FROM PARTICLES TO CONTINUUM
Evolution of micro-structure (isotropic & anisotropic)

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Introduction

- Granular materials are the combination of **discrete** solid (macroscopic) particles
- **many interesting phenomena - can we understand them all together?**

    history-dependence, slow relaxation, creep, shear-localization, “avalanches”, …

    fluid-solid transition => jamming

Examples:




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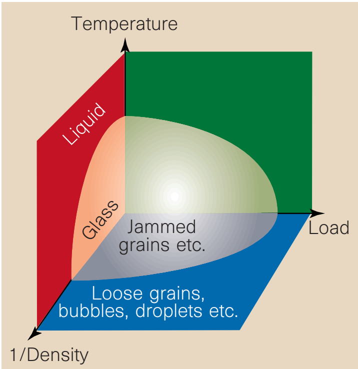
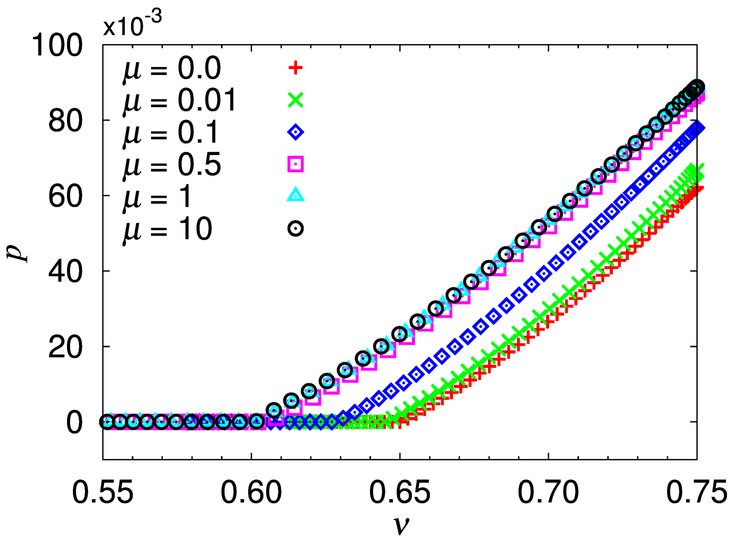
fluid-solid transition => **jamming** “point”

Examples:

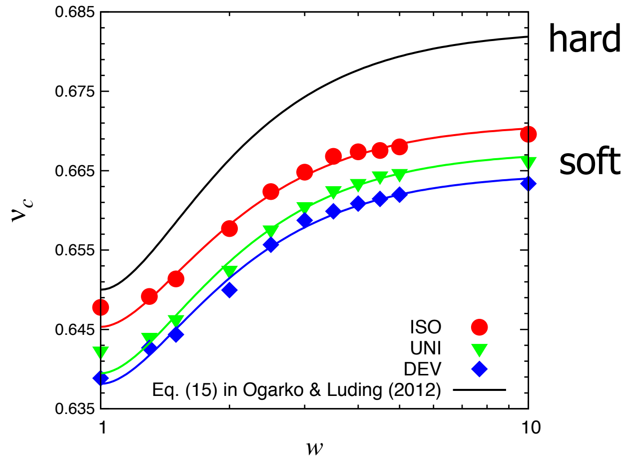
A. Liu and S. Nagel, Nature 396, 1998



Isotropic de-compression; effect of friction



Polydispersity and what's the difference between ISO, UNI and SHEAR?



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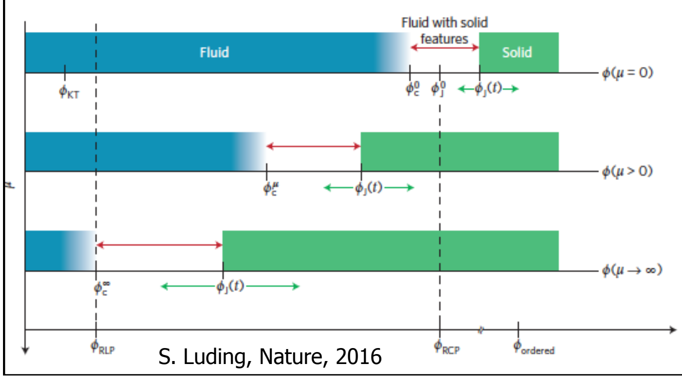
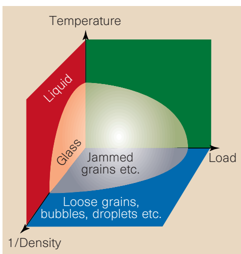
history-dependence, slow relaxation, creep, shear-localization, "avalanches", …

fluid-solid transition => jamming "~~point~~" – no point!



S. Luding, Nature, 2016



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Overview – where do we start?

- Jam-**packed** discrete systems … not a (single) jamming point …
- **Simplest** model system (linear, no friction, no cohesion, no walls)
- **no** dynamics, jiggling, (granular) temperature, Brownian dynamics
- ***microstructure*** + ***dilatancy*** + ***anisotropy*** + ***history***

GOAL:

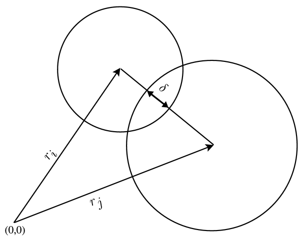
Multi-scale: micro => macro

Macro-scale **continuum model** with **microstructure**

Later: Add friction as a material parameter …

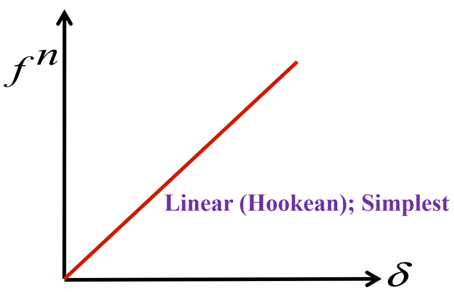
DEM (Discrete element method) = MD

Develop **force – delta (overlap) interaction relation**, when two entities interact



Solve Newton's equation of motion

$$m_i \ddot{\mathbf{r}}_i = F_i + \sum_{j \in N : j \neq i} \mathbf{F}_{ij}$$



Exclude:
nonlinear elastic
nonlinear plastic
Friction
Cohesive

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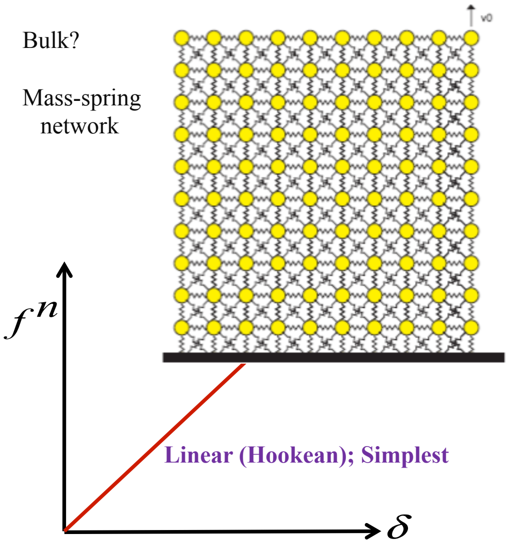
Bulk?

Mass-spring network



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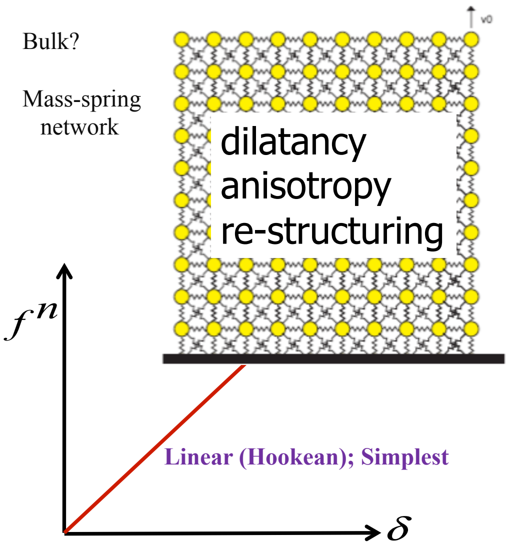

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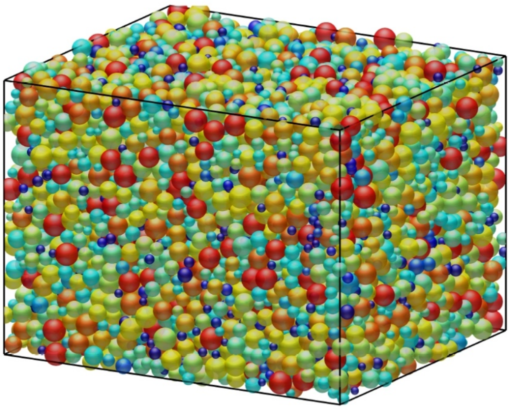
No tension: Simplest Model System (RVE)



- 3D (true) tri-axial periodic box
- Linear visco-elastic contact model

$$f^n = k\delta + \gamma\dot{\delta}$$

- Strain controlled
- Quasi-static deformation
- Polydisperse spheres
- Frictionless samples
- No gravity
- Homogeneous / no walls

Material parameters

Parameter	Symbol	Material A
Number of Particles	N	N= 21^3
Average radius	<r>	<r> = 1 mm
Polydispersity	$w = r_{max}/r_{min}$	3
Particle density	ρ	ρ= 2000 [kg/m^3]
Normal stiffness	k^n	k^n =5.10^8 [kg/s^2]
Normal Viscosity	γ	1 [kg/s]
Background viscosity	γ^b	0.1 [kg/s]

Overview – where do we stand?

- all complexities are removed!

- what remains?

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… and its history / protocol dependence …

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… ISOTROPIC & DEVIATORIC …

Microstructure

… ISOTROPIC & DEVIATORIC …

“packing efficiency” ⇔ Anisotropy

Microstructure – 1st focus on isotropic

… ISOTROPIC & DEVIATORIC …

“packing efficiency” ⇔ ~~Anisotropy~~

Sample Preparation – from the beginning!

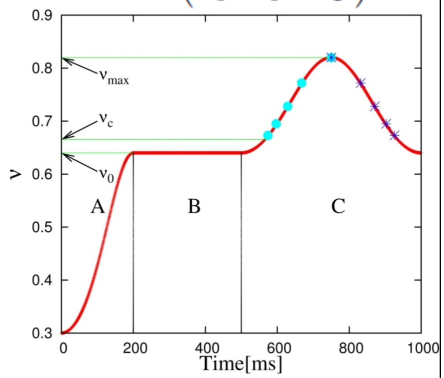
tapping … => accepted procedure …
similar to temperature (isotropic)
or annealing …

or: over-compression

Sample Preparation – from the beginning!

