

F. Alonso-Marroquín*

*ESSCC, The University of Queensland, Qld. 4068, Brisbane, Australia and
National Technical University of Athens, 5 Heroes of Polytechnion, 15773, Athens, Greece*

I. Vardoulakis

National Technical University of Athens, 5 Heroes of Polytechnion, 15773, Athens, Greece

H. J. Herrmann

ICP, University of Stuttgart, Pfaffenwaldring 27, 70569, Stuttgart, Germany

D. Weatherley and P. Mora

ESSCC, The University of Queensland, Qld. 4068, Brisbane, Australia

(Dated: March 15, 2006)

Sliding and rolling are two outstanding deformation modes in granular media. The first one induces frictional dissipation whereas the latter one involves deformation with negligible resistance. Using numerical simulations on two-dimensional shear cells, we investigate the effect of the grain rotation on the energy dissipation and the strength of granular materials under quasistatic shear deformation. Rolling and sliding are quantified in terms of the so-called *Cosserat rotations*. The observed spontaneous formation of vorticity cells and clusters of rotating bearings may provide an explanation for the long standing heat flow paradox of earthquake dynamics.

I. INTRODUCTION

The micromechanics of heat production by friction in granular materials has become an important issue in the study of earthquake mechanics. One of the unresolved controversies in this field is a phenomenon that geophysicists call the heat-flow paradox [1]. According to common sense, when two blocks grind against one another, there should be friction, and that should produce heat. However, measurements of heat flow during earthquakes are unable to detect the amount of heat predicted by simple frictional models. Calculations using the value of rock friction measured in the laboratory, i.e. a typical friction coefficient between 0.6 and 0.9 [2], lead to overestimation of the heat flux. As an example one refers in this context to the heat flow observations made around the San Andreas fault, which show that the effective friction coefficient must be around 0.2 or even less [3]. One possible scenario for the explanation of these observations is the mechanism of heat-induced pore-fluid pressure increase [3–5]. Other mechanisms have been also discussed [1, 6, 7]. At any rate, with or without pressurization, the correct assessment of frictional heat production during shear is a central issue. Here we will address this issue by resorting to the micromechanics of dry granular media representing the gouge, i. e. the shear band consisting of fragmented rock inside the fault zone.

The formation of rolling bearings inside the gouge has been introduced as a possible explanation for a substantial reduction of the effective friction coefficient [6]. This simplified picture assumes that the gouge is filled with

more or less round grains which, as the plates move, can roll on each other thus reducing the amount of frictional dissipation. Granular dynamics simulations [1, 8, 9] and Couette experiments [10] have demonstrated the spontaneous formation of such bearings.

The overall effects of grain rotation are studied here using granular dynamics simulations. We show that particle rotation induces a phase separation in the granular media in terms of three coexisting phases: (1) Vorticity cells, (2) rotational bearings and (3) slip bands. The first two phases reduce significantly the frictional strength and the dissipation with respect to the hypothetical case of simple shear. We quantify these phases in terms of the so-called *Cosserat rotations*. We address the necessity to introduce these variables for the constitutive modeling of fault gouge. In Secs II and III we present the theoretical background and the particle-based model. In Sec. IV the effect of particle rotation on the strength and frictional dissipation is investigated. In Sec. V we calculate the population of the three coexisting phases using the homothetic-antithetic decomposition of the Cosserat rotations.

II. COSSERAT CONTINUUM

In the framework of continuum mechanics, the mathematical description of granular rolling and sliding is a challenging task. We notice first that classical continuum theories introduce the concept of the material point as a representative assembly of grains and ascribes to it only the degrees of freedom of displacement, which in turn are correlated to the displacements of the grains of the assembly. Thus classical continuum theory makes no provision for particle rotation. More recent continuum

*Electronic address: fernando@esscc.uq.edu.au

models include the rotational degrees of freedom by using the so-called Cosserat rotations [11–14]. These are continuum field variables, measuring the relative particle rotations with respect to the rotational part of the displacement-gradient field. The name of these variables gives tribute to the brothers Cosserat (1909) who were the first to propose such a continuum theory. 50 Years after the first publication of the original work [10], the basic kinematics and static concepts of Cosserat continuum were reworked in a milestone paper by Günther [15]. Günther’s paper marks the rebirth of micromechanics in the 1960s. Following this publication, several hundred of papers were published on the subject of micromechanics of granular media [16]. The growing interest in the Cosserat theories in recent years followed the link that was made by Mühlhaus and Vardoulakis [14] between the Cosserat continuum and the onset of shear-bands in granular materials. Observations of particle rotations from particle-based and continuum-based computer models [17] and physical experiments [18] show that inside shear- and interface-bands the particles rotate differently as their neighborhood. These findings demonstrated the necessity to introduce the Cosserat rotations as additional field variables in the shear-band evolution. These new variables involved also a characteristic material length that allows in turn to reproduce the characteristic width of shear bands. This internal length has special significance from the computational point of view, because it resolves the mesh-dependency problems in the Finite Element simulations [19, 20].

At any material point of the Cosserat continuum we assign a velocity \vec{v} and a spin vector $\vec{\omega}$. Accordingly in plane-strain deformation the kinematic fields are: the classical strain-rate tensor, which corresponds to the symmetric part of the average particle velocity :

$$D_{ij} = \frac{1}{2} \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right), \quad (1)$$

and the Cosserat rotation, that is given by the difference between the macro- and micro-rotations:

$$W = \frac{1}{2} \left(\frac{\partial u_x}{\partial y} - \frac{\partial u_y}{\partial x} \right) - \omega, \quad (2)$$

This variable can be calculated as the difference between the rotation of the branch vector - defined as the line connecting particle mass centers - and the rotation of the particle, averaged over all pair contacts in the representative volume element.

III. PARTICLE-BASED MODEL

We will investigate the discrete counterpart of the Cosserat rotations by using granular dynamics simulations. The discrete model consists of disks confined between two horizontal plates. A normal force is applied on

the plates, as they are moved in opposite directions with a constant velocity. Periodic boundary conditions are imposed along the horizontal direction, see Fig. 1. This geometry is a simplified model of a gouge. Real rock gouge consists of non-spherical particles. In the present model we are able to simulate two extreme cases: The first one represents a young fault, which is characterized by a strong interlocking of closely packed rocks in the gouge. This case is simulated by hindering the rotation of the disks. In the second case we allow the particles to rotate without rolling resistance. This is an idealization of mature gouges, where the interlocking and the rock asperities are reduced due to grain fragmentation.

