About elasto-plasticity, anisotropy, dilatancy and an alternative macro-view on jamming under isotropic and deviatoric deformations

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

jamming “~~point~~” – and shear jamming

• Everywhere in nature/industry and used in day-to-day life.

Examples:

Overview – where do we start?

- Jam-**packed** systems … not a (single) jamming point …

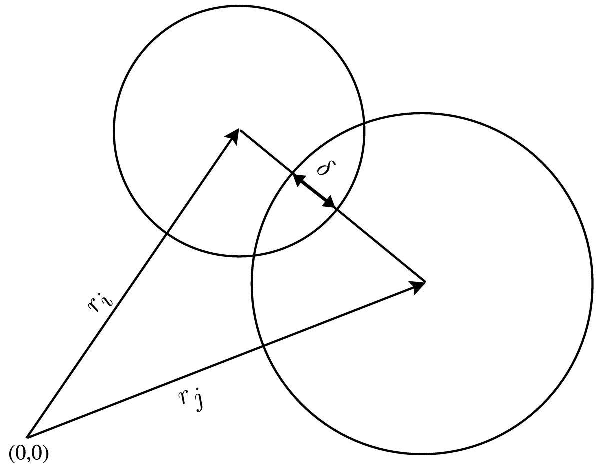
- **Simplest** model system (linear, no friction, no cohesion, no walls)

- **no**(?) dynamics, jiggling, granular temperature, Brownian dynamics

- microstructure+dilatancy+anisotropy+history

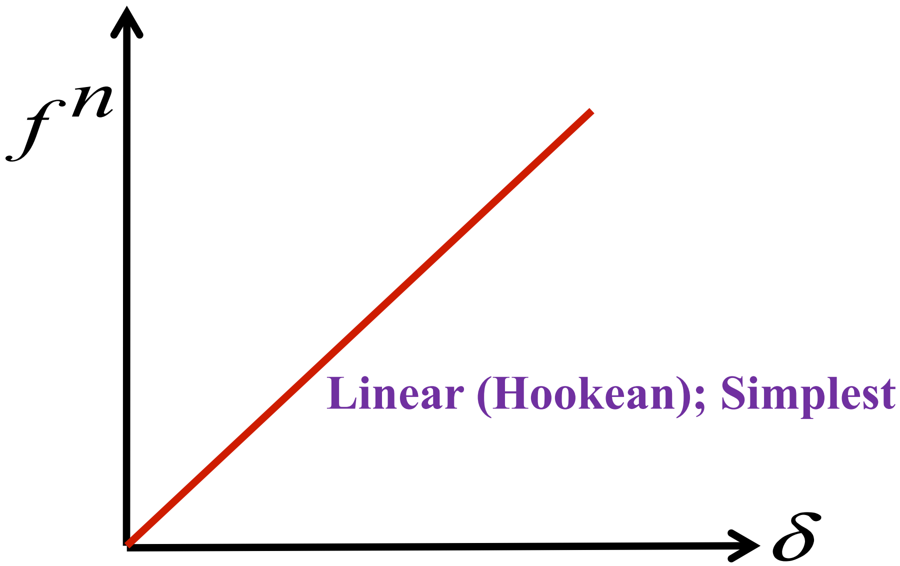
DEM (Discrete element method) = MD

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



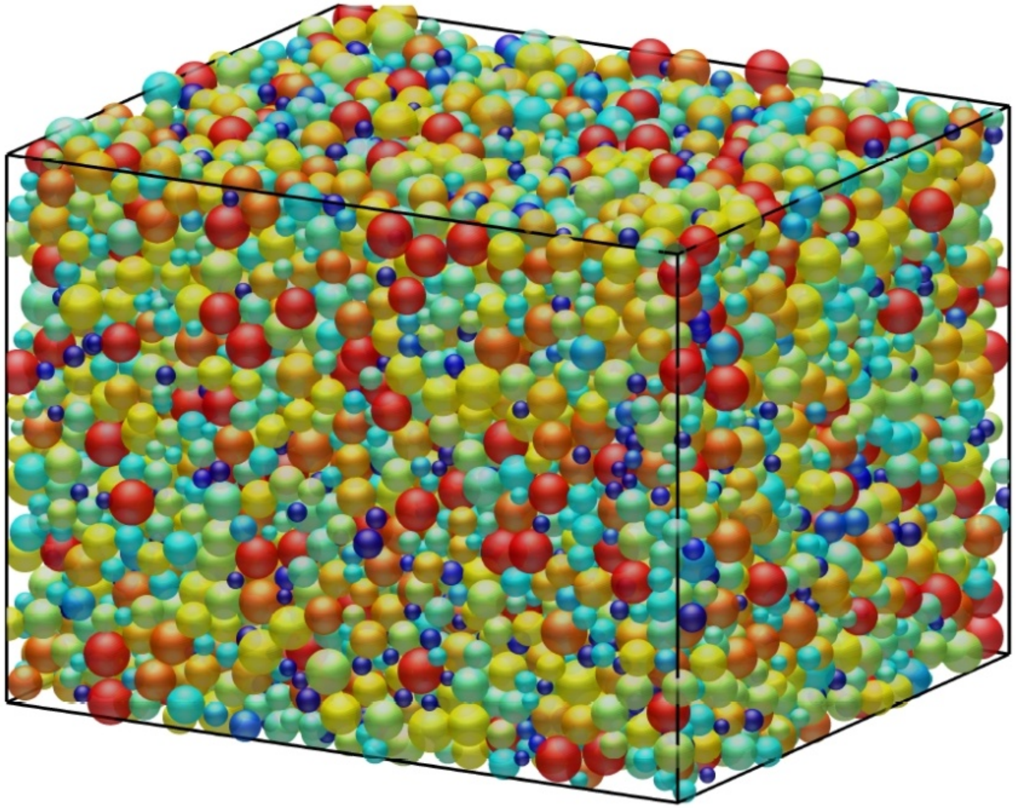
Solve Newton's equation of motion

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



Exclude:
nonlinear elastic
nonlinear plastic
Friction
Cohesive

Simplest Model System



- 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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microstructure!

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microstructure!

… and its history / protocol dependence …

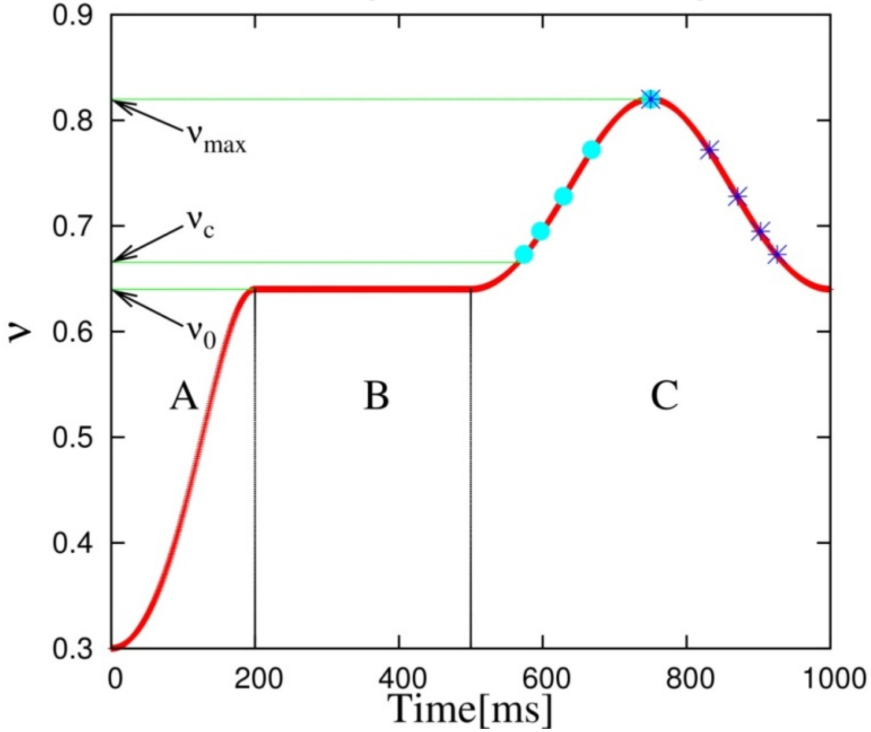
Sample Preparation – from the beginning!

tapping … => accepted procedure …

Sample Preparation – from the beginning!

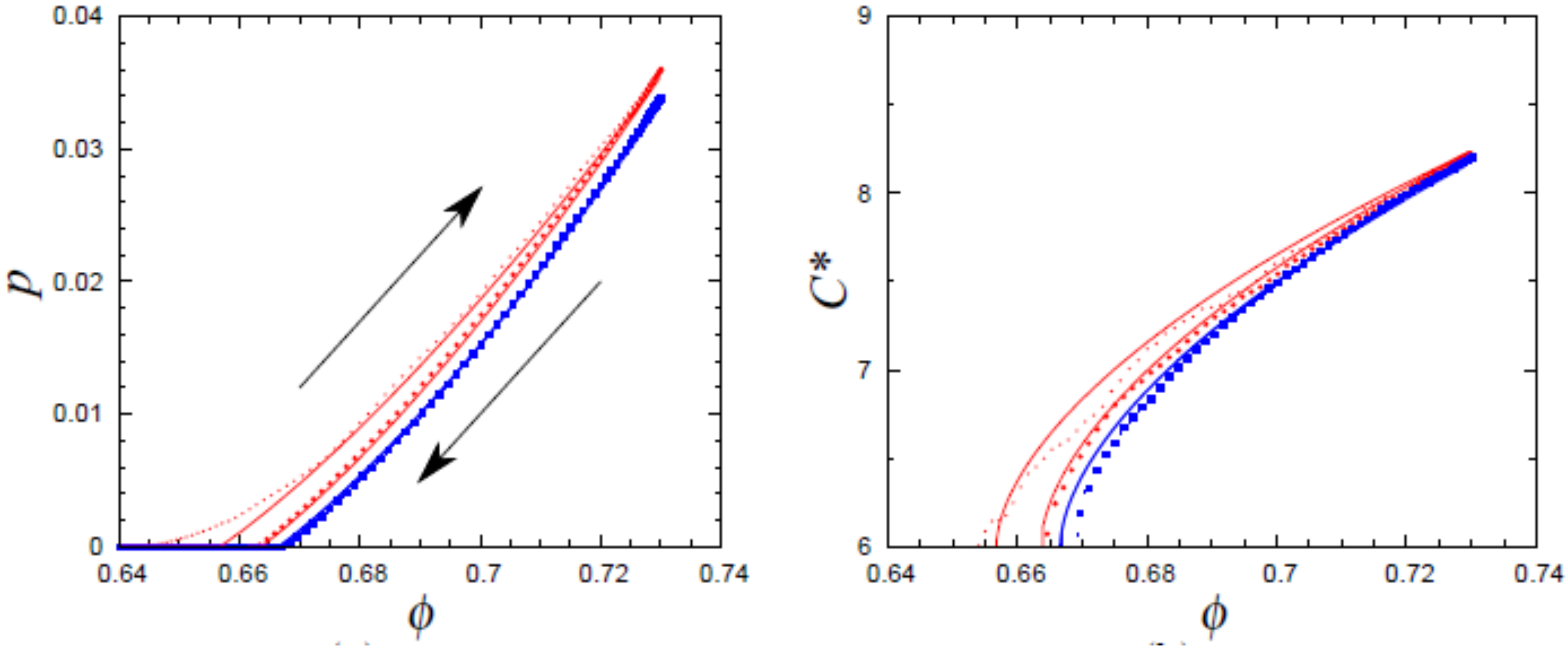
Isotropic Compression and de-compression

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



(cyclic) isotropic deformation

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



Sample Preparation – from the beginning!

Isotropic Compression and de-compression

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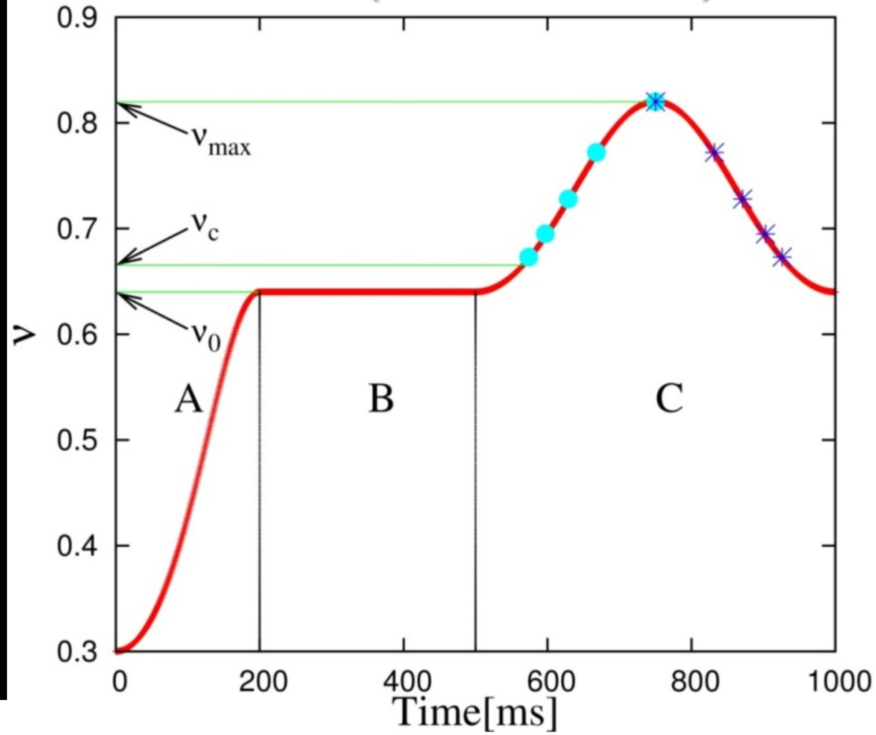
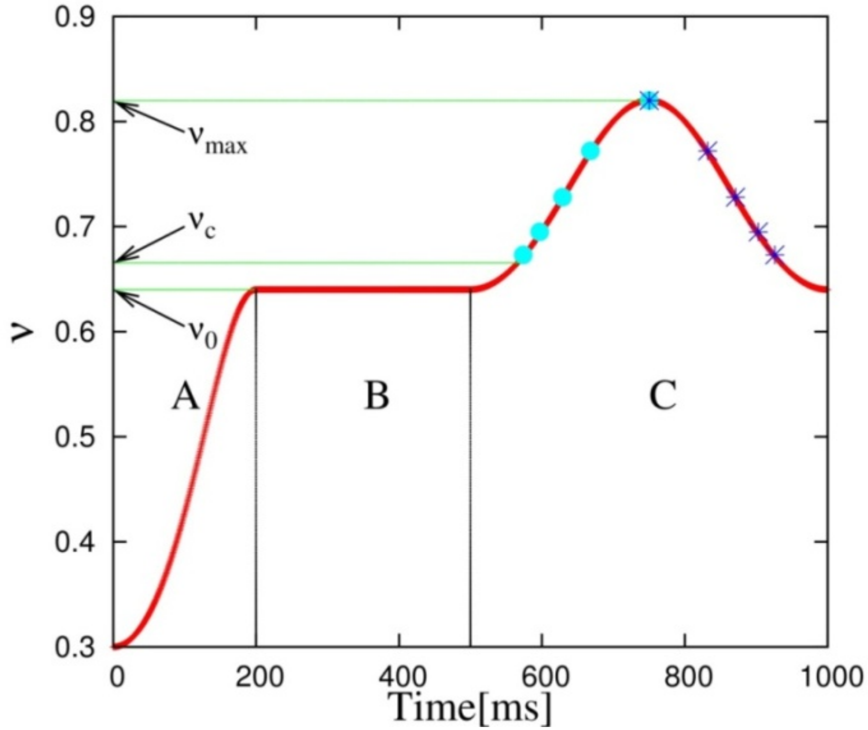


Main Experiments

Two types of deformation:



Cyclic isotropic (de-)compression

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

Cyclic deviatoric (volume-conserving) shear

$$\dot{\mathbf{E}} = \dot{\varepsilon}_{\text{dev}} \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1/2 & 0 \\ 0 & 0 & -1/2 \end{bmatrix}$$

Main Experiment 1 - Cyclic isotropic over-compression

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

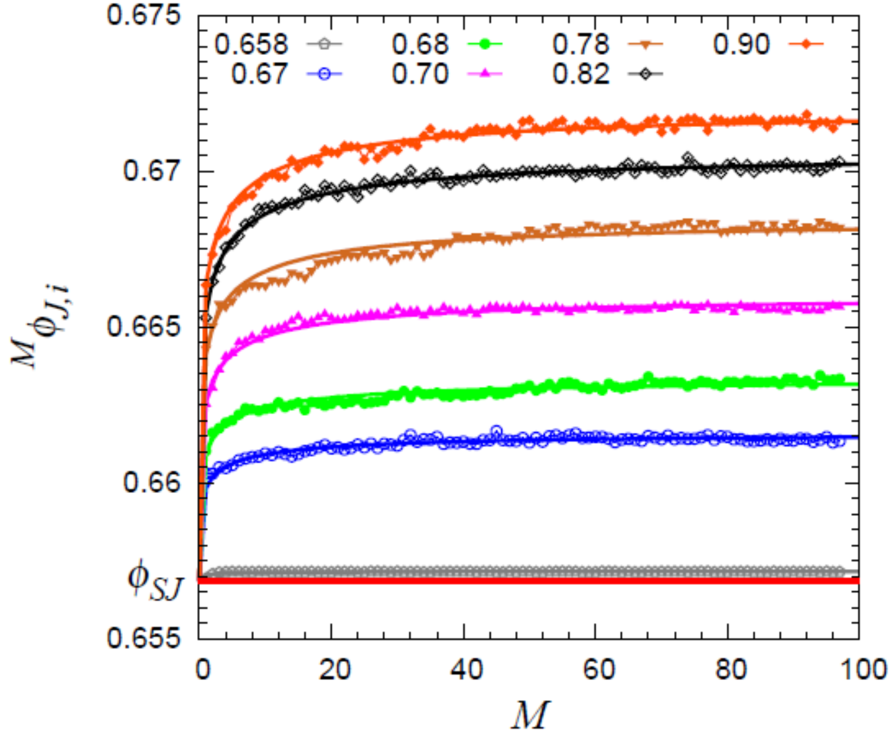
Choose a un-jammed state.
Perform cyclic isotropic (de-)compression for ***M=100*** cycles.

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



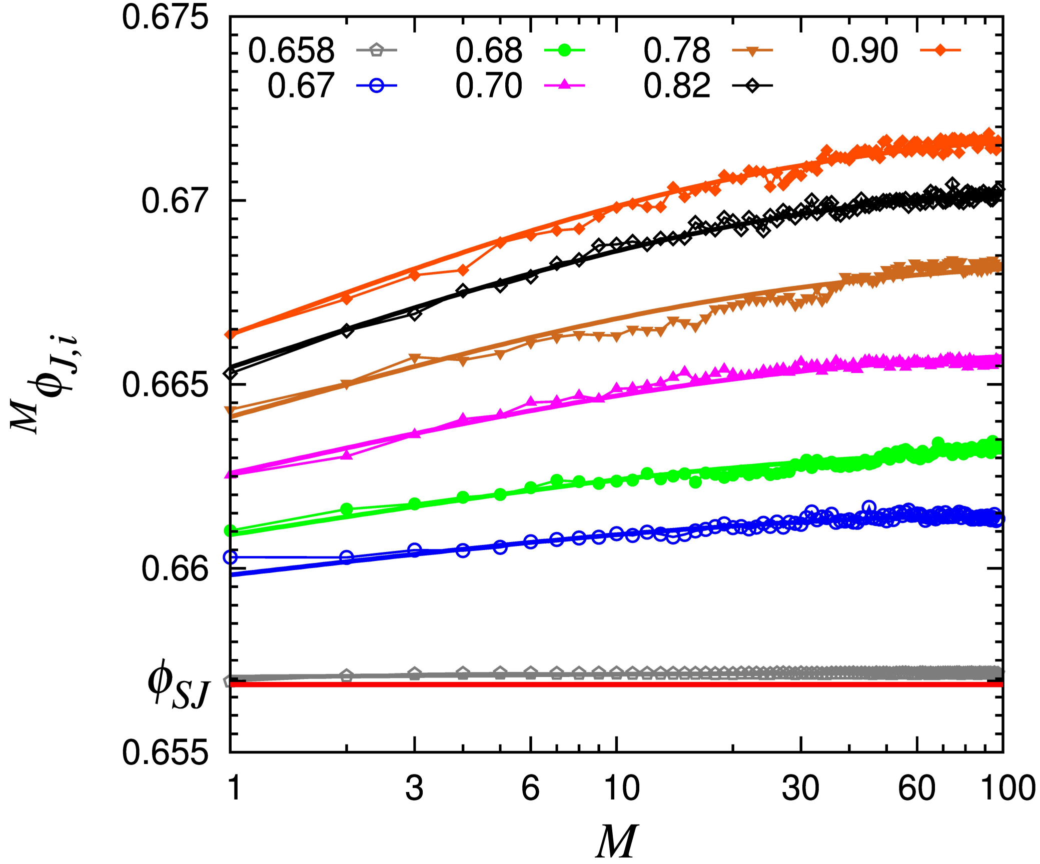
- For higher over-compression, jamming point is higher

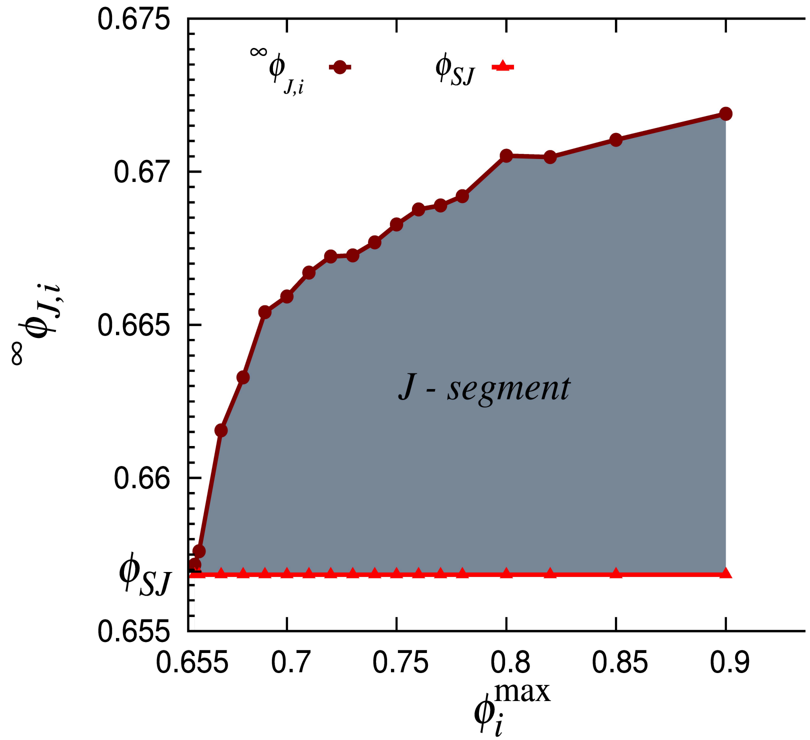
- Jamming point increases (KWW stretched exponential function).

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

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

Evolution of isotropic jamming points





$$^{\infty}\phi_{J,i} = \phi_{SJ} + \alpha_{\max}\left(\phi_i^{\max}/\phi_{SJ} - 1\right)^{\beta}$$

$\phi_{SJ} = 0.6567$ $\mu_i = 1$ $\beta_i = 0.3$ α_{max}=0.02

Message 1

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

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

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

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System with $C^*=Z_{iso}=6$ (frictionless), at $p \Rightarrow 0$
at different densities for different protocols (same material)

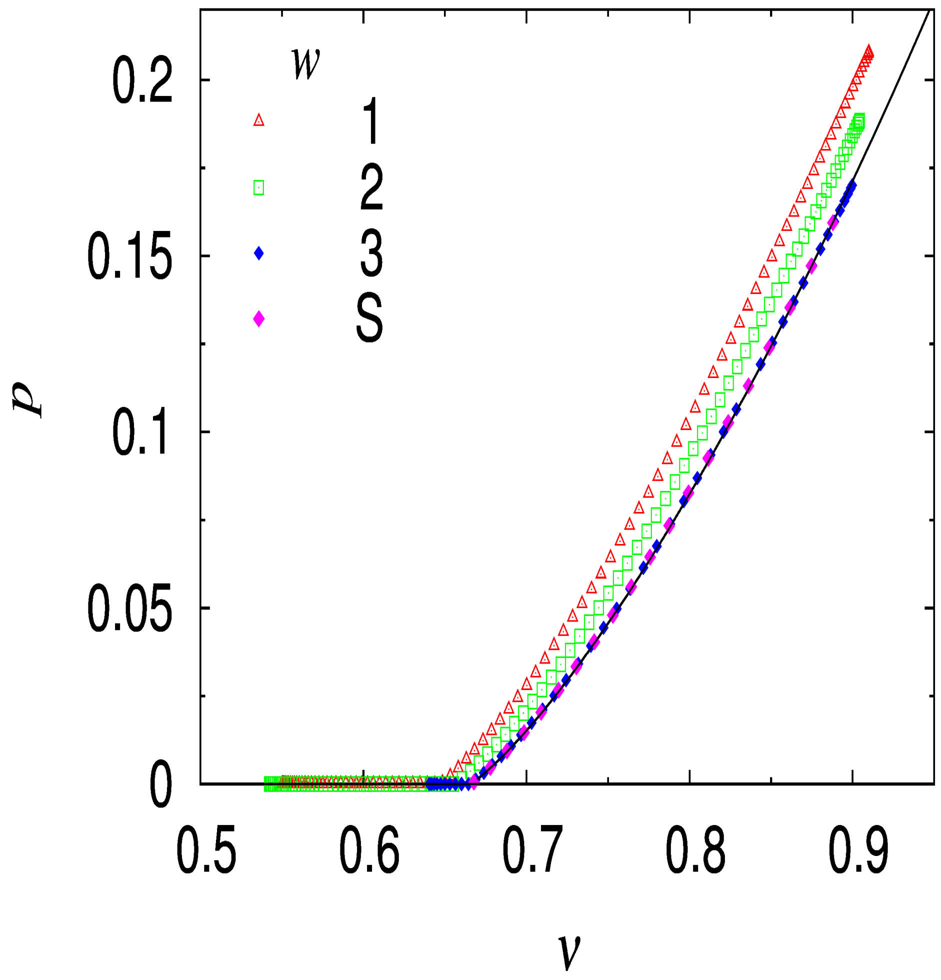
jamming "point" slowly increases!

