Arch generated shear bands in granular systems

ALEX BORDIGNON¹, LUCAS SIGAUD², GEOVAN TAVARES¹, HÉLIO LOPES¹, THOMAS LEWINER¹ AND WELLES MORGADO²

¹ Department of Mathematics — Pontifícia Universidade Católica — Rio de Janeiro — Brazil
² Department of Physics — Pontifícia Universidade Católica — Rio de Janeiro — Brazil


Abstract. We propose an arch based model, on cubic and square lattices, to simulate the internal mobility of grains, in a dense granular system under shear. In this model, the role of the arches in granular transport presents a non-linear dependence on the local values of the stress components that can be modeled geometrically. This non-linearity is very important since a linear dependence on the stress will make the models behave similarly to viscous fluids, which will not reproduce highly interesting properties of the sheared systems such as shear bands. In special, we study a modified Couette flow and find the appearance of shear-bands in accordance with the literature.

Keywords: Shear band. Granular system. Transport properties. Bi-based cuprates.

Figure 1: Images of the computer simulation. a, b and c show three different stages of the simulation, respectively: at the very beginning, where the velocities (represented by arrows) are all randomly distributed along the system, but for the walls (the red arrows); halfway through the simulation, where many rows of cells with the same velocities orientation can be seen; and at the equilibrium state, with almost half of the rows moving one way, half moving the other way, with the shear band being formed at the very center. d shows a zoom of this center area, where the velocity is randomly distributed and its module is almost zero, resulting in a shear band.

1 Introduction

Granular Systems (GS) are very interesting systems due to the large quantity of unusual equilibrium, and non-equilibrium, physical phenomena they exhibit, and also for the possible practical applications they present [1, 2]. A lot of progress has been accomplished during the last couple of decades concerning the state of the art of granular dynamics knowledge [2]. However, that is still quite incomplete. Recently, a new model for the role of the internal elastic and dissipative stresses has been proposed [3]. An interesting aspect of this model is the role played by the elastic stress therein [3], in the sense that, at equilibrium, the elastic stress is responsible for the structural stability of the system, while at non-zero granular temperature ($T_g > 0$: non-equilibrium) plastic transient components (with characteristic time $1/T_g$) of the stress are also present. The stability of the structures formed by the (network of) elastic stresses, during the non-equilibrium phase of the motion, and the role of the plastic stresses are some of the questions we intend to address in the present work.

One of the most important features that GS present is the highly unusual way internal stresses are spatially distributed. Stresses follow mainly along a topological, one dimensional, network of high stress contacts, e.g., the arches. In fact, one could roughly classify the grains as belonging either to the network carrying most of the stresses (arches) or to the mass of relatively loose grains (soft phase) [2]. The role arches play is crucial for the understanding of some non-usual granular behavior, such

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2 Stochastic dynamics for arches

naturally occurs in it. Many dissipative phenomena, such as granular clustering or shear band formation, arise as dissipation minimizing artifacts, truly reducing the total energy dissipation in these systems.

Furthermore, shear bands are narrow regions that cannot be stable for soft viscous-like systems: they might however be associated with the internal spatial discontinuity of stresses in granular systems, most likely due to the presence of arches of forces in the system. The next step is to propose an effective model for the time variation of the arches strength.

2 Stochastic dynamics for arches

We model the role of arches in granular transport for a specific dynamic situation: dense granular systems under external shear. It is a fact that dissipative granular systems can only sustain their motion while an external source provides energy to them. For sheared systems, that energy is provided via work done by the friction forces at the boundaries. How these surface forces can initiate, and maintain, motion in the system’s bulk have direct connection with the action of arches.

In the present model, we represent the system by a rectangular lattice, constituted of cells and their edges. Each cell corresponds to a volume of grains and is assigned a local parameter $\psi_{i,j} = \psi_{i,j}$ (with $i, j$ integers) associated with the local distribution of grains. The grains are not represented individually but only through the cell’s granular mass, via the parameter $\psi_{i,j}$.

