A New Paradigm for Modeling Fault Zone Inelasticity: A coupled granular-bulk framework incorporating spontaneous localization and grain fragmentation

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I. Project Overview

A. Abstract

In the box below, describe the project objectives, methodology, and results obtained and their significance. If this work is a continuation of a multi-year SCEC-funded project, please include major research findings for all previous years in the abstract. (Maximum 250 words.)

The scientific objective of this proposal was to develop a 2D model for inelastic deformation in fault gouge to predict the evolution of grain size and shear banding patterns across a wide range of scales spanning both laboratory-like and field-like conditions. Methodology: We use the Shear Transformation Zone theory to describe viscoplasticity in sheared granular layers. We implement an inhomogeneous version of the theory as a user defined subroutine VUMAT in the finite element software Abaqus and couple it with a finite deformation continuum model based on the updated Lagrangian formulation and Green-Naghdi stress rate. Main results: (1) A working validated implementation of the material subroutine, (2) Identification of brittle to ductile transition in sheared granular materials as a function of initial porosity and grain size, (3) Reproducing complex strain localization patterns while tracking their evolution history. Significance: The proposal is an important step towards developing a theoretically sound framework for inelasticity and shear banding in granular materials accounting for complex structural and loading conditions. It opens new opportunities for multiscale modeling of earthquake ruptures that couple large scale elastodynamics with small scale inelastic processes in fault gouge. Coupling the current formulation with pore fluids will enable investigation of poro-visco-plasticity in fault gouge at a level of details that has not been addressed before.

B. SCEC Annual Science Highlights

Each year, the Science Planning Committee reviews and summarizes SCEC research accomplishments, and presents the results to the SCEC community and funding agencies. Rank (in order of preference) the sections in which you would like your project results to appear. Choose up to 3 working groups from below and re-order them according to your preference ranking.

Fault and Rupture Mechanics (FARM)
Seismology
Computational Science
C. Exemplary Figure

Select one figure from your project report that best exemplifies the significance of the results. The figure may be used in the SCEC Annual Science Highlights and chosen for the cover of the Annual Meeting Proceedings Volume. In the box below, enter the figure number from the project report, figure caption and figure credits.

![Figure](image)

Figure: Evolution of compactivity (a state variable that is in one-to-one-correspondence with porosity) and stress strain response in a sheared granular layer for different initial conditions. [Top]: Contour plots for compactivity in the case of high initial disorder (a) and low initial disorder. In the former case disorder is distributed across the sample and evolves almost uniformly. In the latter, disorder is localized and a shear band emerges. [Bottom] A layer with high initial disorder shows a ductile-like deformation with the stress increasing progressively towards the flow strength (red curve). Low initial disorder yields a brittle behavior and a visible stress drop (blue curve).

D. SCEC Science Priorities

In the box below, please list (in rank order) the SCEC priorities this project has achieved. See https://www.scec.org/research/priorities for list of SCEC research priorities. For example: 6a, 6b, 6c

3a, 3c, 4b, 3e
E. Intellectual Merit

How does the project contribute to the overall intellectual merit of SCEC? For example: How does the research contribute to advancing knowledge and understanding in the field and, more specifically, SCEC research objectives? To what extent has the activity developed creative and original concepts?

The project addresses short-term objectives in Fault and Rock Mechanics (3a, 3c, 4b and 3e) by developing models that quantify the influence of small scale processes on large scale rupture response. A better quantification of this issue will aid long-term objectives in Earthquake Source Physics and Ground Motion, informing models of fault system evolution and dynamics, and physics-based hazard analysis. Understanding the complex behavior of fault zone and its influence on rupture dynamics is also essential for the interpretation of seismic observations and for the problem of seismic inversion. It is also essential for evaluating impacts of future seismic events on Southern California. The proposal develops a unique and novel methodology for modeling gouge viscoelasticity considering grain evolution characteristics, shear band complexity and gouge spatial heterogeneities.

F. Broader Impacts

How does the project contribute to the broader impacts of SCEC as a whole? For example: How well has the activity promoted or supported teaching, training, and learning at your institution or across SCEC? If your project included a SCEC intern, what was his/her contribution? How has your project broadened the participation of underrepresented groups? To what extent has the project enhanced the infrastructure for research and education (e.g., facilities, instrumentation, networks, and partnerships)? What are some possible benefits of the activity to society?

