Simulation of the Frictional Stick-slip Instability

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Abstract An « atomic lattice solid model » is capable of simulating the non-linear dynamical processes associated with earthquakes. Based on molecular dynamics, the lattice solid model consists of a set of interacting particles. Interactions are described through radial pairwise effective potential functions which are chosen to enable the dynamic fracturing and frictional behaviour of solids to be studied. Particles are arranged in a two dimensional triangular lattice. Each particle is linked with its nearest neighbours by elastic bonds which can break irreversibly. A numerical experiment involved two elastic-brittle blocks with rough surfaces being dragged past one another at constant rate. During the experiment, the two blocks are initially locked together by inter-meshing asperities along the two rough surfaces (fault). When the stored elastic energy is large enough to unlock some of these asperities, the two blocks begin to slip past one another. The region of slip propagates as a pulse along the fault which dies away once enough stress has been released. Stick-slip frictional behaviour is observed during these experiments. Particle motion normal to the fault occur during slip with trajectories similar to those observed in stick-slip experiments involving foam rubber blocks. Simulations using a relatively small 256x256 system of particles demonstrated that realistic stick-slip behaviour could be modelled. However, this system size is too small to enable realistic rock surface roughness and fault system geometries to be specified. This would require a huge system of particles (e.g. greater than 100,000,000) to be modelled. Regarding the current rate of increase in computer speeds, it is expected that geophysical simulations involving 100,000,000 particles and 1,000,000 time steps will become feasible within two years.

INTRODUCTION

Molecular dynamics as well as wave propagation are two problems where numerical simulations are a large time consumer. The development of massively parallel computer in the early nineties marks the beginning of large scale numerical simulation in such domains. The "atomic lattice solid model" (Mora and Place, 1993) is based on molecular dynamic principles. It enables non-linear processes such as fracturing, friction and stick-slip instability to be modelled. An algorithm originally developed on a Connection Machine 5, was adapted for the Power Challenge computer. Increase in computer speed and the progressive development of the model should ultimately lead to realistic simulation capabilities of tectonics, earthquakes and physics of rocks.

THE ATOMIC LATTICE SOLID MODEL

The lattice solid model consists of a set of interacting particles which are the smallest indivisible units of the system. Particles are arranged in a two dimensional triangular lattice which corresponds to an isotropic elastic medium (Figure 1). In such a crystalline structure fracture behaviour is anisotropic, so a random lattice must be used if isotropy is an important factor.

Each particle is linked with its nearest neighbours by elastic bonds which break irreversibly after a given breaking separation is exceeded.

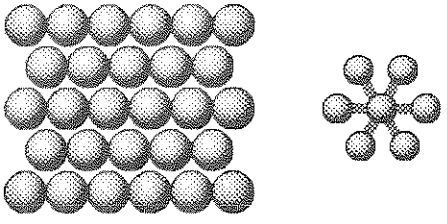

Figure 1: The close-packed 2D lattice

Interactions are described through radial pairwise effective potential functions $V(r)$ where r is the separation between two particles. Bonded particles are attract one another when pulled apart ($r/r_0 \leq 1$) and repel one another when pushed together (dashed line in figure 2). If the breaking separation r_b between two particles is exceeded ($r > r_b$), the potential function is modified to avoid subsequent attraction. The repulsive part of the interaction ($r/r_0 > 1$) remains unchanged (dotted line in figure 2).

This kind of interaction is used in systems which are capable of modelling dynamic fracturing and frictional behaviour (DONZE et al., 1993; LOMDAHL et al., 1993b)

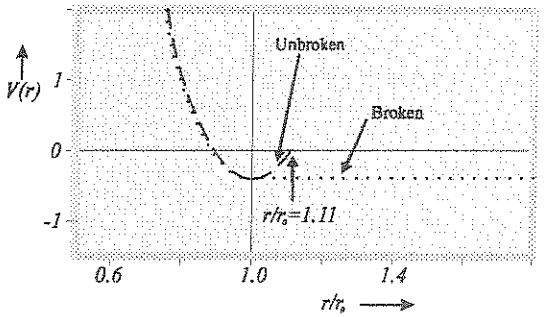

Figure 2: Effective interparticle potentials

This potential function is given by :