We assume that the grains in the bulk of a given cell interact weakly with each other, characteristically of a typical soft phase. The edges of the cells are used to represent the arches, which interact with the grains inside and also in the neighborhood of the cell. These edge-arches, represented by forces along the edges, $F_{i,j}^{x,y,+}$ (where the lower indexes, $i$ and $j$, represent the coordinates of the lattice cell, while the upper indexes, namely $x+$, $x-$, $y+$ and $y-$, refer to the cell border it is referring to with $x+$ the horizontal upper border, $x-$ the horizontal lower border, $y+$ the vertical right-hand border and finally $y-$ the vertical left-hand border), evolve in time by phenomenological rules, and are given an orientation associated with the direction of local mass motion. The orienting of the arches comes from the apparent conflict of trying to describe a strictly local quantity (the stress) by means of a variable associated with a finite range in length. In fact, the granular mobility will depend on the gradients of stress, hence the necessity of orienting the edge-arches.

(a) Branching arches

We need a simple model to explain qualitatively how the edge-arches contribute to the transport of the grains. In two dimensions, the transported mass due to an arch of typical intensity $T$ (in force units) depends on the number of times it branches. Let us assume a typical branching length $L$ where the arch bifurcates into two new arches (see figure 3), of approximate strength $T/2$. The branching proceeds until the arch strength reaches the typical soft phase value for the intergrain force, $f_0$.

We assume that the amount of grains transported are proportional to the area $A$ spanned by the branches. Defining $N$ as the number of branches necessary to bring the stress from $T$ down to $f_0$:

$$f_0 = \frac{T}{2^N} \Rightarrow N = \frac{\ln \frac{T}{f_0}}{\ln 2}.$$ 

Thus the area $A$ above is proportional to $N^2L^2$, and we can write

$$\Delta \psi \propto \pm \ln \frac{|T|}{f_0} \approx \pm \ln \left(1 + \frac{|T|}{f_0}\right),$$

(1)

since, in general, $|T| \gg f_0$. The last modification in Eq. 1 is done for numerical convergence only.

Eq. 1 above should not be viewed as an exact model for transport inside a dense granular system but only as an approximate phenomenological indicator for the correct transport equation. For instance, the non-linear saturation of mass transfer with force strength is a very important ingredient for the appearance of shear bands and probably will be present in better and more sophisticated models.

3 Set-up description

A standard way of studying the effect of shear in a granular system is to use a Couette modified setting [6], composed of a fixed external cylinder (radius $R$) with a fixed external annulus and an internal rotating disk (radius $r$, with $0 < r < R$) at the base (see figure 2). The upper surface is free, with no external stresses applied on it. This experiment is well described in a two dimensional model, due to its symmetries, especially in the case of shallow granular filling, as follows.

By turning on the internal cylindrical surface’s motion, stresses are induced into the granular systems via shear forces, and a clear separation between oppositely moving masses of grains arises, showing a sharp shear band between them. That band is comparatively thin: its thickness is of the order of a few granular diameters.

An interesting transition occurs depending on the filling height ($H$) of the cylinder (in fact it depends on $H/R$) [5]. For a shallow filling depth ($H < R$), the shear band reaches the surface and the internal rotation can be perceived externally as a rotating disk on the top of the system. The radius of the observed upper disk is smaller than the bottom disk and follows closely some theoretical predictions based on the principle of minimum dissipation [6][7]. However, for larger filling depths ($H > R$), the shear band folds on itself and takes on a domed shape, that is also predicted by the same method used in shallow fillings [6][7]. More specifically, the method presented in reference [6] assumes the internal pressure to vary linearly with depth, which is only true for shallow fillings and far away from the side walls, e.g. $R \gg r$. In fact, the dome height is predicted to tend to zero as the filling becomes deeper ($H \rightarrow \infty$) for that model [6]. For realistic length limited systems the mean pressure tends to reach a plateau [4], and so would the dome’s height.

It is important to understand the physical causes of phenomena such as the formation of shear bands and the transitions described above. We can obtain much insight about a system by using the most important physical ingredients in modeling it. This is the idea behind the present model. We applied these ideas to simulate a dense granular system under the set of external shearing condition described above. This model is expected to give good results for large fillings due to the fact that the vertical pressure will be taken care of only in an indirect way, akin to the case when a pressure plateau has already developed.
4 Computer Model

(a) Simple model

The present model is developed in a square-cell lattice. Each lattice cell represents a certain region of the system containing a certain mass of grains.

