Probing sand in the jamming limit

Anita Mehta

(loosely based on

AM, J M Luck, J M Berg, G C Barker, cond-mat/0412763)

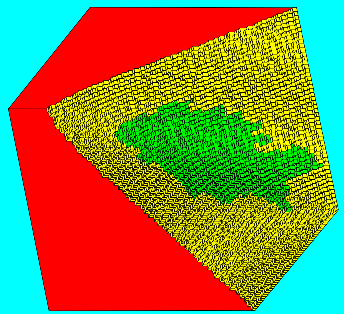
Plan of talk

- Introduction
- Vibrated sand: review of numerical results
- Statistics of bridge geometries
- Granular compaction - sand on random graphs
- Shape matters in granular compaction

Introduction

Sand: athermal complex system with hysteresis and metastability

it avalanches

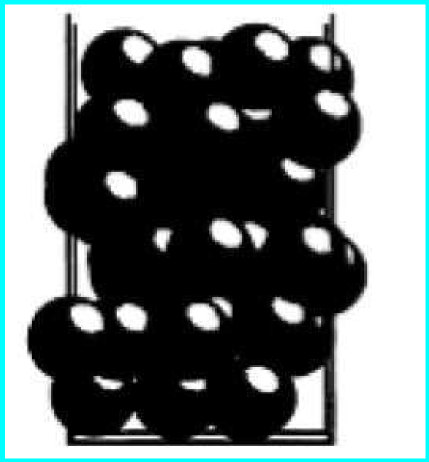


(AM and G C Barker, EPL 1994; AM, J M Luck and R J Needs, PRE 1996; P Biswas et al PRE 1998; AM and G C Barker PRE 1996; AM and G C Barker EPL 2001)

Vibrated sand: review of (some) numerical results

(AM and G C Barker, PRL 1991: G C Barker and AM, PRA 1992, PRE 1993; G C Barker, AM and MJ Grimson PRL 1993)

Algorithm: Hybrid Monte Carlo scheme with stochasticity and cooperativity



- Dilation: free volume introduced homogeneously in vertical direction, stochastic displacements in axial direction.
- Quench: packing recompressed by *hybrid* Monte Carlo, which allows cooperative structures to form.

Plot of volume fraction vs shake intensity

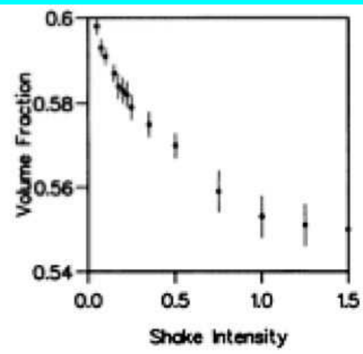
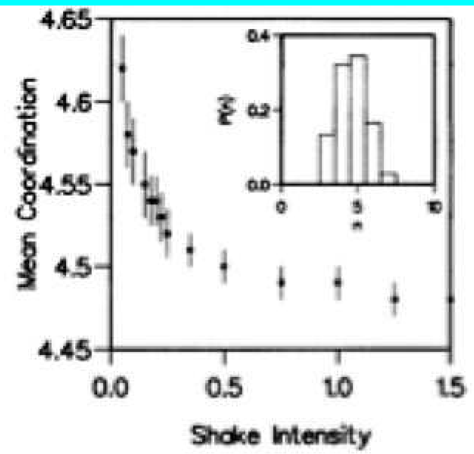


FIG. 4. Steady-state volume fraction of monodisperse hard spheres plotted against the shaking intensity.

Note rise in volume fraction over 0.58 - *collective* effects!

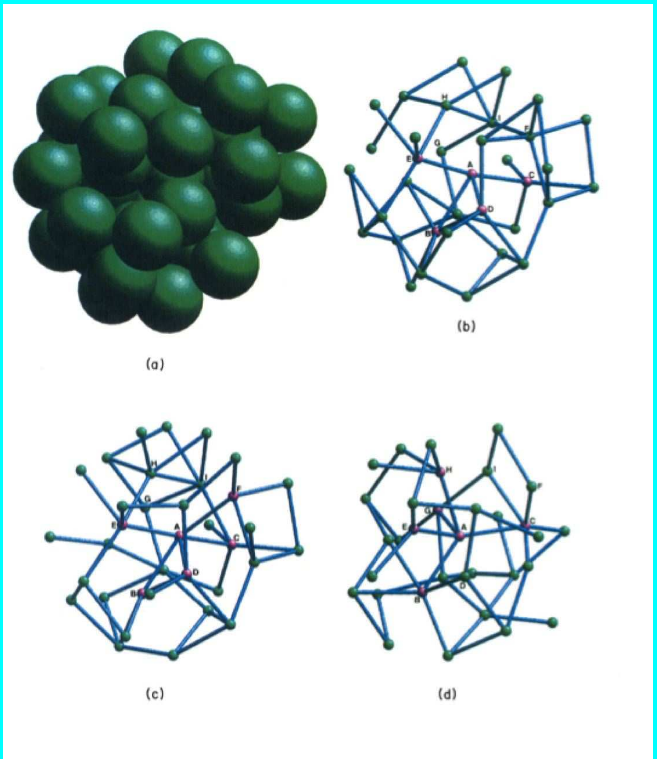
Plot of coordination no. vs shake intensity



Coordination nos. about 4.5 - 'frictional packings'! cf. MD simulations of Silbert et al PRE 2002

Contact networks: how they deform or break!

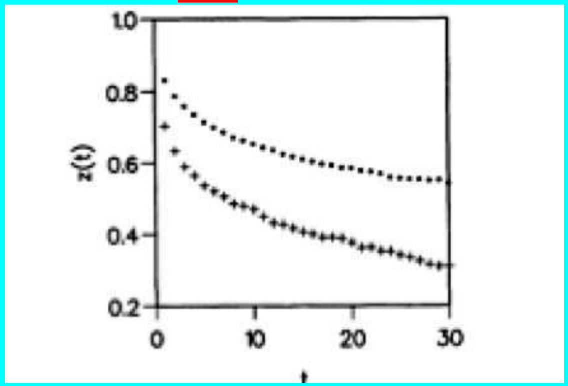
Low vibrational intensities cause contact networks to deform:
High vibrational intensities cause contact networks to break!



