Role of disorder in the yielding transition: an investigation through elasto-plastic models

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Deformation of amorphous solids

Different solids, different behaviors under deformation

Nicolas et al., 2018

In general:

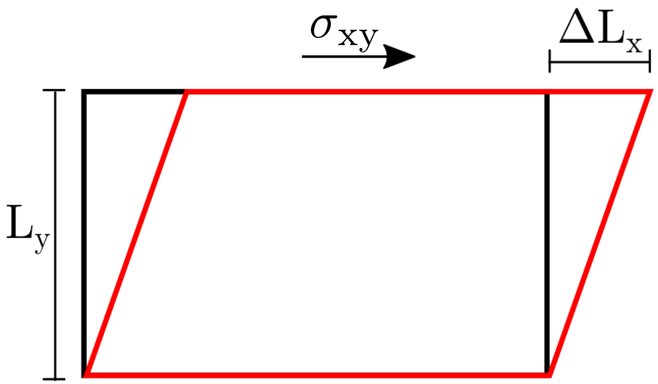
Displacement vector: u_i

Stress tensor: σ_{ij}

Strain tensor:

$$\epsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial j} + \frac{\partial u_j}{\partial i}\right)$$

Our case: simple shear



Scalar variables

Stress: $\sigma = \sigma_{xy}$

Strain: $\gamma = 2\epsilon_{xy} = \frac{\Delta L_x}{L_y}$

Elastic and Plastic regimes

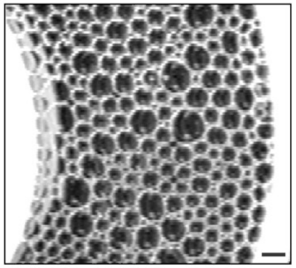
For small deformations, linear elasticity:

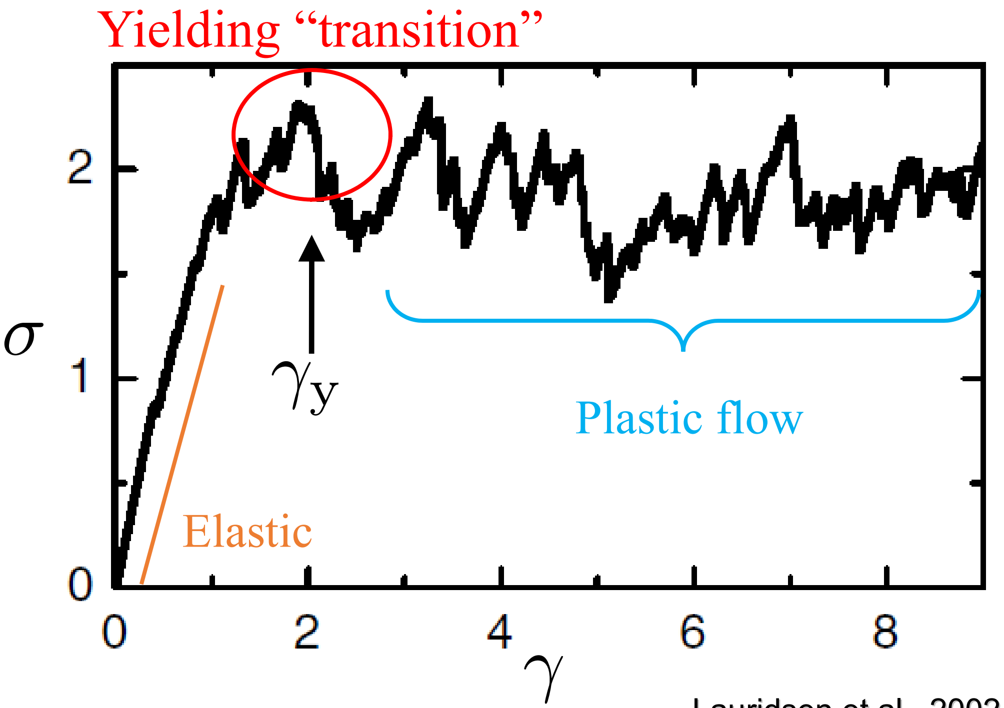
- Stress increases linearly with strain
- If forcing is removed, the solid goes back to the initial state

For large deformations, plastic flow:

- Stress cannot increase (on average) with strain
- Deformation is irreversible

The two regimes are separated by the yielding transition





Lauridsen et al., 2002

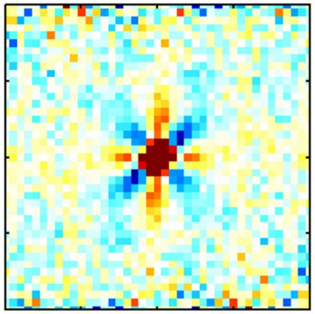
Origin of plasticity and shear banding

Amorphous solids can be very different, but share some common properties.
For example, same origin of plastic events:

Localized rearrangements of few particles (ex. T1 events)

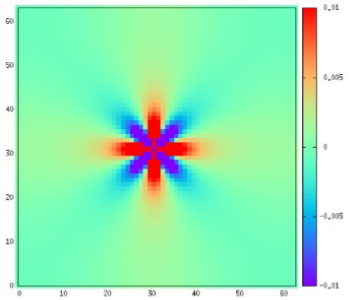
Biance et al., 2009

Strain field generated by plastic events

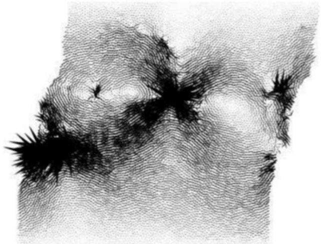


Jensen et al., 2014

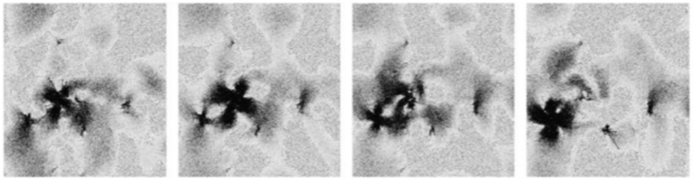
Well captured by the Eshelby kernel



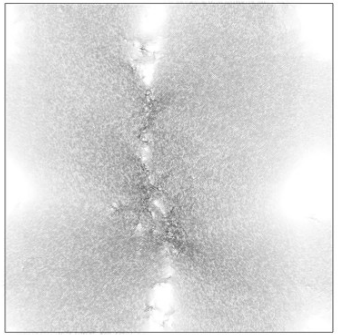
Due to the form of this strain field the events may organize in shear bands



Tanguy et al., 2006



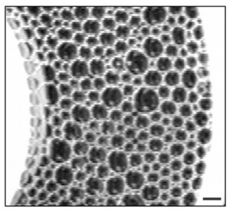
Lemaître et al., 2009



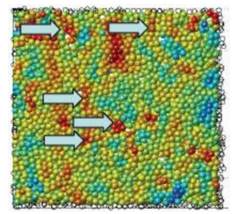
Maloney et al., 2006

Brittle vs ductile materials

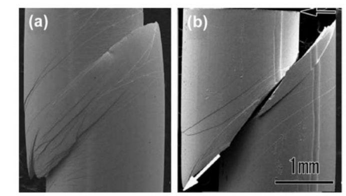
Similar qualitative origin of plasticity, but different behavior under deformation



