Simulating deformations of granular solids under shear

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Abstract

We present MD simulations of shear cells of a densely packed array of polygonal grains in two dimensions. We study the dependence of the shear force on the shear velocity. Generally shear hardening is observed. The dependence of the dilatancy on the shear velocity is measured. We also apply the method to simulate two tectonic plates moving under shear. We find a Gutenberg–Richter-like law with a $b$-value of $(1.02 \pm 0.06)$ in good agreement with geophysical measurements. Shear bands of widths dependent on the confining pressure and the shear velocity are observed.

1. Introduction

The shearing of densely packed granular matter is relevant in soil mechanics, silo design and several contexts in geophysics. Large scale deformations of granitic or sedimentary rocks occur in regions of strong shear stresses in which the material dilates and breaks up into fragments aligned into shearbands if the hydrostatic pressures are sufficiently large [1,2]. On much larger scale tectonic plates slide against each other on a debris of fragments called gouge [3,4]. A two-dimensional realization can be observed when pack-ice breaks up [5]. The determination of friction and dilatancy angles as used in classical Mohr–Coulomb plasticity [6], is commonly done in shear devices called Jenike cells, much used by engineers in powder technology [7].

Due to their simplicity in stress distributions and the relative ease in controlling the externally imposed parameters shear cells have constituted a paradigm to theoretical [8] and numerical [9–13] studies. The concepts of friction can be applied and one speaks of hardening or softening when the friction force increases or decreases with velocity.

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respectively. Dilatancy, i.e. a negative Poisson ratio, is generically present and like in Coulomb's picture the normal force is the dominant parameter.

Various numerical techniques have been used to simulate shear cells. Discritizations of continuum equations like FLAC [14,2] allow one to consider rather large systems but cannot reproduce micromechanical effects due to the particulate character of the material. A very powerful technique simulating the trajectory of each particle known as the Discrete Element Method (DEM) has been introduced by Cundall and Strack [15-19]. It is based on the same principles as Molecular Dynamics (MD) which was originally used to simulate the atoms or molecules of a liquid [20] and now is applied in many fields spanning from the simulation of molecules up to asteroids.

A general overview over MD simulations used in the field of granular materials can be found in [22]. These methods follow the movement of the particles by solving Newton’s equations. This can be done by using for example a Predictor-Corrector scheme or a Leap Frog algorithm. As the time step in such simulations has to be quite small for numerical stability reasons this technique is numerically expensive so that its availability grows with the appearance of more and more powerful computers. The big advantage of numerical simulations is the possibility to look at each physical variable at each time step which might be rather difficult in experimental setups.

In this article we perform simulations with shear cells. The main feature of our model in contrast to previous ones is that we take into account the random shapes of the individual grains described as arbitrary convex polygons. We investigate the dependence of the shear force on the shear velocity and the confining pressure onto the system. An important question is whether the shear force increases or decreases with the shear velocity, i.e. whether one observes shear hardening or shear softening. In Section 2 we describe our computer model in a certain detail. For the reader more interested in the physics, Section 3 contains a description of the numerical experiments which we performed. In Section 4 we present the results of our simulations and in Section 5 we finally conclude.

2. The model

Molecular dynamics simulations of granular media have been widely used [21,22]. Also in the special field of shear cells a rich literature exists about the shearing of spherical particles [10,14,23-26]. Also simulations using non-spherical particles have been performed [27,28]. Walton used non spherical particles to simulate explosions in rocks [29]. In Ref. [30] a model using irregularly shaped convex polygons which is very similar to ours is used in order to simulate brittle fracture. Here the cells are connected to each other and break if the stress between them exceeds a certain limit. A similar model was used by Handley [31] in order to examine uniaxial and biaxial cells. We will compare some of our results with their findings. In [32] a similar model is used to simulate the flow of particles down an inclined chute.

We use a Molecular Dynamics (MD) technique in two dimensions. In order to better
In order to calculate the elastic force between two particles one has to obtain the area of the geometrical overlap. The force point is applied at the center of the connection between the intersection points of the polygons. The direction of the force is perpendicular to this intersection line.

capture the complex structure of real soils we use in our simulation arbitrarily shaped convex polygons interacting with each other elastically, see Fig. 1, instead of spheres. MD is a method that solves Newton’s equations for the translational and rotational motion of the particles:

\[ m_i \ddot{r}_i = \sum_{j=1}^{N} F_{ij} + F_{i}^{ext}, \]  
\[ M_i \ddot{\phi}_i = \sum_{j=1}^{N} L_{ij}, \quad i = 1, \ldots, N. \]

Here \( m_i \) denotes the mass of the particle \( i \), \( r_i \) its coordinate, \( M_i \) its momentum of inertia, \( \phi_i \) its rotation angle and \( F_{i}^{ext} \) external forces which act onto the system, like e.g. gravity. \( F_{ij} \) and \( L_{ij} \) are the force and the torque which are imposed by particle \( j \) on particle \( i \). In our two-dimensional simulation the particles have three degrees of freedom: two for the translational and one for the rotational motion. In order to integrate these differential equations numerically various methods exist, e.g. the Verlet algorithm, the Berendsen–Gunsteren algorithm and the Predictor–Corrector scheme. We use in our simulations a Predictor–Corrector scheme of fifth order [20]. This means we have to keep track of the coordinates and all their derivatives up to fifth order.