(see also T A J Duke, G C Barker and AM, EPL 1990)

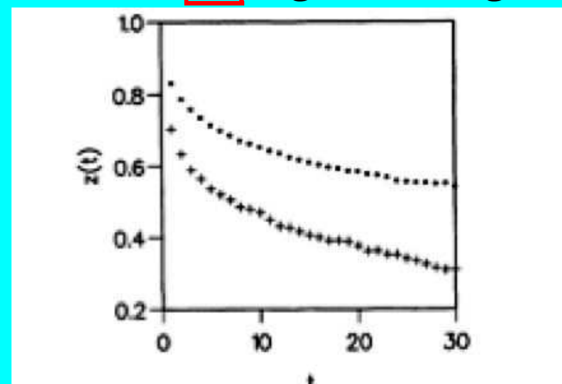
Bridge collapse - the mechanism for compaction near jamming?

- At
  low intensities, contact networks deform ▷ a grain's neighbours stay (almost) the same...

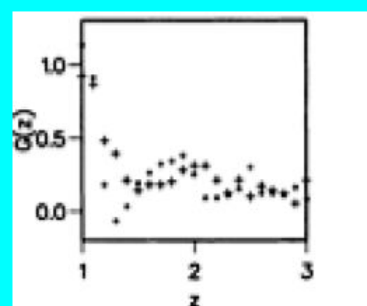


Bridge collapse - the mechanism for compaction near jamming?

- At
  low intensities, contact networks deform ▷ a grain's neighbours stay (almost) the same...

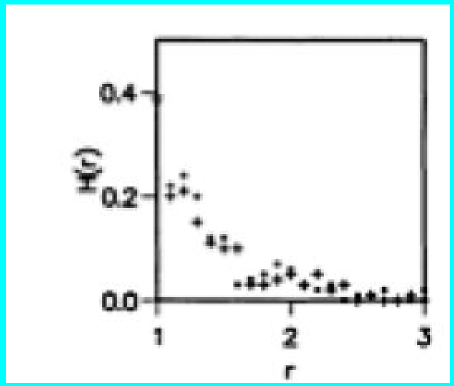


- ..and collapse onto each other causing displacement *anticorrelations*!

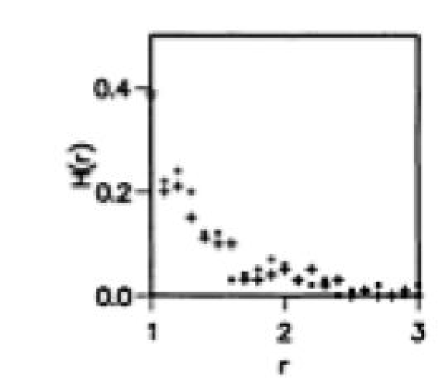


- A major mechanism for compaction near jamming is **bridge collapse**; 'sharper' bridges (which trap more void space) collapse into 'flatter' ones.
  (G C Barker and AM, PRE 1993)

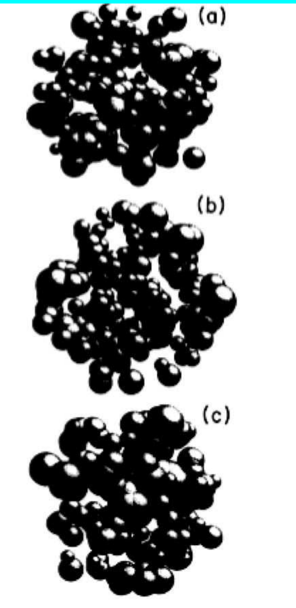
What about horizontal displacement correlations?



What about horizontal displacement correlations?



The void space at different amplitudes



Note that the void space gets connected at large amplitudes!

Is there spontaneous crystallisation?

Spontaneous crystallisation can occur by nucleation near the jamming limit for a specific range of intensities

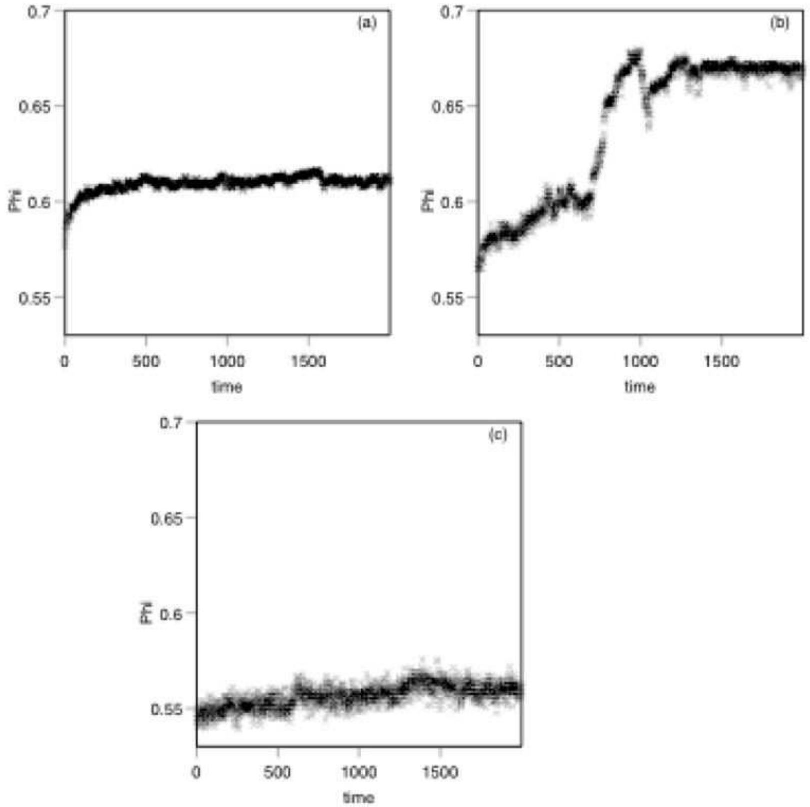


Figure 1. Plots of packing fraction ϕ versus time t for (a) $A = 0.05$, (b) $A = 0.5$, (c) $A = 1.2$. Note the approach to crystallization in (b).

