Outlook:

• What’s Stat. Mech. theory of dense Granular Media (GM) and why Edwards introduced it

• Our current understanding of such a theory (from experiments and models)

• What we learn from it about the physics of GM (Phase Diagram, Equation of State, ...)

Granular Media (GM)

Examples of granular media are: powders, sands, rice, ...

- they are dissipative, non-thermal systems:
  \[ d > 1 \mu m \Rightarrow mgd >> k_B T \]


- Macroscopic properties of GM at rest are characterized by a few control parameters.
- As much as in thermal systems, macrostates correspond to many microstates, i.e., mechanically stable configurations.
Experiments in Chicago (Nagel et al. 1998)

- Experimental set-up for tapping dynamics: \( \Gamma = \frac{(\text{peak acceler.})}{\text{gravity}} \)

- Packing fraction, \( \phi \), as a function of the shake amplitude, \( \Gamma \).

(see also exp.s by D’Anna et al. 2001; Bideau et al. 2002; “flow taps” by Swinney et al. 2005)
Edwards’ approach to GM

- Granular media are found, at rest, in mechanically stable microstates. In Edwards approach to GM one uses the “standard machinery” of Stat. Mech. where averages are only over mechanically stable states.

- E.g., in the canonical ensemble (given average energy) the probability, $P_r$, of a microstate $r$ with energy, $E_r$, is:
  
a) $P_r \propto e^{-\beta_{conf} E_r}$ if $r$ is “mechanically stable”;
  
b) else $P_r = 0$.

$$T_{conf} = \beta_{conf}^{-1} \leftarrow \text{configurational temp.}$$

$$\beta_{conf} = \frac{\partial \ln \Omega}{\partial E}$$

$\Omega(E)$ is the number of “mechanically stable states” with $E$.

- The system at rest has: $T_{bath} = 0$ and $T_{conf} = \beta_{conf}^{-1} \neq 0$
Test of the Stat. Mech. scenario

We have to show that for any observable $Q$:

a) “Thermodynamics”

\[ \Gamma \quad \tau_0 \quad \longrightarrow \quad t \]

\[ \bar{Q} = \frac{1}{\Delta t} \sum_{t} Q(t) \]

$\bar{Q}$ is not “history” dependent; for instance, for a given energy, $e$, there is only one value $\bar{Q}(e)$.

b) “Statistical Mechanics”

\[ P_r \propto e^{-\beta_{conf} E_r} \quad \implies \langle Q \rangle = \sum_r Q_r P_r \]

Time and Ensemble Averages must coincide: $\bar{Q}(e) = \langle Q \rangle(e)$
Schematic Models and Dynamics

(Nicodemi, Coniglio, Herrmann 1997; ...)

Grains → draw a lattice → round grains

- **Hard Spheres** on a cubic lattice:

\[ H = H_{HC} + g \sum_i m_i z_i \]

Hard Core + Gravity

- Monte Carlo taps dynamics:

shaking “off” \( \iff T_{bath} = 0 \)
shaking “on” \( \iff T_{bath} = T_{\Gamma} > 0 \)

Tap **amplitude**: \( T_{\Gamma} \)
Tap **duration**: \( \tau_0 \)
The energy, $e$, is a good thermodynamic parameter; $T_\Gamma$ is not.
Connection of $T_{conf}$ and $T_{\Gamma}$

Use the equilibrium FDR:

$$\frac{\partial E}{\partial \beta_{conf}} = \Delta E^2$$

to evaluate $T_{conf}(E)$ by integration

$$\beta_{conf} = \beta_{conf}^0 - \int \frac{dE}{\Delta E^2}$$

$\Rightarrow$ $E(T_{conf})$ and $T_{conf}(T_{\Gamma}, \tau_0)$

Analog. $\frac{\partial \phi}{\partial X} = \Delta \phi^2 \quad \Rightarrow \quad X = X_0 - \int \frac{d\phi}{\Delta \phi^2} \quad \Rightarrow \quad \phi(X)$, where $\phi =$ vol. fraction, $X =$ “compactivity”.

