A concept of Discrete Element Method based on overlapping regions of spherical particles for modelling solid body behaviour

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Abstract

The aim of this paper is to formulate a new concept of Discrete Element Method (DEM) dedicated to solid body mechanics. The new method is to be an answer to the disadvantages of the classic DEM, which are evident in computer simulations of small solid body objects but less important in the case of rock or powder mechanics. The creation of a computer code implementing the new algorithms is an integral part of the research. The paper presents the basic assumptions of the new method but omits implementation details. At the time of writing, the computer program has been in its pre-alpha phase and no results of computer simulations have been available. The proposed version of the method has been named DEM D+.

Keywords: Discrete Element Method, DEM, solid body mechanics, computer modelling

1. Introduction

Considering a solid body as a continuum we assume that it consists of an infinite set of independent closely adjacent elements of infinitesimal volume *dV*, which shapes depend mainly on a chosen coordinate system (Fig. 1a). In the Discrete Element Method (DEM) this assumption is different. The solid body is perceived as an assembly of *N* rigid elements (Fig. 1b) of finite volume V_i $(i=1..N)$. In the latter case, spherical elements are preferred due to simplicity in the management of model geometry. In both cases interactions between elements are introduced that are just execution of physical laws. Next, by the means of mathematical analysis (continuum) or direct computer simulation (discrete model), the behaviour of the solid is obtained as a result of designed geometry and introduced interactions. The common feature of the two methods is that they do not describe the true material, but merely represent its approximation. The purpose of this research is to elaborate a discrete model of a solid body capable of emulate the behaviour of a real solid body under external factors in the way of direct computer simulation. The starting point for the author has been classic DEM method but the new method is based on different assumptions.

The author's goals are: 1) simplification the process of building the model, 2) limiting the number of parameters describing the model, 3) modelling only 3D objects.

2. Foundations of the method

2.1. Mezostructure

In the classic DEM approach the solid body is represented with spherical particles, which are tangential to their neighbours (Fig. 1c). Often limited tolerance of penetration or remoteness is applied. Whereas in the propound model neighbouring spheres overlap and thus have common parts (Fig. 2a). The common parts, called overlaps, are very important components of the new model. The overlaps are bonds, that is the regions where interactions between particles take place. Confronting both models it easy to notice that classical model introduces artificial porosity (Fig. 1c, 1), which does not exist in the new model (Fig. 2a, 1). However the new model is still capable of handling porosity (Fig. 2a, 2). Forming a plane borders of the specimen is a problem in classic DEM (Fig. 1c, 2) but not in DEM D+ (Fig. 2a, 3), where any sphere can be adjusted to a plane easily. The next important problem is creating a model fitting an assumed grading curve or from a photo of a real material. Both operations are easer in the new model because the overlaps means big tolerance in a packing algorithms. In the same way splitting one particle into a set of smaller ones can be handled effortlessly in the new method.

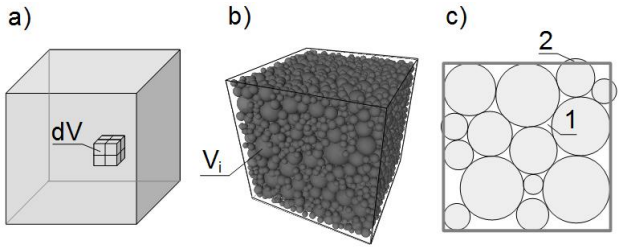

Figure 1: Conceptual models of a solid body: a) continuous medium, b) assembly of rigid spherical elements c) close up on the structure in classic DEM version. Description in the text.

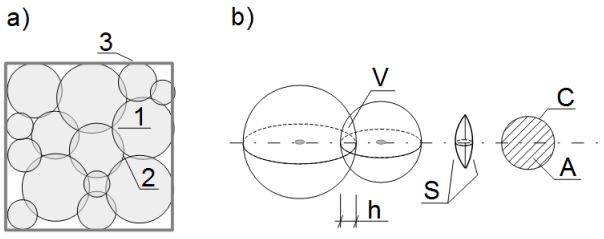

Figure 2: The structure of material in DEM D+ version: a) set of particles, b) close up on the overlap of two spheres. Description in the text.

Figure 2b shows a common part of two spheres in facile penetration. The facile penetration means that none of the spheres includes the centre of the other one. Studying the geometry of the intersection region, we can state that the interaction should be a function of: depth of the penetration *h*, volume of the common part *V*, surface of the common part *S*, area *A* and perimeter *C* of the cross section area of the common part .

2.2. Interactions

A computer model of any material in DEM D+ consist of a mezostructure and interactions between its elements. If the model is correct the whole specimen should emerge macroscopic effects such as: elongation, shortening, Poisson effect, bending, buckling, cracking and the like.

In the case of the continuum model the analysis of deformation reduces to finding change in geometry of every randomly chosen three points A,B,C (Fig. 3a). The point A is the middle point. Then deformation is 1) the change in the distances A↔B and A↔C and 2) the change in the angle B←A→C. Importing the well know technique into the mezostructure we need to find every trio of bonded spherical particles A,B,C (Fig. 3b). In the example the particle A is a middle one. Then the deformation is a cognately: 1) the change in the distances A↔B and A↔C and 2) the change in the angle B←A→C. The changes in distances induce axial forces N between particles (Fig. 3c) while the change in the angle the transverse forces T (Fig. 3d). In both cases the forces equilibrate. They are able to restore the initial configuration but unable to move the body as a whole.