Our model is composed of two concentric rings, each rotating in a different direction, with granular material between them. This is simulated by a medium divided as a lattice of square cells, which can contain up to $N$ grains each. This lattice has periodic boundary conditions on its horizontal limits, representing a section of the system (or two ‘open rings’), and constant velocity conditions at the inferior and superior limits, representing the two cylinders walls. On each side of each cell a force appears due to the formation and transportation of arches. These forces are responsible for the correlated movement of grains between cells and, therefore, inside the medium.

At the start of our simulation, only the cells at the far bottom or far top of the lattice have any kind of velocities or applied forces. The whole lattice starts with an isotropic distribution of grains. The cells at the inferior and superior lines have fixed velocities: it equals zero at the $y$ direction, and a constant $v$ at the $x$ direction (but with different signals for the inferior and superior lines). This simulates a glued layer of grains at the moving walls, where the grains and the wall move with the same velocity. This movement of grains, as well as their random diffusion pattern, forms arches, which cause the appearance of forces and the transportation of granular material.

We simulate this interaction between grains by applying a force at the borderline between two cells - in both directions, a force for each cell, as can be seen in Figure 4 - that suffers the influence from both the forces in its vicinity and the grain density in its neighbor cells. At each time step $\tau$, the forces are calculated again accordingly to the equations shown below. This simulates arches appearing along the edges of the lattice, in-between the cells, which are responsible for the grains transport and, in consequence, the appearance of shear bands.

As a first step, we will test our working hypothesis of square-lattices and arch branching by means of a simplified model. Therefore, we only take into account the action of neighboring forces in a direct way. Hence, in equations (2) all we do is to take a simple averaging over the forces that are on the same direction and have direct connection with the force we are looking at, assuming that it roughly mimics the behavior of real arches in the material. For instance, for $F_{x,i,j}^\pm$ (besides itself) the relevant contributions come from the forces immediately before and after the location $(i,j)$, and along the same straight line, respectively $F_{i,j-1}^\pm$ and $F_{i,j+1}^\pm$, associated with the direct force transmission; the parallel force applied at the same cell, but on the opposite wall ($F_{j,i}^\pm$), since it can ease (if both forces have the same signal) or hamper (if they have opposite signals) the transport of grains by the transmission of its effect through the soft phase; kinetic friction with the adjacent cell via $F_{i-1,j}^\pm$; and the force itself ($F_{i,j}^\pm$).

Therefore, our ‘test model’ can be described by this simple set of equations:

$$
F_{x,i,j}^\pm(t + \tau) = \frac{F_{x,i,j+1}^\pm(t) + F_{x,i,j-1}^\pm(t) + F_{x,j-1,i}^\pm(t) + F_{x,j+1,i}^\pm(t) + F_{x,i,j}^\pm(t)}{5} + \eta_{x,i,j}^\pm(t),
$$

Equation (2)

\[ F_{x,i,j}^e (t + \tau) = \frac{F_{x,i,j+1}(t) + F_{x,i,j-1}(t) + F_{x,i,j}^+(t) + F_{x,i,j}^+(t) + F_{x,i,j}^+(t)}{5} + \eta_{i,j}^x (t), \]  
\[ F_{y,i,j}^e (t + \tau) = \frac{F_{y,i+1,j}(t) + F_{y,i-1,j}(t) + F_{y,i,j}^+(t) + F_{y,i,j}^+(t) + F_{y,i,j}^+(t)}{5} + \eta_{i,j}^y (t), \]  
\[ F_{y,i,j}^e (t + \tau) = \frac{F_{y,i+1,j}(t) + F_{y,i-1,j}(t) + F_{y,i,j}^+(t) + F_{y,i,j}^+(t) + F_{y,i,j}^+(t)}{5} + \eta_{i,j}^y (t), \]  
\[ \Delta \psi_{ij} = K \ln(k_f |F_{R,i,j}| + 1) + \eta_{ij}^y (t), \]  
where \( K \) sets the time scale (\( K=0.1 \)), \( k_f \) is the force scale (\( k_f = 20 \)), the \( \eta \)'s are randomly generated numbers (through a normal distribution, with mean \( \mu = 0 \) and variance \( \sigma^2 \)), \( \psi \) is the density function of the grain cells and \( F_{R}^i \) is the resultant of the arch forces applied on the edges of the \((i,j)\) cell and calculated for both directions separately. The change in \( \psi_{ij} \) given by the model of section 2.1, as shown in equation (1).