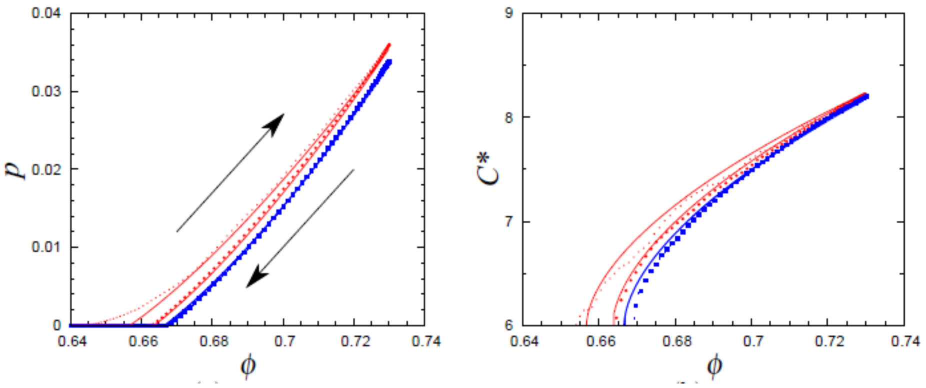
Isotropic Compression and de-compression

$$\dot{\mathbf{E}} = \dot{\epsilon}_v \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$



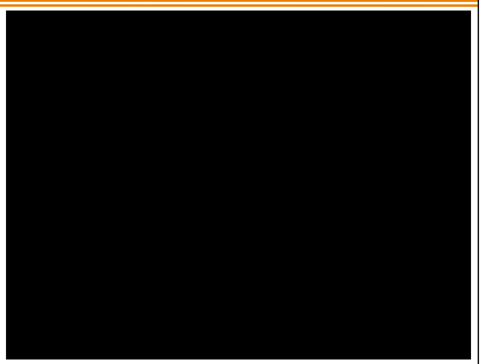
(cyclic) isotropic deformation

- Intermediate cyclic over-compression (amplitude 0.73)
- red: 1st cycle … blue: 100th cycle …



Main Experiment 1 - **Cyclic isotropic over-compression**

$$\dot{\mathbf{E}} = \dot{\epsilon}_v \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$



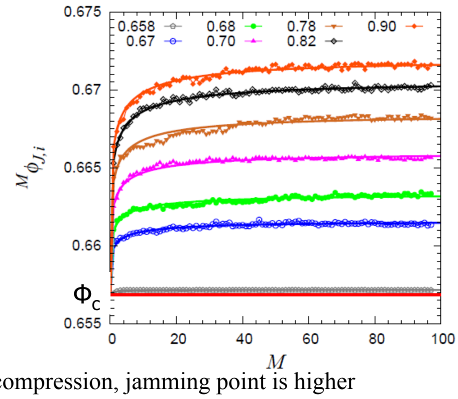
Choose a un-jammed state.
Perform cyclic isotropic (de-)compression for ***M=100*** cycles.

Perform for different over-compression amplitudes. $\phi_i^{\max}$

Measure the jamming point ${}^{\bar{M}}\phi_{J,i} = \phi_J(M, \phi_i^{\max})$

N. Kumar and S. Luding, preprint (2014); O.I. Imole et al. *KONA (2013)*

Main Experiment 1 - Cyclic isotropic over-compression



- For higher over-compression, jamming point is higher

- Jamming point increases (KWW stretched exponential function).

$$\boxed{{}^M\phi_{J,i} := \phi_J(\phi_i^{\max}, M) = {}^\infty\phi_{J,i} - ({}^\infty\phi_{J,i} - \Phi_c)\exp\left[-(M/\mu_i)^{\beta_i}\right]}$$

- Minimum value is achieved $\phi_{SJ} = 0.6567$ $\mu_i = 1$ $\beta_i = 0.3$

Message 1

response of **microstructure** to **isotropic deformations**!

- a new state variable is needed!
=> take e.g. coordination number, z, C^*, …
But: at p=0, there is no information in C^*=6!

- p>0: "efficiency" of packing high ~ coordination number low

- proposal: use the jamming "point" itself as state variable!
i.e. the density at which the system un-jams
or loses mechanical stability (stress free reference)

Message 1

response of **microstructure** to **isotropic deformations**!

- a new state variable is needed! use: Φ_J
- *proposal*: use the jamming "point" itself as state variable!

Response to tapping/annealing or over-compression:

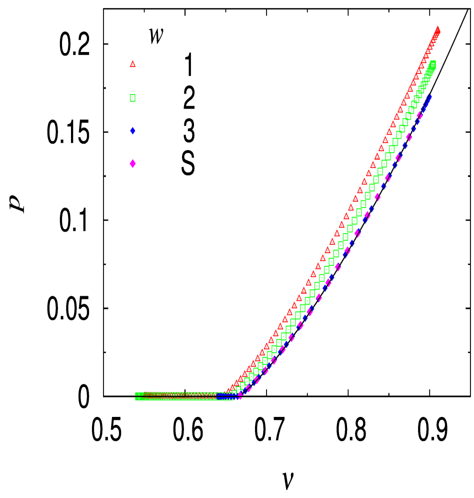
=> **jamming "point" density slowly increases!**

Constitutive model for Pressure

$$p = p(v, \ldots)$$

Isotropic compression – Pressure

$$p = p_0 \frac{\nu C}{\nu_c} (-\varepsilon_v) [1 - \gamma_p(-\varepsilon_v)]$$



What's the point? Almost linear!

$$p^* = \frac{p\nu_c}{\nu C} = p_0(-\varepsilon_v) [1 - \gamma_p(-\varepsilon_v)] \qquad \varepsilon_v = -\ln\left(\frac{\nu}{\nu_c}\right)$$

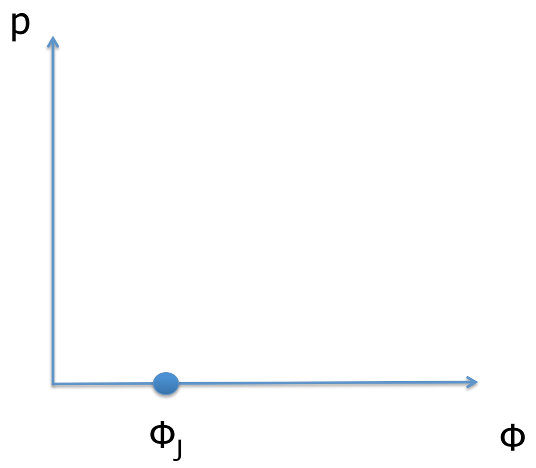
There are some material constants (depend on polydispersity, friction)
Like:

$$p_0, \gamma_p << 1, C_0 = 6, C_1, \alpha \approx 0.56, g_3 \approx O(1), \phi_r, \phi_v, \ldots \text{ and } \ldots \nu_c$$

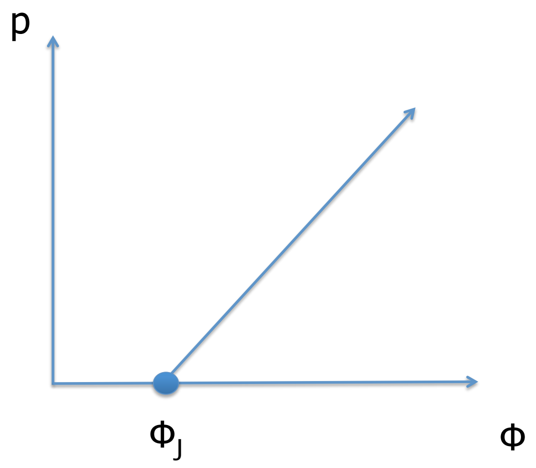
How to calibrate/measure them – done …
(some of them are even known analytically)

$$p_0, C_0 = 6, g_3 \approx O(1)$$

Tapping = coffee-experiment!
homework – do it yourself



Tapping "isotropic"



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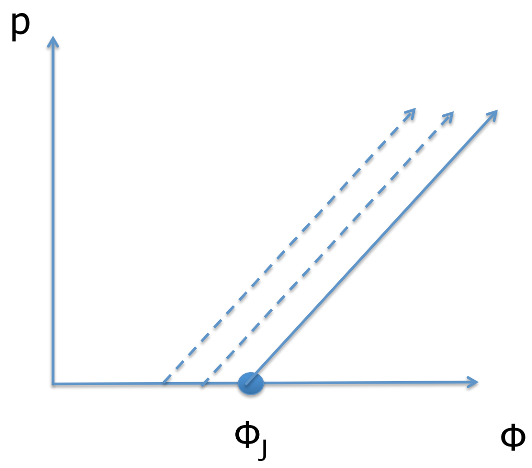
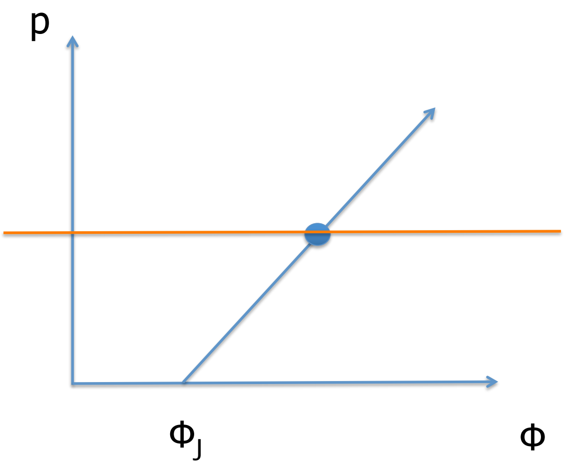


BC “isobaric” + tapping



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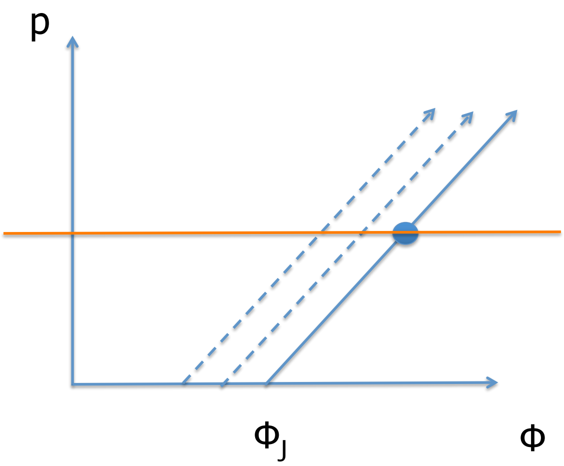

