Theoretical Model of Granular Compaction

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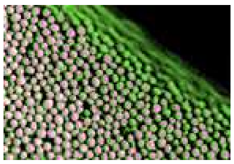
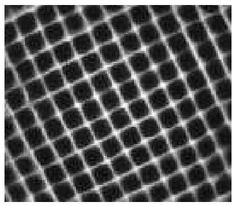
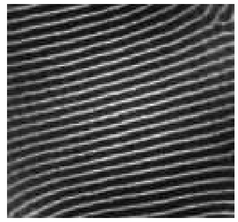
Theory: Grossman, Zhou (Chicago), Krapivsky (Boston)
Experiment: Knight, Nowak, Jaeger, Nagel (Chicago)

Observations

- Avalanches in sand piles — Bak ,Jaeger 89
- Size segregation — Knight 93
- Force chains — Coppersmith 95
- Clustering — Gollub 97
- Compaction — Knight 95
- Pattern formation — Swinney 95
- Solitary waves — Umbanhowar 95
- Convection rolls — Ehrics 95

Rich and intriguing behavior

Theoretical Issues

- Fluid Mechanics: Flow properties.

  How to express pressure, equation of state, stress tensor, boundary conditions?

  Averaging problematic - macroscopic grains

- Statistical Mechanics: Collective properties.

  Thermal fluctuations negligible ($T \equiv 0$)

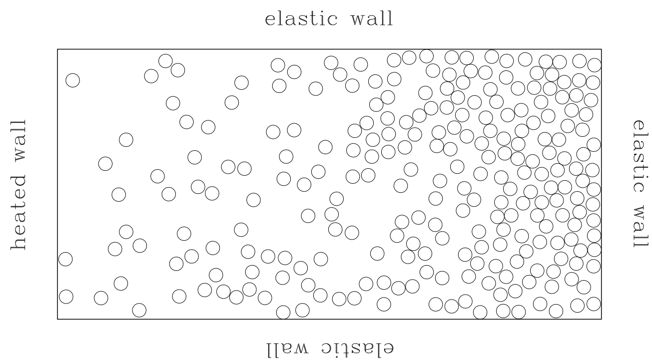
  Gas/Liquid/Solid behavior

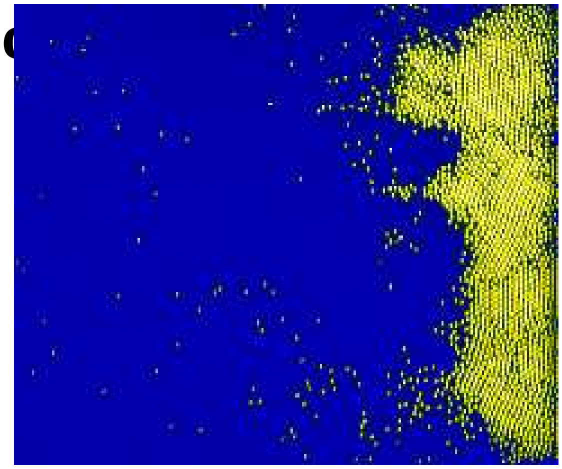
- Mechanics: Grain-Grain interaction

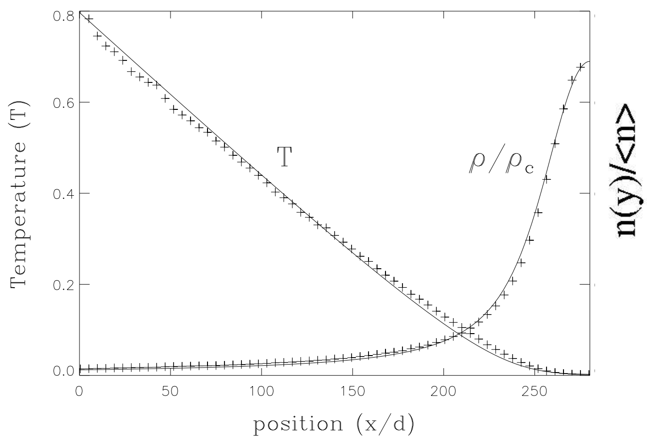
  Molecular Dynamics: inelastic collisions

