Application the particle method in problems of mechanics deformable media

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Abstract. The work implemented method of deformation of ground-based particle method, which is a collection of mineral grains, which are linked to some system of forces on the contact areas between the mineral particles. Two-parameter potential Lennard-Jones and it is modified version were selected for describing the behavior of ground. Some model problems of straining layer of ground in the gravity field was decided. The calculations were performed on a heterogeneous computing cluster, on each of the seven components that were installed on three GPU AMD Radeon HD 7970.

1. Introduction
Currently, most of the computational methods based on sampling the area by finite element and finite difference methods [1–10]. This approach has proven itself in the solution the problems of deformation complex heterogeneous environments of different nature. However, there is extensive class of problems, in which the loading of the medium is accompanied by the destruction of multiple fragments and slippage, intensive mass transfer, including mass mixing effects, etc. Using the mesh approach meets with considerable difficulties in solving such problems. A promising class of numerical methods of solid mechanics, adapted for modelling the destruction is a particle method. It should be noted, that in the modern sense of the term “particle method” is a collective and includes very diverse numerical methods, as belonging to the classical representatives of the discrete approach to mechanics and meshless numerical algorithms for solving equations of continuum mechanics (for example particle method in cells [11], smoothed particles method [12], SPAM [13], etc.). Moreover, in the present some current implementations conventional numerical methods, such as finite dotted element method (particle finite element method [18]) often carry to the particle methods. It should be noted, that the particle method formed by methods well-known method of molecular dynamics is used for studying the response of medium at the atomic level [14]. At the same time, the possibilities of atomic description for modelling the behavior of rigid body in interest from the point of view of engineering applications of spatial and temporal scales are extremely limited. Now, the interatomic interaction potentials for the majority of materials are known cannot be said about the potentials to describe the behavior of deformable continuous media, especially shear. One of the important advantages of the particle method is that we can do a small amount of information about the properties of the material. Complex mechanical processes can be modelling by using simple Lennard-Jones potential.
2. Formulation of the problem

Consider the aggregate from $N$ of material particles interacting with each other in a potential field. Particle motion is described by the definitly equation of motion in this method

$$m\ddot{r}_k = \sum_{n=1}^{N} \Phi(r_{kn})r_{kn} + \sum_{n=1}^{N} \Psi(r_{kn}, v_{kn})r_{kn} + \Phi(r_{kn}) + \Psi(r_{kn}, v_{kn})$$

where $r_k$ and $v_k$ – position vectors and velocity of k-particle,

$m$ – mass of particle, $\Phi(r), \Psi(r, v)$ describe conservative and non-conservative component of the interaction between the nearby particles, $\Phi(r)$ and $\Psi(r, v)$ describe external conservative and non-conservative force field. Conservative component of interaction $\Phi(r)$ we can find, according to the formula:

$$\Phi^{\text{def}}(r) = \frac{1}{r} f(r), \quad f(r) = -\Pi(r),$$

where $f(r)$ – scalar potential force, $\Pi(r)$ – interaction potential. Non-conservative force $\Psi(r, v)$ allows to describe dissipation of energy. We consider the pair potential $\Pi(r)$, interaction force $f(r)$ appropriating to this potential is defined as

$$f(r) = -\Pi(r).$$

The most promising technology to simulate particle method in environments with different rheology and to solve problems, where the set of particles is large enough are heterogeneous computing clusters using graphics accelerators (GPU). One GPU device is equivalent about 50 Xeon CPUs for solving problems such as: calculation P-waves, S-waves propagation [15]. However, this technique has certain limitations on the amount of memory available, since the internal GPU memory devices much smaller than traditional RAM cluster nodes. For calculations on graphic accelerators used a library with open source VexCL, because this library simplifies the development of applications and strives to reduce amount of boilerplate code needed to develop GPU applications [16-18]. The calculations were implemented on a heterogeneous computing cluster. On each of the seven nodes in the cluster set of three GPU AMD Radeon HD 7970.

For comparison the proposed approaches to the solution problems of deformation and destruction of the soil, two different solutions have been implemented algorithm [19-21]. In the first case we selected Lennard-Jones potential, and the power options for interaction which takes the form of

$$D = 4 \times 10^5, \quad a = 0.4r, \quad f(r) = \frac{12D}{r} \left(\frac{a}{r}\right)^3 - \left(\frac{a}{r}\right)^6.$$

In the second case used a “modified” the potential, parameters and the interaction force for which takes the form of

$$D = 10^5, \quad a = 0.4 \times 1.28r, \quad f(r) = \frac{D}{r} \left[12\left(\frac{a}{r}\right)^3 - 36\left(\frac{a}{r}\right)^6 + 14.4\left(\frac{a}{r}\right)^9 + 6\left(\frac{a}{r}\right)^6\right].$$

3. Numerical example

For illustration the possibilities of the proposed “modified” potential (as compared to the Lennard-Jones potential), two model problems have been solve. The first task of the soil layer is initially formed on a perfectly rigid obstacle, the central part of which at some time $t=20$ (it should be noted, that the time is a dummy variable and does not correspond to the real, and the decision itself is a quality) instantly disappears. The layer of soil under its own weight flexes, causing its partial destruction. Figure 1 shows a configuration that acquires the compactor mass during bending and partial destruction, depending on the time for the Lennard-Jones and “modified” potential, respectively.
Figure 1. The configuration of the compactor mass during bending and partial destruction, depending on the time for the Lennard-Jones and “modified” potential.

Figure 2. The distribution of per-frame velocity amplitude in the ground, modeling by “modified” potential and Lennard-Jones potential.

The second problem in the formed layer of the ground to a particle material situated in the middle of the lower border of soil is applied some initial vertical offset, which leads to the occurrence and propagation of waves in the computational domain. Figures 2 show the distribution of per-frame velocity amplitude in the ground, modeling by “modified” potential and Lennard-Jones potential, respectively. It may be noted, that using a “modified” potential can observe not only the P-wave in the ground, but and S-wave, while using Lennard-Jones S-wave is not observed.
4. Conclusion
In our work was carried particle method, which give us opportunity to investigate the interaction of a system of material points that are in a potential field. For describing the motion of the material points was used the system equations of motion. The integration is performed with using the algorithm Verlet. The problem of deformation and partial destruction of the soil mass, located in the gravity field, as well as the problem of wave propagation in a ground massif, caused some local perturbation of the computational domain were solved on the basis of the Lennard-Jones potential and the introduction of a new “modified” potential. Analysis of the results shows that the using the “modified” potential allows to realize the process of brittle disruption in the ground, while the Lennard-Jones potential allows you to reproduce only ductile disruption. In addition, in modeling the behavior of soil with Lennard-Jones potential wave propagation occur on the hydromechanical model (without shear wave), whereas the using of “modified” potential allows you to model tension-compression and shear waves.

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