Summary of Session 1:

Micro-physics underlying earthquake nucleation and frictional behaviour of complex fault zones: observations and simulation

Terry Tullis [(1)], Peter Mora[(2)], Julia Morgan[(3)], and Teruo Yamashita[(4)]

(1) Department of Geological Sciences, Brown Universiity, Providence, RI 02912-1846, USA (e-mail: Terry_Tullis@brown.edu; phone: +1 401 863-3829, fax: +1 401 863-2058). (2) QUAKES, Department of Earth Sciences, The University of Queensland, Brisbane, 40072, Qld, Australia (e-mail: mora@earth.uq.edu.au; phone: +61 7 3365-2128, fax: +61 7 3365-7347). (3) Department of Geology and Geophysics, MS-126, Rice University, 6100 Main Street, Houston, TX, USA (e-mail:morganj@rice.edu; phone: +1 713 348-6330, fax: +1 713 348-5214). (4) Teruo Yamashita, Earthquake Research Instiitute, University of Tokyo, Yayoi 1-1-1, Bunkyo-ku, Tokyo, 113-0032, Japan (e-mail: tyama@eri.u-tokyo.ac.jp; phone: +81-3 5841-5699, fax: +81-3 5841-5693.

Session issues and questions

Modeling of frictional behavior and the nucleation of unstable slip have been simulated using a variety of numerical models such as particle and lattice models. Session 1 aimed to evaluate the status of such studies and the extent to which they have been or can be successful in understanding earthquake physics. Major questions considered were:

- What is the current status of understanding of earthquake nucleation and fault zone behaviour using microscopic simulation methods?
- What are the possibilities, challenges and potential limitations of microscopic simulation approaches?

Questions discussed included: What physics needs to be added to the models to make them more realistic? How do the results of 2D and 3D modeling compare? How do the results of using different methods compare? How do the results compare with other data sets such as laboratory experiments and field observations of fault zones and earthquakes? What new insights are being, or can be, gained of fault zone dynamics and earthquake nucleation using microscopic simulation models? The questions were considered in two subdivisions of session 1:

Session 1-I:	Processes in gouge-filled shear zones, and
Session 1-II:	Nucleation of unstable slip or catastrophic failure.

Summary of activities

Working Group 1 (WG1) had four formal activities at the 2nd ACES workshop: Session 1-I, Session 1-II, and Session 1-P, all on Tuesday, 17 October 2000, at which all in attendance at the ACES meeting were present, and a smaller Working Group Meeting of all interested participants on Wednesday, 18 October, 2000. This was documented by Julia Morgan. During the two oral sessions, 1-I and 1-II, a brief overview of each poster to be presented in Session 1-P was also given.

Papers presented

Processes in gouge-filled shear zones

1. *Simulations of shear in gouge zones*, E. Aharonov and D.W. Sparks
2. *Anatomy of a slip event in an idealized fault gouge*, D.W. Sparks & E. Aharonov
3. *Distinct element simulations of granular shear zones*, micromechanical controls on shear zone strength and stability, J. Morgan
4. *Simulation of the influence of rate and state dependent friction on the macroscopic behaviour of complex fault zones with the Lattice Solid Model*, S. Abe, J. H. Dieterich, P. Mora and D. Place
5. *Three dimensional particle based modelling of frictional behaviour in shear zones*, H. Sakaguchi , A. Makinouchi and H-B Mühlhaus
6. *An optimistic interpretation of friction law from thermal-mechanical coupling in shear deformation of viscoelastic material*, M. Kameyama, T. Hori, P.R. Cummins, S. Hirano, T. Baba, K. Uhira and Y. Kaneda

Nucleation of unstable slip or catastrophic failure

1. *Damage localization, sensitivity of energy release and catastrophe transition*, Y-L. Bai, H-L. Li, F-J. Ke and M-F. Xia
2. *Simulation of Load-Unload Response Ratio using the Lattice Solid Model*, Y-C. Wang, P. Mora, D. Place and X-C. Yin
3. *Microscopic simulation of stress correlation evolution: implication for the Critical Point Hypothesis for earthquakes*, P. Mora and D. Place
4. *Experimental study of seismic short-imminent precursory mechanism by new methods and techniques*, Z-Y. Xu, R-H. Yang, J-M. Zhao, Y-Y. Wang, P-L. Li, B. Wang, S-R. Mei, B-H. Xiong, Z-R. Wang, X-X. Lu, L-Y. Zhong, Y-G. Zhang and C-L. She
5. *Aftershock occurrence due to fluid migration in a fault zone*, T. Yamashita

Overview of papers and discussions

Many interesting papers were presented and much lively discussion occurred during sessions 1-I, 1-II and 1-P. Following is brief overview of some of the points of the presentations and discussions.

