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**
- **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

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

- Parameters depend on \( \Gamma \) only
- Robust behavior - independent of grain type, grain size, container geometry, etc.

What causes logarithmic relaxation?
**Heuristic picture**

\[ \rho = \frac{V}{V + V_0} \quad \text{or} \quad V_0 = V \frac{1 - \rho}{\rho} \]

**Assumption: Cooperative rearrangement**

\[ NV_0 = V \quad \text{or} \quad N = \frac{\rho}{1 - \rho} \]

**Assumption: Exponential rearrangement time**

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

\[ \rho(t) \equiv 1 - \frac{1}{\ln t} \]

**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

\[ P(x, t) = \text{Density of } x\text{-size voids at time } t \]

\[ 1 = \int dx(x + 1)P(x, t) \quad \rho(t) = \int dxP(x, t) \]

**Master equation:**

\[
\frac{\partial P(x)}{\partial t} = 2k_+ \int \limits_{x+1} dyP(y) - 2k_-P(x) + \theta(x-1) \left[ \frac{k_-}{\rho(t)} \int \limits_{0}^{x-1} dyP(y)P(x-1-y) - k_+(x-1)P(x) \right]
\]

**Density rate equation:**

\[
\frac{\partial \rho(t)}{\partial t} = -k_-\rho(t) + k_+ \int \limits_{1} dx(x - 1)P(x, t)
\]

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

\[ \sigma^2 = \rho_\infty (1 - \rho_\infty)^2 / L \quad \beta = 2 \]

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:** $\rho_\infty = 0.7718$, $\sigma^2 = 4.05 \times 10^{-5}$.

\[ P(\rho - \rho_\infty) \text{ versus } (\rho - \rho_\infty)^2 \text{sgn}(\rho - \rho_\infty) \]

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 \((k_- \to 0)\)

\[ \rho(t) \approx 1 - \frac{1}{\ln k_+ t} \]

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

\[ \rho(t) \approx \begin{cases} 1 - \frac{1}{\ln k_+ t} & t \ll \tau \\ \rho_\infty - A e^{-t/\tau} & t \gg \tau \end{cases} \]

Slow density relaxation
The sticking probability

Total adsorption rate

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

Reduced adsorption rate \( k_{+} \rightarrow k_{+}s(\rho) \)

Sticking probability

\[ s(\rho) = e^{-N} \quad N = \frac{\rho}{1 - \rho} \]

Heuristic picture is exact in 1D

Cooperative behavior in dense limit
Spectrum of density fluctuations

Definition

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

Leading behavior

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

For noninteracting dilute case, linear theory, \( \text{PSD}(f) \propto [1 + (f/f_0)^2] \), 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)