AM and G C Barker, J Phys. Cond. Mat. 2000

Note the difference in ordering!

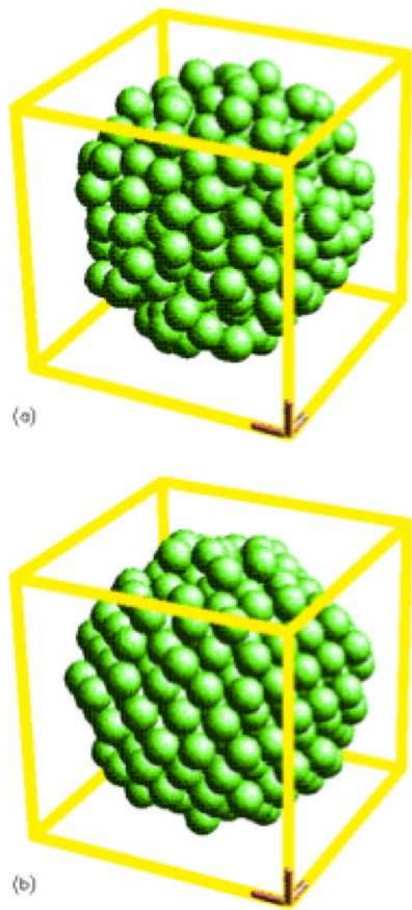


Figure 2. An example of typical clusters obtained after 2000 time steps for (a) $A = 0.05$, (b) $A = 0.5$. Note the crystalline-like ordering in the second case.

(This figure can be viewed in colour in the electronic version of the article; see www.iop.org)

Statistics of bridge geometries

AM, J M Luck and G C Barker, JSTAT 2004.

Bridges can be classified as simple...

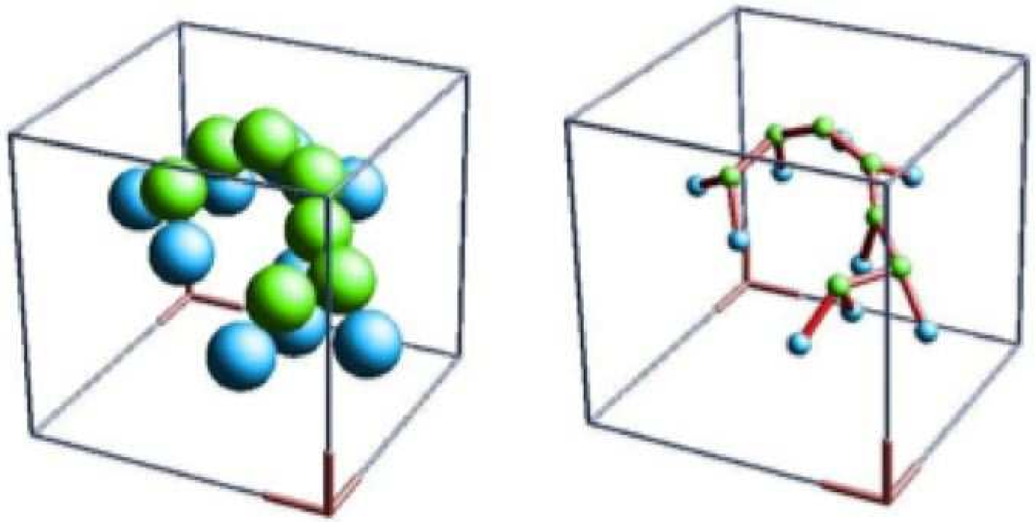


Figure 2. A seven particle *linear bridge* with nine base particles (left), and the corresponding contact network (right). Thus $n = 7$ and $n_b = 9 = 7 + 2$.

...or complex

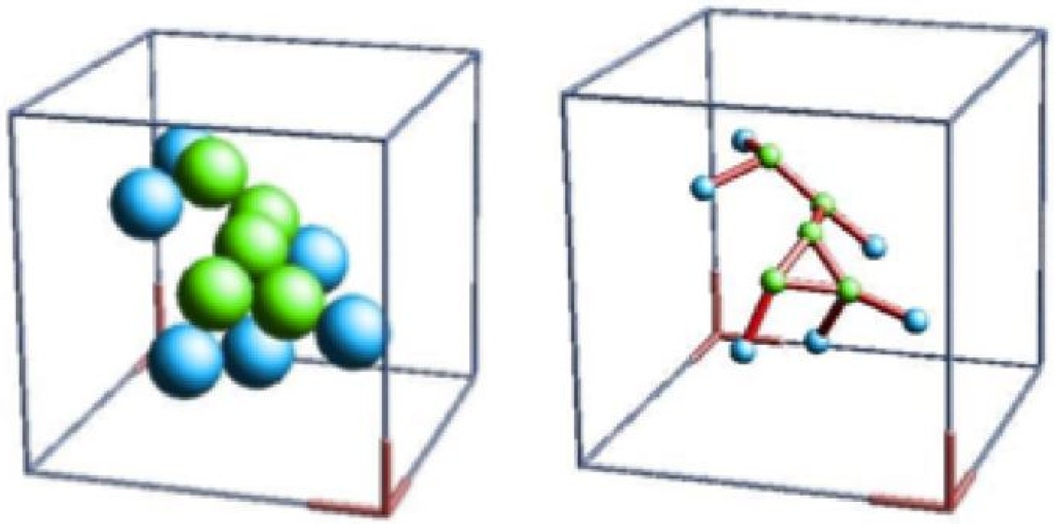


Figure 1. A five particle *complex bridge*, with six base particles (left), and the corresponding contact network (right). Thus $n = 5$ and $n_b = 6 < 5 + 2$.

- Linear bridges are exponentially distributed ($P(n) \sim \exp(-an)$) and look like self-avoiding walks with d between 2 and 3.
- Complex bridges dominate after $n \approx 8$, and look like $3d$ critical percolation clusters: $P(n) \sim n^{-\tau}$ with $\tau \sim 2$.
- Asymptotically, long linear bridges are domes, with flat bases.
- Linear bridges grow diffusively in the vertical, and superdiffusively in the horizontal directions.