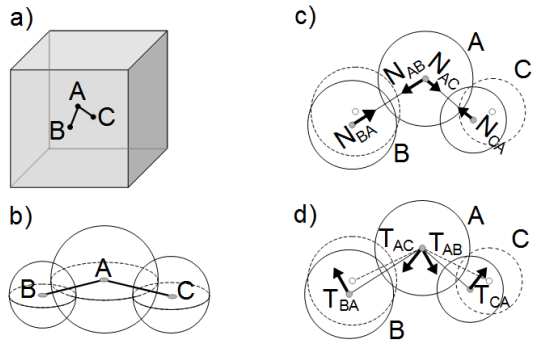

Figure 3: The conception of deformation of a solid body a) continuum, b) mezostructure. The interaction between a trio of particles: c) axial, d) transverse.

The effect of the axial interaction is occurring of two pairs of forces between particles A–B and A–C (Fig. 3c). One pair is two forces laying on the same line connecting centres of the particles, with the same magnitude and opposite orientation. It is assumed that the magnitude of the forces depends of a stiffness parameter E (analogy to Young's modulus), the change in the volume of overlap ΔV and its area A (Fig.2b):

$$N = E \cdot n(\Delta V) \cdot A, \quad (1)$$

where: $n(\Delta V)=\alpha_0+\alpha_1\Delta V+\alpha_2\Delta V^2+...$ is a dimensionless function of the axial interaction.

The effect of the transverse interaction is occurring of two couples of forces (Fig. 3d), which moments cancel out. It is assumed that the magnitude of each moment depends of a stiffness parameter G (analogy to shear modulus), the change of the angle B←A→C denoted as $\Delta\Theta$ and a sum of velocity of both overlaps $\Sigma V=V_{AB}+V_{AC}$:

$$M = T \cdot d = G \cdot t(\Delta\Theta) \cdot \Sigma V, \quad (2)$$

where: $t(\Delta\Theta)=\beta_0+\beta_1\Delta\Theta+\beta_2\Delta\Theta^2+...$ is a dimensionless function of the transversal interaction, d –arm of a force couple.

2.3. Internal friction

The effect of the interaction forces is the change in the configuration of the mezostructure. The change means movement of each particle under external and internal forces. Before the forces balance the particles move. Each particle moves in the presence of its neighbours (Fig.4a). The selected particle indicated by 1 has near neighbours 2 and remote neighbours 3. In every simulation step the movement of particle 1 is small and influences neighbours type 2 only. During movement the particle 1 undergoes resistance R that comes from near neighbours type 2. The resistance is the force that is opposite directed to the velocity of the particle u. The magnitude of the force is proposed to be:

$$R = C \cdot \Sigma V \cdot u, \quad (1)$$

where: C -friction coefficient, ΣV - sum of volume of overlaps of the particle 1 with particles type 2 (here: $\Sigma V=V_1+V_2+..+V_6$).

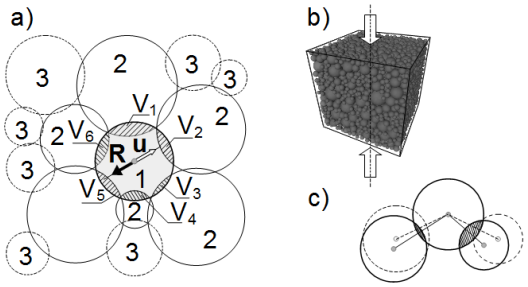

Figure 4: a) Internal friction of a selected particle (shaded). b) External action on the mezostructure. c) Deformation of selected trio of particles. Description in the text.

2.4. Fracture

Any external influence (Fig. 4b) results in the change of the configuration of the mezostrucure, which rearranges in order to withstand the influence i.e. balance the forces acting on each particle. The cost of the rearrangement is storing energy in the structure. The stored energy let resume the initial configuration after the external influence disappears. However, in the case of overstepping the limit of energy stored, the mezostructure brakes and the energy converts into kinetic energy of the particles. The energy is assumed to be stored in the volume of the overlaps but capability of taking on the energy is limited. It should be noted here that the volumes change during the simulation. They can increase in compression and decrease in tension (Fig. 4c).

3. Research program

The effect of the work on the DEM D+ method is a computer program of the same name. Alas at the time of writing the paper the program has been in its the pre-alpha phase and no results of computer simulations have been available. The research program in the first stage is going to be devoted to recognized the behaviour of the designed mezostructure e.g. relation between E and G stiffness parameters and Young's and shear modulus as well as the influence of an initial structure on the behaviour. The initial structure is a spatial distribution of spheres and overlaps. The next stage of the research will be devoted to modelling of engineering problems such as machining cutting, pulling anchor or reinforced concrete destruction.

At the stage of research work the first goals (enumerated 1,2,3 in the Introduction paragraph) have been achieved.

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