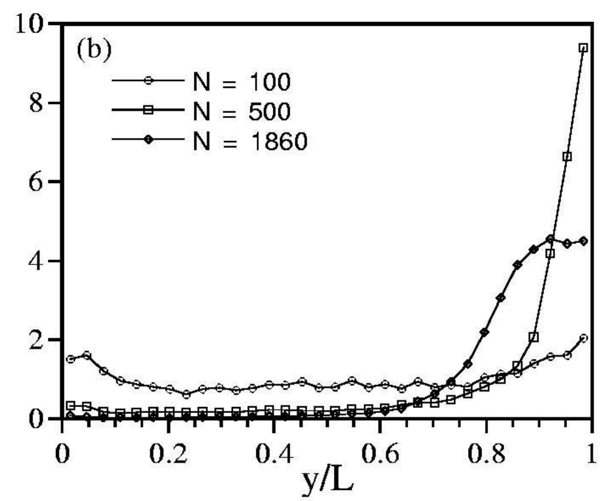
Theory is incomplete

Granular Fl









- Experiment - spherical steel particles Gollub 97
- Theory - energy balance eqn. $dq/dx = -I$. Approximate hard spheres equation of state $P = \rho T \frac{\rho_c+\rho}{\rho_c-\rho}$, etc.

Agreement - Theory, Simulation, Experiment

Compaction

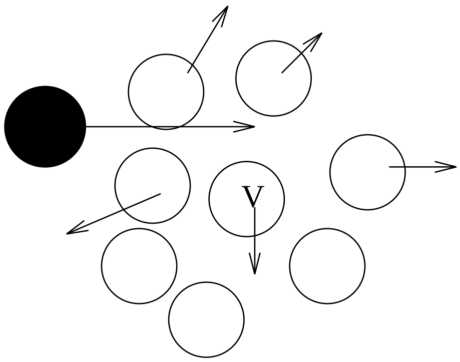
- Uniform, simple system
- Probes the density - a fundamental quantity
- Slow density relaxation Knight 95

$$\rho(t) = \rho_\infty - \frac{\rho_\infty - \rho_0}{1 + B\ln(t/\tau)}$$

- Parameters depend on Γ only
- Robust behavior - independent of grain type, grain size, container geometry, etc.

What causes logarithmic relaxation?

Heuristic picture



$$\begin{aligned} \rho &= \text{volume fraction} \\ V &= \text{particle volume} \\ V_0 &= \text{pore volume/particle} \end{aligned}$$

$$\rho = \frac{V}{V + V_0} \qquad \text{or} \qquad V_0 = V\frac{1-\rho}{\rho}$$

Assumption: Cooperative rearrangement

$$NV_0 = V \qquad \text{or} \qquad N = \frac{\rho}{1-\rho}$$

Assumption: Exponential rearrangement time

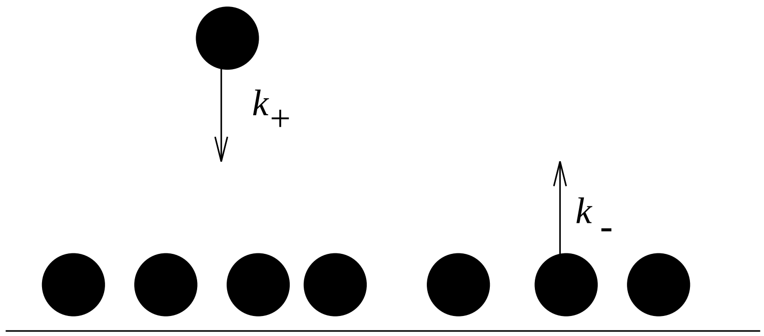
$$T = e^N = e^{\frac{\rho}{1-\rho}}$$

$$\frac{d\rho}{dt} \propto (1-\rho)\frac{1}{T} = (1-\rho)e^{-\frac{\rho}{1-\rho}}$$

$$\rho(t) \cong 1 - \frac{1}{\ln t}$$

Volume exclusion causes slow relaxation

The "parking" model



- 1D Adsorption-desorption process
- Adsorption subject to volume constrains
- Desorption not restricted
- Detailed balance satisfied
- System reaches equilibrium steady state