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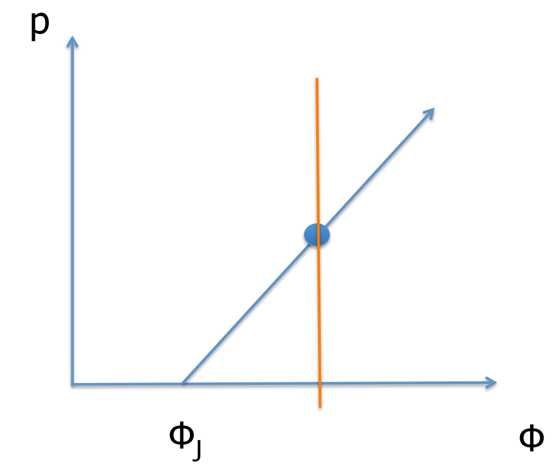

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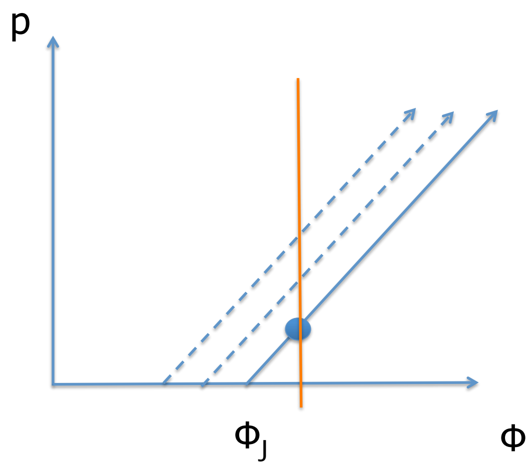
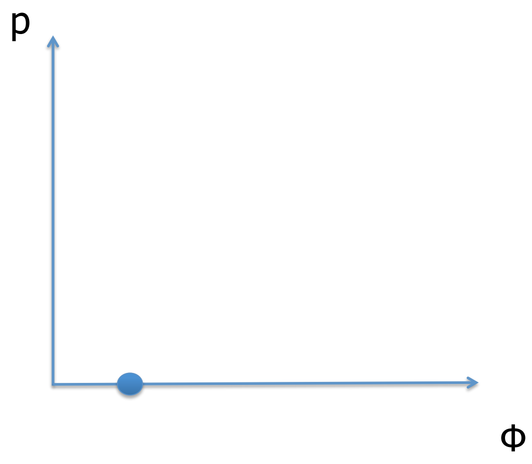


Isotropic (de)compression
(like in the particle simulations before)



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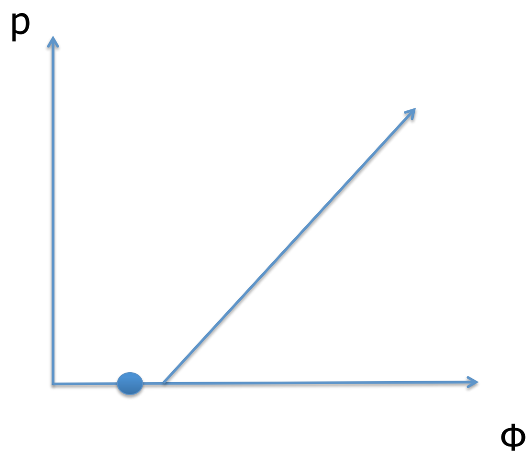

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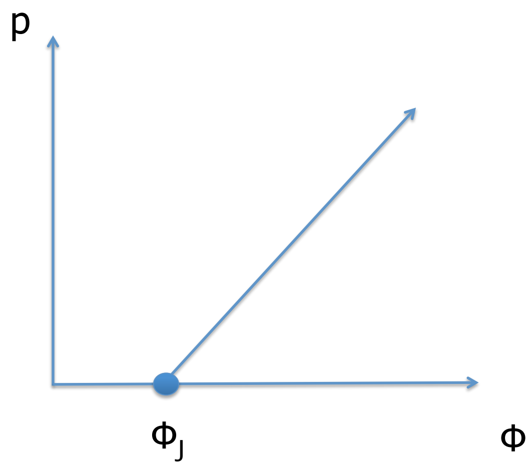
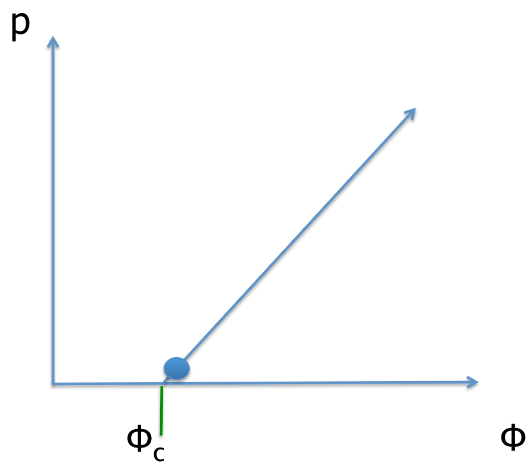


Isotropic compression



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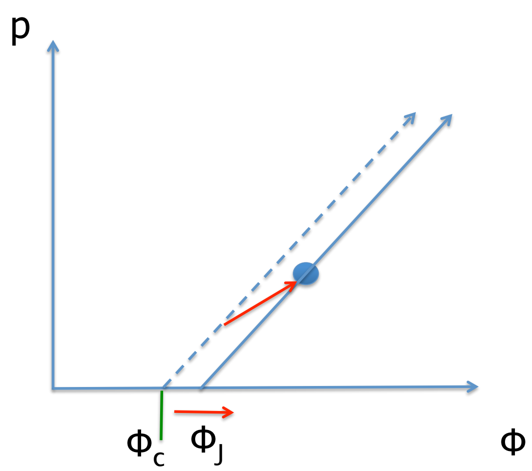

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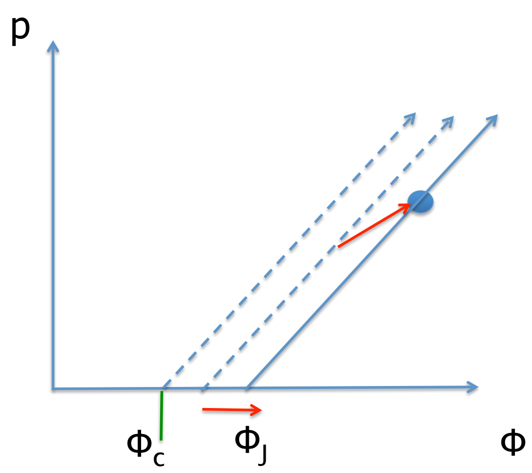

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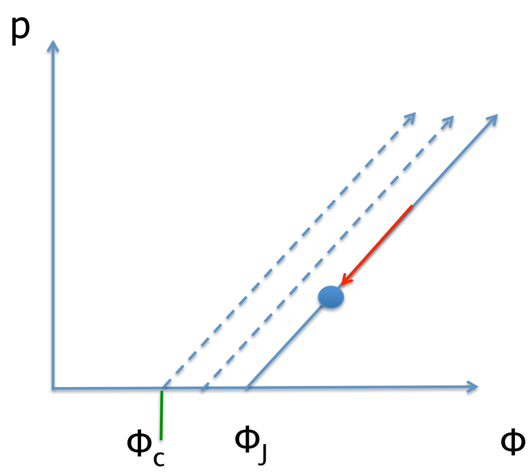

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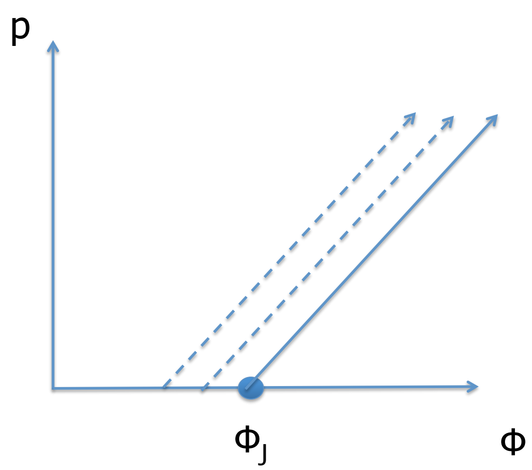
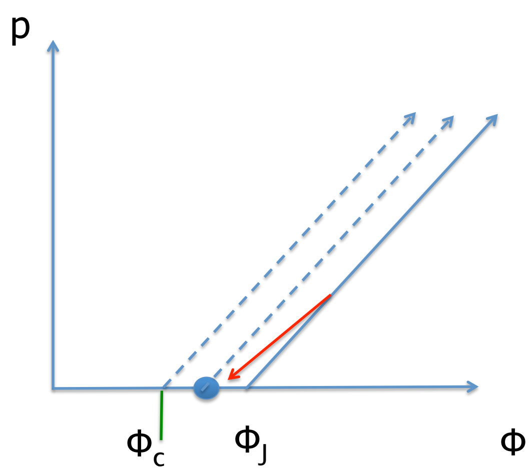
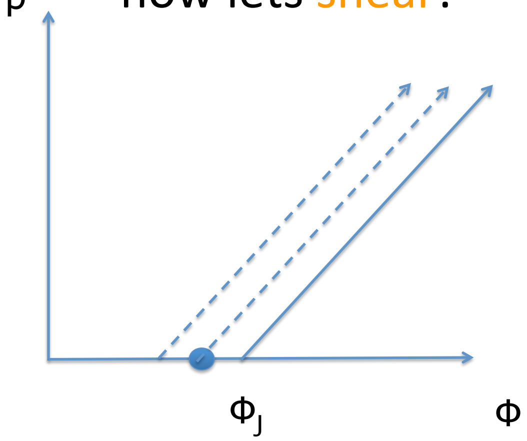


Isotropic (de)compression to an unjammed state



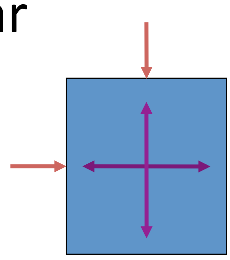
Isotropic (de)compression to an unjammed state now lets shear!



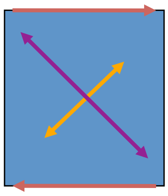
Isotropy <-> Shear

- no shear = compression or extension

$$\varepsilon = \begin{pmatrix} \varepsilon_V & 0 \\ 0 & \varepsilon_V \end{pmatrix}$$



Anisotropy <-> Shear ?



- Simple shear

$$\varepsilon=\begin{pmatrix}0 & 2\varepsilon_s\\ 0 & 0\end{pmatrix}=\begin{pmatrix}0 & \varepsilon_s\\ -\varepsilon_s & 0\end{pmatrix}+\begin{pmatrix}0 & \varepsilon_s\\ \varepsilon_s & 0\end{pmatrix}$$

Rotation + symmetric shear

Anisotropy <-> Shear ?

