Micro and macro aspects of the elastoplastic behaviour of sand piles

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Abstract We use a discrete element method to simulate the dynamics of granulates made up from arbitrarily shaped particles. Static and dynamic friction are accounted for in our force laws, which enables us to simulate the relaxation of (two-dimensional) sand piles to their final static state. Depending on the growth history, a dip in the pressure under a heap may or may not appear. Properties of the relaxed state are measured and averaged numerically to obtain the values of field quantitities pertinent for a continuum description. In particular, we show that it is possible to obtain not only stresses but also displacements in the heap, by judicious use of an adiabatic relaxation experiment, in which gravity is slowly changed. Hence the full set of variables of the theory of elasticity is available, allowing comparison with elastoplastic models for granular aggregates. A surprising finding is the behaviour of the material density in a heap with dip, which increases where the pressure is minimum.

1 Introduction

In spite of their importance in applications, it is fair to say that there is as yet no fundamental understanding of granular materials. Such an understanding might manifest itself in a general continuum theory, applicable to the majority of granular assemblies, without the need of ad hoc assumptions for each new system considered. Even though continuum descriptions have been applied extensively to model granular materials, especially in the engineering community [1,2], neither are these based on a microscopic theory nor is their predictive power for new experiments on granulates impressive. In the physics community, continuum descriptions are based either on balance equations [3] or on symmetry considerations [4], i.e., on general principles that are not specific to the granular state, so these ideas may yield important constraints for a microscopic theory but cannot stand in its place. For static assemblies, phenomenological closure relations [5] as well as elastoplastic models [6] have been used in macroscale calculations of the stress tensor, leading to different stress distributions in a sand pile.

The pressure distribution under a sand pile is not independent of the conditions of its creation. Rather, in some cases the pressure exhibits a minimum below the tip of the sand pile whereas in others, it does not. Which behaviour is observed depends strongly on the characteristics of the granulate, especially the size and shape distribution of the particles. Moreover, it depends on the construction history of the sand pile, so two piles consisting of the same material may have different stress distributions. If grains are dropped from a point source, there usually is a pressure minimum; if they are dropped layerwise, then there is no minimum. This phenomenon has been observed both in experimental sand heaps [7] and in numerical simulations [8].

The counterintuitive behaviour of the stress distribution under a sand pile may be traced back to the fact that the aggregate consists of particles that can be considered rigid to a good approximation and that do not stick together, i.e., the material is noncohesive. The pile will nevertheless be able to show elastic or plastic responses to external loads, as the particles can rearrange under pressure to fill voids more completely, so there will be a finite macroscopic deformation resulting from a finite load. Since the only effects that hold the pile together near its surface are friction and geometric constraints, the free surface of the heap has a tendency to flow, which means that in its vicinity *plastic* behaviour should be anticipated.

On the other hand, deep inside the pile, *elastic* behaviour is not necessarily to be expected, if mechanical aspects suggested by analogies from the field of structural rigidity are considered [9]. A network of rotatable bars is flexible (= hypostatic), isostatic or overconstrained (= hyperstatic), depending on whether the number of bars connecting vertices is smaller than, equal to, or larger than, the number needed to maintain stable equilibrium. If the links between touching grains in a sand pile are considered as the "bars" of a network, then the noncohesive nature of the granular constituents allows only bars under compression, which rules out the possibility of an overconstrained network, leaving the sand pile to be either hypostatic or isostatic. Arguments based on the different scaling behaviour of self-stresses and imposed stresses [9] seemed to imply isostaticity for granular matter loaded only by its own weight. Then the average coordination number z of grains would have to correspond exactly to a critical value z^{crit} (6 in two dimensions for frictionless non-circular particles and 3 with friction). The mechanical equilibrium conditions of isostatic structures lead to hyperbolic field equations, whereas static elasticity is described by elliptic equations.

However, it has been pointed out that load and geometry are not independent [10] in sand piles, and the distinction should be between isostatic and non-isostatic *problems* rather than *structures* [10,11]. Solutions of isostatic problems with prescribed load may lead to hypostatic structures, describable by elliptic equations, hence the introduction of effective elastic coefficients may be meaningful [10].