For the Predictor–Corrector scheme it is necessary to calculate the forces which act onto the particles. We will treat our particles as elastic bodies. We include a dissipation term in order to capture the possibility of energy loss during collisions and a friction term. So the total force between two particles can be written as

\[ F_{ij} = F_{ij}^N \cdot n + F_{ij}^T \cdot t, \]

where \( F_{ij}^N \) is the part of the force in the normal direction \( n \) and \( F_{ij}^T \) is the part in the tangential direction \( t \). The normal and tangential direction are defined by the touching interface which will be explained below.
In the case of spherical particles one can easily derive a formula which gives the elastic force between two particles as a function of the geometrical overlap distance. In the case of polygonal particles however the situation is more complex. No analytical formula exists for the exact solution of the force between two polygonal particles. So one has to use numerical methods like for example the finite element method (FEM). This would be very expensive in computer time. Hence we prefer an approximative but fast method. We consider an elastic force \(-YA/L_c\) proportional to the overlap area \(A\) (Poisson elasticity) [30] and the inverse particle radius \(1/L_c\) as will be discussed later.

\(F_{ij}^N\) contains the elastic and the damping term. \(F_{ij}^{\text{T}}\) contains the term responsible for the tangential friction:

\[
F_{ij}^N = -\frac{YA}{L_c} - m_{ij}^{\text{eff}} \cdot \gamma_N \cdot u_{\text{rel}}^N, \tag{4}
\]

\[
F_{ij}^{\text{T}} = -\min \left( m_{ij}^{\text{eff}} \gamma_N |u_{\text{rel}}^T|, \mu |F_{ij}^N| \right), \tag{5}
\]

\[
u_{\text{rel}} = v_j - v_i, \tag{6}
\]

\[
m_{ij}^{\text{eff}} = \frac{m_i \cdot m_j}{m_i + m_j}, \tag{7}
\]

with the Young modulus \(Y\), the damping coefficient \(\gamma_N\) and the friction coefficients \(\gamma_T\) and \(\mu\). Eq. (6) defines the relative velocity of the surfaces of the particles at the point of contact and Eq. (7) gives the effective mass. Eq. (5) takes the Coulomb friction law into account [15,33].

The damping parameter \(\gamma_N\) is related to the coefficient of restitution which can be experimentally measured. The coefficient of restitution \(\varepsilon\) is defined as the ratio of the energy after a collision to the energy before the collision, hence it always has values between zero and one. The connection between the experimental parameter \(\varepsilon\) and the parameter \(\gamma_N\) is defined by the relation [22],

\[
\varepsilon = \exp \left( \frac{-\pi \gamma_N}{\sqrt{\omega_0^2 - \gamma_N^2}} \right). \tag{8}
\]

A damping parameter of \(\gamma_N = 0\) is equivalent to a restitution coefficient \(\varepsilon = 1\), while with a damping coefficient of \(\gamma_N = \infty\) one would simulate a coefficient of restitution of zero. \(\omega_0\) denotes the eigen-frequency of the elastic material. It is given by

\[
\omega_0 = \sqrt{\frac{k}{m_{\text{eff}}}}. \tag{9}
\]

where \(m_{\text{eff}}\) is the reduced mass and \(k\) denotes the spring constant which in our model is approximately \(k = (Y/L_c)\) cm².

We continue by explaining the elastic term of Eq. (4) in more detail. We do not allow the particles in our simulation to deform like e.g. in the Finite Element Method (FEM). This makes the simulation much faster but has the drawback of treating the interaction between two particles in an approximate way.
Fig. 2. In cases where polygons with small angles interact with each other it might happen that there are more than two intersection points. One chooses the pair of points with the largest distance from each other.

As the particles are not deformable they will overlap when they approach each other. We use the size and the shape of this geometrical overlap to get the elastic forces between the particles. To get the overlap polygon, i.e. the part of the plane which belongs to both particles, one has to calculate the intersection points between all edges of particle $i$ and all edges of particle $j$. Usually, there will be either zero intersection points which means that the two particles do not interact or there will be two intersection points as shown in Fig. 1. In pathological cases there can be more than two intersection points (see Fig. 2). These cases have to be treated in a special manner as we will explain later.

If there are two intersection points we proceed in the following way: To get the point at which the elastic force vector acts, take the line which connects the two intersection points which we treat as the contact interface between the two particles and choose the center of this line. The direction of the force is chosen to be perpendicular to this line (see Fig. 1). The elastic force is chosen to be proportional to the overlap area divided by a characteristic length. This correction by a characteristic length $L_C$ is necessary to reflect the fact that the spring constant is proportional to the elastic modulus divided by the rest length of the spring. In our case the characteristic length is not well defined because of the irregular shape of the polygons. We chose for $L_C$ the diameter of a circle which is of the same area as the polygon.

To calculate the overlap area and the force vector $F$ the intersection points between all edges of cell $i$ and cell $j$ must be determined. Note that it is possible to save some computer time by considering that not every pair of edges has to be treated. If one constructs the circles containing the edges of polygon $i$ and the smallest circle which contains the entire polygon $j$ one notes that intersections are only possible if the corresponding circles overlap.

