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Assessment of PhD Thesis of

Piotr Klejment

Institute of Geophysics, Polish Academy of Sciences

Title

The Microscopic Insight into Fracturing of Brittle Materials

with the Discrete Element Method

In his thesis the goal of Mr. Klejment is to use the discrete element method (DEM) to obtain a microscopic understanding of the fracture of heterogeneous materials relevant for geological processes. In nature, geo-materials undergo deformation and fracture due to several loading conditions, notably under compression, shear, and tensile loading. The heterogeneity omnipresent in the composition and disordered microstructure of materials play a decisive role in the nucleation and propagation of cracks, and in the emergence of the ultimate failure of the system. The relation of these microscopic details to the overall material properties such as Young modulus or ultimate fracture strength is still not completely understood.

Research efforts are focused in two main directions: Mr. Klejment studies the fracture of heterogeneous brittle materials in three standard tests of engineering. i.e. uniaxial compression and elongation, furthermore, he performs so-called Brazilian tests. Additionally, he investigates the calving of glaciers focusing on the propagation of waves in ice and in the underlying water.

The topic of the thesis is absolutely timely, and it has an importance for the understanding of the emergence of catastrophic failures in geosystems such as landslides and earthquakes, furthermore, for the monitoring of the time evolution of the ice mass world-wide. Studies on glacier calving is indispensable since the calving of marine terminating glaciers and ice shelves has the major contribution to the rise of the ocean level.

The subject is strongly interdisciplinary, it requires the simultaneous application of mechanics, rheology, fracture mechanics, computational physics, and geophysics.

The main methodological element of the research is the application of the discrete element method. During the past 30 years, also thanks to the rapid development of computer power, DEM has become a very efficient modelling and simulation approach, which has gained widespread applications across disciplines. DEM is based on the physical discretization of materials, where discrete elements represent material units with well-defined physical properties. Prescribing proper inter-particle interactions, DEM can capture various types of materials' behavior. The method has a high flexibility in representing loading and boundary conditions, as well. DEM provides an adequate environment to achieve the goals of the research program of Mr. Klejment, since it provides an efficient way of relating microscopic materials' parameters to macroscopic characteristics through simulated measurements.

In his work, Mr. Klejment used a freely accessible DEM code, called ESyS-Particle, which has proven very successful in the scientific literature. Still implementing the specific materials and loading conditions, and performing computer simulation on supercomputers, is a rather demanding job.

The revised thesis is organized in for main chapters: at the beginning a short introductory chapter gives an overview of the motivations of the work, outlines the main challenges faced, explains the basic theoretical methods and numerical techniques used in the investigations, and highlights the most important results. It is followed by a summary of the basics of fracture mechanics. A brief introduction is given by chapter 2 to the discrete element method complemented by the presentation of the ESyS-Particle program package. The actual work of the candidate is presented in detail separated in two chapters, one devoted to the fracture of heterogeneous brittle materials, and another one to the calving of glaciers. The thesis is closed by an extended summary of the results. I found it very useful that the details of simulations, and technicalities (including details of the usage of a supercomputer) are collected in the appendix.

The literature review of the revised theses was extended, it is based on more than 170 references including several review articles and monographs, and highlighting the most important publications of the field. These references show the comprehensive knowledge of the candidate with the ability to unveil wider relationships of phenomena.

The research is entirely of theoretical nature. The candidate studied the fracture of brittle heterogeneous materials under three different loading conditions with the aim to relate microscopic, particle level parameters of the model to the macroscale physical quantities and overall behavior of the sample. DEM simulations were performed in the framework of ESys-Particle varying several parameters such as the size of the particles of the discretization, the material density, the microscopic Young modulus, and cohesion. Under compression and elongation, the authors concluded that the material density has a minor effect on the elastic behavior. The macroscopic Young modulus is almost entirely determined by the microscopic Young modulus of inter-particle bonding, while the ultimate strength of the sample is controlled by the microscopic cohesion.

The most appealing result is achieved in the case of the Brazilian test where the size of the particles, especially, the lower cutoff of the particle size, is found to have a strong effect on the critical load, the system can withstand. The effect could be cast into a scaling law which may trigger further studies in the scientific community. Additionally, the different regimes of the deformation and fracture process identified based on the displacement and kinetic energies of particles are also interesting novel findings.

In the second part of the research program, Mr. Klejment developed a simplified model of glacier calving, where the break off of ice chunks from the glacier body not supported by soil or water can be studied. This study analyzed the signals recorded by accelerometers focusing on the wave propagation in ice and in water where the ice fragments arrive. Several interesting, and somewhat counter intuitive findings have been obtained numerically. The well-established simulation environment, the careful testing of the simulations, and the data presented in the figures of the revised thesis give strong support for the statements of the author.

The thesis is very well written in English, only a few misspellings or small grammatical problems can be identified. In the revised thesis the candidate managed to further clarify the presentation of the research performed. The motivations, numerical measurements, and main findings are now very clearly formulated, the main points are easily accessible for the reader. The numerical data presented in the figures support the arguments of the candidate.

The high academic standard of the thesis is shown by the fact that the simulations performed on the fracture of brittle materials and the model development and studies on glacier ice calving form a well-designed research program, which led to a couple of interesting findings. The significance of the results is underlined by the fact that they have been presented at several prestigious conferences including Particles and Fatigue conference series. The results were published in 5 papers in peer reviewed journals and proceedings volumes where the candidate is always the first author.

In summary, the thesis in its revised form is a very nice summary of a well thought research program with several interesting outcomes. It fulfills the academic standards and requirements of a PhD, hence, in case of a successful defense, I recommend the PhD degree for Mr. Piotr Klejment.

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