LA MECCANICA STATISTICA DEI MATERIALI GRANULARI

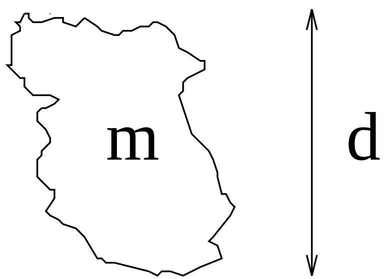
A. Coniglio, A. de Candia, A. Fierro,
Mario Nicodemi, M. Pica Ciamarra, M. Tarzia

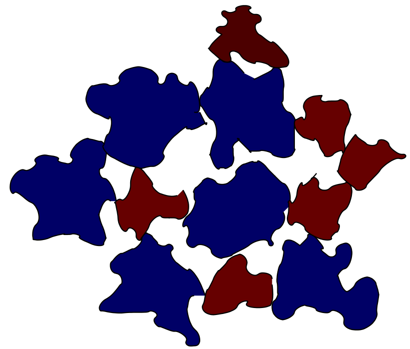
Piano del seminario:

- i Mezzi Granulari (Granular Media, GM): sistemi non termici;
- la Meccanica Statistica dei GM e la teoria di Edwards;
- la scoperta del diagramma di fase dei GM e la spiegazione dei fenomeni di segregazione di taglia.

Napoli, 8 Ottobre 2004

□ Granular Media (GM)



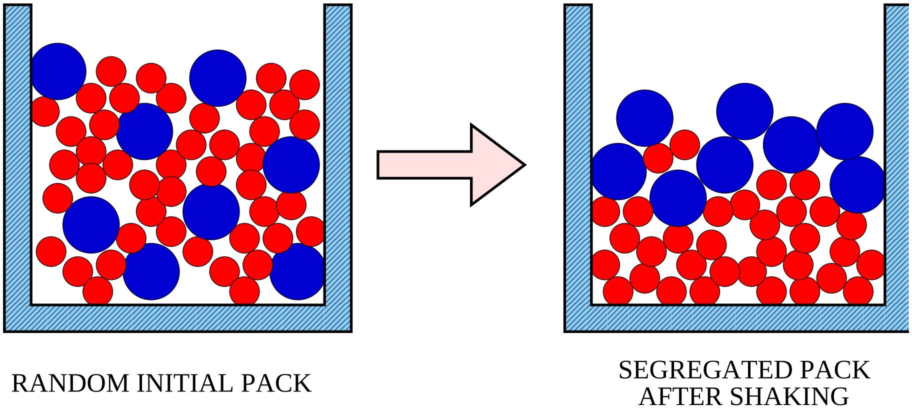


Examples of granular media are: powders, sand, corn-flakes, aspirins, etc...

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

since $d > 1\mu m \quad \Longrightarrow \quad \boxed{mgd >> k_B T}$

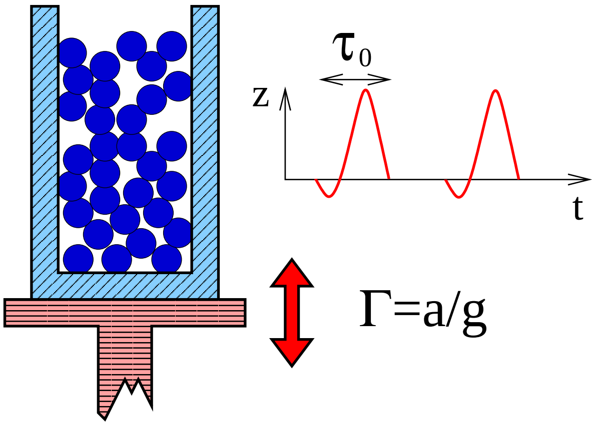
☐ Size segregation



In presence of shaking a granular system is not randomized, but its components tend to separate:

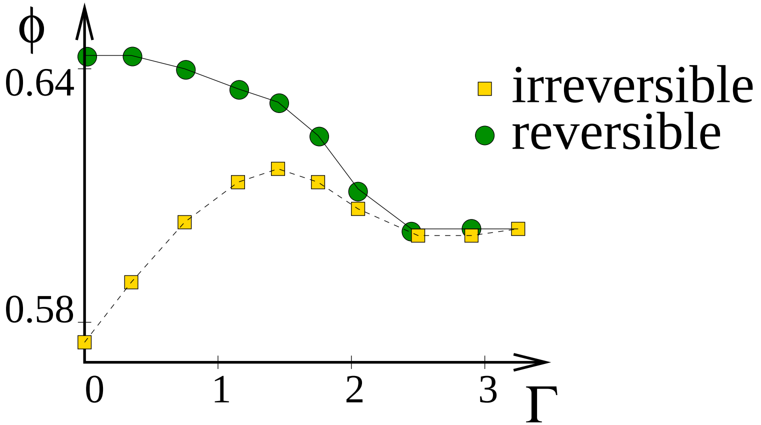
- BNE, "Brazil nut effect": large grains above;
- RBNE, "reverse Brazil nut effect": large grains below.
  (Hong,Quinn&Luding 2001)

☐ Experiments in Chicago (Nagel et al. 1998)



- **Experimental set-up.**
  Γ=*(peak acceler.)/gravity*

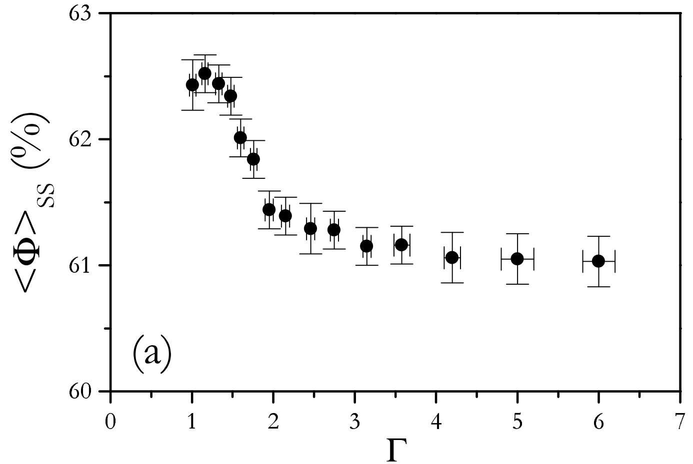
- **Packing fraction**, ϕ,
  as a function of the
  shake amplitude, Γ.

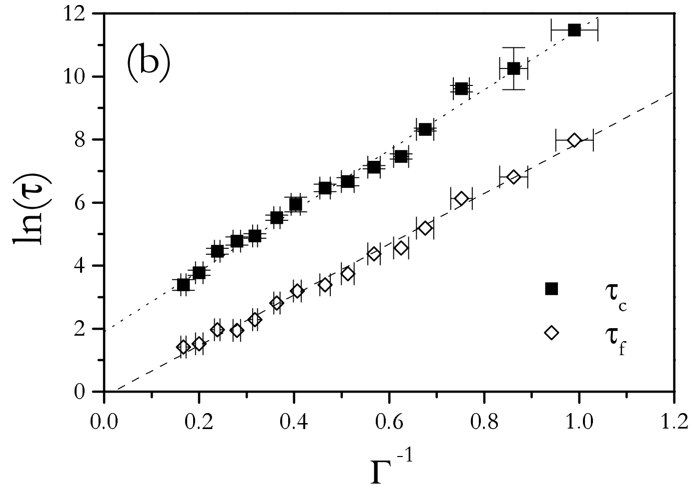


☐ Experiments in Rennes (Philippe&Bideau 2002)

- **Packing fraction**, ϕ, at stationarity as a function of the shaking amplitude, Γ

- Characteristic **time scale**, τ, to reach stationarity as a function of $1/\Gamma$





□ Macro and Micro-States

- 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.

- In thermal systems the space of microstates is explored by the presence of a finite T_{bath}, and in granular media (where, at rest, $T_{bath} = 0$) by an external drive ($\mathbf{\Gamma} \Leftrightarrow T_{bath} > 0$).

□ An important question (Edwards 1989)

What's the probability, P_r, to find the "mechanically stable state" r? P_r allows to substitute *time* with *ensemble averages*.

□ Edwards' approach to GM

(Edwards 1989, Nicodemi 1999, Coniglio&Nicodemi 2001)

- Granular media are found, at rest, in mechanically stable microstates. In Edwards' Stat. Mech. of GM, averages are only over these mechanically stable states with a flat measure.