In order to investigate the matter, we perform numerical simulations, in which a sand pile is constructed from several thousand convex polygonal particles with varying shapes, sizes and edge numbers. The particles are poured from either a point source, which regularly leads to a pressure minimum under the pile or a line source. We use a discrete-element method with soft but shape-invariant particles: two particles in contact with each other are allowed to interpenetrate partially. On the one hand, it would be inefficient to solve the elastic equations for each collision between pairs of nonrigid particles, on the other, to implement an eventdriven code allowing the (desirable) solution of the equations of motion for rigid particles would be too cumbersome with polygonal particles.

2 Simulation method

We solve the equations of motion following from the balances of momenta and angular momenta of the particles, using a fifth-order Gear predictor-corrector method [12]. Colliding particles overlap. Forces are then calculated from the geometric characteristics overlap area and contact length (defined as the distance between the two points of intersection of the overlapping polygons) using the relative velocities of the two particles. The calculation involves phenomenological elastic constants as well as model parameters for friction and viscous damping. Details are given in [8].

In two dimensions, the momentum balance provides two equations per particle, the angular momentum balance one:

$$m_i \ddot{\mathbf{r}}_i = \sum_{j=1}^{n} \mathbf{F}_{ij} + \mathbf{G}_i \,, \qquad I_i \ddot{\varphi} = \sum_{j=1}^{n} L_{ij} \,. \tag{1}$$

Here, the subscript i runs over all the particles, the subscript j over all the contacts of particle i with other particles. That is, forces and torques are exchanged between particles only if they touch. Hence we have short-range forces, viz. contact forces. $\mathbf{G}_\mathrm{i}$ is the force acting on particle i due to external fields, in our case just gravitation, $\mathbf{F}_\mathrm{ij}$ the force created by the particle touching particle i in contact j.

The force calculation is the most time-consuming part of the algorithm. Of course, advantage is taken of the short-range nature of the forces by calculating only non-vanishing forces, i.e., forces between particles that are really in contact with each other. To achieve fast contact determination in a time that is proportional to the number of particles (not to its square), independent of the complexity, i.e., number of edges of the particles, algorithms from virtual reality and computational geometry were adapted. These use bounding boxes and Voronoi regions to determine overlaps of particles [8].

2.1 Stress calculation

Once we have the forces, we can compute stresses. It is easy to derive a formula for the average stress obtained in a homogeneous polygonal particle [13], assuming that the forces given in the contact points act on the corresponding edge of the polygon:

$$\sigma_{ij}^{p} = \frac{1}{V^{p}} \sum_{c=1}^{m} x_i^c f_j^c \,, \tag{2}$$

where x_i^c is i-th component of the branch vector pointing from the center of mass of the particle to the contact point c, and f_j^c is the j-th component of the total force in that contact point. V^p is the volume of particle p (actually an area, since we are in 2D) .

Expression (2) may be interpreted as the stress tensor associated with a single particle. This microscopic stress would not be a convenient means to describe the macroscopic sandpile, as it fluctuates wildly within a volume containing a few sand grains. In fact, it is undefined in the voids between the grains. Hence, for a continuum description, we need to average microscopic stresses. A representative volume element (RVE) is introduced via the requirement that the average becomes size independent, if the volume is taken equal to this value or larger. We find that box sizes containing 100-200 particles are sufficient to serve as RVE.

The averaged stress tensor was evaluated throughout the sand pile; typically, we represent it via a plot of tensor components as a function of the lateral coordinate x of the pile for layers of given heights y_1, y_2, ... y_n.

2.1 Determining strains

While the calculation of stresses is rather straightforward, this is not true for strains. In fact, even the definition of strain is problematic after assuming particles to be essentially rigid. For this reason, most macroscopic descriptions proposed in the last few years try to get by without using strain at all. Whether this approach can be successful in the long run remains to be seen. In any case, even if it may be difficult or impossible to determine strains in *experiments* on sand piles, this is not so in a *simulation*.

We define strains with respect to a hypothetical reference state of zero gravity and a sand pile identical to the one at ambient gravity, except for slightly displaced particle centers; i.e., in the reference state, no particle rearrangements that modify neighbourhood relationships should be present in comparison with the actual state. We obtain the reference state from the ambient one by slowly changing gravity. In principle, it is not necessary to go down to zero gravity, as long as the strains increase linearly with the gravity level – one may then extrapolate to zero from the knowledge of the positions of the particle centers of mass at two arbitrary different gravity levels. But it is necessary to let the sand pile approach a rest state after a reduction of gravity. Moreover, linearity has to be checked by looking at different gravity levels.

