SCEC 2013 Progress Report:
Compactivity, comminution, heating and disorder – the physics of granular fault gouge

PI: Professor Jean M. Carlson
Department of Physics
University of California, Santa Barbara

Overview and Accomplishments

In this reporting period we continued our work investigating the physics of plastic deformation and strain localization and the corresponding implications for dynamic earthquake problems. We are extending Shear Transformation Zone (STZ) theory to include new features, previously omitted in the model, and have begun a series of direct comparisons to laboratory experiments involving frictional weakening, shear banding, and auto-acoustic compaction. These new features are expected to be important to earthquake physics at multiple scales. Our work addresses several SCEC priority science objectives in Fault and Rupture Mechanics (3c,3e and 4b) by developing physical constitutive laws for the fault zone, and evaluating their impact on rupture dynamics, faulting, and energy balance.

We accomplished the following:

- We combined the STZ theory with fracture mechanics to describe grain fragmentation in shear flow. We have shown that the resulting dynamics for grain size reduction shares common qualitative features with those seen in several simulations – namely, that grain splitting dominates at small shear strains and grain abrasion dominates at large slip displacements. We have also found a feedback between strain localization and grain fragmentation which explains the formation of a thin gouge layer with particles with characteristic size several orders of magnitude smaller than those outside the shear band.
- We generalized the STZ theory to include temperature dependence of material properties such as the yield stress to capture additional causes of weakening and localization. We have applied our results to fit high-speed frictional experiments and make predictions for steady and transient frictional response of sheared gouge layers.
- We have developed a preliminary thermodynamic model that explicitly takes into account additional dissipative mechanisms and system-specific features such as inter-particle friction, vibration generated by acoustic waves, and shape effects, which are found in experiments to have important implications on the dynamics of faulting and rupture.

This work builds upon our accomplishments on previous SCEC projects which resulted in a reformulation of the STZ theory for hard-core materials of which granular fault gouge is a prime example [Lieou and Langer, 2012], and focused on small scale physics of strain localization [Manning et al, 2009; Daub and Carlson, 2009], and the impact of strain localization on fault scale dynamic ruptures (Daub et al, 2008; Daub and Carlson, 2010) and energy partitioning [Hermundstad et al, 2010].

Funds from the project were used to support the training and education of graduate student Charles Lieou at UCSB, who is expected to complete his PhD June, 2015. We also continue our collaboration with Professor Ahmed Elbanna, who has recently begun as an Assistant Professor at University if Illinois in Champaign-Urbanna.

Comparisons with Discrete Element Models:

We have been able to show quantitative agreement between STZ theory and discrete element simulations results (Figure 1), thereby validating our theoretical framework.

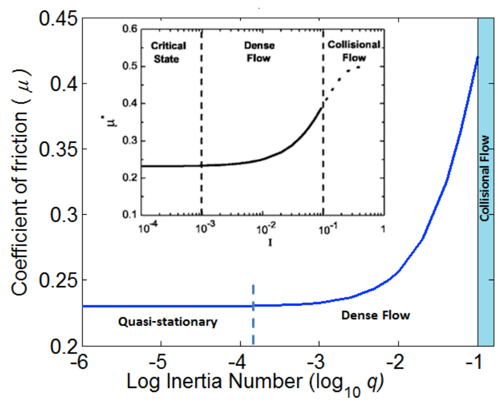

Figure 1: Predictions of STZ theory for the rheology of a sheared granular system. Inset shows results from molecular dynamic simulations [da Cruz et al., 2005, reprinted with permission]. The inertial number is represented by the symbol I in the inset, and q in the main figure.

Grain fragmentation:

In our most recent publication that seeks to account for grain fragmentation in sheared fault gouge [Lieou, Elbanna and Carlson, 2014], we combined the shear-transformation-zone (STZ) theory of amorphous plasticity [Lieou and Langer, 2012], adapted to hard-core materials such as gouge particles [Edwards and Oakeshott 1989a, 1989b; Mehta and Edwards, 1090; Edwards, 1990], with basic fracture mechanics.

As before, the compactivity, the measure of configurational disorder in a granular packing, governs the density of STZ's – flow defects where irreversible granular rearrangements take place and account for macroscopic shear deformation. To account for grain fragmentation, however, the grain size becomes a dynamical variable. The rate of grain size reduction is posited to be proportional to the shear rate – which measure the number of interaction events between grains – and inversely proportional to the surface energy per unit area. In addition, it is constrained by a threshold pressure, determined based on the assumption that the characteristic flaw size on a grain is proportional to its size, and that this determines the threshold pressure below which grain fragmentation becomes rare, as seen in several experiments and simulations [Mair and Abe, 2011; Mair and Marone, 2012; Mair, Frye and Marone, 2002].