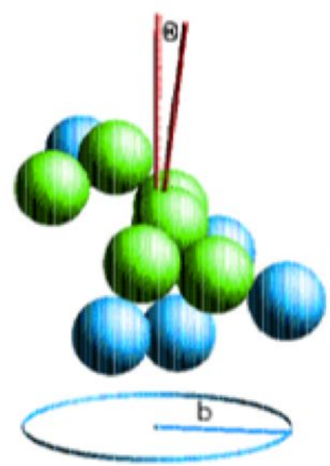


Figure 3. Definition of the angle Θ and the base extension b of a bridge. The main axis makes an angle Θ with the z-axis; the base extension b is the projection of the radius of gyration of the bridge on the x-y plane.

cf. experiments of To et al PRL 2001

Distributions of base extensions of linear bridges (through which any forces would be transmitted in the normal direction)...

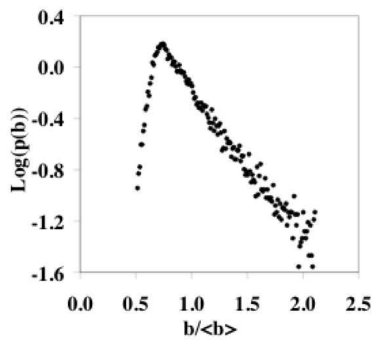


Figure 4. Distribution of base extensions of bridges, for $\Phi = 0.58$.

Distributions of base extensions of linear bridges (through which any forces would be transmitted in the normal direction)...

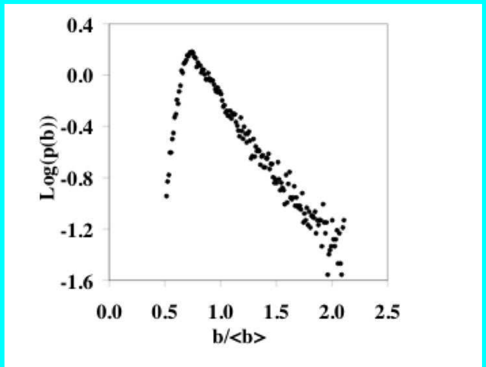


Figure 4. Distribution of base extensions of bridges, for $\Phi = 0.58$.

... resemble experimental distributions of normal forces in shaken granular media!

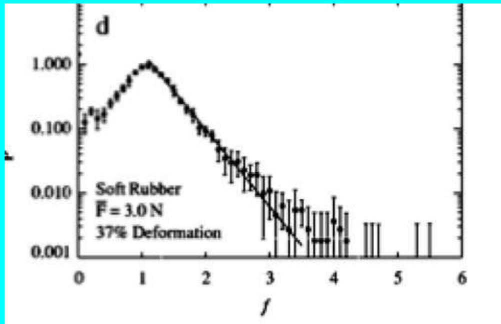


FIG. 2. $P(f)$ with varying particle hardness. Probability distri-

Erikson et al PRE 2002.

Distributions of base extensions of linear bridges (through which any forces would be transmitted in the normal direction)...

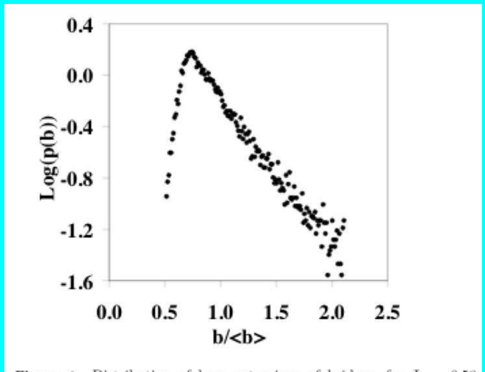


Figure 4. Distribution of base extensions of bridges, for $\Phi = 0.58$.

... resemble experimental distributions of normal forces in shaken granular media!

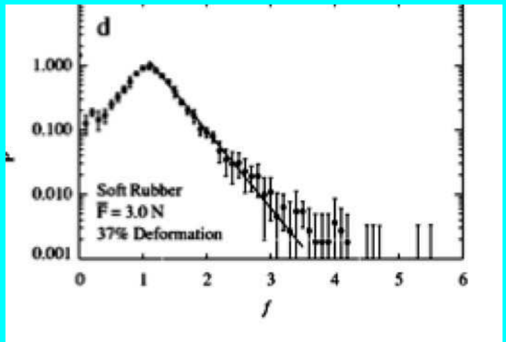


FIG. 2. $P(f)$ with varying particle hardness. Probability distri-

Erikson et al PRE 2002.

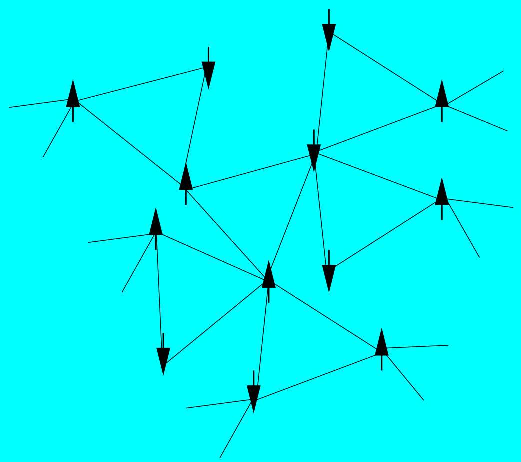
Speculate: Linear bridges ≡ force chains?

Granular compaction: sand on random graphs

J M Berg and AM, EPL 2001, PRE 2002.

The model

- Put grains/spins at vertices of random graphs - ▷ full disorder with finite connectivity!

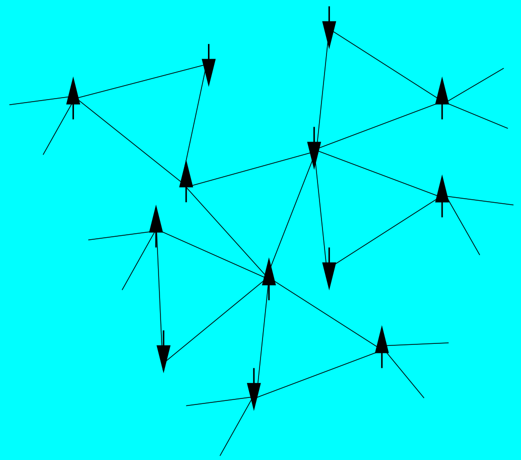


Granular compaction: sand on random graphs

J M Berg and AM, EPL 2001, PRE 2002.