Figure 1 shows effective elastic constants determined using the stress tensor evaluated according to the prescription of the last subsection and the strain tensor obtained by variation of gravity and measurement of the ensuing displacements.

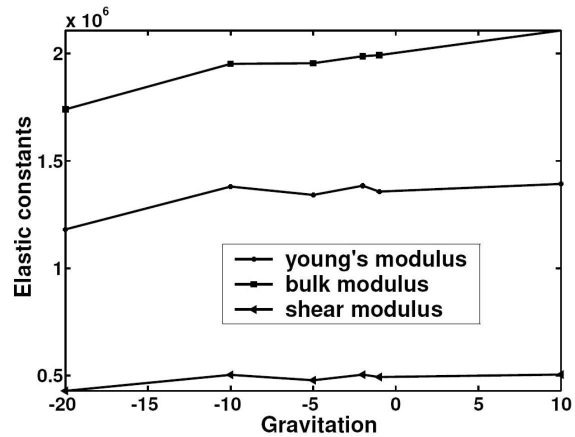


Fig. 1: Elastic moduli evaluated using displacement vectors as obtained from different changes of the gravitational acceleration. Zero corresponds to the ambient value of *g* (9.81 m/s^2), the figures give the change in percent, used in the calculation of displacements. The Young modulus for a single particle was taken to be 10^7 N/m.

It appears that too large a change of gravity leads to topological rearrangements of particles and plastic deformations of the sandpile. Nevertheless, there is a range of gravity levels g of about 10% about the ambient level, in which strains change linearly, meaning that essentially no rearrangements of this type have taken place and the ideal zero-gravity limit can be defined by extrapolation. Hence, our strain measurements are obtained by a meaningful procedure. The appropriate RVE for strain averaging turns out to have the same size as the one for stress averaging.

3 Analytic descriptions

Next we would like to briefly describe two macroscopic approaches based on analytic descriptions [5,6] the quality of which we have checked with our simulations. All analytic approaches for sand pile physics have to respect the basic law of mechanical equilibrium, which in two dimensions reads

$$\begin{aligned} \partial_x \sigma_{xx} + \partial_y \sigma_{xy} &= 0 \\ \partial_x \sigma_{xy} + \partial_y \sigma_{yy} &= -\rho g \end{aligned} \tag{3}$$

where ρ is the density of the sand pile, taken constant in these theories. In our simulation, we have to evaluate this density as the product of the particle density, which is fixed, and the local volume fraction of the sand pile.

Moreover, it is generally agreed that the *surface* of a sand pile is in a state of incipient failure, i.e., it corresponds to a slip plane. Using this assumption, one can show that the normal-component free-interface condition $\sigma_{nn} = 0$ leads to the vanishing of *all* stress components (i.e. $\sigma_{nt} = 0$ and $\sigma_{tt} = 0$). This follows directly from the Mohr-Coulomb yield criterion

$$(\sigma_{xx} - \sigma_{yy})^2 + 4\sigma_{xy}^2 - (\sigma_{xx} + \sigma_{yy})^2 \sin^2\varphi = 0\,, \tag{4}$$

applied in a coordinate system with x parallel to the surface (i.e., replace $x \to t$, $y \to n$ in (4)). Herein, φ is the internal friction angle (related to the friction coefficient μ via $\tan\varphi = \mu$). The assumption of incipient failure provides stress boundary conditions at the surface of the sand pile.

Because the two field equations are insufficient to determine the three stress components σ_{xx}, σ_{xy}, and σ_{yy}, a third equation, a so-called closure relation, is needed. In elasticity, this is a constitutive relation connecting stresses and strains.

Usually, it is then stated in the literature that for sand piles displacement fields are not available, which is true experimentally and also for the macroscopic analysis, as it does not have access to the microscopic particle displacements. Moreover, it is argued that for rigid particles these displacements are not meaningful. Both rigidity and Coulomb friction contribute to static indeterminacy of the pile.

