DEM simulation of comminution: Fragmentation and size distribution

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Abstract. ESyS_Particle, the 3-D Discrete Element Model, is used to model the fracture process and the size distribution of rock fragmentation under two different loading conditions: 1) Slow uni-axial compression of a ball aggregate which consists of small bonded particles; 2) Impact of a ball consisting of bonded particles to a stiff wall. We reproduce the realistic fracture patterns, such as meridional cracks under slow loading and secondary cracks under fast loading. A transition from damage to fragmentation as impact velocity increases is observed. The latter one is characterized by generation of fines and a power law distribution of fragment sizes.

Keywords: Discrete Element model, fragmentation, size distribution.
PACS: 45.70

INTRODUCTION

Rock fracture and fragmentation play very importance roles in mining industry. In process of comminution, an important issue is to determine how the input energy is related to fragment size distribution. Laboratory tests are essential to investigate the fragmentation patterns and the energy budget associated to these processes. However, in experiments it is difficult to quantify how the input energy is transformed in dissipation, acoustic waves and surface energy. Numerical models, such as Discrete Element Method, do not have this limitation because it is easy to access to the micromechanical data associated to fracture. With the recent advances of large scale simulations, numerical simulations represent an attractive alternative, as they provide detailed information on breaking of bonds and size distribution of the fragments that are not easily accessible in experiments.

As a first step to understand fragmentation phenomenon, we use our Discrete Element software, ESyS_Particle, to model fracture of a sphere sample under two different loading conditions. We reproduce the realistic fracture patterns and fragment size distribution.

ESYS_PARTICLE

ESyS Particle is a 3-D paralleled Discrete Element Model (DEM) developed in ESSCC, the University of Queensland. It is suitable to model brittle rock fractures and earthquake process [1]. There are several major differences between the ESyS_Particle and the other existing DEMs. First, in the ESyS_Particle, the unit quaternion $q = q_0 + q_1 i + q_2 j + q_3 k$ is used to describe explicitly the orientations of particles. The quaternion represents a one-step rotation around the vector $q_1\hat{i} + q_2\hat{j} + q_3\hat{k}$ with a rotation angle of $2\,\mathbf{arccos}(q_0)$. At each time step the dynamic Euler equations and quaternion equations are integrated such that the orientation of each particle is uniquely known [2, 3].

The second important difference is that a full set of interactions are included. There are three kinds of interactions in ESyS_Particle: bonded interaction, solely normal repulsive interaction and cohesionless frictional interaction [3]. A special emphasis is on the bonded interaction in which all three interactions (normal, shearing forces and bending moment) in 2D and six (normal, shearing forces, bending and twisting moment) in 3D are transmitted between each bonded particle pair [2, 3].

The third one is the way of updating forces and torques caused by the relative movements between two particles. In other existing DEMs, the incremental method is used to update the interactions between particles. Instead of the incremental method, ESyS_Particle uses the Finite Deformation Method, in which the total relative (translational and rotational) displacements are calculated at each time step [5].

Using quaternion algebra, we proved that [3] an arbitrary rotation between two rigid bodies or two coordinate systems cannot be decomposed into three order independent rotations around three orthogonal axes. However it can be decomposed into two rotations, which correspond to the relative twisting and bending between two bodies in our model. The two rotations are sequence-independent. The beauty of this sequence-independent decomposition is that it respects the physical law and it is guaranteed that forces and torques decided by such a two-step rotation are unique. Numerical results show that when dealing with finite rotations of particles, the incremental method is not as stable and accurate as the method used in our model [3]. We also use a different criterion to judge the breakage of bonds [2] and study how the spring stiffnesses should be chosen [4]. Realistic fracture patterns are reproduced using the ESyS_Particle [5]. Figure 1 shows the 3D fracture pattern of a brittle rock-like material under uni-axial compression.

