STATISTICAL MECHANICS OF DENSE GRANULAR MEDIA

A. Coniglio, A. Fierro, **Mario Nicodemi**,
M. Pica Ciamarra, M. Tarzia

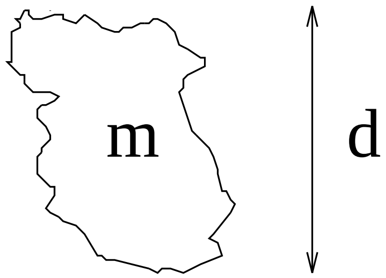
Universitá di Napoli "Federico II"

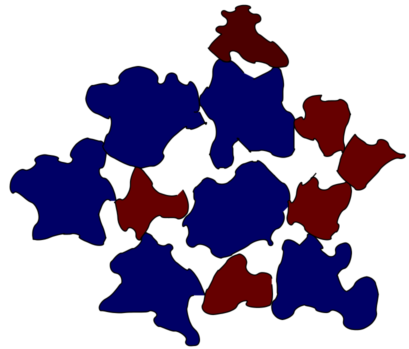
Outlook:

- 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, ...)

See review by Richard, Nicodemi, Delannay, Ribière, Bideau, *Nature Materials* **4** 121 (2005),
February 2005 Nat. Mat. Highlight *"Compaction in a sand box"*

☐ Granular Media (GM)





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

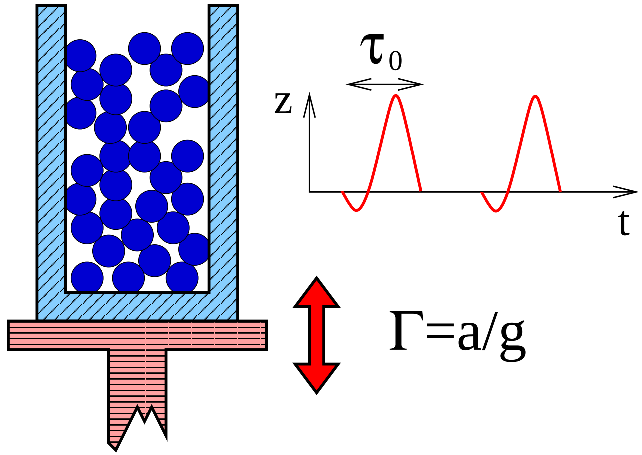
- they are **dissipative**, **non-thermal** systems:

$$d > 1\mu m \implies \boxed{mgd >> k_B T}$$

Is Statistical Mechanics suited for dense GM ? (Edwards 1989)

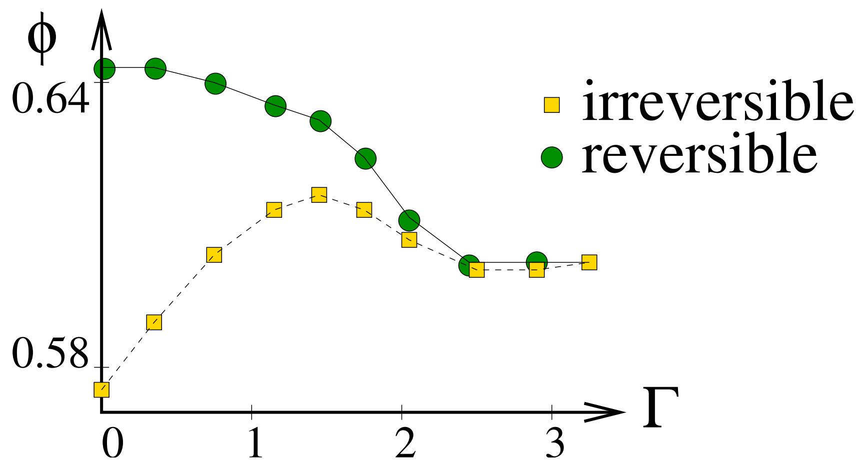
- Macroscopic properties of GM at rest are characterized by a few control parameters.
- As much as in thermal systems, macrostates correspond to many microstates, i.e., mechanically stable configurations.