The activity contributed to the training of 1 graduate student Xiao Ma who is currently conducting his PhD at UIUC on inelasticity in amorphous solids. The activity supported the PI’s travel to attend the annual meeting and continue his interactions/ explore new collaboration opportunities with other SCEC scientists. The computational methods developed as part of this proposal have applications beyond fault mechanics as it is relevant to analyzing deformation and failure in a broad range of amorphous materials including metallic glasses and lithium ion batteries. The activity contributes to SCEC efforts in developing fundamental models for multiscale deformation in fault zones which will enhance our physics based earthquake rupture simulations and improve our ground motion prediction tools on the long run. This will contribute to combating the heavy toll that earthquakes take on our society through making better informed decisions in the context of seismic hazard and risks.

G. Project Publications

All publications and presentations of the work funded must be entered in the SCEC Publications database. Log in at http://www.scec.org/user/login and select the Publications button to enter the SCEC Publications System. Please either (a) update a publication record you previously submitted or (b) add new publication record(s) as needed. If you have any problems, please email web@scec.org for assistance.

These papers are in submission and has been partially funded by this proposal:


II. Technical Report

The scientific objective of this proposal is to investigate the influence of the small scale processes within sheared gouge (e.g. comminution and shear banding) on the multiscale evolution of fault zone morphology (e.g. width, and grain size distribution) and dynamic rupture propagation. For this purpose, we use a 2D version of the Shear Transformation Zone (STZ) theory to formulate a constitutive description of granular systems with breakable grains and strain localization potential. Then, we will integrate this constitutive model into a computational framework for finite deformation using the finite element software ABAQUS.

The long term goal of this research is to provide a consistent framework for the evolution of fault zone topology and off-fault damage generation and healing over multiple earthquake events. To achieve this objective, several computational and theoretical challenges have to be addressed. These include: (1) a more fundamental understanding of the behavior of fault gouge, particularly its potential for fragmentation, localization, and its response to high frequency oscillations emitted from the rupture tip; (2) development of a computational framework in which granular and continuum phases of material coexist with the abilities of resolving the different spatial and time scales associated with gouge deformation and the wave propagation in intact rocks; (3) development of a computational framework capable of resolving the slow tectonic loading during the inter-seismic period and the rapid elastoplastic co-seismic response; and (4) a flexible adaptive mesh refinement framework to resolve evolving localization and distributed damage features as a function of progressive loading.

For the previous funding period we focused primarily on development of a 2D multiscale model for fault gouge to predict the evolution of grain size and shear banding patterns.

Applicability to SCEC4 Research Objectives: The project addresses short-term objectives in Fault and Rock Mechanics (3a, 3c, 4b and 3e) by developing models that quantifies the influence of small scale processes on large scale rupture response. A better quantification of this issue will aid long-term objectives in Earthquake Source Physics and Ground Motion, informing models of fault system evolution and dynamics, and physics-based hazard analysis. Understanding the complex behavior of fault zone and its influence on rupture dynamics is also essential for the interpretation of seismic observations and for the problem of seismic inversion. It is also essential for evaluating impacts of future seismic events on Southern California.

Motivation and relevance to Southern California and beyond: The upper portion of the crust contains a hierarchy of structural features that span a wide range of length scales [Scholz, 1990]. These features not only influence the different phases of the seismic cycle but also evolve in response to the spatio-temporal complexity of earthquake ruptures [Scholz, 1990; Lapusta et al., 2000 and references therein; Aki and Richards, 2002]. Small-scale instabilities at the gouge scale may evolve into large-scale instabilities at the fault scale. Moreover, fault mechanics, earthquake dynamics and rupture termination processes are linked to the physical properties of

Figure 1: Fault zone complexity. Fault system for Landers 1992 showing a hierarchy of features and secondary faults generate on the extensional side of the parent faults [Poliakov et al., 2002].
fault zones. A unified framework for modeling fault gouge deformation coupled with seismic and aseismic loading condition is a key to resolving many outstanding geophysical problems such as the heat flow paradox [Sibson, 1973; Lachenbruch, 1980], variation of fault zone thickness with depth [Scholz, 1988], the depth of the seismogenic zone, scaling of stress drops in earthquakes as well as estimates of seismic efficiency and energy partitioning [Kanamori and Heaton, 2000, and references therein]. These problems are particularly relevant in a region like Southern California in which a complex system of faults exist and extensive field studies have been carried out for characterizing the multiscale nature of this complexity, including damage density variations, properties of low velocity fault zones, statistics of fault branches, and surface roughness. Seismological observations also suggest that these features alter ground motion patterns. Hence, the problems addressed in this proposal, as well as their future extensions, are not only theoretically significant, but they also have important practical implications in the analysis of seismic hazard and risk.