The discrete model is a 2D implementation of the Lattice Solid Model [1, 21, 22]. This is a suitable platform to investigate the dynamics of fault gouge via granular dynamics simulations. Two disks of radii R_i and R_j interact when the distance between their centers of mass r_{ij} is less than the sum of their radii. Their interaction is given by the viscoelastic contact force

$$\vec{f}^c = k_n \Delta x_n \vec{n} + k_t \Delta x_t \vec{t} + \delta_0 m (\gamma_n v_n^c \vec{n} + \gamma_t v_t^c \vec{t}) \quad (3)$$

The first two terms are elastic forces, and the last two are viscous forces. The unit normal vector \vec{n} points in the direction of the vector connecting the center of mass of the two disks. The tangential vector \vec{t} is taken perpendicular to \vec{n} . The elastic material constants are the normal k_n and tangential k_t grain contact stiffnesses. The normal elastic deformation is the overlapping length $\Delta x_n = R_i + R_j - r_{ij}$. The tangential elastic deformation is chosen to be consistent with the Coulomb sliding condition as follows: When two particles come into contact we set $\Delta x_t = 0$. Then, at each time t , we guess a new value for the tangential elastic deformation as:

$$\Delta x_t^p(t) = \Delta x_t(t - dt) + v_t^c dt, \quad (4)$$

where v_t^c is the tangential relative velocity at the contact:

$$v_t^c = \omega_i R_i + \omega_j R_j + (\vec{v}_i - \vec{v}_j) \cdot \vec{t}. \quad (5)$$

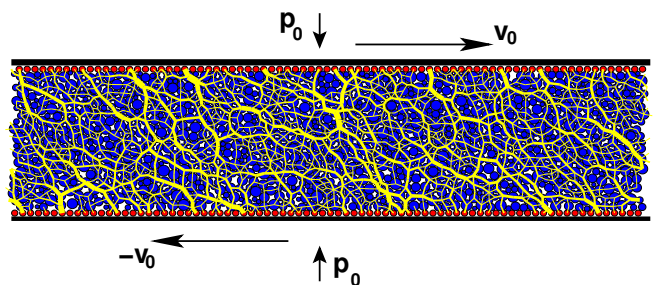


FIG. 1: Contact network in the shear cell at critical state. The lines represent the branch vectors; the width of the lines the normal contact force.

Here \vec{v}_i is the velocity and ω_i is the angular velocity of the particles in contact. The predicted value of elastic deformation should be corrected to satisfy the Coulomb sliding condition $|f_t^e| < \mu f_n^e$, where f_t^e and f_n^e are the tangential and normal component of the elastic force and μ is the friction coefficient. This condition equates to:

$$\Delta x_t(t) = \text{sign}(\Delta x_t^p(t)) \min\left(\frac{\mu k_n \Delta x_n(t)}{k_t}, |\Delta x_t^p|\right). \quad (6)$$

The viscous force in Eq. (3) assures the restitution between colliding particles. γ_n and γ_t are coefficients of viscosity, and the harmonic mean $m = (1/m_i + 1/m_j)^{-1}$ is the effective mass of the disks. The normal and tangential components of the relative velocity at the contacts are $v_n^c = (\vec{v}_i - \vec{v}_j) \cdot \vec{n}$ and v_t^c given by Eq. (5). The factor $\delta_0 = \Delta x_n/R_0$ is included in Eq. 3, to guarantee continuity of the viscous force during collision. R_0 is the averaged radius of the disks.

The roughness of the driving plates is modeled by attaching particles to it. Their vertical displacement is controlled with a simple viscoelastic force $f^b = k_n \delta + \gamma_n m_i v_n^c$, where δ is the overlapping length and v_n^c is the relative normal velocity. The attached disks are not allowed to rotate and their horizontal velocity is set to the velocity of the plates.

Each contact contributes to a direct force \vec{f}^c and a torque $\tau^c = R_i \vec{f}^c \cdot \vec{t}$ in the equation of motions. The model does not include gravitational forces, but a viscous force $\vec{f}_i^v = \gamma m_i \vec{v}_i$ and a torque $\tau = \gamma m_i R_i^2 \omega_i$ is included for each particle. This viscous forces allow relaxation of particles without contacts. We use the Verlet method for solving the equations of motion [23].

The efficiency of the simulation is mainly determined by the method of contact detection. Our method searches in each step the contacts in a list of *neighbours* that is called a Verlet List. This list is constructed by taking the pair particles whose distance of their center of mass satisfies the constraint $r^{ij} < R_i + R_j + \delta$. The Verlet List is updated when the maximal displacement of the particles since the last update is larger than $\delta/2$. The parameter δ is chosen by making a compromise between the storage (size of the Verlet List) and the compute time (frequency of list updates). A Linked Cell algorithm is used to allow a rapid calculation of the new Verlet List [24].

The material constants of the model are the normal stiffness $k_n = 1$; the tangential stiffness $k_t = 0.1$; the normal $\gamma_n = 0.001$ and tangential $\gamma_t = 0.0001$ damping frequency and the body viscosity $\gamma = 0.0001$. The density of the disks $\rho = 1$; and the friction coefficient whose default value is $\mu = 0.5$. The control parameters are the applied pressure $p_0 = 0.001$, and the velocity of the plates $v_0 = 10^{-6}$. The time step is $\Delta t = 0.05$. The most relevant parameter of this model is the ratio between the shear velocity v_0 and the velocity of compressional waves, which in our model is $v_p \sim R_0 \sqrt{k_n/m}$. In our simulation $v_p \sim 1$ so that $v_p/v_0 \sim 10^6$. This value

should be compared to the ratio in realistic fault zones, where $v_p \sim 1 \text{ Km/s}$ and $v_0 \sim 1 \text{ cm/year}$ leading to a factor of $v_p/v_0 \sim 10^{10}$. To remedy this discrepancy of time scales we use the quasistatic limit: The velocity is chosen low enough so that the reduction of it by half affects the effective friction coefficient by less than 5%.

IV. EFFECT OF PARTICLE ROTATION

Here we address the question of how particle rotation affects the mechanical response of the shear cell. Simulation of shear cells with rotating and non-rotating disks are compared by calculating the power dissipation and the stress ratio at the limit of large shear deformation. Each shear cell consists of 1600 disks with random sizes between $0.5R_0$ and $1.5R_0$. The length of the cells is $80R_0$. We start from a loose packing that is compressed by applying a constant pressure at the top plate. After a short collisional regime the sample reaches an equilibrium configuration where the kinetic energy decreases exponentially with time. After this stage the sample is sheared by applying a horizontal velocity v_0 at the top plate and $-v_0$ at the bottom. The simulations are performed by taking microscopic friction coefficients between 0.0001 and 8. These values should be compared with the friction of realistic materials, which ranges from 0.0001 for super-lubricated surfaces to 1.2 for rubber-concrete contact surfaces.