Ignores: mechanical stability

Realistic: excluded volume interaction

Theory

$P(x,t) =$ Density of x-size voids at time t

$$1 = \int dx (x+1) P(x,t) \qquad \rho(t) = \int dx P(x,t)$$

Master equation:

$$\frac{\partial P(x)}{\partial t} = 2k_+ \int_{x+1} dy P(y) - 2k_- P(x)$$
$$+\theta(x-1)\left[\frac{k_-}{\rho(t)}\int_0^{x-1} dy P(y) P(x-1-y) - k_+(x-1)P(x)\right]$$

Density rate equation:

$$\frac{\partial \rho(t)}{\partial t} = -k_- \rho(t) + k_+ \int_1 dx (x-1) P(x,t)$$

Convolution term assumes voids are uncorrelated (exact in equilibrium)

Exact Equilibrium Properties

Exponential void distribution

$$P_\infty(x) = \frac{\rho_\infty^2}{1-\rho_\infty} \exp\left[-\frac{\rho_\infty}{1-\rho_\infty} x\right]$$

Sticking Probability

$$S(\rho_\infty) = \exp\left[-\frac{\rho_\infty}{1-\rho_\infty}\right]$$

Gaussian Density Distribution

$$P_\infty(\rho) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(\rho-\rho_\infty)^2}{2\sigma^2}\right]$$

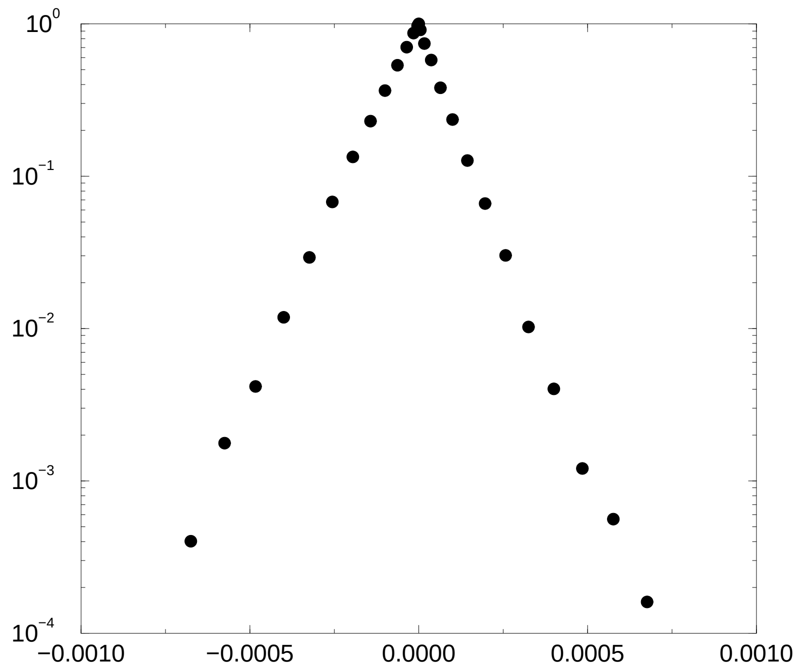
Variance decreases with density

$$\sigma^2 = \rho_\infty(1-\rho_\infty)^2/L \qquad \beta = 2$$

$\boxed{\text{Volume exclusion dominates at high densities}}$

Monte Carlo simulations

- Parameters: $k = 10^2$, $L = 10^3$.
- Theory: $\rho_\infty = 0.7719$, $\sigma^2 = 4.01 \times 10^{-5}$.
- Simulations: $\rho_\infty = 0.7718$, $\sigma^2 = 4.05 \times 10^{-5}$.