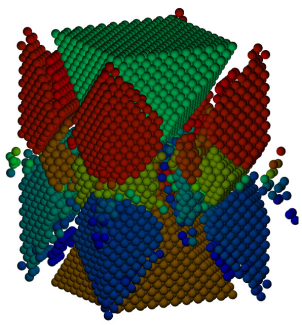

FIGURE 1. Fracture pattern of a 3-D brittle rock-like material under uni-axial compression.

FRACTURE PATTERNS AND SIZE DISTRIBUTION

In ESyS_Particle, the breakage of a bond is an explicit representation of a small fracture event. Under loading some bonds begin to break, while others are still linked. At certain time intervals we output information of the particle pairs which are still bonded. An algorithm is developed to identify which particles belong to a group (fragment). The idea is that if two particles are bonded, they belong to the same fragment. If another particle is bonded to any of the particles in the group, it joins the group. This process repeats until a particle is not bonded to any of the particles in the existing groups, then it starts a new group. If two particles from two different fragments are found to be linked, then the two fragments are combined into one. In this way all particles can be grouped to corresponding groups. By calculating the volume of each fragment, the size distribution can be obtained.

Fragmentation size distribution under slow uni-axial compression

Figure 2 shows fracture patterns of a sphere consisting of 29117 bonded particles under a slow uni-axial compression driven by two rigid walls. The colors represent horizontal displacements, and discontinuities in colors show the formation of fractures. Close to two contact zones with the rigid walls, two circular, flatten areas are observed. Detailed studies show that they are two cone shaped fragile regions, formed mainly by shear fractures. Four meridional cracks are clearly seen, which are caused by tensile fractures. This kind of pattern is also observed in laboratory tests [6].

Figure 3 shows the fragmentation size distribution of Figure 2 at four different loading stages. It plots the number of fragments within each volume size bin. As time increases, the size of the largest fragments decreases and percentages of medium fragments increase, indicating continuing fracture. We do not observe a good power law distribution since there are relatively more large and small pieces. In some literatures the percentage of particles bigger (or smaller) than certain volume is plotted against the volume sizes [7], which can be obtained by integration from Figure 3.

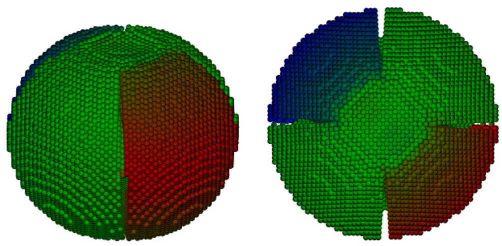

FIGURE 2. Fracture pattern of a sphere under slow loading, side view (left), top view (right). Colors represent displacement, so that discontinuities of the color show the fractures.

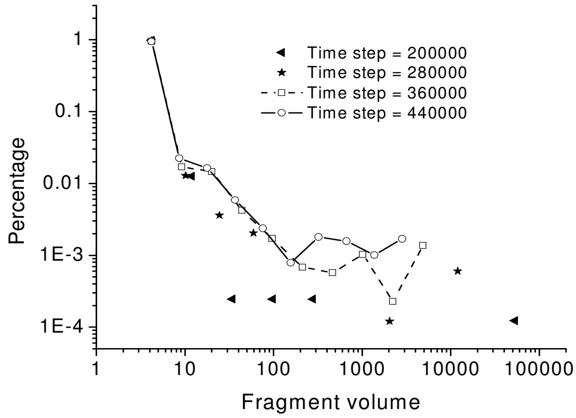

FIGURE 3. Fragment size distribution of Figure 2.

Size distribution under fast loading: impact fracture of a ball to a rigid wall

Figure 4 shows four snapshots of fracture patterns of a ball after impacting a rigid wall at different velocities. When the velocity is small (v = 7.5 units), only slight damage occurs with several meridional cracks, and the ball mainly keeps its integrity. But with increase of velocities, the specimen breaks into more, smaller pieces, and latitudinal secondary cracks develop.

