A small-scale numerical study of fault slip mechanisms using DEM

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1. Introduction - Context
2. Sample generation and numerical modelling
3. Results on granular gouge behaviour
4. Perspectives and conclusions
1- Introduction - Context
1. Introduction - Context

What is induced seismicity?

Injection well

Recuperation well

Hydraulic stimulation

Induced micro-seismicity

Slip reactivation into the existing faults

Increase of pore pressure

Granular gouge

Hot Rocks

Cold water

Steam

Power generation

Enhanced Geothermal Systems

Tectonic context due to pre-existing stress field

Depth: 3-4 km

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1. Introduction - Context

What are the parameters influencing slipping?

- Type of rock
- Confining Stress
- Temperature
- Shearing velocity
- Interactions
  - Cohesion
  - Friction
- Grains
  - Size of grains
  - Shape of grains
  - Initial solid fraction
- Granular materials
  - Size of grains
  - Granular distribution
- Fluid
  - Viscosity
  - Pore pressure
- Rock
  - Roughness
  - Hardness
  - Porosity
- Porosity

(Talebi & Cornet, 1987), (Bourouis & Bernard, 2007), (Mair & Marone, 1999)
(Morgan & Boettcher, 1999), (Sammis et al., 1987), (Muto et al., 2015), (Biegel et al., 1989), (Chris Marone & Scholz, 1989)
(Guo & Morgan, 2004), (Mair et al., 2002), (Santamarina & Cho, 2004), (Mair et al., 2002), (Anthony & Marone, 2005)
(Dorostkar et al., 2017a), (Dorostkar et al., 2017b), (M. Violay et al., 2014), (Acosta et al., 2018), (Cornelio et al., 2019), (Di Toro et al., 2018), (Noël et al., 2019), (Bourouis & Bernard, 2007), (Cornet, 2015), (Olgaard & Brace, 1983), (Brace et Martin, 1968)
(Zhao, 2013), (Guo & Morgan, 2004), (Byerlee & Brace, 1968), (Mair & Marone, 1999)
(Neuville et al. 2010), (Griggs et al., 1960), (Rabinowicz, 1965), (Stesky, 1978)
(Dorostkar et al., 2018), (Rognon et al., 2008)
1. Introduction - Context

Overview of the investigated parameters

What is the influence of inter-particular friction within the gouge?

- What is the role of cohesion? What does cohesion represent in reality and how can we simulate its effect?
- What is the influence of cohesion on the mechanical behavior of a granular fault gouge and on the energy budget of the system?
- Is the energy budget well defined and exhaustive? How can we enrich energy budget definition?

We will focus on
1. Introduction - Context

**How to model a granular fault gouge?**

Discrete Element modelling – 2D – Granular and faceted shapes

- $\sigma$: Constant Normal stress
- $v$: Imposed slip velocity
- Bonded Mohr-Coulomb Law (interparticular Cohesion and friction)
- Fixed body 1
- Periodic boundary conditions

What is the influence of cohesion within the gouge?
2 – Sample generation and numerical modelling

Packing2D  →  MELODY

Granular sample generation
Developed on Matlab

Discrete Element Modelling
Matlab and C++

Documented and free access

(Mollon & Zhao, 2013)

(Mollon, 2016), (Mollon, 2018a), (Mollon, 2018b)
2. Numerical modelling and sample generation

2.1- Packing2D

Generation of a realistic packing of grains with complex and angular shapes.

- Fourier-Voronoï method (2D) or (3D)
- Complex particle shapes
- Anisotropic orientation possible

Mollon and Zhao, 2014
2. Numerical modelling and sample generation

2.1- Packing2D

**Step 1: Generation of a Voronoï Tessellation**

- Creation of the domain (w x L)
- Division of the domain into N small cells
- Evaluation of the target size distribution

**How to create a packing of grains?**

Bounded Voronoï tessellation

Inverse Monte-Carlo Method
2. Numerical modelling and sample generation

2.1- Packing2D

Step 2: Spectrum of morphological descriptors, Fourier descriptors

Discrete Fourier spectrum of the signal \{A_n, B_n\}, fourier series:

\[ r_i(\theta_i) = r_o + \sum_{n=1}^{N} [A_n \cos(n\theta) + B_n \sin(n\theta)] \quad (\text{with } r_o \text{ average radius}) \]

Normalized amplitude for each harmonics \( n \):

\[ D_n = \frac{\sqrt{A_n^2 + B_n^2}}{r_o} \quad \text{“Fourier descriptor”} \]

N harmonics = N points to discretized the contour of grains.

Inverse Fourier transform \( \rightarrow \) grain shape

How to create a packing of grains?
2. Numerical modelling and sample generation

2.1- Packing2D

How to create a packing of grains?

Step 3: Cell filling

Generated grain with Fourier spectrum

Reproduces target properties (size, orientation, target solid fraction...)