Our results indicate that grain size reduction is most rapid upon the onset of irreversible plastic deformation, and slow down significantly afterwards (Figure 2a); this feature corroborates with the results of the Mair and Abe simulations [2011] which show that grain splitting dominates at the early stages, while grain abrasion becomes prominent at large shear strains. Under generic assumptions on the rate-strengthening behavior of the material itself, grain fragmentation is shown to provide significant weakening at large shear rates (Figure 2b), even though it accounts for only a small fraction of energy dissipation. More importantly, we found that a small perturbation in the compactivity, or configurational disorder, profile across the material results in the formation of a shear band, where particles experience the most severe comminution (Figures 2c and d). This provides an explanation for the formation of a thin layer of gouge particles.

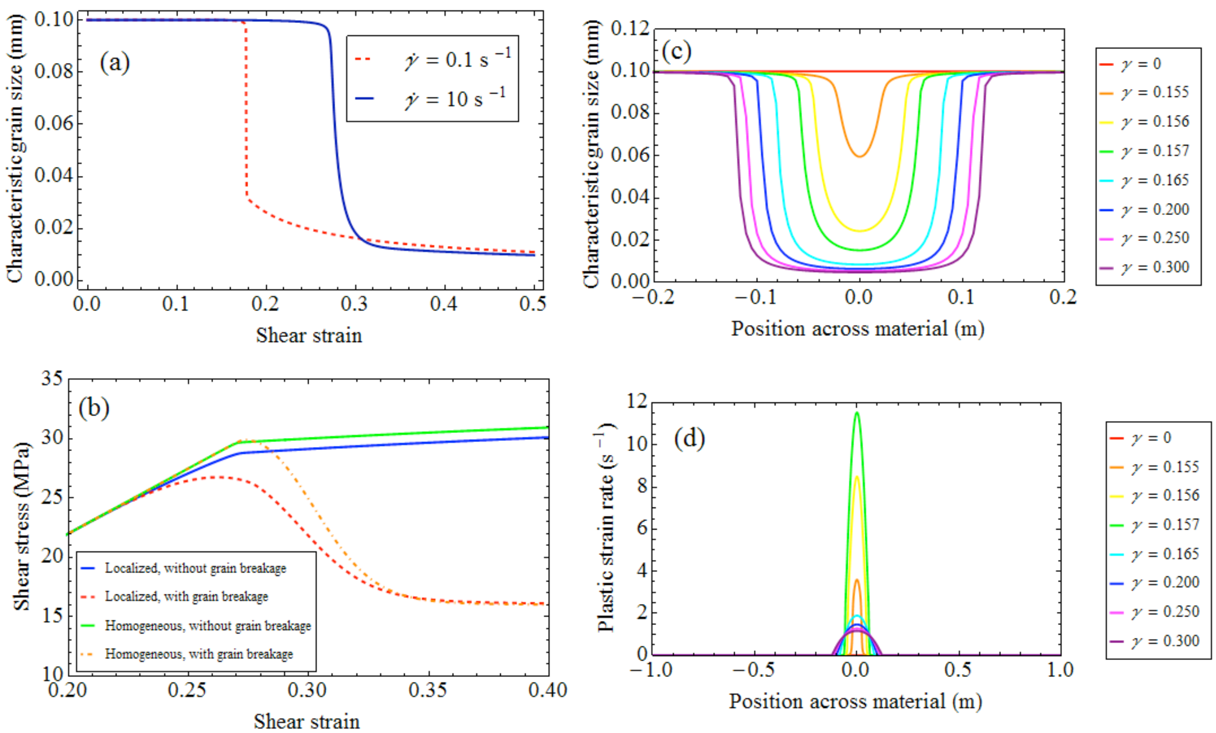

Figure 2: (a) Temporal evolution of characteristic grain size showing that grain comminution is most severe at the early stage, immediately upon the onset of irreversible plastic deformation. It slows down dramatically afterwards, suggestive of the dominance of grain abrasion at later stages. (b) At a fast shear rate, grain fragmentation significantly reduces the flow stress, under generic assumptions on the rate-strengthening behavior of the material. Strain localization also provides another weakening mechanism. (c) Sample grain size profile (close-up) and (d) Shear rate profile across the material, at various shear strain displacements. There is a feedback between shear localization and grain fragmentation accounting for the formation of a thin gouge layer at the shear band. Note the difference in horizontal scale.

