Fluctuations and State Variables in (Boundary) Driven Granular Materials

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Granular materials fail

**industrial transport/mixing**
- fail at higher rates than fluid systems
- run below their design capacity
- costs $

**natural systems**
- erosion
- earthquakes
- snow/rock avalanches

How can we **describe the state of a granular system?** (... in order to make accurate predictions about its future behavior?)
### Solid?
- Sustains forces via force chains

### Liquid?
- Flows have shear-banding

### Gas?
- Requires energy input; clustering instabilities
Granules ≠ Macroscopic Molecules

- athermal: $k_B T \sim 10^{-12} mgh$
- dissipative (friction & collisions)
- poor separation of micro- and macroscopic scales
- large spatial and temporal inhomogeneities
- history-dependence due to frictional contacts
Which granular state variables matter?

**Particles**
- global packing fraction
- local packing fraction
- packing fluctuations
- velocity fluctuations
- orientation/texture
- particle-size distribution
- ...

\[ \phi \]

**Stress**
- boundary stress
- local stress
- stress fluctuations
- orientation/texture
- ...

high \( \phi \)  
low \( \phi \)
Exponential Force Distribution

Mueth, Jaeger, & Nagel
PRE (1998)

Majmudar & Behringer
Nature (2005)

rare, extreme
S E C T. V I I.

De Motu per Fluida propagato.

Prop. XLI. Theor. XXXI.

Pressio non propagatur per Fluidum secundum lineas rectas, nisi ubi particula Fluidi in directum jacent.

Si jaceant particulae a, b, c, d, e in linea recta, potest quidem pressio directe propagari ab a ad e; at particula e urgetur particulas oblique potitus f & g oblique, & particula illae f & g non sustinebunt pressionem illatam, nisi sustineantur a particulis ulterioribus b & k; quatenus autem sustineantur, premunt particulas sustinentes; & haec non sustinebunt pressionem nisi sustineantur.
Force Chains in Other Systems

Simulation of stress distribution in a polymer network under strain

Fluorescent dye measurement of forces on 10 micron liquid droplets
“Temperature” as a State Variable?

- kinetic theory
- entropy & energy
- fluctuation-dissipation

\[ k_B T = \frac{1}{2} m \langle (v - \bar{v})^2 \rangle \]

\[ \frac{1}{T} = \frac{\partial S}{\partial E} \]

\[ C(t) = -k_B T R(t) \]

Do these “temperatures” measure the same thing?

Do they tell us anything meaningful about the state of the system?
Boltzmann

Energy is conserved
Temperature equilibrates
\( \Omega(E) \) counts valid states

\[ e^{-\frac{E}{k_B T}} \]

\[ S = k_B \ln \Omega(E) \]

\[ \frac{1}{T} = \frac{\partial S}{\partial E} \]

\[ C_v = \frac{d \langle E \rangle}{d T} = \frac{1}{k_B T^2} \langle dE^2 \rangle \]

Edwards

Volume is conserved
Compactivity equilibrates
\( \Omega(V) \) counts mechanically-stable states

\[ e^{-\frac{V}{X}} \]

\[ S = k_E \ln \Omega(V) \]

\[ \frac{1}{X} = \frac{\partial S}{\partial V} \]

\[ \frac{d \langle V \rangle}{d X} = \frac{1}{X^2} \langle dV^2 \rangle \]

[Edwards & Oakeshott 1989]
2D granular systems


- can (more easily) obtain complete information about particle positions and stresses than in 3D
- comparison with 3D allows tests of dependence on dimensionality
Creating a dense granular fluid

- 3 boundary conditions (CP, CV, EQ)
- 3 interparticle frictions & coefficients of restitution
- Amorphous vs. ordered
Injecting energy

bumper frequency = 10 Hz
Intermittency

Longhi, Easwar, Menon *PRL*(2002)
Ferguson & Chakraborty *PRE*(2006)
Injecting energy

average kinetic energy/particle

\[ \frac{E}{N} [\mu J] \]

\( \phi \)

- CP, \( \mu = 0.5 \)
- CP, \( \mu = 0.85 \)
- CV, \( \mu = 0.5 \), crystal
- CV, \( \mu = 0.5 \)
What state variables equilibrate between two subsystems in contact?
• constant total volume
• $N$ is same on both sides
• vary $N$ by removal of triplets

Does $\lambda = 1/2$ ?