Constitutive model for Pressure

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

Isotropic compression – Pressure

$$p = p_0 \frac{\nu C}{\nu_c}(-\varepsilon_{\mathrm{v}})\left[1 - \gamma_p(-\varepsilon_{\mathrm{v}})\right]$$



Isotropic compression – Pressure

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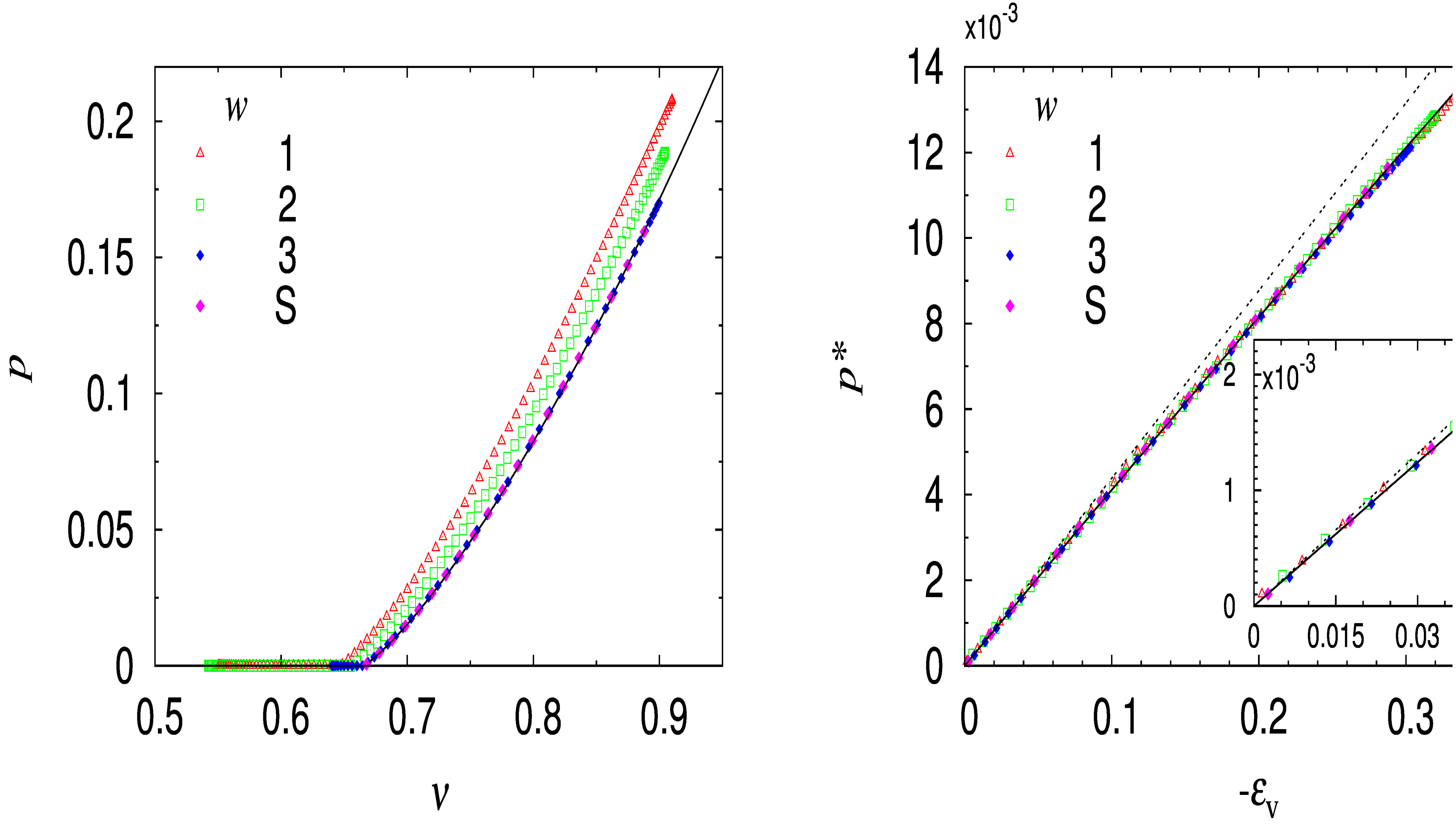

Constitutive model for Pressure

linear ☺

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

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

What's the point?

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

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

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

What's the point?

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

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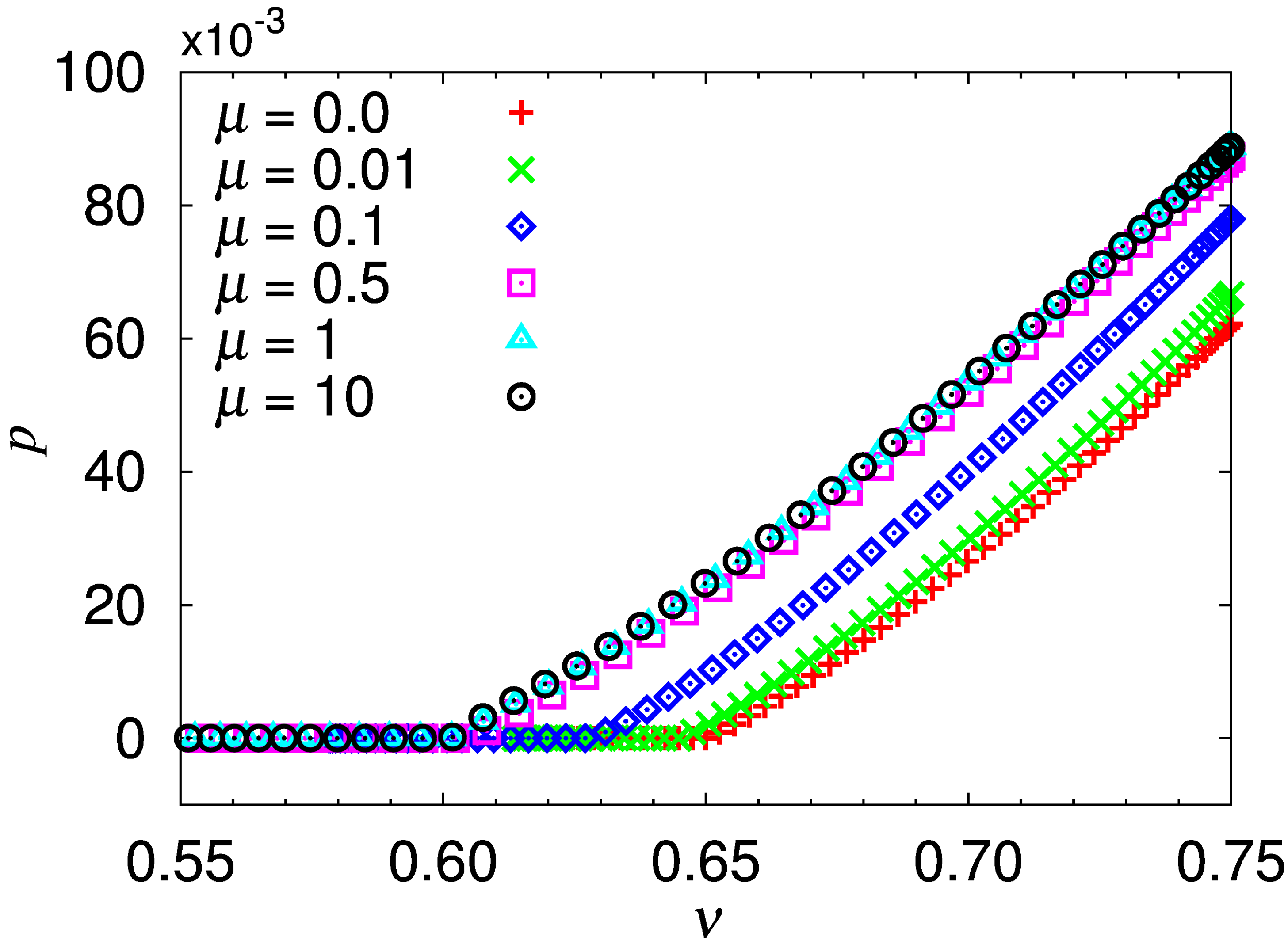
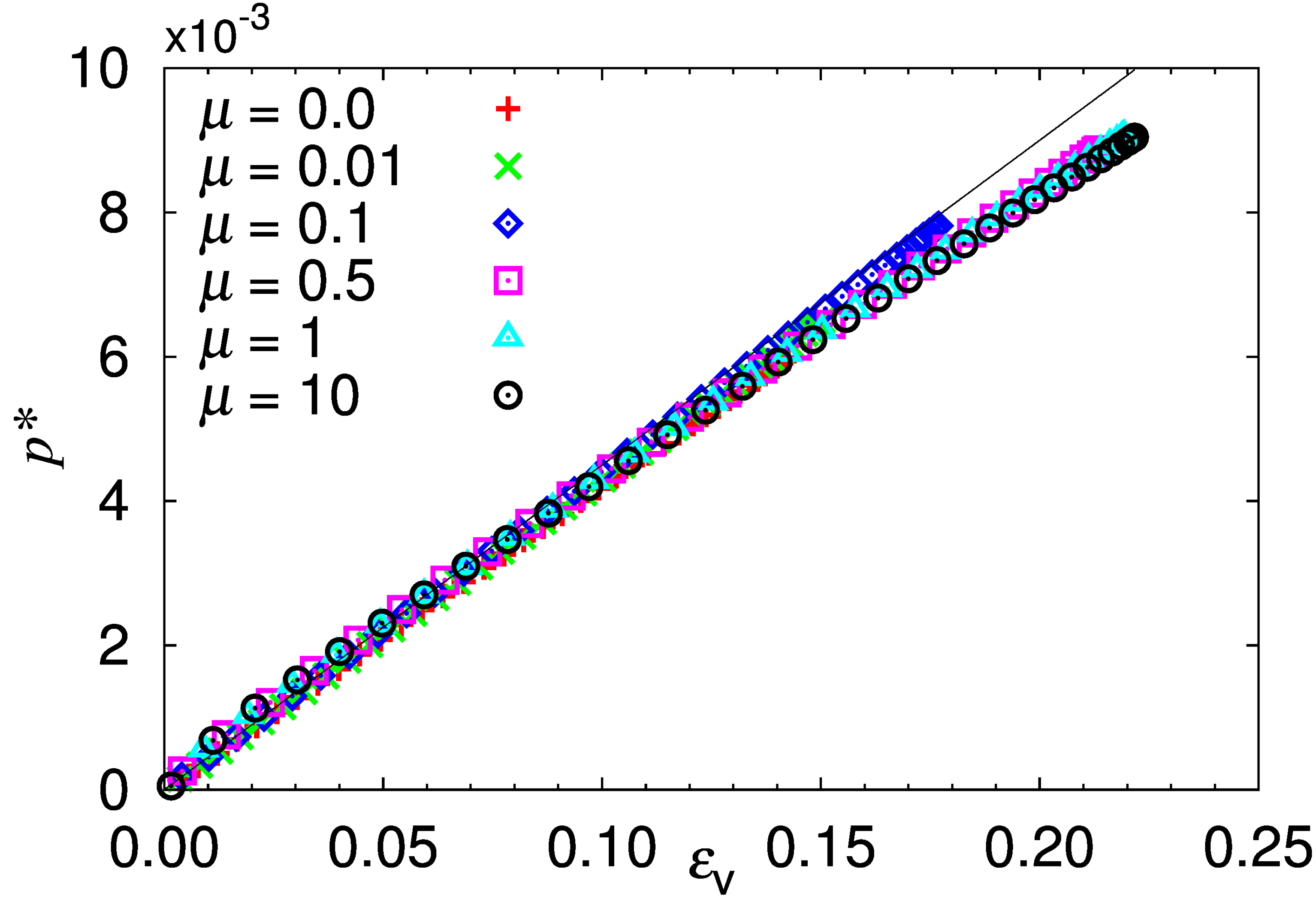
How to calibrate/measure them – done …
(some of them are even known analytically)

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

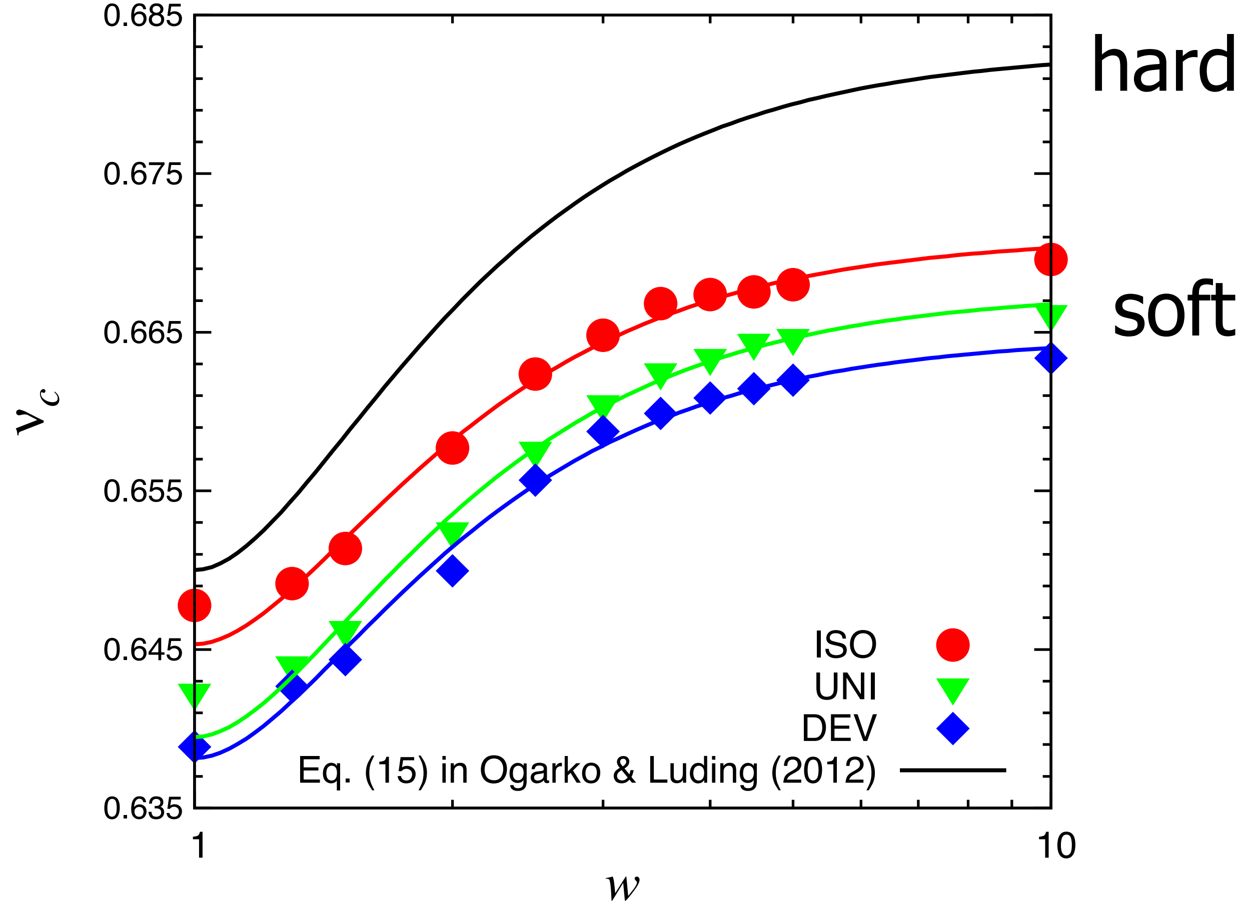
Isotropic de-compression M=1; effect of friction



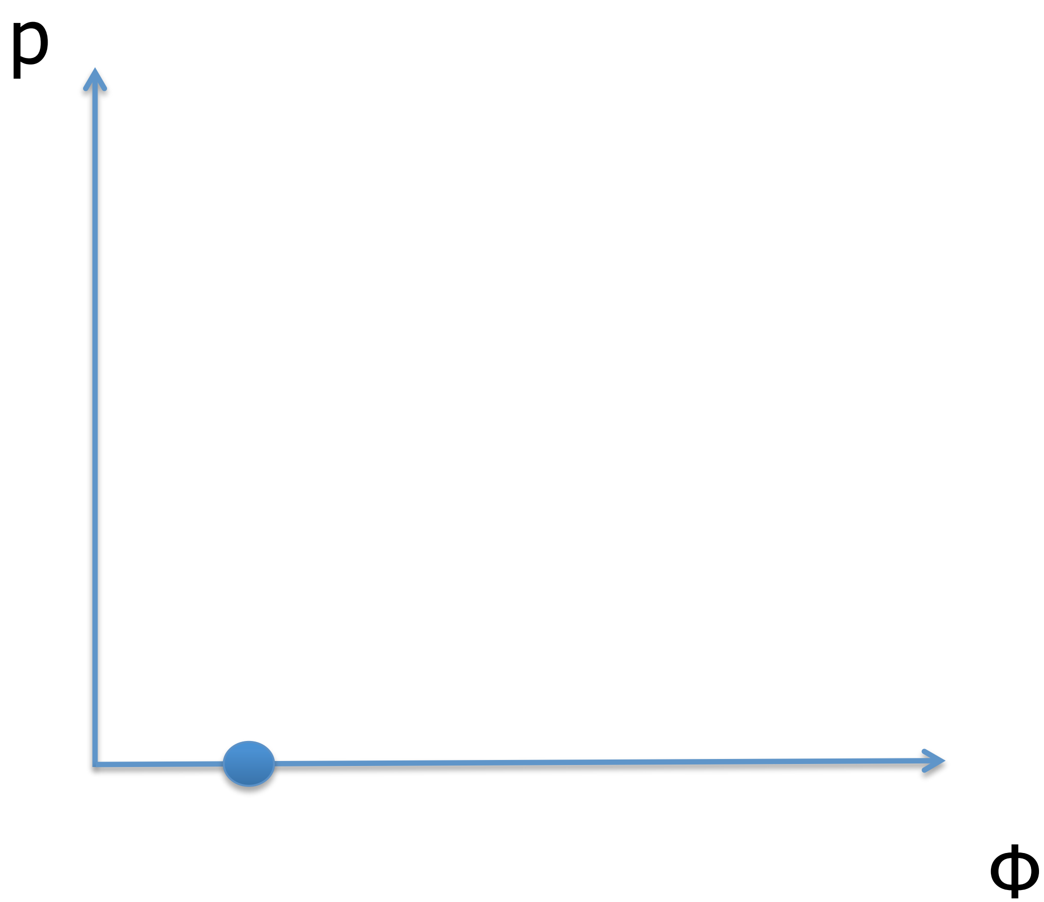
Isotropic de-compression; effect of friction



Polydispersity and whats the difference between ISO and SHEAR?



Isotropic (de)compression



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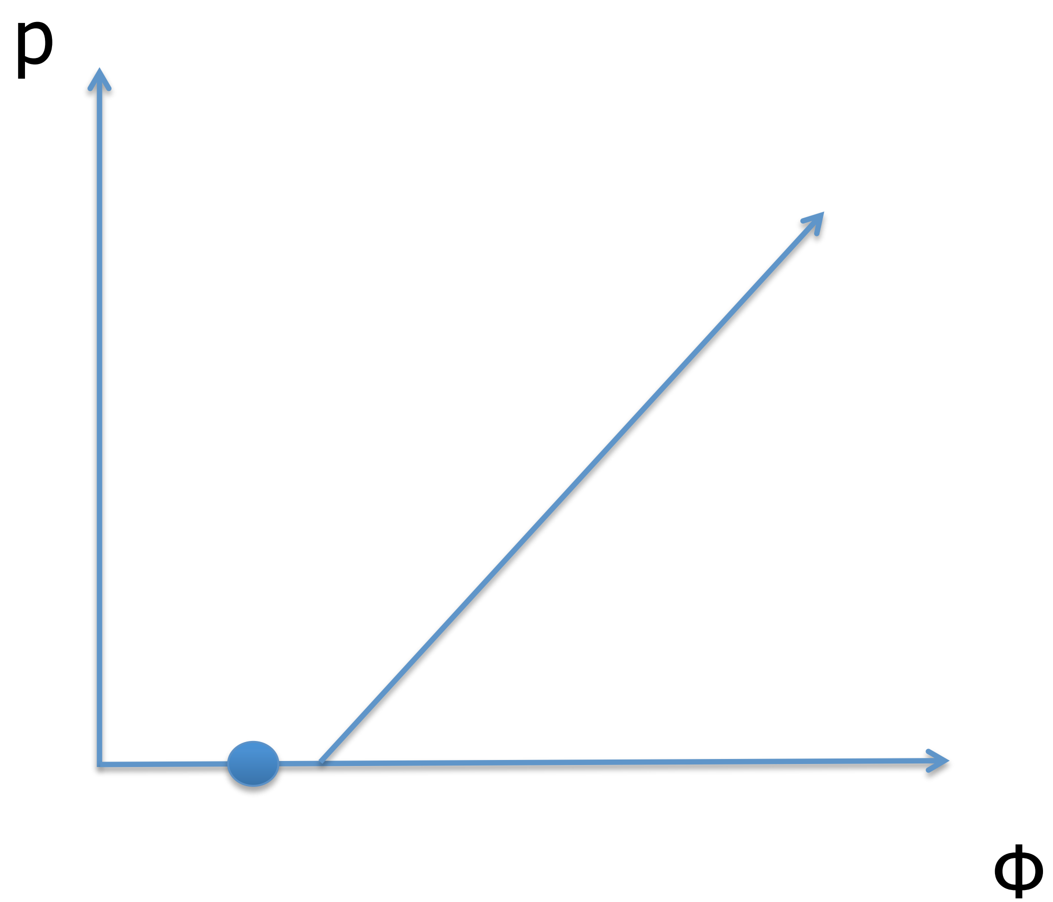

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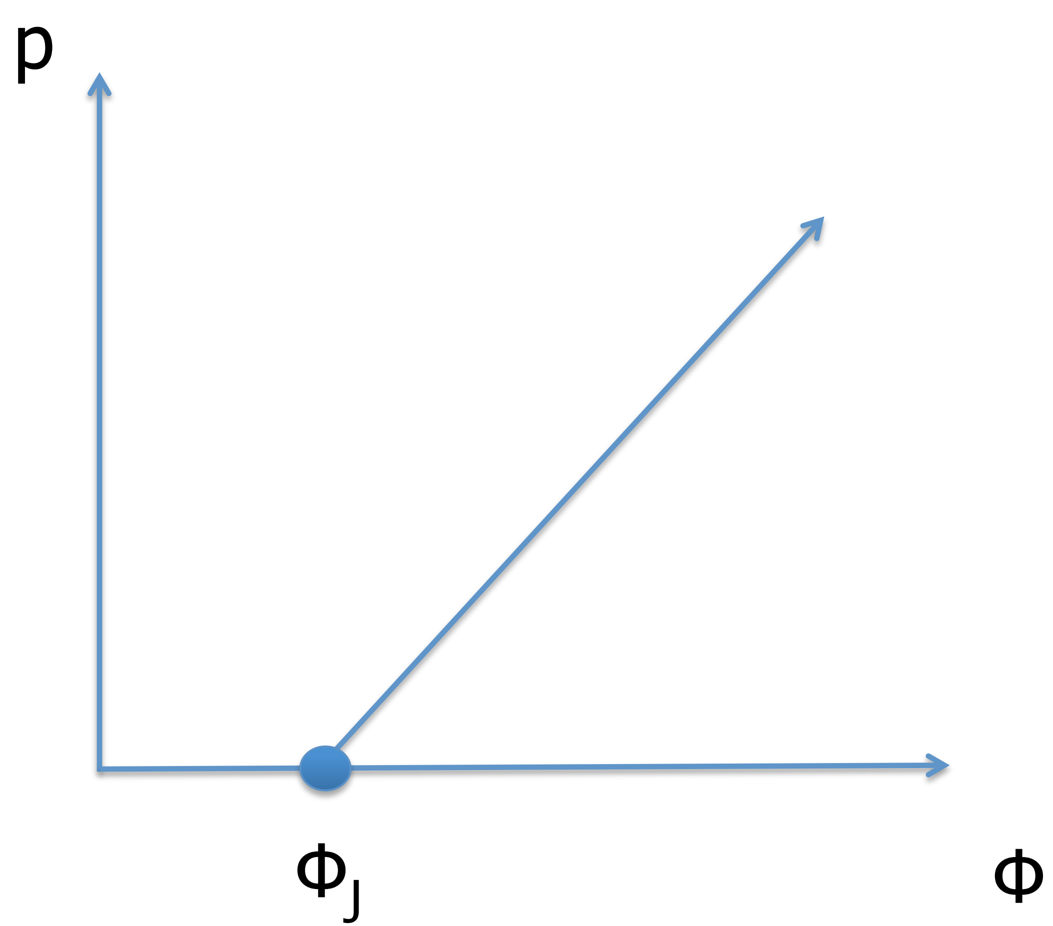