(b) Complete Model

In order to take into account the effects of static friction in the boundaries and the force feedback from the mass of the soft phase grains into the arches we propose a new model, to be defined in the following. This model also incorporates the feedback mechanism between mass-arch strength. Several new parameters are introduced: the parameters \( \alpha \) and \( \beta \) will take care of internal anisotropies (in our calculations we make \( \alpha = \beta = 1 \) for the self-reinforcing average term in the equations below; \( c_1 (=0.03) \) is a small coupling term accounting for the kinetic friction between neighboring cells where the Heaviside function will indicate the direction of the kinetic friction force, due to the relative sliding of the neighboring cells; \( c_2 (=0.1) \) controls the compressive interaction between neighbors’ soft phases and its influence in the strengthening-weakening of the arch stress intensity. This is in fact done by the “penalty” term in energy (controlled by \( c_2 \)) that is associated with the exponentials (an arbitrary constant in the argument of the exponential is not shown) of the mass density difference between neighbors. It penalizes trying excessively to fill (or empty) cells in expense of their neighbors. The small \( \epsilon \) prevents spurious numerical divergences. In the following, we show with more detail the behavior of the terms mentioned above.

As in realistic systems, the segments of arches immediately before and after a given segment interact with a calculated force via direct contact (the first and second terms of equations (2-5)). We maintain hereafter the same approach of the simpler model: a simple average over both of them. The other term of the former equations, the force at the opposite wall of the same cell, also gives a direct contribution, though of a different nature. This happens because the other two represent arches connected by direct contact, while this one reflects the influence of the forces on opposite walls of the same cell on the transport of the granular material inside. To take this difference into account, their contribution is pondered by the constants \( \alpha \) and \( \beta \) - where \( \alpha \) depends only on the material properties of the grains, while \( \beta \) depends not only on these properties, but also on the density and the medium: if the medium is more dense, the influence of this force will be bigger, and vice-versa. To simplify the computer model, we make \( \beta \) dependent only on the initial conditions of the system, instead of a step-by-step calculation based on the density of each individual cell. It is, for sure, an oversimplification, but without it the simulation runs would take too long.

The friction between the neighboring cells is taken into account now by means of a Heaviside step-function. We consider that the friction is a function of the effective kinetic friction coefficient \( (c_1) \), and the Heaviside step-function defines if the friction is working for or against the granular movement. This sign is given by the value of the Heaviside-function of the difference between the forces and subtracting 1/2 (for example, \( [\theta (F_{x,i,j}^e(t) - F_{x,i,j}^e(t)) \) \( - \frac{1}{2} \]) would result in \(-1/2\) if the forces have opposite signals and \(+1/2\) otherwise). We then have the means of taking into account the direct contribution caused by the friction, with that kinetic friction increasing or reducing the forces sustained by the arches.

Another problem we address is that of describing the physical properties of the medium without looking to what is happening in the “soft phase” inside the cell. To improve the model, we now include a term dependent on the cell densities, which accomplishes two things: first, it gives a contribution to the force relative to the grain quantities inside the cell, and, second, it takes into account that each cell has a physical limit of a certain number \( N \) of grains inside of it.
maximum capacity, then it can’t be filled with any more grains. If there are any grains in adjacent cells that have to move there, then they are stuck at their original place - creating clusters. Since we do not attempt to describe the behavior of the soft phase, it is hard to know beforehand how relevant this term will be to our simulations - that’s why we include a constant parameter $c_2$, so that we can increase or decrease the relevance of the densities to the overall behavior of the arches.

