Modeling of deformation of ground media on the basis of the particle method in a two-dimensional formulation

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Abstract. A two-dimensional version of the soil deformation method based on the particle method is implemented in this paper. For describing the behavior of a continuous medium, the previously used two-parameter "modified" Lennard-Jones interaction potential was chosen. A number of model problems describing the loss of stability of the soil embankment in the field of gravity and the destruction of the soil under the action of the liquid phase are solved.

1. Introduction
At present, most of the computational methods are based on the discretization of the region, most often the finite-element and finite-difference techniques [1-12]. Such an approach has perfectly proved itself in solving problems of deformation of complex heterogeneous media of various nature. However, there is a wide class of problems in which the loading of the medium is accompanied by multiple destruction and slippage of fragments, intensive mass transfer, including the effects of mixing masses, etc. When solving such problems, the use of the grid approach is very difficult. A promising class of numerical methods for the mechanics of a deformable solid body, adapted for modeling fracture, are particle methods [13-18].

One of the promising applications of the particle method is hydraulic fracturing, which is currently considered one of the most effective technologies for intensifying oil and gas production, both in traditional reservoirs and in low-permeability reservoirs known as shale hydrocarbons. The theoretical basis for calculating the resulting crack was laid by Christianovich and Zheltov [19]. Somewhat later Perkins and Kern [20] proposed another model for calculating a fissure. Nowadays, these models are currently used in applied fracture design systems. The models of Khristianovich-Zheltov and Perkins-Kern give a rather simplified performance development of the fissure of fracturing; in particular, they do not take into account the vertical and lateral heterogeneity of the reservoir according to mechanical characteristics, as well as the presence of natural fracturing. In addition, in real conditions we know the geological environment with some, sometimes rather large, uncertainty. Insufficient reliability of the design in conditions of stochastic character of the geological environment requires the control of the fracturing process to determine the actual characteristics of the fracture HF and the planning of further activities for the development of the well. Nowadays, the most commonly used monitoring method is the recording of microseismic activity accompanying the formation of a fracture by recording microseismic waves in neighboring wells [21] or from the earth's surface [22]. However, known analytical models do not relate the intensity of microseisms to the parameters of the crack, which makes interpretation difficult. More realistic models for calculating fracture propagation require
the use of numerical multi-model numerical models that take into account the elastic interaction, fracture mechanics, fluid flow in the fracture and filtration processes in the formation.

An approach based on the Lagrange method is known [23], which allows numerical modeling of both hydraulic fracturing (HF) of a formation and generated microseismic waves within the framework of one numerical model. This makes it possible to increase the realistic modeling of the hydraulic fracturing process, in a complex geological environment. This also makes it possible to determine by calculation the dependence of the resulting microseismic waves on the characteristics of the fracture HF and thus increase the adequacy of the interpretation of microseismic methods of fracturing control of HF. Methods of numerical simulation of fracturing processes require the use of high-performance computing systems. At present, high-performance computing systems are increasingly equipped with computational accelerators based on GPGPUs, which are systems with mass parallelism (SIMD). SIMD architecture effectively implements simple linear algorithms without branching. Thus, to effectively model the fracturing process of HF, it is desirable to implement it as simply as possible. The method of discrete elements is used in [23]. According to this paper, the method of discrete elements gives quite realistic models of the behavior of the destruction of continuous media and the propagation of elastic waves. The method of discrete elements has a relatively complex algorithm, which includes, at each step of the simulation, the determination of the contacting elements, the calculation of the contact areas between them, and the calculation of the interaction forces.

We know a simpler approach based on the Lagrange method, based on the representation of the particles of the medium by nonstructural points interacting with each other on the basis of a potential that depends only on the distance between the points. This approach is called molecular dynamics and is widely used in computational chemistry, nanoparticle mechanics, and astrophysics. The attractiveness of this method lies in the computational simplicity. The method of molecular dynamics is based on the same type of calculations of potential forces between points. These calculations are well implemented on systems with mass parallelism. Modeling of the fracturing process should include modeling of fluid flow, including in pore channels, modeling of fracture and formation of seismic waves, including shear waves. There are known works on the molecular dynamics modeling of fluid flow of different scale, from macro-scale modeling by the well known method of large particles to nanopores [24]. The work on modeling the destruction of solids by the molecular dynamics method using the Lennard-Jones interaction potential has been conducted for a long time [17], however, high-energy supersonic processes are investigated in them, where brittle fracture plays no appreciable role. In this paper, we investigate the possibility of simulating less energy processes of brittle fracture and the formation of seismic waves in modeling the fracturing process.

The modern development of computer technology, including parallel computing systems, provides ample opportunities for modeling continuous media at the micro level. In recent years, such modeling is carried out on the basis of the particle method. The particle method is that a continuous medium is represented as a set of interacting material particles. As such particles can act as atoms and, molecules of matter, and mineral particles of ground materials. At present, the potentials of interatomic interaction for most materials are known, which can not be said about the potentials for describing the behavior of deformed continuous media, especially shear ones. One of the important advantages of the particle method is that much less information about the properties of the material is needed when using it. Complex mechanical processes can be modeled in some way using the simple Lennard-Jones potential. To describe each of these effects, a separate theory is required, while in particle modeling, these effects are obtained by integrating the equations of motion.