☐ Experiments in Chicago (Nagel et al. 1998)



- Experimental set-up for **tapping dynamics**: Γ=*(peak acceler.)/gravity*

- **Packing fraction**, ϕ, as a function of the shake amplitude, Γ.



(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 $P_r = 0$.

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

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

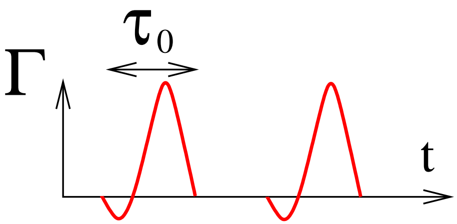
$\Omega(E)$ is the number of "mechanically stable states" with E.

- 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"



TIME AVERAGES

$$\Longrightarrow \overline{Q} = \frac{1}{\Delta t} \sum_t Q(t)$$

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

b) "Statistical Mechanics"

ENSEMBLE AVERAGES

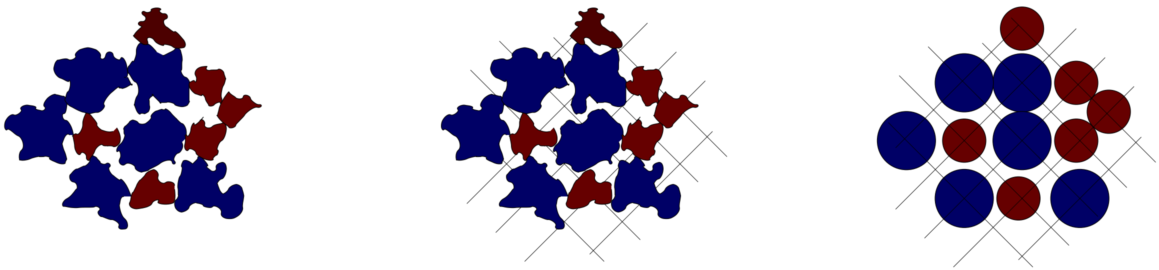
$$P_r \propto e^{-\beta_{conf} E_r} \qquad \Longrightarrow \langle Q \rangle = \sum_r Q_r P_r$$

Time and *Ensemble Averages* must coincide: $\underline{\overline{Q}(e) = \langle Q \rangle (e)}$

□ Schematic Models and Dynamics

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

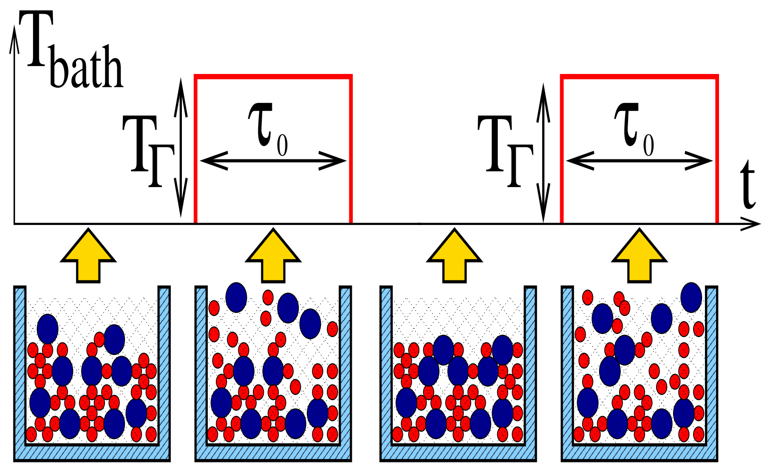
Grains $\longrightarrow$ **draw a lattice** $\longrightarrow$ **round grains**



