The importance of the third dimension in granular shear

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Abstract

[1] We present new numerical results showing the importance of the third dimension in simulations of granular shear. Our 3-D numerical models of gouge layers under shear exhibit friction levels notably higher than 2-D models and values that approach those of recent laboratory experiments on spherical beads. Fluctuations in friction are directly related to grain reorganization normal to shear. In 3-D, these fluctuations are reduced due to significant particle motion in the third dimension, leading to a steady frictional sliding curve. Since these fluctuations are small compared with 2-D models, our 3-D simulation offers potential to investigate small amplitude but extremely important second order rate and state friction effects that fundamentally control the strength and stability of fault zones.

[2] Earthquakes commonly occur on faults containing gouge; therefore investigating the processes operating in gouge sheared under stress is extremely relevant to earthquake and fault mechanics. Laboratory shearing experiments [e.g., Marone, 1998; Beeler et al., 1996] conducted on thin granular layers have been useful in elucidating how loading conditions and perturbations influence friction (see Scholz [1998] and Marone [1998] for recent summaries).

[3] Similar studies can be conducted using discontinuum numerical models in which the shear zone is represented by an assembly of particles that can move independently [Aharonov and Sparks, 2002; Antonellini and Pollard, 1995; Mora and Place, 1998; Morgan and Boettcher, 1999; Scott, 1996]. These models can yield informative insights into micromechanical processes operating in simulated fault zones by allowing direct observation of particle motions, stresses and interactions during shearing. The models also help isolate the influence of material characteristics such as interparticle friction, particle size distribution [Morgan, 1999], effect of normal stress [Aharonov and Sparks, 1999] or particle angularity [Mora and Place, 1998].

[4] Validation of numerical models through laboratory experiments is essential to determining whether the model behavior approaches reality [Wawersik, 2000]. Only after models have been shown to accurately reproduce laboratory results can they be used to simulate more complex, field-scale geosystems such as tectonic faulting and earthquakes.

[5] Recent attempts have been made to bridge the gap between numerical models and the natural fault systems by conducting highly idealized laboratory investigations (e.g. perfectly spherical particles or two-dimensional rods [Frye and Marone, 2002; Mair et al., 2002]). These experiments have highlighted the importance of particle characteristics and dimensionality in frictional response.

[6] We present new results from 3-D numerical modeling of shear in granular materials. We show that 3-D numerical models exhibit higher friction with smaller fluctuations than those in 2-D. Results agree well with recent laboratory work conducted under idealized conditions, validating the general aspects of our approach and offering the potential for incorporating further complexity.

1. Introduction

[7] The distinct element method [Cundall and Strack, 1979] has been used extensively to model granular shear zones. This approach considers an assembly of perfect, indestructible cylindrical (2-D) or spherical (3-D) particles that interact only at points of contact. An explicit solution scheme is used that updates particle positions and contact forces each time step.

[8] Particle and contact micro-properties are prescribed and the resulting macroscopic response is measured. The laws governing interactions between particles are simple, however interactions between large numbers of particles lead to interesting complex behavior.

[9] For the research presented here, the Particle Flow Code in 3 Dimensions (PFC3D) is used [Itasca Consulting Group, 1999] with a Hertz-Mindlin contact model [Cundall, 1988]. The shear force at a contact is limited by specified coefficient of friction. If the shear force is overcome then stable sliding occurs at the contact. The Hertz-Mindlin contact model was thought to be a more realistic representation of contact behavior than a linear, Hookian model, however with the values of normal stress and contact stiffness presented here, the difference in observed macro frictional behavior is minimal.

[10] The simulated layers are created by filling a 6-sided shape with a random assembly of particles (see Figure 1). Particle microproperties are assigned (see Table 1), then the assembly is compacted to the desired isotropic stress state of 5 MPa (Figure 1a). Particle properties and the loading geometry are comparable to recent laboratory experiments [e.g., Frye and Marone, 2002].

[11] Shearing is horizontal and the top and bottom boundaries are comprised of a controlled layer of particles to provide roughness (Figure 1). A servo-control mecha-
nism is activated at the top boundary particles to adjust vertical velocities thereby maintaining the desired (constant) normal stress. The bottom boundary is fixed. During a numerical experiment, the top boundary is driven at a constant horizontal velocity to apply shear to the particle layer. The two side boundaries perpendicular to the direction of shear are periodic such that particles exit from one side and reappear on the other. The other two boundaries (parallel to the direction of shear) are fixed, frictionless walls.

A suite of numerical models were run, including several 2-D simulations, to test the robustness of the results and the sensitivity to a range of input parameters. The influence of the 3rd dimension and the effect of using different particle sizes are described in section 3.

3. Results

A 3-D model after 100% shear strain (Figure 1b) shows a continuous marker band indicating that strain is evenly distributed throughout the layer without any obvious localization features. The frictional response of this model and a similar 2-D model are presented in Figure 2a. For the 2-D numerical model, sliding friction has mean value of 0.3 and exhibits large fluctuations (between 0.2 and 0.38) as a function of sliding. These observations agree well with previous 2-D numerical results [e.g., Morgan, 1999], and with 2-D laboratory experiments [Frye and Marone, 2002].