In this proposal we focused on two key processes in fault gouge deformation: (1) grain comminution, and (2) strain localization. We will account for several factors relevant to the mechanics of fault zones including (i) the grain size distribution and its evolution [Sammis et al., 1987], (ii) generation of off-fault damage [Rice et al., 2005], and (iii) partitioning of slip between localized and distributed modes [Shimamoto, 1986, Chester et al., 1993, 1998, 2004, 2005]. The unique aspect of this proposal is the recognition that these mechanisms are strongly coupled and proposing a physics-based framework that unifies them. An outcome of the proposal is identification of few key mechanisms that contribute to brittle-ductile transition in gouge layers as a result of this strong feedback.

Our starting point is the realization that shear deformation in granular material occurs by means of particle rearrangements, either through rolling or sliding. At high normal stresses, grain breakage may become necessary to facilitate further sliding. Furthermore, strain localization may be triggered by the presence of static or dynamic heterogeneities in the material. The shear transformation zone (STZ) theory, a non-equilibrium statistical thermodynamics framework for describing non-affine irreversible transformations associated with granular rearrangements in amorphous materials, will be our primary tool in providing a micromechanics model for inelasticity at small scales. The premise is that inelastic strain occurs only at rare localized spots known as shear transformation zones (STZs). These STZs are defect-like structures associated with extra free volume that facilitate irreversible non-affine rearrangements of the particles. Each STZ transition event generates a finite amount of local plastic strain. Overall, the macroscopic plastic strain is the cumulative result of many local events. An effective temperature, which evolves according to the laws of thermodynamics, governs the density of the STZs and provides a measure of the system disorder that is in one-to-one correspondence with the system porosity. The theory has been successfully applied to shear deformation in a variety of systems, including granular fault gouge [Daub and Carlson, 2008; Daub et al., 2008; Daub and Carlson, 2010; Hermundstad et al., 2010; Lieou et al., 2014a, 2014b, 2015; Elbanna and Carlson, 2014; Kothari and Elbanna, 2016], and glassy materials [Falk and Langer, 1998, 2000; Langer and Manning, 2007; Manning et al., 2009]. More recently the theory reproduced the non-monotonic volume changes as a function of strain rate observed in granular material experiments subjected to shear and vibration [Lieou et al., 2015a, der Elst, 2014]. Figure 1 shows results from successful applications of the theory.
Koplik and earthquake setup [e.g. Xia et al., 2004] but with fault gouge, may come into play for cohesive fault gouge. To test this hypothesis, new experimental setups, as well as fault zone models, are required. At steady state (See red curve in tensile stresses not high enough (incorporated in our model as a limit on gouge tensile strength) the developed geneities the shear band dynamics will compressive within and outside the plastic regions. On the other hand, in the presence of significant inelastic dilation (e.g. in sands) the stress remains locally expanding plastic zone and the surrounding elastic domain as shearing progresses (Fig. 3). On the other hand, in the presence of significant inelastic dilation (e.g. in sands) the stress remains locally compressive within and outside the plastic regions. As a consequence for this local stress heterogeneities the shear band dynamics will be different in both cases (Fig. 4). Moreover, if cohesion is not high enough (incorporated in our model as a limit on gouge tensile strength) the developed tensile stresses may lead to mode I fractures (or cavitation) with an almost complete loss of strength at steady state (See red curve in Fig. 5). None of these observations is possible in a simplified 1D fault zone model. Cavitation has been widely studied in hyperelastic [Lopez-Pamies et al., 2011] as well as elastoplastic solids [Koplik and Needleman, 1988]. We argue that similar phenomena may come into play for cohesive fault gouge. To test this hypothesis, new experimental setups, shifting from rotary shear geometry to either the simple shear geometry or to the laboratory earthquake setup [e.g. Xia et al., 2004] but with fault gouge, are required.

Fig. 2: Examples of successful applications of STZ theory that go beyond classical rate and state law. (a) Predictions of STZ theory for the rheology of sheared granular system [Elbanna and Carlson, 2014]. Insert shows results from molecular dynamic simulations [daCruz et al., 2005]. (b) Predictions of localization patterns from computational models with STZ theory (top) [Elbanna and Ma, 2015] consistent with the schematic complex patterns observed in the lab (bottom) [Marone, 1998]. Note the different shear sense. Boundary, Riedel and Y-bands develop naturally. The angle between the complementary shear bands will depend on inelastic volume expansion coefficient (which gives rise to pressure sensitivity).