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

$$\mathcal{H} \;=\; \mathcal{H}_{HC} \;+\; g\sum_i m_i\, z_i$$

Hard Core + **Gravity**



- Monte Carlo **taps dynamics**:

shaking "off" $\Leftrightarrow T_{bath} = 0$

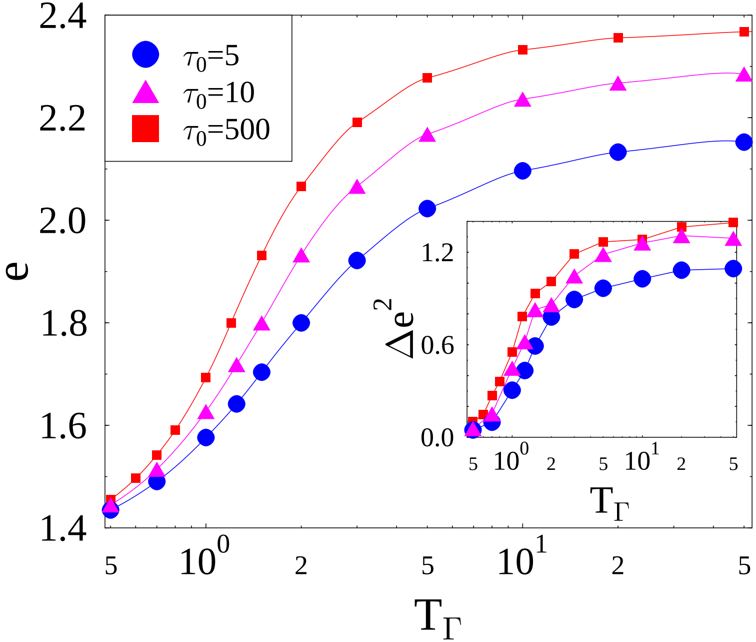
shaking "on" $\Leftrightarrow T_{bath} = T_\Gamma > 0$