$$V(r)=\begin{cases} V_0+\frac{1}{2}k(r-r_0)^2, & r\le R \\ V(R), & r>R \end{cases} \quad (1)$$

where the range is :

$$R=R(t)=\begin{cases} r_b, & r(\tau)\le r_b \quad \text{for all } \tau<t \\ r_0, & \text{otherwise} \end{cases} \quad (2)$$

and :

$$V_0=-\tfrac{1}{2}k(r_b-r_0)^2 \quad (3)$$

The force on a particle n due to a particle m is derived from the potential energy function, and given by :

$$F''_{nm}=\begin{cases} -k(r-r_0)\,e_r, & r\le R \\ 0, & r>R \end{cases} \quad (4)$$

where the distance between the two particles n and m , is :

$$r=r_{nm}=\left|x_n-x_m\right| \quad (5)$$

and the unit vector is :

$$e_r=\frac{x_n-x_m}{r} \quad (6)$$

The total force F' on a particle n is given by :

$$F'_n=\sum_{m\neq n}F''_{nm} \quad (7)$$

A viscosity, ν, is introduced to damp the energy from the closed system. The total force on particle n is now given by :

$$F_n=F'_n-\nu\,\dot{x}_n \quad (8)$$

Particle positions, velocities and accelerations are extrapolated by numerical integration using a finite difference scheme. The acceleration is given by :

$$\ddot{x}_n(t)=F_n(t)/M_n \quad (9)$$

Positions and velocities for the next time step are computed from :

$$x_n(t+\Delta t)=x_n(t)+\Delta t\,\dot{x}_n(t)+\frac{\Delta t^2}{2}\ddot{x}_n(t) \quad (10)$$

and :

$$\dot{x}_n(t+\Delta t)=\dot{x}_n(t)+\Delta t\,\frac{\ddot{x}_n(t)+\ddot{x}_n(t+\Delta t)}{2} \quad (11)$$

The value of time step Δt determines the precision of the numerical integration. The final value of the time step must be inversely proportional to the maximum speed of information propagation.

NUMERICAL EXPERIMENT

A numerical experiment represents two elastic-brittle blocks with rough surfaces (a fault) being dragged past one another at a constant rate (Figure 3). The entire system consists of 256x256 particles. Each block is attached to a rigid driving plate. The fault has a resolution of three particles in y direction. Circular conditions are apply in the x direction.

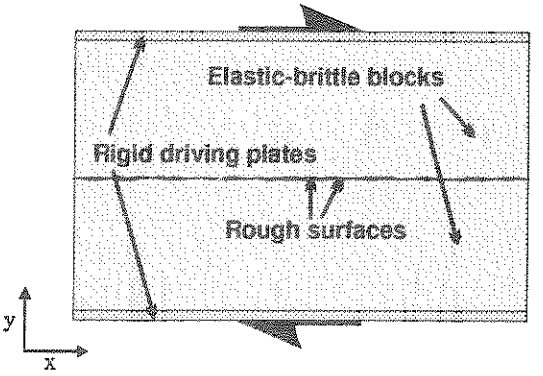

Figure 3: Lattice setup for the numerical experiment.

The system is pre-stressed in y direction to maintain the two blocks in contact (i.e. a stress equivalent to 10 Kbars is maintained on the solid), and the rigid plates are pushed at a constant speed of 0.025% of the compressional wave speed (~1 in this system of units). Time step for the numerical integration is 0.2 unit of time, and computations were made for 100,000 time steps which correspond to 20,000 units of time.

During the experiment, the two blocks are initially locked together by inter-meshing asperities along the two rough surfaces (fault). When the stored elastic energy is large enough to unlock some of these asperities, the two blocks begin to slip past one another. The region of slip propagates as a pulse along the fault which dies away once enough stress has been released. This cycle of energy build-up and slip repeats, simulating stick-slip frictional behaviour. The frictional force of the medium is given by the difference between the average force on the two driving plates (Figure 4).