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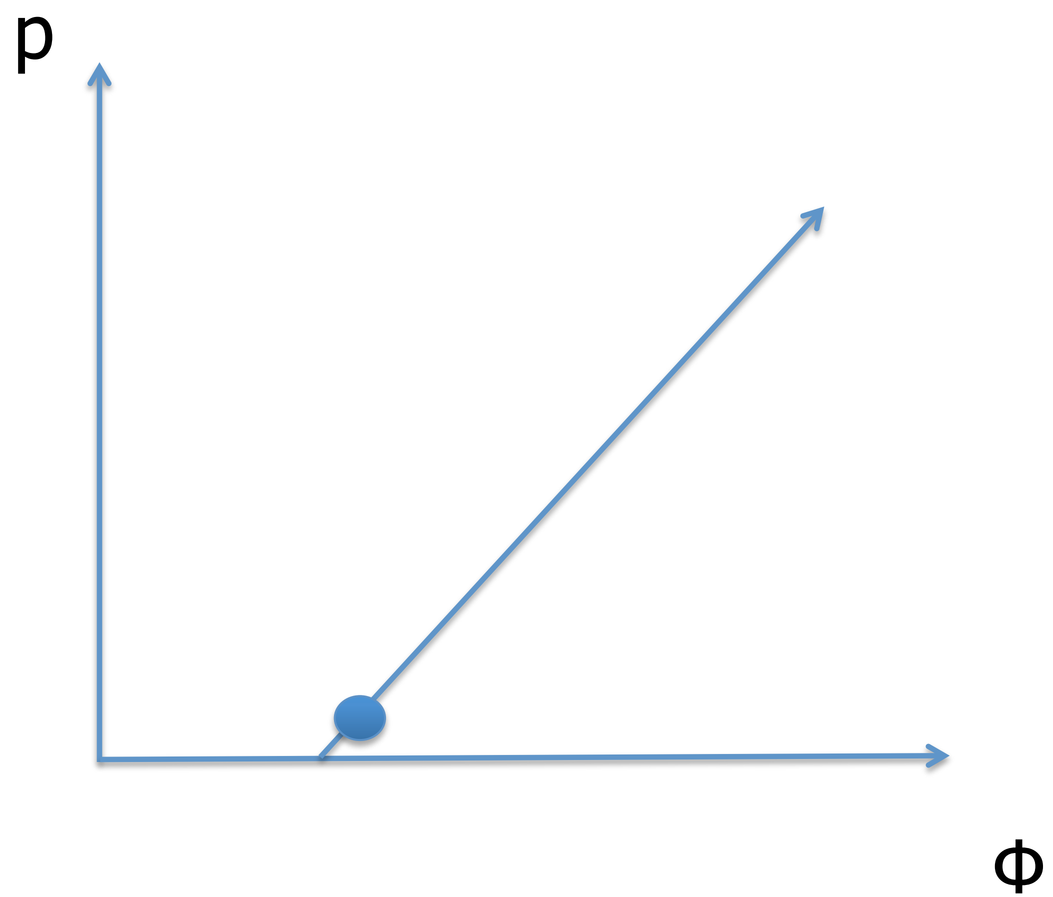

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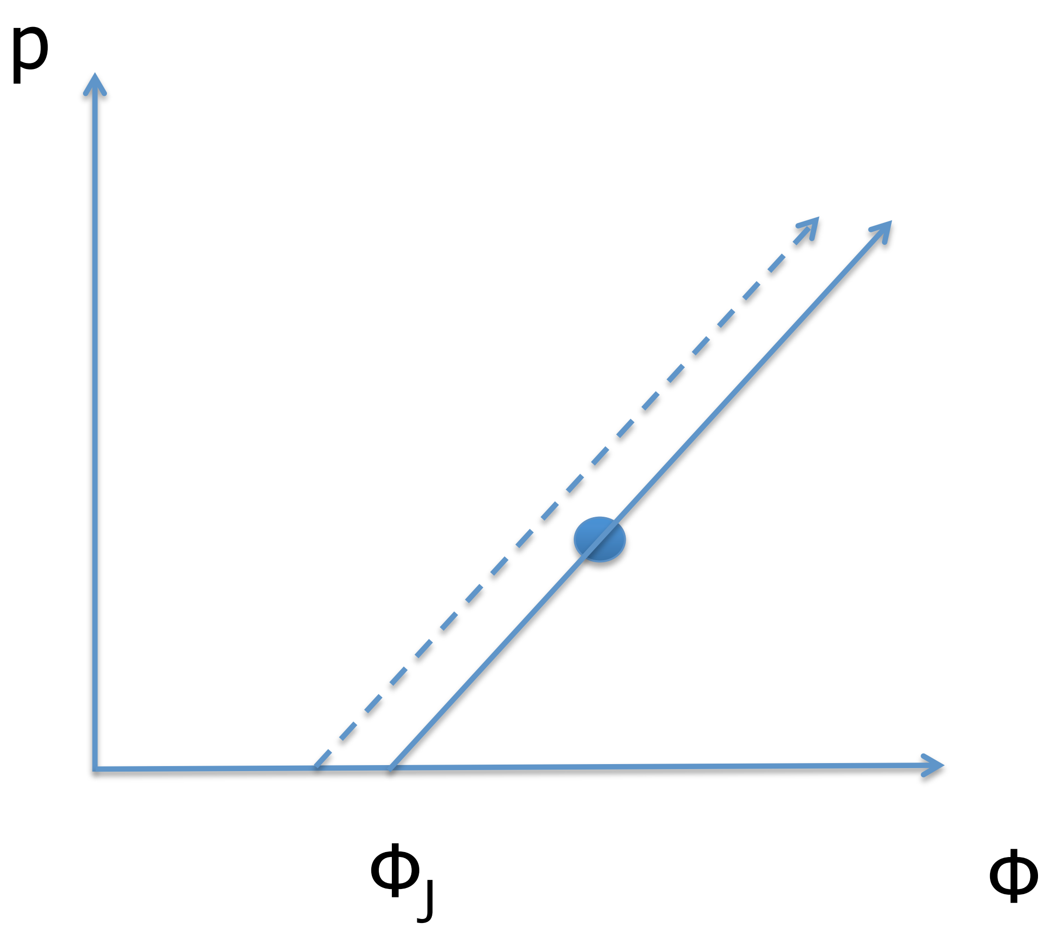

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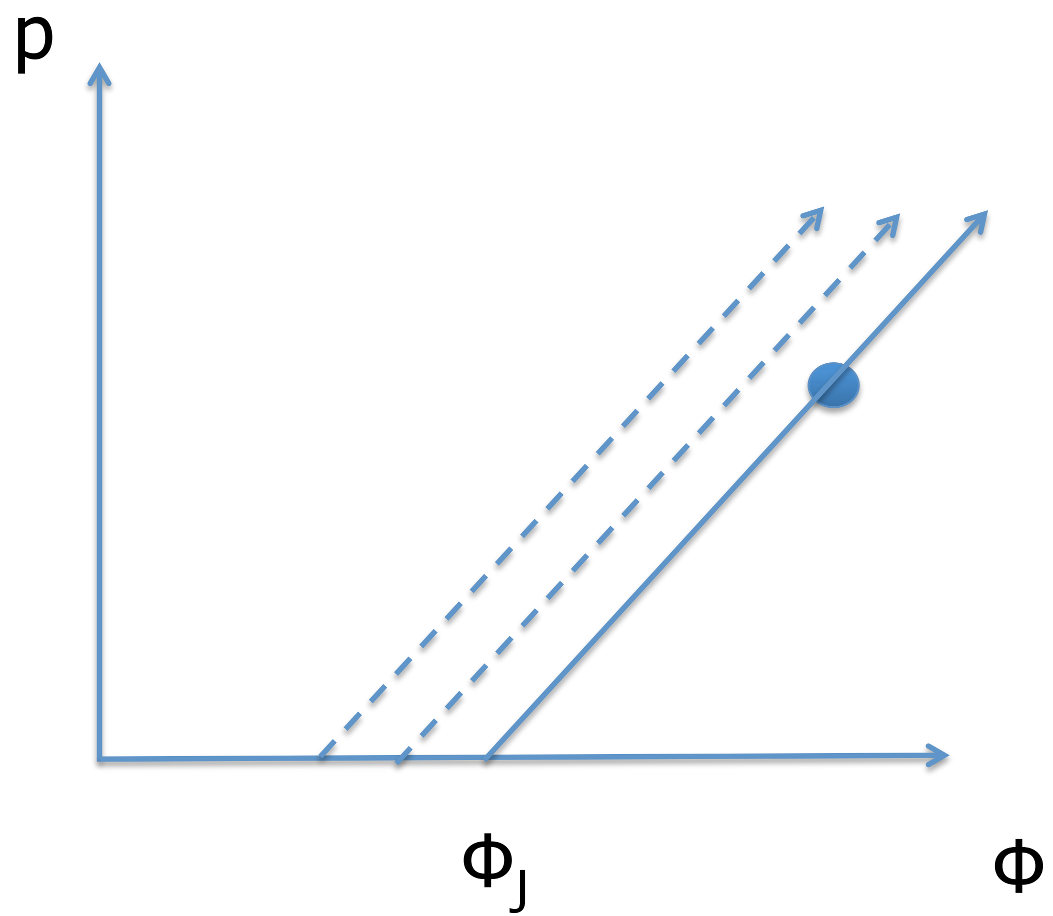

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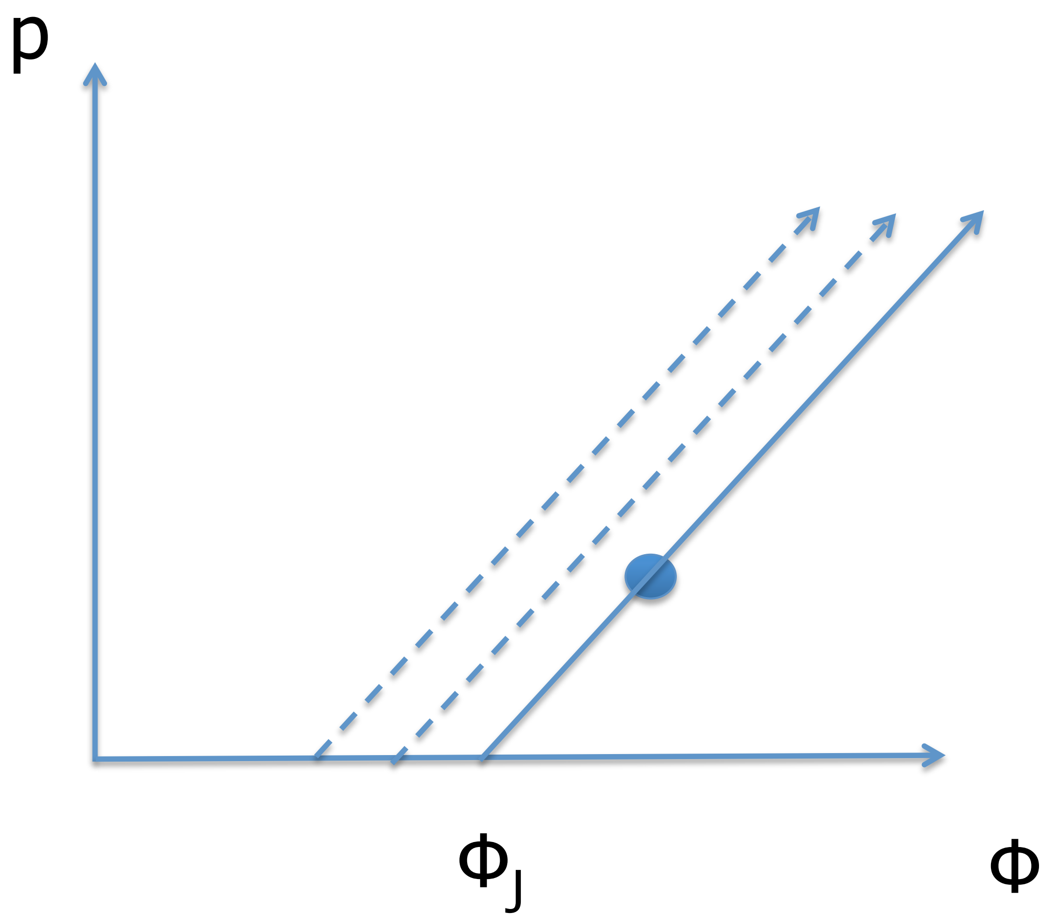
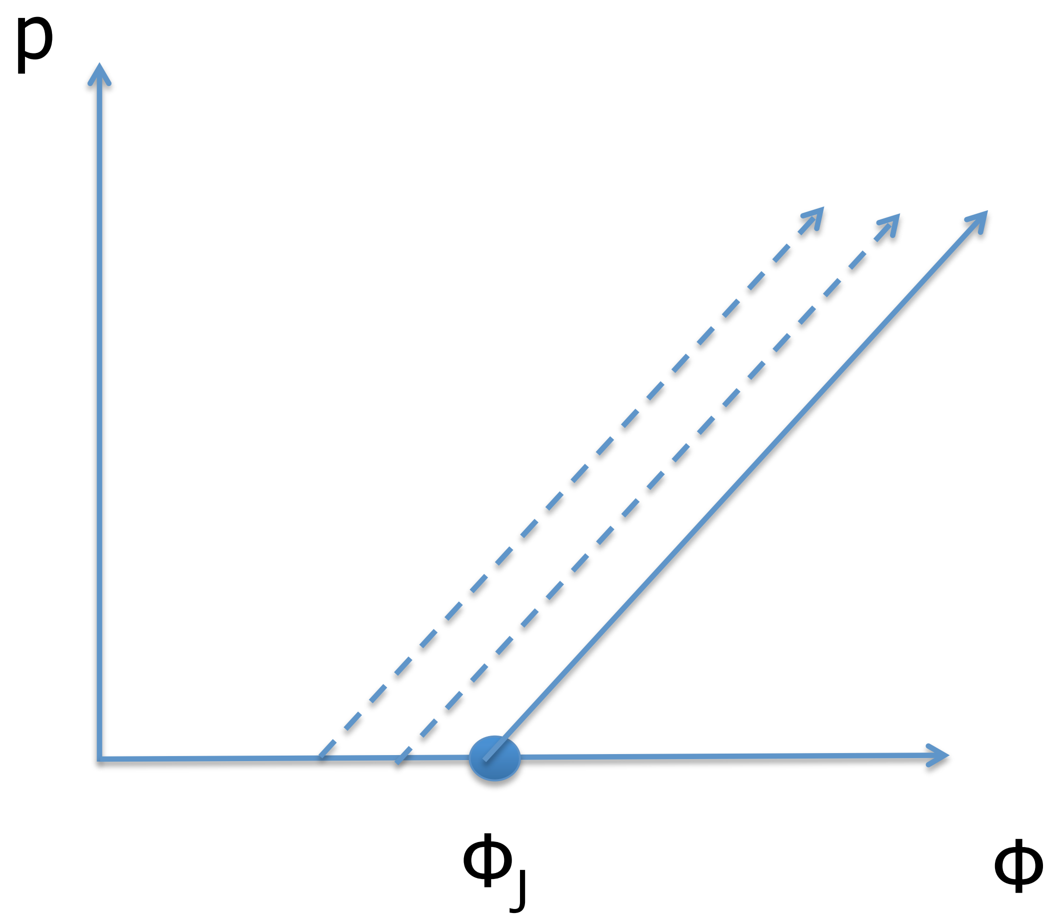
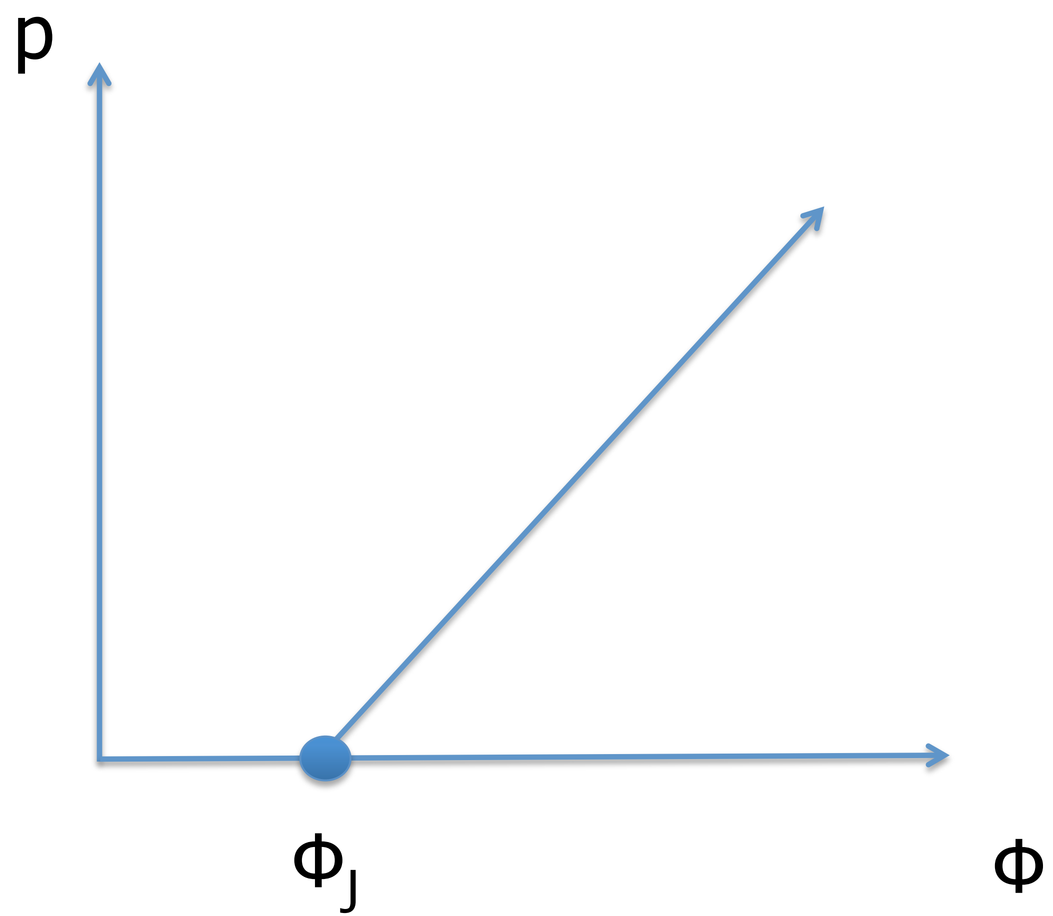


Isotropic (de)compression



Tapping "isotropic"



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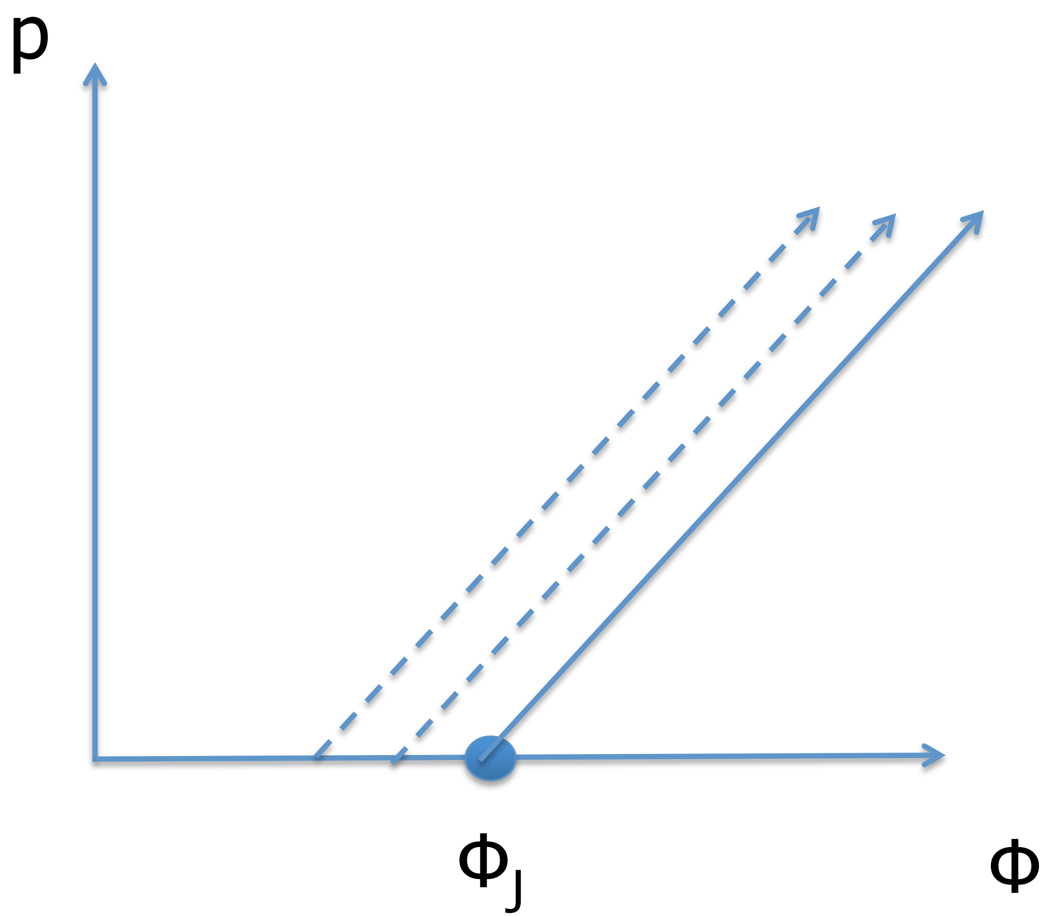
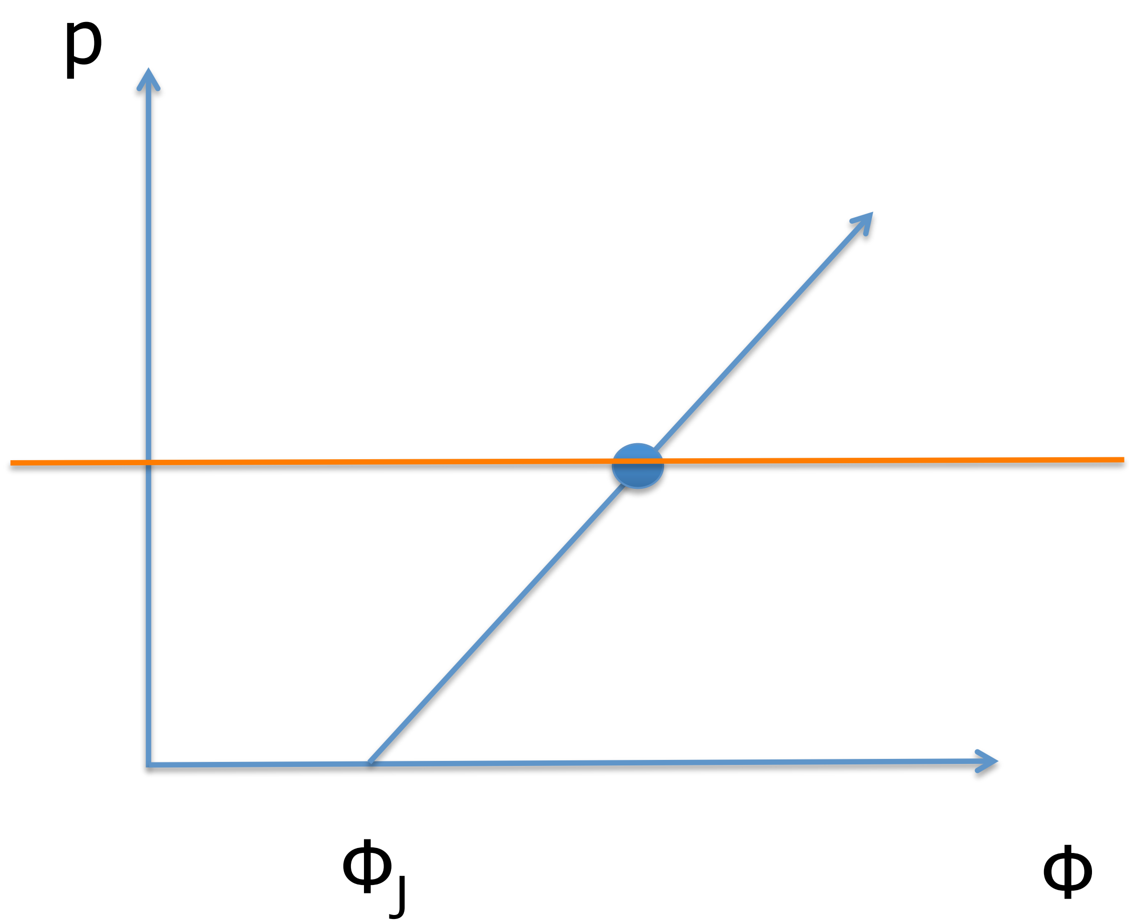