The model

- Put grains/spins at vertices of random graphs - ▷ full disorder with finite connectivity!



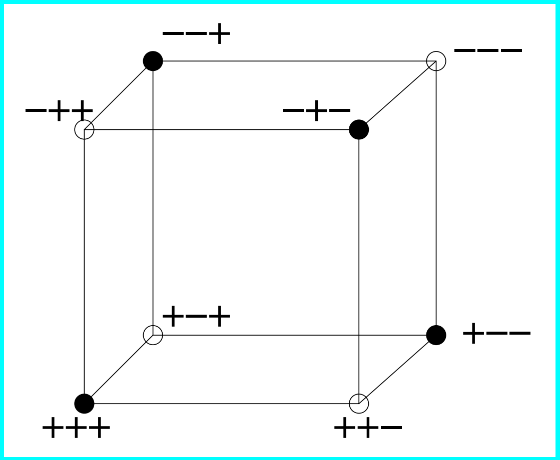
- Use 3-spin model $V = -\rho N = -\sum_{i<j<k} C_{ijk} S_i S_j S_k$ with $C_{ijk} = 1(0)$ denoting presence/absence of plaquette connecting sites i, j, k and $S = \pm 1$ grain orientations
- Get fluctuating local connectivities
- Need to minimise V leads to frustration!

Slow dynamics and metastability emerge...

- Global ground state $+++$ but locally, $--+, -+-, +--$ also good!
- Competition between global and local *void minimisation* leads to slow dynamics.

Slow dynamics and metastability emerge...

- Global ground state $+ + +$ but locally, $- - +, - + -, + - -$ also good!
- Competition between global and local *void minimisation* leads to slow dynamics.



- two spin flips required to take plaquette from one metastable state to another - 'energy' barrier crossed!

  cf. bridge collapse ▷ granular compaction! (AM and G C Barker, PRL 1991)

Modelling tapping at intensity Γ

(thermal tapping as in G C Barker and AM, PRA 1992)

- Dilation ▷
  grain i flipped w. prob. 1 if s_i antiparallel to local field h_i,
  w. prob. $\exp(-h_i/\Gamma)$ if parallel,
  w. prob. 0.5 if $h_i = 0$ - rattlers!

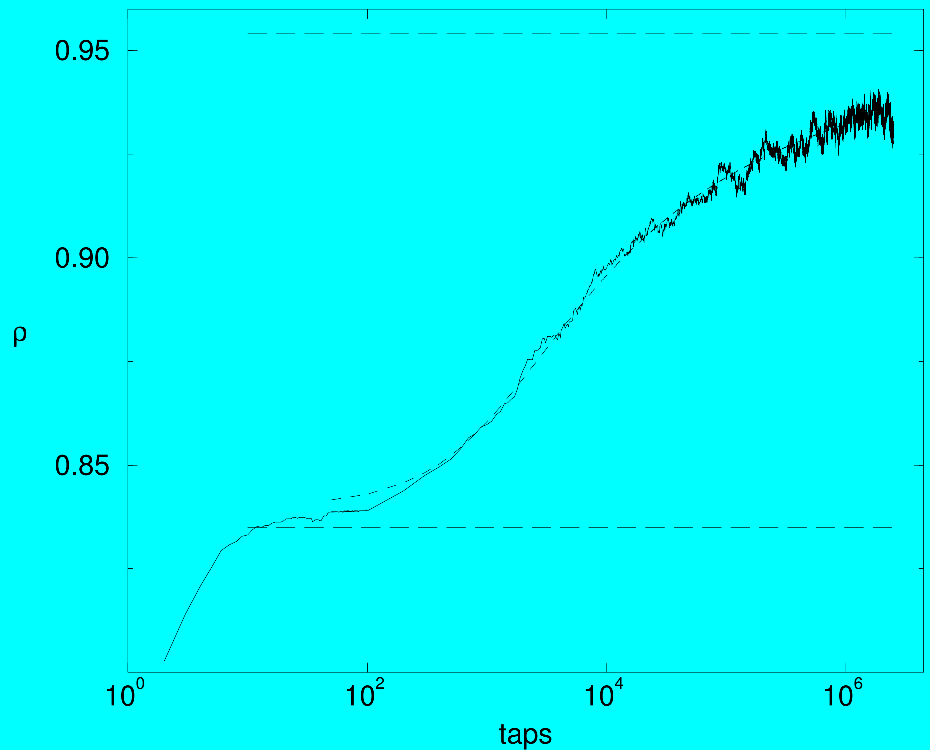
- Quench till blocked state reached

▷ Sites with large h_i are highly constrained ▷ thermal tapping!

Results

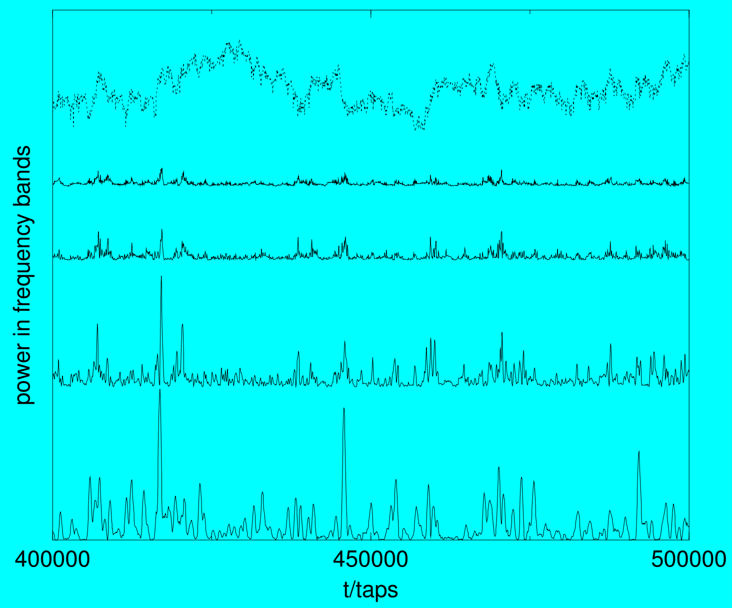
The Compaction curve

- fast dynamics until single-particle relaxation threshold
- slow dynamics with logarithmic relaxation
- systemwide density fluctuations