Granular sample

Circular grains

Angular grains

Voronoï cell
2. Numerical modelling and sample generation

2.2- MELODY 2D

Discretized Element Method = DEM

- To compute motions of a large number of particles
- Every particle is considered as a body with dynamic equations
- Interactions with other bodies

**MELODY = Multibody Element-free Open code for Dynamic simulation** (Mollon, 2018)

Represent in the same digital frame the first and 3rd bodies with their deformation and dynamics

- to keep the discontinuity of the 3rd body => Multi-body
- to take into account the inertial and damping effect => dynamic
2. Numerical modelling and sample generation

2.2- MELODY 2D

What is MELODY, what differences?

Mesh-free shape functions
(for compliant bodies)

COMPLIANT BODY

RIGID BODY

Centre of mass
Contact node
Field nodes
Contact segment

Mesh-free shape functions
(for compliant bodies)
2. Numerical modelling and sample generation

2.2 - MELODY 2D

What is MELODY, what differences?

Small interpenetrations

$$F_n = \begin{cases} 0 & \text{si } \delta_n > 0 \\ -k_n \cdot \delta_n - \gamma_n \cdot \frac{d\delta_n}{dt} & \text{si } \delta_n < 0 \end{cases}$$

$$F_t = \begin{cases} -k_t \cdot \delta_t & | -k_t \cdot \delta_t | \leq \mu \cdot F_n \\ \text{sign}(-k_t \cdot \delta_t) \cdot \mu \cdot F_n & | -k_t \cdot \delta_t | > \mu \cdot F_n \end{cases}$$

Rigid grains → High numerical stiffness

Optimized proximity and contact detection → 3 steps of contact detection
2. Numerical modelling and sample generation

2.3- Gouge model assumptions

**Shape and geometry of the model**

- Angular shapes of particles: higher friction coefficient and different global behaviour from circular particles (Mair et al., 2002), (Guo et al., 2004). Validation with DEM

- Size of the model: 2D, 2mm x 20mm
- Wavelength of the wall roughness: sinusoidal

**Rigid particles and bodies**

Micromechanical point of view, deformation represented by numerical stiffness and interpenetration between particles. Less calculation cost. No fragmentation.

**Contact detection and interaction**

- Dry contacts: understand mechanism without water and test the effect of cohesion.
- Bonded Mohr-Coulomb contact law:
  - Unbroken bond: constant value of cohesion
  - Broken bond: only inter-particular friction (µ micro = 0.5)

At the beginning of the experiment, all the particles in contact receive a percentage of cohesion. Once broken, a cohesive contact cannot be cohesive anymore.
2. Numerical modelling and sample generation

2.4- Procedures and boundary conditions

\[ \sigma : 40 \text{ MPa} \]

\[ v : 1 \text{ m/s} \]

\[ \text{density} = 2600 \text{ kg/m}^3 \]

Number of particles: 4959
Size of particles: 27 – 260 µm
Fractal distribution of grains

Fixed body 1

Law: « Bonded Mohr-Coulomb »
Cohesion and friction between the different bodies in contact.

Numerical stiffness and damping

Inter-particular friction and cohesion
3 – Results on granular gouge behaviour
3. Results on granular gouge behavior

3.1- Initial solid fraction without cohesion

Solid fraction vs mechanical behaviour

Two kinds of initial samples: dense and mid dense samples
→ Two mechanical behaviours

Macroscopic friction

\[ \mu(t) = \frac{F_T(t)}{F_N(t)} \]

Solid fraction

\[ SF = \frac{S_{grains}}{S_{gouge}} \]

With \[ S_{gouge} = S_{grains} + S_{void} \]

Dense sample, SF=0.89
Mid-dense sample, SF=0.84

Graph 1: Shearing experiment of a granular fault gouge (a) Friction coefficient in function of the slip of the upper rock wall (m) - (b) Gouge width (m) in function of the slip of the upper rock wall (m) - for dense and mid-dense sample
3. Results on granular gouge behavior

3.2- Role of inter-particular cohesion

What is the effect of cohesion on granular gouge behavior? Cohesion is a difficult parameter to observe and to quantify and even more to follow during experiments. People have already tried to describe cohesion, from lab experiments or simulations (Rognon et al., 2008) with numerical cohesion or (Dorostkar et al., 2018) to represent capillary bridges. Here we try to bring some new knowledge on this parameter.

We decided to consider cohesion as a cementation we can find within a gouge, representing mineral matrix between particles.

Main differences with previous studies

• To use angular and faceted shapes instead of circular shapes
• To follow cohesion during the experiment
• To extract the energy budget from the breakage of cohesion bonds

Cohesion quantification:

(Friedman et al., 1972) defined maximum cohesion and apparent surface energy of rocks, the energy needed to propagate a stable tensile fracture inside the rock. The higher apparent surface energy is found for the Chilhowee quartzite with a value of $U = 62 \, J.m^2$. We consider this energy as the maximum energy, where cohesion recovers 100% of grains perimeter.

We express cohesion as a percentage of cohesion $X \%$ inside the model, compared to the maximum cohesion found in our model for an energy $U$.

