Modelling rock grain interactions at the meso-scale to study the micro and macro-physics of rocks: simplicity vs complexity

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Abstract

The particle-based lattice solid model developed to study the physics of rocks and the non-linear dynamics of earthquakes has been refined by incorporating intrinsic friction between particles. The model provides a means to study frictional heat generation, fault zone evolution and localisation phenomena. A modified velocity-Verlat scheme is developed that allows friction to be precisely modelled. This is a difficult computational problem given that a discontinuity must be accurately simulated by the numerical approach (ie. the transition from static to dynamical frictional behaviour). An efficient numerical integration is achieved by using an adaptive adjustment of the time step increment. This approach is compared with another numerical approach developed by P. Cundall which specifies different proprieties at the particle scale while simulating materials with the same macroscopic properties as the lattice solid model. The increase of super-computer performance allows one to: (1) simulate a larger number of particles with simple interactions at the particle scale or, (2) specify more complex interactions at the particle scale such that the correct macroscopic behaviour is simulated. This enables more realistic simulations to be achieved such that phenomena occurring at various scales can be modelled and hence, may lead to an improved understanding of earthquake precursory phenomena and dynamics.

Introduction

The "lattice solid model" (Mora, 1992[1]) consists of a lattice of interacting particles and was motivated by the molecular dynamics method. The model is similar to the Discrete Element Model proposed by Cundall and Strack, 1979[2] but offers a greater precision in the calculation of the frictional forces (cf. Place and Mora, 1999[3]). The model was developed in order to study fracturing (Mora and Place, 1993[4]), wave propagation in complex discontinuous media, faulting (Donzé et al., 1994[5]), the stick-slip instability which is responsible for earthquakes (Mora and Place, 1994[6]), heat generation (Mora and Place, 1998[7]) and localisation phenomena (Place and Mora, 1998[8]).

In order to quantitatively study heat generation and to simulate frictional behaviour (including the transition between static and dynamical behaviour), frictional forces must be "accurately" computed and the discontinuity between static and dynamical behaviour must be modelled. Heat is generated when two surfaces are slipping past one another (ie. the frictional behaviour is dynamic). When the surfaces are locked (ie. the frictional behaviour is static) no heat should be generated. The transition between static and dynamic frictional behaviour is also an important consideration. Due to the time discretisation, only linear processes can be simulated within a finite time step. However, within a time step, discontinuities in the force on a particle may occur and these must be take into account before proceeding to the next time step. Ignoring these discontinuities (that is assuming they occur only at the instant between two time steps) can yield an incorrect frictional behaviour.

The lattice solid model

The particles in the lattice solid model interact with one another in a similar way as particles in short range molecular dynamics. Particles specify the smallest indivisible units of the system and in the following, represent building blocks of rock that are approximately grain size in diameter. This approach enables the non-linear behavior of discontinuous solids such as rocks to be simulated with relative simplicity.

Particles in consolidated regions are arranged in a two dimensional triangular lattice and linked by elastic bonds. Bonds can break if the separation exceeds a given threshold r_{cut}. A bond, acting as a spring, exerts a normal force on the two bonded particles given by

$$\mathbf{F}_{ij} = k(r_0 - r_{ij})\mathbf{e}_{ij} \quad , \tag{1}$$

where k is the spring constant, r_0 is the equilibrium separation, r_{ij} is the separation between particle i and particle j, and $\mathbf{e}_{ij}$ is the unit vector pointing from particle i to j.

A viscosity is introduced in order to damp reflected waves from the edges of the lattice. The viscous forces are proportional to the particle velocities and are given by

$$\mathbf{F}_i^{\nu} = -\nu\dot{\mathbf{x}}_i \quad , \tag{2}$$

where ν is the viscosity coefficient and $\dot{\mathbf{x}}_i$ the velocity of particle i. The viscosity is frequency independent and does not not fundamentally alter the dynamics of the system if carefully chosen (Mora and Place, 1994[6]).

In addition, a frictional force is added to unbonded particles which come into contact. The frictional force opposes the direction of slip and its magnitude is no greater than the dynamical frictional force given by

$$F_{ij}^F = \frac{\mu}{r_0}|\mathbf{F}_{ij}| \quad , \tag{3}$$

where μ is the coefficient of friction and $\mathbf{F}_{ij}$ is the normal force (Eq. (1)) between particle i and j. The dynamical frictional forces and the static frictional forces (e.g. the force required to stop slip between particles) are computed using an approach involving the resolution of a nonlinear system (Place and Mora, 1999[3]).