All samples reach a limit state for large shear deformation. This state resembles the so-called critical state of soil mechanics [25]. As shown the Fig. 2, the stress and the void ratio reach a constant value besides some fluctuations. These fluctuations result from the characteristic stick-slip dynamics of the shear cell: In the stick phase, the elastic energy is stored in force chains. These chains build up during the slow relative motion of the plates. The elastic energy is released in form of *quakes*. Each quake corresponds to the collapse of a force chain which is reflected by an abrupt drop of the macroscopic stress and a sudden compaction of the sample. The collapse of force chains leads to reorganization of the particles and hence acoustic emission. This is detected from the acceleration of a single particle in the sample, see part (d) of Fig. 2. Between two quakes the buckling of forces chains leads to an overall elastoplastic response with constant increase of void ratio.

The strength of the shear cell in the critical state can be quantified by an effective friction coefficient $\mu^* = F_t/F_n$. Here F_n and F_t are the normal and tangential force acting on the top plate. Part (a) of Fig. 2 shows the time evolution of μ^* . Typically this value increases in the interval between two quakes, and it drops during the quakes, leading to time fluctuations which are of the same order as the time average value $\mu_s = \bar{\mu}^*$.

The dependence of μ_s on the microscopic friction coefficient for rotating and non-rotating disks is plotted in part (a) of Fig. 3. For small values of μ the strength

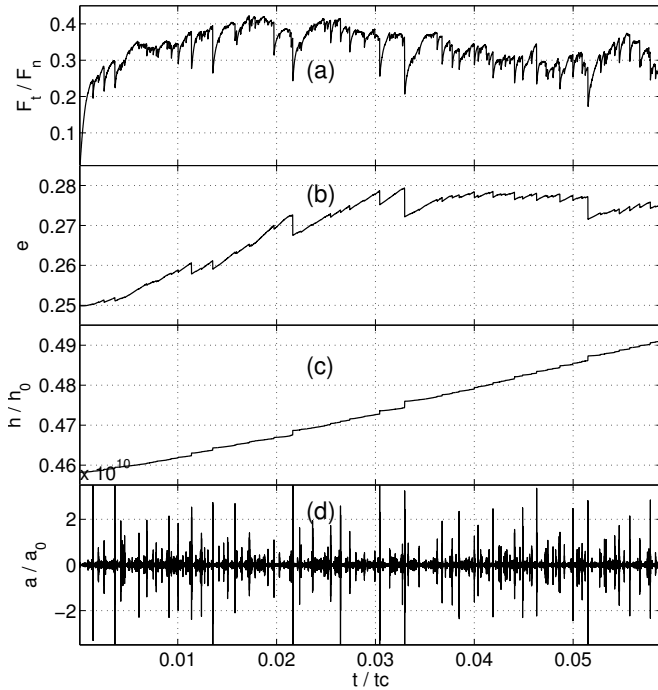


FIG. 2: Time profiles of (a) ratio between the normal and tangential force acting on the plates, (b) void ratio, calculated as $e = (A - A_d)/A_d$, where A is the area of the cell and A_d is the total area occupied by disks, (c) frictional dissipation normalized by $h_0 = Lp_0v_0t_c$ and (d) acceleration of one disk in the center of the cell, normalized by $a_0 = L/t_c^2$. The time is normalized by $t_c = L/v_0$

of the shear cells is not affected by grain rotation. In both cases the effective friction coefficient is larger than μ . This is due to the addition of an interlocking strength component to the shearing friction component. In the limit case $\mu \rightarrow 0$ the effective friction tends to 0.1, showing that interparticle friction is not the only origin of the macroscopic frictional behavior of granular materials.

For large values of μ particle rotation has a significant effects on the strength of the shear cell. Particularly, in the range $0.28 < \mu < 1.42$ samples with rotating disks have a macroscopic friction coefficient lower than the contact friction coefficient. On the other hand, the macroscopic friction coefficient is larger than the contact friction coefficient for non-rotating disks. In the limit $\mu \rightarrow \infty$, the strength of both samples tends to a constant value, This value is 0.34 for rotating disks samples and 1.43 for non-rotating disks.

We now turn to the effect of grain rotation on dissipation. Energy loss in the sample results from frictional and viscous dissipation. In our simulations, viscous dissipation takes place only in the collisional regime, which applies only during the phase of sample preparation. In the quasistatic phase and as the sample reaches the critical state, the frictional dissipation is at least three orders of magnitude larger than the viscous dissipation. There-

fore the produced heat can be calculated as:

$$h = \int P(t)dt, \quad (7)$$

where P is frictional power dissipation. This quantity is calculated as the sum of the tangential force times the sliding velocity of all the contacts.

$$P(t) = \sum_c f_t^c (v_t^c - \frac{d(\Delta x_t^c)}{dt}), \quad (8)$$

where f_t^c is the tangential contact force; v_t^c the tangential relative velocity at the contact and Δx_t^c the elastic part of the tangential displacement as defined by Eq. (6). The heat versus time is plotted in part (c) of Fig. 2 for

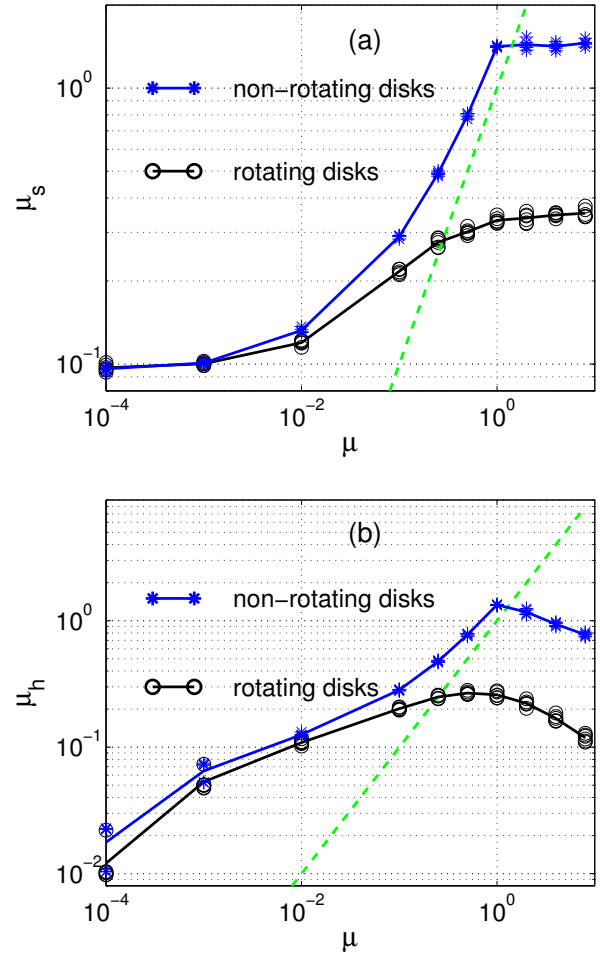


FIG. 3: Dependence of the (a) effective friction coefficient and (b) frictional power coefficient on the microscopic friction coefficient for rotating and non-rotating particles. Data of five different samples are superposed. Solid lines represent the linear interpolation around the averaged value. dashed line corresponds to $\mu_s = \mu$ and $\mu_h = \mu$.