One of the points raised during the discussion of several of these papers was the apparently important role played by reduction of particle size in the deformation of real granular aggregates at the conditions where earthquakes occur. To what extent simulation of extensive grain breakage can be achieved in the models, and how much difference it might make on the results, are important questions to focus on. These questions also relate to the influence of particle shapes in the models. How do these compare with those in laboratory experiments and in natural fault zones, and how might particle shapes affect behavior such as the extent of particle rolling versus sliding and breaking?

One category of papers in Session 1 involved various implementations of models that simulate assemblages of discrete particles. The different authors generally use different force laws for particle-particle interactions (friction, bond-breaking etc), numerical approach, constraints on rotation of the grains, and so on. In addition, different models may have different capabilities such as to simulate fluid processes or thermal effects, and these are generally simulated using different approximations and assumptions. There is general agreement that the extent to which the different assumptions affect the results needs to be better understood. A second category of papers did not involve particle-based modeling and ranged from theoretical to laboratory studies. The first group of papers summarized below lie in this particle-based model category.

Particle-based simulation papers

A pair of papers were given by E. Aharonov and D.W. Sparks. They used a molecular-dynamics based discrete element model to study the behavior of granular materials. One of their principal observations is that they observe two modes of deformation that they characterise as “solid-like” and “fluidised”. The former is characterised by switches between distributed shear and localised internal or boundary shear bands occurring at random times and at random depths within the layer, whereas the latter is characterised by persistent localised shear along the shearing boundary layer. Interestingly, strength of the aggregate for the two modes was not significantly different, although the fluidised mode resulted in slightly higher apparent friction. The fluidised mode is favored by increasing slip velocity, increasing size of the box, and decreasing normal stress. In terms of micromechanics of grain-to-grain contacts, the fluidised and solid-like states differ significantly. During stick slip events, the micro-mechanical characterisation of the material seems to transfer from the solid-like mode to the fluidised mode. Ways in which the slip velocity is able to influence the behavior in this model are time dependence of forces (ie. the normal velocity dependant damping term used here) or inertial contributions such as those implicit in dynamical mechanisms such as acoustic fluidisation (Melosh) or bouncing (Mora & Place), and those that may affect time dependence processes of grain rearrangements. Thus, switching between the two modes may involve the damping term, changes in the relative contributions of surface and normal forces, or dynamics of particle rearrangements. Study of models using different amounts of damping and particles of different mass combined with movies to study the detailed dynamics and evolution of grain arrangements could help to distinguish between these possibilities. Mora mentioned mode-switching behavior in the earlier lattice-solid simulations which Ahranov noted to be consistent with what Ahranov and Sparks call “solid-like" deformation”. In the lattice solid work, grains in a gouge layer rearranged themselves (self-organized) after a long time at high normal stress from a mode of distributed slip where grain sliding was favoured to one where slip occurs in a narrow and weak boundary shear where grain rolling was favored.

Shear in the boundary layer involved more rolling and less sliding – and consequently resulted in much less heat and lower apparent friction thereby potentially explaining the heat-flow paradox. This significant decrease in apparent friction was not seen in the Ahranov and Sparks experiments. This is an important difference that should be systematically explored to develop an understanding of its origin. One possibility could be grain shapes as Mora and Place used grains of various shapes with a regular and high surface roughness, whereas Sparks and Ahranov use smooth round particles. Other possibilities are differences in experimental conditions and setup such as normal stress, length of simulation, gouge layer makeup etc., or differences in numerical implementations of friction (ie. Mora and Place solve a system to stop slip between surface particles of grains whereas the Distinct Element Method introduces a shear rigidity of particles and effectively allows surfaces of particles to stretch until static friction is overcome). Discussions on the possibility for slip to occur on high stress contacts as well as primarily low stress contacts ensued.