The initial conditions are the same as in our former model. The equations for the forces applied at the grains of each cell are:

$$ F_{i,j}^{x+}(t + \tau) = \frac{\alpha \left[ \frac{F_{i,j+1}(t) + F_{i,j-1}(t)}{2} \right] + \beta F_{i,j}^{x-}(t)}{\alpha + \beta} + c_1 \left[ \theta \left( F_{i,j+1}^{x-}(t) - F_{i,j}^{x+}(t) \right) - \frac{1}{2} \right] + c_2 \left\{ \left[ \psi_{i,j+1} - \psi_{i,j} \right] e^{\left( |\psi_{i,j+1} - \psi_{i,j}| \right)} + \left[ \psi_{i,j-1} - \psi_{i,j} \right] e^{\left( |\psi_{i,j-1} - \psi_{i,j}| \right)} \right\} + \eta_{i,j}^{x+}(t), \tag{7} $$

$$ F_{i,j}^{x-}(t + \tau) = \frac{\alpha \left[ \frac{F_{i,j+1}(t) + F_{i,j-1}(t)}{2} \right] + \beta F_{i,j}^{x+}(t)}{\alpha + \beta} + c_1 \left[ \theta \left( F_{i,j+1}^{x+}(t) - F_{i,j}^{x-}(t) \right) - \frac{1}{2} \right] + c_2 \left\{ \left[ \psi_{i,j+1} - \psi_{i,j} \right] e^{\left( |\psi_{i,j+1} - \psi_{i,j}| \right)} + \left[ \psi_{i,j-1} - \psi_{i,j} \right] e^{\left( |\psi_{i,j-1} - \psi_{i,j}| \right)} \right\} + \eta_{i,j}^{x-}(t), \tag{8} $$

$$ F_{i,j}^{y+}(t + \tau) = \frac{\alpha \left[ \frac{F_{i+1,j}(t) + F_{i-1,j}(t)}{2} \right] + \beta F_{i,j}^{y-}(t)}{\alpha + \beta} + c_1 \left[ \theta \left( F_{i+1,j}^{y-}(t) - F_{i,j}^{y+}(t) \right) - \frac{1}{2} \right] + c_2 \left\{ \left[ \psi_{i+1,j} - \psi_{i,j} \right] e^{\left( |\psi_{i+1,j} - \psi_{i,j}| \right)} + \left[ \psi_{i-1,j} - \psi_{i,j} \right] e^{\left( |\psi_{i-1,j} - \psi_{i,j}| \right)} \right\} + \eta_{i,j}^{y+}(t), \tag{9} $$

$$ F_{i,j}^{y-}(t + \tau) = \frac{\alpha \left[ \frac{F_{i+1,j}(t) + F_{i-1,j}(t)}{2} \right] + \beta F_{i,j}^{y+}(t)}{\alpha + \beta} + c_1 \left[ \theta \left( F_{i+1,j}^{y+}(t) - F_{i,j}^{y-}(t) \right) - \frac{1}{2} \right] + c_2 \left\{ \left[ \psi_{i+1,j} - \psi_{i,j} \right] e^{\left( |\psi_{i+1,j} - \psi_{i,j}| \right)} + \left[ \psi_{i-1,j} - \psi_{i,j} \right] e^{\left( |\psi_{i-1,j} - \psi_{i,j}| \right)} \right\} + \eta_{i,j}^{y-}(t), \tag{10} $$

where the values of the constants above are the same as those of Eq. [5].

On the special case where one of the shear forces on the wall equals zero, we had to account for the static friction, at least on the earlier steps of the simulation. To do that, we have only to look at the friction terms on the equation for the force at the cell border in contact with the wall. We then force it to be exactly equal to the force on the opposite border until this force reaches a threshold $F_0$ (e.g., if we look at the cell $i, j$ in contact with the non-moving inferior wall, then $F_{i,j}^{x-} = F_{i,j}^{x+}$ for $F_{i,j}^{x-} < F_0$). Afterwards, the force follows the regular equation. This forces a condition of no transportation of grains laterally between cells, simulating the static friction.