BC “isobaric” + tapping



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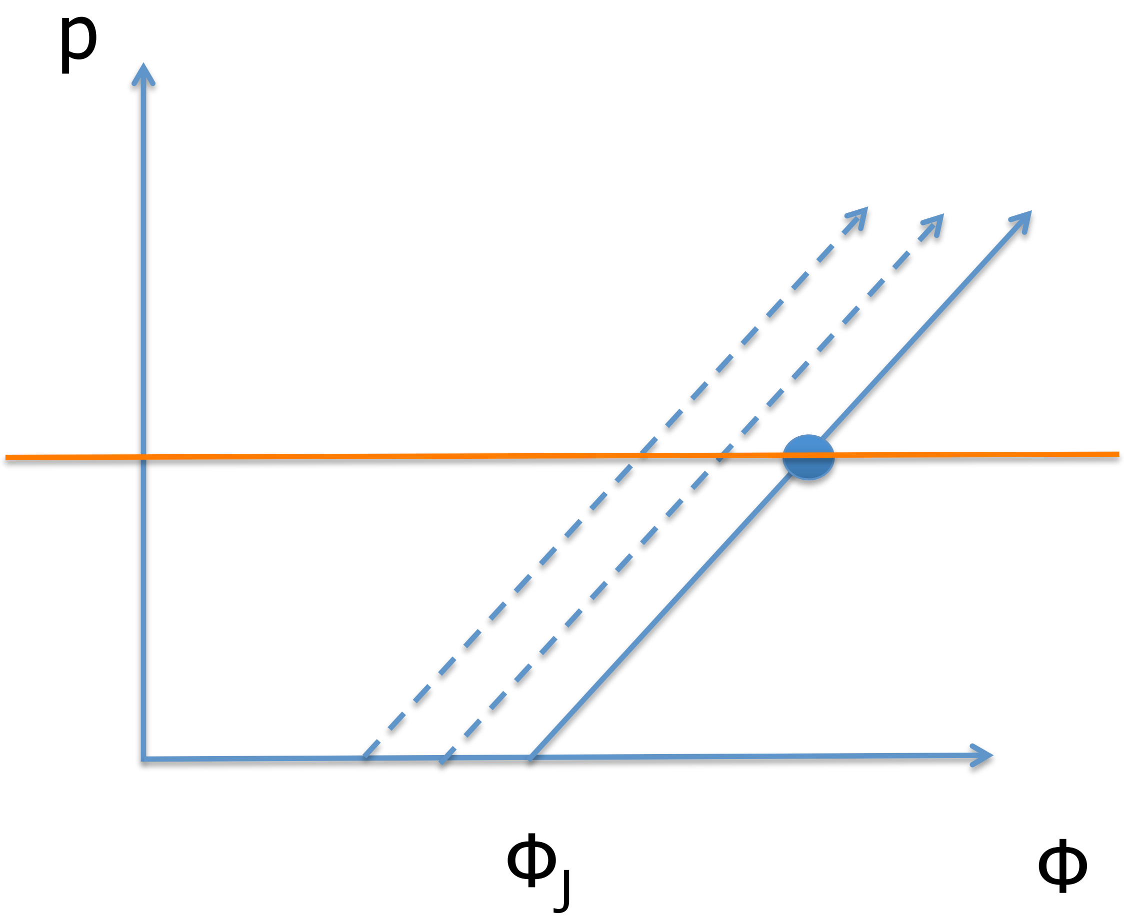
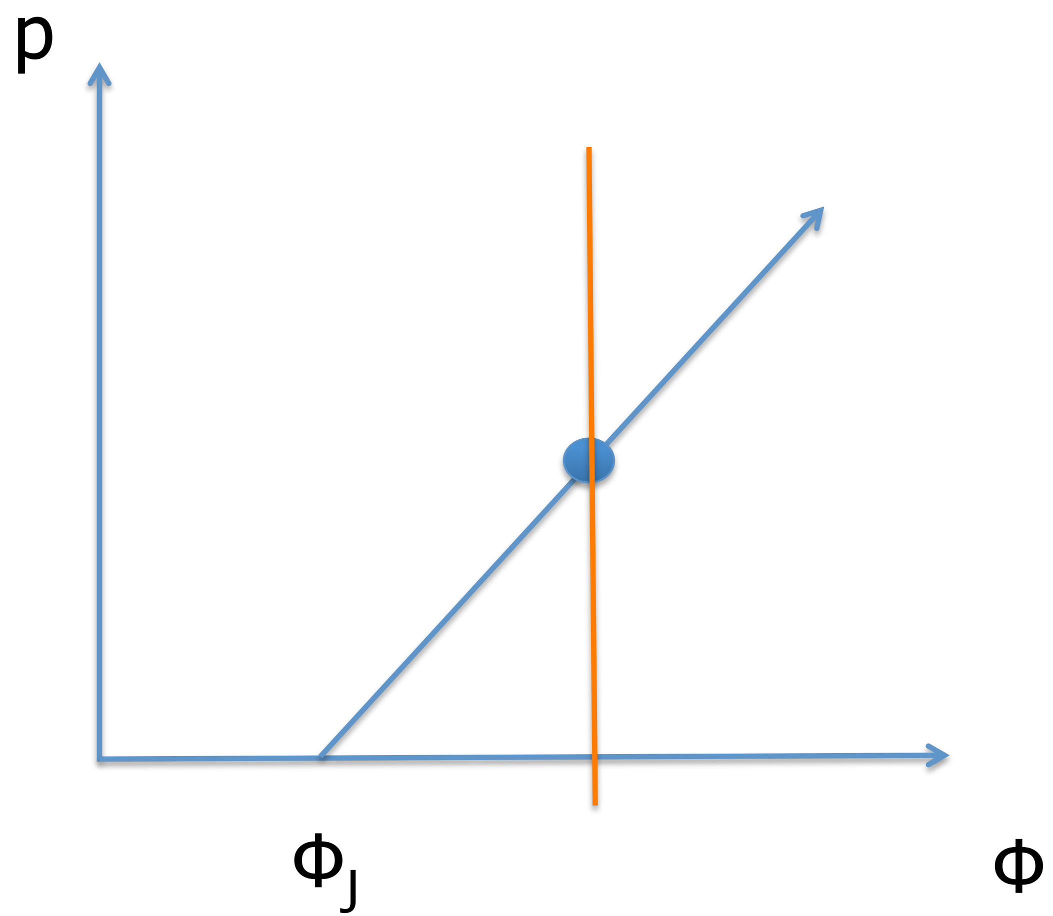


BC "isochoric" + tapping



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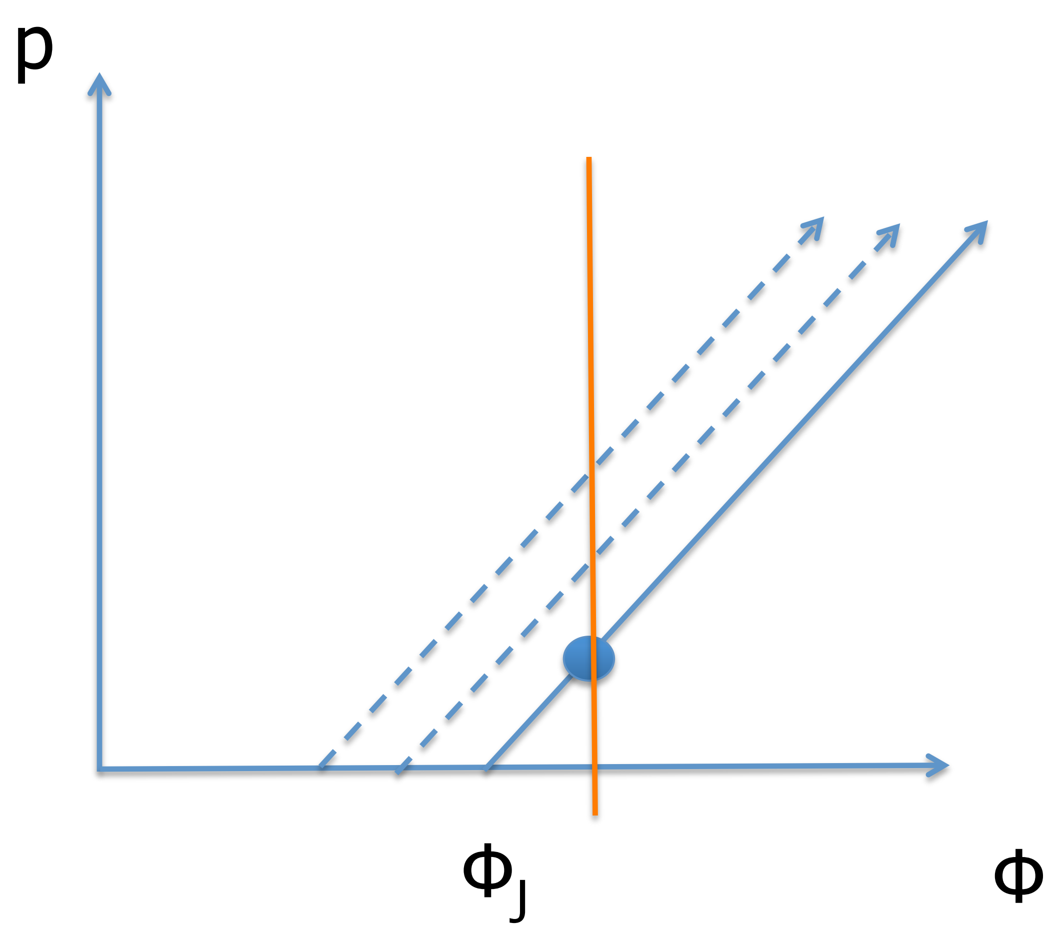
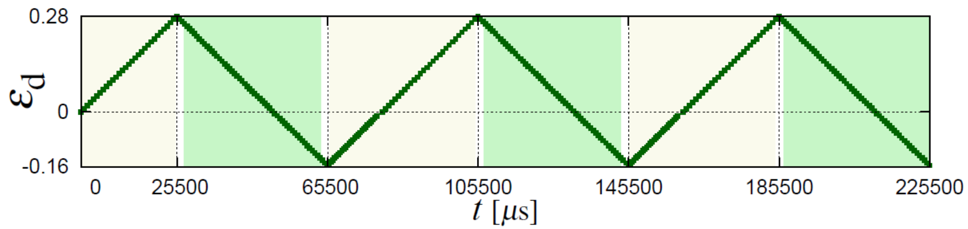


Main Experiment 2 – Shear (volume-conserving)

$$\dot{\mathbf{E}} = \dot{\varepsilon}_{\mathrm{dev}} \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1/2 & 0 \\ 0 & 0 & -1/2 \end{bmatrix}$$

2 => 3 cyclic: see later …



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

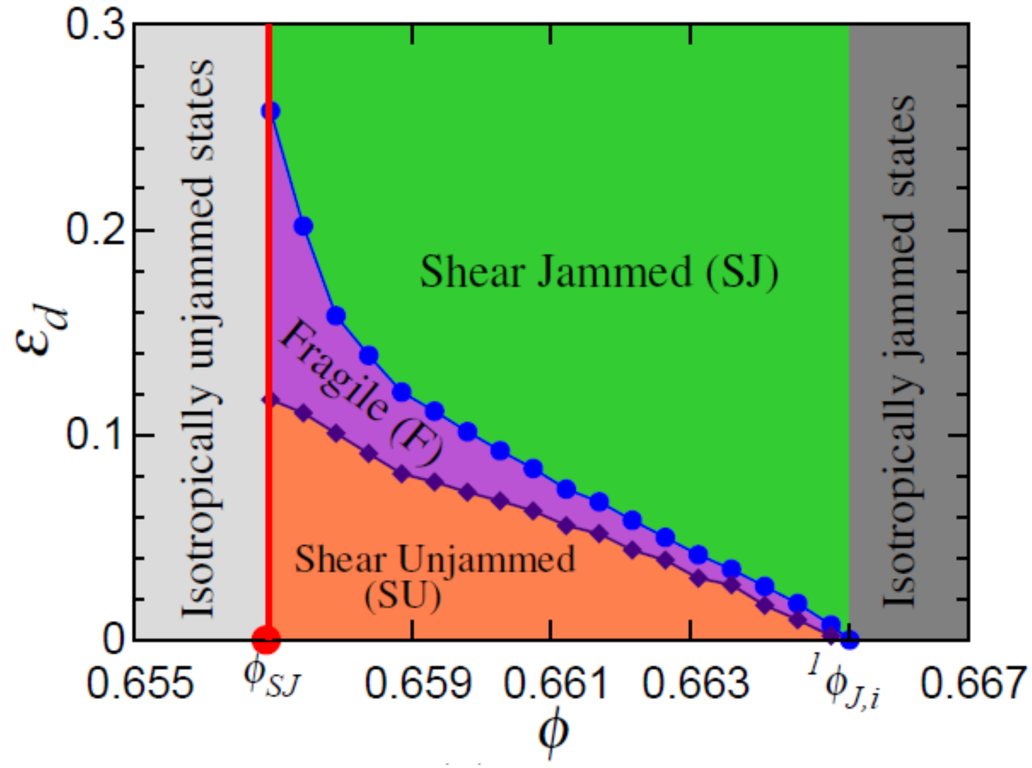
Perform deviatoric (volume conserving) shear deformation to strain 0.28.

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?

Message 2

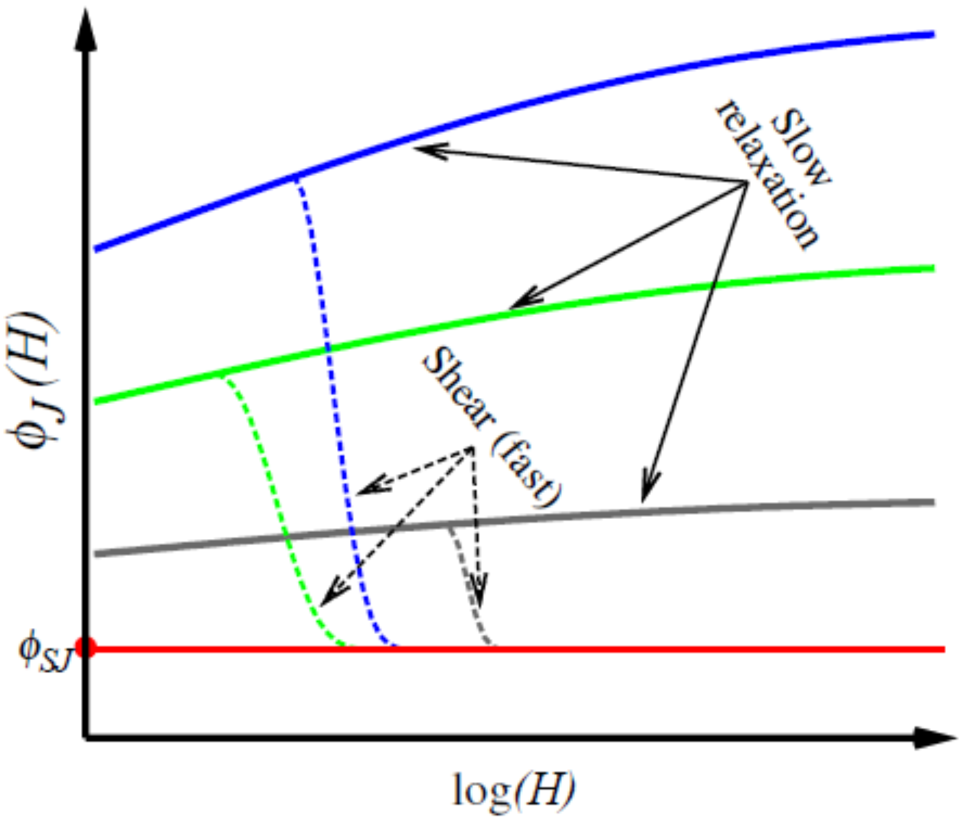
response of **microstructure** to **isotropic deformations**!

- a new state variable is needed!
- isotropic deformation leads to an increase of Φ_J (slow)

response of **microstructure** to **deviatoric/shear deformations**!

- no new state variable is needed!
- deviatoric deformation leads to a decrease of Φ_J (fast)

Connecting the two Experiments



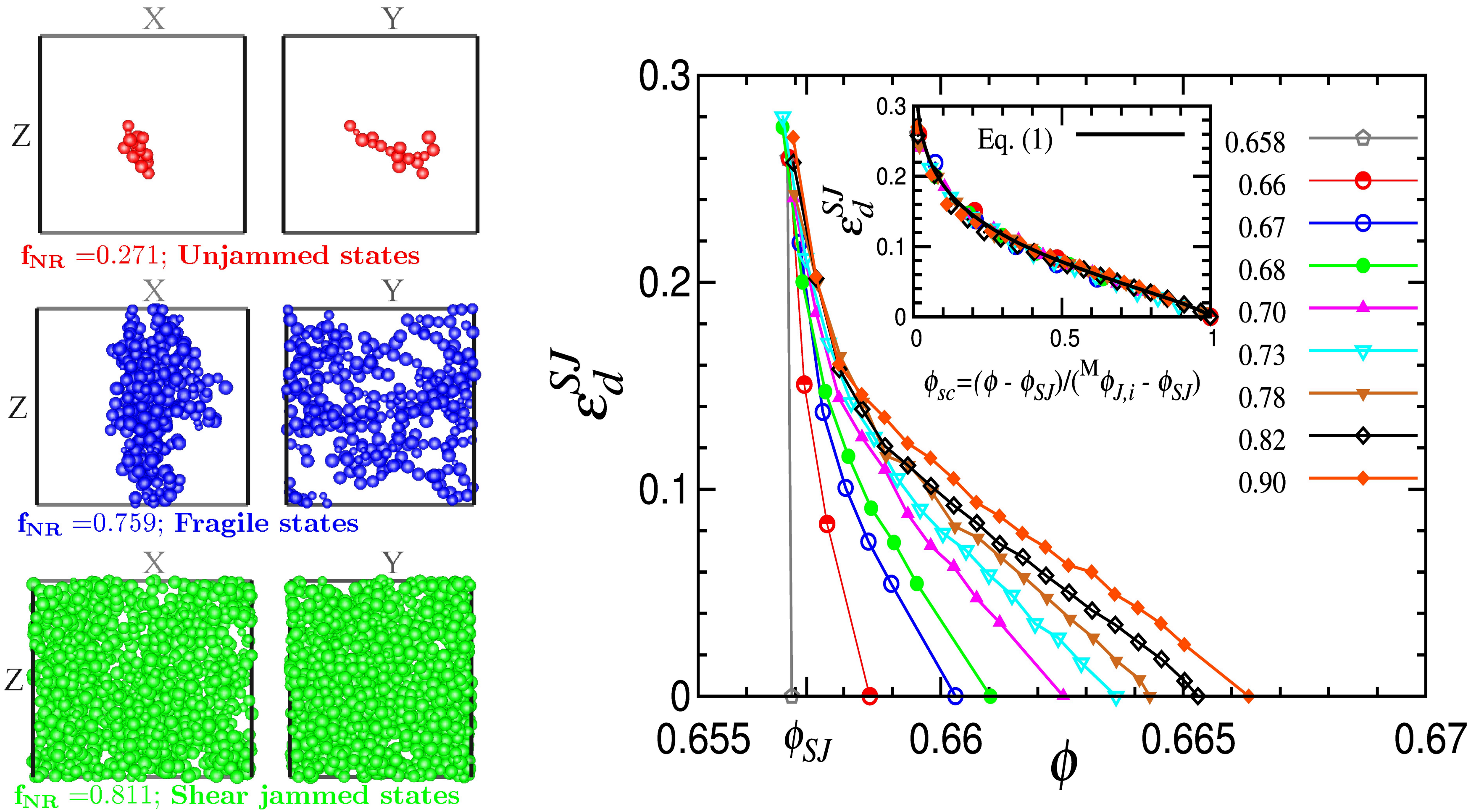
- Combining the two history-dependencies,
  by superposing the two limit experiments: isotropic and pure shear deformation.
- Rate of increase in the jamming point by isotropic deformation
  is much slower than the rate of decrease by pure shear.
- Ultimate lower bound, defined as the shear-jamming density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

Main Experiment 2.5 – Shear (volume-conserving)

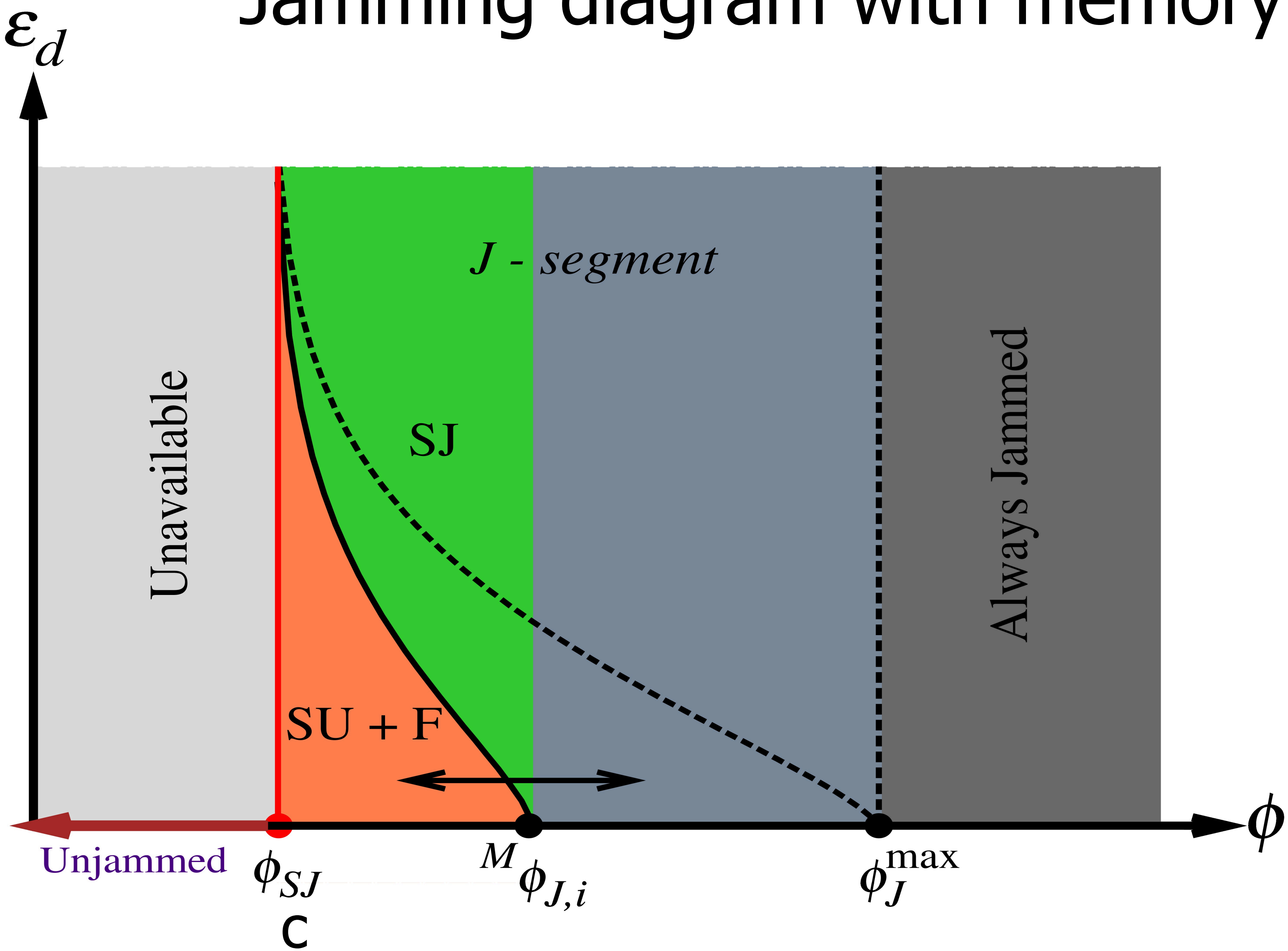
How to measure the shear strain needed to jam the system, based on different history.