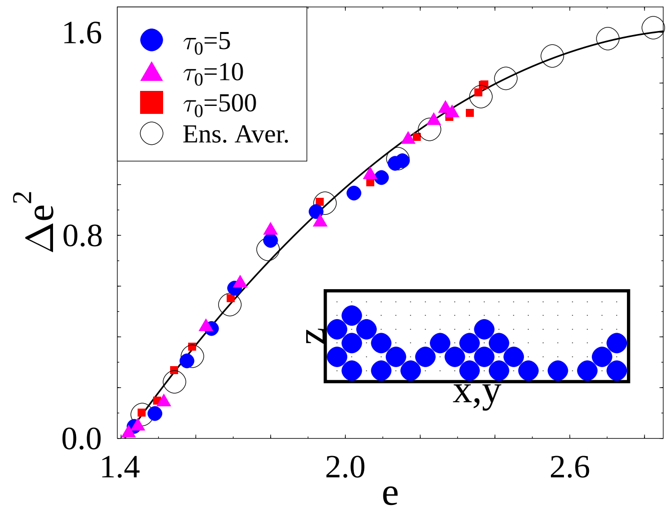
Tap *amplitude*: $\mathbf{T_\Gamma}$

Tap *duration*: $\tau_\mathbf{0}$

□ Stat. Mech. scenario: monodisperse HS

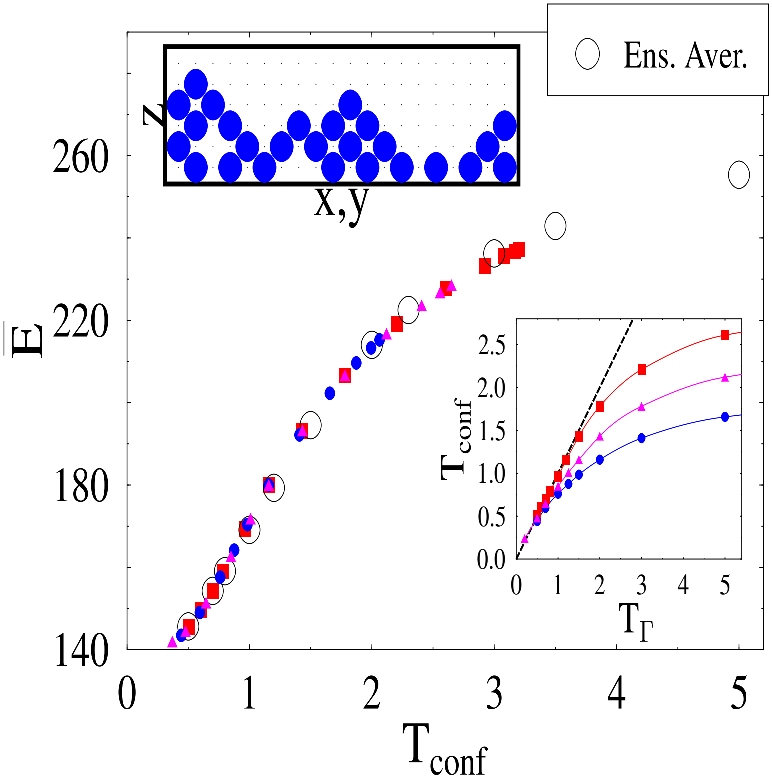
(Coniglio, Fierro, Nicodemi 2001)





- The **energy**, e, is a **good** thermodynamic parameter; $\mathbf{T_\Gamma}$ is **not**.

☐ Connection of T_{conf} and T_Γ



Use the ***equilibrium*** **FDR**:

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

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

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

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

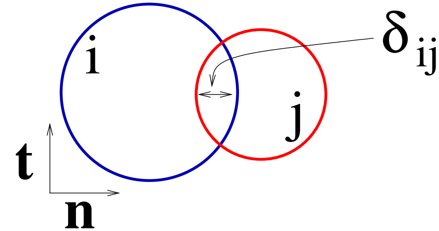
Analog. $-\frac{\partial \phi}{\partial X} = \Delta \phi^2 \Longrightarrow X = X_0 - \int \frac{d\phi}{\Delta \phi^2} \Longrightarrow \phi(X)$, where $\phi =$ vol. fraction, $X =$ "compactivity".

(Edwards 1989; Nagel et al. 1995; Coniglio&Nicodemi 2000; Swinney et al. 2005)

□ 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, posit.s $\mathbf{r}_i$, $\mathbf{r}_j$, vel.s $\mathbf{v}_i$, $\mathbf{v}_j$ and angular vel.s ω_i, ω_j) interact when they overlap via normal and tangential forces (Silbert et al. 2001):

$$\mathbf{F}_{n_{ij}} = \left(\frac{\delta_{ij}}{d}\right)^{\alpha} (k_n \delta_{ij} \mathbf{n}_{ij} - \gamma_n m_{\text{red}} \mathbf{v}_{n_{ij}})$$
$$\mathbf{F}_{t_{ij}} = \left(\frac{\delta_{ij}}{d}\right)^{\alpha} (-k_t \mathbf{u}_{tij} \mathbf{t}_{ij} - \gamma_t m_{\text{red}} \mathbf{v}_{t_{ij}})$$

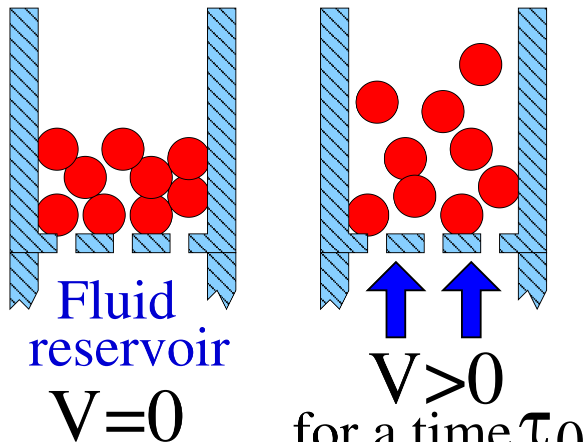


where $k_{n,t}, \gamma_{n,t}$ = elastic, viscoel. const.s, $m_{eff} = m_i m_j/(m_i + m_j)$, $\alpha = 0$ and the rate of change of the tangential displacement $\mathbf{u}_{t_{ij}}$ is: $d\mathbf{u}_{t_{ij}}/dt = \mathbf{v}_{t_{ij}} - (\mathbf{u}_{t_{ij}} \cdot \mathbf{v}_{ij})\mathbf{r}_{ij}/r_{ij}^2$