The intersection points have to be calculated for the remaining pairs of edges. Each point $S_i$ ($S_j$) belonging to an edge of polygon $i$ ($j$) obeys the equation

$$S_i = E_i + \alpha_i v_i,$$

(10)
\[ S_j = E_j + \alpha_j v_j. \]  \hspace{1cm} (11)

Here \( E_i \) and \( E_j \) denote the coordinates of the sites belonging to polygon \( i \) and \( j \), \( v_i \) is the vector which connects \( E_i \) with its neighbor \( F_i \) in counterclockwise orientation and \( v_j \) is the corresponding vector for polygon \( j \). \( \alpha_i \) and \( \alpha_j \) are parameters between 0 and 1. An intersection point between both edges has to fulfill the following two equations:

\[ E_{i,x} + \alpha_i v_{i,x} = E_{j,x} + \alpha_j v_{j,x}, \]  \hspace{1cm} (12)
\[ E_{i,y} + \alpha_i v_{i,y} = E_{j,y} + \alpha_j v_{j,y}. \]  \hspace{1cm} (13)

For the parameters \( \alpha_i \) and \( \alpha_j \) one obtains

\[ \alpha_i = \frac{1}{\Delta} (v_{j,x} d_y - v_{j,y} d_x), \]  \hspace{1cm} (14)
\[ \alpha_j = \frac{1}{\Delta} (v_{i,x} d_y - v_{i,y} d_x). \]  \hspace{1cm} (15)

Here the \( \Delta \) is defined as

\[ \Delta = \begin{vmatrix} v_{i,x} & v_{j,x} \\ v_{i,y} & v_{j,y} \end{vmatrix} \]  \hspace{1cm} (16)

and \( d_x \) and \( d_y \) are given by

\[ d_x = E_{i,x} - E_{j,x}, \]  \hspace{1cm} (17)
\[ d_y = E_{i,y} - E_{j,y}. \]  \hspace{1cm} (18)

An intersection point only exists if \( \alpha_i \) and \( \alpha_j \) both are in the interval between 0 and 1.

In normal cases one finds either zero intersection points which means that no elastic force between the corresponding polygons exists or one finds two intersection points. In pathological situations however it is possible that there are more than two intersection points. This might happen for example if two corners with small angles penetrate each other like in Fig. 2. This behavior does not correspond to any physical situation. In that case we reduce the number of points to two by the following method: For each pair of points the distance from each other is calculated and the pair of points with the largest distance is chosen as shown in Fig. 2. Then the algorithm continues as in the case of two intersection points as described above.

Let us call the two intersection points \( P_1 \) and \( P_2 \) and define a direction such that the oriented area between the vector \( \vec{C_iC_j} \) connecting the centers of mass of the two particles and the vector \( \vec{P_1P_2} \) joining the two intersection points with each other is non-negative,

\[ \det(\vec{C_iC_j}, \vec{P_1P_2}) \geq 0. \]  \hspace{1cm} (19)

This is necessary to have a unique orientation. We find the overlap polygon by starting at \( P_1 \) and searching counterclockwise all sites of the overlap polygon by going from one site to the next until one ends up again at the starting point \( P_1 \). Starting at \( P_1 \) one first goes counterclockwise along polygon \( i \) and then takes all sites of the overlap polygon
until one reaches the edge which contains the second intersection point \( P_2 \) with polygon \( j \). Take the point \( P_2 \) as the next site of the overlap polygon and switch to the boundary of polygon \( j \). Following the boundary of polygon \( j \) go in counterclockwise orientation and take the next sites of the overlap polygon until the first intersection point \( P_1 \) is reached again. In this way we have constructed a list of the sites of the overlap polygon in counterclockwise orientation starting and ending in the intersection point \( P_1 \). The area of this overlap polygon is calculated by subdividing it into triangles and summing up the areas of these triangles. The area of each of these triangles is simply given by half the amount of the vector product of two of its spanning vectors. The force point \( P_F \) is the center of the contact interface line which connects \( P_1 \) and \( P_2 \):

\[
P_F = \frac{1}{2} (P_2 - P_1).
\]

We define the line connecting \( P_1 \) with \( P_2 \) as the touching interface and choose the force vector \( F \) perpendicular to \((P_2 - P_1)\). Note that the calculation of the overlap area is very time consuming as compared to the calculations needed for molecular dynamics with spheres. For this reason, MD with irregularly shaped polygons is about ten times slower than MD with spherical particles. On a workstation like a Sparc 10 one reaches a speed of about 3000 particle updates per second. About 70% of the computer time is used for the calculation of the overlap polygons.

We divide the solid into grains by a Voronoi cellular structure. The initial configuration of our experiment has a packing fraction of unity, see Fig. 3, i.e. the plane is completely filled with particles leaving no voids. A Voronoi construction is a random tessellation of the plane into convex polygons. This is obtained by first putting a random set of points into the plane and then assigning each point the part of the plane which is nearer to it than to any other point. In our case we use a so called vectorizable random lattice [34] which is a Voronoi tessellation with slightly reduced disorder. It is defined by choosing in each cell of a regular square lattice one point randomly within a central area of size \( a \). This has the advantage of making the program faster and does not introduce anisotropies as long as one does not decrease the tunable parameter \( a \) beyond a certain threshold. In [35] several programs are described which generate such tessellation in a fast way. In fact the generation of these lattices is so fast (about 10000 polygons in one second on a typical workstation), that it is not necessary to save initial configurations, but one might generate them again at the beginning of each simulation.

The number of neighbours of each cell is limited [34] which is an advantage for the MD simulation. The maximum distance at which neighbors can be found is three units of the original underlying square lattice. Hence one has to examine all polygons belonging to the original square cells with a distance of three or less.