A paper by Abe et al. introduced rate-and-state dependent friction on individual contacts in the lattice solid model with the goal of enabling studies of how this laboratory derived microphysics at grain contacts would affect the bulk response of a gouge layer. This seems to be a very promising area. However, the work done so far shows that the behavior can be complex and much more work is required to obtain more statistically significant results. Preliminary numerical experiments were presented involving shearing elastic samples containing a fault defined as either bare surfaces in contact or rough surfaces separated by a gouge layer. Experiments similar to laboratory slide-hold-slide experiments were conducted to study the evolution in effective apparent friction after a holding event. Bare surface experiments yielded results consistent with those expected for the rate-and-state friction parameters for grain contacts and validated the numerical implementation. Gouge layer experiments showed that surface roughness strongly affects the effective fault zone behavior with a slower evolution (i.e. larger D_c) being observed for rougher surfaces. This result is consistent with laboratory observations.

A summary of results using the distinct element method with different distributions of particle sizes in a shear zone was presented by J. Morgan. As seen in nature and laboratory experiments, two sets of Riedel shear zones form. In the models, these zones show an opposite sense of rotation of the grains comprising them in the expected sense. Changes in the value of friction between grains in these models had relatively little effect on the macroscopic friction coefficient of the aggregate but altered the amount of particle rolling observed. Considerable rolling occurs in the simulations, and a key result is that the arrangement of rolling particles depends strongly on the particle size distribution (PSD) of the assemblage. Morgan showed that an increase in the relative abundance of small particles in the system led to self-organization of rolling particles that minimized macroscopic friction. This observation supports the hypothesis that cataclasis in real fault zones leads to an optimal PSD for shearing materials. One interesting unanswered question is how much rolling occurs among grains in real gouge materials? The simulations with considerable rolling tend to have much lower macroscopic friction than do the laboratory samples. Does this mean that little rolling occurs in the laboratory samples, perhaps because the grains are more angular? Or is it that rolling is important in the lab samples too, but for some reason results in higher observed macroscopic friction? Or does rolling occur for some real faults and explain the heat flow paradox but not in the laboratory, and if so, what is the reason? Is it because special gouge geometry is needed and could develop only through a very long self-organization process as proposed by Mora and Place, or is there another reason? Extensive discussions ensued and results were compared to lattice solid simulations by Mora and Place in which self-organization had also resulted in low friction. They noted the lack of sensitivity of macroscopic friction in lattice solid simulations arguing that a "self-regulation" mechanism controlled the balance between rolling, sliding and grain breakdown such that a nearly constant effective friction is normally maintained. The normal lattice solid effective friction of around 0.6 was much higher than 0.2–0.3 values obtained in Morgan's DEM results. However, in special cases, the effective friction in DEM and lattice solid simulations are comparable. Namely, friction values of 0.6 were shown by Morgan for stick-slip experiments conducted using compliant shear zone boundaries and low friction values of around 0.2–0.3 are obtained in lattice solid simulations for special self-organizing gouge configurations or when round lattice solid particles are modeled rather than rough and angular unbreakable grains. Discussion ensued about limitations in the present DEM and lattice solid implementations leading to agreement of the importance of modeling grain breakage and a wider range of particle sizes and grain shapes.

Impressive three-dimensional simulations of a triaxial compression experiment were presented by H. Sakaguchi et al. using a discrete element method. A very cogent philosophical review was presented on the need and elegance of particle-based models for simulating rock fracture and frictional behaviour of shear zones. This was the only 3D modeling presented in this session although other particle codes – the DEM and lattice solid model codes – also have 3D capabilities. It will be very interesting to compare the results of such 3D models for simple shear geometry with the results of 2D simple shear models being studied by other authors in this session.