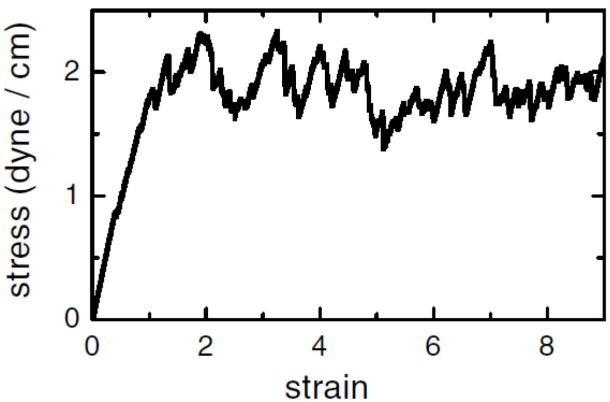
Lauridsen et al., 2002



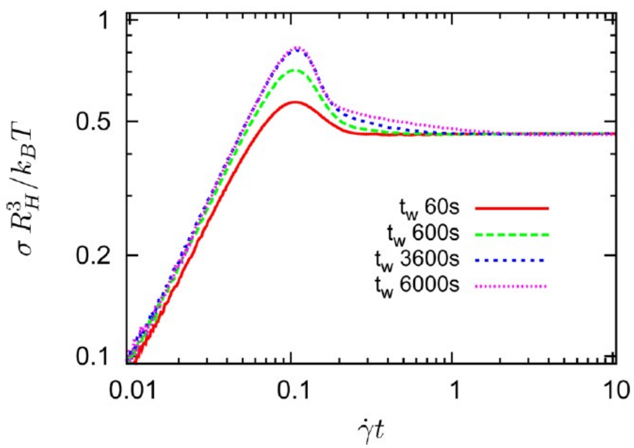
Amann et al., 2013



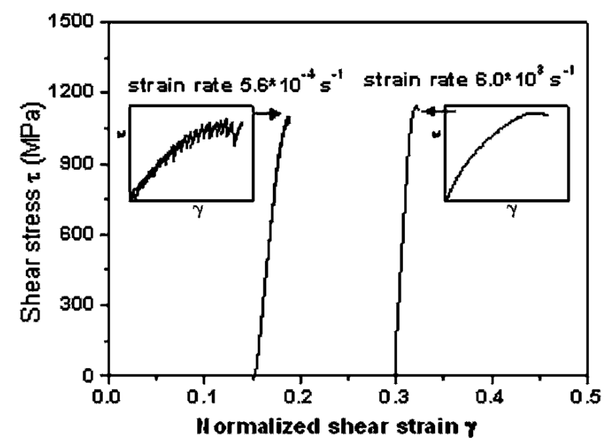
Song et al., 2008



Monotonic crossover
(Ductile)



Mild stress overshoot
(Ductile)



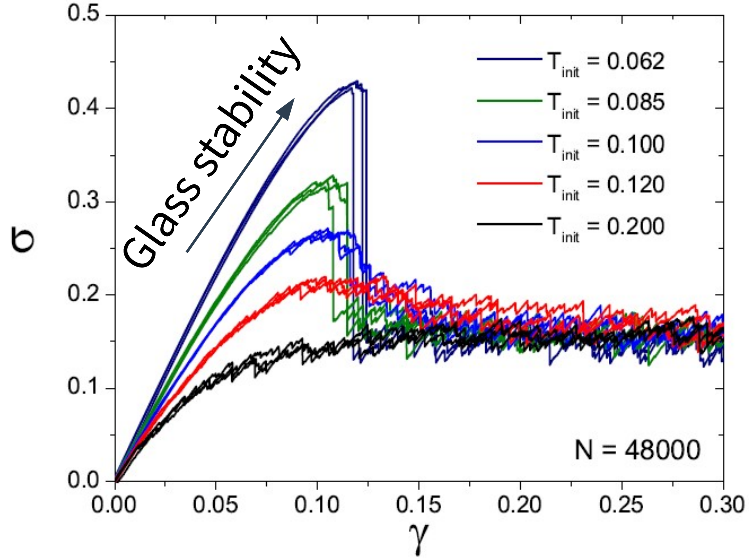
Discontinuous stress
drop and shear band
(Brittle)

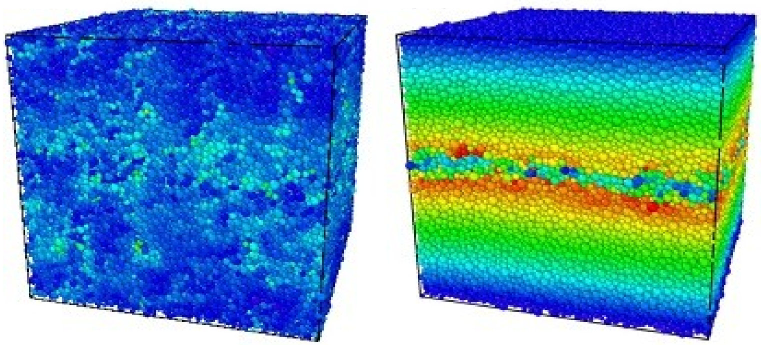
Liu et al., 2005

If same type of plasticity, what distinguishes brittle and ductile?

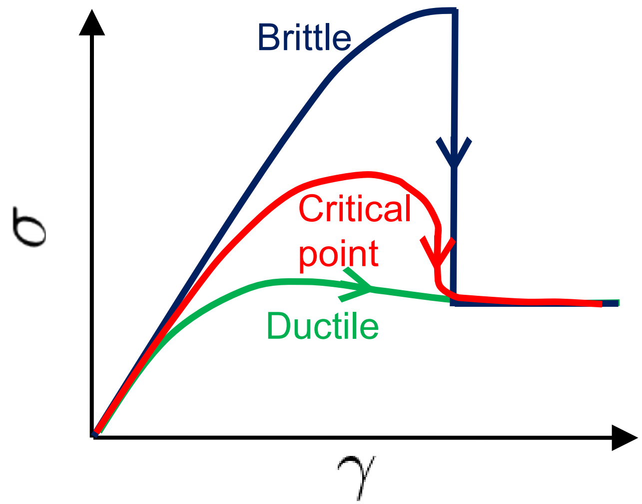
Results from Molecular Dynamics simulations

From Molecular Dynamics (MD) simulations we see that the preparation of the solid affects its behavior under deformation





A critical point between brittle and ductile yielding.