In order to find the neighbors in the MD simulation it is natural to use a linked cell algorithm. We use as linked cells the same square cells which were used to construct the initial configuration. To find all neighbors of one particle we determine inside which cell it is positioned and examine all linked cells within an integer distance of three units. In our shear simulations the velocities of the cells are rather small, so that cells change their linked cells only rarely. Therefore it is sufficient to update the neighborhood list only
Fig. 3. A Voronoi tessellation of $16 \times 16$ cells as we used it in our simulations. Also shown are the random points which define the tessellation and the underlying square lattice.

every tenth time step. To make the neighbor list as short as possible, a radius around the center of mass is stored for each particle which defines the smallest circle containing the whole particle. Each time when the neighborhood list is updated it is checked if the circles defined in this way overlap each other (which is a fast operation). Only if they do the particle is included into the neighborhood list. This method reduces the length of the neighbor list, but still some pairs exist which correspond to non overlapping cells.

3. The numerical experiment

With the model described above, it is possible to perform a variety of different experiments with particles moving and colliding in the two-dimensional plane. For example, the clogging of hoppers has been examined using quadratical, rectangular and more complicated shaped particles [36].

Here we want to examine the behaviour of particles in a shear cell, similar to the Jenike cell, described in [7]. This is a cylindrical device which contains granular particles. The
Fig. 4. The shear cell which we use in our numerical experiments. A normal force $F_N$ acts on the top and the bottom of the device. Both are sheared against each other with a total shear velocity $V_S$, which leads to a horizontal shear force $F_S$ acting against the shear direction.

top and bottom are sheared against each other and pressed together by a tunable normal force. The shear cell we use in the simulation is depicted in Fig. 4. In the horizontal direction we use periodic boundary conditions in order to simulate the cylindrical setup. Fixed boundary conditions are implemented at the top and bottom.

During the simulation the top and bottom layer of polygons (representing the walls of the shear cell) are moved against each other with a fixed shear velocity $v_S$ under a fixed normal force $F_N$. The particles of these layers are glued together. The boundary conditions are imposed in such a manner that the cells of the top and bottom layers are not able to rotate or displace against each other. The horizontal force acting on average on these two layers will undergo wide fluctuations, as shown in Fig. 5. At the beginning of the simulation the average value of this force will be large and decrease with time until it reaches a saturation value $F_S$ which will be measured. It takes about $10^5$ time steps to reach this saturation value in the simulation. We also measure the dilatancy $D_Y$ of the system, i.e. the vertical increase of the distance between the lower and upper walls. This results from the fact that at the beginning the packing fraction of the system is unity and decreases with time because after deformation the polygons will not fit into each other so perfectly anymore. This behaviour of granular media is well known and is quantitatively captured by a negative Poisson ratio. We also measure the angle of dilatancy, observe shear bands and measure their widths. Finally, we use our simulation as a model for earthquakes created in shear zones and measure the number of earthquake events and their dependence on their strengths.

For small systems the fluctuations and the error bars of our measurements are rather large. If one wants to improve the statistics of the results one has to use either larger
systems or one has to average over many smaller systems. Using larger systems to look into size effects is not so relevant in this case since no critical fluctuations occur here. We prefer the second method since it is very convenient to do on a parallel supercomputer like the INTEL Paragon of the ZAM (Institute for Applied Mathematics) in the KFA Jülich or on the CM5 of the GMD in Bonn. We use the farming method, i.e. the same program runs on a variety of nodes with different initial setups. In our case we used a system of 16 times 16 cells. 32 copies of the system ran with different seeds for the Voronoi generator, i.e. with differently shaped Voronoi cells, on the nodes of the supercomputer which corresponds to 8192 cells. This averaging reduces the fluctuations considerably as seen in Figs. 6 and 7. One such run took about four hours on an Intel 860i processor.

4. Results

4.1. Dependence of shear force and dilatancy on shear velocity

In Fig. 8 we present a time sequence of a typical simulation of a shear experiment. At time \( T = 0 \) s the cell is in its completely ordered initial state with packing fraction one and dilatancy zero. When one begins to shear the system the dilatancy grows, i.e. the system grows in its vertical dimension (\( T = 0.1 \) s). In the next figure one can observe that some cells in the center of the shear cell begin to rotate (\( T = 0.2 \) s) while the cells near the top and bottom layer do not rotate. In the last picture of this sequence it is clearly visible that there is a localized zone with rotated cells in the center of the system, while the upper and lower parts are still in their initial ordered states and have not been rotated. So the shearing of a granular system produces a localised zone which
we can interpretate as a shear band. We will determine how the width of this shear band depends on the normal force and on the shear velocity.

We measured the dependence of the shear force versus the shear velocity. We used in all our simulations a fixed Young modulus of 1 MPa. This is quite small compared to real sand or rock which has a Young modulus of several GPa. In MD simulations the time step which is necessary to ensure numerical stability and energy conservation is inversely proportional to the square root of the Young modulus. A Young modulus of several GPa would be too costly with respect of computer time. We can, however, achieve equivalent results by rescaling the time scales. On the other hand a Young
Fig. 8. Sequence of snapshots of a shear cell experiment. At time $T = 0$ s the system is still completely ordered, the packing fraction is 1. At $T = 0.1$ s the system begins to dilate. Then at $T = 0.2$ s and more clearly at $T = 0.4$ s a localized zone near the center of the system begins to occur where cells rotate. The arrows in the cells indicate their orientation as compared to the one at $T = 0$ s.

modulus of 1 MPa is still high enough to ensure that the geometrical overlap between the particles amounts to only a few percent of their diameter which is the essential criterion for getting trustworthy results. Simulations with Young moduli in the range of GPa and very small strains have been performed by Handley [31].

