Relation of Structure and History of Granular Sediments

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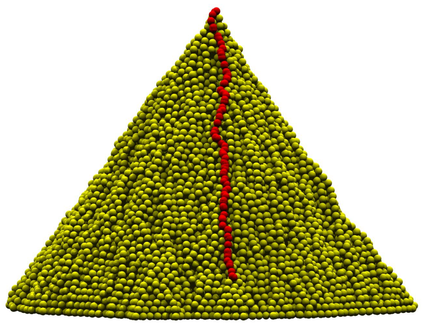
We study the coordination numbers of inhomogeneously grown three-dimensional sediments. The resulting packings have spatially varying coordination numbers determined by the historical surface profile. Higher than average coordination numbers correspond to convex surface and lower than average to concave surface. We derive equation relating historical surface profile to spatial filed of coordinatio numbers.

Visscher-Bolsterli model, [1]

Assumptions:
• Particles are dropped one by one
• They follow the path of steepest descent
• They are immobilised at stable position

The red particle is dropped from the top a heap. It follows the steepest descent path until it reaches a stable position.

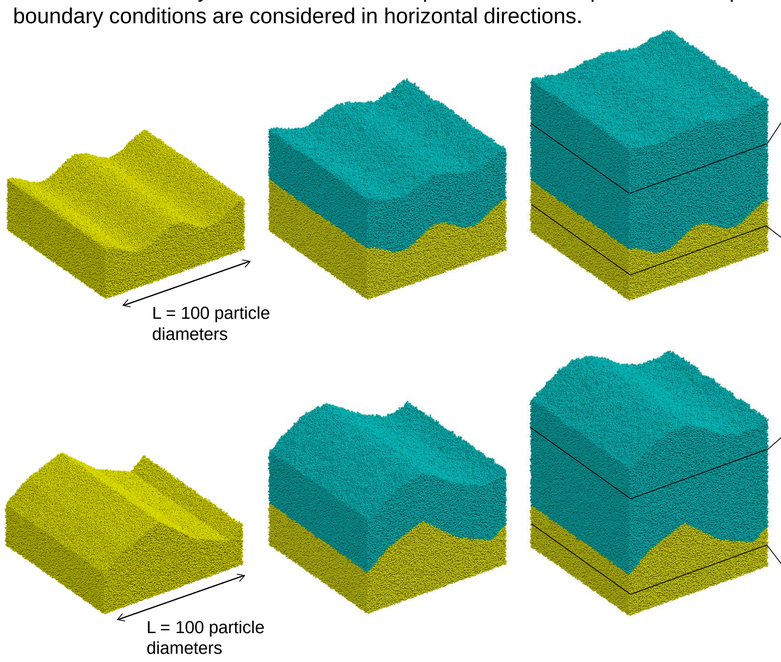


Single particle dynamics is composed of the motion on a straight straight line (falling) and rotation (rolling). This model can be implemented in an event – driven way, and due to its speed tens of millions of particles can be simulated.

Each particle makes three contacts in its stable position, and therefore the average contact number is 6.

Coordination numbers in inhomogeneous sediments

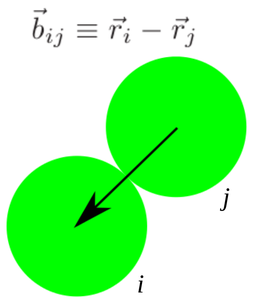
In order to create an inhomogeneous sediment we drop the particles with uniform flux onto an initially non-flat surface. All particles have equal size and periodic boundary conditions are considered in horizontal directions.



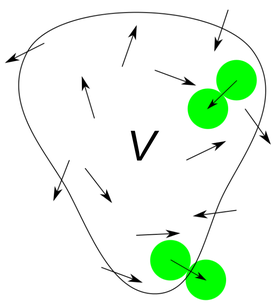
Initial surface, cut from a homogeneous packing | N = 400000 added particles | N = 800000 added particles | distribution of coordination numbers averaged over 100 sediments

Convex surface increases coordination numbers, while concave decreases. Similar effect has been observed in related systems, [2-4].

Average contact numbers in the bulk



Bond: vector pointing from newer to older particle.



Arbitrary volume inside of the bulk of the packing. Some bonds are within the volume, while others cross its surface.

$$\langle c \rangle = \frac{6N_V + k^+ - k^-}{N_V} \qquad \text{... (1)}$$

Average coordination number $\langle c \rangle$ inside of the volume *V* deviates from 6 due to bonds that cross the surface of the volume. The volume contains N_V particles. k^+ and k^- are the number of bonds entering the volume and exiting the volume, respectively.

The bonds in the bulk have various orientations, but it is possible to define a field of bonds, $\vec{b}$, obtained by averaging bonds in a small volume relative to the scale on which inhomogeneity in the packing appears, but much larger than the volume of a particle. Under the assumption of constant density, which is a good approximation in Visscher-Bolsterli packings, the differential form of equation (1) becomes:

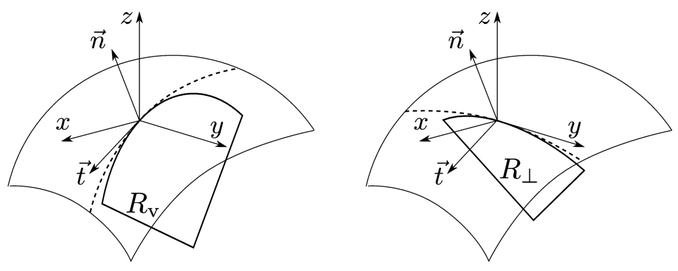
$$c = 6 - 3\nabla\vec{b} \qquad \text{... (2)}$$

Explicit relation between the surface profile and coordination numbers

Under the assumption of slowly evolving surface and linear relation between the horizontal component of the bond field on the tilt angle, the relation (3) can be rewritten as:

$$c = 6 + 3s\left(\frac{1}{\cos(\alpha)}\frac{1}{R_v} + \frac{\alpha}{\sin(\alpha)}\frac{1}{R_\perp}\right) \qquad \text{... (5)}$$

where the curvature R_v is in the direction of the steepest descent, and $R_\perp$ normal to the direction of steepest descent:



Positive curvature increases contact numbers while concave decreases.