Uses of particle-based models were also presented for purposes other than study of shear zone dynamics and evolution. In one instance, Wang et al. used the lattice solid model to study the Load-Unload Response ratio (LURR) approach for earthquake prediction. These simulations involved adding a sinusoidal stress fluctuation on constant strain-rate or stress-rate compression experiment of an intact sample approaching failure. For many participants at the meeting, this was the first introduction to the concept of LURR and its possible utility for predicting earthquakes. LURR arose again in session 6 when LURR values were calculated using earthquake data from China and Australia to study the relation between Accelerating Moment Release and LURR critical regions. The idea underlying the LURR approach is that near the failure stress of a rock or the crust, the behavior is non-linear and differs depending on whether small stress excursions, such as those due to earth tides, add to or subtract from the overall load. The LURR response, measured as seismic energy or Benioff strain release during loading compared to unloading therefore provides a possible measure for proximity to catastrophic failure. The simulations suggested that the nonlinear behavior in models can be somewhat variable since high LURR preceded catastrophic failure significantly in a strain-controlled experiment whereas in a stress-controlled experiment, high LURR values appeared to detect the onset of failure. These results suggest LURR may provide a good predictor of the unstable regime preceding failure in stress driven systems. Further simulation studies are a promising approach to investigate the physical mechanisms underlying the LURR earthquake prediction concept.

On a related theme, the lattice solid model was used by P. Mora and D. Place to evaluate whether the lead-up to large earthquakes is similar to the approach to a critical point in which long-range stress correlations increase as failure approaches. Such behavior would make it more likely that intermediate-term earthquake prediction could be possible because the crust would not always be at the critical point, but would approach it before large earthquakes and retreat from it after large earthquakes. Two kinds of simulations were studied. One involved a shear zone consisting of a granular layer where ruptures may occur on any internal surface, and the second involved an intact sample being compressed resulting in development of a multiple fracture system. An evolution in the correlation function consistent with the Critical Point Hypothesis for earthquakes is observed in the first case. In the second, a similar evolution is observed only after multiple fractures had developed. The observation in the model of an approach and retreat from criticality through the evolution in the stress correlation function offers encouragement for intermediate-term earthquake prediction. The results suggest a well-developed interacting fault system may be a requirement for Critical-Point-like system dynamics in which intermediate-term forecasting is achievable.

Four other papers were presented in the sessions of WG1 that did not involve using particle based modeling. The first, authored by Y. L. Bai et al., involved modeling of a 2D network in which damage localization lead to a catastrophe transition. This localization can also lead to an increased sensitivity of energy released by small events to changes in stress. Thus the non-linearity of response embodied in this critical sensitivity is similar to the non-linearity involved in the LURR mentioned above. The two features prior to a catastrophic transition of damage localization and critical sensitivity both related to a cascade of damage coalescence. These features were suggested as two crosschecking precursors of large earthquakes.

Another non-particle model was that by Kameyama et al., a one dimensional model of shearing of a material for which the flow law is a power law with thermal activation, such as is found in laboratory experiments studying ductile flow. The spatial evolution of stress and temperature were studied as a function of time using a finite difference approach. Unstable slip occurred in this model from thermo-mechanical coupling at higher boundary-condition velocities. Higher velocities were required for the instability with increasing ambient temperature, so the model predicts a transition to stable slip with increasing temperate at depth in seismogenic zones.

An experimental study of short-term signals preceding failure of plexiglass was conducted by Xu et al. They employed holographic interfereometry and seismometers with response up to 20KHz and found nonlinear effects as the samples approached failure.

Aftershock migration was modeled by T. Yamashita who investigated the role that fluid diffusion can play. The model involved migration of fluid away from a high-pressure source at the hypocenter of the main shock, the rupture of which is assumed to have caused the main shock. Although other models can produce similar results, this model offers one way to explain spatial migration of aftershocks as well as Omori's law.

Working Group meeting and proposed future activities

Introduction

Working Group 1 met over dinner on Wednesday 10/18; eight people attended the session: Terry Tullis, Peter Mora, Jim Dieterich, Dave Sparks, Einat Aharanov, Julia Morgan, David Place, and Steffen Abe. This group included most of the people working on discrete element or particle dynamics (PD) simulations of shearing fault gouge; absent was Hide Sakaguchi from CSIRO, who needed to depart prior to the WG meeting. The presence of two experimentalists, Tullis and Dieterich, ensured that the discussion addressed physical observations as well as numerical concerns. Several other members of WG1 were not present at this gathering, so their input could not be taken into account and their concerns may not be adequately covered here.