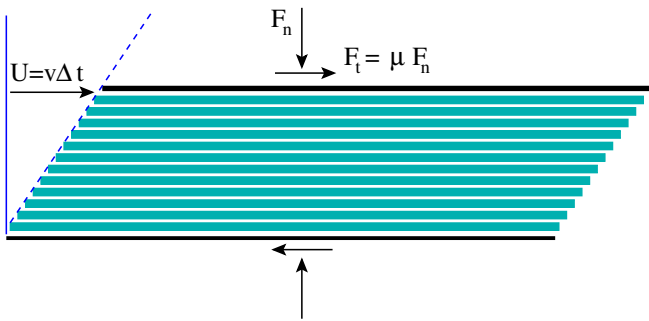


FIG. 4: Simple shear model of gouge deformation.

rotating particles with $\mu = 0.5$. The general trend of the heat is to increase slowly between two quakes, and rapidly during quakes.

The calculated heat should be compared to the theoretical energy dissipation of simple shear, which reads:

$$h_{th} = \mu F_n v \Delta t, \quad (9)$$

where μ is the microscopic friction coefficient, F_n the normal force on the plates, $v = 2v_0$ the relative velocity of the plates and Δt is the time interval. The value of Eq. (9) is calculated according to the model shown in Fig. 4. This model corresponds to the simple shear of a multilaminate with interlaminate friction equal to μ . To compare this value to the calculated power dissipation $P(t)$, we introduce the frictional power coefficient as $\mu_h = P(t)/P_0$, where $P_0 = F_n v$ and $P(t)$ is the time average along the critical state regime. Note that $\mu_h = \mu$ when the measured heat coincides with the theoretical value.

Part (b) of Fig 3 shows the dependency of the frictional power coefficient on μ . Heat production assumes a maximal value at $\mu = 0.5$ for rotating particles and $\mu = 1.0$ for non-rotating particles. In both cases the dissipation tends to decrease for $\mu \rightarrow 0$ and $\mu \rightarrow \infty$. In the first case because $f_t \rightarrow 0$ and in the second case because the fraction of sliding contacts is very small for large microscopic friction coefficients.

For small values of μ heat production is not affected by particle rotation, but for larger values it is affected by almost one order of magnitude. In both cases heat production is quantitatively different from the value of simple shear. Small friction coefficients lead to a dissipation larger than the theoretical one. This is due to the large population of sliding contacts in this regime, and their relative orientation with respect to the principal direction of load, which leads to tangential forces larger than the expected value for simple shear. For large friction coefficients few contacts can reach the sliding condition, so that the dissipation is much lower than that one expected for simple shear.

The displacement field confirms that the picture of simple shear (Fig. 4) is also not supported. In part (a) of Fig. 5 we plot the displacement field for non-rotating

particles when $\mu = 0.5$. We observe the formation of blocks of particles moving approximately as a whole. The boundaries between these blocks are not flat, but curved. This produces strong interlocking, that explains the considerable increase of the strength of the material with respect to simple shear. Note that these blocks can not slide against each other for very long without changing shape. The reorganization of these structures appears by means of large quakes. These quakes change completely the displacement fields, even when the position of the particles stays approximately the same.

If the particles are allowed to rotate, vorticities appear spontaneously. They are shown in part (b) of Fig 5. These vorticities are accompanied by strong temporal fluctuations of the displacement field, but they can appear and disappear intermittently in the same zone. The vorticity field has been observed in many numerical simulations [26, 27]. It resembles to some extent the turbulent regime observed in fluids, but their dynamics is quite different [28]: Fluids under slow motion present a laminar regime where the mass displacements can be considered as simple shear. On the other hand, our shear cells develop large vorticities even in the quasi-static regime, ruling out the simple shear deformation regime. The short lifetime of these vorticities, typically the same as the interval between two large quakes, contrasts to the large lifetime of the eddies in turbulent flow. Thermal measurements in dynamic shear-banding on metals also reveals that homogeneous shear is not possible and vortices are the rule [29].

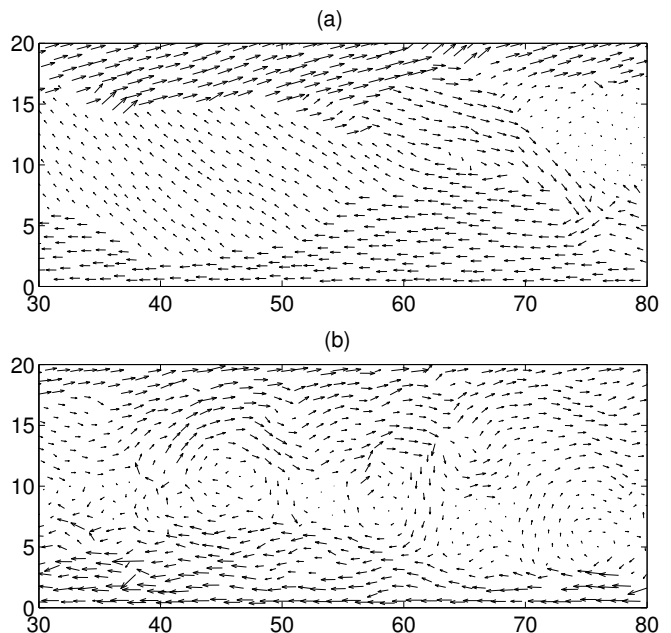


FIG. 5: Snapshot of the displacement field for (a) non-rotating and (b) rotating grains. The friction coefficient is $\mu = 0.5$.

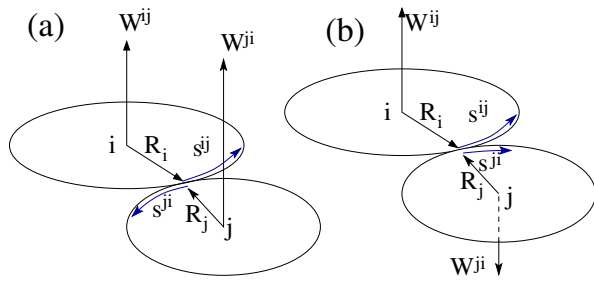


FIG. 6: homothetic (a) and antithetic (b) couple of the Cosserat rotations.

The spatial distribution of vorticity cells, when combined with the distribution of rolling, provides a novel picture of bearings: Inside vorticity cells all particles rotate as a rigid body, whereas the space between the vorticity cells is characterized by intense relative rotations. This leads to clusters of rotational bearings and zones of intense slippage. We will quantify the contribution of these modes to global deformation by performing a kinematic decomposition of the contact deformation. This decomposition will distinguish rolling from sliding and from the rigid body motion of the vorticity cells.