-Using percolation method (when strong force chain is percolated through the whole system)

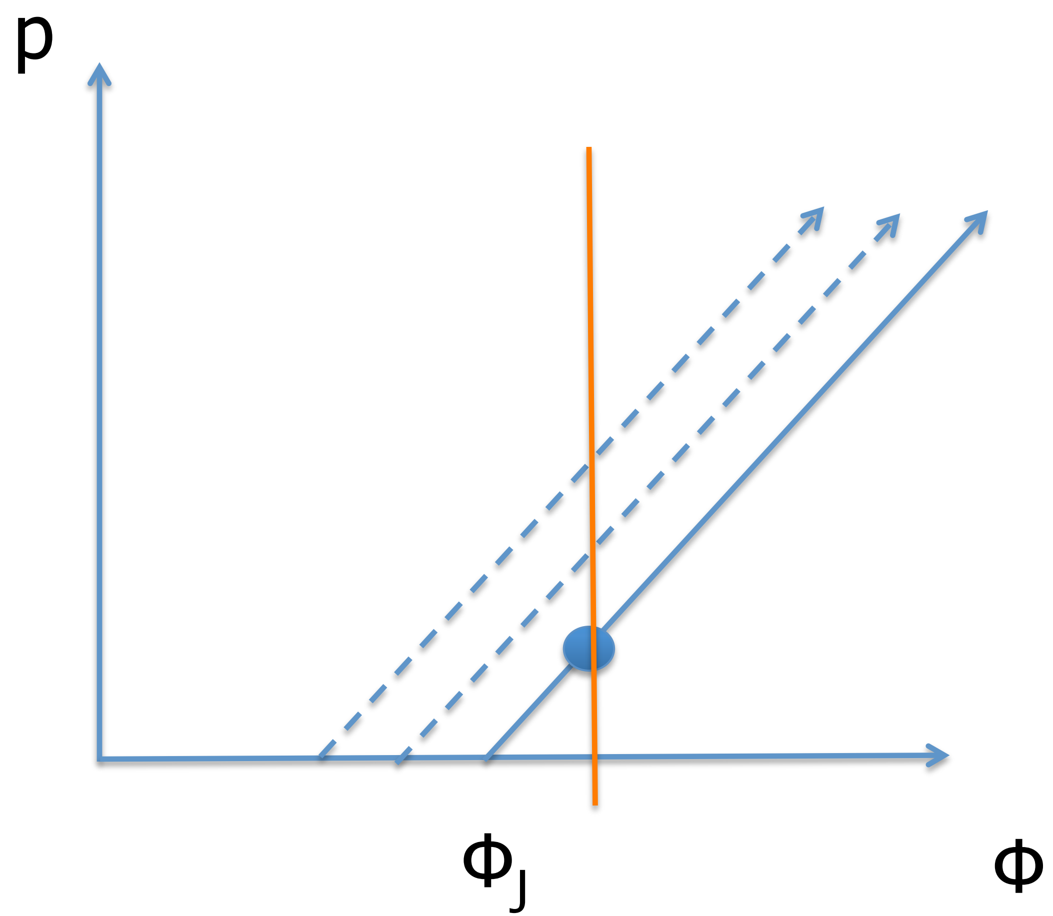
Jamming by application of shear



Jamming diagram with memory



BC "isochoric" shear



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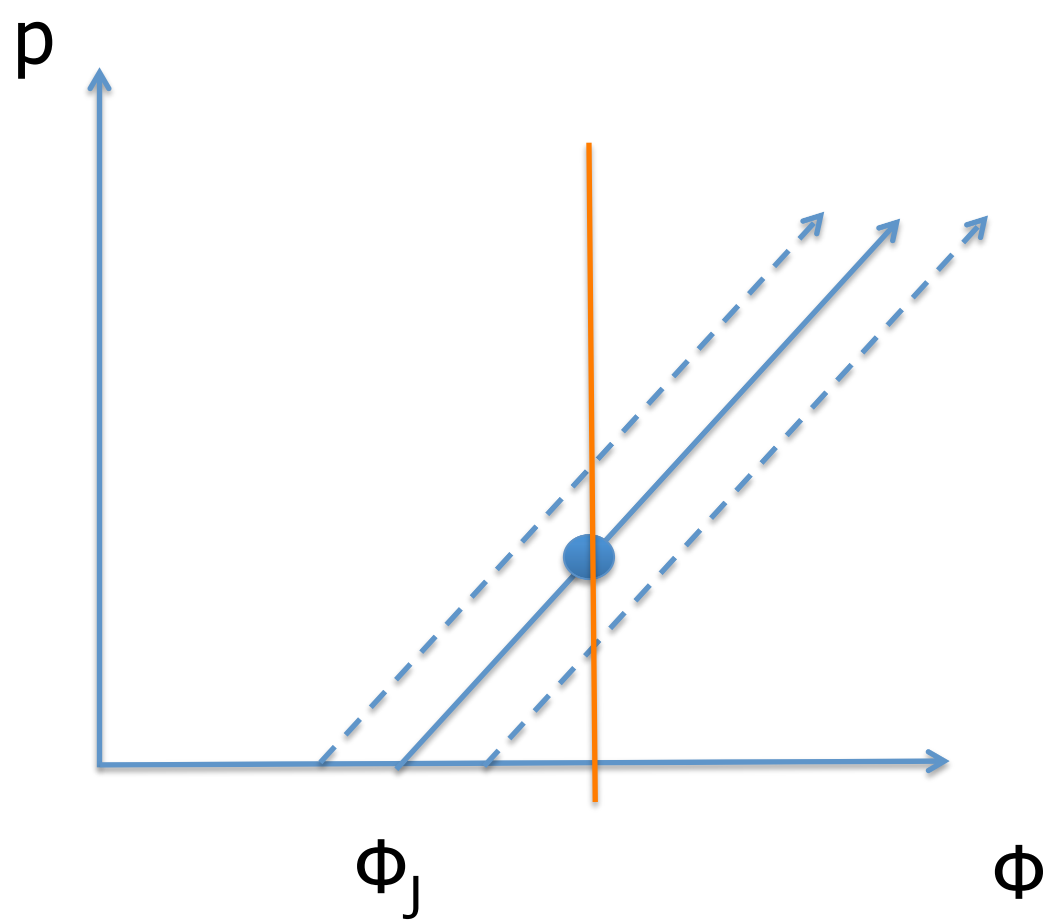
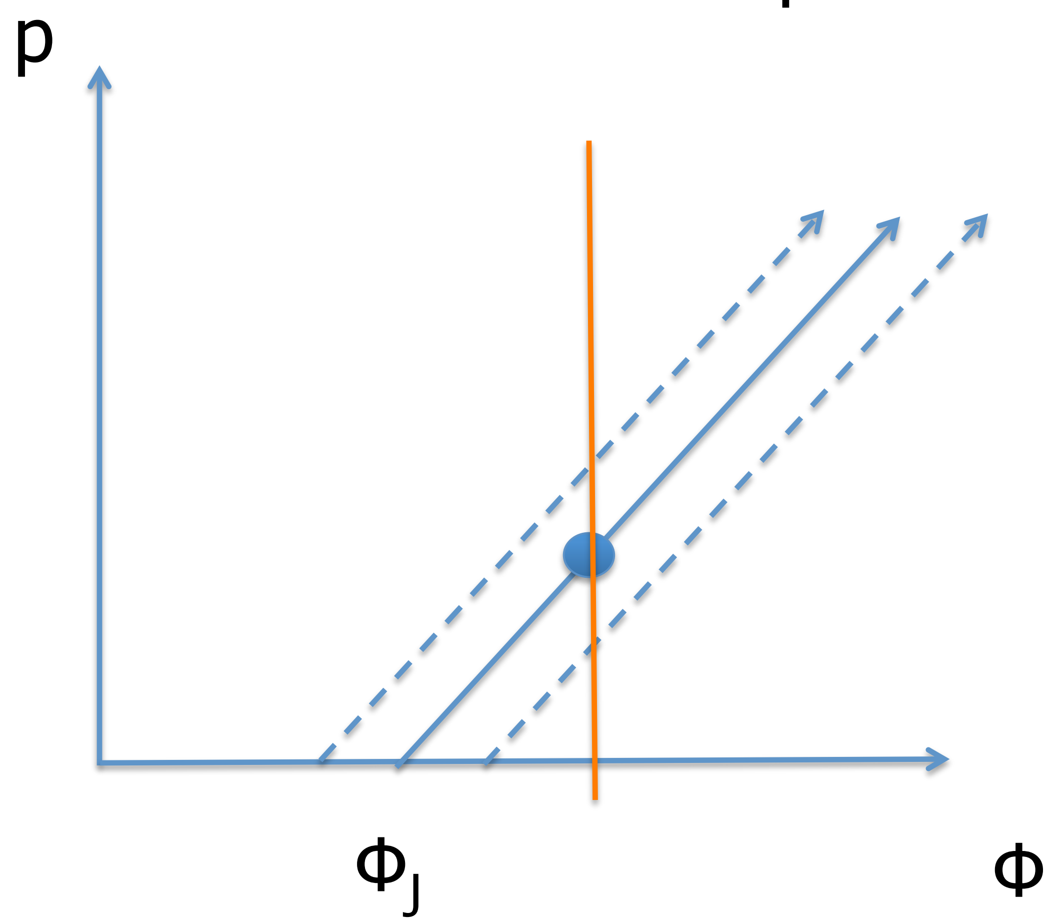


BC "isochoric" shear

i.e. pressure-dilatancy



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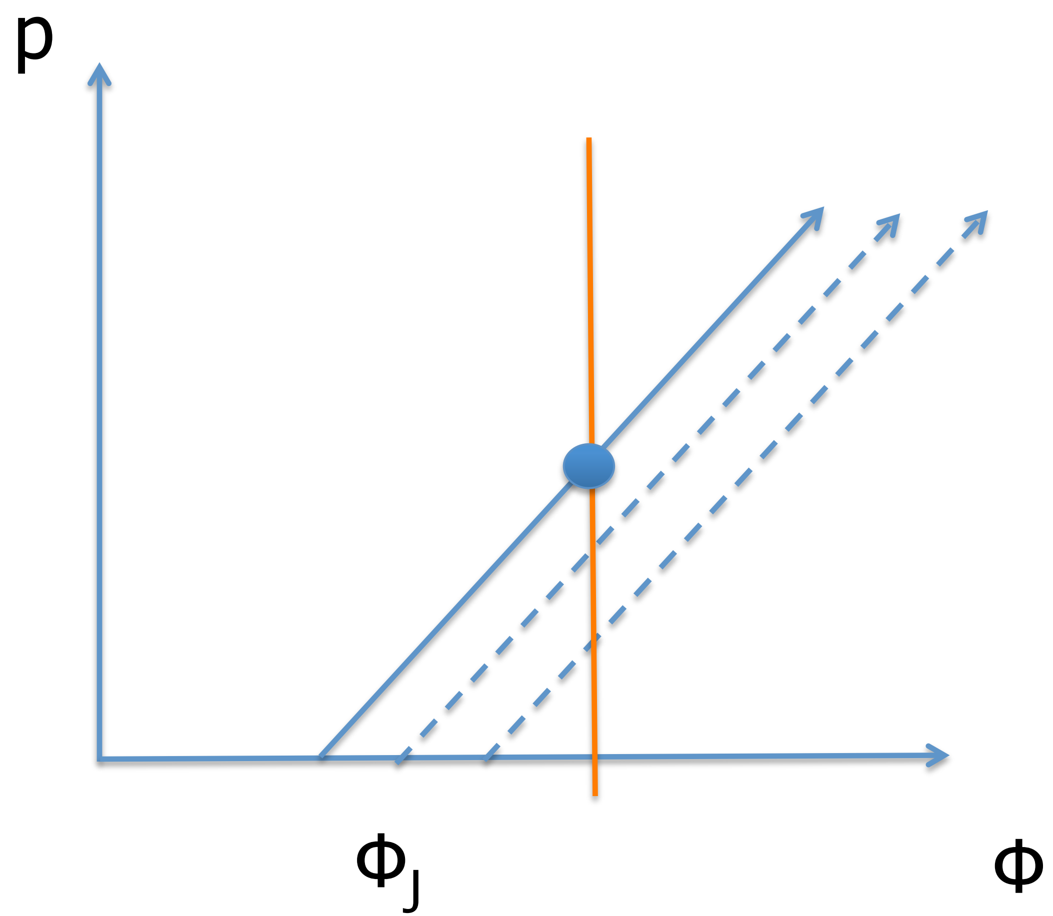
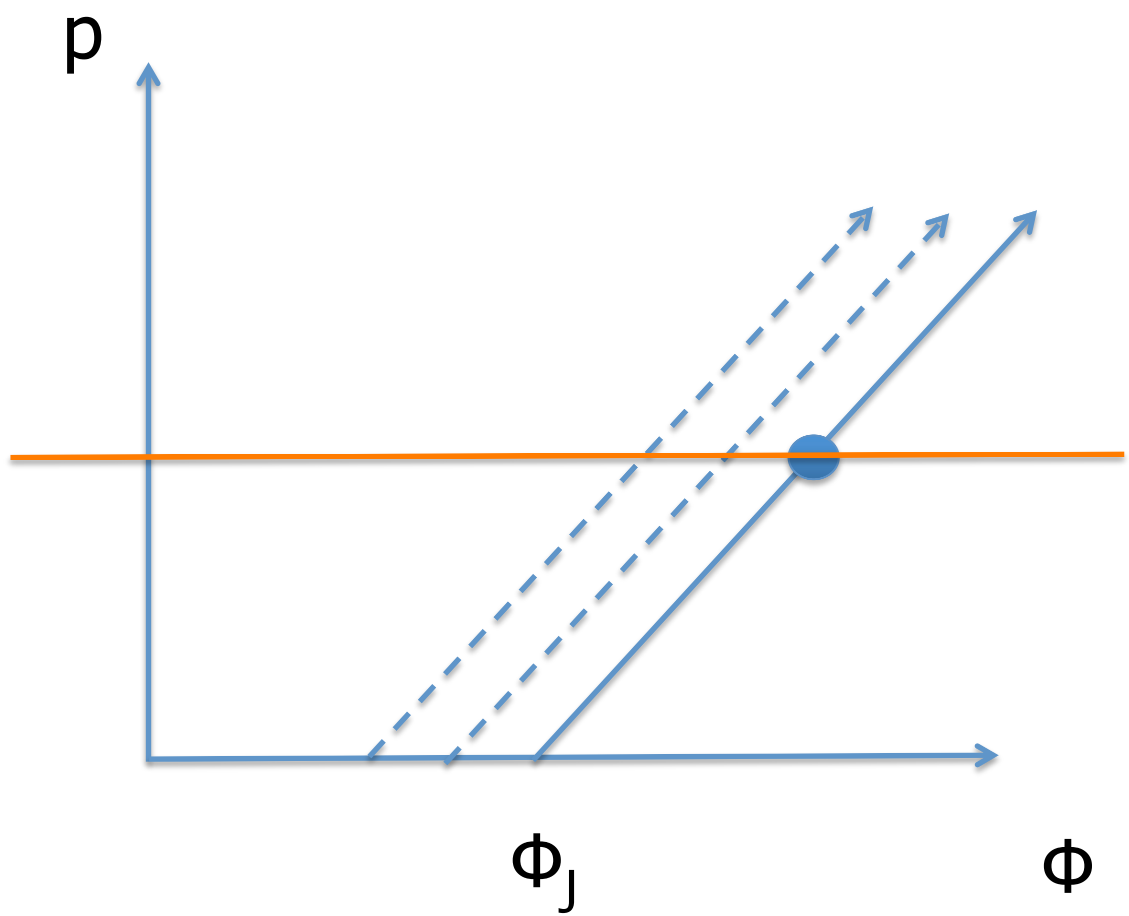
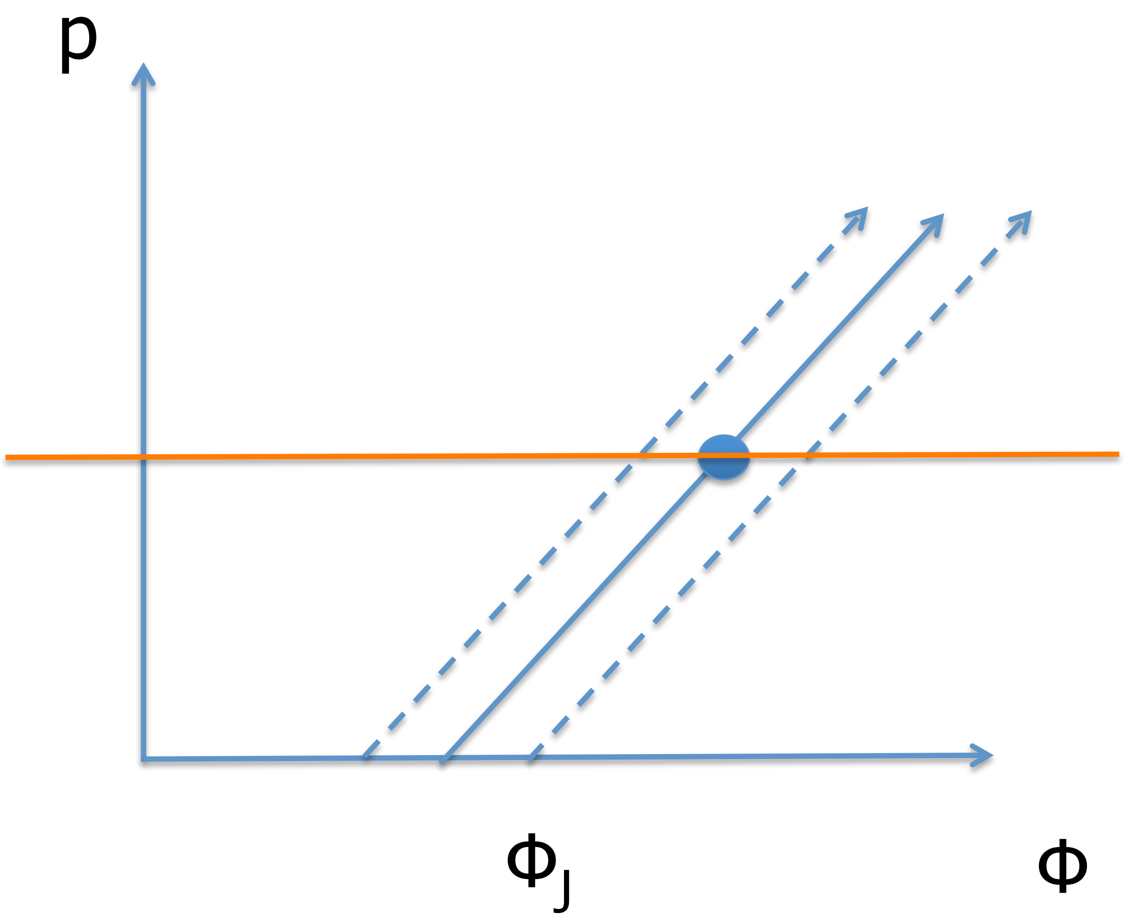


BC “isobaric” shear



BC "isobaric" shear



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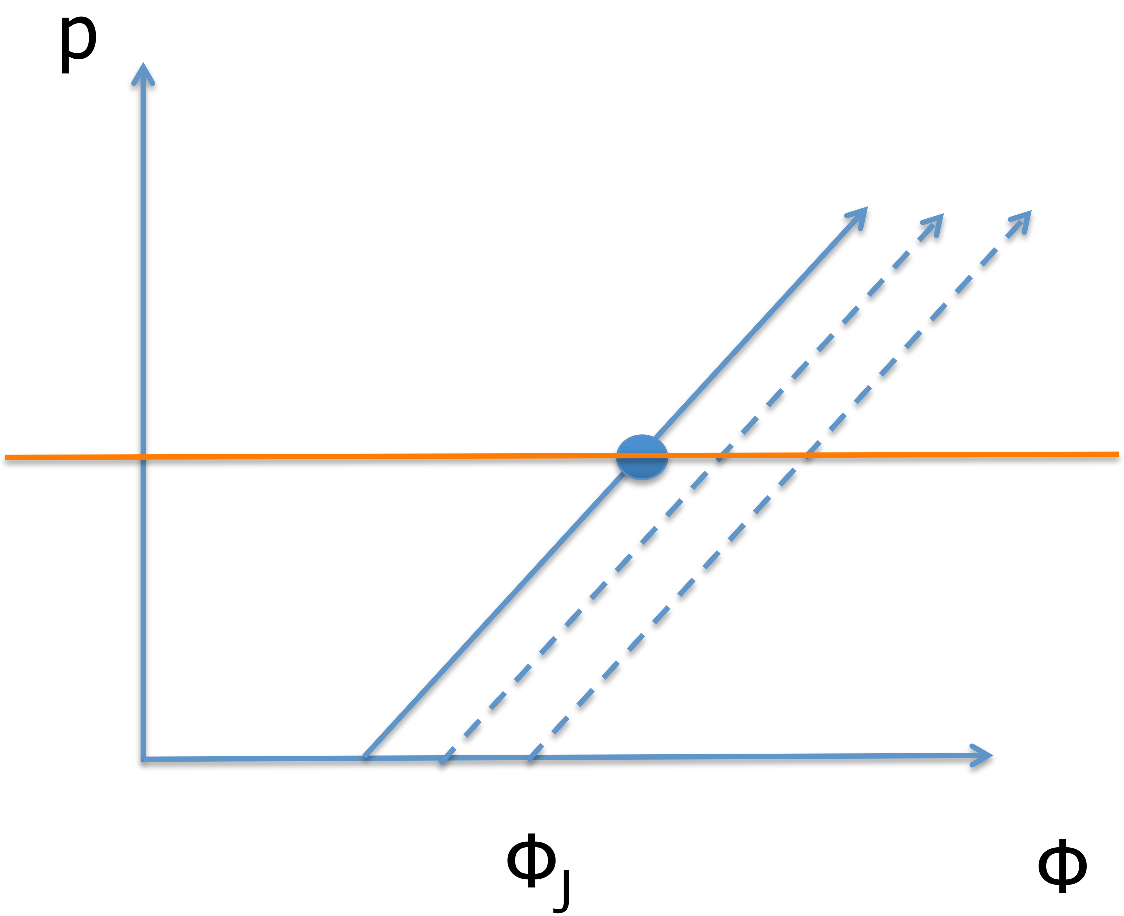

