REPORT

On the doctoral thesis of Mr Vaclav SMILAUER entitled

Cohesive Particle Model using Discrete Element Method on The Yade Platform

Presented for the degree of Doctor to
Czech Technical University in Prague, Faculty of Civil Engineering
&
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1. Subject of the thesis and description of the problem

Materials like concrete, masonry, ceramic, jointed rocks or any cohesive geo materials are ideal candidates for modelling as discrete systems after material disintegration or cracks initiation have started. The length scale of interest for the mechanical behaviour is then similar to that of the discontinuity spacing. In that, the inability of classical continuum models to reproduce correctly the phenomena associated with discontinuous material behaviour like strain localization at crack initiation directly led to the development of discrete models. In summary, the discrete element method can be classified as a family of related numerical techniques specifically designed to solve problems in applied mechanics that exhibit gross discontinuous material and geometrical behaviour. In many of these discontinuous situations, continuity constraints are either inappropriate or relaxed because of the physics of the problem. Hence, they are either intractable or very difficult to analyze with procedures based upon continuum principles, such as conventional methods like FEM.
Although several commercial DEM codes are on the market, the use of an open source research code was preferred since it provides by far more possibilities for code advancements and implementations. Only the open-source character guarantees the working environment needed for an implementation of several tools necessary to gauge the different ways to treat the difficult tasks outlined above (discrete particle approach, crack appearance and propagation which are taken into account and managed through the contact forces).

Thus the work presented in this thesis, is a most welcome and appropriate contribution towards elucidate a very complicated and pressing problem. The subject is interesting and practical, the obtained results and the given tools may lead to an improvement of the simulation of strain localisation, failure and fragmentation in cohesive geo materials.

2. Description of the thesis and comments

The thesis is divided in two parts. The first part concerns mechanics, this part of the dissertation falls well into the area of my expertise. In chapter 1, the DEM is situated amongst other modelling techniques. Even if the key characteristic points are presented and commented, the reviewer would have appreciated to see in this chapter, the state-of-the-art concerning the concrete models developed in the DEM area, followed by a short paragraph which gives the problem statement and the goal and scope of the work, and the motivations explicated more clearly, justifying some new researches in these domains.

The failure mechanisms of geo materials are characterized by complex failure modes and show a highly anisotropic bias due to their inhomogeneous microstructure. Since localization phenomena like cracks or shear bands occur, the material cannot be treated as continuous in the usual manner. The discontinuous nature of failure in geo materials demands an adequate and reliable numerical simulation model like the discrete element method (DEM). The attraction of DEM simulations of continua is attributable to the fact that the appropriate complexity (localization, pattern formation, etc.) appears as an emergent feature, without the need for it to be programmed explicitly. Based on simple contact laws and a limited number of arbitrary parameters a particularly rich behaviour is obtained. But the reviewer is not sure that the mesh/length dependence of the strain, encountered in continuum models in the context of the FEM, is completely inhibited in the DEM. This problem is typically solved by introduction of localization limiters, i.e. continuum models that include an internal length scale and yield mesh-independent results. This is discussed by Hillerborg et al. or van Mier. Usual enhancements of continuum formulations are based on the introduction of localization limiters. Typical examples are non-local integral-, gradient or viscous models. The internal length scales the width of arising localization zones and yields to mesh insensitive simulation results. What about the DEM and the mesh dependence in the cracked regime?

Then, the DEM is formulated mathematically in chapter 2, in particular, a specific algorithm, aiming the stabilization of the response even with large rotation speeds or time increment approaching stability limit, was built by the author.

Chapter 3 presents the concrete model formulated in the DEM framework and implemented in Yade. The paradox is that the model was derived by applying concepts from continuum mechanics (plasticity, damage, viscosity) onto discrete particles. It was tested on standard material tests, thanks to a calibration procedure proposed by the author. The results are good and the main features are captured like softening in tension in the post-peak regime, confinement effect, strain rate dependence in tension and compression. Generally, a simple one-step algorithm that yields an explicit solution for the corrected stress state is only possible if linear yield surfaces (MohrCoulomb plasticity model for example), linear plastic potentials and linear softening evolution laws are chosen. But in this case the results don't match with the experiment ones. Here an extension of the linear plastic surface by a logarithmic surface in the compression part is proposed to better capture confinement effect and to prevent shear locking under extreme compression. This artefact conducts apparently to a better description of the behaviour even if possible amelioration could be made. Since the failure mechanisms dominated by shear and tension differ substantially in geomaterials, it is advisable in the reviewer point of view to model them separately. This implies the bounding of the elastic domain by two distinct failure surfaces, usually termed two- or in the general case multi-surface plasticity. This of coarse conducts to singularities appearance in the failure surface at the intersection of different failure surface segments and conduct generally to the difficulty to define a unique flow direction. But the solution of this problem is nowadays well known.

The other chapters give an excellent overview of Yade platform. This huge amount of work concerns all the available tools and guidelines for a neophyte user or an expert who wants to built a model of structure or material simulations on Yade's platform. These developments highlight the know-how acquired by the author. This second part of the thesis presents both tools, the methodology, and the way to uses them and gives the reader a clear development of understanding. The exposition is well planned, moving from the simplest cases, progressively towards the most complex ones.

3. Evaluation of the thesis

This research thesis is based on a thorough understanding of the difficult field of DEM applied to cohesive geo materials, more precisely concrete material and it uses analytical, computational and informatics developments in a well-balanced and integrated manner to achieve a large contribution. The match achieved between different analytical techniques and between computational analysis and informatics and architecture's languages, shows great competence in the use of all these research methods.

The thesis undertakes in the difficult field of concrete material failure and presents a large body of both computational and analytical new work. It contains minor shortcomings, but the complete work is of a good intellectual standard.

This thesis is most worthy of the degree of Doctor. I strongly recommend that Mr Vaclav Smilauer be awarded the Ph.D degrees of both University Joseph Fourier University in Grenoble and Czech Technical University in Prague.

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