Cascades

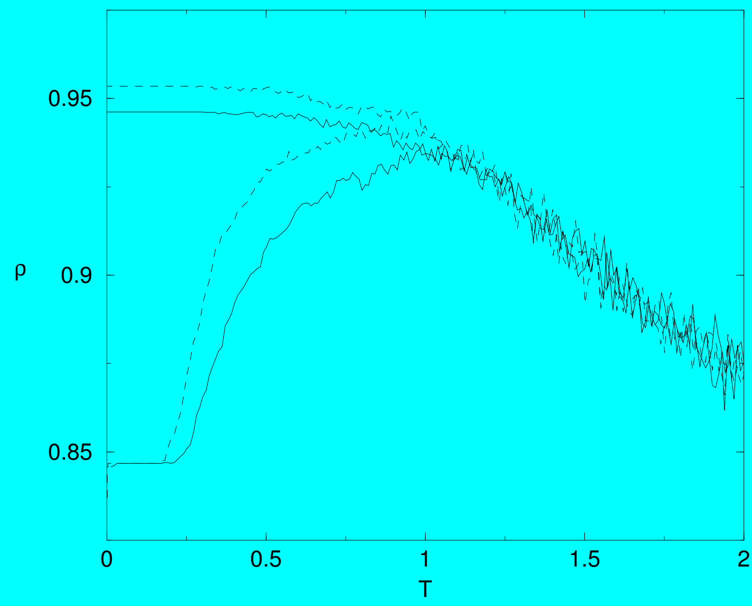
- Density fluctuations analysed (following Nowak et al, PRE 1998)



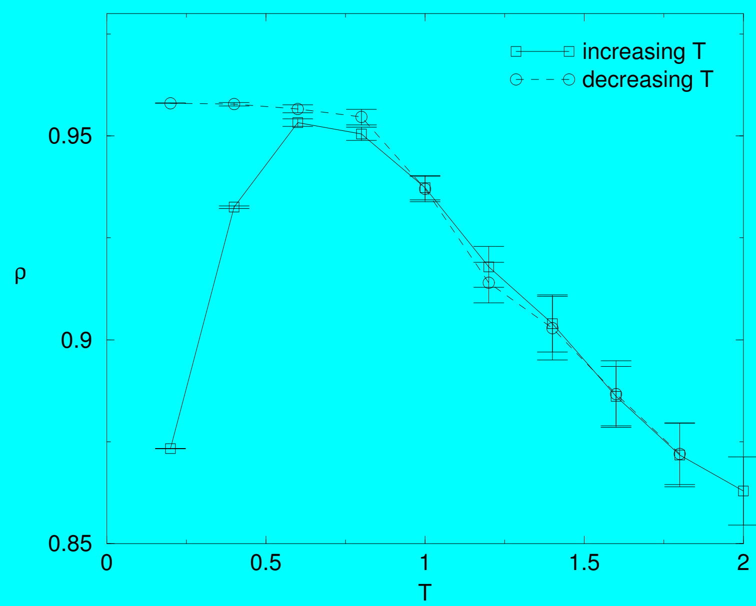
- ▷ a cascade mechanism of compaction!
- grains release other grains, so correlations over all scales!

Amplitude cycling

- Grains tapped at amplitude Γ for a time τ, then at $\Gamma + \delta\Gamma$ and so on...
- Control parameter $\delta\Gamma/\tau$ - measure of 'equilibration'
- Most models predict 'crystallisation' (not realised experimentally, cf Nowak et al PRE 1998....)



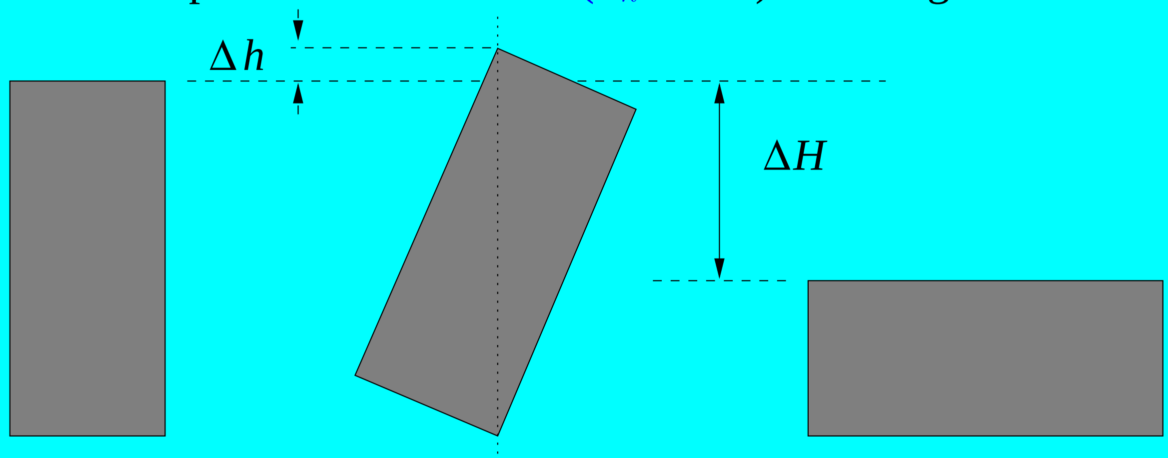
...with pinning of immobile grains, our model jams!!!



