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## On the role of boundary conditions in particle-based numerical simulations of brittle failure

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Brittle failure is a complex phenomenon involving nonlinear interactions within brittle media and trans-scale coalescence of cracks. The macroscopic constitutive behaviour of brittle media is a combination of both the intact strength of the constituent minerals and the frictional strength of pre-existing discontinuities within the medium. Simulating brittle failure using continuum-based numerical methods is challenging both from a mathematical standpoint, to define appropriate nonlinear constitutive laws, and a computational standpoint, requiring adaptive re-meshing to properly characterise the propagation of cracks within the numerical domain in many instances.

A popular alternative numerical method is the Discrete Element Method (DEM). The DEM represents a brittle medium as an assembly of spherical particles connected via brittle-elastic springs (called bonds). At each timestep, the net force acting on each particle is computed and Newton's Laws are integrated to update particle positions and velocities. External forces are applied to the assembly via elastic interactions between boundary particles and movable walls. Although conceptually simple, the DEM has proven popular for numerical studies on brittle failure since it does not require complex constitutive laws and expensive re-meshing algorithms to mimic aspects of the phenomenology of brittle failure.

In a series of high-resolution DEM simulations involving uniaxial compressive failure of cylindrical samples, the patterns of broken bonds have been closely examined. Using typical methods to apply stress to the samples, broken bonds are distributed uniformly throughout the sample and only during late stages of failure do wide shear bands develop which cause the sample to fragment. To simulate localised crack coalescence and formation of realistic fracture surfaces, a new type of boundary condition has been developed. Rather than monotonically increasing the stress applied to the sample, the loading rate is reduced as bonds break and the compressive strength of the sample begins to degrade. The extreme sensitivity of brittle failure patterns in DEM simulations to the boundary conditions is a surprising result with broad implications for the application of the DEM to understand brittle failure of heterogeneous media.