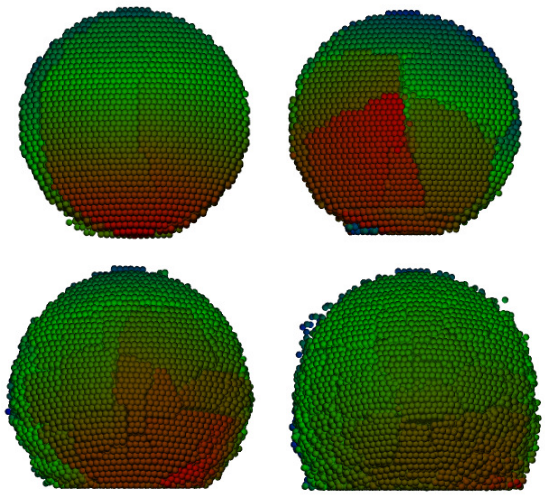

FIGURE 4. Fracture pattern of a sphere under impact, V=7.5 units (top left), 10 (top right), 20 (bottom left), and 30 (bottom right).

The fragmentation size distribution can be found in Figure 5. Good power law distributions are observed for nearly four orders of magnitude in volume. Generally it is observed that higher impacting velocity means more fragments, higher percentage of small pieces, lower percentage of large pieces and reduced sizes of the largest pieces, indicating the important role of input energy.

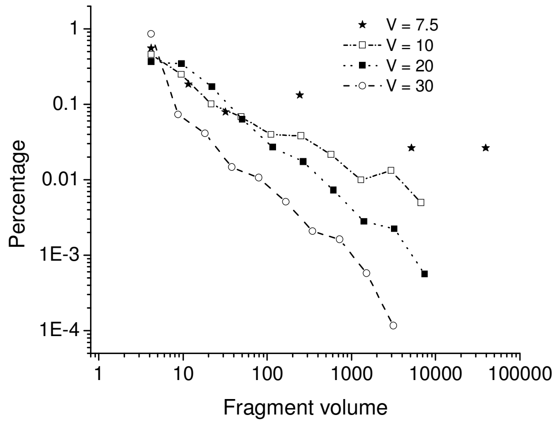

FIGURE 5. Fragment size distribution of Figure 4.

SUMMARY AND DISCUSSIONS

We presented simulation results of brittle fracture of rock-like materials under two types of loading conditions: the fracture of a sphere under slow uni-axial compression and dynamic fracture of a sphere colliding with a rigid wall. The realistic fracture patterns, such as meridional cracks and secondary cracks, are well reproduced.

A numerical algorithm was developed to calculate the size of fragments. We do not obtain power law size distribution in case of slow uni-axial loading, but good power law distributions are observed for nearly four orders of magnitude in volume in case of impact.

The origin of the power laws distributions of size is still not clear. Previous studies based on percolation clusters of broken bonds were successful to explain the power laws, but they failed in the prediction of the exponents [8]. The larger deviations for large fragments were also reported by other studies [6]. Some even suggested that coarse and fine fragments obey two different power law distributions [6]. Based on numerical experiments [7] it is suggested that the coarser fragments result from cracks propagated from the loading/impact zone, whereas the finer fragments result from secondary fragments created perpendicular to the fractured surfaces.

Others questions need to be answered in the future studies: Are the deviations from the power law for large and small fragments caused partly by the size effects, or is it caused by different physical mechanisms? How do the geometrical packing of the sample and initial size distribution of particles effect the calculated fragmentation size distribution? Besides, the studies in this paper are still rudimentary and qualitative. The model is still not an accurate representation of a rock sample yet since some parameters, such as the size, porosity, grain size and macroscopic elasticity etc, are not strictly chosen according to a specific type of rock. This is why in Figure 4 and 5 there is no detailed units for velocities and volumes. Also there are no pre-existed flaws in the rock at this stage. Accurate calibration and large scale simulations are required to investigate these problems in the future.

ACKNOWLEDGMENTS

We thank for the support of the ACcESS and AuScope project. FAM is supported by the Australian Research Council (project number DP0772409) and the University of Queensland Early Carrier Grant.

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