Two kinds of initial samples:

• Dense SF=0,89
• Mid-dense SF=0,84
3. Results on granular gouge behavior

3.2- Role of inter-particular cohesion

Friction curve comparison between dense and mid-dense sample in function of the upper wall displacement – (b) Zoom in on the friction peak

Two kinds of initial samples:
- Dense SF=0.89
- Mid-dense SF=0.84

For a denser sample?
- Higher friction peak $\mu_p$ for the same % of cohesion
- Different peak shape
- Different initial slope
- Different critical slip distance
- Same average friction coefficient in the steady-state zone (0,5)
- Higher dilatancy rate
3. Results on granular gouge behavior

3.2- Role of inter-particular cohesion

Non-cohesive behaviours [0–10% cohesion]:
- almost all cohesive bonds break at the beginning and give way to a Mohr-Coulomb contact law with inter-particular friction only.
- Behaviour very close to a non-cohesive gouge respectively for dense and mid-dense sample.

Cohesive behaviours [>10% cohesion]:
- Some cohesive bonds remains intact during the beginning of shearing.
- Cohesion modifies the initial state of compaction and the energy that the system must provide to break the tangled and cohesive grains.
- High cohesion contacts occur between agglomerates of cohesive grains, changing the whole geometry and PSD of the gouge.
3. Results on granular gouge behavior

3.2- Role of inter-particular cohesion

Different fracturation behaviours inside the granular gouge. For 40% of cohesion:

- Dense: shear bands in the direction of force chains, increase of porosity inside the sample. Clusters of cohesive grains.
  - Mid-dense: Shearing localization at the bottom of the sample. Big cohesive zone in the upper part of the gouge.

→ Initial solid fraction of the sample changes packing of particles, and thus the application of cohesion. Shear bands do not follow the same patterns.
3. Results on granular gouge behavior

3.2- Role of inter-particular cohesion

**Energy Budget – new definition**

**Example for a mid-dense sample – 40% cohesion**

- **Dilatancy contribution** = from the dilation of the gouge.
- **Damage contribution** = from the energy used to break cohesive bonds.
- **Frictional contribution** = from the inner friction between particles.
3. Results on granular gouge behavior

3.2 - Role of inter-particular cohesion

Frictional Energy \geq\ Dilatancy Energy \geq\ Decohesion Energy

Energy Budget – new definition

**Dense sample:** more energy needed after 40% cohesion. But cohesion doesn’t seem to have a big influence on energy budget.

**Mid-dense sample:** energy needed by the system decreases from 0 to 100% cohesion, getting closer to the energy needed by a denser sample.

What part in Fracture Energy? How can we relate this new Energy budget and Fracture Energy?
3. Results on granular gouge behavior

3.2- Role of inter-particular cohesion

- **For small or non-cohesive gouge** [0 – 10% cohesion]
  Mechanical behaviour of the granular gouge is similar between 0 and 10% cohesion, we can conclude that the effect of cohesion is negligible below 10% for the given experimental conditions. Cohesive bonds break very quickly when the upper wall is set in motion, reducing the tests to standard tests without cohesion. Normal stress and imposed velocity on the upper rock wall generate larger efforts in the gouge than the inter-particular cohesion.

- **For cohesive gouge** [>10% cohesion]
  The observed peak of friction is much more important because, before expanding, the system must be able to break cohesive bonds. Once the sample is "fractured", the gouge will expand and tend towards an average friction value on steady-state part, similar to the one observed for cases without cohesion. Cohesive bonds are however always present after the friction peak, maintaining clusters of cohesive grains inside the gouge. Solid fraction decreases in the case of a very cohesive gouge, and fracture opening can lead to a more permeable gouge.

- Friction differences between dense and mid-dense sample increase with a higher percentage of cohesion. A denser sample presents higher friction coefficient, but shear band localisation tend to break the gouge in a different way. (Marone et al 1990) remind us that granular fault gouges involving dilation during shear produce velocity-strengthening frictional behaviour. (Beeler et al, 1996) also reported that friction velocity can be related to dilatancy rate. Strengthening behaviour is observed for higher dilatancy and Riedel shear bands R1. However, a higher cohesion seems to bring closer energy budget of dense and mid-dense samples.

- Cohesion also increases this strengthening behaviour, cementing the initial sample. Knowing the cohesion within the gouge can let us have a better idea of the strengthening or weakening behaviour of a granular fault gouge. Studying more in details friction peak could give us information about dynamic of the gouge, and link microstructures to seismic and aseismic behaviours.
4- Conclusion and perspectives

- 2D Discrete Element modelling with angular and faceted shapes
- Role of cohesion in the mechanical behaviour of the granular gouge
  - A certain percentage of cohesion is needed to affect the gouge (>10%)
  - The increase of cohesion changes fracturation mechanisms inside the granular gouge and leads to brittle behaviours.
  - During the peak zone, the energy budget of the gouge get closer for dense and mid-dense samples after 40% of cohesion.
- On-going work on a new definition of energy budget and fracture energy linked to micro-mechanical behaviour

- Next:
  - Represent mineral matrix between particles, and study the shear band localisation
  - Rock walls need to be deformable to represent stiffness of the loading apparatus
    → New model with elastic medium and pressure gradient to simulate the increase of pore pressure and observation of slip triggering
Bibliography

Bibliography