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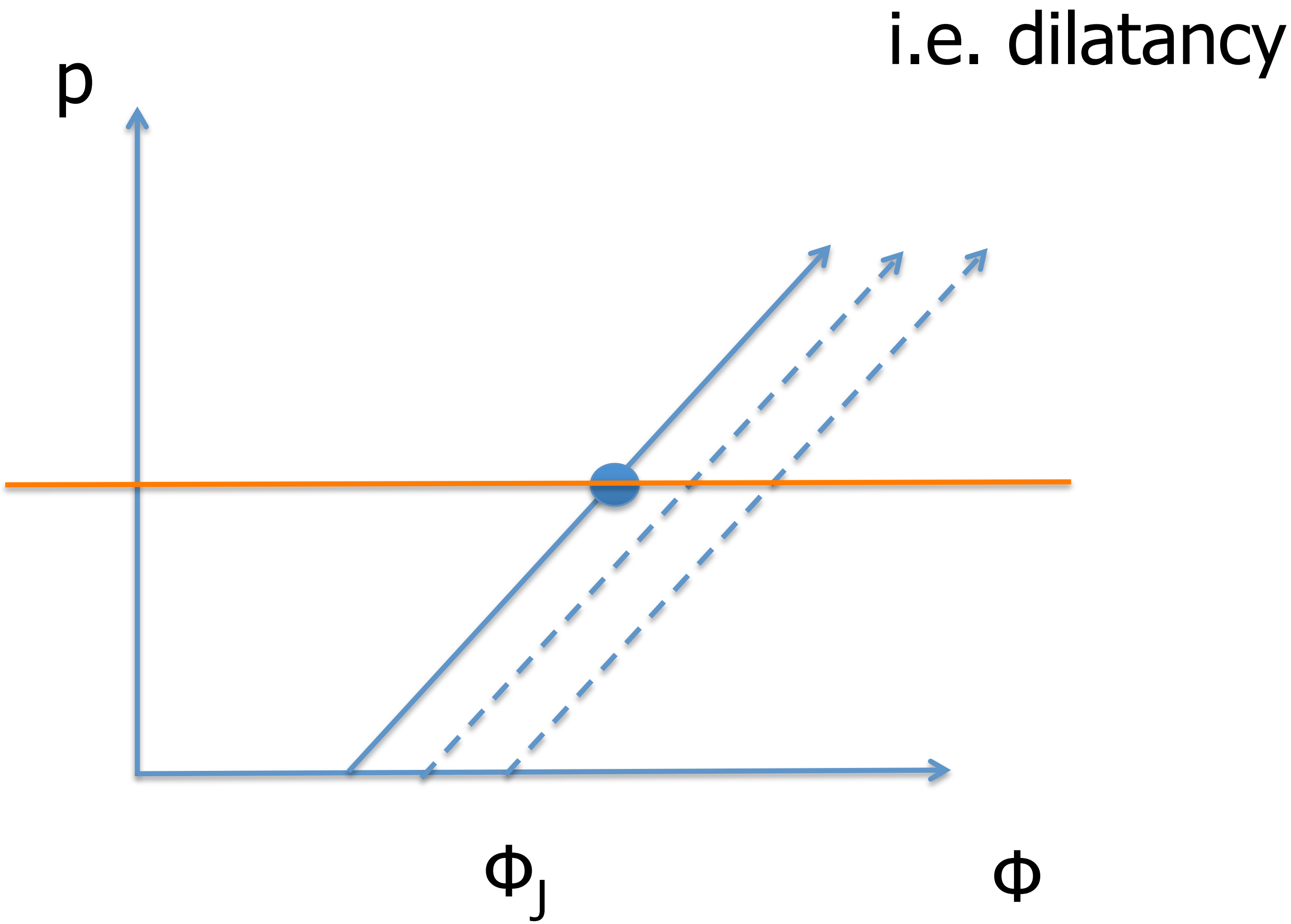
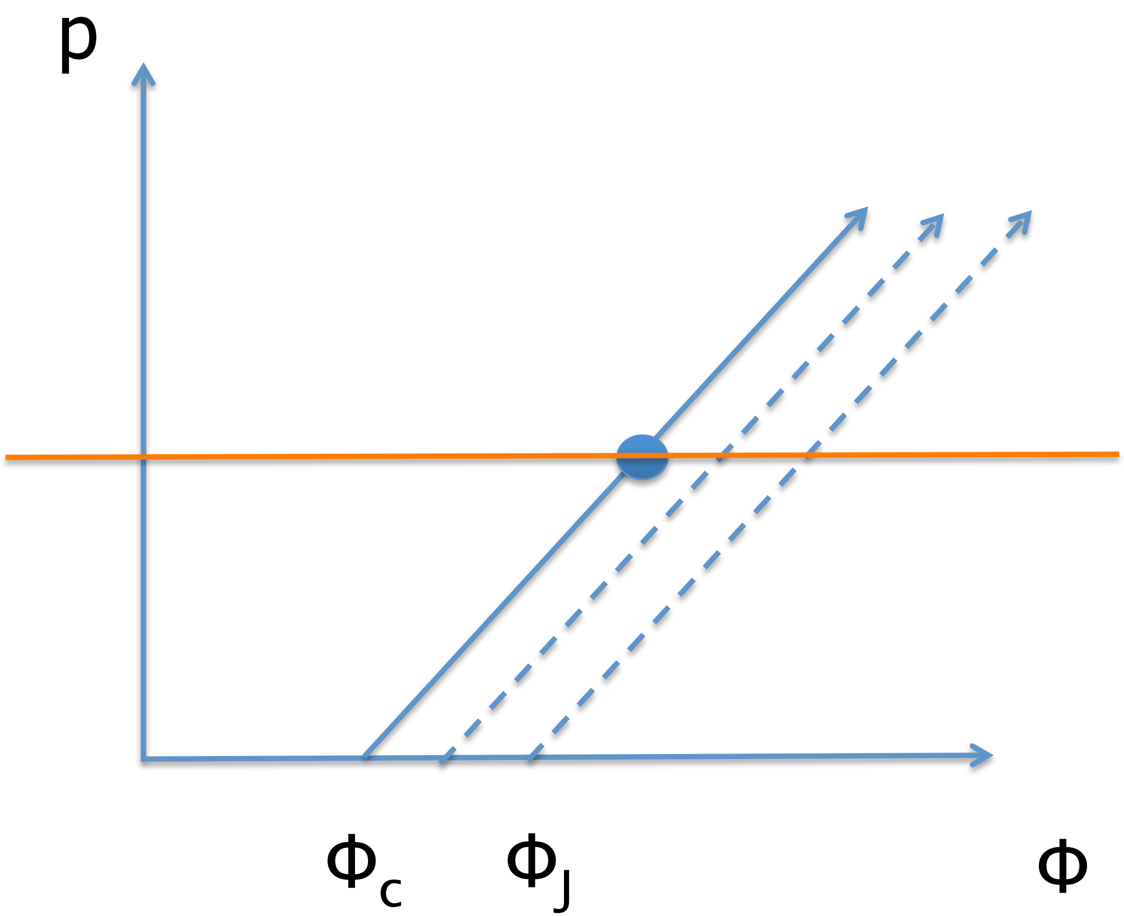
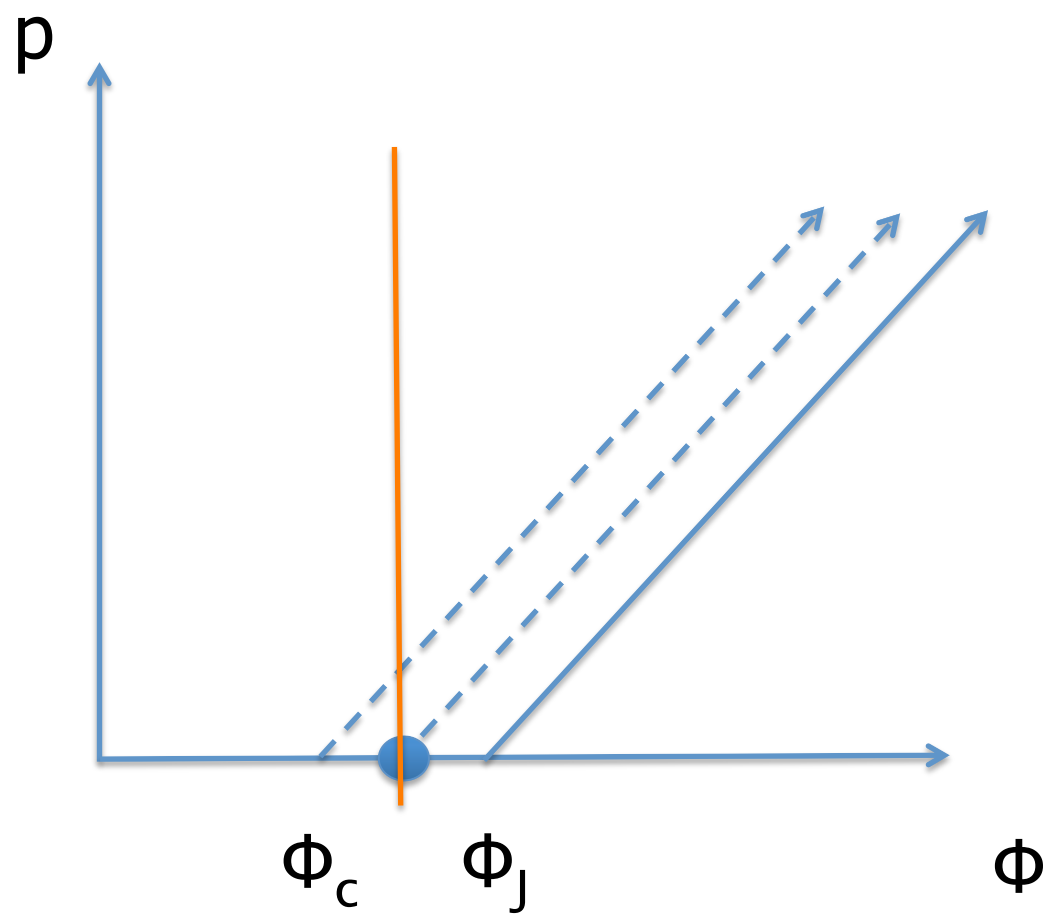


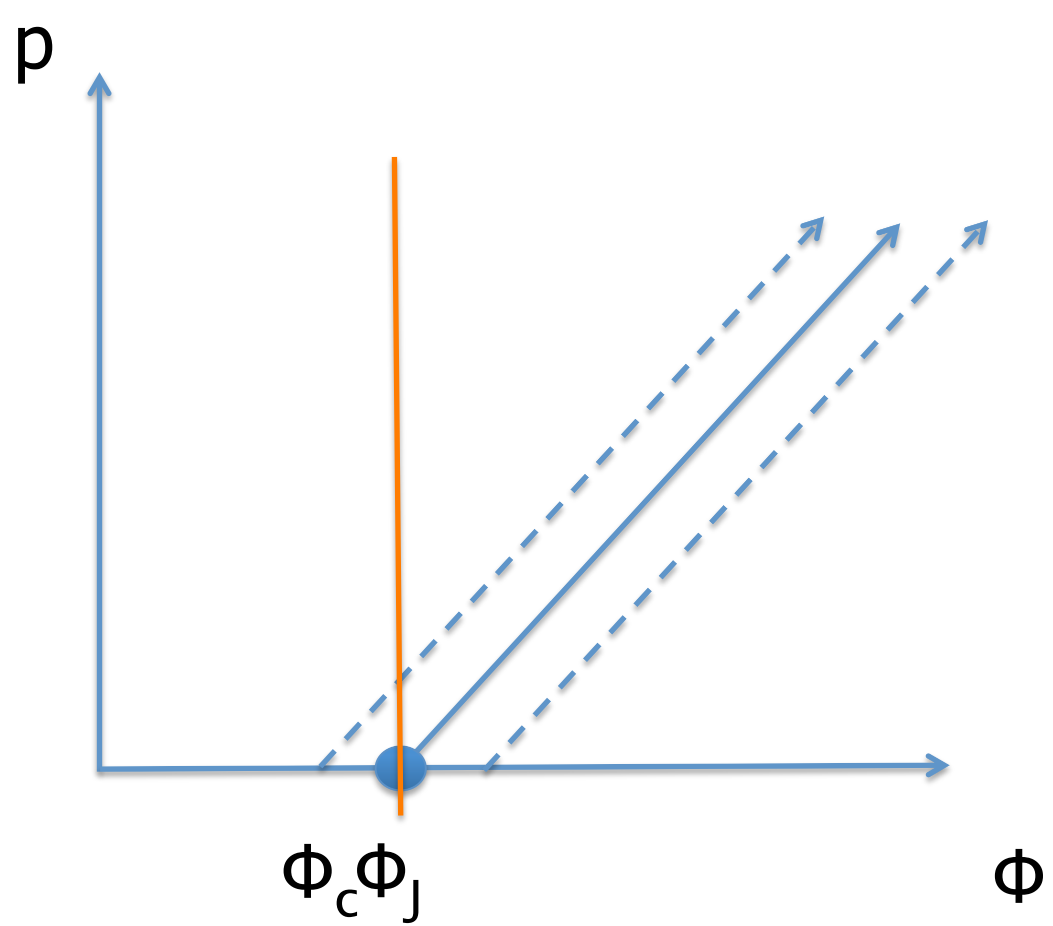
BC "isobaric" shear



BC "isochoric" shear-jamming



BC "isochoric" shear-jamming



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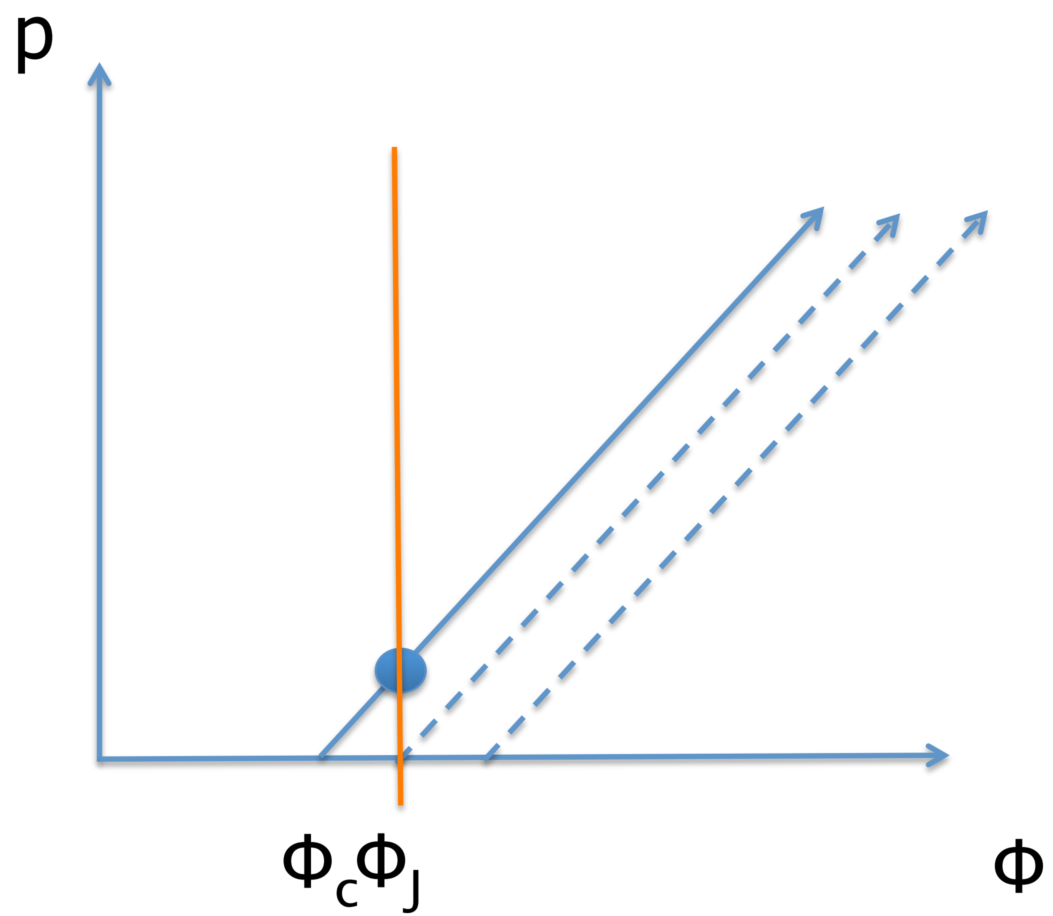
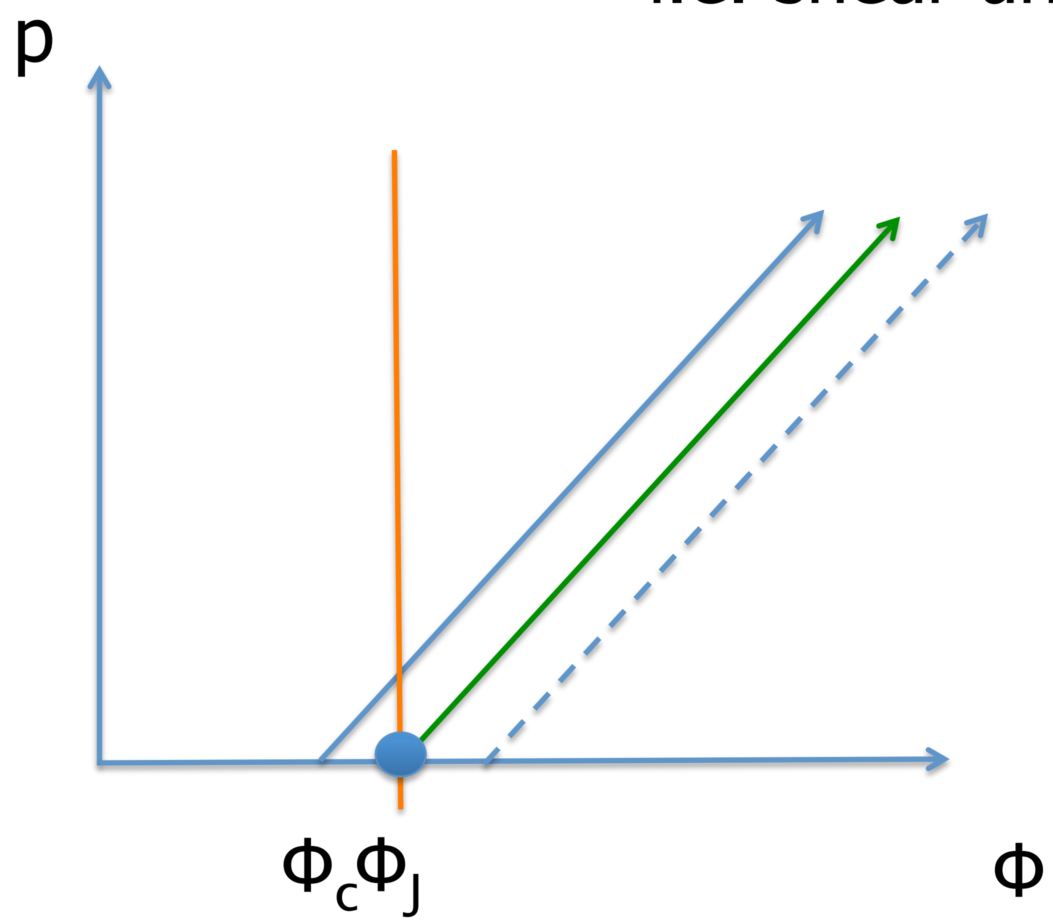
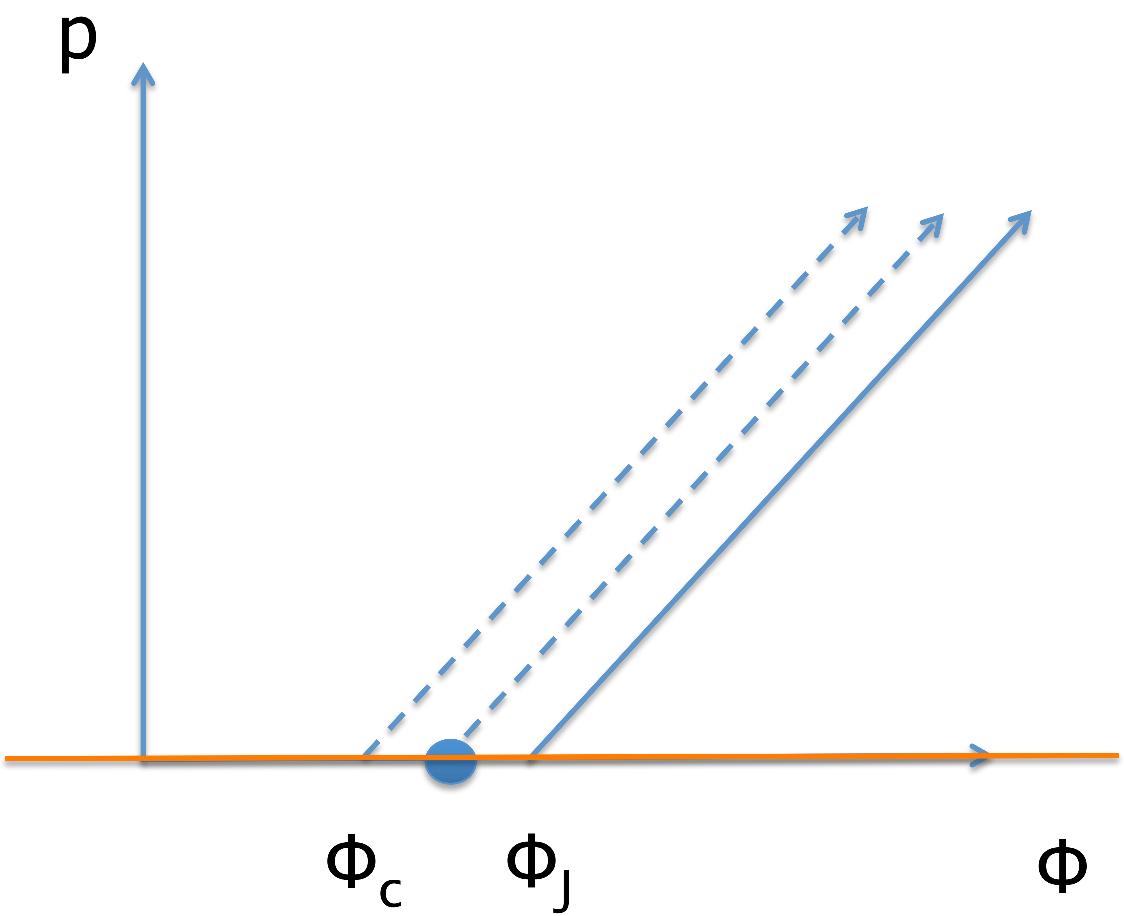