V. MEASURE OF ROLLING

Several definitions of rolling can be found in the literature [30–32]. They are taken as measures of contact deformation for each pair of interacting particles. Kuhn and Bagi decompose the degrees of freedom of the two particles into rigid body motion and objective motion [31]. Then the rolling is defined as the average of the objective translation at each side of the contact point [32]. Based on these studies, we introduce a new definition of rolling in terms of the rotation and translation of the particles in contact. This definition will be consistent with the fact that rolling allows deformation in the assembly without frictional dissipation or accumulation of elastic energy.

Let us suppose that at time t two particles indexed by i and j are in contact, and they stay in contact during an infinitesimal time interval dt afterward. We introduce a system of coordinates \vec{n}^{ij} , \vec{t}^{ij} , \vec{z}^{ij} attached to the contact. The unit normal vector \vec{n}^{ij} connects the center of mass of the particle i to that of the particle j :

$$\vec{n}^{ij} = \frac{\vec{x}_j(t) - \vec{x}_i(t)}{|\vec{x}_j(t) - \vec{x}_i(t)|} \approx \frac{\vec{x}_j(t) - \vec{x}_i(t)}{R_i + R_j}. \quad (10)$$

The latter approximation is valid when $\Delta x_n \ll d$, where Δx_n is the overlapping length and d the characteristic diameter of the disks. The unit vector \vec{z}^{ij} is perpendicular to the plane of the disks, and the unit tangential vector satisfies $\vec{t}^{ij} = \vec{z}^{ij} \times \vec{n}^{ij}$.

Let us consider two points attached to each particle, in a region infinitesimally near to the contact point. The tangential velocity of these points are given in terms of the linear \vec{v}_k and angular ω_k velocities of the particles:

$$\begin{aligned} v_{i,t}^c &= \vec{v}_i \cdot \vec{t} + \omega_i R_i \\ v_{j,t}^c &= \vec{v}_j \cdot \vec{t} - \omega_j R_j. \end{aligned} \quad (11)$$

Let us take the movement of the branch vector. i.e the vector connecting the center of mass of the two particles. The tangential component of the velocity of a point attached to the branch vector at the contact will be called *rigid body velocity*:

$$V_{rb}^{ij} = \frac{(\vec{v}_i R_j + \vec{v}_j R_i) \cdot \vec{t}}{R_i + R_j}. \quad (12)$$

If the two particles move as a rigid body, the velocity coincides with Eqs. (11). Otherwise there is a relative velocity between the two points attached to the particles. This velocity can be calculated by subtracting the rigid body like velocity of Eq. (12) from the contact velocities of Eqs. (11):

$$\begin{aligned} s^{ij} &= v_{i,t}^c - V_{rb}^{ij} \\ s^{ji} &= v_{j,t}^c - V_{rb}^{ij} \end{aligned} \quad (13)$$

These velocities can be given in terms of linear and angular velocities by using Eqs. (11) and (12):

$$\begin{aligned} s^{ij} &= \omega_i R_i - \frac{R_i}{R_i + R_j} (\vec{v}_j - \vec{v}_i) \cdot \vec{t}^{ij}, \\ s^{ji} &= -\omega_j R_j + \frac{R_j}{R_i + R_j} (\vec{v}_j - \vec{v}_i) \cdot \vec{t}^{ij}. \end{aligned} \quad (14)$$

They will be called *objective velocities* of the two particles at the contact. These velocities are *objective* in the sense that their magnitude is unaffected by the common rigid-body motion of the particle pair. In particular, these measures are not affected by a change of the reference frame. The objective velocities vanish if, and only if, the two particles move as a rigid body. Otherwise the objective velocities involve rolling, sliding or accumulation of shear strain at the contact.

We will relate these *objective velocities* to the aforementioned Cosserat-continuum rotations. At the micromechanical level, the later are defined as the relative rotation of the particle with respect to the rotation of the branch vector around the axis parallel to \vec{z}^{ij} at the contact point [33]:

$$\begin{aligned} W^{ij} &= \omega_i - \Omega^{ij}, \\ W^{ji} &= \omega_j - \Omega^{ij} \end{aligned} \quad (15)$$

where ϕ_i is the angular velocity of the particle i with radius R_i . Ω^{ij} is the rotational velocity of the branch vector:

$$\Omega^{ij} = \frac{(\vec{v}_i - \vec{v}_j) \cdot \vec{t}^{ij}}{R_i + R_j} \quad (16)$$

Replacing Eq. (16) into Eqs. (15) and comparing the result with Eqs. (14) we obtain a relation between the Cosserat rotations and the objective velocities.

$$s^{ij} = R_i W^{ij} \quad s^{ji} = -R_j W^{ji} \quad (17)$$

These equations provide an interesting connection between the relative orientation of the Cosserat rotation and rolling: When the Cosserat rotations are in a *homothetic couple* as shown part (a) of Fig. 6, the objective velocities s^{ij} and s^{ji} have opposite signs. In this case, depending on whether the contact is or not in the sliding condition, the contact deformation result either in frictional dissipation or in accumulation of elastic energy, without rolling deformation. Homothetic couples appear in several cases: If the two disks in contact rotate in the same sense without linear velocity, the Cosserat rotations reads $W^{ij} = \omega_i$ and $W^{ji} = \omega_j$. If the particles do not rotate, the Cosserat rotations are given by $W^{ij} = W^{ji} = \Omega^{ij}$. In both cases they are in a homothetic couple, and hence there is no rolling deformation.

The appearance of rolling between the particles is linked to the *antithetic couple* of the Cosserat rotations. This couple is shown in part (b) of Fig. 6. In this case the rolling is given by the common part of the objective velocities, i. e. $\min(|s^{ij}|, |s^{ji}|)$. In particular, if the Cosserat rotations satisfy $W_i R_i + W_j R_j = 0$ both grains have the same objective velocity. Therefore the contact deformation does not accumulate elastic deformation or produce frictional dissipation, and hence the deformation corresponds to pure rolling.