In the 3-D model, sliding friction is enhanced to a mean level of $\frac{1}{24}$ of 0.4. This supports the hypothesis that friction is higher in 3-D than 2-D due to an extra dimension of grain interaction (sliding, rolling, dilation and compaction) during shear [Frye and Marone, 2002].

Variations in friction in the 3-D model are significantly smaller than in the 2-D case, ranging between 0.38 and 0.43. These fluctuations are associated with dilation and compaction of the granular layer during shear. Figure 2b highlights the clear connection between the amplitude of friction fluctuations, and dilatancy rate ($dh/dx$ where $h$ is the layer thickness and $x$ is the shear displacement) for the 2-D and 3-D models.

Figure 3 summarizes the macroscopic friction characteristics for a series of 2-D and 3-D models with different particle sizes (see Table 1). The systematic differences between 2-D and 3-D models, discussed above, are clear and reproducible and the models compare favorably to laboratory results. For a given case (2-D or 3-D), particle size has little effect on average friction although smaller particles tend to produce reduced frictional fluctuations. The influence of adding a 3rd dimension to the models is clearly much stronger than that induced by changes in particle size (at least over the range shown).

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Table 1. Laboratory and Numerical Experiments

<table>
<thead>
<tr>
<th>Experiment</th>
<th>Description</th>
<th>Mean Particle Diameter ($\mu$m) (±1 std. dev)</th>
<th>Mean macro friction (±1 std. dev)</th>
</tr>
</thead>
<tbody>
<tr>
<td>T007</td>
<td>3-D model</td>
<td>191 (±16.5)</td>
<td>0.403 (±0.015)</td>
</tr>
<tr>
<td>T001</td>
<td>3-D model</td>
<td>254 (±22)</td>
<td>0.407 (±0.010)</td>
</tr>
<tr>
<td>T009</td>
<td>3-D model</td>
<td>381 (±33)</td>
<td>0.409 (±0.021)</td>
</tr>
<tr>
<td>T012</td>
<td>3-D model</td>
<td>508 (±44)</td>
<td>0.404 (±0.017)</td>
</tr>
<tr>
<td>m349</td>
<td>3-D lab study (glass beads)</td>
<td>105–149</td>
<td>0.473$^a$</td>
</tr>
<tr>
<td>m301</td>
<td>3-D lab study (angular sand)</td>
<td>50–150</td>
<td>0.644$^a$</td>
</tr>
<tr>
<td>T102</td>
<td>2-D model</td>
<td>127 (±11)</td>
<td>0.292 (±0.037)</td>
</tr>
<tr>
<td>T103</td>
<td>2-D model</td>
<td>191 (±16.5)</td>
<td>0.322 (±0.072)</td>
</tr>
<tr>
<td>T101</td>
<td>2-D model</td>
<td>254 (±22)</td>
<td>0.287 (±0.057)</td>
</tr>
<tr>
<td>T104</td>
<td>2-D model</td>
<td>381 (±33)</td>
<td>0.313 (±0.089)</td>
</tr>
<tr>
<td>m518</td>
<td>2-D lab study (glass rods)</td>
<td>1000</td>
<td>0.274 (±0.053)</td>
</tr>
</tbody>
</table>

Modeled particles and glass beads have a shear modulus of 22.0 GPa, Poisson’s ratio of 0.25 and a Gaussian size distribution. Interparticle friction of modeled particles is 0.5. Normal stress is 5 MPa for all tests except m518, for which $\sigma_n = 1$ MPa. Experimental data is from [Mair et al., 2002] and [Frye and Marone, 2002].

$^a$Peak values given instead of mean.

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Figure 1. (a) 3-D numerical model (T001) after isotropic compaction (5 MPa) but prior to shear. A vertical marker band is shown. The layer is 3.7 mm thick (z dimension) by 6.9 mm in the x and y dimensions. The average particle diameter is 254 $\mu$m. Shear stress is applied by moving the top layer in the positive x direction. The bottom layer is fixed. (b) The model after 100% shear strain. The top boundary layer has been stripped off to enable viewing of the marker band.

Figure 2. (a) Friction versus shear displacement for 2-D and 3-D models of shear in granular layers. Laboratory data is also shown for spherical beads and angular sand from Mair et al. [2002]. (b) Friction and dilatancy rate ($dh/dx$ where $h$ is the layer thickness and $x$ is the shear displacement) for the 2-D and 3-D models.

Figure 3. A 3-D model of granular shear (T001) after isotropic compaction (5 MPa) but prior to shear. A vertical marker band is shown.
The observed fluctuations are likely related to the number of layers of free grains. Clearly 3-D models will have significantly more free layers for the same particle size. It is possible that a 2-D model with extremely small particles could yield small fluctuations like the 3-D models, however this would reproduce the observed macro results without capturing the important micromechanisms producing the observations.