BC “isochoric” shear-reversal

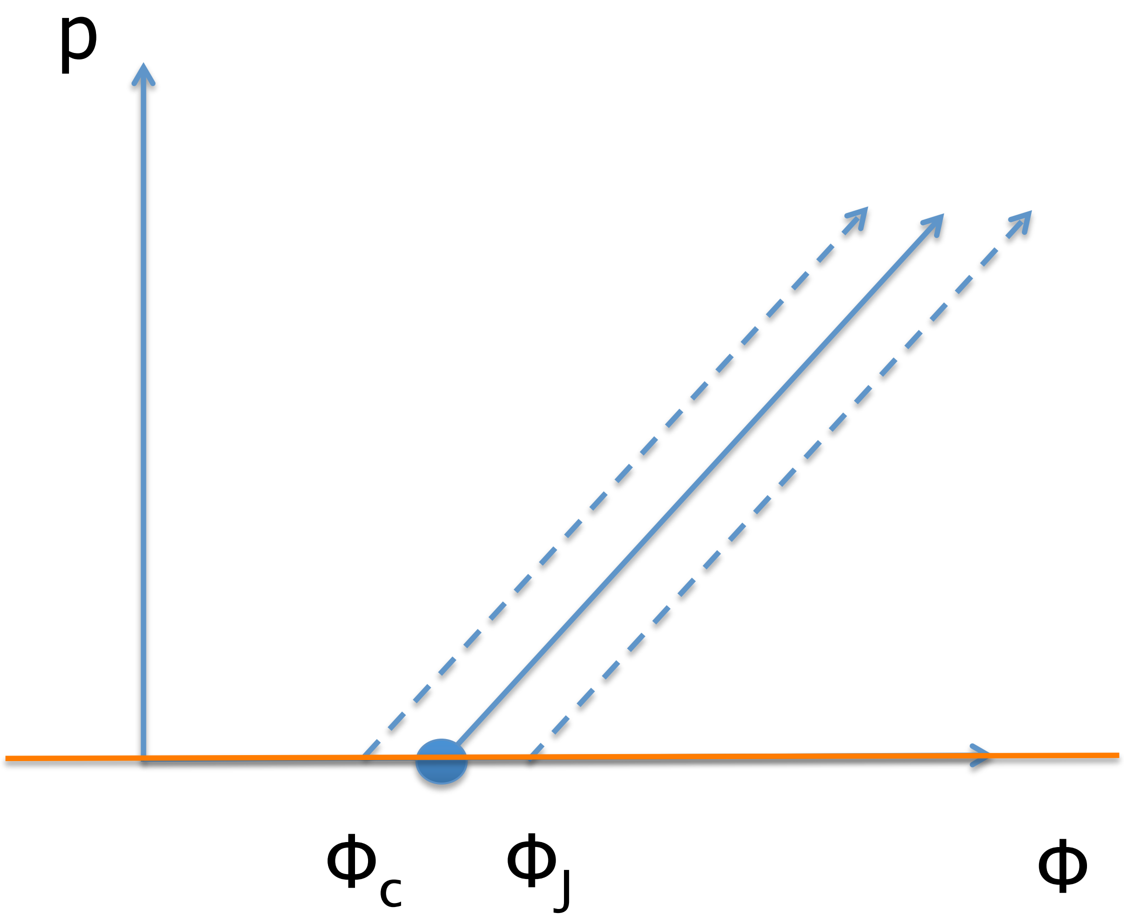
i.e. shear un-jamming



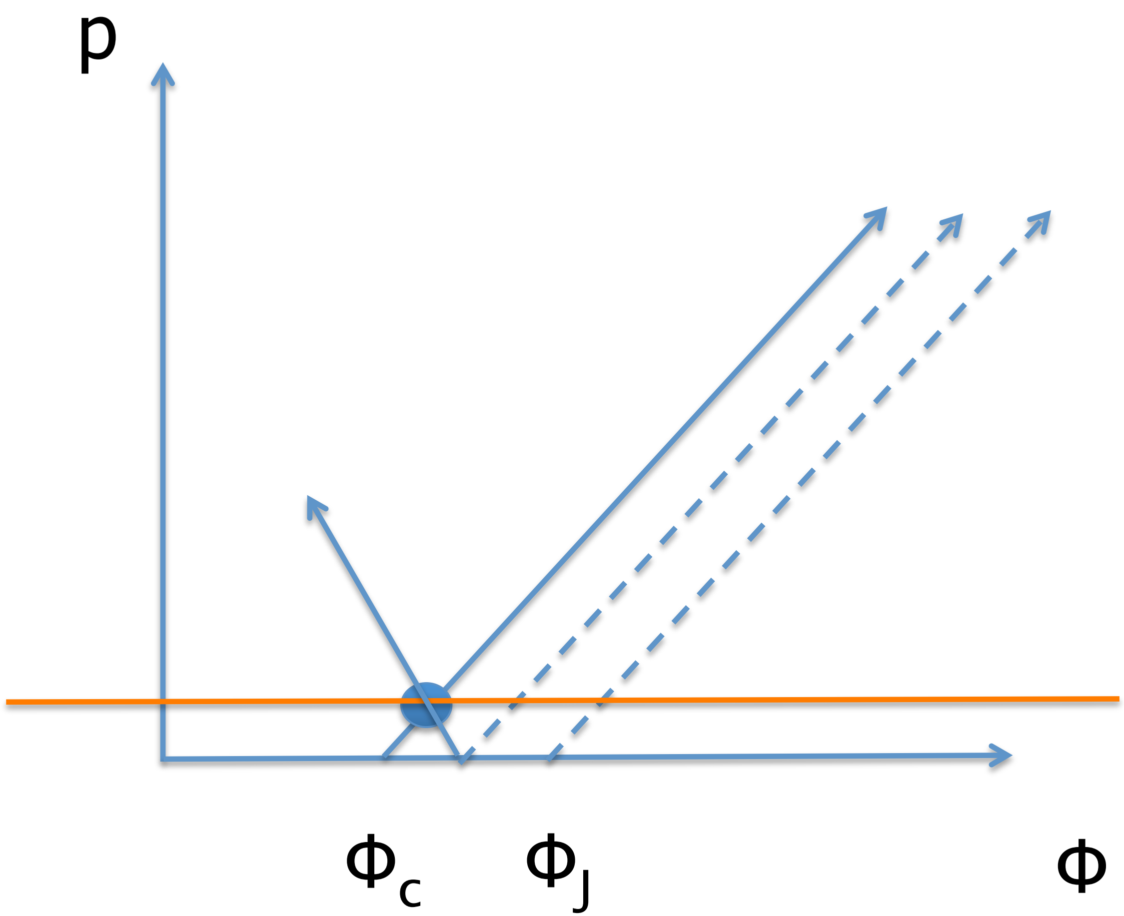
BC “isobaric” shear-jamming



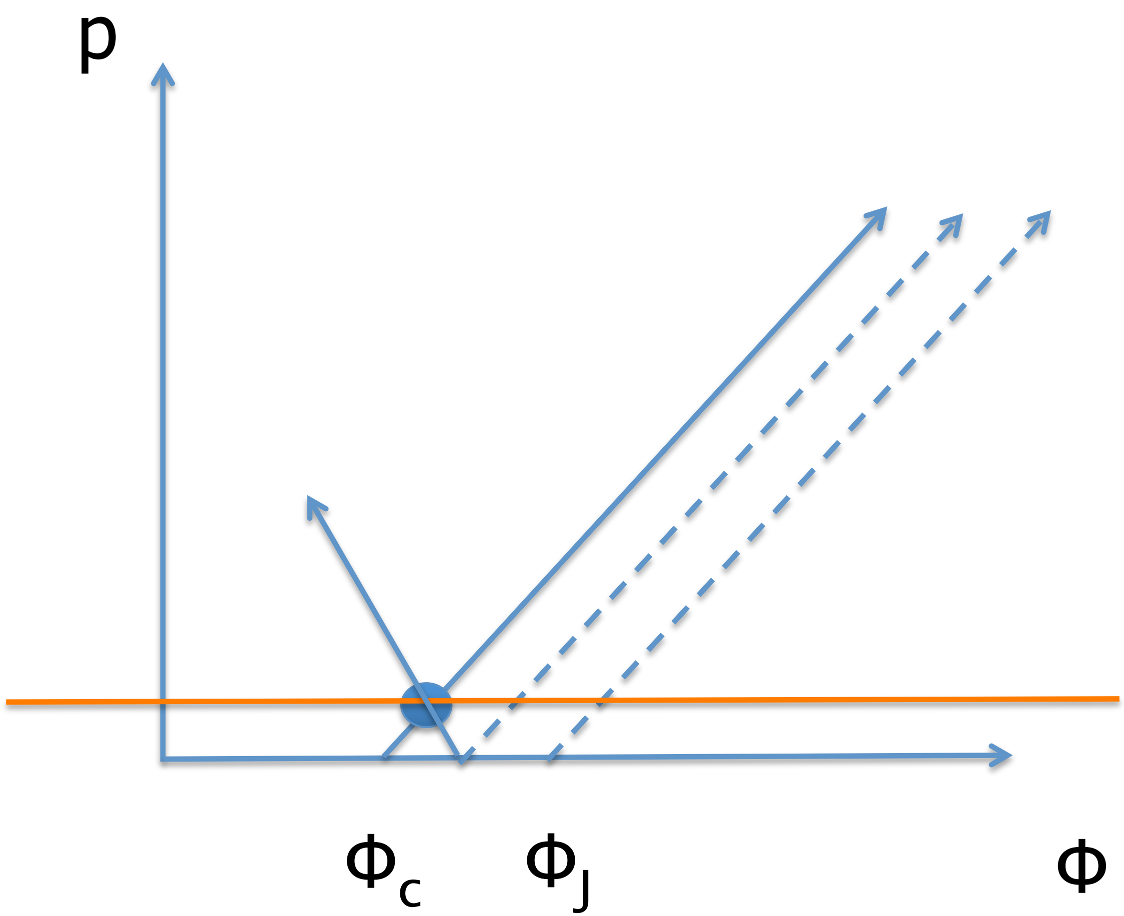
BC "isobaric" shear-jamming



BC "non-isobaric" shear-jamming

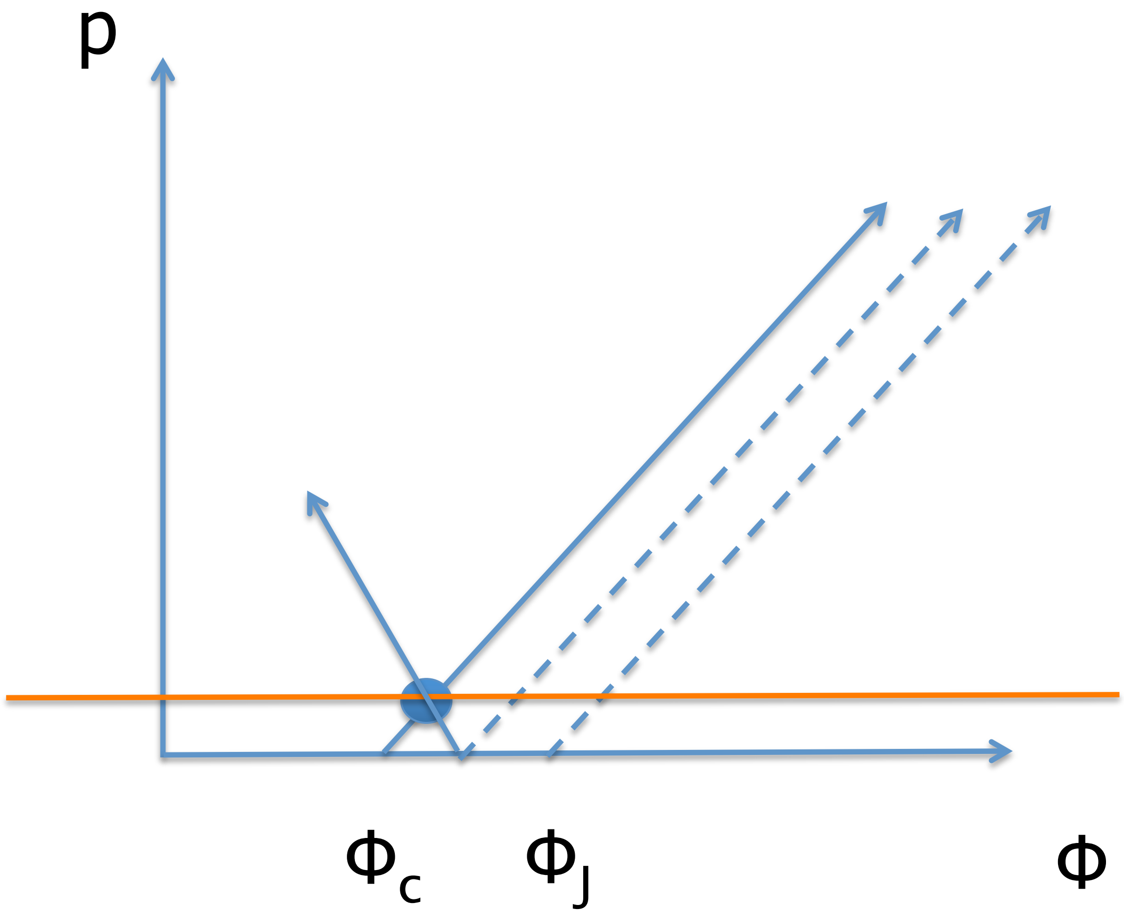


NOW – we are elastic

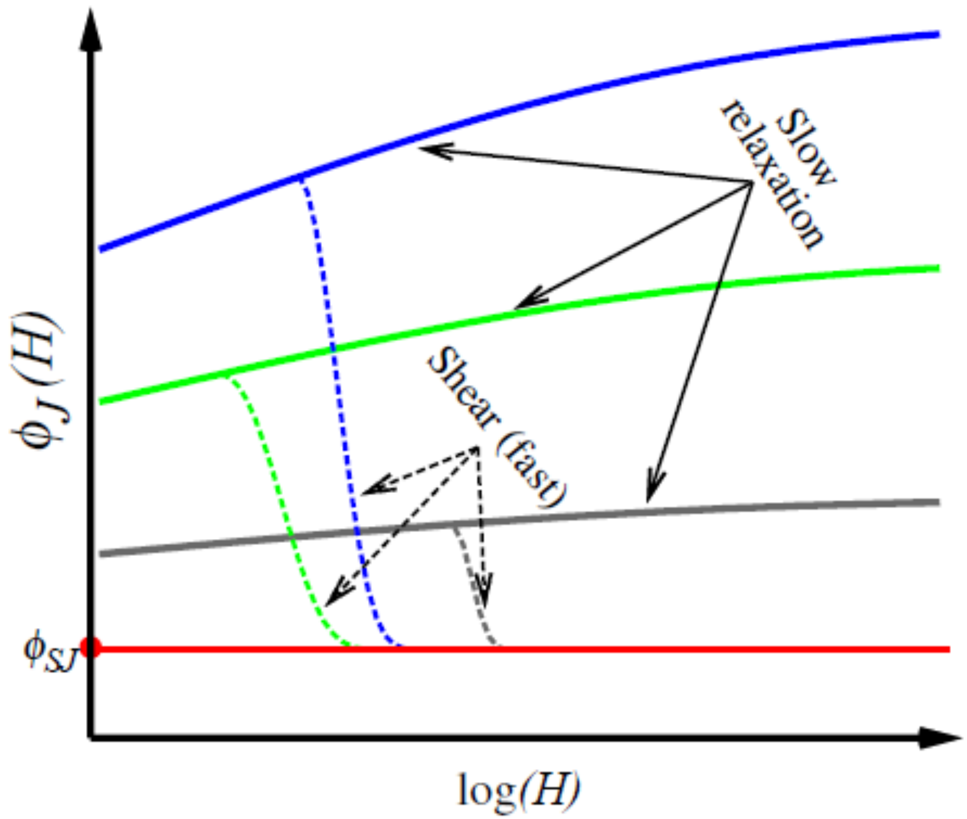


NOW – we are elastic

finite N, p + tiny ε



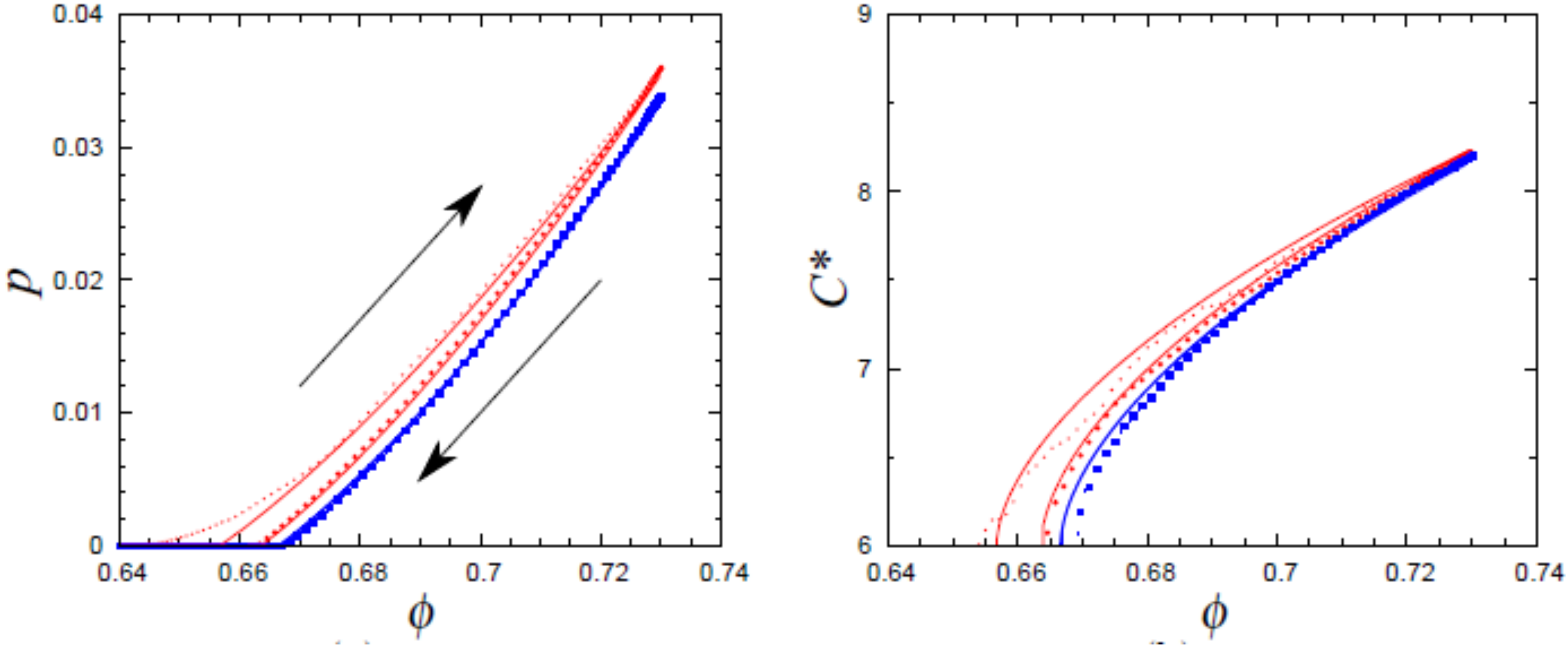
Connecting the two Experiments



- Combining 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

Predictive power – cyclic isotropic deformation

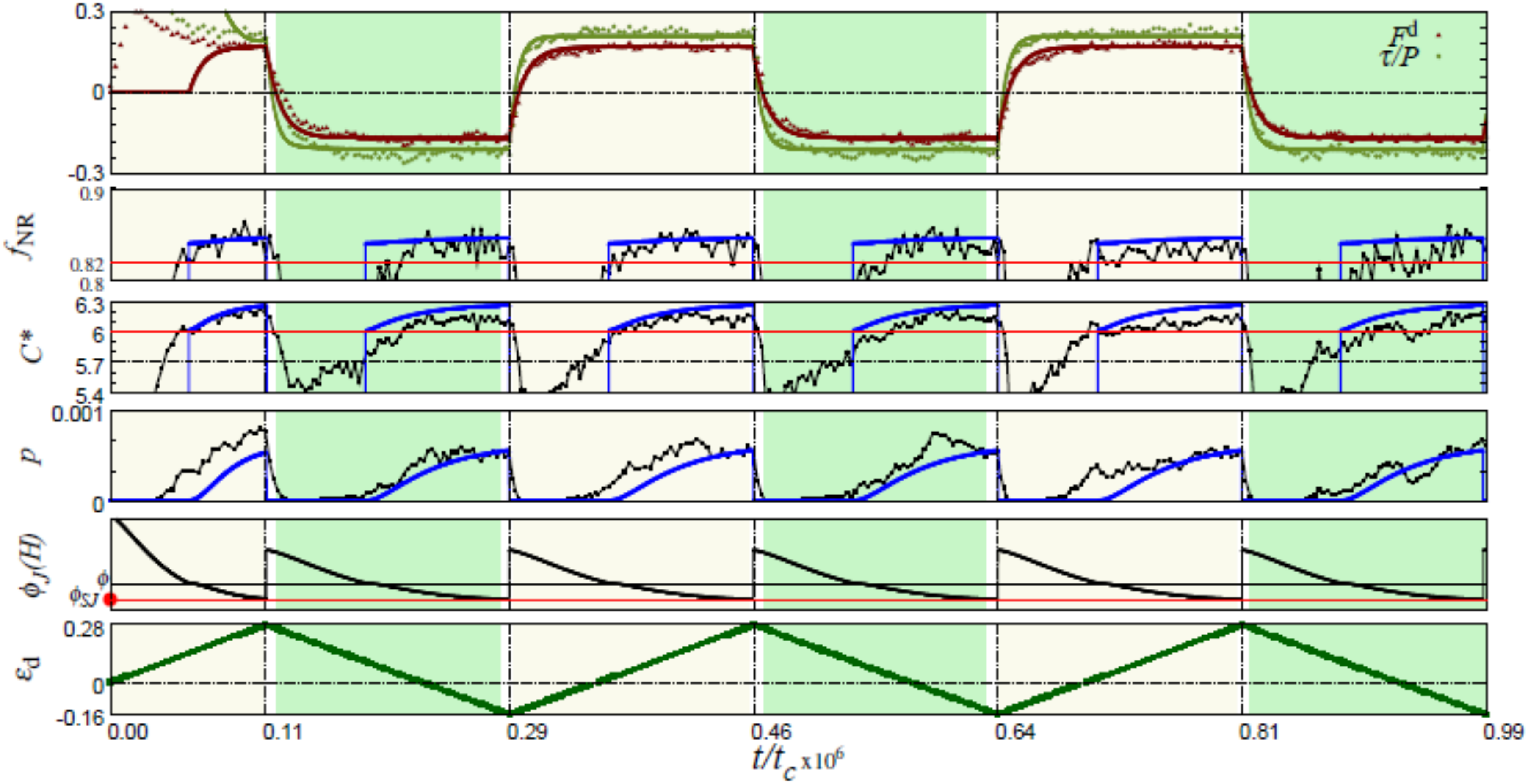
- Intermediate cyclic over-compression (amplitude 0.73) for 100 cycles.



-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 pure shear deformation

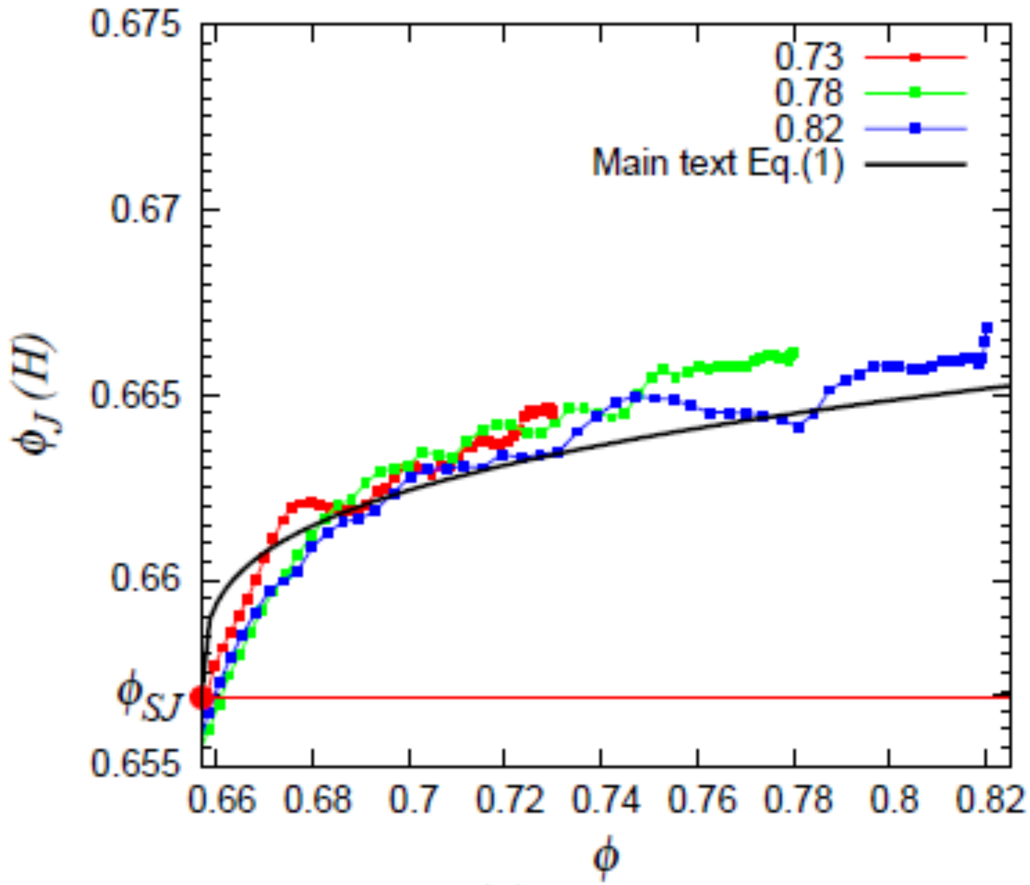
- Cyclic shear for 3 cycles (after the first loading, system forgets history).



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

Something for experimentalists

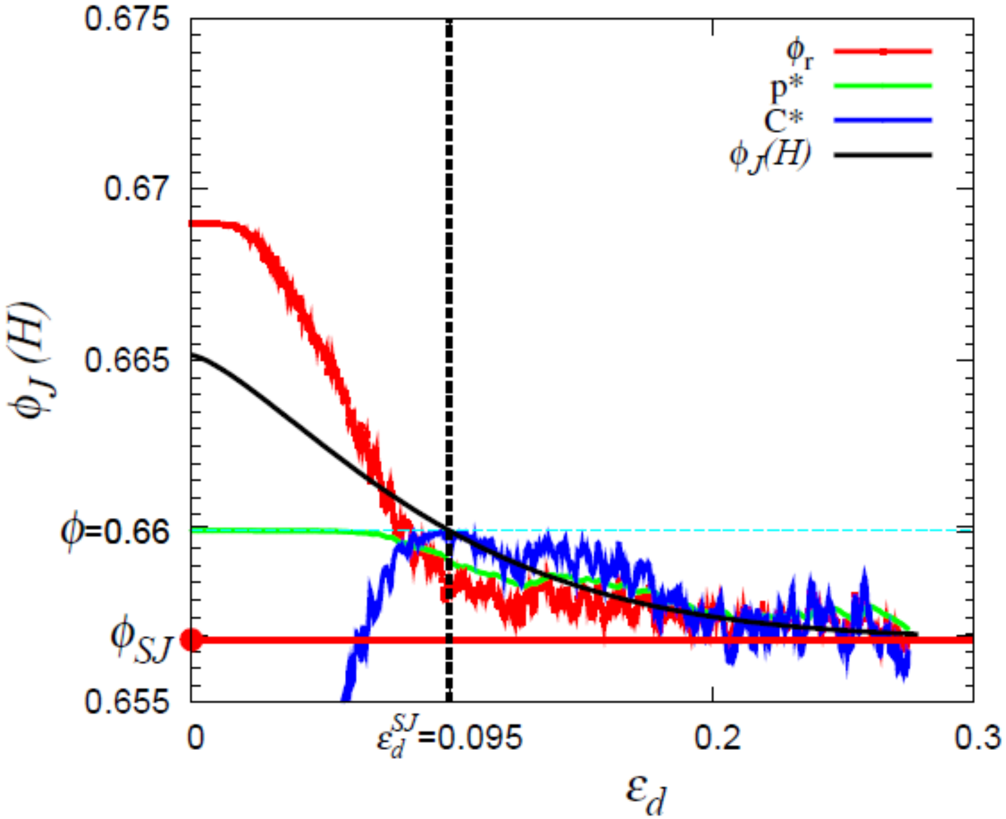
Measuring jamming points from the accessible macroscopic quantities – easiest pressure ☺