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

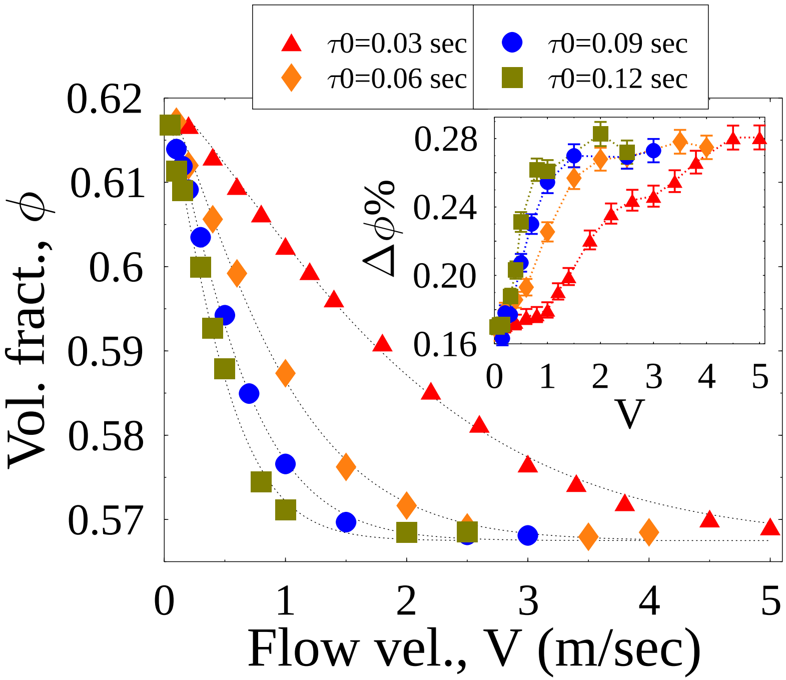
$$\mathbf{F}_i = -\frac{\gamma}{(1-\Phi)^{\xi}}(\mathbf{v}_i - \mathbf{V}_{fluid}) + m_i \mathbf{g}$$

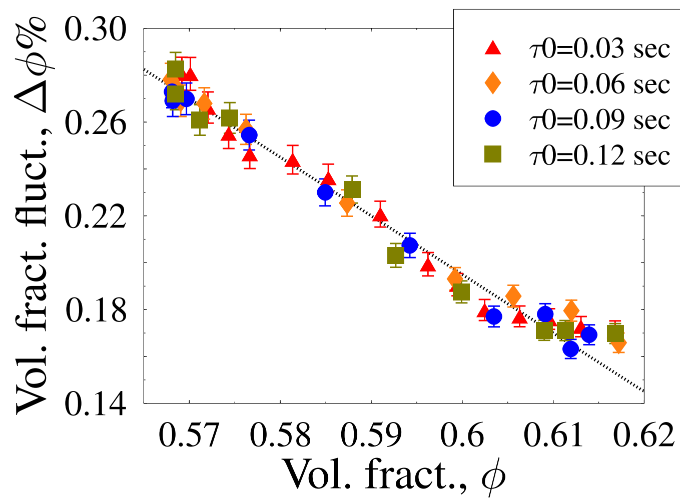
where Φ is the local packing fraction (P. Sánchez et al. 2004, C. Crowe 1998).



☐ Stat. Mech. scenario in MD “flow taps”

(Pica Ciamarra, Coniglio, Nicodemi 2005)





- The **volume fraction**, ϕ, is a **good** thermodynamic parameter; The flow velocity, **V**, is **not**.

