements (see, e.g., [13]) gives rise to the formation of reflected and refracted waves. In all cases under consideration, the results of our calculations showed no significant distortion of wave fronts (Fig. 2). Nor did we observe significant secondary (reflected, refracted, or conical) waves.

Thus, the results of numerical simulation of the propagation of elastic waves in a combined medium modeled using the continuum and discrete approaches confirmed the possibility of jointly using these methods for description of the elastic behavior of complex media. Good prospects of the proposed approach and algorithms of its realization were confirmed by the results of test calculations, which showed that no artificial or induced effects arise even in cases of complex, dynamically developing elastic displacements in a complex medium with a free surface. The proposed method can be especially useful for solving problems involving numerical simulation of the behavior of complex media with strongly different physical properties of components. Such problems are not only considered in materials science and machine building but also frequently encountered in problems of geomechanics and the mechanics of soils and rocks.

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