The numerical integration is based on a modified velocity Verlat scheme which uses a half time-step integration approach (Place and Mora, 1998[3]). This approach

allows the discontinuity in particle frictional behavior to be precisely captured (e.g. transition between static and dynamic frictional states).

The total energy of the system is computed at each time step as the sum of the kinetic energy, the energy lost to the artificial viscosity (which we normally consider as lost energy of the radiated waves), the energy lost due to bond breaking (fracture energy), the work done by frictional forces (heat generated) and the energy added into the system (e.g. to maintain a constant pressure and speed of the driving plates). The total energy is verified to remain constant within an error of 1% after 1,000,000 time steps.

The lattice solid approach seeks the static frictional force such that no slip is allowed when two surfaces are locked by static friction. The approach consists of resolving a nonlinear system to compute the effective frictional forces that must be applied during a time step. Frictional forces are computed such that the transition between static and dynamic behaviour is captured within a time step by introducing intermediate states when particles are bouncing (when the direction of slip reverses but slip does not stop), starting to slip, or stopping.

Particle properties

To enable isotropic fracturing and to obtain more realistic small-scale behaviour, particles are grouped into "grains" of different sizes and shapes. Bonds, linking particles inside a grain, are set to be much stronger than bonds that link particles belonging to different grains (ie. grains are made of material stronger than the overall strength of the material being modelled). Grains can be considered as the smallest indivisible units of the system.

Rotational dynamics is simulated at the grain scale as a consequence of linear momentum conservation of the bonded particles in a grain although it is not modelled at the particle scale. Furthermore, grouping of particles into grains allows isotropic fracturing to be modelled. This is because grains can be made of a variable number of particles, and hence have different sizes and shapes.

Grains of rocks are deformed when subjected to a shear stress. These deformations can be modelled at the particle scale by introducing a "soft" shear constraint at the particle scale (ie. the particle has a shear elasticity). This approach has been developed by Cundall and co-workers, (Cundall & Strack, 1979[2]) and introduces a shear stiffness at the particle scale. The shear stiffness should be chosen such that the elastic properties remain unchanged (ie. such that Poisson's ratio σ of the solid being modelled is $\sigma = 1/3$ as for real rocks). In our model, a "rigid" shear constraint is used. Hence particles are rigid and cannot be deformed when subjected to shear stress. By grouping particles to form grains, deformations can effectively take place when bonds inside a grain are stretched or compressed.

Discussion

Particle interactions are specified such that the correct macroscopic behaviour is simulated. Particles require only a few input parameters (size, normal elasticity and coefficient of friction) and complexity is a consequence of the lattice arrangement. Grains in the model represent grains of rock and interact accordingly where shear

elasticity and moment of inertia are the two principal emergent properties at this scale. However, because the smallest indivisible unit of the system is now composed of a few particles, this approach requires a large number of particles to simulate the same number of grains of rock. Typically, using 128×128 particles and in order to have a sufficient number of grains, grains are composed of only a small number of particles. Another approach would be to specify at the particle scale a shear elasticity and a moment of inertia (as in the D.E.M. developed by P. Cundall). This approach allows the scale of the numerical experiment to be increased but requires a greater number of input parameters and may not correctly simulate some phenomena occurring at the grain scale which now represents the lower limit of the model scale.

In the process of fracturing, grains of rocks can break down eventually until the grain sizes reach a lower limit. This may be micron or smaller sizes where plastic deformation may take place rather than fracturing, but in principle could go down to sizes of a few molecules or even that of individual molecules. Therefore, the interaction between grains will change depending on the scale.

By rubbing two rough surfaces kinetic energy is generated. At a microscopic scale, this kinetic energy is present as lattice vibrations quantised into phonons that obey the diffusion equation (ie. heat). This effect of surface roughness at the microscopic scale is modelled using a friction law. Hence a "discontinuity" is introduced where at the microscopic scale, only heat is generated and at the macroscopic scale, high frequency vibrations generate no heat.

Ultimately, interactions between particles must be specified such that phenomena occurring at various scales can be simulated. This may include friction and plastic deformation that occurs at a microscopic scale up to fractures and interaction of different fault systems that occurs at a macroscopic scale. Increases in super-computer power allow larger model size to be used. This, with the progressive development of the model, will allow phenomena occurring at various scales to be simulated which may lead to an improved understanding of earthquake precursory phenomena and dynamics.

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