In the general case the objective velocities should be decomposed into rolling and dislocation. The first one results in:

$$V_{roll}^{ij} = \begin{cases} 0 & \text{homothetic couple} \\ \min(|s^{ij}|, |s^{ji}|) \text{sign}(s^{ij}) & \text{antithetic couple,} \end{cases} \quad (18)$$

and the dislocation is given by the difference of the objective velocities:

$$V_{dis}^{ij} = s^{ij} - s^{ji}. \quad (19)$$

Using the identity $s^{ij} - s^{ji} = v_{i,t}^c - v_{j,t}^c$, it is easy to prove that the dislocation velocity corresponds to the relative tangential velocity defined in Eq. (5). In the limit of rigid disks, where elastic deformation at the contact is absent, the dislocation velocity coincides with the sliding velocity. In granular dynamics an elastic shear deformation is allowed, so that the sliding velocity is given by:

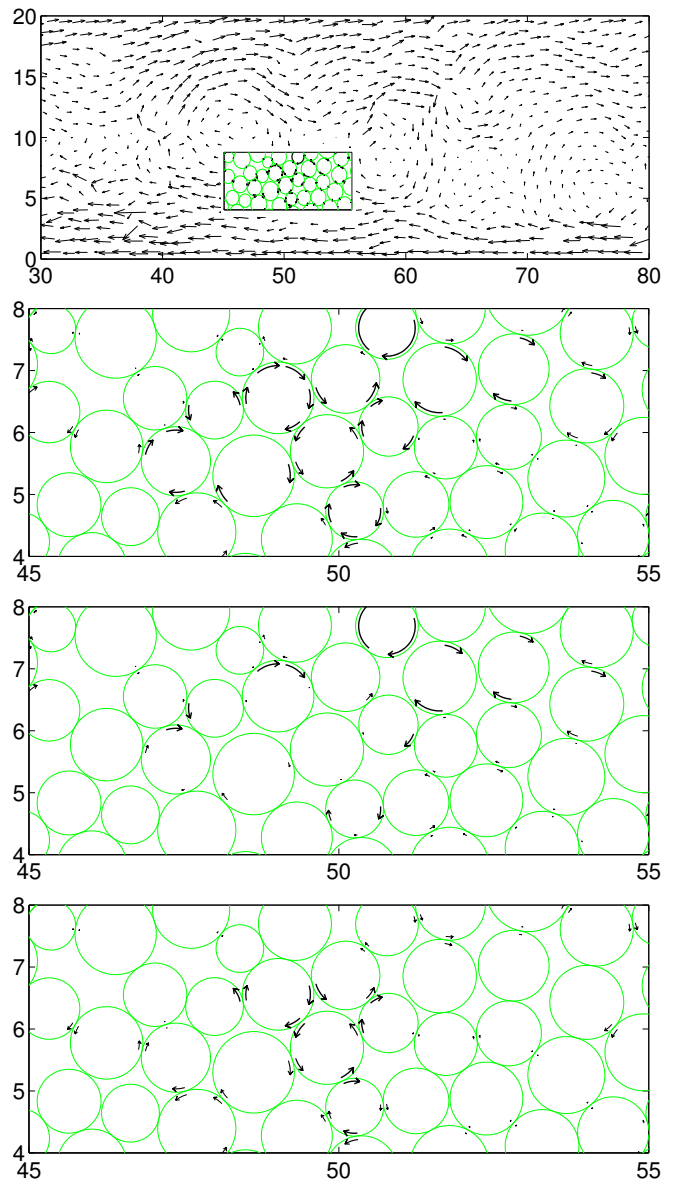


FIG. 7: Snapshot of (a) vorticity field, (b) objective velocities at the contacts as shown the inset in part (a), and their decomposition in (c) dislocation and (d) rolling. The sample consists of rotating grains with $\mu = 0.5$.

$$V_{slid}^{ij} = V_{disl}^{ij} - \frac{d(\Delta x_t)}{dt}, \quad (20)$$

where Δx_t is the elastic part of the tangential displacement at the contact, that is given by Eq. (6). According to Eq. (8) the sliding velocity times the tangential force corresponds to the frictional dissipation. The second term of Eq. 20 involves accumulation of elastic energy.

The Cosserat rotations turn out to be a suitable *or-*

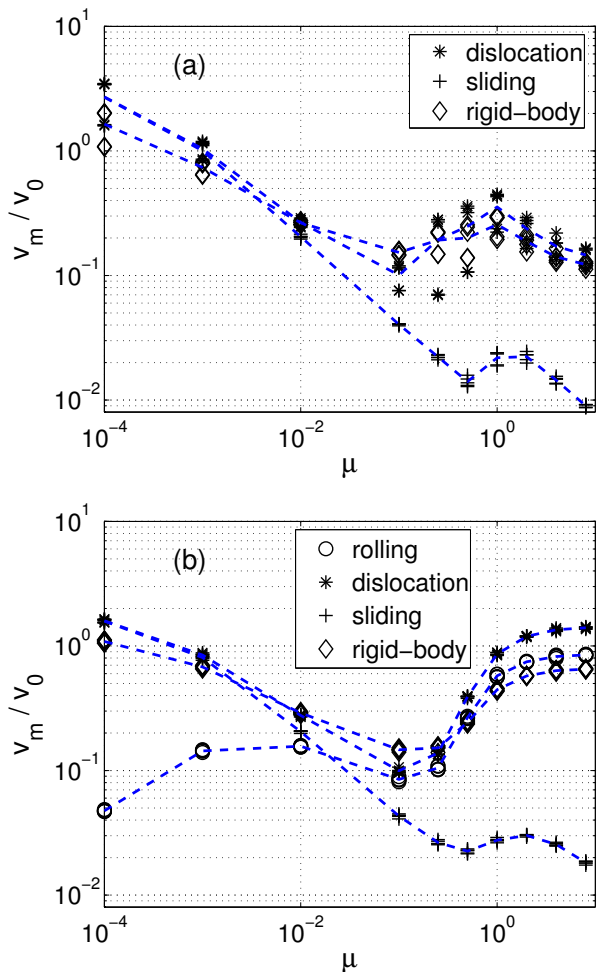


FIG. 8: Decomposition of kinematic roles for (a) non-rotating and (b) rotating particles, as function of μ . They are calculated from the average of the absolute value of the rolling, dislocation, sliding and rigid body velocities at the contacts. Data of five different samples are superposed.

der parameter to describe the vorticities and bearings in the shear deformation: As shown in Fig. 7, the spatial distribution of these structures is not just random, but strong correlations appear in form of three coexisting phases: (1) Vorticity cells, where the particles rotate almost as a whole, so that the Cosserat rotation is vanishingly small, (2) clusters of particles with intense rolling (rotational bearings), where the Cosserat rotations are antithetic, and (3) zones between particles with intense dislocation (microbands), characterized by homothetic couples of the Cosserat rotations. Microbands induce frictional dissipation and accumulation of elastic energy, whereas the rotational bearings accommodate the vorticity cells to make them more compatible with the imposed kinematic boundary conditions.

The microscopic friction coefficient can serve as a control parameter of the relative population of these three

phases. This is shown in Fig. 8 for (a) non-rotating and (b) rotating particles. In both cases the sliding displacement and rigid body velocities are the dominant deformation modes for small values of μ . In this regime, the dislocation velocity coincides with the sliding velocity, because almost all the contacts are in the sliding condition. Deformation in this case is characterized by small clusters of particles moving against each other through microbands of intense sliding. For rotating particles the rolling is much lower than the other deformation modes, whereas the rolling is absent for non-rotating grains.