- Simple shear

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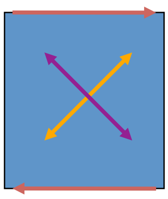
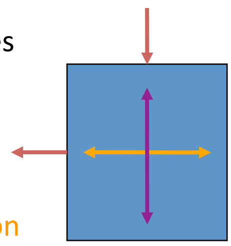
Rotation + symmetric shear



- Rotate symmetric shear tensor by 45 degrees

$$R_{45}\cdot\begin{pmatrix}0 & \varepsilon_s\\ \varepsilon_s & 0\end{pmatrix}\cdot R_{45}^T=\begin{pmatrix}\varepsilon_s & 0\\ 0 & -\varepsilon_s\end{pmatrix}$$

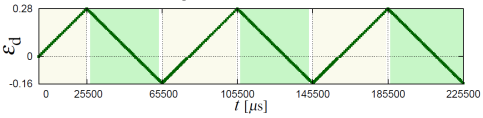


- biaxial=pure “shear”: compression+extension

Main Experiment 2 – Shear (volume-conserving)

$$\dot{\mathbf{E}} = \dot{\varepsilon}_{\mathrm{dev}} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

2 => 3 cyclic: see later …



Choose un-jammed states (with different preparation history).

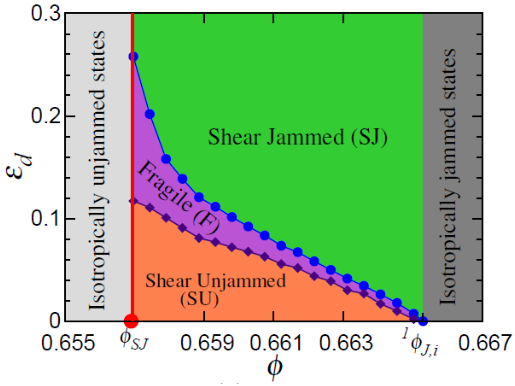
Perform deviatoric (volume conserving) shear deformation to strain 0.28.

Measure the shear strain needed to jam the system.

Main Experiment 2 – Shear (volume-conserving)

Three stages observed: Shear Unjammed → Fragile → Shear jammed

Minimum volume fraction, below which incite shear is needed to jam the system.

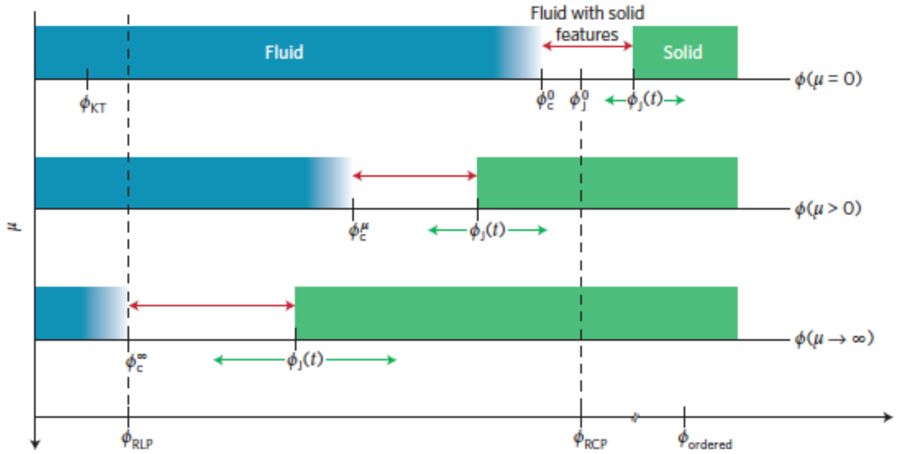


For one over-compression amplitude (one history).

How does it look for many different histories?

So much for the jamming point …

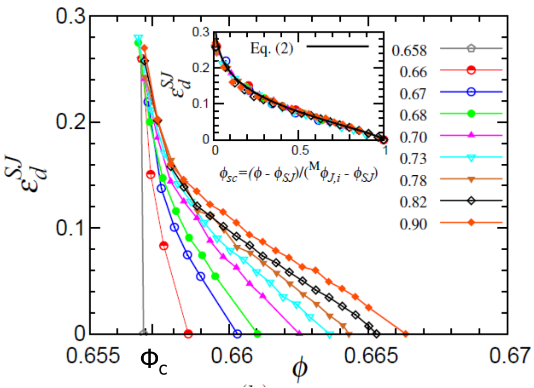
• **fluid-solid transition => jamming "~~point~~"** – no point!



S. Luding, Nature, 2016

Main Experiment 2.5 – **Shear (volume-conserving)**

Many different histories



Collapse on a master curve using

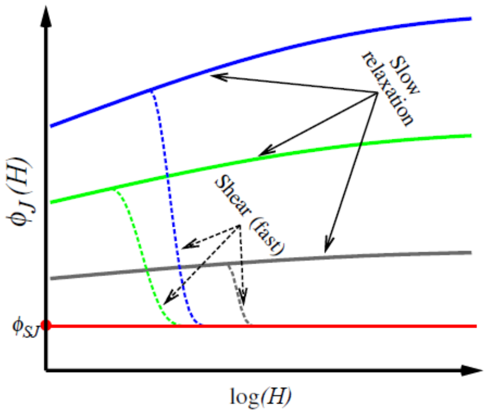
$$\left(\varepsilon_d^{SJ}/\varepsilon_d^0\right)^\alpha = -\log \phi_{sc} = -\log\left(\frac{\phi - \Phi_c}{{}^M\phi_{J,i} - \Phi_c}\right)$$

Message 2

response of **microstructure** to **isotropic deformations**!
- a new state variable is needed! use: Φ_J
- isotropic deformation leads to an <u>increase</u> of Φ_J (***slow***)

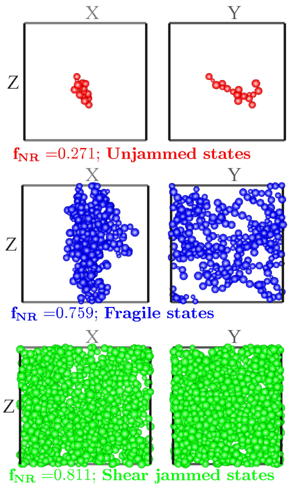
response of **microstructure** to **deviatoric/shear deformations**!
- no new state variable is needed! (use struture F_{dev})
- deviatoric deformation leads to a <u>decrease</u> of Φ_J (***fast***)

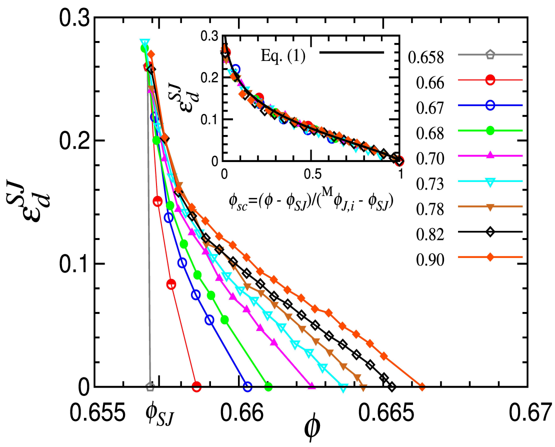
Connecting the two Experiments



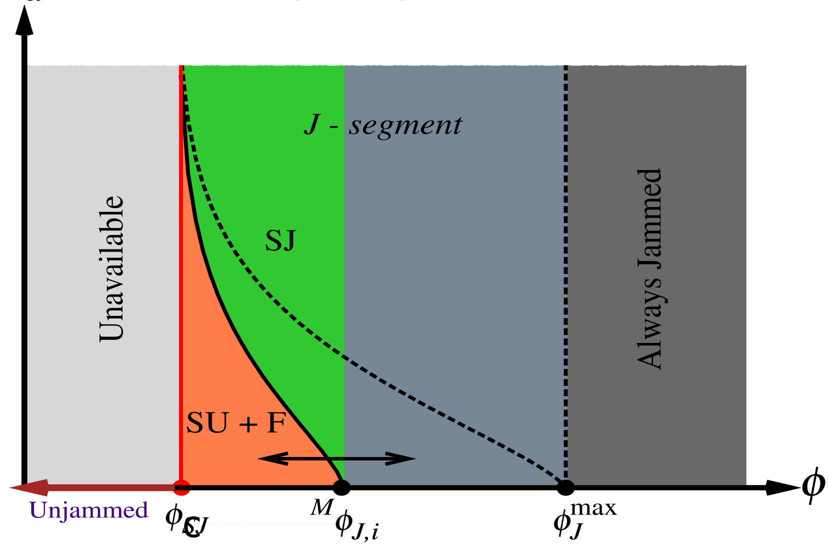
- Combine the two history-dependencies, by *superposing* the two limit experiments: isotropic and pure shear deformation.
- Rate of increase in the jamming point by isotropic deformation is much *slower* than the rate of decrease by pure shear.
- Ultimate lower bound, defined as the shear-jamming density … minimal jamming point reached

Jamming by application of shear

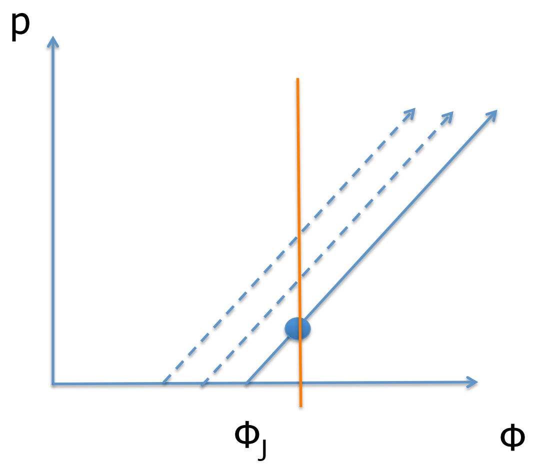




Jamming diagram with memory



BC “isochoric” shear



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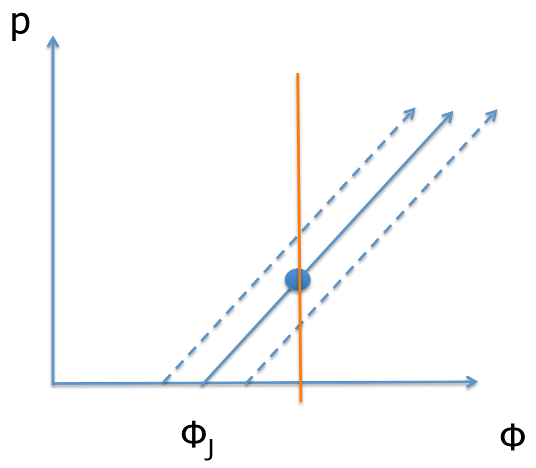