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5 Results

The results obtained by our computer simulations agree with the experimental results found in the literature. In both models (the simple and the complete one), we built the model as an infinite array of grains between two walls, simulating this condition by using a rectangular medium with periodic conditions at the side walls. The density profile at the beginning is isotropic, with each grain cell filled up to fifty percent of its maximum capacity. The top and bottom walls are subjected to forces in opposite directions, creating, therefore, a shear. The grain cells between the top and bottom walls begin with no forces or transportation rate whatsoever. We then wait for the system to evolve naturally - the grains begin to be transported between the lattice cells due to random movement (the random term in our equations) and to the forces applied along the cell edges (creating the arches and the stress propagation - and, in consequence, the force transmission they cause), and after it reaches equilibrium we inspect the velocity and density fields and analyze the medium behavior. Images of the computer simulation can be seen in Figure 5.

Even our simple computer model, with a complete lack of refinement of the force equation, shows that our modeling of the medium as a group of square cells, with the arches forming in between them, is already good enough to reproduce a real system, as can be seen in figure 5. We present the results for three configurations: $F_1 = F_2$, $F_1 > F_2$ and $F_2 = 0$, where $F_1$ and $F_2$ being the forces applied respectively to each non periodic wall of the system. It is interesting to note that the shear band observed in the velocity profile is very sensitive to the forces applied to the walls, exactly as they’re supposed to be. At

Figure 5: Graphics of velocity (in module) and density profile for three different configurations (with the same set of parameters) of our computer model: $F_1 = F_2$ (red), $F_1 > F_2$ (green) and $F_2 = 0$ (blue). It is easy to see a shear band-like formation in the first graphic, while the second graphic tells us the density of grains inside the cells remains constant throughout the medium.
the extreme case where one of the walls does not move, the shear band is formed at the wall of the medium. And the density profile shows that the medium remains basically isotropic. During the simulation, it can be observed, as the system evolves, that sometimes a small agglomeration (regions where the density of the grain cells reach above levels above 60 percent of its capacity) is formed, but it quickly dissolves, even in the neighborhood of the shear band. Therefore, it can be concluded that its role is but a fluctuation of the system.

Let us observe that the frictionless simplified model is not as good to mimic what happens in the experimental settings as the complete one, since it can be seen in figure 5 that the case of zero velocity external wall ($F_2 = 0$) the shear band is located at the wall. The complete model is much more consistent since in figure 6 we see that a large mass of grains adjoining the stationary wall has zero velocity, as expected.

When we include the refinements proposed in our complete model, the shear band formation becomes much more pronounced and realistic. As we can see in figures 6 and 7 the graphics show a clear shear band formation, which varies accordingly with the forces we assign to the moving walls, reproducing the experimental data found in the literature. Not only that, with the addition of the kinetic friction and transport terms, the simulations run much more smoothly than on the simpler model, avoiding any kind of agglomerations.

It can be seen that the formation observed is much more shear band-like than on the previous model, specially at the case where $F_2 = 0$ (with the shear band forming close to the wall, but not AT the wall, as the former model seemed to imply). And it is also important to notice that, although a variation of the model parameters may influence the characteristics of the equilibrium state (shear band included), the behavior of the system, its kinematical properties and the physics behind it (in particular, the shear band formation itself), remain unchanged - showing that the parameters do not interfere with the proposed physical description of the system.

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Figure 7: Graphics of average velocity module (first column) and average density (second column) profiles for three different configurations of our computer model 2, respectively from top to bottom: \( F_1 = F_2, F_1 = 2F_2 \) and \( F_2 = 0 \) (see text). The graphics are averaged for all tested configurations of the simulation parameters. It is easy to see the shear band formation - in all three cases - in the first column, while the second column tells us that there are no formation of clusters and that the density of the cells remains constant throughout the medium.

6 Conclusions

Summarizing, our proposed new arch-based model to describe the collective behavior of dense granular material systems seems to yield satisfying results. Our two-dimensional square-latticed model, although a rough approximation of a real, free arch-forming system, presents us with fairly good results, which describe with surprising accuracy the qualitative behavior of dense granular systems under shear - in particular, the shear band formation. The quantitative behavior is not possible to simulate on such a general model, since it is highly dependent on specific granular properties (e.g. size, friction coefficient, etc.). But, on our complete model, by a simple variation of the equation parameters, these granular conditions can be easily reproduced. But the important notion to have in mind is that this simple model shows that arches may have a much more important role in the behavior of non-static dense granular systems than previously assumed, since such phenomena are so well reproduced.

References