- Thus, 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 $P_r = 0$.

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

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

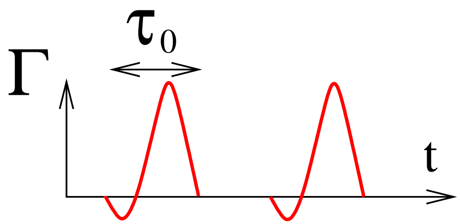
$\Omega(E)$ is the number of "mechanically stable states" with E.

- The system at rest has: $T_{bath} = 0$ and $T_{conf} = \beta_{conf}^{-1} \neq 0$

☐ Test of Edwards' 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

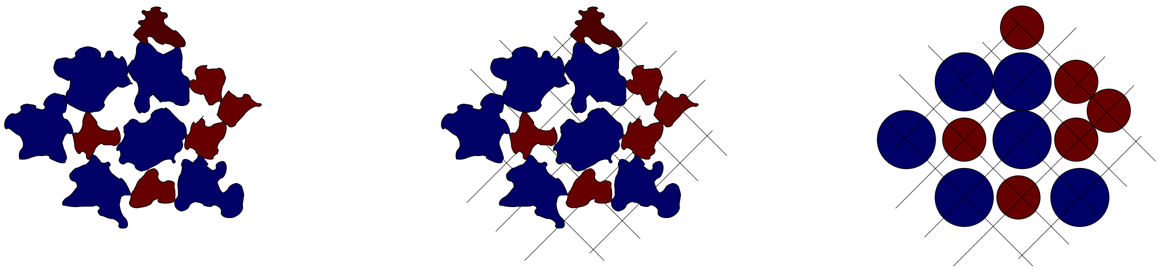
$$P_r \propto e^{-\beta_{conf} E_r} \qquad \Longrightarrow \langle Q \rangle = \sum_r Q_r P_r$$

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

□ Schematic Models and Dynamics

(Nicodemi,Coniglio,Herrmann 1997)

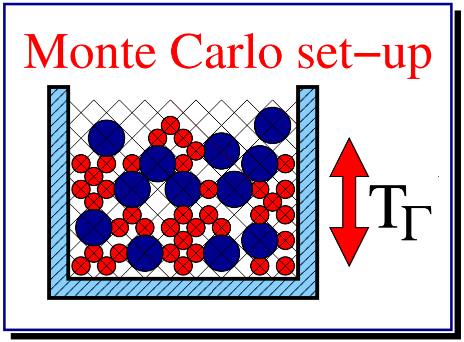
Grains $\longrightarrow$ **draw a lattice** $\longrightarrow$ **round grains**



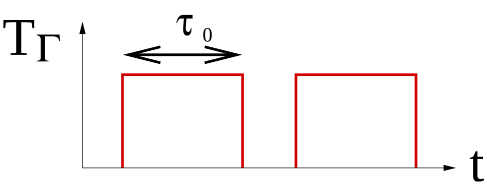
- **Hard Spheres** on a cubic lattice:

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

Hard Core + Gravity



- Monte Carlo **"taps" dynamics**:

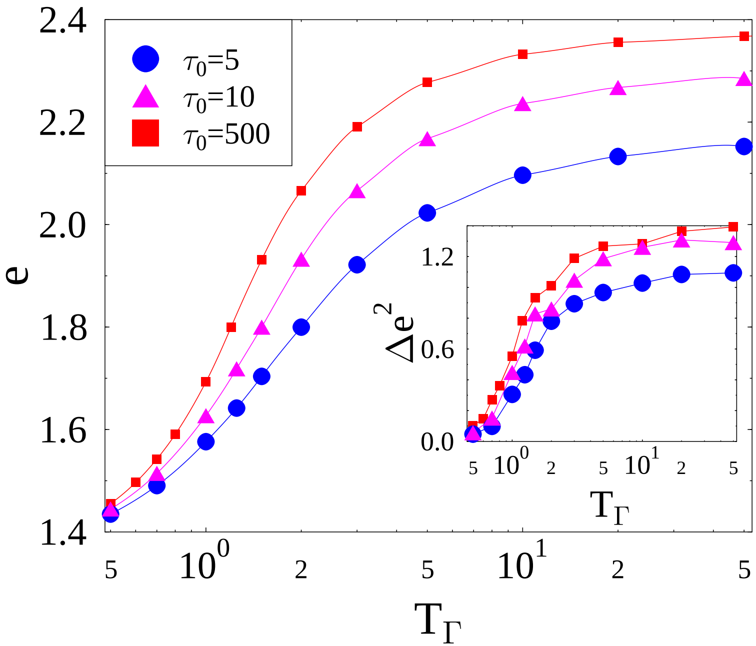


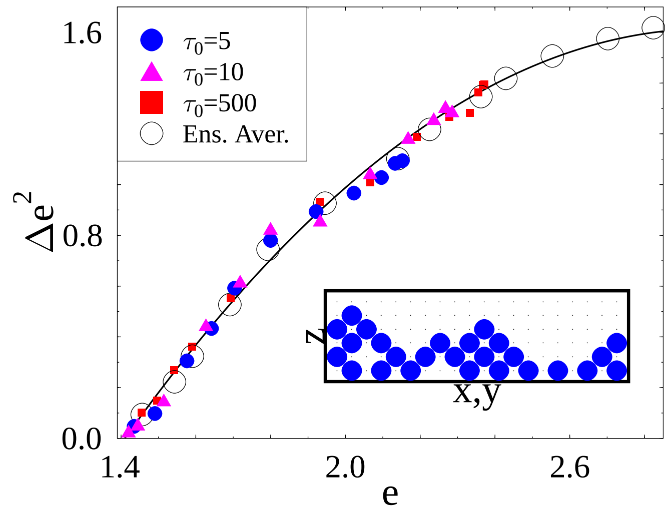
Tap <u>*amplitude*</u>: T_Γ ($\leftrightarrow \Gamma = a/g$ of exp.s)

Tap <u>*duration*</u>: τ_0 ($\leftrightarrow \omega^{-1}$ of experiments)

☐ Edwards' scenario: monodisperse HS

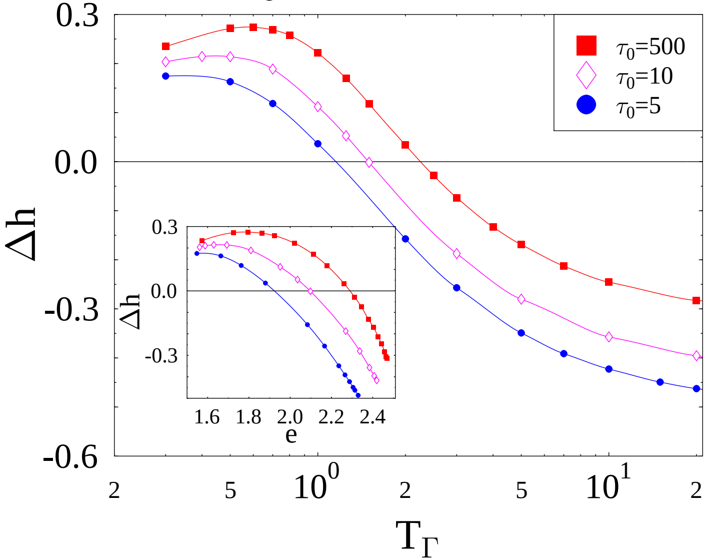
(Coniglio, Fierro, Nicodemi 2001)

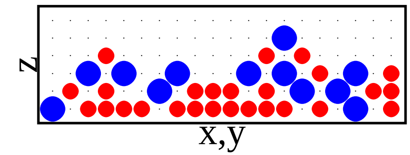




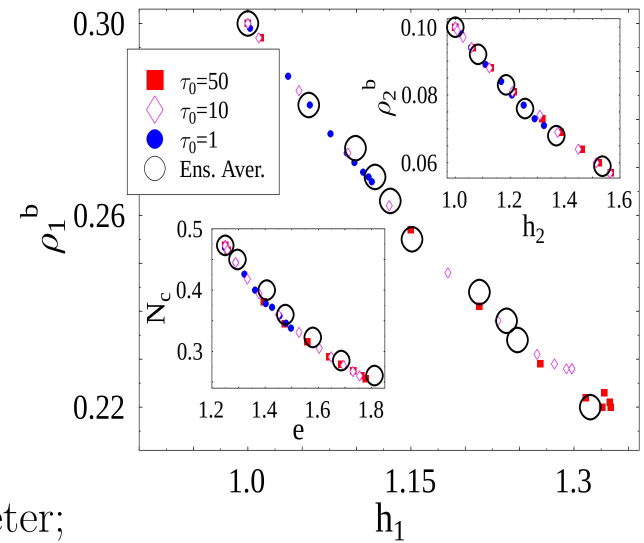
- The **energy**, e, is a **good** thermodynamic parameter; $\mathbf{T_\Gamma}$ is **not**.