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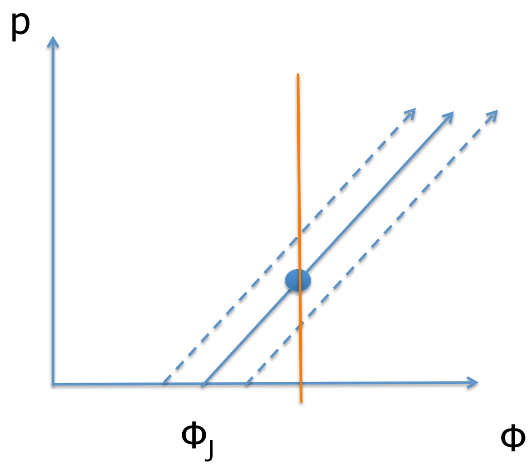
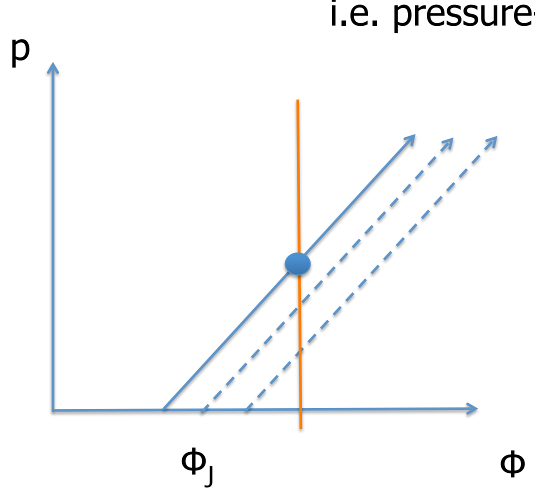
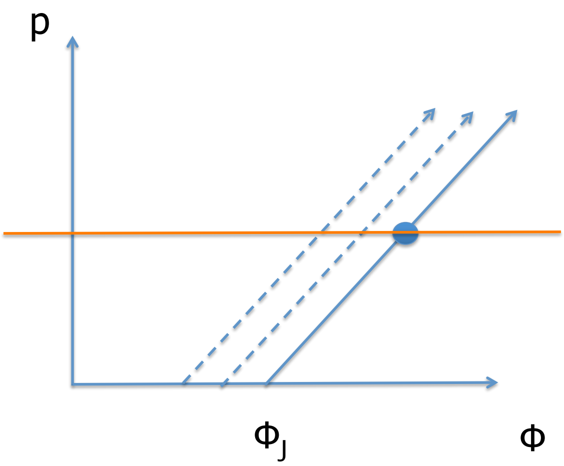


BC “isochoric” shear

i.e. pressure-dilatancy



BC “isobaric” shear



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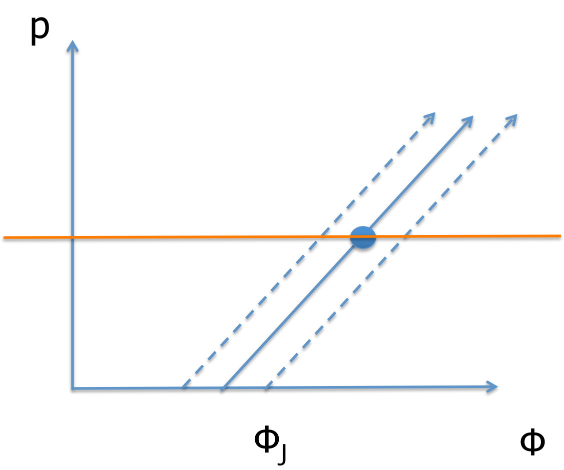
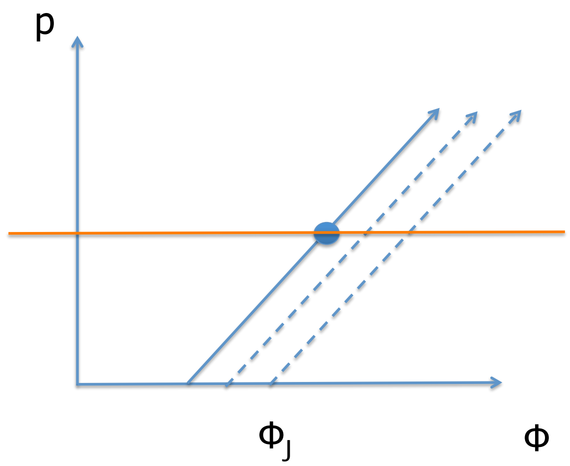
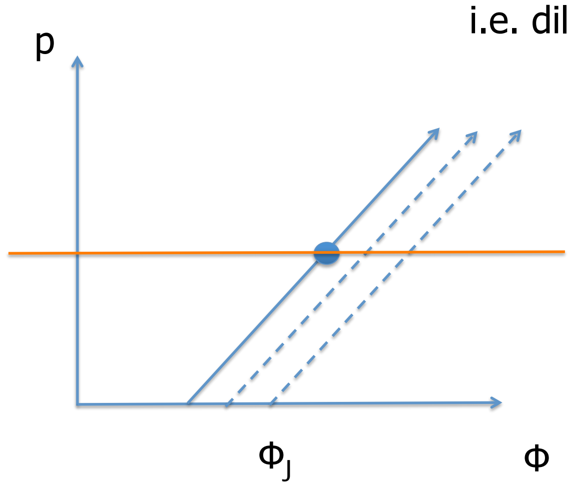


BC “isobaric” shear

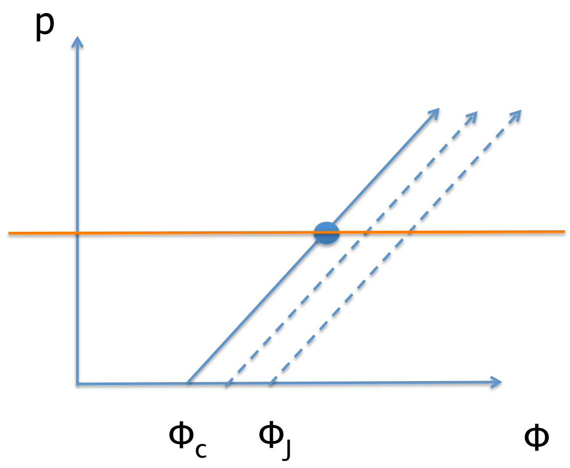


BC “isobaric” shear

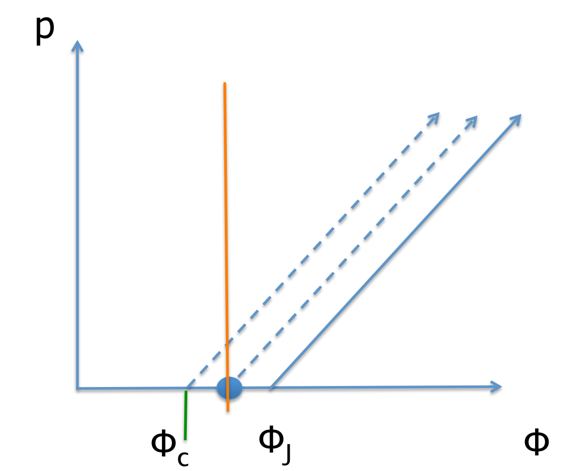
i.e. dilatancy



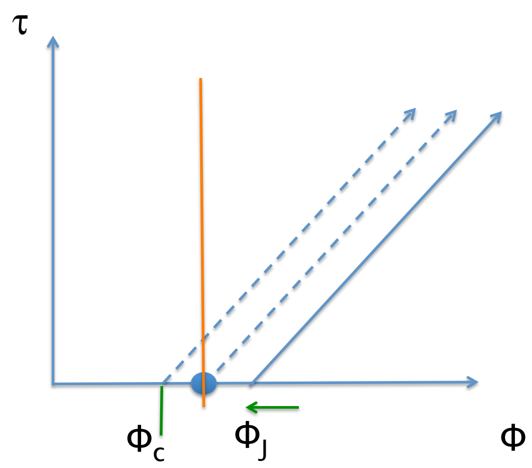
BC "isobaric" shear



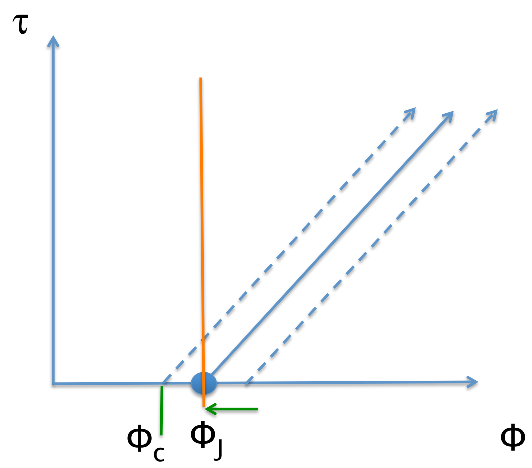
BC "isochoric" shear-jamming like in the particle simulations before!