Macroscopic states: piston statistics

Non-Equilibrium, but Steady-State

- stationary states with equal average pressure
- gaussian statistics
- mean and variance changes with N
Macroscopic states: average volume

- \( \lambda \leq \frac{1}{2} \rightarrow \text{Side 1} \) (large friction) is denser
- Material properties matter

\( <\lambda> \rightarrow \) solid-like (onset of caging)
Measuring diffusion

\[ \sigma^2 = 4Dt \]

diffusion coefficient

Dynamics slow down

- high $\phi$: structural relaxation time increases over several orders of magnitude & diffusion drops to zero $\rightarrow$ “caging”
- diffusion coefficient takes the same value in each subsystem $\rightarrow$ equilibration of something?
What equilibrates?

\[ D = \frac{kT}{\text{drag}} \]

\[ \text{drag} \propto \mu \]

\[ \mu_1 \neq \mu_2 \rightarrow T_1 \neq T_2 \]
Packing fraction fluctuations

- Packing fraction fluctuations set by average packing fraction
- Particle properties don't matter !!!

Jamming for static particles
Majmudar et al, PRL (2007)
Lechenault et al, EPL (2008)
O'Hern et al, PRE (2003)

- \( \mu_1 = 0.85 \)
- \( \mu_2 = 0.5 \)

Just how universal is this relationship between mean and variance of $\phi$?
Lots of similar results in the literature

Aste EPJB (2008): 3d, jammed, exp + sim, local

Schröter et al PRE (2005): 3d, jammed, exp, global


Makse PRL (2008): 3d, jammed, sim, coarse-grained


Lechenault/Daniels (2010): 2d, driven, exp, local
$P(\phi)$ doesn't care about $\mu$ and BC

Voro++
Rycroft et. al. 2006

Puckett, Lechenault & Daniels PRE (2011)
$P(\phi)$ doesn't care about $\mu$ and BC
Why does \( P(\phi) \) depend on mean \( \phi \)?

**Edwards idea:**
\[
S = k_E \ln \Omega(V)
\]

- **high \( \phi \)**: zero variance, one valid configuration
- **low \( \phi \)**: more variance, many valid configurations
Granocentric model of jammed emulsions

draw particles from $P(r)$ until next one doesn't fit

contacts: $s = 0$
neighbors: $s = \delta$
(assign to 41%)

Broad distribution of separations
Local model

- \( P(r) = \) bidisperse (large, small particles)
- \( P(s) = \) measured from experiment
- random walk to fill angular space
- add local cell volumes from each neighbor to calculate \( \phi \)
- repeat for \( 10^4 \) central particles
Observations from experiment

Puckett, Lechenault & Daniels PRE (2011)
\( \mathcal{P} \exp(s) \) reproduces \( \sigma^2(\phi) \)
Geometry matters

- Variance of $P(\phi)$ falls with increasing $\phi$
  - Independent of $P(s)$, dimensionality, friction, above/below jamming, ...
  - Mean-field-like model ('granocentric') is sufficient to explain effect

- **Scarcity of angular space controls $P(\phi)$**
  - Edwards-like, but for non-mechanically-stable states
Can these states be described by analogy to a thermodynamic gas?

Kiri Nichol
(Leiden)
Velocities are not Maxwell-Boltzmann
Bumpers provide “thermal” bath

E/N [µJ]

CP, \( \mu = 0.5 \)

CV, \( \mu = 0.5 \), crystal

CP, \( \mu = 0.85 \)

CV, \( \mu = 0.5 \)
 Equipartition

\[
\langle E \rangle = \frac{1}{2} m \bar{v}_x^2 + \frac{1}{2} m \bar{v}_y^2 + \frac{1}{2} I \bar{\omega}^2
\]

\[
\langle E \rangle = E_{tr} + E_{rot}
\]

small, all, large

CV bare

CP banded

CP bare

2/3
Boyle's Law

Equation of State

\[ P(\overline{A} - A^*) = \overline{E}(1 + \chi) \]
Evaluating “temperatures”

- **kinetic theory**
  \[ kT = \frac{1}{2} m \langle (v - \bar{v})^2 \rangle \]

- **entropy & energy**
  \[ \frac{1}{X} = \frac{\partial S}{\partial V} \quad (Edwards) \]

- **fluctuation-dissipation**
  \[ C(t) = -kT R(t) \]
How useful are “thermodynamics” and statistical physics?

**Thermal-like**
- diffusive behavior
- Boyle's law with van der Waals-like EOS
- energy equipartition for rotational/translational degrees of freedom

**Not thermal-like**
- same diffusion constant @ different μ → different T?
- large/small equipartition fails
- non-Maxwell-Boltzmann velocity distribution

**Edwards-like**
- scarcity of angular space is a key control
Thanks!

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