Relation between the historical surface profile, bond orientations and coordination numbers

To obtain a relation between the field of coordination numbers and historical surface profile we rewite eq. (2):

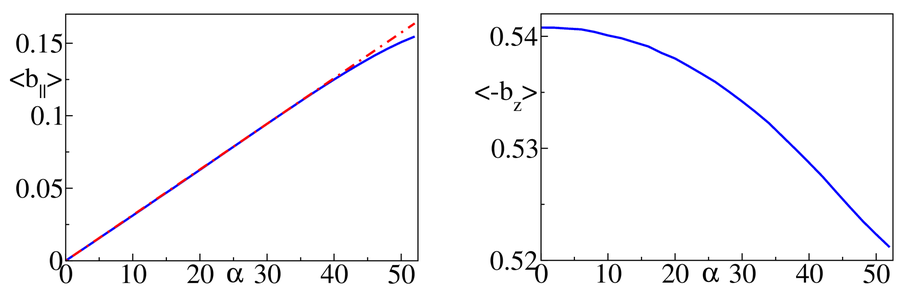
$$c(\vec{r}) = 6 - 3\mathrm{tr}\left(\frac{\partial\vec{\theta}}{\partial\vec{r}}\frac{\partial\vec{b}}{\partial\vec{\theta}}\right) \qquad \text{... (3)}$$

where $\vec{\theta} = (\alpha, \beta)$ corresponds to unit vector normal to the surface of the packing, with a being polar with respect to the vertical and b being the azimuthal angle.

The field of bonds b can be written in the form:

$$\vec{b} = \left(-\cos\beta b_{\parallel}(\alpha), -\sin\beta b_{\parallel}(\alpha), b_z(\alpha)\right) \qquad \text{... (4)}$$

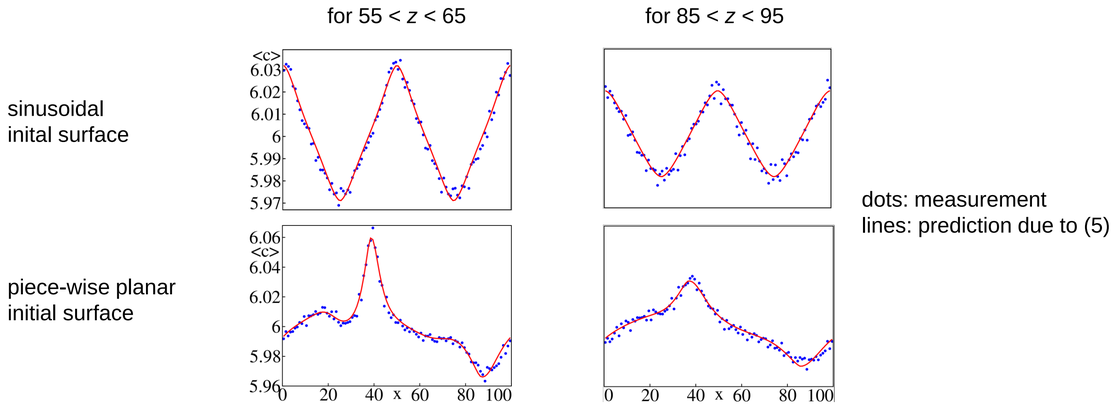
Where $b_{\parallel}$ is the absolute of the projection of $\vec{b}$ to xy plane and b_z is the vertical component. If $b_{\parallel}$ and b_z are known, we can solve eq. (3) to obtain $c(\vec{\theta}, \partial\vec{\theta}/\partial\vec{r})$. We obtain $b_{\parallel}$ and b_z numerically from a sedimentation onto a plane tilted by a.



We find that $b_{\parallel} \approx s\,\alpha$, with $s = (0.1803 \pm 0.0001)$, while the b_z component varies little with tilt.

Quantitative check of the relation (5)

In order to check the relation between the surface profile and coordination numbers, eq. (5), we calculate the evolution of the surface profile using the Edwards-Wilkinson equation without fluctuations [5]. The result is then computed using the obtained surface profile and its local tilts and curvatures. We consider systems rendered above and find a good agreement between predicted and measured coordination numbers.



References:
[1] W. M. Visscher and M. Bolsterli, Nature **239**, 504 (1972).
[2] C. H. Bennet, J. Appl. Phys. **43**, 2727 (1972)
[3] L. F. Liu, Z. P. Zhang, and A. B. Yu, Physica A **268**, 433 (1999).
[4] N. Topic, J. A. C. Gallas and T. Pöschel, Phys. Rev. Lett. **109**, 128001 (2012).
[5] S. F. Edwards and D. R. Wilkinson, Proc. R. Soc. London, Ser. A **381**, 17 (1982)

We studied the coordination numbers in inhomogeneous sediments. In numerical experiments we found that the average coordination number is larger than average of 6 where the surface is convex, and smaller than 6 where the surface is concave.The relation (5) alows to determine the field of coordination numbers inside 3D packings from the observation of the surface profile during the process of sedimentation.