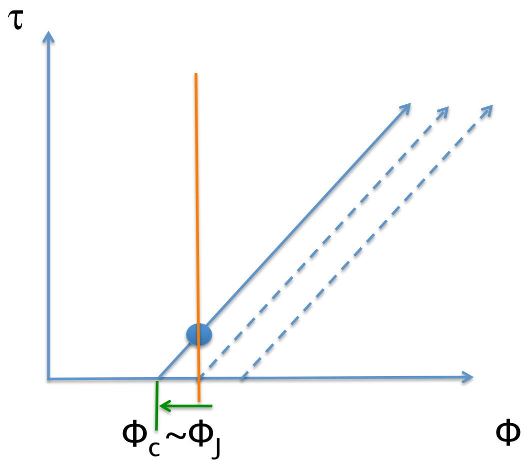
BC isochoric shear



BC isochoric shear-jamming

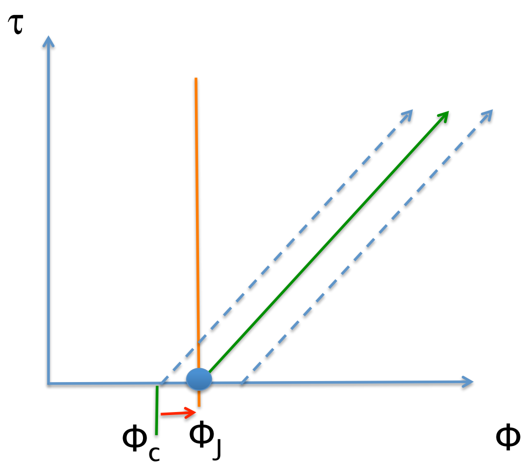


BC isochoric shear-jamming

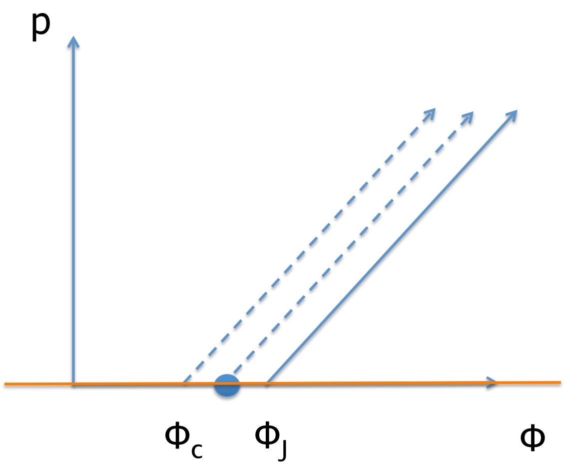


BC isochoric shear-reversal

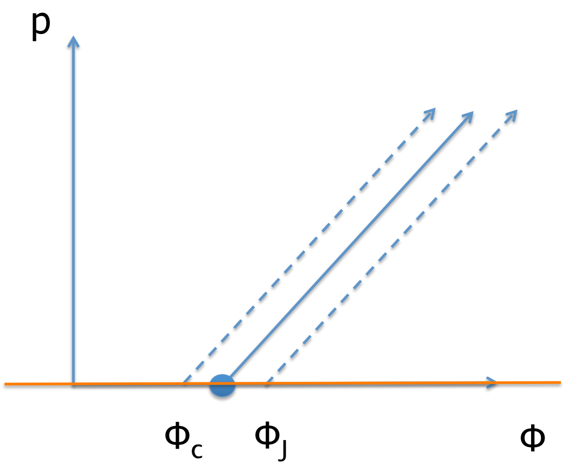
i.e. shear un-jamming



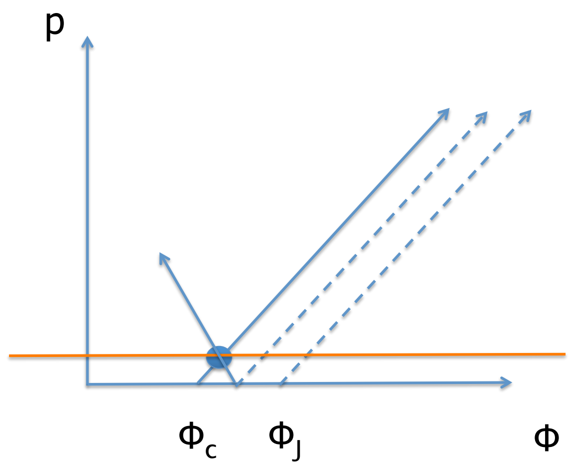
BC "isobaric" shear-jamming



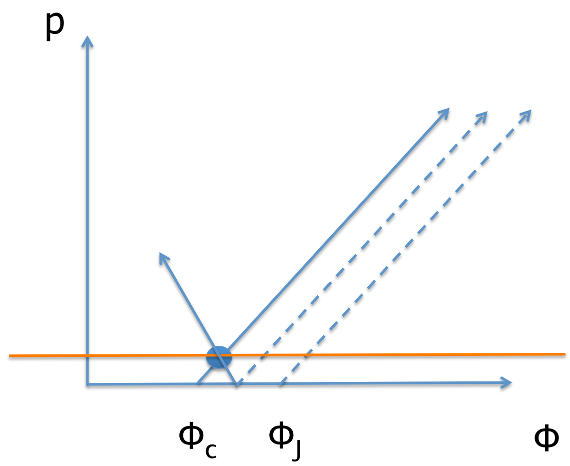
BC "isobaric" shear-jamming



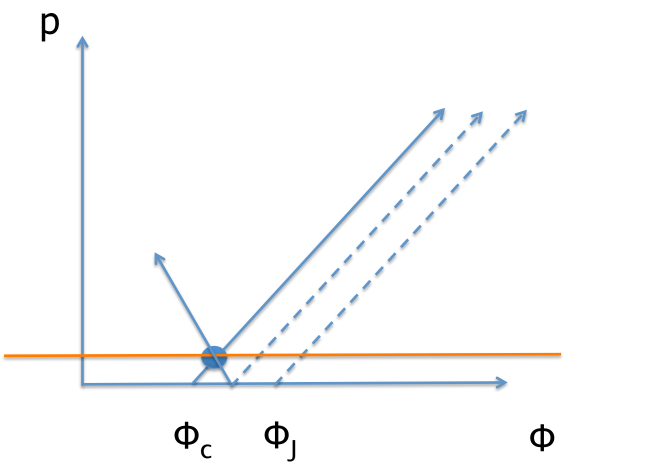
BC “non-isobaric” shear-jamming



NOW – we are elastic



NOW – we are elastic



Connecting the two Experiments

1: $^{M}\phi_{J,i} := \phi_J(\phi_i^{\max}, M) = {}^{\infty}\phi_{J,i} - ({}^{\infty}\phi_{J,i} - \phi_{SJ}) \exp\left[-(M/\mu_i)^{\beta_i}\right]$

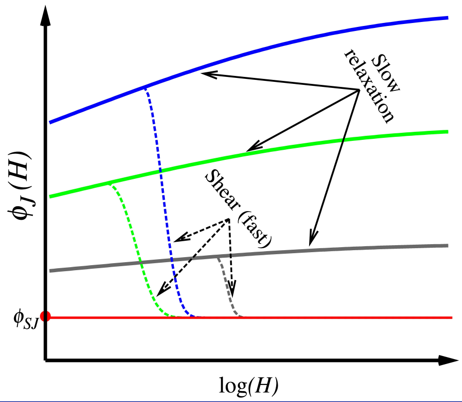
2: $$\left(\varepsilon_d^{SJ}/\varepsilon_d^0\right)^{\alpha} = -\log\phi_{sc} = -\log\left(\frac{\phi - \phi_{SJ}}{^{M}\phi_{J,i} - \phi_{SJ}}\right)$$

α=1.37 and ε_d^{SJ}=0.10

$$\phi_J(\varepsilon_d) = \phi_{SJ} + (\phi - \phi_{SJ}) \exp\left[\left(\frac{\left(\varepsilon_d^{SJ}\right)^{\alpha} - \left(\varepsilon_d\right)^{\alpha}}{\left(\varepsilon_d^0\right)^{\alpha}}\right)\right]$$

Evolution of jamming points with history

$$^{M}\phi_{J,i} := \phi_J(\phi_i^{\max}, M) = {}^{\infty}\phi_{J,i} - ({}^{\infty}\phi_{J,i} - \phi_{SJ}) \exp\left[-(M/\mu_i)^{\beta_i}\right]$$



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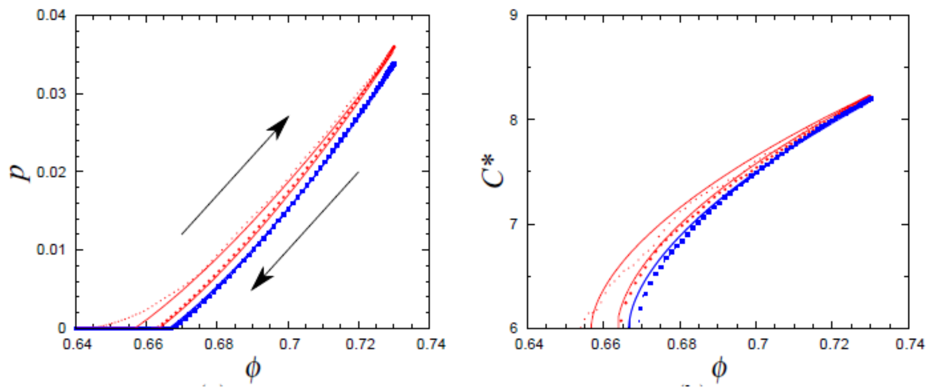
Predictive power – cyclic isotropic deformation

- Intermediate cyclic over-compression (amplitude 0.73) for 100 cycles.



-Well predicted isotropic - pressure and coordination number (during loading and un-loading).
- Only by adding motion of jamming-point in the constitutive model.
- Curves saturate for large cycles for loading and un-loading and is also predicted.

Predictive power – cyclic isotropic deformation

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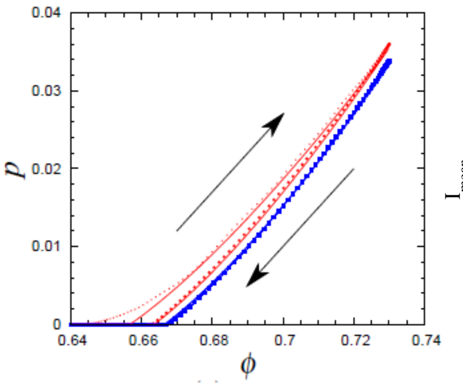
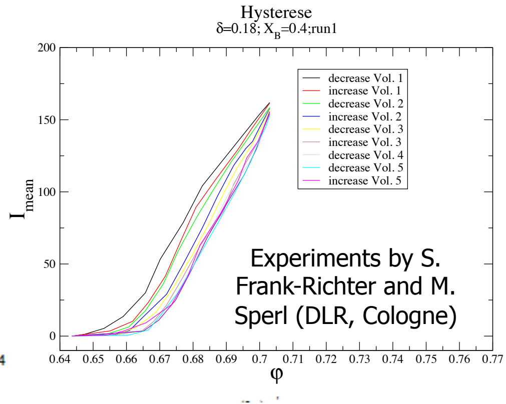




-Well predicted isotropic - pressure and coordination number (during loading and un-loading).
- Only by adding motion of jamming-point in the constitutive model.
- Curves saturate for large cycles for loading and un-loading and is also predicted.