□ A mean field theory (Tarzia et al. 2004)

- The **partition function**: $Z = \sum_r \mathrm{e}^{-\beta_{conf}\mathcal{H}(r)} \cdot \Pi_r$

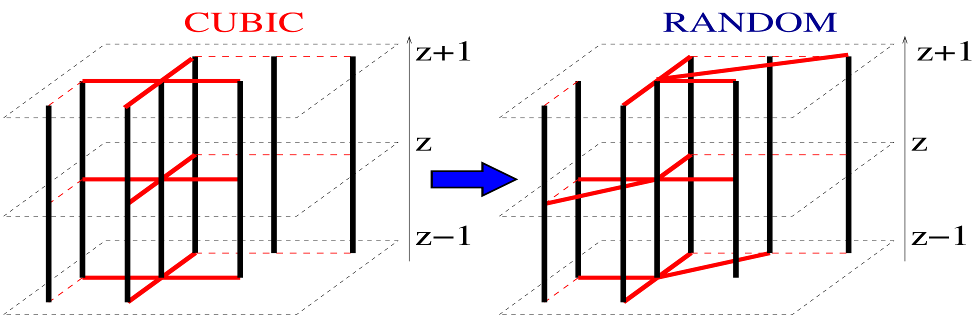
  where $\Pi_r = 1$ if r is a "stable state"; else $\Pi_r = 0$.

- For **hard spheres** on a lattice Π_r has a tractable expression:

  $\Pi_r = \lim_{K\to\infty} \exp\{-K \sum_z \mathcal{H}_{CONF}(z)\}$ 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 hight 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").