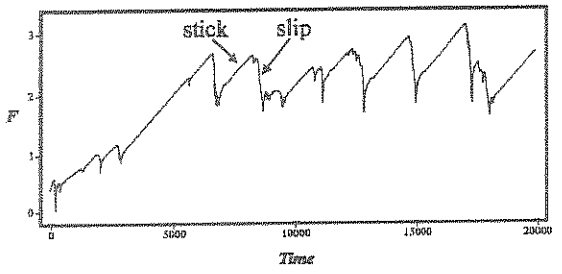

Figure 4: Frictional force

This first part of the simulation (prior the 5000th unit of time) corresponds to the initialisation where the force increases until a critical point. Displacement often occurred as large stick-slip events and also as multiple small stick-slip events (time step ~11000). Foreshocks are also observed (time step ~13000).

Particle motions normal to the fault occur during slip with trajectories similar to those observed in stick-slip experiments involving foam rubber blocks. Slip occurs as a pulse which propagates along the fault. Fault surfaces jump apart during the passage of the slip pulse. Additional work is required to determine whether or not the slip pulses relate to the interface waves proposed by Brune et al. (1993) to explain the heat-flow paradox and if the slip pulses are capable of inducing a significant local reduction of the normal stress.

COMPUTER REQUIREMENTS

Simulations using a relatively small 256x256 system of particles demonstrated that realistic stick-slip behaviour could be modelled. However, this system size is too small to enable realistic rock surface roughness and fault system geometries to be specified. For instance, the 256x256 system allows the fault to have a resolution of three particles, while a fault resolution of 40 particles, necessary to simulate more realistic rock surface roughness, would require a system of 4096x4096 particles.

The initialisation time required to load the system to the critical point increases with the fault roughness and the system size: 20,000 time steps for 256x256 particles and more than 200,000 time steps for 1024x1024 particles. Even if the initialisation time can be reduce by pre-shearing the blocks, the simulation, after the system is loaded, still needs at least 100,000 time steps for a complete simulation with 256x256 particles. Therefore, larger models will require more time steps.

The atomic lattice solid algorithm has been optimised for an SGI Power Challenge (5.7 Gflops super computer composed of 16 nodes and 6 Gb of memory), and is capable of simulating a system of 16 millions of particles. Figure 5 shows the performance for different model sizes (compared to maximum computer speed) using up to eight nodes.

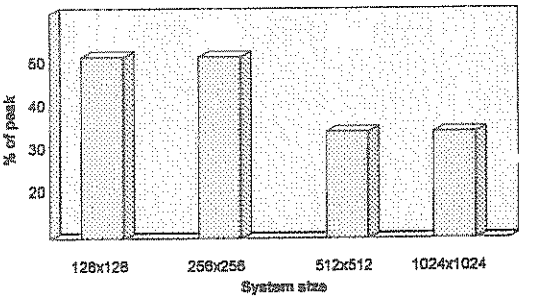

Figure 5: Algorithm performance

Due to the computer architecture the performance decreases when the system size exceeds 100,000 particles. Power Challenge has a global memory shared by all the processors to minimise conflict when several processors access the same data. Each node has an extra memory (cache memory) used like a buffer between the processor and the memory. Best performances are obtained when all data resides in the cache memory, so the computer does not have to swap data between the cache and

the global memory. This is the case, when the simulation uses less than 100,000 particles.

The algorithm speed is proportional to the number of processors used. However a simulation involving 4096x4096 particles will require 5 months of computation and 4 Gb of memory for 1,000,000 time steps. In comparison, a 1024 node Connection Machine 5 (128 Gflops computer) is capable of modelling up to 100 million particles for 10,000 time steps in 4 days, for the case of short range molecular dynamics (Lomdahl et al., 1993).

The present algorithm is capable of simulating relatively large systems (more than 4 million particles), but needs to be refined to enable more realistic rock surface roughnesses. Computational time may be reduced by modifying the algorithm during periods of stick or periods of aseismic slip.

CONCLUSIONS

Frictional behaviour has been simulated by modelling a 2D system of particles without introducing friction between particles. Stick-slip events are observed during an experiment involving two elastic-brittle blocks with rough surfaces being dragged past one another at a constant rate. Particles have normal motion to the fault during a slip phase, suggesting that slip pulses decrease the normal stress, and interface waves may exist that could explain the heat flow paradox.. Simulations involving 4096x4096 particles are now feasible enabling more realistic surface roughnesses. Future work is required to address issues regarding the slip pulses and to enable experiments with larger systems of particles.

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