Constitutive Model: Anisotropy Model

Isotropy (before) + Anisotropy F_{dev}

$$\begin{aligned}
\delta P^* &= 3B\delta\varepsilon_v + \boxed{A_1} S_\sigma \delta\varepsilon_{dev}, \\
\delta\sigma^*_{dev} &= 3\boxed{A_2}\delta\varepsilon_v + G^{oct} S_\sigma \delta\varepsilon_{dev}, \\
\delta F_{dev} &= \beta_F \operatorname{sign}(\varepsilon_{dev})\, F^{max}_{dev} S_F \delta\varepsilon_{dev}
\end{aligned}$$

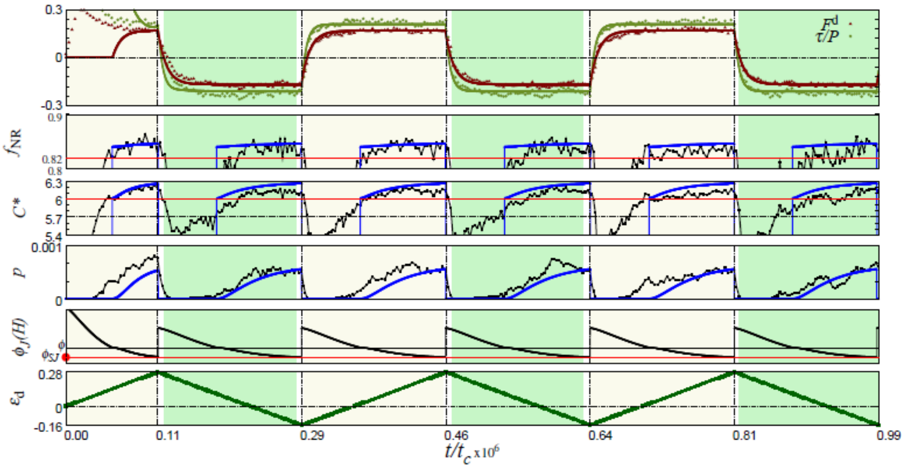
Due to A_1 and A_2, the model provides a **cross coupling** between the two types of stress and strain in the model

Need to define - Initial state and the deformation path

… then integrate the incremental evolution …

Predictive power – cyclic pure shear deformation

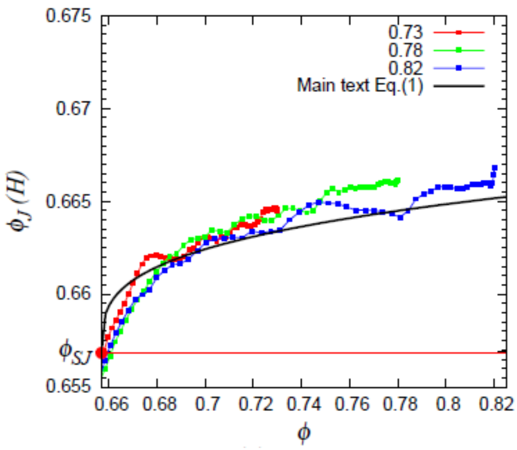
- Cyclic shear for 3 cycles (after the first loading, system forgets history).



- Quantities like – fraction of non-rattlers, coordination number, pressure – by mainly modifying the constitutive model with non-constant jamming point.

Something for experimentalists

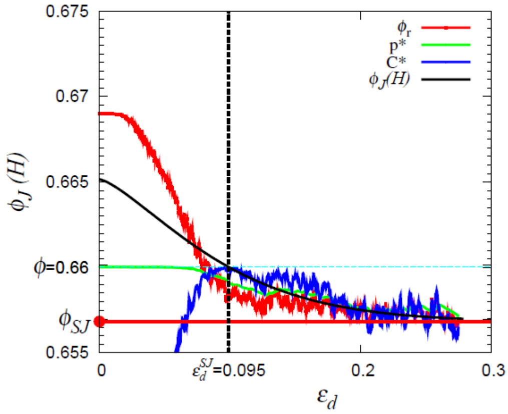
Measuring jamming points from the accessible macroscopic quantities – easiest pressure ☺



During isotropic deformation at three different amplitudes,
and extracting it from pressure … comparison with the theoretical framework

Something for experimentalists

Measuring jamming points from the accessible macroscopic quantities – easiest pressure ☺

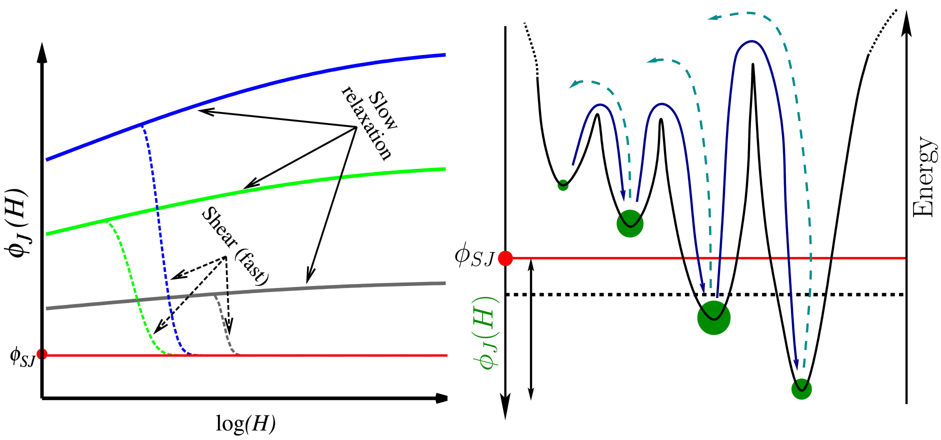


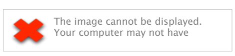
$$\frac{p\nu_c}{\nu C} = p_0(-\varepsilon_v)\,[1-\gamma_p(-\varepsilon_v)]$$

$$\varepsilon_v = -\ln\left(\frac{v}{v_c}\right)$$

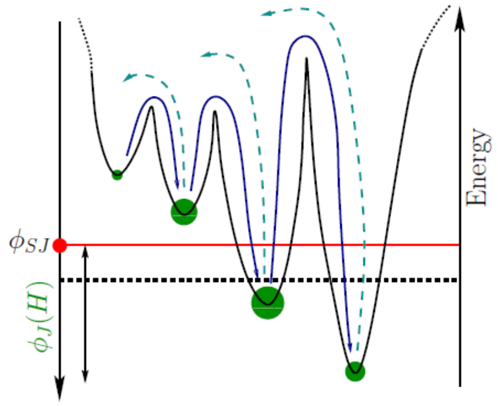
During shear deformation, and extracting it from pressure, coordination number.
Comparison with the theoretical framework

Evolution of jamming points with history





Explanation – Energy landscape



- Isotropic deformation – leads to an increase in local and total jamming point, wheras the shear deformation decreases it…

- Deeper valleys with higher barriers, can be achieved with higher over-compression.

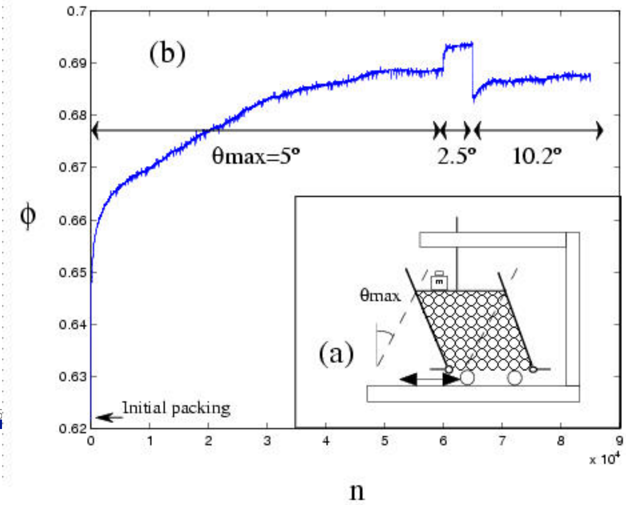
Minimal meso-statistical model

- Experiment (O. Pouliquen, Marseille)
- & Model (developed during my visit)
- Results
  - Slow compaction
  - Cyclic compaction
- Summary
- Next steps ?

22.03.2016

Experiments

- Dense, monodisperse periodic shear

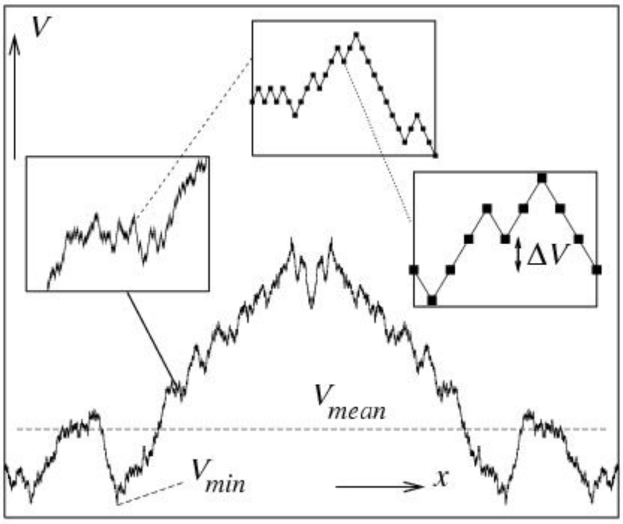


22.03.2016

Model

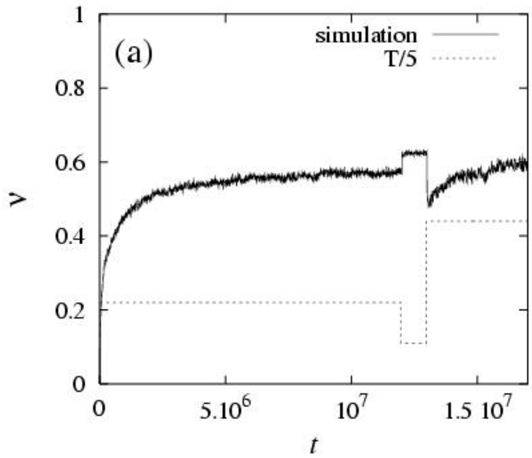
- Packing:
  - Local configuration?
  - Energy landscape
  - Potential energy → Density
- Particles:
  - Explore the energy landscape
  - Random walk = Sinai Diffusion