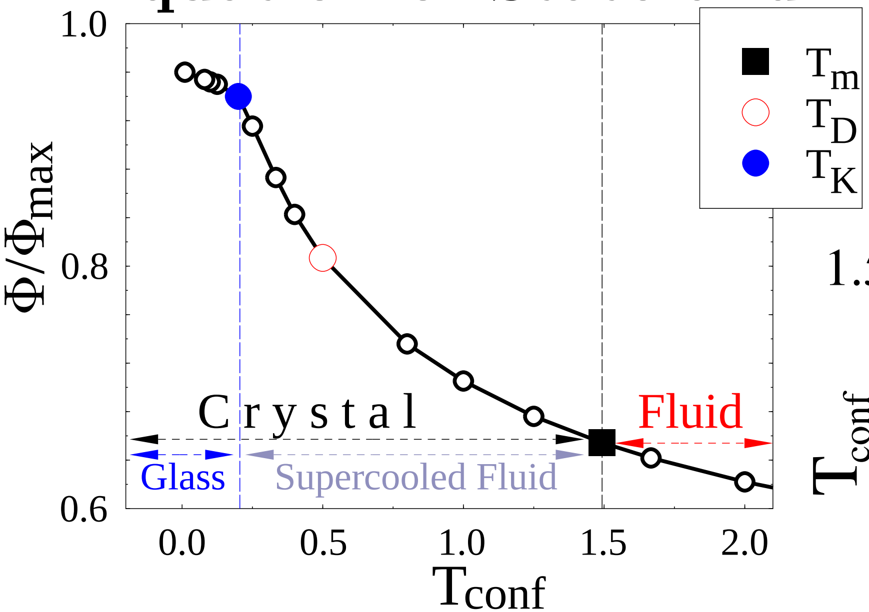


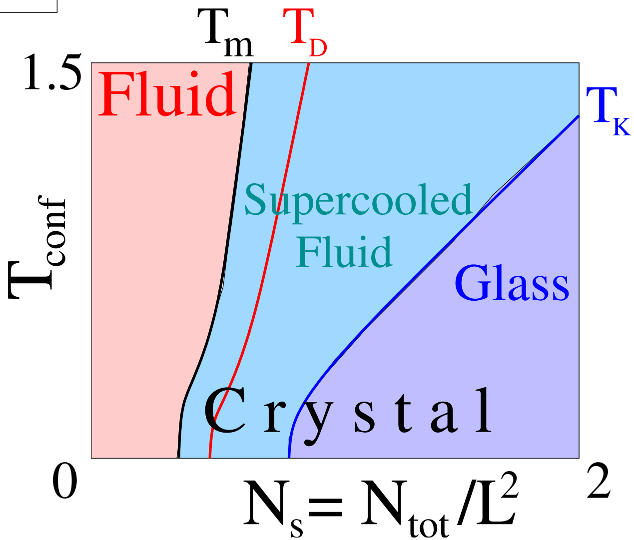
There is a "box" with H layers z=1,...H

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

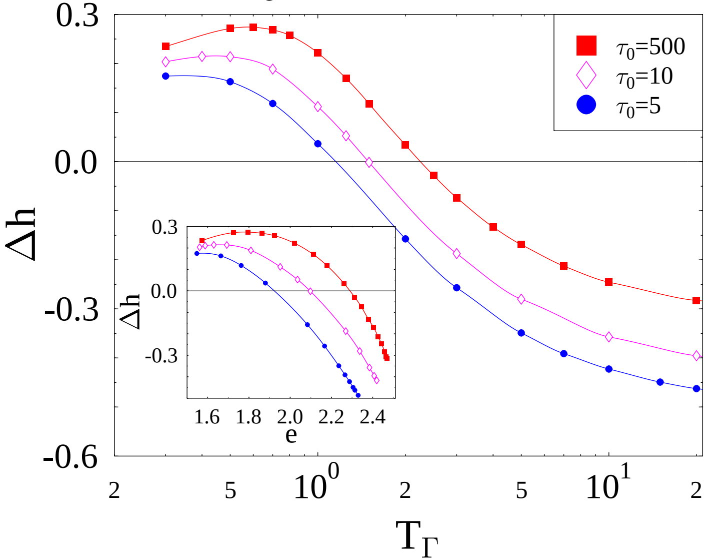
□ Equation of State and Phase Diagram



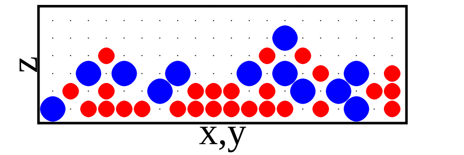


- $\mathbf{T_m}$: **Fluid** to **Crystal** transition line
- $\mathbf{T_K}$: *Supercooled Fluid* to *Glass* transition (metastable phases)
- $\mathbf{T_D}$: dynamical crossover line

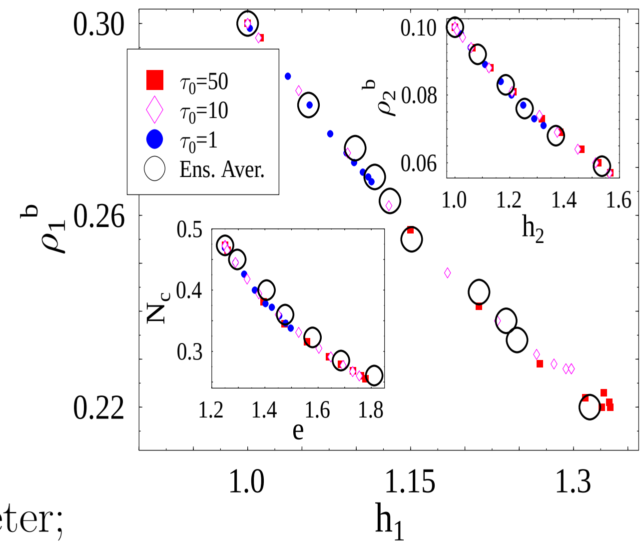
☐ Binary mixture



$\Delta h = h_1 - h_2$ difference of species heights;
N_c = contacts between "large" grains;
ρ_1^b, ρ_2^b = densities on the bottom layer.



Mass densities: $\rho_2 = \rho_1$; Radii: $R_2 > R_1$



- e is **not** the only thermod. parameter;
- h_1 and h_2 are enough $\Longrightarrow$ **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 ϕ (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, ...