Objectives

- Correctly simulate and understand the micro-mechanics controlling fault strength, fault stability, deformation behavior, nucleation and failure, in particular in the presence of fault gouge.
- Develop general constitutive relationships (maps) of fault behavior under a broad range of conditions.
- Extrapolate such relationships to geologic conditions that cannot be adequately examined or simulated in the laboratory.
- Use the models to probe system behaviours and the onset to catastrophic failure.

Issues Discussed

- Establishment of reference library of initial systems.
- Calibration of particle dynamics techniques.
- Validation of simulations by comparisons with lab experiments and field observations.
- Comparison of 2D and 3D simulations.
- Coupled particle dynamics and fluid flow simulations.
- Coupling micro- to macro-scale simulations.
- Meeting of WG1 in August 2001.

Summary of Discussions

Establishment of reference library of initial systems

By some methods, the initialization of particle configurations for numerical simulations of granular systems is a time and CPU consuming process. Several methods are used by the groups involved in PD simulations, including (a) systematic placement of particles of given sizes, generating an effectively “crystallized” assemblage, (b) random placement of particles of a given particle size distribution (PSD) with progressive infilling of pore spaces to generate an in-situ assemblage with a specified porosity, and (c) random placement of particles of a given particle size distribution (PSD) in an oversized domain followed by consolidation to a specified mean stress.

It was proposed and agreed to create a library of initialized particle configurations, contributed by the various PD modeling groups, that could be used and reused by all groups. The advantages of this include standardization of initial conditions for comparison of results of different modeling methods, as well as timesavings in setting up each experiment. Given the significant differences in the ways numerical experiments are set-up and carried out by the several groups currently, defining and developing such standard initial particle configurations will take some time. A committee of representatives of each modeling group was developed to oversee this effort; members include David Place, Julia Morgan, Dave Sparks and Hide Sakaguchi.

Calibration of particle dynamics techniques

A second concern, raised especially by non-modeling representatives at the working group meeting, is the need to “calibrate”, or compare results of, PD techniques being used by the several groups. In particular, at least two different standards are currently in use by the representatives at this meeting: the Lattice Solid Method (LSM) developed by Peter Mora and David Place, and Distinct Element Method (DEM) encoded originally as TRUBAL by Pater Cundall and Otto Strack. The latter code and its derivatives (PFC-2D, 3D) are being used widely within the geologic, engineering, and rock mechanics communities, so an extensive literature comparing numerical and laboratory experiments exists.

The conceptual idea is that of “benchmarking” the PD simulations, comparing simulation results to analytical descriptions as is commonly done to validate FEM and other continuum simulation techniques. Unfortunately, this concept does not apply directly to simulations of granular materials, because few exact analytical descriptions are available. Nonetheless, it is possible to make comparisons among simulations carried out on similar (or identical) assemblages with similar (or identical) boundary conditions – “blind tests”. It was decided that several simple tests would be defined to compare the output of the various PD methods. These are discussed below.

However, in discussion it was recognized that major differences exist in how PD is implemented and granular shear experiments carried out by the various groups; this will make direct comparisons difficult at this time. Major differences include: contact laws used to determine inter-particle forces, presence or absence of rotational dynamics of particles, damping of particle velocities to simulate inelastic processes at particle contacts, methods for generating initial particle configuration (see above), types of shear zone walls, boundary conditions applied to the shearing system, numerical approach to implement frictional interactions. In an effort to facilitate code standardization, or at least the exchange of ideas about PD implementation and algorithm development, Morgan agreed to share with others the TRUBAL code that has been available to the public for many years. Similarly, QUAKES is making available the virtual environment software (LSMearth) for the lattice solid model of Mora and Place for collaborative work under ACES.

Validation of simulations by comparison with lab experiments and field observations

A related issue is that of “validating” the PD methodologies by comparing numerical experiments to laboratory experiments and field observations. Such comparisons are critical before we attempt to apply our numerical results to the interpretation of fault deformation processes. It was noted that this task may prove difficult, not only because of differences in how PD is implemented in various codes, but because quite often data and interpretations of both laboratory experiments and faults in the field are contradictory. For this reason, it is particularly important that we focus at first on simple systems for which most parameters are reasonably constrained; this effort must be carried out cooperatively with experimentalists and field geologists.