For large friction coefficients the sliding velocity becomes negligible, because few contacts are able to reach the sliding condition. In this regime, depending on whether the particles are or not allowed to rotate, the population of the deformation modes is quite different: for non-rotating particles, the contact deformation is dominated by rigid-body motion and elastic dislocation. The latter one builds up elastic energy that is liberated in the form of strong quakes. The dependence of dislocation and rigid-body motion on μ is fairly weak. This reflects a self organization of the shear cells, characterized by a non-dependency of the effective friction coefficient on μ , already shown in part (a) of Fig. 3.

For rotating grains and large friction coefficients rolling plays a relevant role, as shown part (b) of Fig. 8. The deformation is dominated by rigid-body motion (due to the vorticities), rolling (due to the rotational bearings) and elastic dislocation (due to building of force chains). The self organization of the shear cells is given by the fact that rolling and vorticities are not affected by a change in the microscopic friction coefficient. The sliding turns out to be much smaller than the other modes, because only few contacts can reach the sliding condition. Therefore the dislocation results almost completely in accumulation of elastic energy that is released in the form of quakes.

The details of the dynamics of one quake is shown in Fig. 9. We use a friction coefficient of $\mu = 0.5$. We observe a small time interval (shock) characterized by a sudden decrease of the effective friction coefficient, along with an abrupt compaction and a rapid generation of heat. This is followed by a longer time interval (after-shock) given by an exponential decay of microseismic activity with almost no frictional dissipation. More details of the structure of the quake are visible by calculating the time evolution of the contact modes of deformation. Part (e) of Fig. 9 shows that most of the contact deformation at the shock corresponds to rolling and rigid body deformation. In the after-shock the sliding velocities become vanishing small, whereas the other modes decay exponentially. Acoustic waves are generated at the point where the force chain fails. These waves travel through the sample and they are reflected as they reach the plates. After many reflections they become uncorrelated, which removes almost all contacts from the sliding condition. Therefore sliding velocity modes are not active in the aftershock, whereas the other modes decay exponentially in form of uncorrelated oscillations.

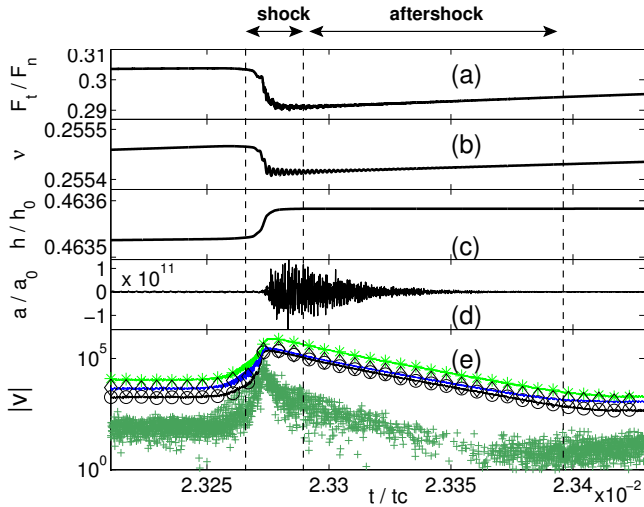


FIG. 9: Time evolution of (a) stress, (b) void ratio, (c) frictional dissipation, and (d) acoustic emission at the center of the sample. (e) Average of the absolute value of rolling (circles), dislocation (asterisks), sliding (crosses) and rigid body velocities (diamonds). The sample consists of rotating particles with $\mu = 0.5$.

As far as earthquakes is concerned, it is remarkable that only a minute part of the contact deformation during the quake corresponds to sliding. This leads to an effective friction coefficient around 0.25 which is lower than the contact friction coefficient of $\mu = 0.5$, see part (b) of Fig. 3. Therefore the introduction of rolling in the gouge dynamics could potentially explain the Heat Flow Paradox.

VI. CONCLUDING REMARKS

The most important contribution of this work is to show that spontaneous formation of vorticity cells assisted by rotational bearings is the mechanism of reduction of strength and frictional dissipation in shear cells. For the range of rock friction of $\mu = 0.6-0.9$, the effective friction coefficient increases from $\mu_s = 0.3$ to $\mu_s = 0.35$, whereas the frictional power coefficient decreases from $\mu_h = 0.28$ to $\mu_h = 0.22$. These results could explain the heat flow anomalies in fault gouges, where the macroscopic friction coefficient, as deduced from heat flow observations, is around one order of magnitude lower than the rock friction [3]. The existence of such rotational patterns confirm earlier speculations about the effect of rolling in the reduction of heat production by means of a self-organization process in fault gouge [1].

The effective friction coefficient and frictional power coefficient are strongly dependent on particle rotation. This reflects the necessity to introduce rotational degrees

of freedom in the continuum description of fault gouge. As deduced from the deformation field at the contacts, the Cosserat continuum approach should be consistent with the observed three phase separation of kinematic modes: (1) vorticity cells, where the Cosserat rotations are absent; (2) Bearings given by antithetic couple of the Cosserat rotations, and therefore a pronounced rolling at the contacts; and (3) microbands of homothetic couples, with pronounced dislocations, and hence, strong accumulation of elastic energy and high frictional dissipation. This description requires an extension of the existing Cosserat continuum models, which consider only homothetic couples of the Cosserat rotations [19, 20]. As far as dissipation is concerned, besides the Cauchy stress tensor, a couple stress tensor should be introduced as an additional static variable of the enhanced continuum, entering as the energetically dual counterpart of the gradient of the homothetic part of the Cosserat rotations [11, 13, 14, 34]. In this context numerical simulations can be used as a virtual laboratory to assist the development of micromechanical constitutive models.

An improved constitutive law for fault gouge will require integration of not only rolling, but also the contribution of grain fragmentation to the energy budget. Observations of fault zones suggest that earthquakes can pulverize rocks in the gouge [7]. This leads to a fractal grain size distribution and an increase of the gouge surface area. Some important issues concerning the heat flow paradox should be considered: Does fracture energy play an important role in the earthquake energy balance? and do such fractal gouges develop vortical structures and rotating bearings?.

There are also some aspects about the aseismicity of fault zones which deserve detailed study in a future work. Vortical structures and rotating bearings promote a coherent deformation which remains during two quakes. These may inhibit the large events we observe in samples with non-rotating grains. The dynamics of these rotational patterns will be significant in the understanding the enigmatic aseismic creep, where two tectonic plates move against each other without accumulating elastic energy or generating earthquakes [35, 36].

Acknowledgments

We thank S. Latham, H. Mühlhaus, A. Tordesillas, K. Bagi, H. Sakaguchi, Y. C. Wang and F. Froio for helpful discussions and acknowledge the support of the European DIGA project HPRN-CT-2002-00220 and the Australian Computational Earth Systems Simulator (ACcESS). HJH acknowledges support from the German-Israeli Foundation grant No.I-795-166.01/2003. Simulations were performed on the ACcESS SGI Altix 3700 supercomputer.