A closure relation between the stress components is then sought for and postulated, to remove this static indeterminacy. Different approaches differ in their postulates concerning this "constitutive" relation. A common assumption of several theories is *radial stress field scaling* (RSF), which seems to be verified in experiments and is essentially based on the idea, that the stress fields of geometricalla similar piles should be the same up to a scale factor. Mathematically, this reads

$$\sigma_{ij} = \rho g y\, s_{ij}\left(\frac{x}{y\cot\varphi}\right)\,. \tag{5}$$

One can then reduce the equilibrium equations to ordinary differential equations, once a closure relation has been found. (In three dimensions, several closure relations are needed – the expression for the divergence of the stress tensor yields only three equations, whereas the stress tensor has six independent components.)

A theory that created a lot of stir in the 90s is due to Wittmer, Cates, and Claudin [5]. They considered a continuous family of closure relations of the form

$$\sigma_{ww} = K\sigma_{uu}\,, \tag{6}$$

where K is a constant, and σ_{ww} and σ_{uu} are the principal stress components along two orthogonal directions w and u, oriented at a prescribed fixed angle (the parameter of the family) with respect to the basic xy coordinate system. These models are called OSL models; OSL stands for "oriented stress linearity". The most interesting of these models as it seemed to be justifiable more easily as a natural form incorporating the construction history of the sand pile, is the so-called *fixed-principal axis* model (FPA). It is given by $K = 1$ and the angle of the coordinate axis, along which σ_{uu} is to be measured, being equal to $\tau = (\pi-\varphi)/2$. This model can be derived more intuitively by assuming that the principal axes of the stress tensor take the fixed directions $\pm\psi$ on both sides of the central axis of the sand pile, where $\psi = (\pi\text{-}2\varphi)/4$, hence the name FPA. The FPA model leads to a pronounced dip in the pressure distribution under the tip of the sand pile.

Part of the debate about the model came from the fact, that with a closure relation such as (6), the field equations for the stress tensor became hyperbolic throughout the volume of the whole sand pile (corresponding to isostaticity).

A much more conventional approach is the elastoplastic theory by Didwania, Cantelaube, and Goddard [6]. They note that near the surface of the pile, plastic behaviour is to be expected, and the closure relation is simply given by Mohr's yield criterion, Eq. (4).

Near the center of the pile, they assume that there is linearly elastic behaviour. The absence of measurable displacements is not a problem, as one can derive within linear elasticity stress compatibility relations, from which the elastic moduli scale out, so the limit $E \to \infty$ can be easily taken. In two dimensions, there is just one such relationship. It takes the form

$$\sigma_{xx,yy} + \sigma_{yy,xx} - 2\sigma_{xy,xy} = 0 \,, \tag{7}$$

and if it is imposed, rigid-body indeterminacy is removed. Whenever a plastic region touches an elastic one, there are boundary conditions, requiring continuity of stresses but allowing discontinuous derivatives. When two elastic regions touch each other with nonmatching stress derivatives, an infinitely thin layer of a yield region is assumed between them, along which equation (4) holds.

Cantelaube et al. assume RSF scaling as well. They obtain solutions which in the outer plastic domain obey the field equations (3) and (4), which FPA does near the sand pile surface, too, but strongly differ from FPA behaviour in the elastic core. For symmetric sand wedges, the shape of the inner domain is that of an isosceles triangle with a steeper base angle ($\hat{\beta}$) or a smaller tip angle. They find three discrete solutions, of which one has a pressure minimum. Once the angle of repose φ of the pile is fixed, the theory contains no free parameters. For later reference, we write their solution here. The expressions for the elastic domain are

$$\sigma_{\mathrm{xx}} = (a_2 - 1)y, \qquad \sigma_{\mathrm{yy}} = (a_1 - 1)y + b_1|x|, \qquad \sigma_{\mathrm{xy}} = -a_1 x, \tag{8}$$

those for the plastic domain ($\beta = \pi/2\text{-}\varphi$)

$$\sigma_{\mathrm{xx}} = a_{11}\left[\frac{|x|}{\tan\beta} - y\right], \quad \sigma_{\mathrm{yy}} = a_{22}\left[\frac{|x|}{\tan\beta} - y\right], \quad \sigma_{\mathrm{xy}} = a_{12}\left[\frac{|x|}{\tan\beta} - y\right]. \tag{9}$$

4 Simulation results

To convey an impression of a typical result for a numerical aggregate obtained in a sand pile simulation, we show a final state of a computation comprising a few thousand particles dropped from a point source (this is the hopper above the pile).

