Summary of Session 3.2: Particle-based methods (LS, Distinct Element, MD) to simulate fault microphysics

David Place

QUAKES, Department of Earth Sciences, The University of Queensland, Brisbane, Australia (e-mail: place@shake2.earthsciences.uq.edu.au; phone: +61-7-3365-2176; fax: +61-7-3365-7347).

Goals

Particle-based models require a large number of particles and an enormous number of computations. Parallel computers provide the means to perform these calculations. However, because of the large number of particles, special algorithms are necessary to efficiently perform such simulations. The goals of the session "Particle-based methods (LS, Distinct Element, MD) to simulate fault microphysics" were (1) to expose the computational problems that arise from particle-based methods (such as the construction of particles assembly and the localisation of near neighbours interactions) and (2) to provide solutions to these computational problems together with a mechanism to implement them on a parallel computer.

Outcomes

To allow large scale simulations to be performed, a high performance must be obtained when implementing a model. This is achieved by refining the model according to the computer architecture and by developing algorithms that use the full potential of the given parallel super-computer.

Computational requirements

Geophysical particle-based models aim to study dynamic processes at various scales ranging from the microscopic scale (such as nucleation processes) to the macroscopic scale over long time intervals (such as interaction of faults in a fault system for multiple fault ruptures representative of centuries of seismic activity). Hence, the time discretisation (i.e. the time step increment) must be sufficiently small to capture microscopic and/or macroscopic dynamic processes and the simulation must be run for a long enough period of time. Consequently, simulations at geological scale may require a few billion time steps or more. For this reason, large scale simulation of

geophysical processes will require not only millions of particles but also billions of time steps. Currently, super-computers are far from achieving high enough performances for these problems. Hence, models must be improved and new techniques developed in order to enable large scale simulations to be performed.

In the lattice solid model (Place and Mora, 1999[1]) the main techniques that have been developed to enable large scale simulations are the introduction of a half time-step integration scheme, the use of a time-dependent time-step increment and also optimisation and parallelisation of the computer code. Although these refinement allow a gain of a factor of three in the total computational time, only relatively small system can be used. Because synthetic earthquake events are very localised, the use of a space dependent time-step increment would allow the simulation of large systems without excessive computational requirements. Another approach to enable large scale simulation would be to use a more mesoscopic approach where more complex interactions are defined at the particle scale.

Mesoscopic approach

In a model based on the Discrete Element Method and the Lattice Solid Model, Wang and co-workers (Wang et al.,1999[3]) used a mesoscopic approach where elasticity, rotation, torque and friction are modelled at the particle scale. Although it permits more complexity to be obtained than a microscopic approach the calibration of the model is more complex. For both approaches, if the simulations are not scale dependant, the calibrations can be performed using the self similarity of the model, where observations from numerical experiments are used to set the input parameters.

Lattice construction

The initial problem that arises with particle based models is the assemblage of particles when using a random distribution. The algorithm that specifies the initial particle positions and how particles are connected together is time consuming because it involves a huge number (e.g. millions or billions) of particles. The major problems are (1) to construct a close packed lattice and (2) to find an arrangement not far from equilibrium so that the simulation can reach its equilibrium state in a short period of time[1]. Using a regular lattice (for instance a triangular lattice in 2D), a close packed distribution is easily obtained. Hence, one approach is to use "macro-grains" composed of several particles arranged in a regular lattice and to randomly distribute the macro-grains (Sakaguchi and Mühlhaus, 1999[2], Place and Mora, 1999[1]). This approach requires a large number of particles since grains of rock are composed of up to a few hundred particles. But, this allow to model isotropic fracturing since a regular lattice or grid has a strong effect on the behaviour of a simulation: when a 2D triangular lattice rotated by 90 degrees, different fracture process behaviours are observed during numerical uni-axial or bi-axial compression experiments.

[1]Before starting the numerical experiment, the initial state must in a stable equilibrium so that no artificial perturbations are introduced in the simulation.

Pore fluid and solid interactions coupling

In the coupling of pore fluid and solid interactions, the computational requirements for the calculation of fluid pressure effectively limits the model size. The resolution of the grid to compute fluid flow has to be sufficiently small to allow the forces exerted on particles to be computed. The precision required for fluid flow and solid deformation calculations are different, hence, different time steps can be used for fluid flow and solid deformation calculations to minimize the computational needs.

References

[1] Place D. and Mora P., 1999, *Modelling rock grain interactions at a meso-scale to study the micro and macro-physics of rocks: simplicity vs. complexity,* in: this volume, 83-87 (Brisbane, Qld, Australia).

[2] Sakaguchi H. and Mühlhaus H.B., 1999, *Hybrid modelling of coupled pore fluid-solid deformation problems,* in: this volume, 99-101 (Brisbane, Qld, Australia).

[3] Wang Y.C., Yin X.C., Chen X.Z., Peng K.Y. and Song Z.P., 1999, *Simulation of rock failure and earthquake process on meso-scopic scale,* in: this volume, 385–388 (Brisbane, Qld, Australia).