- [1] P. Mora and D. Place. The weakness of earthquake faults. *Geophys. Res. Lett.*, 26:123–126, 1999.
- [2] J. Byerlee. Friction of rocks. *Pure and Applied Geophysics*, 116(4-5):615–626, 1978.
- [3] A. H. Lachenbruch and J. H. Sass. Heat flow from cañon pass, fault strength, and tectonic implications. *J. Geophys. Res.*, 97(B4):4995–5015, 1992.
- [4] J. Rise. Heating and weakening of faults during earthquake slip. *J. Geophys. Res.*, 2006. in print.
- [5] J. Sulem, I. Vardoulakis, H. Ouffroukh, M. Boulon, and J. Hans. Experimental characterization of the thermo-mechanical properties of the aigion fault gouge. *Geoscience*, 336:455–466, 2004.
- [6] R. Mahmoodi-Baran, H. J. Herrmann, and N. Rivier. Space-filling bearings in three dimensions. *Phys. Rev. Lett.*, 92(4):044301, 2004.
- [7] B. Wilson, T. Dewers, Z. Reches, and J. Brune. Particle size and energetics of gouge from earthquake rupture zones. *nature*, 434:749–752, 2005.
- [8] J. A. Astrom, H. J. Herrmann, and J. Timonen. Granular packings and fault zones. *Phys. Rev. Lett.*, 84:4638–4641, 2000.
- [9] A. Zervos, I. Vardoulakis, M. Jean, and P. Lerat. Numerical investigation of granular kinematics. *Mechanics of Cohesive-Frictional Materials*, 5:305–324, 2000.
- [10] C. T. Veje, D. W. Howell, and R. P. Behringer. Kinematics of a two-dimensional granular couette experiment at the transition to shearing. *Phys. Rev. E*, 59(1):739–745, 1999.
- [11] W. Ehlers, E. Ramm, S. Diebels, and G. A. D’Addetta. From particle ensembles to cosserat continua: homogenization of contact forces towards stresses and couple stresses. *I. J. Solids Struct.*, 40(24):6681–6702, 2003.
- [12] I. Vardoulakis and J. Sulem. *Bifurcation analysis in geomechanics*, chapter 8, pages 281–283. Blakie Academic & Professional, London, 1995.
- [13] F. Froio and I. Vardoulakis. A continuum-like description of granular media. In *Powders & Grains 2005*, pages 135–139, Leiden, 2005. Balkema.
- [14] H.-B. Mühlhaus and I. Vardoulakis. The thickness of shear bands in granular materials. *Géotechnique*, 37:271–283, 1987.
- [15] W. Guenther. Zur Statik und Kinematik des Cosseratschen Kontinuums. In *Abhandlungen der Braunschweigischen Wissenschaftlichen Gesellschaft*, volume 10, pages 195–213, Goettingen, 1958. Boltze.
- [16] M. Satake. Some considerations on the mechanics of granular materials. In *IUTAM Symposium on the Mechanics of Generalized Continua*, pages 156–159, Freudenstadt-Stuttgart, 1967.
- [17] P. Papanastasiou and I. Vardoulakis. Bifurcation analysis of deep boreholes: II. scale effect. *Int. J. Num. Anal. Meth. Geomechanics*, 13:183–198, 1989.
- [18] P. Lerat. *Etude de l’Interface entre un Milieu Solide et un Milieu Granulaire à l’Aide d’ un Nouvel Appareil de Cisaillement Simple Annulaire*. PhD thesis, ENPC, Champs-sur-Marne, France, 1996.
- [19] P. Papanastasiou and I. Vardoulakis. Numerical treatment of progressive localization in relation to borehole instability. *Int. J. Num. Anal. Meth. Geomechanics*, 16(6):389–424, 1992.
- [20] J. Techman and E. Bauer. Numerical simulation of shear band formation with a polar hypoplastic constitutive model. *Computers and Geotechnics*, 19(3):221–244, 1996.
- [21] P. Mora and D. Place. Simulation of the frictional stick-slip instability. *Pageoph.*, 143:61–87, 1994.
- [22] S. Latham, S. Abe, and P. Mora. Macroscopic friction response of rotational and non-rotational lattice solid models in 2d and 3d. In *Powders & Grains 2005*, pages 213–217, Leiden, 2005. Balkema.
- [23] M. P. Allen and D. J. Tildesley. *Computer Simulation of Liquids*. Oxford University Press, Oxford, 1987.
- [24] T. Poeschel and T. Schwager. *Computational Granular dynamics*, chapter 2.4, pages 61–65. Springer, Berlin, 2004.
- [25] D. M. Wood. *Soil behaviour and critical state soil mechanics*. ISBN: 0-521-33782-8, Cambridge, 1990.
- [26] H. Sakagushi A. Murakami and T. Hasegawa. Dislocation, vortex and couple stress in the formation of shear bands under trap-door problems. *Soils and Found.*, 123-135(1), 1997.
- [27] M. R. Kuhn. Structured deformation in granular materials. *Mech. Mater.*, 21:407–429, 1999.
- [28] F. Radjai and S. Roux. Turbulent-like fluctuations in quasistatic flow of granular media. *Phys. Rev. Lett.*, 89(6):064302, 2002.
- [29] P. R. Guduru, R. Ravichandram, and A. J. Rosakis. Observations of transient high temperature vortical microstructures in solid during adiabatic shear banding. *Phys. Rev. E*, 64:036128, 2001.
- [30] H. M. Shodja and E. G. Nezami. A micromechanical study of rolling and sliding contacts in assemblies of oval granules. *Int. J. Numer. Anal. Meth. Geomech.*, 27:403–424, 2003.
- [31] M. R. Kuhn and K. Bagi. Alternative definition of particle rolling in a granular assembly. *J. Eng. Mech.*, 130(7):826–835, 2004.
- [32] K. Bagi and M. R. Kuhn. A definition of particle rolling in a granular assembly in terms of particle translations and rotations. *J. Appl. Mech.*, 71:493–501, 2004.
- [33] I. Vardoulakis and J. Sulem. *Bifurcation analysis in geomechanics*. Blakie Academic & Professional, London, 1995.
- [34] A. Tordesillas, S. D. C. Walsh, and B. S. Gardiner. Bridging the length scales: Micromechanics of granular media. *BIT Numerical Mathematics*, 44:539–556, 2004.
- [35] C. H. Scholz. Earthquakes and friction laws. *Nature*, 391:37–42, 1998.
- [36] T. I. Melbourne and F. H. Weeb. Slow but not quite silent. *Science*, 300:1886–1887, 2003.