Figure 2 shows that the reduced friction fluctuations in 3-D are due to smaller changes in layer thickness required to accommodate shear. The third dimension means that particles have greater freedom to re-organize ‘out-of-plane’. Figure 4 demonstrates this, showing velocities of individual particles during shearing (viewed from above). There is significant motion of particles in directions not parallel to the shearing direction indicating ‘out-of-plane’ motion is a common phenomenon for accommodating the shear strain. This motion is clearly not permitted in the 2-D case.

To quantitatively examine this effect, the average x, y and z particle velocities were calculated for each of the models at 100% strain. It was found that the average velocities perpendicular to shear (RMS of y and z velocities) were 25–45% of the average velocity in the shear direction (x-velocity) for both 2-D and 3-D models. In 2-D, all of the shear-perpendicular strain is the z-direction. Whereas in 3-D, this strain is being accommodated (roughly equally) in each of the directions (y and z) perpendicular to shear.

4. Discussion

Figures 2 and 3 show graphical comparisons of 3-D modeling and laboratory results. The level of friction attained in the 3-D numerical model approaches the frictional strength of 3-D spherical beads sheared in the laboratory under similar loading conditions. However, unlike the laboratory data that show highly repetitive stick slip [Mair et al., 2002], our numerical results indicate stable sliding at a relatively constant level. Increasing particle size in the models (see Figure 3) produced larger friction fluctuations but the magnitude and character of these fluctuations still differed significantly from the laboratory stick-slip observations.

When angular gouge is sheared in the laboratory under similar conditions, no stick-slip motion is observed (see Figure 2). Therefore certain special conditions are required for the stick-slip phenomenon including the use of spherical grains with a narrow size distribution. These conditions were replicated closely in the numerical experiments however stick-slip motion was not observed.

One possible explanation is that the numerical models are loaded by a constant velocity boundary, which essentially simulates a loading frame of infinite stiffness. It is well known that a more compliant loading frame increases the potential of observing stick-slip motion. Therefore, to reproduce the stick-slip behavior observed in the laboratory, more realistic boundary conditions may be required.

Another contributing factor is likely the lack of time-dependent processes in the model. In the laboratory, the size of stress drops increase systematically with recurrence interval (ie stick time between events) indicating that a time dependent healing process is operating between dynamic slip events [see Mair et al., 2002]. Our numerical model has no time dependent processes (e.g., contact healing) therefore it is not surprising that it does not imitate this behavior. The current model is more representative of a fault being sheared at infinite velocity, hence laboratory and model results would converge (i.e. exhibit stable sliding) at very high loading rates [see Berman et al., 1996; Karner and Marone, 2000].

Stick slip motion associated with first order, purely geometric effects has been produced in 2-D numerical models when clusters of bonded particles make up the shear zone [Mora and Place, 1998] or when rolling of particles is inhibited [Morgan, 2003]. Particle geometry and resulting distribution of stress across 3-D granular layers is clearly also an important factor influencing stick slip in the laboratory [Mair et al., 2002]. However, the time dependent nature of stick slip cycles emanating from extremely simple 3-D geometries (unbroken spherical beads) in the laboratory...
suggests that 2nd order grain-scale healing processes are fundamentally important [Mair, in prep 2003].

[25] Attempts have recently been made to add 2nd order rate and state dependent effects to 2-D numerical models [Abe et al., 2002; Igami et al., 2002; Morgan, 2003]. This is a welcome step forward and has been successful in qualitatively reproducing certain aspects of laboratory rate and state friction. One issue however, is that these subtle second order effects are masked by the large fluctuations in sliding friction caused by geometric interactions as grains bounce over each other. In the 3-D model presented here, natural variations in macroscopic friction are small (compared to the 2-D case) therefore we have the potential to isolate 2nd order changes in friction associated with rate and state effects and thereby assess the relative importance of 1st order geometry and 2nd order healing mechanisms. We propose therefore that 3-D models are essential for investigation of these important 2nd order frictional effects.

5. Conclusions

[26] New 3-D numerical modeling has revealed that out-of-plane particle motion is extremely relevant to understanding the mechanical behavior of granular material under shear. In 3-D models, levels of friction are higher than in 2-D, comparing favorably to results of recent laboratory experiments on spherical particles. 2-D and 3-D models show that friction fluctuations are directly associated with grain reorganization (normal to shear), however the normal component of these processes is small in the 3-D case (since much motion occurs out of plane), leading to almost constant levels of friction. Changing the particle size has little effect on this behavior.

[27] Currently, our 3-D models do not reproduce the stick slip instability seen in laboratory tests on spherical beads, however this is likely a limitation due to the constant velocity boundary condition and a lack of time dependent healing mechanisms. We propose that a 3-D approach may be vital in isolating the influence of 2nd order grain contact processes, potentially responsible for rate and state dependent friction, from 1st order geometrical interactions. This is currently not discernible in 2-D due to the large amplitude geometric fluctuations in friction.

[28] The next step in this research will be to increase the complexity (and realism) of the model by including other mechanisms (healing, grain angularity, grain crushing) to assess the importance of these to the earthquake process. The models can then be used to examine internal mechanism such as force chain fabrics, particle velocities and accelerations, microseismicity and evolution of microstructure.

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References