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 ☺

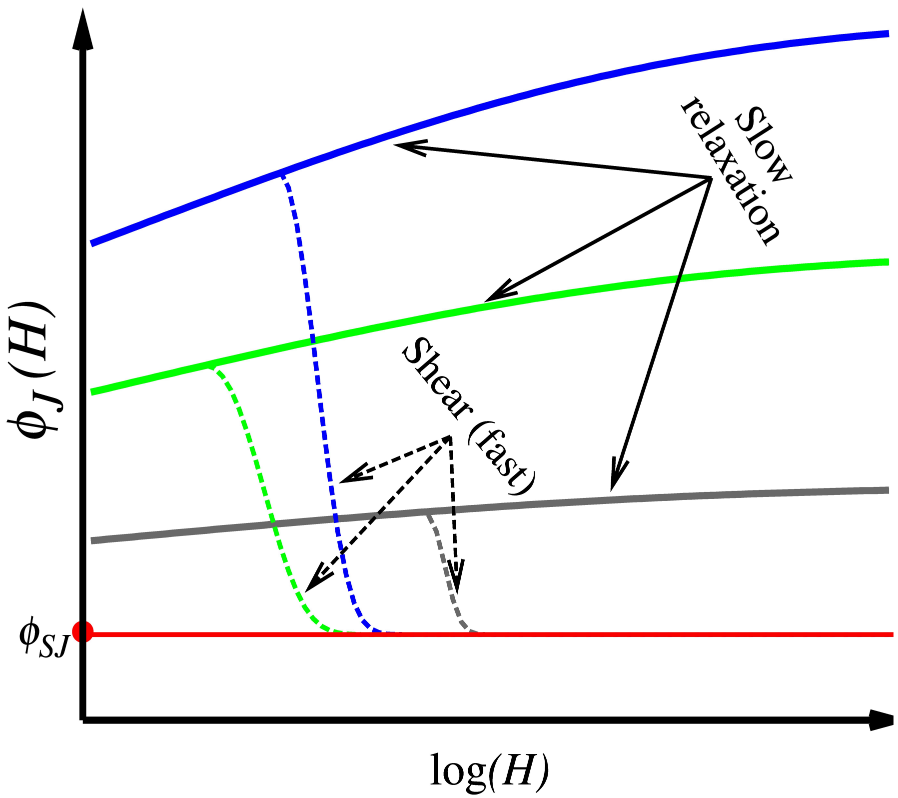


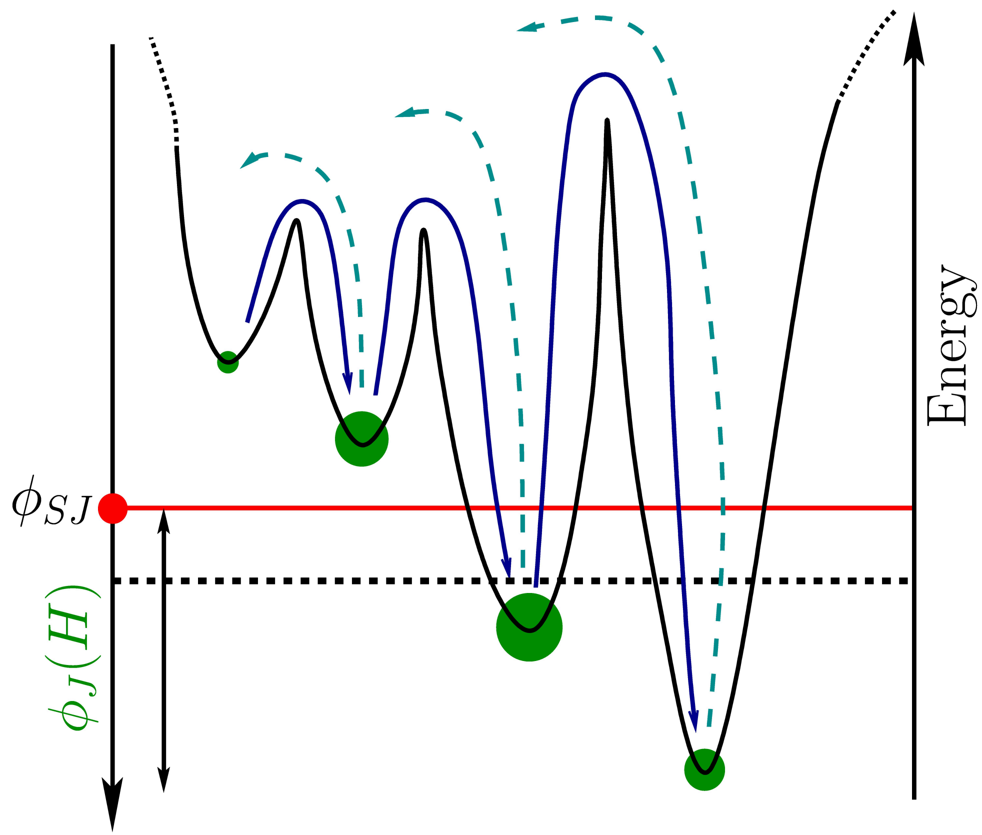
$$\frac{p\nu_c}{\nu C} = p_0(-\varepsilon_\mathrm{v})\left[1 - \gamma_p(-\varepsilon_\mathrm{v})\right]$$

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

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

Evolution of jamming points with history





Summary

there is:

- **dilatancy** in frictionless packings (Jean-Noel)
- **elasticity** (reversible) plasticity (irreversible) (Bulbul)
- **shear-jamming** in frictionless packs (Bob)
- new isotropic-state-variable! (for macro-view)

=> the jamming density $\Phi(H)$

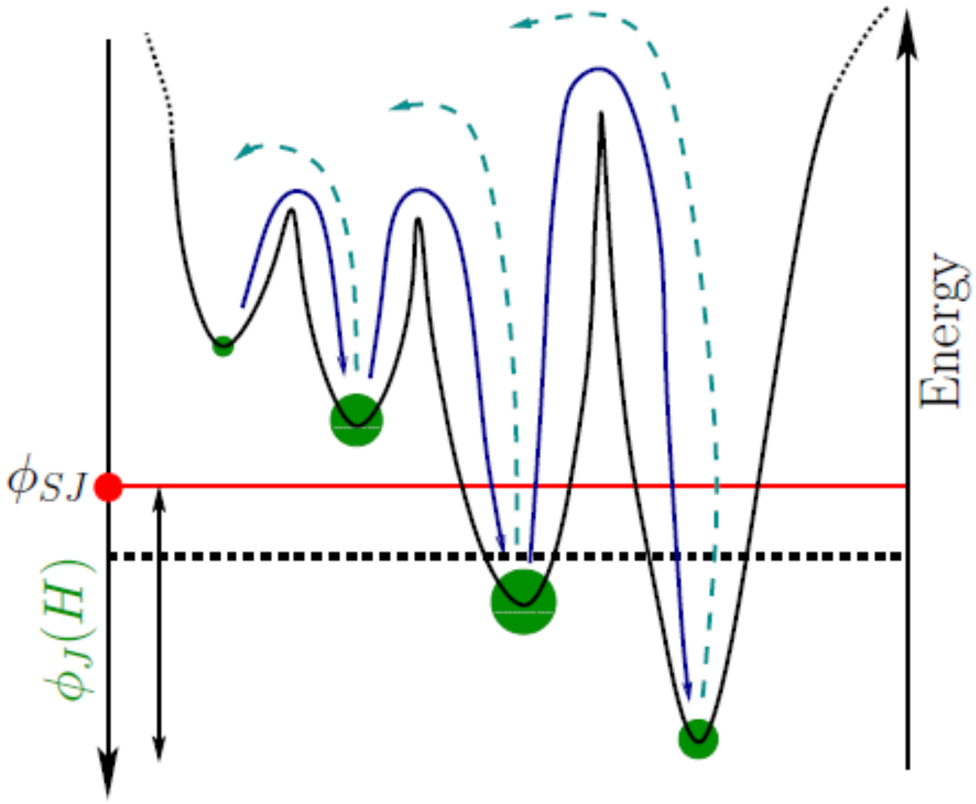
… or an other related quantity

- energy-landscape model explains all ☺

open issues?

- system size dependence? (Corey?)

Explanation – Energy landscape



- Isotropic deformation – leads to an increase in local and total jamming point, while the shear deformation decreases it.
- Deeper valleys with higher barriers, can be achieved with higher over-compression.

Compaction: A minimal model

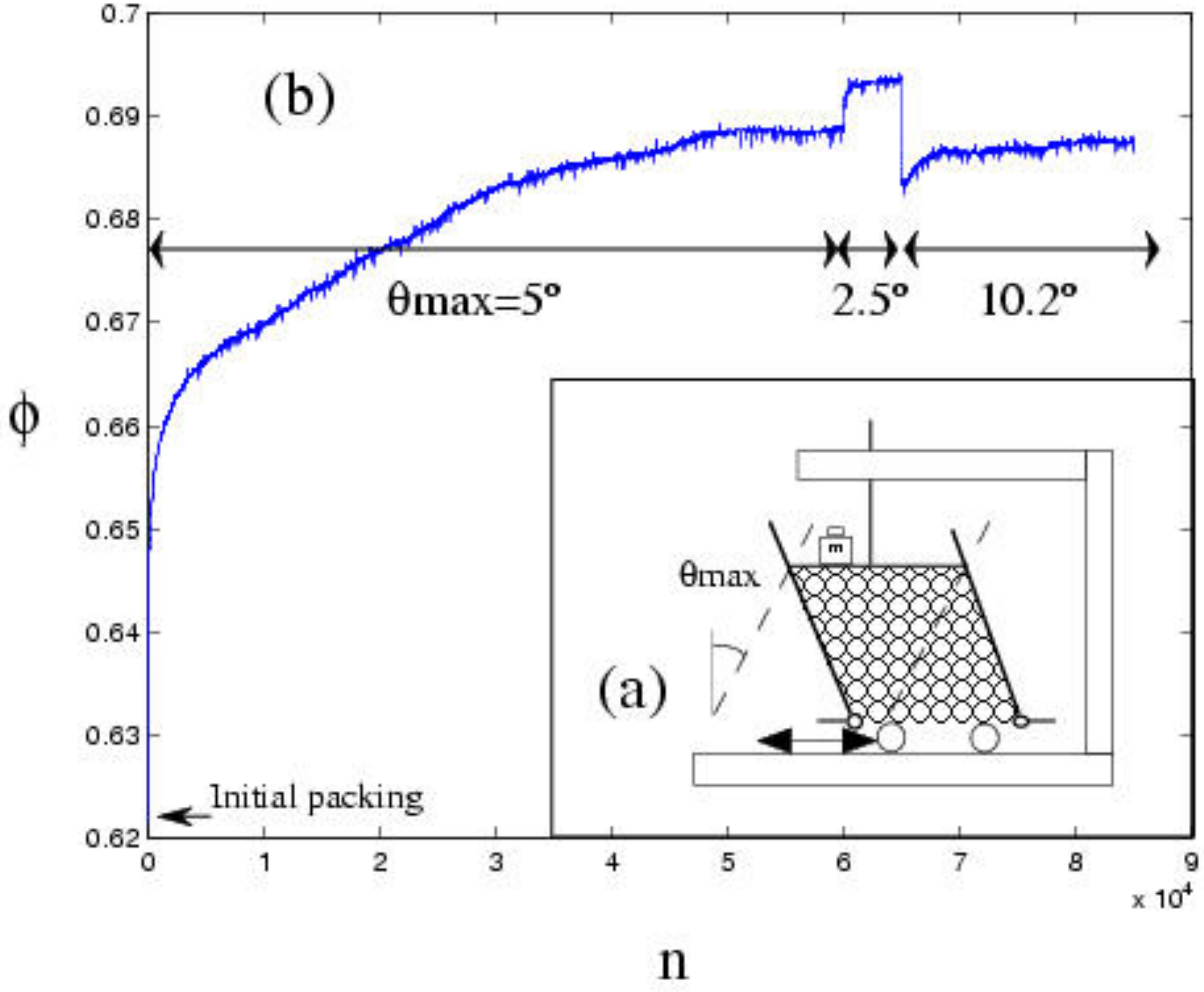
Stefan Luding
Particle Technology
DelftChemTech, TUDelft

Overview

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

Experiments

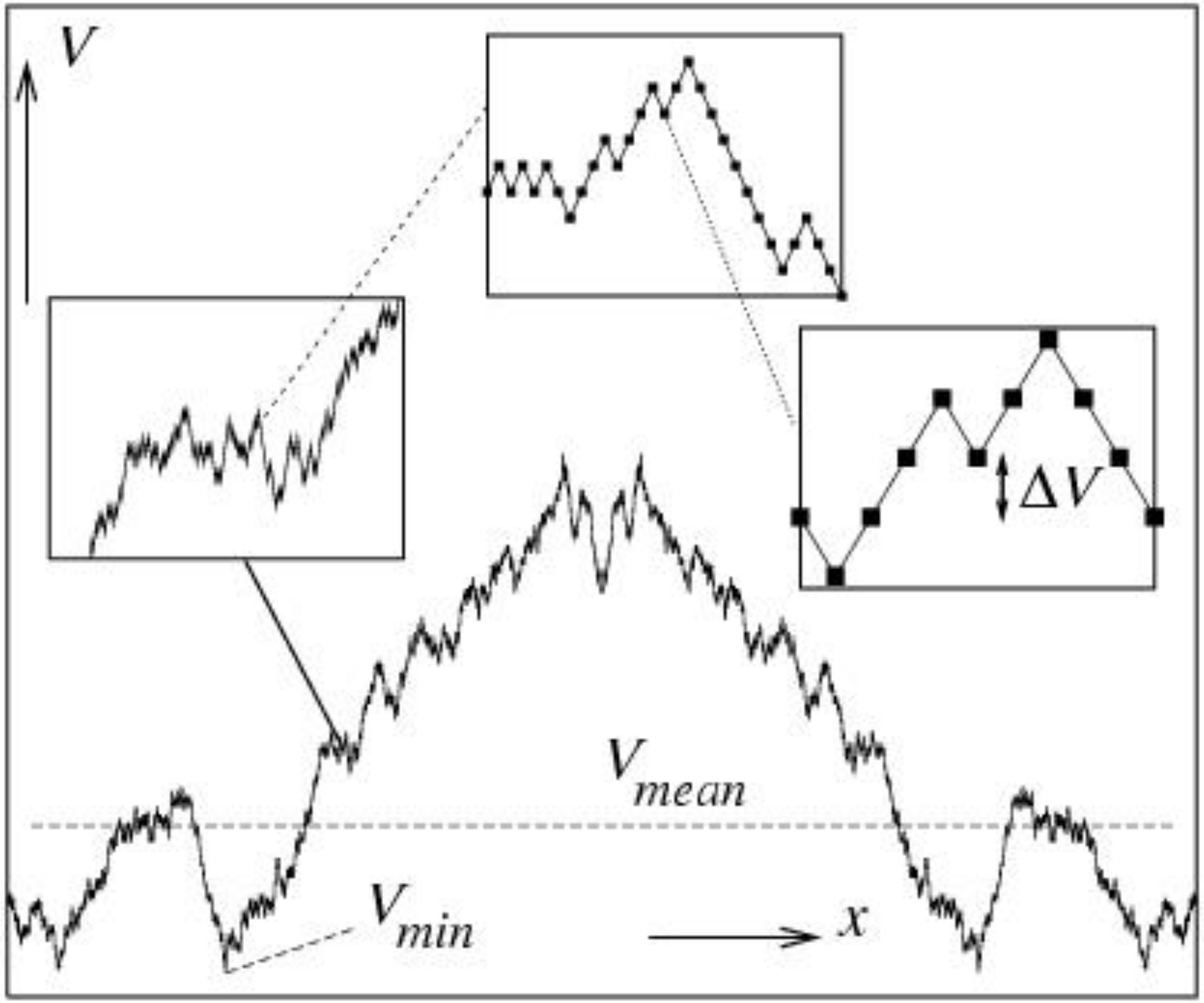
- Dense, monodisperse periodic shear



Model

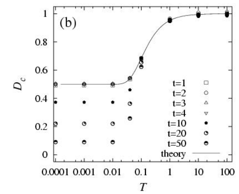
- Packing:
  - Local configuration?
  - Energy landscape
  - Potential energy → Density
- Particles:
  - Explore the energy landscape
  - Random walk = Sinai Diffusion

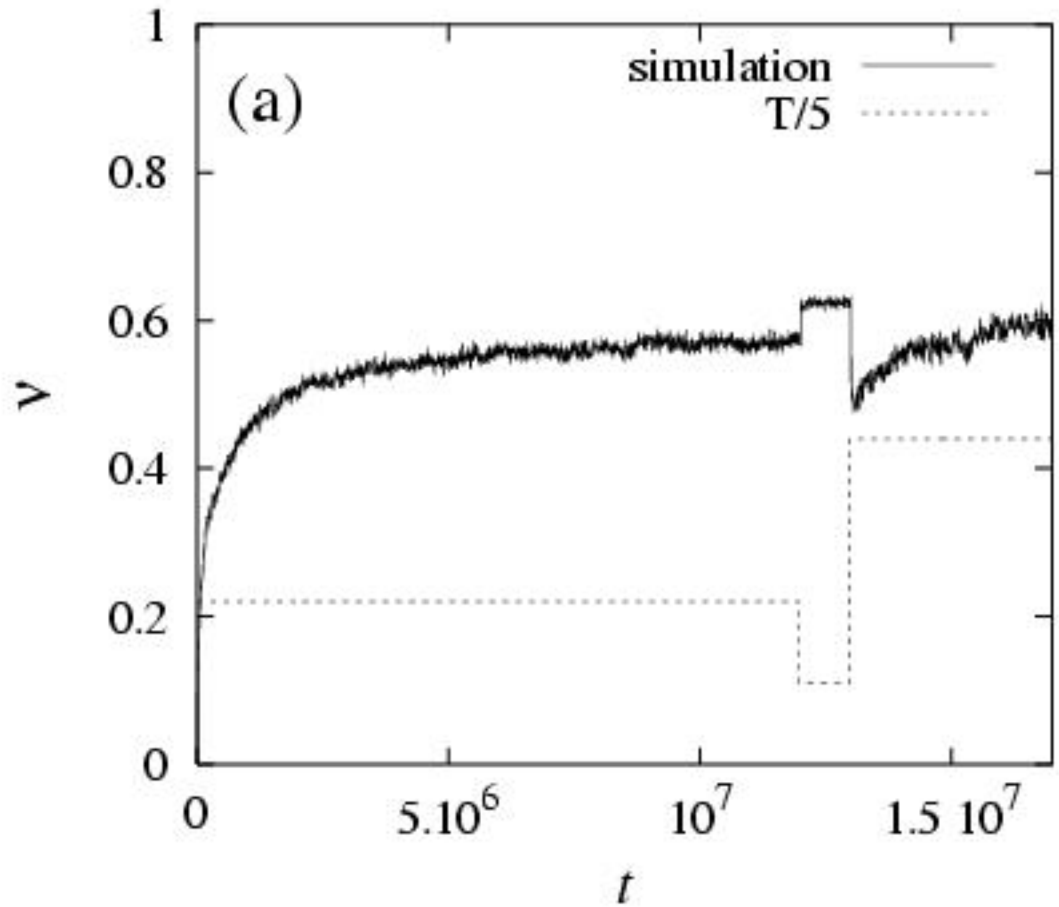
Model



Slow compaction

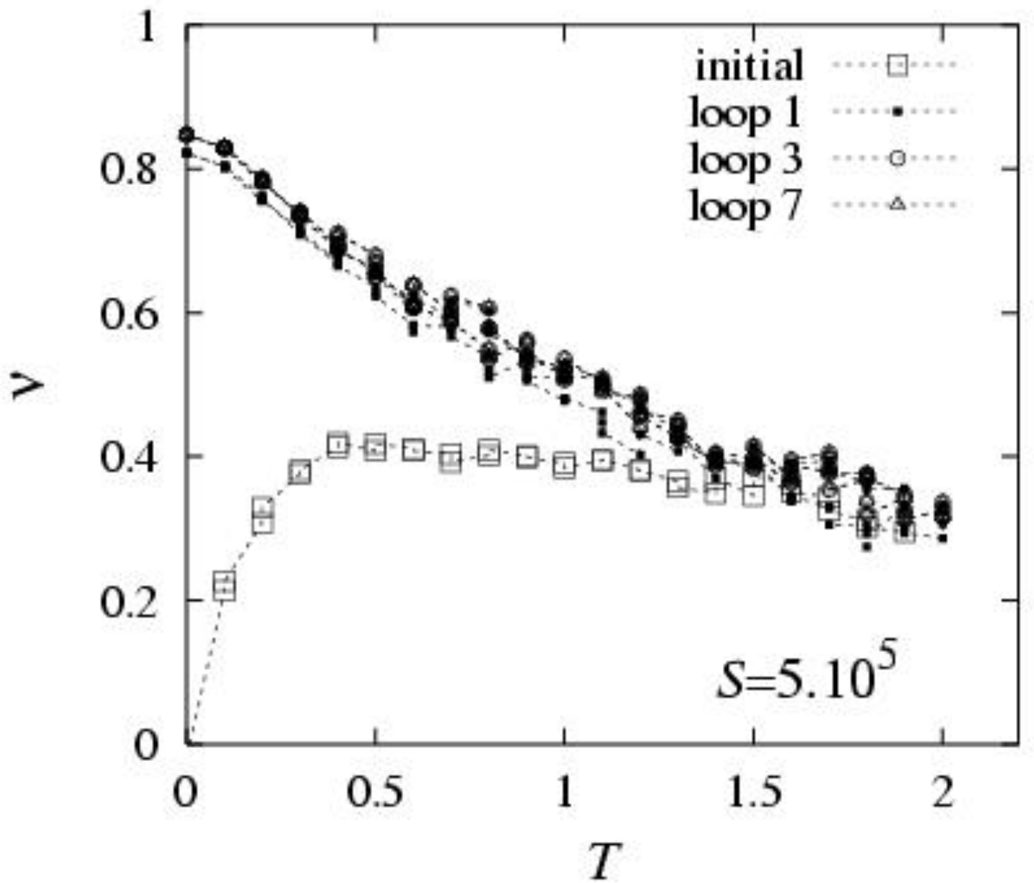
- Experiment vs. model simulation



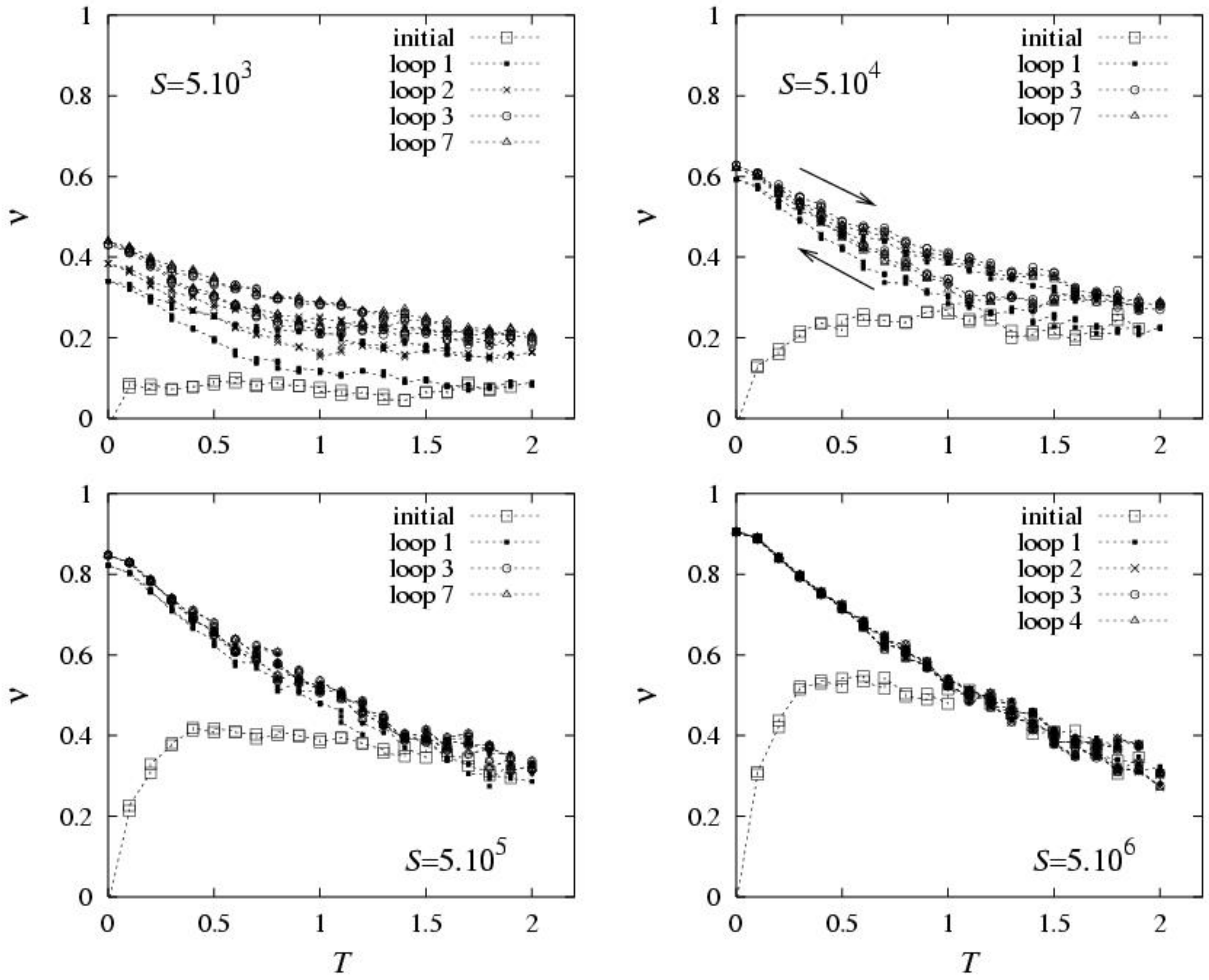


$$\nu = 1 - \frac{E - V_{\min}}{V_{\text{mean}} - V_{\min}}$$

Cyclic compaction



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



S=5.10^3
initial
loop 1
loop 2
loop 3
loop 7
S=5.10^4
S=5.10^5
S=5.10^6
loop 4
v
T
0
0.2
0.4
0.6
0.8
1
0.5
1.5
2

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 ?