Several types of reference experiments were discussed by the group: (a) Two particle collisions define a simple binary system that has been explored experimentally and described analytically; a simple numerical test can be carried out to verify numerical implementations of contact laws, force determination, and particle rotations. (b) Standard geotechnical tests provide simple problems for which there is a wealth of laboratory data (and some empirical constitutive relationships) with which to compare results - e.g., uniaxial consolidation, load-unload tests, triaxial deformation. (c) Shear tests define the heart of the matter for WG1, and comparisons can be made of experiments carried out under various loading conditions, interparticle friction relationships, etc. It will be important to be able to reproduce documented shear strength, sliding behavior, and observed deformational fabrics to ensure that the simulations are capturing the process. (d) Fluidization experiments, as described by Aharanov and Sparks in this volume, offer the possibility of relating granular simulation results to a theoretical description; do the different numerical techniques yield the same mechanical conditions for the solid to fluid transition?

Tullis offered to organize a session at the WG1 meeting in August 2001 where all interested parties can show and view petrographic thin sections of deformed samples. He will try to arrange to have a high-quality petrographic microscope on hand with a good computer-interfaced digital camera system so several people can view the samples simultaneously and so digital images can be produced and given to any interested participants. His lab has produced a large number of thin sections of samples from friction experiments with displacements varying from a few mm to over a meter. Both gouge produced by sliding initially bare surfaces, and simulated gouge that has been sheared are available in the collection, and a considerable variety of rock types are represented. Hopefully others with samples from both experimental and natural faults will attend and bring their samples. The great variety of features in the deformed samples provide a useful comparison with what can now be done with PD modeling and provide a basis for discussing what are the important features to try to include in the models.

The committee defined above will attempt to define standard tests that can be used to “tune” and validate simulations, in cooperation with experimentalists present at the meeting (Tullis and Dieterich) and other interested parties. Ideally, we can have comparisons in hand by the next WG1 meeting in August 2001 (see below). Julia Morgan agreed to oversee this effort.

Comparison of 2D and 3D simulations

Most PD simulations carried out to explore fault processes and gouge deformation have been conducted in 2D, even though real faults are 3D features. 2D approximations allow for efficient computation, and yield important insights into granular processes, but they may fail in reproduce granular behaviors that are strongly influenced by out-of-plane interactions. For example, particles in 3D systems will have contacts out of the plane of transport that can increase the strength of the assemblage and reduce tendency for interparticle rolling. Direct comparison of numerical experimental results with lab results is really best done on 3D rather than 2D assemblages. This issue was addressed only briefly; all of the codes are able to carry out 3D simulations, but due to the CPU time and memory required, this has not been done. No clear agreement was made, but it is reasonable to expect that such simulations will be under way by August 2001, and can be commence being compared with comparable 2D assemblages.

Coupled particle dynamics and fluid flow simulations

Pore fluids and fluid pressure gradients are known to influence rock and sediment strength and deformation. Coupling fluid flow and particle dynamics in simulations of fault zones is a very important avenue for future research. Several methods exist by which to do this; for example, Hide Sakaguchi has developed a method that maps changes in pore spaces resulting in pore pressure changes for triads of particles in 2D, allowing fluid pressures to propagate through an assemblage. Abe et al. model fluid flow directly in a lattice or on a separate finite-difference grid interpolating pressures onto the lattice (Abe et al, 2000). Alternative approaches average over more particles to generate a pore pressure field over the assemblage. Again, no consensus was reached as to how or when to include pore fluid pressures in simulations of shearing granular assemblages, but it seems to be an area of on-going research. A difficulty that was noted is in how to calculate dynamically evolving permeability and porosity.

Coupling micro to macro-scale simulations

This topic was addressed during the workshop meeting by several papers in the special session for WG5 – Computational environment and algorithms – on collaborative work between Australia and Japan (eg. Hazama and Place; Iizuka, Place and Hazama). This is an area of research and development that is commencing and it is hoped that initial results will be ready at the next major ACES workshop in 2002.

Meeting of WG1 in August 2001

It was decided that WG1 would meet in August 2001 in Ojai, California, at which time we will review our progress and determine future directions.