Shape matters in granular compaction

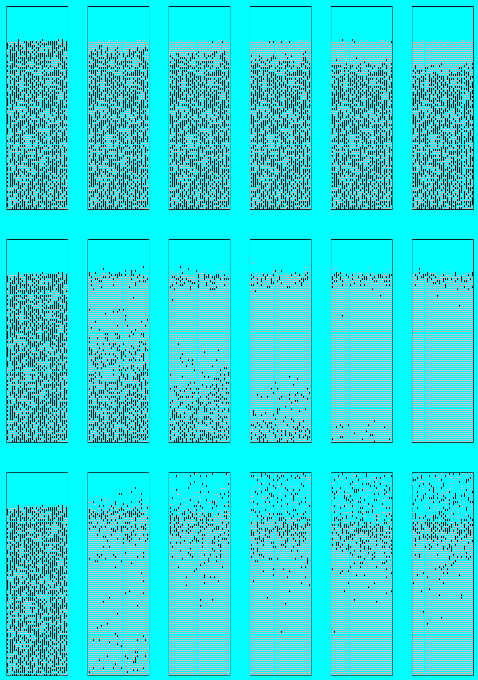
Simplest model - shaking a box of sand
P F Stadler, AM and J M Luck, EPL 2000.

- NxM sites in a box: two possible orientations ($\sigma_n = \pm 1$) of each grain

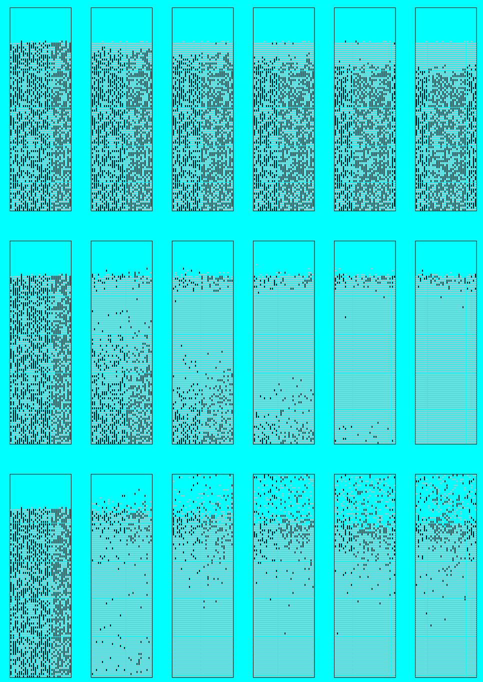


- Grains can fly, fall or flip
- The deeper the grain in the box, the less likely it is to flip!

- Get fluidised, intermediate and 'glassy' regimes



- Get fluidised, intermediate and 'glassy' regimes



- ...but 'glassy' regime isn't **really** glassy - no intergrain interactions... ▷ modify model!

Introduce interactions based on orientation of grains in a column of N grains:
AM and J M Luck, JPA 2003, EPJB 2004.

- Each disordered grain leaves a **void space** ε on the site it occupies
- **(Ir)rational** ε $\boxed{\triangleright}$ **(ir)regular grains**: the effect of shape
- Transition probability $w(\sigma_n = \pm \to \sigma_n = \mp) = \exp(-n/\xi_{\rm dyn} \mp h_n/\Gamma)$
- $\xi_{\rm dyn}$ dynamical length, Γ vibration intensity
- Ordering field $h_n = \varepsilon\, m_n^- - m_n^+$
  with m_n^+ no. of $+$ grains above grain n
  and m_n^- no. of $-$ grains above grain n

Introduce interactions based on orientation of grains in a column of N grains:
AM and J M Luck, JPA 2003, EPJB 2004.

- Each disordered grain leaves a **void space** ε on the site it occupies
- **(Ir)rational** ε $\boxed{\triangleright}$ **(ir)regular grains**: the effect of shape
- Transition probability $w(\sigma_n = \pm \to \sigma_n = \mp) = \exp(-n/\xi_{\rm dyn} \mp h_n/\Gamma)$
- $\xi_{\rm dyn}$ dynamical length, Γ vibration intensity
- Ordering field $h_n = \varepsilon\, m_n^- - m_n^+$
  with m_n^+ no. of $+$ grains above grain n
  and m_n^- no. of $-$ grains above grain n

- h_n **is just excess void space!** see e.g. Brown and Richards 1969
- Transition from order to disorder for grain n *hindered* by no. of voids above it.

Ground states

- For irrational ε, all h_n are non-zero

  ▷ **Unique quasiperiodic ground state for irregular grains!**

Ground states

- For irrational ε, all h_n are non-zero

  ▷ **Unique quasiperiodic ground state for irregular grains!**

- For rational $\varepsilon = p/q$, h_n can vanish!

  ▷ perfect packing when n multiple of period $p + q$.

  ▷ **Highly degenerate ground states for regular grains!**

Ground states

- For irrational ε, all h_n are non-zero
  ▷ **Unique quasiperiodic ground state for irregular grains!**

- For rational $\varepsilon = p/q$, h_n can vanish!
  ▷ perfect packing when n multiple of period $p + q$.
  ▷ **Highly degenerate ground states for regular grains!**

- **Simple example for regular grains:**
  For $\varepsilon = 1/2$, dynamics chooses $+ - -$ and $- + -$ as units of perfect packing
  ▷ two 'half' voids from each $-$ grain filled by $+$ grain.

Zero-temperature dynamics - irregular grains, irrational ε

- Dynamical rule $\sigma_n = \mathrm{sign}\ h_n$
- Irrational ground state optimal, imperfect and quickly retrieved
- Ordered layer grows ballistically $L(t) \approx V(\varepsilon)\, t$, for $L \ll \xi_{\rm dyn}$
- For $L(t) \sim \xi_{\rm dyn}$, logarithmic slowing down retrieved
  ▷ $L(t) \approx \xi_{\rm dyn} \ln t$

Zero-temperature dynamics - irregular grains, irrational ε

- Dynamical rule $\sigma_n = \text{sign}\ h_n$
- Irrational ground state optimal, imperfect and quickly retrieved
- Ordered layer grows ballistically $L(t) \approx V(\varepsilon)\, t$, for $L \ll \xi_{\text{dyn}}$
- For $L(t) \sim \xi_{\text{dyn}}$, logarithmic slowing down retrieved
  ▷ $L(t) \approx \xi_{\text{dyn}} \ln t$