2. **Formulation of the problem**

The motion of the aggregate of material particles interacting in a potential field can be described on the basis of the following equation of motion

\[ m \ddot{r}_k = \sum_{i=1}^{N} \frac{1}{r_{ki}} f (r_{ki}) r_{ki} + \nabla \varphi (r_{ki}), \]

(1)
where \( \mathbf{r}_k \) – radius vector \( k \)-th particle
\[
\mathbf{r}_{kn} = \mathbf{r}_k - \mathbf{r}_n, \tag{2}
\]

\( m \) – mass of particle, \( \varphi(r) \) describes an external conservative force field, energy dissipation was not taken into account. We consider the pair potential \( \Pi(r) \), force of interaction \( f(r) \) corresponding to it is defined as
\[
f(r) = -\frac{\Pi'(r)}{r}. \tag{3}
\]

For describing the interaction of material particles of a deformed medium (soil), we used the "modified" Lennard-Jones potential [25, 26], the parameters and interaction force for which were taken in the form
\[
D = 10^4, a = 0.4 \times 1.28r, f(r) = \frac{D}{r} \left[ 12 \left( \frac{a}{r} \right)^2 - 36 \left( \frac{a}{r} \right)^4 + 14.4 \left( \frac{a}{r} \right)^6 + 6 \left( \frac{a}{r} \right)^8 \right]. \tag{4}
\]

To describe the deformation of the liquid phase, we used the Lennard-Jones potential, the parameters and the interaction force for which were taken in the form:
\[
D = 4 \times 10^4, a = 0.4r, f(r) = \frac{12D}{r} \left[ \left( \frac{a}{r} \right)^2 - \left( \frac{a}{r} \right)^6 \right]. \tag{5}
\]

3. Numerical example

To illustrate the possibilities of the implemented methodology, two model problems were solved, for which the qualitative character of the deformation of the soil massif, the possibility of its destruction and loss of stability of slopes, is determined, so a certain arbitrariness was allowed in choosing the parameters of the Lennard-Jones potential. The parameters of the "modified" Lennard-Jones potential were selected on the basis of the parameters of the ordinary Lennard-Jones potential, starting from the qualitative condition of the appearance of a shear wave when considering the problem of propagation of seismic waves in a geological environment [26]. In the first task, the soil layer modeled by 800 particles is initially formed between two absolutely rigid barriers. After the "packing" of material particles in the form of a rectangle, the lateral obstacles instantly disappear and the layer of soil under the influence of its own weight creeps, resulting in its partial destruction. Figures 1-4 show the final configurations, which acquire a soil massif in the process of loss of stability and partial destruction, depending on the magnitude of acceleration of gravity \( 0.5g, 0.8g, 0.85g \) and \( g \) respectively) using the Lennard-Jones potential and the "modified" Lennard-Jones potential.

In the second task, a soil layer defined by 1000-th material points with a rectangular notch formed by absolutely rigid walls is formed (Fig. 5). In the cavity rectangular area consisting of 200 particles a system of material particles is formed, representing the liquid phase failure. At some point in time, the lower wall that bounds the liquid phase disappears instantaneously, and the fluid under pressure pours into the ground. The so-called hydraulic fracturing of the formation is being realized. Figures 6-9 show the different cases of the soil breaking out with a liquid phase, when the magnitude of acceleration of gravity - \( 0.9g, 1.1g \) respectively.
Figure 1. The final configuration of the soil layer after the process of sample destruction for the Lennard-Jones potential (b) and its modified version (a) when the magnitude of acceleration of gravity - 0.5g.

Figure 2. The final configuration of the soil layer after the process of sample destruction for the Lennard-Jones potential (b) and its modified version (a) when the magnitude of acceleration of gravity - 0.8g.

Figure 3. The final configuration of the soil layer after the process of sample destruction for the Lennard-Jones potential (b) and its modified version (a) when the magnitude of acceleration of gravity - 0.85g.
Figure 4. The final configuration of the soil layer after the process of sample destruction for the Lennard-Jones potential (b) and its modified version (a) when the magnitude of acceleration of gravity - $g$.

Figure 5. Initial position of the solid and liquid phases.

Figure 6. Fracturing process and soil degradation when the magnitude of acceleration of gravity - $0.9g$.

Figure 7. Fracturing process and soil degradation when the magnitude of acceleration of gravity - $g$.

Figure 8. Fracturing process and soil degradation when the magnitude of acceleration of gravity - $1.1g$. 
4. Conclusion

Analysis of the results shows that the use of the "modified" Lennard-Jones potential to describe the ground phase allows the brittle fracture process to be realized in the ground, whereas the Lennard-Jones potential will allow reproducing only viscous fracture. In the work, studies were carried out to identify the parameters of the "modified" Lennard-Jones potential, but it should be noted that these parameters are difficult to find numerically for an adequate description of the deformation of real earth. In the future, a comprehensive analysis of the "modified terms" of the potential should be carried out on the basis of a comparison of the results of solving the simplest problems for different chilas of the material particles used. It is also worth noting that the "modified" potential shows itself well in the modeling of a deformable solid medium. It can be seen from the experiments that the process of cracks formation takes place, which shows that the modified potential is really capable of describing the brittle properties of the medium.

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