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Investigations on the role of microstructure in brittle failure using discrete element simulations

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It is generally accepted that brittle failure is a process by which pre-existing and newly-initiated microcracks coalesce to form macroscopic fractures that ultimately fragment rock specimens. Crack growth has also been shown to be influenced by the mineral texture and porosity of the rock, in addition to the rate at which loads are applied. Despite a wealth of data supporting these observations, it remains difficult to quantitatively characterise the role of microstructure in brittle failure via field or laboratory studies for various practical reasons. Numerical simulation of brittle failure provides an alternative avenue in this respect although computational limitations have to date, precluded in-depth numerical investigations.

The Discrete Element Method (DEM; Cundall and Strack, 1979) is a popular choice for numerical modelling of brittle failure, as crack formation and coalescence is modelled naturally without need for the complex constitutive laws or re-meshing techniques typically required for continuum-based methods. In the DEM, rock specimens are represented as an assembly of indivisible spherical particles connected to nearest neighbours via brittle-elastic beams which impart forces and moments upon one-another as particles move relative to each other. By applying boundary forces and solving Newton's laws for each particle, elastic deformation and brittle failure may be simulated (Potyondy and Cundall, 2004). Although some calibration of the model parameters governing the properties of particles and beams is required, realistic macroscopic brittle-elastic behaviour may be simulated (Schopfer et al., 2009). The primary limitation of the DEM lies in the computation time required to simulate specimens of sufficiently high resolution using timestep increments on the order of nanoseconds. An implementation of the DEM designed for execution on parallel supercomputers called ESyS-Particle (https://launchpad.net/esys-particle/) has been used for this research. Due to the weak scalability of its DEM engine (Latham et al., 2004; Weatherley et al., 2010), brittle failure simulations involving tens of millions of particles may be executed in reasonable time on cluster supercomputers. This alleviates the computational burden sufficiently to permit control experiments to study the influence of microstructure upon the macroscopic elastic properties and brittle failure mechanisms of rock specimens.

By randomly removing a prescribed fraction of particles prior to simulations, it is demonstrated that porosity plays a key role in shear localisation within specimens undergoing uniaxial compression. Low porosity typically results in significant distributed micro-cracking throughout the specimen prior to development of a broad fragmented shear zone bisecting the specimen. By contrast, a moderate porosity of 10-15% eliminates much of the precursory distributed damage with the localisation of a single narrow shear fracture resulting in failure of the specimen. Investigations on the influence of pre-existing cracks and mineral texture upon the failure characteristics of DEM rock specimens are also underway, the results of which will be presented at the meeting.