Auto-acoustic Compaction:

The concept of compactivity is closely related to that of porosity, often measured in experiments for sheared fault gouge [Neimijer et al., 2010]. On this front, we have started preliminary work on analyzing the anomalous, reversible shear thinning behavior – the so-called "auto-acoustic compaction" – observed in angular sand particles sheared at intermediate rates [Van der Elst et al., 2012]. Our present speculation is as follows:

- Interparticle friction introduces an extra dissipative mechanism that may result in free volume reduction under some circumstances. Based on the existing framework of two-subsystem nonequilibrium statistical thermodynamics [Lieou and Langer, 2012; Bouchbinder and Langer, 2009], we have developed a preliminary model that adds a "frictional thermal subsystem" to the two existing thermodynamic subsystems. The ability to account for the flow of heat and entropy of the three subsystems, when properly coupled together to describe the interparticle frictional heating and the shear-induced mechanical vibration, may predict compactivity reduction and hence volume compaction under some circumstances.

- The possibility of angular grains to interlock with one another, thereby reducing configurational volume, is an extra complication that may be modeled within the three-subsystems framework, using an extra two-state internal variable that pertains to the kinetic subsystem and describes the degree of grain interlocking. In this manner, it may be possible to account for vibration-induced compaction at small shear rates, as seen in the experiments by van der Elst et al. [2012], as well as the effect of tapping alone [Nowak et al, 1998, Daniels and Behringer, 2005, 2006]. In effect, the disorder state variables that describe the effects of tapping and shearing are two compactivities that fall out of equilibrium with each other. Interlocking becomes prominent below a certain critical "kinetic compactivity", resulting in volume reduction, in analogy to the spontaneous magnetization of an Ising ferromagnet below a critical temperature.

Temperature Dependent Material Properties:

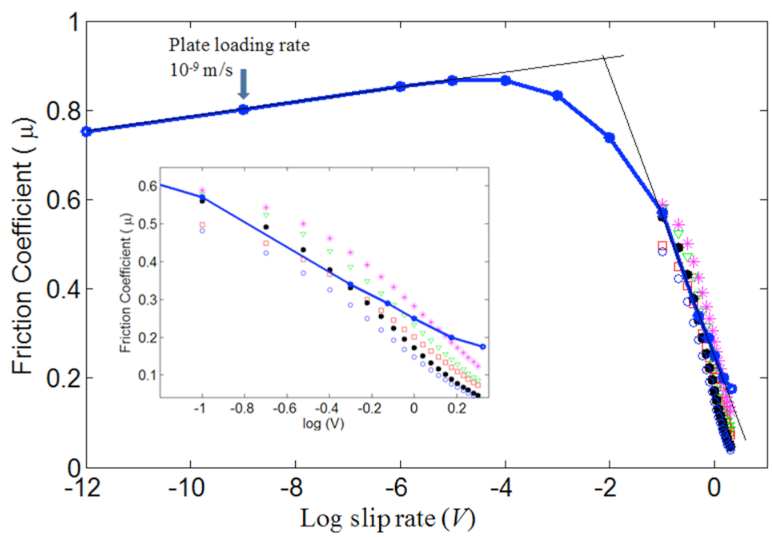

Figure 3: Steady state friction coefficient as a function of slip rate (layer thickness = 1mm) at a temperature of 300 K. The blue curve represents the prediction of our model. Scattered points represent the experimental data from Sone and Shimamoto [2009], and different colors correspond to different parameter values. The theoretical model did not account for the strain localization observed experimentally. This led to the slight discrepancy between the model predictions and the experiments at the highest slip rates.

We developed a model for sheared gouge layers, within the framework of STZ theory, that accounts for the local increase in temperature at the grain contacts during sliding. We tracked the temperature evolution at the grain contacts using a one dimensional heat diffusion equation. At low temperatures, the strength of the asperities is limited by the flow strength, as predicted by dislocation creep models. At high temperatures, some grains may partially melt leading to the degradation of the asperity strength. Our model predicts a logarithmic rate dependence of the steady state shear stress in the quasi-static regime. In the dense flow regime the frictional strength decreases rapidly with increasing slip rate due to the effect of thermal softening at the granular interfaces. The predictions of the model for friction at large slip rates lie within the range of experimental observations by Sone and Shimamoto (Figure 3)

The transient response following a step in strain rate includes a direct effect and a subsequent evolution to steady state, both of which depend on the magnitude and direction of the velocity step (Figure 4). The model links low-speed and high-speed frictional response of gouge layers, and provides an essential ingredient for multiscale modeling of earthquake ruptures with enhanced coseismic weakening.