□ Binary mixture





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



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

- e is **not** the only thermod. parameter;
- h_1 and h_2 are enough $\Longrightarrow$ **two configurational temperatures** exist:

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

☐ A mean field calculation

- Hard spheres on a lattice. The Hamiltonian is:

$$\mathcal{H} \quad = \quad \mathcal{H}_{HC}(\{n_i(z)\}) \;\; + \;\; mg\sum_i n_i(z)z$$

Hard Core + **Gravity**

The variable $n_i(z)$ is 1 (resp. 0) when site i at hight z is filled by a grain (resp. empty).

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

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

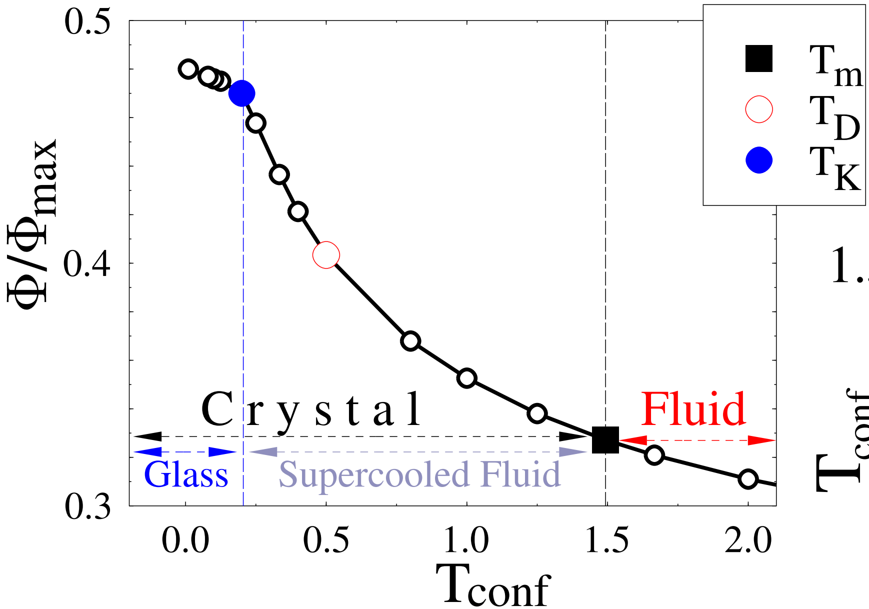
A tractable expression for Π_r can be found:

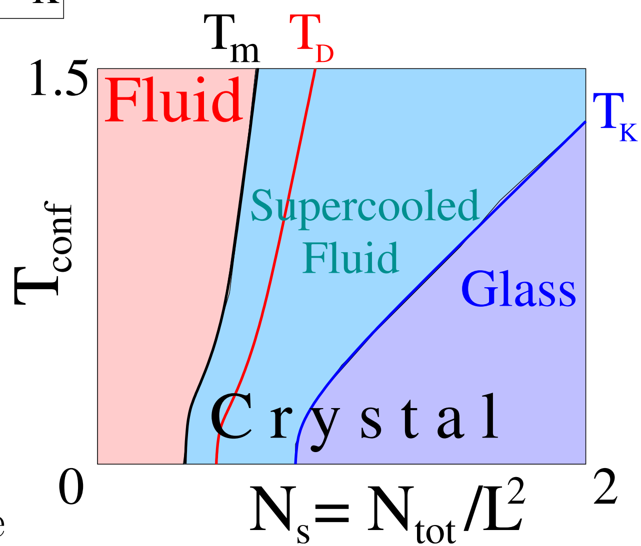
$\Pi_r = \lim_{K\to\infty} \exp\{-K\sum_z \mathcal{H}_{CONF}(z)\}$ where $\mathcal{H}_{CONF}(z) = \sum_i \delta_{n_i(z),1}\delta_{n_i(z-1),0}\delta_{n_i(z-2),0}$

- A mean field analytic calculation ("Bethe approx.") of Z in this model is shown to be possible!