In all simulation sequences we observe shear force weakening with time, cf. Fig. 6. Just at the beginning of the simulation a strong increase is observed which corresponds to the high amount of force needed to destroy the initially densely packed ordered structure of the Voronoi cells. This can be interpreted as a static friction and is in fact an effect of the "geometrical" friction caused by the polygonal shape. After some time the shear force needed to maintain the fixed shear velocity decreases and saturates against a fixed value.

In Fig. 7 the dilatancy of the shear cell is plotted versus the simulation time. At the
beginning of the simulation the increase in the dilatancy is very high. This is also a geometrical effect: Shearing imposes rotation of cells. But as the cells are not spherical the system has to dilate when rotating. After a short time a localised shear zone has been created and the slope in the dilatancy versus time decreases, finally saturating at a constant value. The fact that the time evolution of the shear force and the dilatancy saturate allows us to take the saturated value as the uniquely defined value for a given shear velocity.

We measure the saturation values for the shear force and the dilatancy and examine the dependence on the shear velocity. In Fig. 9 the shear force is plotted versus the shear velocity for four different normal forces. We observe in all cases shear hardening, i.e. the shear force increases with the shear velocity. The behavior of this dependence is different for low and high velocities. There is a threshold value between 10 and 20 cm/s where the behavior of the curve changes. We will try to explain this change later. The second part of the curve (above 20 cm/s) can be fitted to a power law, with an exponent of about 0.16. In Fig. 10 the shear force is depicted versus the shear force in a double logarithmic plot. The diagrams are nearly straight lines and are compared with a line of slope 0.16.

We can see from Fig. 11 that for higher normal forces one needs higher shear forces to obtain a certain shear velocity. This is intuitively clear because as we have seen the shear cell has to be dilated to be sheared. The higher the normal forces the more force one needs for this dilation. In order to capture the quantitative behavior of this dependence the curves are fitted. In Fig. 11 the shear force is plotted in a log–log plot versus the normal force. One gets straight lines with a slope of 0.77. As a guide to the eye a curve of the form \( F_S = F_N^{0.77} \) is also plotted. Hence, the dependence of the shear force \( F_S \) on the normal force \( F_N \) and the shear velocity \( v_S \) in the regime of large velocities can be written as
Fig. 10. Shear force in dyn versus shear velocity in cm/s for four different normal forces (○ = 2.5 Mdyn, + = 10 Mdyn, □ = 20 Mdyn and × = 40 Mdyn) in a log–log plot. The curves can be fitted well to a power law of the form $F_S \propto u_S^{0.16}$, which is also shown in comparison.

Fig. 11. Shear force in dyn versus normal force in dyn for six different shearing velocities in a log–log plot. The curves can be fitted to a power-law with exponent 0.766. For comparison the curve $F_S = F_N^{0.766}$ is also plotted.

\[ F_S \propto u_S^a F_N^b, \tag{21} \]

with the exponents $a \approx 0.16$ and $b \approx 0.77$.

In Fig. 12 the dependence of the dilatancy versus shear velocity is depicted for the four normal forces which we examined. The dilatancy increases monotonically with the shear velocity. Again, one can distinguish between two regimes with a different behavior. The boundary between the two regimes is again marked by a shear velocity value of about 10–20 cm/s. In both regimes the dependence between (saturated) dilatancy and shear
velocity is more or less linear. In the regime of low shear velocities the slope is larger than in the regime of high shear velocities. In both regimes the slope of the dilatancy as well as the dilatancy itself are higher for lower values of the normal forces. This is intuitively clear because the normal force acts against the dilatation of the system. The slope of the dilatancy in the high velocity regime is inversely proportional to the square root of the normal force,

$$
\frac{dD_Y}{dV_S} \propto \frac{1}{\sqrt{F_N}}.
$$

This is shown in Fig. 13 where the slope of the dilatancy $dD_Y/dV_S$ in the high velocity regime of the curve is plotted versus the normal force in a log–log plot. For comparison the curve $1/\sqrt{F_N}$ is also depicted. Both curves are parallel to each other.

We also measured the angle of dilatancy $\Psi$. This is the angle between the horizontal and the trajectory of one fixed point of the top or bottom layer, i.e. the angle of the slope of the dilatancy versus the displacement of the shear cell. First we checked if this angle is uniquely defined. For a fixed normal force we plot in Fig. 14 the dilatancy versus the strain $\epsilon$. We get curves with three parts I, II and III, see Fig. 14. In the first part the dilatancy is negative because at the beginning of the simulation the cell is just compressed elastically. In part II the curve is roughly linear. In part III the curve saturates slowly against a fixed value. In Fig. 15 we plot the normal force versus strain for different shear velocities. Parts I and II of all the curves collapse to a unique curve so that the angle of dilatancy is well defined. It is taken from the linear part II of the curve. We obtain for the four different normal forces the following angles $\Psi$ of dilatancy:
Fig. 13. The slope of the dilatancy versus shear velocity in the saturated regime in dyn/(cm/s) in a log-log plot against the normal force. This curve can be fitted to $F_N^{-1/2}$. The straight line is a guide to the eye of slope $-\frac{1}{2}$.