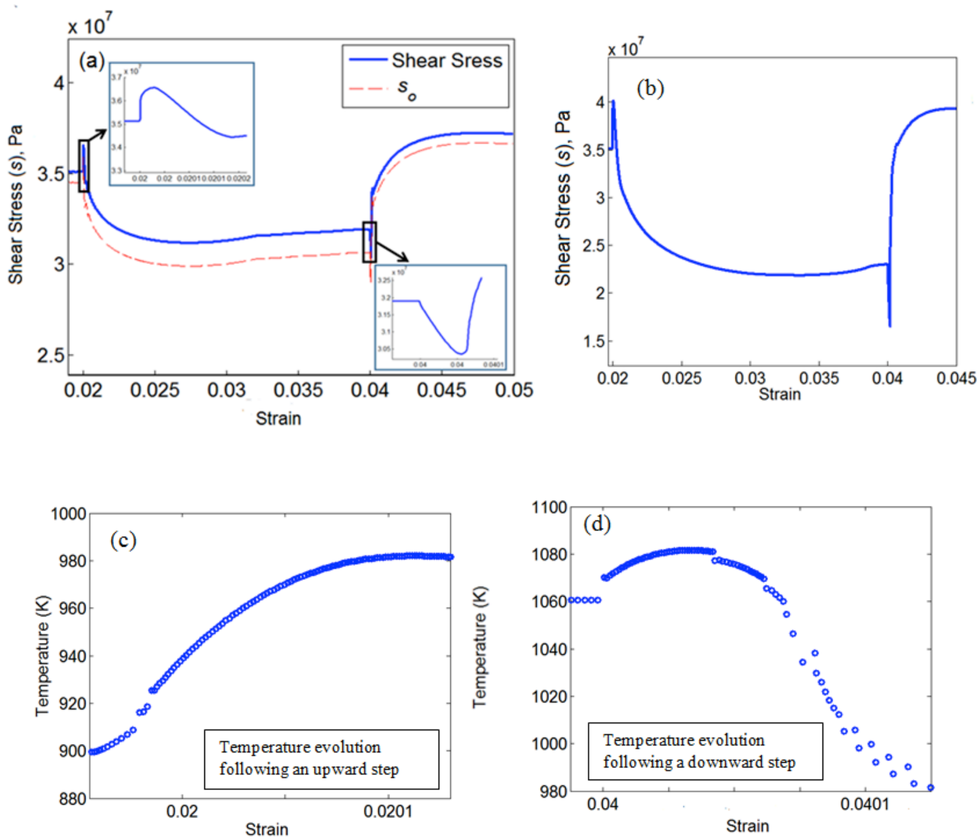

Figure 4: Results for a velocity stepping numerical experiment. (a) Evolution of shear stress and minimum flow stress s_o. In the upward step, the strain rate is doubled. After reaching steady state the strain rate was reduced to its original value. Inserts show a magnified plot for the variation of shear stress immediately following the step. Steady state stress is reached after the downward step at strains greater than 0.05 (not shown here). (b) Evolution of shear stress in a pair of strain rate stepping experiment in which the strain rate ration is 10 (0.1) in the upward (downward) step. (c) Evolution of contact temperature immediately following an upward step in velocity corresponding to Fig. 4(a) (d) Evolution of contact temperature immediately following a downward step in velocity corresponding to Fig. 4(a).

The combination of mechanisms including granular rearrangement, thermal softening, and shear banding within our STZ framework will be necessary to interpret such experimental observations and quantify frictional processes at the seismic scale more precisely.

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Lieou, C. K. C., J. S. Langer, A. E. Elbanna, and J. M. Carlson, Non-equilibrium thermodynamics in sheared hard-sphere materials, Poster presentation at Gordon Research Conference on Granular and Granular-fluid Flow, Davidson, NC (2012); and at the SCEC Annual Meeting, Palm Springs, CA (2012).

Elbanna, A. E., C. K. C. Lieou, and J. M. Carlson, Strong velocity weakening and energy partition in a model of sheared dry gouge with thermally varying material properties, Poster presentation at the SCEC Annual Meeting, Palm Springs, CA (2012).

Lieou, C. K. C., A. E. Elbanna, and J. M. Carlson, Grain fragmentation in sheared granular flow: Weakening effects, energy dissipation, and strain localization, Poster presentation at the SCEC Annual Meeting, Palm Springs, CA (2013).

Elbanna, A. E., C. K. C. Lieou. X. Ma, and J. M. Carlson, Towards a Unified Framework For Modeling Fault Zone Evolution: From Particles Comminution to Secondary Faults Branching, Poster presentation at the American Geophysics Union Fall Meeting, San Francisco, CA (2013)

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Publications

Elbanna, A. E. and J. M. Carlson (2014), Strong velocity weakening and energy partition in a model of sheared dry gouge with thermally varying material properties, submitted to Journal of Geophysical Reseach. (http://arxiv.org/abs/1402.1127)

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