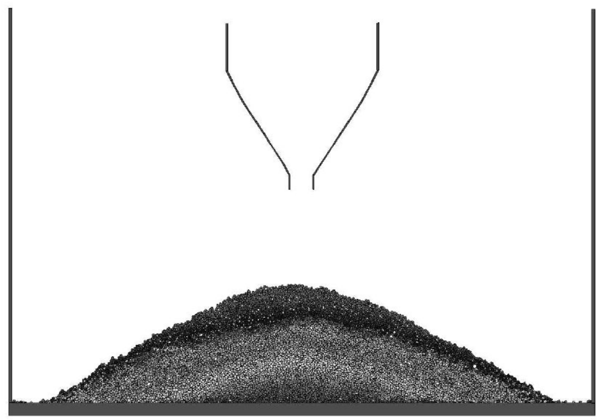
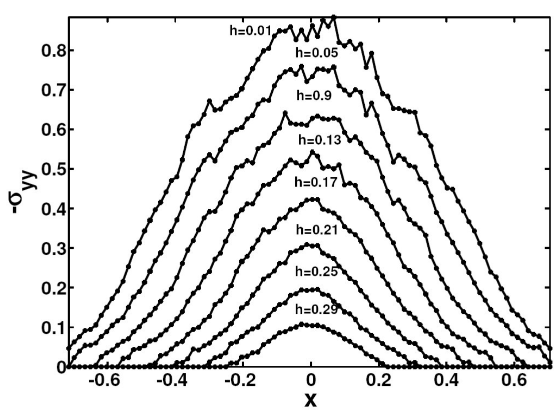
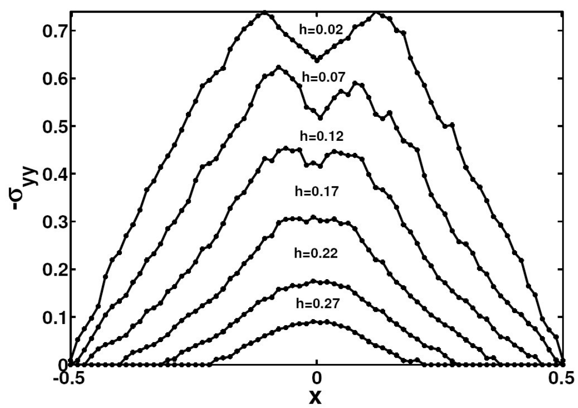


Fig. 2: Simulated sand pile. The walls and the hopper are made of immobile specially shaped particles. Different gray levels correspond to particles dropped at different times. The number of polygon edges varies between 6 and 8.

Next we display the distributions of vertical stress components obtained in layerwise deposition (line source) and in deposition from a central position (point source). Both results are averages over a number of simulations.



a)



b)

Fig. 3: Distribution of “pressure” on horizontal cuts at different heights through a simulated sandpile. a) sand piles constructed from a line source (average over 6 piles of 6600 particles each), b) sand piles deposited from a point source (average over 7 piles of 8000 particles each). The topmost curves correspond to the lowest cuts and vice versa.

The next figure shows the effect of particle shape. Here, roughly elliptic particles with a ratio of major and minor axis of 2 were used, whereas the particles leading to Fig. 3 were inscribed into circles. The “dip” in the pressure distribution becomes significantly more pronounced for elliptic particles. We also determined the orientational distribution of the elliptic particles. Their alignment is mostly horizontal, as one would expect.

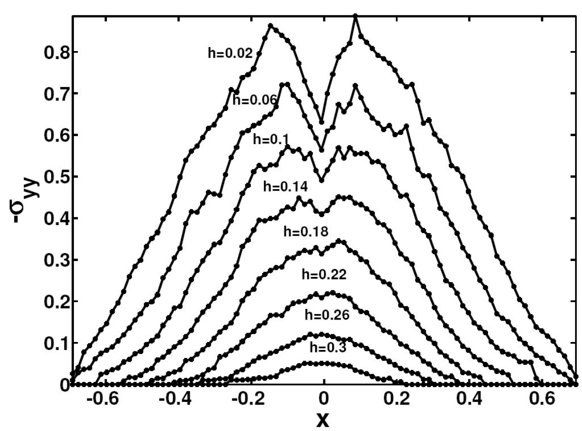


Fig. 4: Pressure distribution under sand pile constructed from elliptic particles. Average over 7 piles with 8000 particles each.