Fig. 14. Dilatancy in cm versus displacement in cm for $\gamma = 1$ MPa and four different normal forces ($\Diamond = 2.5$ Mdyn, $+ = 10$ Mdyn, $\Box = 20$ Mdyn and $\times = 40$ Mdyn). The curves consist of three parts: In part I the dilatancy is negative because the system is compressed elastically at the beginning of the simulation, then follows the linear part II where the angle of dilatancy has to be measured and finally the curve saturates in part III toward a constant value.

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<td>1.1</td>
</tr>
</tbody>
</table>
Fig. 15. Dilatancy versus displacement in one diagram for different shear velocities. The beginning of the curves collapse very well onto one single curve, so that we can extract a uniquely defined angle of dilatancy.

The data show significant dependence from the confining pressure as has been also observed by Handley [31]. One notices that when the confining pressure is of the same order of magnitude as Young's modulus of the particle the angle of dilatancy becomes very small because the particles are strongly compressed (corresponding to a big overlap of the polygons). This is confirmed by experiments with rocks under high compression, [38] and [39]. In comparison to dilation experiments on granular media our values for small confining pressures are rather high because our initial packing fraction is unity. To simulate granular media it might be better to use a smaller initial packing fraction. One could do this for example by removing some of the cells, thus creating holes. Another way would be to shrink all cells by a certain amount.

4.2. Localization

To examine localised rotation of cells we divide the shear cell into horizontal layers parallel to the top and bottom layer. For each layer the total rotations of all cells inside this layer are added up. By total rotation we mean the rotation of a cell since the beginning of the simulation. In Fig. 16 we show the total rotation within the layers versus the normalized distance from the bottom layer for four different shear velocities after a fixed time. A normalized distance of 0 corresponds to the bottom and a normalized distance of 1 to the top layer. For shear velocities of 2 cm/s and 10 cm/s the total rotation of cells has a peak in the center of the cell and decreases to zero at the bottom and top of the cell. Hence there is a localised zone in the center region of the shear cell where rotation takes place. In the outer regions the amount of rotation is much smaller. Fig. 16 is like all our results an average over 32 systems of size 16 × 16. If one regards one single simulation sequence the localisation phenomenon is even clearer. In the simulation sequence in Fig. 8 one recognizes that there is a localised zone in the center
of the system and in the upper and lower part the cells do not move at all. A relative translation is always accompanied by a relative rotation of the cells. The upper and lower part are bulk blocks and the shear movement of the cell is localized in the shear band in the center of the system. This result is in good agreement with shear experiments with sand and rocks where one generically finds localized shear bands [40]. The fact that in Fig. 16 the rotation close to the walls is not exactly zero, but only decreases continuously to zero results from the averaging process we use. The shear band is not always created exactly in the center of the shear cell but is sometimes shifted a little bit to the upper or lower wall because the position where the first fracture takes place depends on the special geometry of the system.

From the curves for shear velocities of 20 cm/s and 30 cm/s in Fig. 8 one notices that the localization disappears for higher shear velocities until the motion spreads over the whole shear cell. For 30 cm/s the localization has disappeared completely and the effect has even reversed to some degree, i.e. cells near the center have rotated less than near the boundaries.

In Fig. 17 where the relative width $W$ of the localized zone versus shear velocity is depicted one observes that there is a threshold for the shear velocity above which the localization nearly disappears. We defined $W$ as the width of the zone within which the rotation is larger than half the amount of the largest rotation. If we compare the width of the localized zone and the dilatancy versus shear velocity with each other one observes that the threshold where the localization disappears is at the same value where the slope of the dilatancy decreases, see Fig. 18. This can be understood by considering that the cells dilate the system in order to rotate. So the increase of the dilatancy with the shear velocity must be high until a localized region is formed in which all cells take part in the rotation. Above this value the slopes in Fig. 18 are smaller in agreement
Fig. 17. The relative width of the shear band versus the shear velocity for the four normal forces (\(\phi = 2.5\) Mdyn, + = 10 Mdyn, □ = 20 Mdyn and × = 40 Mdyn) after 12 seconds.

Fig. 18. Dilatancy (upper curve) versus shear velocity compared with total rotation (lower curve) versus shear velocity. The thresholds for the change in curvature for the dilatancy and for the disappearance of localization are nearly identical.

with Ref. [40]. One also observes that the higher the normal force on the system the stronger the localization is, i.e. the higher the normal force the smaller the width of the shear band. This fact has also been experimentally observed by von Kármán [41]. He performed biaxial tests on marble under different confining pressures and found a transition to plasticity for high confining pressures.

As one looks closer at Fig. 17 one finds that a small amount of localization remains even in the saturated regime. The remaining localization is larger for higher normal forces.

A continuum mechanical computer simulation using the FLAC technique [2] showed
that shear bands are generated spontaneously if a large block of material is sheared. In this article a large number of shear bands was observed. The continuum approach is able to simulate material on a large scale but has the drawback that the micromechanical aspects are only treated phenomenologically. Our method is in some sense complementary to the one they used because it treats the micromechanical aspects but is not able to simulate large systems because of limitations in computer time. Nevertheless the findings complement each other in the way that our shear cell can be regarded as a small part of systems.