Key Results:

Our investigations of 2D fault gouge viscoplasticity models unravel some interesting physical phenomena that were not apparent from the 1D studies. An example of this is shown in Fig 2b where complex shear localization patterns (including boundary, Riedel and Y-shears) naturally develop, in a numerical experiment of shearing a gouge layer between two rigid plates, in agreement with experimental observations. A 1D model is capable of only capturing the Y-shear and thus misses the more complete picture of shear band nucleation and propagation. This complex evolution of shear bands turns out to play an important role in strength evolution. In particular, and unexpectedly, we have observed that in the absence of significant inelastic volume changes (i.e. in the limit of isochoric plasticity, as in the case of some clays), regions of tensile mean stress may develop at the early stages of strain localization. These are observed at the boundary between the slowly expanding plastic zone and the surrounding elastic domain as shearing progresses (Fig. 3). On the other hand, in the presence of significant inelastic dilation (e.g. in sands) the stress remains locally compressive within and outside the plastic regions. As a consequence for this local stress heterogeneities the shear band dynamics will be different in both cases (Fig. 4). Moreover, if cohesion is not high enough (incorporated in our model as a limit on gouge tensile strength) the developed tensile stresses may lead to mode I fractures (or cavitation) with an almost complete loss of strength at steady state (See red curve in Fig. 5). None of these observations is possible in a simplified 1D fault zone model. Cavitation has been widely studied in hyperelastic [Lopez-Pamies et al., 2011] as well as elastoplastic solids [Koplik and Needleman, 1988]. We argue that similar phenomena may come into play for cohesive fault gouge. To test this hypothesis, new experimental setups, shifting from rotary shear geometry to either the simple shear geometry or to the laboratory earthquake setup [e.g. Xia et al., 2004] but with fault gouge, are required.
Fig. 3: Distribution of hydrostatic stress in a gouge layer with limited dilatancy that is sheared at $\dot{\gamma} = 1/\text{sec}$, and pressure 25 MPa between two parallel rigid plates. Periodic boundary conditions are imposed on the lateral edges. Areas with tensile mean stress (red/orange) develop at the boundary of the expanding plastic region (the circular domain in the center of the insert).

Fig. 4: Early stages of shear band development in a gouge layer that has (a) limited dilatancy but high cohesion, (b) high dilatancy. The contours represent values of the effective temperature which measure the degree of disorder (indicative of porosity) in the system. Shear sense is right lateral in both cases. The cohesive layer exhibit a pair of almost orthogonal shear bands while the highly dilatant layer shows a thicker shear band. The orientation of the shear bands is significantly different hinting at different local stress fields.

Furthermore, the current theoretical formulation enables us to investigate the influence of grain size and initial state on the gouge response. Figure 5a shows suggests that the gouge behavior may transition from a brittle (rapid strength drop with progressive slip) to a ductile response (gradually approaching the flow stress) as the grain size is reduced. Moreover, the initial porosity is also found to have a strong influence on the shear behavior; an initially loose layer (high disorder) will compact and deform in a ductile way whereas an initially compacted layer (low disorder) will dilate and exhibit a quasi-brittle response (Fig. 5b). These observations suggest that our computational work has the potential to provide new insights into several phenomena associated with fault gouge deformation including changes in the slip weakening distance, variations in peak and flow strength as well as transition from brittle to ductile behavior as a function of pressure and grain size [Ma and Elbanna, 2016].
Future Work: We plan to extend our current formulation that enables tracking volume changes in sheared granular layer to include pore fluids. Our current investigations aim at the Development of a 2D model for fault gouge poro-visco-elasto-plasticity. This will be done by coupling the continuum STZ viscoplasticity framework with pore fluid diffusion models. Furthermore, we plan to develop computational model in which the 2D gouge layer, either drained or undrained, is subjected to vibrations either from an external source or vibrations that are internally generated due to local frictional and fracture processes.

Fig. 5: Stress, slip response for a sheared gouge Layer with different effective volume expansion coefficient $\alpha$. The response with $\alpha = 10^{-4}$ is very close to the isochoric plasticity predictions. If the tensile strength is low, the gouge start developing mode I normal to the direction of minimum tensile stresses. (Fig. 2) and the peak strength and flow stress are significantly reduced (red curve). On the other hand, a more dilative layer $\alpha = 5 \times 10^{-3}$ will not experience local tensile stress formation. It will deform plastically over a larger slip weakening distance.

Fig. 6: Brittle to ductile transition in sheared gouge layer. (a) Effect of grain size: smaller grain size leads to more ductile response. (b) Effect of disorder: Less initial disorder leads to brittle response.
References