$P(\rho - \rho_\infty)$ versus $(\rho - \rho_\infty)^2 \mathrm{sgn}(\rho - \rho_\infty)$

$\boxed{\text{Theoretical predictions verified numerically}}$

Relaxation Properties

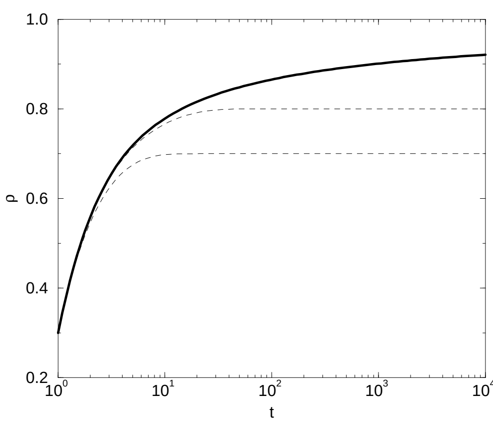
Quasistatic (near equilibrium) approximation

$$\frac{\partial \rho(t)}{\partial t} = -k_- \rho(t) + k_+(1-\rho)\exp\left[-\frac{\rho}{1-\rho}\right]$$

I Desorption-limited case $(k_- \to 0)$

$$\rho(t) \cong 1 - \frac{1}{\ln k_+ t}$$

II Finite k_- $\tau = (L/k_- \rho_\infty)\sigma^2 = (1-\rho_\infty)^2/k_-$



$$\rho(t) \cong \begin{cases} 1 - \frac{1}{\ln k_+ t} & t \ll \tau \\ \rho_\infty - Ae^{-t/\tau} & t \gg \tau \end{cases}$$

Slow density relaxation

The sticking probability

Total adsorption rate

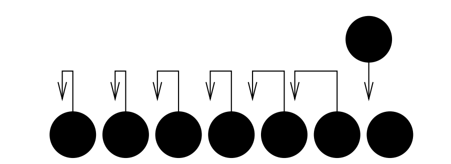
$$\int_1 dx(x-1)P_\infty(x) = k_+(1-\rho_\infty)\exp\left[-\frac{\rho_\infty}{1-\rho_\infty}\right]$$

Reduced adsorption rate $k_+ \to k_+ s(\rho)$

Sticking probability

$$s(\rho) = e^{-N} \qquad N = \frac{\rho}{1-\rho}$$

Heuristic picture is exact in 1D



Cooperative behavior in dense limit

Spectrum of density fluctuations

Definition

$$\mathsf{PSD}(f) = \left| \int d\tau e^{if\tau} \langle \rho(t)\rho(t+\tau) \rangle \right|^2$$

Leading behavior

$$\mathsf{PSD}(f) \cong \begin{cases} f^0 & f \ll f_L \\ f^{-\alpha} & f_L \ll f \ll f_H \\ f^{-2} & f_H \ll f \end{cases}$$

For noninteracting dilute case, linear theory, $\mathsf{PSD}(f) \propto [1 + (f/f_0)^2]$, with $f_0 = \tau^{-1} = k_+ + k_-$

In general, still open problem. Reasonable that $f_L \approx k_-$ and $f_H \approx k_+$

Similar noise spectrum for finite system Monte Carlo and experimental data

Conclusions

- Compaction dominated by exponentially rare grain size voids
- Growing time scales associated with cooperative bead rearrangements
- Argument is general - should hold for aspherical grains or horizontal tapping
- Gaussian density fluctuations

Outlook

- Fluctuations spectrum
- **Experiment** - measure local density
- **Experiment** - 2D (crystalline structure)

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