MD simulations of “flow taps”

In our MD simulations of grains in a 3D box pulsed by a fluid flow, two grains (with diameters $d_i$, posit. s $r_i$, $r_j$, vel. s $v_i$, $v_j$ and angular vel. s $\omega_i$, $\omega_j$) interact when they overlap via normal and tangential forces (Silbert et al. 2001):

$$F_{n_{ij}} = \left( \frac{\delta_{ij}}{d} \right)^\alpha \left( k_n \delta_{ij} n_{ij} - \gamma_n m_{\text{red}} v_{n_{ij}} \right)$$

$$F_{t_{ij}} = \left( \frac{\delta_{ij}}{d} \right)^\alpha \left( -k_t u_{t_{ij}} t_{ij} - \gamma_t m_{\text{red}} v_{t_{ij}} \right)$$

where $k_n, \gamma_n, k_t, \gamma_t = \text{elastic, viscoel. const.s}$, $m_{\text{eff}} = m_i m_j / (m_i + m_j)$, $\alpha = 0$ and the rate of change of the tangential displacement $u_{t_{ij}}$ is: $du_{t_{ij}}/dt = v_{t_{ij}} - (u_{t_{ij}} \cdot v_{ij}) r_{ij} / r_{ij}^2$.

Grain $i$, under gravity, interacts with the fluid via a viscus force:

$$F_i = -\frac{\gamma}{(1-\Phi)^\xi} (v_i - V_{\text{fluid}}) + m_i g$$

where $\Phi$ is the local packing fraction (P. Sánchez et al. 2004, C. Crowe 1998).
- The **volume fraction**, $\phi$, is a **good** thermodynamic parameter; The flow velocity, $V$, is **not**.
A mean field theory (Tarzia et al. 2004)

- The partition function:
  \[ Z = \sum_r e^{-\beta_{conf} \mathcal{H}(r)} \cdot \Pi_r \]
  where \( \Pi_r = 1 \) if \( r \) is a “stable state”; else \( \Pi_r = 0 \).

- For hard spheres on a lattice \( \Pi_r \) has a tractable expression:
  \( \Pi_r = \lim_{K \to \infty} \exp \left\{ -K \sum_z \mathcal{H}_{CONF}(z) \right\} \) where \( \mathcal{H}_{CONF}(z) = \sum_i \delta_{n_i(z),1} \delta_{n_i(z-1),0} \delta_{n_i(z-2),0} \)
  \( \mathcal{H} = \mathcal{H}_{HC} \{ n_i \} + mg \sum n_i(z)z \) and \( n_i(z) = 0,1 \) if site \( i \) at height \( z \) is empty, filled by a grain.

- For hard spheres on a random lattice a mean field analytic calculation of \( Z \) is possible (“Bethe approx.” or Mézard&Parisi’s “cavity method”).

There is a "box" with 
H layers  \( z=1,...,H \)

Each layer is a random graph with a given connectivity

Each site at layer \( z \) is also connected to a site in \( z-1 \) and \( z+1 \)
- $T_m$: Fluid to Crystal transition line
- $T_K$: Supercooled Fluid to Glass transition (metastable phases)
- $T_D$: dynamical crossover line

$N_s = N_{\text{tot}} / L^2$
**Binary mixture**

\[ \Delta h = h_1 - h_2 \] difference of species heights; 
\[ N_c = \text{contacts between “large” grains;} \]
\[ \rho_1^b, \rho_2^b = \text{densities on the bottom layer.} \]

- \( e \) is **not** the only thermod. parameter;
- \( h_1 \) and \( h_2 \) are enough \( \implies \text{two configurational temperatures exist:} \)

\[ \beta_1 = \frac{\partial \ln \Omega(E_1, E_2)}{\partial E_1} \quad \beta_2 = \frac{\partial \ln \Omega(E_1, E_2)}{\partial E_2} \]
Conclusions

The picture has just begun to be assessed:

- Simple models, and some exp.s, support Edwards’ approach to dense GM, at least as a first good approx. (Edwards et al.; Kurchan et al.; Brey et al.; Dean et al.; Nagel et al.; Bideau et al.; D’Anna; Swinney et al.; ...);

- A comprehensive Stat. Mech. description of “thermodynamic” and dynamical properties of dense GM is emerging;

- A unified framework appears of “jamming” in glasses and granular media (see Liu&Nagel “jamming phase diagram”).

Many relevant open questions ahead:

- Is a “thermodynamic” description of dense GM possible? For instance, is \( \phi \) (or \( e \)) found to be a good thermod. parameter in experiments?

- Are Stat. Mech. approaches ground? (general validity? basic justifications? how to predict a priori the number of independent param.s needed? ...)

- Need for deeper tests of theory: experimental phase diagram, eq. of state, fluct.-dis. relations, mix/segregation transitions, ...