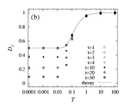
Model



Slow compaction

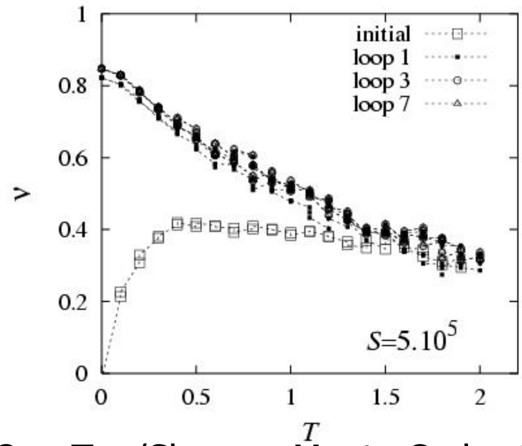
- Experiment vs. model simulation



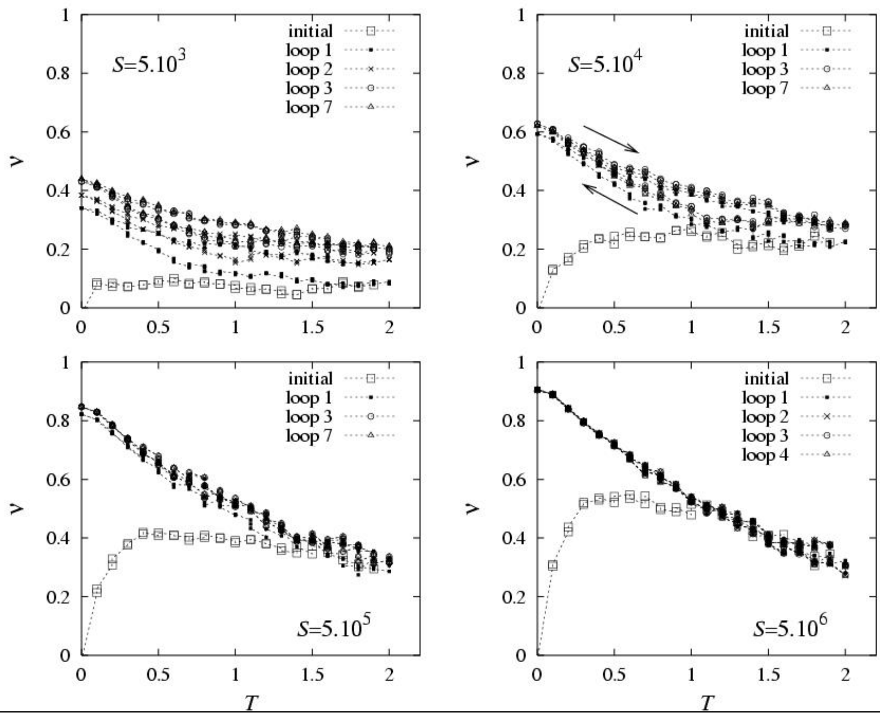


$$\nu = 1 - \frac{E - V_{\text{min}}}{V_{\text{mean}} - V_{\text{min}}}$$

Cyclic compaction



- One Tap/Shear = Monte Carlo step
- Tapping Amplitude = Temperature



Summary

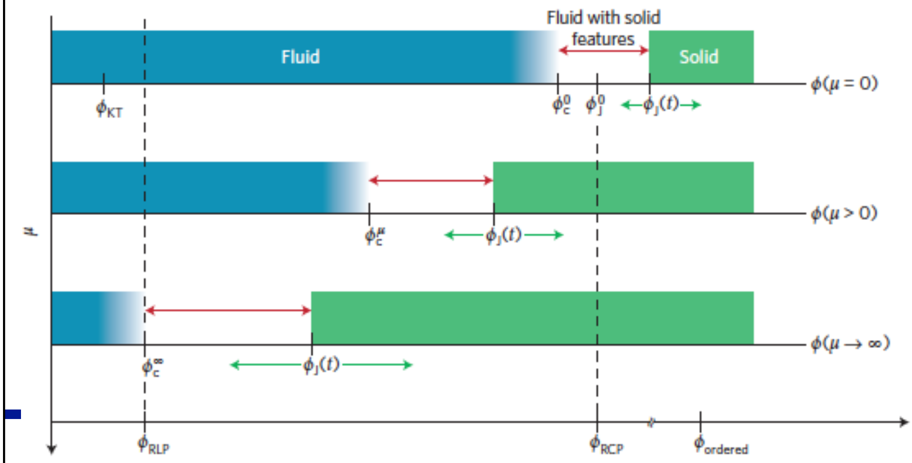
- Minimal (?) model
- Define configuration energy landscape
- Tap/Shear = Explore landscape
- Experimental phenomenology

Next Steps

- How to get the energy landscape ?
- Temperature = ?
- Monte Carlo time-scale ?
- Correlations ?
- Energy landscape as function of
  system parameters ?

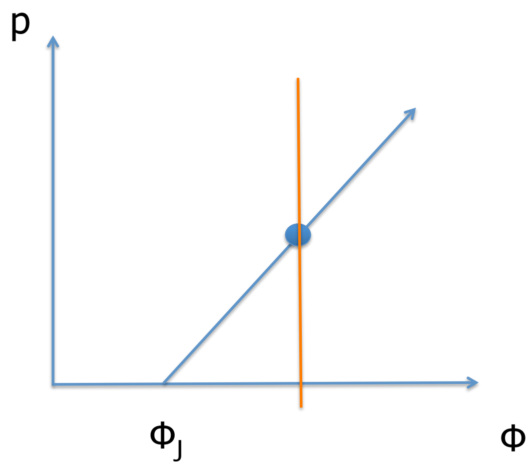
So much for the jamming point …

• **fluid-solid transition => jamming** "~~point~~" – no point!

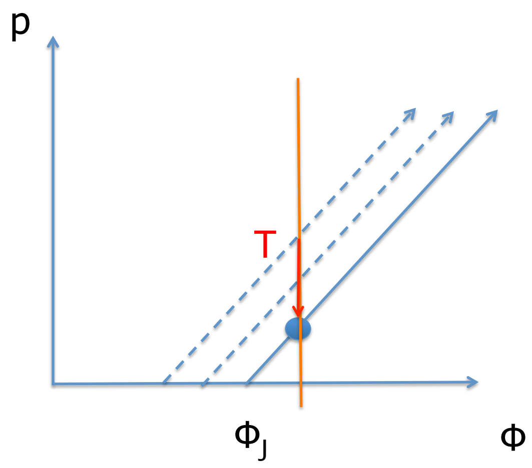


S. Luding, Nature, 2016

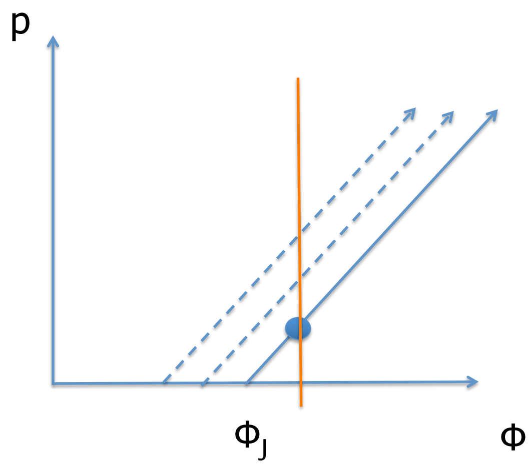
BC "isochoric" + tapping equivalent to ***temperature***



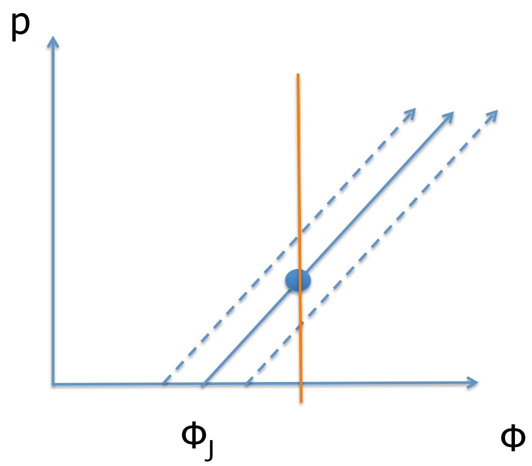
BC “isochoric” – relaxation/creep



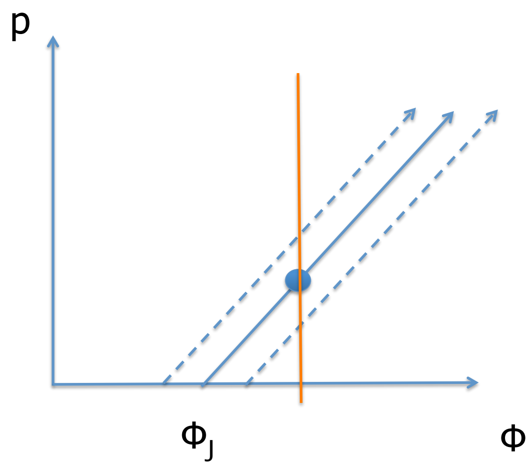
BC “isochoric” shear



BC “isochoric” shear



BC “isochoric” shear



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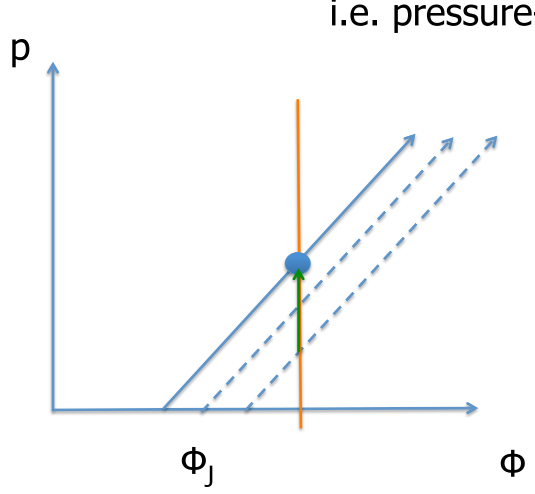
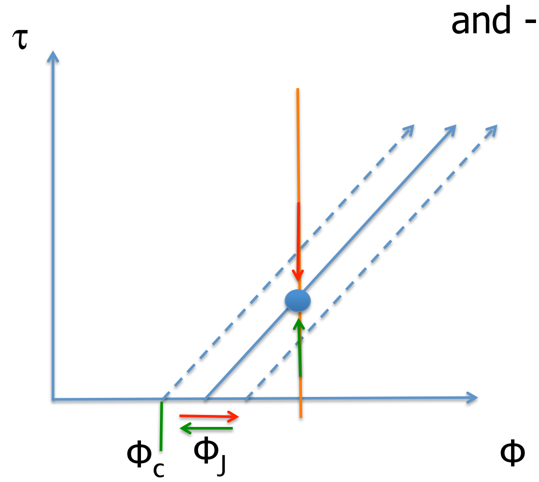


Equilibrium: shear + T

i.e. pressure-dilatancy
and -relaxation



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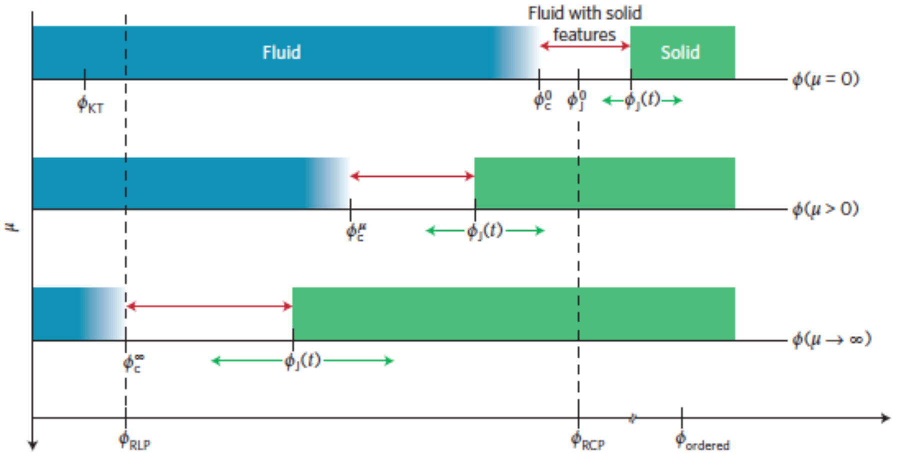

S. Luding, Nature, 2016