New formulation of the deformable discrete element method

Description for the general public

Enormous technological and scientific progress we observe nowadays would be impossible without computer simulations. One of important applications of computer simulations is design of new materials and prediction of materials behaviour during manufacturing processes and at work conditions. Because of new needs and growing expectations there is need of continuous development of numerical methods which provide theoretical framework for computer programs.

One of the methods which is increasingly important in material modelling is the discrete element method (DEM). In this method, a material is represented by a large assembly of particles (discrete elements) interacting with one another by contact forces. Discrete elements can be of arbitrary shape. The most simple, but also the most efficient, is the formulation using cylindrical and spherical particles, and this formulation will be investigated in the present project. In a simple way, the DEM takes into account material microstructure and discontinuities such as fractures either existing in the material or appearing under an applied loading. The DEM is a powerful tool to model material failure. It is a powerful tool for predicting the behaviour of materials such as soils, rocks, concrete, ceramics, powders and other natural and man-made materials.

In the standard DEM formulation, particles are treated as pseudo-rigid elements and the deformation is assumed to be localized at the particle-to-particle contacts. The contact model in this method plays the role of a micromechanical material model. An adequate contact model with appropriate parameters should yield a required macroscopic behaviour.

Appropriate representation of the macroscopic properties in the DEM, however, is still a challenge. There are some limitations in micro–macro relationships due to the assumption of rigidity of discrete elements. In this project, we propose a new formulation of the discrete element method with deformable elements, which should cure some of the drawbacks of the standard DEM. The main idea consists in introducing a global mode of particle deformation in addition to the localized deformation. Incorporation of additional deformation mode should improve representation of deformation mechanisms in materials and extend range of macroscopic properties which can be obtained. Research work in this project encompasses formulation of theoretical models, development and implementation of numerical algorithms, verification theoretical and experimental validation of the new numerical models.

The new formulation will enhance the DEM methodology, which is an important tool for scientific investigation as well as for the solution of practical engineering problems in many branches of industry important for economic and social development such as civil engineering, mining, chemical industry, material science, agriculture, pharmaceutical industry and many others.