5 Comparison with theory

Our first observation in attempting to confront our data to theoretical results is that the orientation distribution of the principal axes of the stress tensor is varying smoothly throughout the sand pile. This rules out the FPA model as a quantitative predictor. Some of the less plausible OSL models give a better fit with our data. An example is shown in Fig. 5. For a given angle of repose, there is a relationship between the two parameters K and τ, so this is essentially a one-parameter fit.

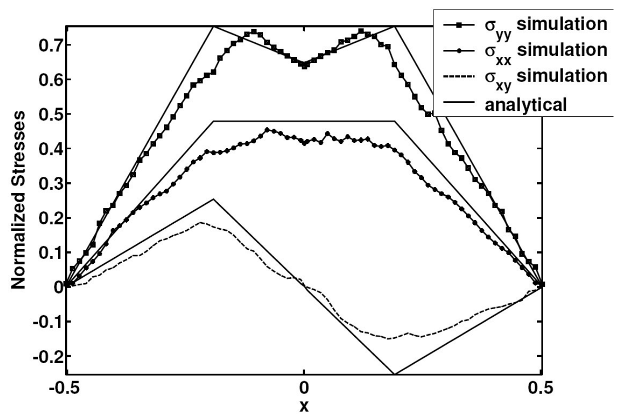
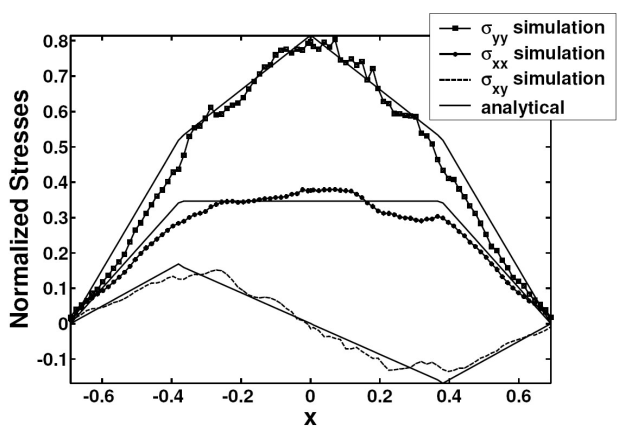
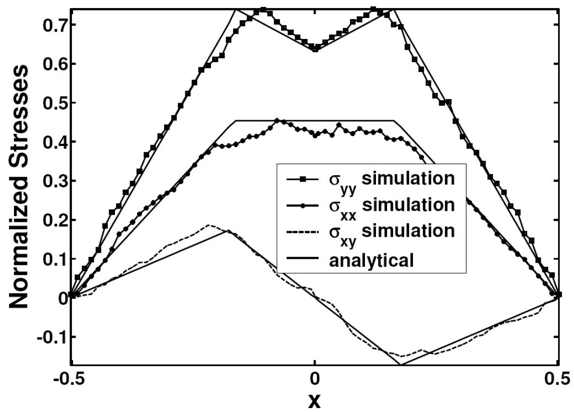


Fig. 5: Fit of the components of the (negative) stress tensor predicted by the OSL model to the point source simulations. Parameter values obtained: K=1.4, τ = 85°.

As soon as we need to fit, however, we get comparable or better quality from fits to the elastoplastic model by Cantelaube et al. [6], to which we will turn now.



a)



b)

Fig. 6: Comparison of simulation data with predictions from elastoplastic theory [6]. Shown components of the (negative) stress tensor are evaluated at the bottom of the pile. a) sand piles from line source, b) point source (compare with corresponding curves from Fig. 3).