4.3. Earthquakes

The lithosphere is the outer layer of the earth mantle which has a thickness of approximately 100 km. According to modern theories of plate tectonics the lithosphere consists of a number of about twenty big plates, called tectonic [42] plates, which move relatively to each other. Their relative velocity is very small, namely in the range of a few centimetres per year. These tectonic plates are driven by forces which are generated in the interior of the earth. The earth consists of three layers. The innermost part is the solid core which consists of heavy rock material. The inner mantle of the earth is fluid while the outer mantle consists of solid rock material. At the boundary between the inner and outer mantle the decay of radioactive material produces heat which is transported to the surface by convection rolls. The tectonic plates are driven by these convection rolls.

Depending on the relative motion of the tectonic plates there are three possible situations. In the first case they move apart from each other as seen for example in the middle ocean rifts where new sea floor is continuously produced. If one plate moves into another one it could be subducted beneath the other one, thereby uplifting it. An example for this situation is the Andean subduction zone. The third possibility is the shearing of one plate along another as is the case for example between the Pacific and the North American plate. This movement is responsible for the San Andreas fault along the West Coast of North America. Another example is the Motagua fault where the North American and the Caribbean plate are sliding along each other. Our program is able to simulate a shear zone but not the first two cases because this would require including the third dimension. The shearing of two tectonic plates represents a very similar situation as a shear cell, just on a geophysical scale.

The movement of tectonic plates against each other is the origin of earthquake and volcanic activity. This fact is impressively evidenced through a plot of the distribution of earthquakes and volcanoes on a world map [43]. Nearly all points – each representing an earthquake – mark the border of the tectonic plates. Many large earthquakes take place for example in Japan where three tectonic plates touch each other or on the San Andreas fault where two tectonic plates shear along each other. We change our model by not allowing the system to dilate which captures the geophysical situation in a better way.
Fig. 19. A snapshot of the earthquake simulation with $64 \times 64$ cells after two million simulation steps. Cells which have rotated by more than three degrees are shaded grey. As one can see the fault zone is very narrow having an average thickness of only two or three cells.

The polygons of our shear cell represent large rocks in the region between two tectonic plates. The upper and lower boundaries are parts of the plates which are sheared against each other. We performed computer runs with $32 \times 32$ and $64 \times 64$ polygons. The size of each cell is of the order of 1 km, so the complete region taken into account had a size of $320 \times 320$ and $640 \times 640$ km. In Fig. 19 we see how faults localize. We chose the following simulation parameters:

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Unit</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density</td>
<td>$\rho$</td>
<td>g/cm$^3$</td>
<td>5</td>
</tr>
<tr>
<td>Young modulus</td>
<td>$\gamma$</td>
<td>dyn/cm$^2$</td>
<td>$10^{11}$</td>
</tr>
<tr>
<td>Dissipation</td>
<td>$\gamma_N$</td>
<td>s$^{-1}$</td>
<td>0.1</td>
</tr>
<tr>
<td>Dynamic friction</td>
<td>$\gamma_T$</td>
<td>s$^{-1}$</td>
<td>0.1</td>
</tr>
<tr>
<td>Coulomb friction</td>
<td>$\mu$</td>
<td>1</td>
<td>0.5</td>
</tr>
<tr>
<td>Time step</td>
<td>$dt$</td>
<td>s</td>
<td>0.005</td>
</tr>
</tbody>
</table>

Altogether we performed $2 \times 10^6$ time steps, the first $10^6$ to reach some steady state and the next $10^6$ to perform measurements. If one plots the kinetic energy of one particle against time one obtains a figure like Fig. 20 which shows a big number of bigger and smaller peaks. As earthquakes we define sudden movements of particles, so that every local energy minimum defines the beginning and the following maximum the end of an earthquake. The energy difference between these values is the energy which is
Fig. 20. Logarithm of the kinetic energy of one cell (sum of all three degrees of freedom) versus time. We interpret one event (earthquake) as the energy difference between a minimum and the following maximum because this is the stored elastic energy which is released during the event.

released during the earthquake and is a measure for its strength. In our simulations the dissipation parameter was 0.1 s\(^{-1}\), which means that the kinetic energy drops to \(1/e\) of its maximum after 10 s. This is a realistic value compared to real earthquakes. The Young modulus of 10 GPa is in the range of values for rock materials and hence also a realistic value. Our shear velocity was 100 cm/s and is nine orders of magnitude too high compared to the velocity of tectonic plates. Which means that we can simulate in one day on the computer about one million years of tectonic activity. We simulated a time of about three hours. Unfortunately, simulations with realistic shear velocities are not feasible because of the high amount of computer time required.

We analyse the distribution of the number of earthquakes versus their strength. The strength \(M\) of earthquakes is defined by their magnitude which is given by the decadic logarithm of the maximum of the curve which is plotted by a seismograph at a given distance from the earthquake [44]. In many earthquake regions this distribution follows a power law,

\[
N \propto 10^{-Mb},
\]  

(23)

where the exponent, the so called \(b\)-value, is around 1 [44]. It has been estimated [42] that one order in the magnitude is equivalent to a factor of about \(10^{3/2} \approx 31\) in the dissipated energy. This means that a log–log plot of the number of earthquake events per cell versus their energy should give a straight line with a slope of \(-1.5\). In Fig. 21 the earthquake statistics for the simulation with \(32 \times 32\) cells is depicted. We observe a power law with an exponent of \(-1.41\) which is equivalent to a \(b\)-value of 0.96. The power law holds over nearly five orders of magnitude and the \(b\)-value is in excellent agreement with the expected value of 1.0. This is also in good agreement with other, simpler, one and two-dimensional earthquake models using blocks connected to each other with
springs which feel friction with the floor on which they are gliding [3,45,46]. True asymptotic power law behaviour is obtained in earthquake models with self organized criticality (SOC) [47].