Preview of rationals: **Perfect ground states, irretrievably lost!**

Zero-temperature dynamics - regular grains, rational ε

- Local field h_n may vanish in $\sigma_n = \text{sign}\ h_n$

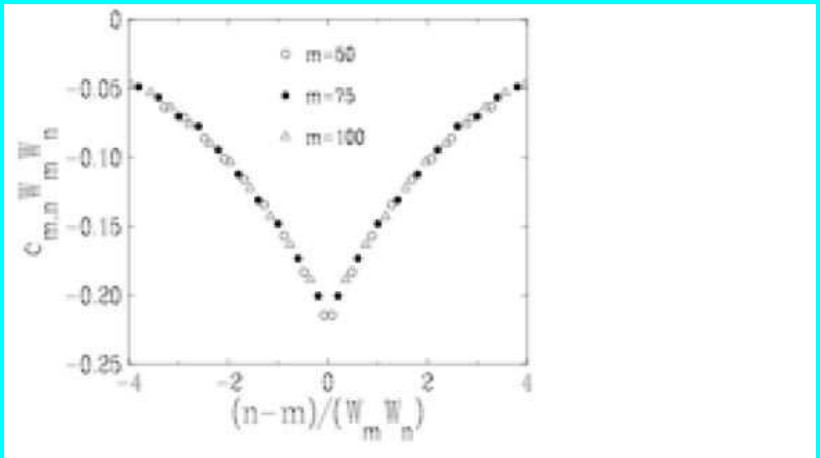
- Rational ground state **perfect and (all) too easily lost!**

- Get stochastic dynamics at *zero* temperature
  $\triangleright$ system relaxes to non-trivial steady state !!!

- Unbounded fluctuations of h_n $\triangleright$ Density fluctuations seen in experiments of Nagel et al, Nowak et al, 1992 -!

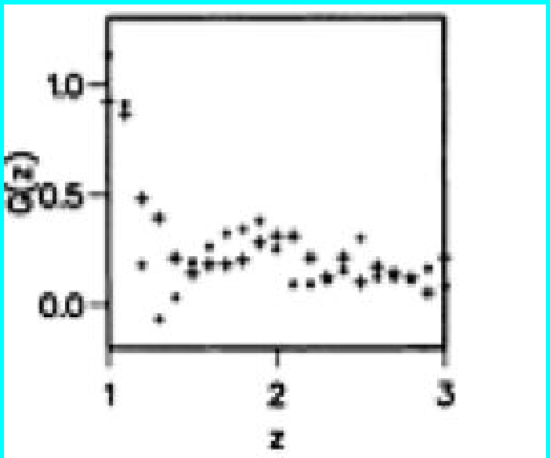
- KEY RESULT: **Anomalous roughening law** $W_n^2 = \langle h_n^2 \rangle \approx A\, n^{2/3}$

▷ **Grain displacements fully anticorrelated!**

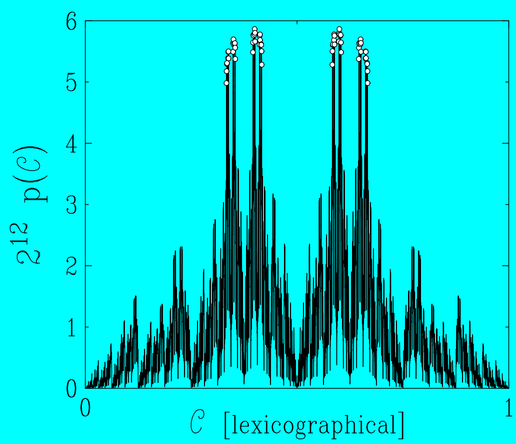


....reminiscent of anticorrelations in longitudinal displacement-displacement correlations in the jamming limit...

G C Barker and AM Phys Rev A 1992

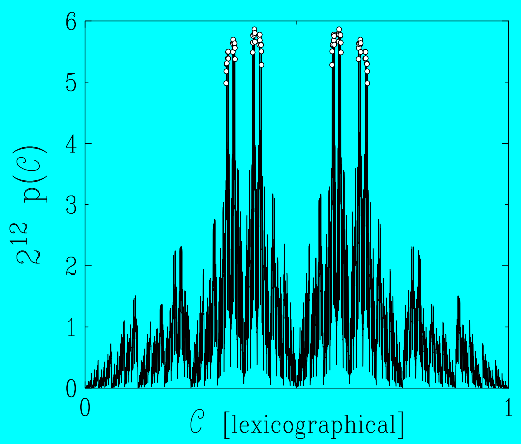


Ground state entropy for regular grains, rational ε



- Extremely rugged landscape of microscopic entropy (as it should be for compaction near jamming)
- Some configurations clearly visited far more often than others! ▷ ground states!

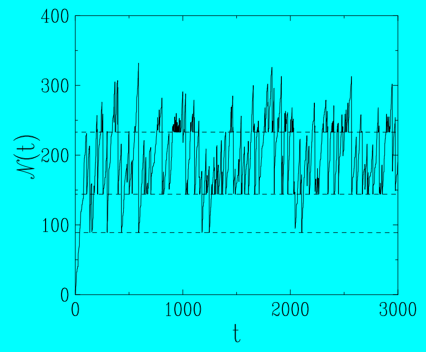
Ground state entropy for regular grains, rational ε



- Extremely rugged landscape of microscopic entropy (as it should be for compaction near jamming)
- Some configurations clearly visited far more often than others! ▷ ground states!
- Macroscopic entropy agrees with **Edwards' flatness** hypothesis!! (Edwards 1989)

Intermittency in low-temperature dynamics

Boundary Layer Position $\mathcal{N}(t)$, for a temperature $\Gamma = 0.003$



- Ordering length $\langle \mathcal{N} \rangle$ diverges at low T - excitations more and more rare - $\langle \mathcal{N} \rangle \sim 1/(\Gamma |\ln \Gamma|)$
- Finite-temperature equivalent of 'zero-temperature' length $\xi_{\rm dyn}$ which divides an ordered boundary layer from a lower (bulk) disordered region.
- Seen in experiments of Clement et al, 2003