The theory predicts that the sum of the parameters a_{11} and a_{22} from Eq. (9) must be equal to 2, a relationship that may serve as a consistency check. For the piles on the right panel of Fig. 6, we find $a_{11} = 1.23$ and $a_{22} = 0.78$, so the relationship is satisfied to better than 1%. If we consider the elastoplastic approach as a theory with a fit parameter, the agreement with the simulations is quite satisfactory. However, for symmetric sand piles the theory does not contain any free parameters. In particular, it predicts the angle $\hat{\beta}$, which for $\varphi = 28°$, the angle of repose in our simulations from a point source, should be 22° for the solution producing a dip, but is obtained as 35° from the fit. For the case of the solution producing a plateau, appropriately describing sand piles constructed from a line source, the agreement is surprisingly good: both the theoretical and fitted angle are 49°.

A reason why the theory does not work as well for the solution that is discontinuous at the center of the pile is that its assumption of a yield line along the axis of the pile is not really satisfied. This can be seen from Fig. 7, where we evaluated the expression on the left-hand side of Eq. (4), which should become zero in the plastic regions. Clearly, it approaches zero far from the center of the pile (x = 0), so the existence of plastic regions near the surface of the pile can be confirmed (though not their triangular shape), but there is little indication of singular behaviour of the expression near the center of the pile. For the plateau solution, there is no such singular behaviour even in the theory, which may explain why it works so well.

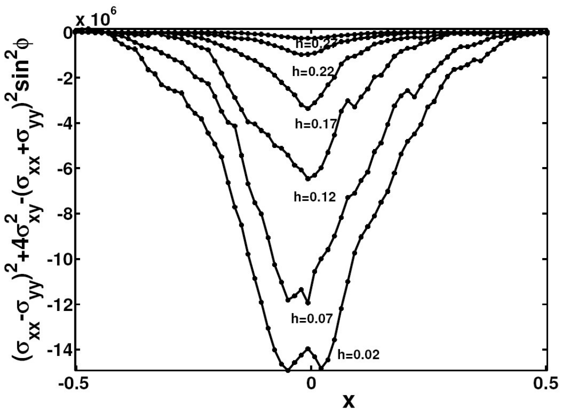


Fig. 7: The Coulomb-Mohr expression (4) evaluated for the average over sand piles from the right panel of Fig. 6.

6 Conclusions

To conclude, we have performed simulations of two-dimensional granular aggregates consisting of convex polygons and measured microscopic force distributions of the resulting “sand piles”. Via averaging over representative volume elements, for which a sufficient size was determined to contain 100-200 particles, we have determined stress and strain distributions. To obtain a measure for strain, the sand-pile was allowed to relax under reduction or increase of gravity.

For a point source, we find, not unexpectedly, that the pressure is not only minimum at the bottom layer, but also in higher layers of the pile. However, it disappears in layers near the tip of the pile. The density profile of sand piles was also measured; we observe it to have a maximum where the pressure is minimum, a somewhat unexpected result, as it suggests the presence of a mechanical instability.

A similar pressure minimum was not obtained in piles poured from a line source, which demonstrates that the simulation reproduces pressure distributions corresponding to different experimental protocols. Dynamically, the two cases differ by the appearance of avalanches during the build-up of a pile from a point source, and their absence for layer-by-layer deposition.

While it may be difficult or impossible to determine the *strain* tensor in an experimental sand pile, it is feasible to obtain a reasonable approximation to it from simulations. We define the strain with respect to a hypothetical reference state of zero gravity. This reference state may be generated from the static pile obtained in a simulation, by slowly changing gravity and following the particle trajectories during the ensuing load change. Then, it is easy to compute the macroscopic strain tensor by averaging over an RVE. It turns out that the size of the RVE we need for converged strain tensors is the same as for stress tensors.

Comparison with simple analytic theories [5,6] for the macroscopic mechanical behaviour of a sand pile shows that these theories have certain deficiencies. Radical departures from convential approaches such as the introduction of almost ad hoc closure relations [5] seem unnecessary, as an equally good or better fit of the data is obtained by a simple elastoplastic model [6]. Nevertheless, reality is not as simple as these models. One ingredient missing in all the models that use stresses only, is possible density variations in the sand pile.

As an outlook, it may be said that the consideration of varying density naturally leads to the idea that the internal texture of the pile is important and that a macroscopic description therefore probably has to go beyond a simple description in terms of stresses and must introduce additional variables such as fabric tensors. There have been some recent developments in this regard [14]. The question is then of course, how to calculate a macroscopic fabric tensor to close the theoretical description.

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