The simulation with $64 \times 64$ cells gave a $b$-value of 1.07. The reason for the slight discrepancy is not very clear. It is possible that finite size effects are responsible. More simulation runs with different parameters have to be performed. Unfortunately, a big amount of computer effort is needed for this kind of simulations. For example the run with 64 times 64 cells took about 20 days on a Sparc 10 workstation.

We always see a rich structure of aftershocks and if we turn to Fig. 22 which is a magnification of Fig. 20 we recognize that in some cases there are also precursor events before a larger earthquake. However there are no precursor events in the case of the largest earthquake in Fig. 20 at about time step 130000.

The shear bands which are created in our simulations (with no dilatancy allowed) differ from shear bands of numerical experiments where dilatancy is allowed. As one can observe in Fig. 19 the width of the shear band is always very small (only a few layers of cells large). It is created spontaneously after the system is sheared by an amount corresponding to the diameter of two or three cells. The fault zone is parallel to the top and bottom layer. It is not necessarily positioned exactly in the center of the shear cell but can deviate because of the irregularity of the initial configuration. After a fault zone has opened it remains always at the same position. This is in very good agreement with the fact that the San Andreas fault has been at about the same position for a very long time. We can regard the shear experiment without dilatancy as a situation with very high confining pressure. This fits very well with our observation that the localisation increases with the normal force.
Fig. 22. Magnification of a part of the data of Fig. 20, but this time in linear scale. One finds a rich structure of aftershocks after an event and in this case also a number of precursors.

5. Conclusion

We presented a numerical model, similar to the one of Potapov et al. [30] to simulate shearing of granular media in two dimensions. With that model we investigated shear cells and found that there is an important difference in taking randomly shaped polygons as grains instead of spheres as is usually done and which gives anisotropic responses due to the existence of a regular triangular lattice [12]. The first results we got are qualitatively in good agreement with experiments. Especially the observation of shear bands and the correct value for the $b$-value in the Gutenberg–Richter-law are very promising results. In comparison to MD simulations with spherical particles it is a step forward to use irregularly shaped polygons in order to simulate real grains or rocks. The model has also been successfully used to examine the clogging of hoppers with more realistically shaped particles than spheres [36]. But many other applications are possible.

First, the program can also been modified to simulate real fracture processes. For this purpose it is necessary to connect the particles among each other by bonds which are able to break. We connected the particles by elastic beams. These are objects with three degrees of freedom, i.e. they can be elongated and compressed, sheared and bent. This kind of elastic objects have been used by engineers for a long time to simulate continua and fracture processes [48]. By combining MD with irregularly shaped polygons with the beam method it is possible to simulate fracturing of heterogeneous solids. We defined thresholds for elongation, compression and bending above which a beam breaks, i.e. is removed. We tried some simple fracture experiments where we simulated a solid block of cells connected to each other by beams. Then we gave one cell on the surface of the block a high velocity directed inside the block simulating for instance the impact of a hammer. Depending on the velocity of this particle we observed that the block is more
Fig. 23. Fracture experiments simulating a concrete block composed of elastic grains fixed to each other by elastic beams. The beams break if their distortions exceed a certain threshold. One particle at the lower middle part of the block is given a high velocity directed inside the block. Here the velocity of this particle is 300 m/s. We see snapshots of an evolving system at $t = 0.0001$ s, $t = 0.001$ s and $t = 0.005$ s.

or less destroyed as shown in Figs. 23 and 24. The fracture pattern and the distribution of the fragments looks very much as in real fracture experiments. But still much work has to be done to adjust the parameters to experimental situations in particular the ones defining the breaking criterion of a beam. In [37] particles with an inner structure were simulated by connecting four triangles with beams to each other. The damping was implemented in this case by using beams with a dash-pot instead of using the parameter $\gamma_N$. In this way it is in principle possible to build very complex particles consisting of
Fig. 24. The same experiment as in the previous figure but with an initial velocity of 400 m/s of the accelerated particle. Again we show snapshots for the time at $t = 0.0001$ s, $t = 0.001$ s and $t = 0.005$ s. This time the destruction is much stronger and more and larger fragments are generated.

simple elementary cells.

We also incorporated the possibility of inserting new beams trying to capture sintering and healing processes, i.e. the possibility that two particles are melted together to one if the confining pressure is high enough. But again there are new parameters which have to be fitted. In principle it would be possible for example to shear with this program a block of material which originally does not contain any fractures. After some time fracturing would occur and some fractures would be healed again until one reaches a
steady state. From geophysical observations [49] it is known that one gets a power-law if one depicts the number of fracture lines against their lengths in a log–log plot. The exponent of this power law is found to be between 1.4 and 1.6. Numerical simulations on larger scales have been able [2] to reproduce these observations. Another application of this program could be to examine the dependence of the packing fraction on the geometric aspects of the powder grains that one obtains in sintering processes.

A very important improvement would be writing a three-dimensional programme which simulates arbitrarily shaped polyhedrons. A drawback of our two-dimensional simulation is that we do not know how far the omission of the third dimension influences our results. But at the moment such simulations would be much too expensive in calculation time. Not only are the calculations in three dimensions more complicated (six differential equations instead of three, polyhedrons much more complicated than polygons) but one also needs many more particles to simulate equivalent sizes. Nevertheless the results obtained until now are promising and encouraging to work further into this direction.

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