□ Equation of State and Phase Diagram

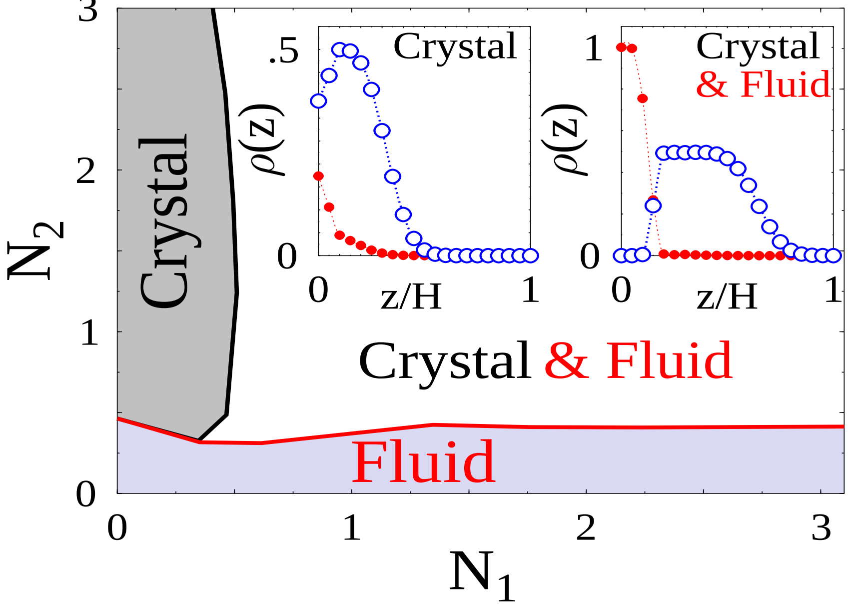
(Coniglio, de Candia, Fierro, Nicodemi & Tarzia 2003)

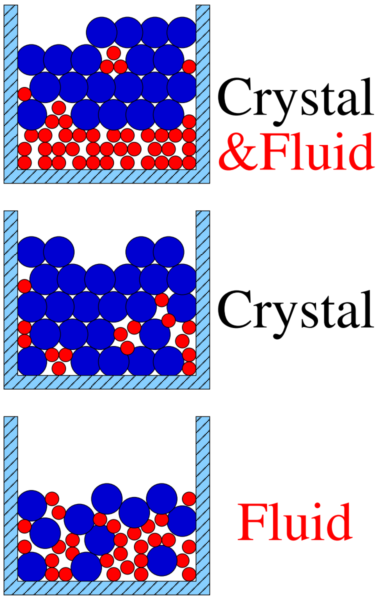




- $\mathbf{T_m}$: **Fluid** to **Crystal** transition line
- $\mathbf{T_K}$: *Supercooled Fluid* to *Glass* transition (metastable phases)
- $\mathbf{T_D}$: dynamical crossover line

☐ Mechanisms of segregation





Phase diagram in the plane (N_1, N_2) of a mixture in 3D
$(N_1, N_2$ = num. of small, large grains per unit surface)

$$\frac{m_1 g d_1}{T_{conf1}} > \frac{m_2 g d_2}{T_{conf2}}$$

Two basic mechanisms (no "hydrodynamics" here):

- *Weak segregation/mixing*: **"geometric"** effects within a given phase
  (e.g., more stable states with small grains below)

- *Strong segregation*: **phase separation** due to phase transitions

□ Conclusioni

- Comincia oggi a farsi strada l'idea di poter descrivere materiali non termici, come i mezzi granulari, con teorie di Meccanica Statistica.

- Lo studio dei limiti di validitá dell'approccio di Edwards é appena agli inizi. Emerge, peró, per la prima volta una teoria unitaria della fisica dei mezzi granulari: dal loro "diagramma di fase", alle proprietá "vetrose", ai fenomeni di segregazione di taglia.

- Si comincia a comprendere l'*universalitá* di fenomeni (come transizioni di fase, "jamming", ...) osservati in sistemi molto diversi tra loro: dai "vetri strutturali", ai "vetri di spin" sino ai materiali granulari.