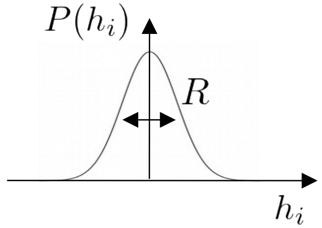


Ozawa et al., 2018

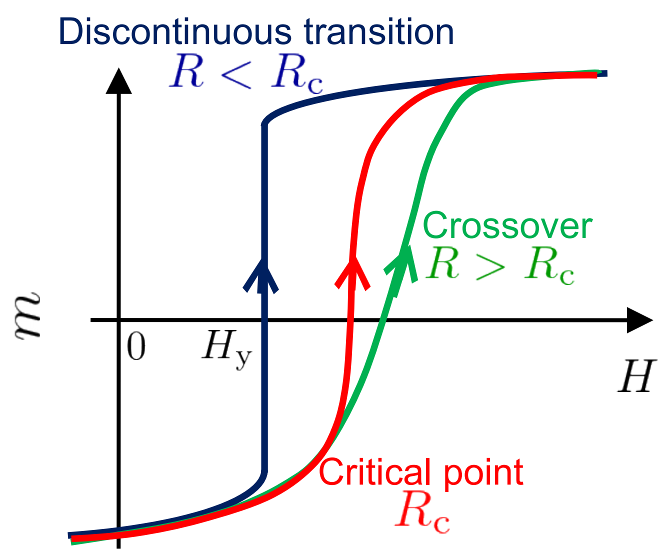
An analogy: the Random Field Ising Model

Behavior similar to the athermal Random Field Ising Model (RFIM) under quasistatic driving.
Described by the Hamiltonian:

$$\mathcal{H}(\{s_i\}) = -J \sum_{\langle i,j \rangle} s_i s_j - \sum_i (h_i + H) s_i \quad \text{with} \quad s_i = \pm 1, \; h_i \sim \mathcal{N}(0, R)$$



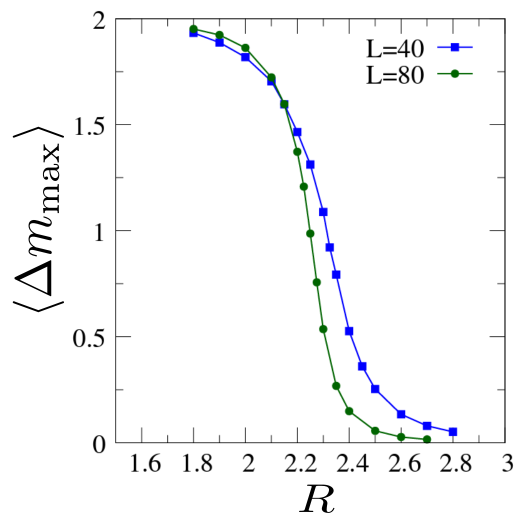
The system-averaged magnetization $m = \frac{1}{N} \sum_{i=1}^{N} s_i$ increases with the external field H in a way that depends on R

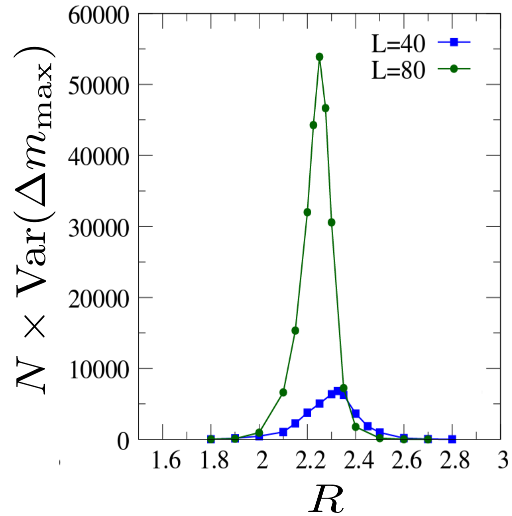


Natterman, 1997
Sethna et al., 2005

An analogy: the Random Field Ising Model

To capture the critical point one can measure the largest jump in the magnetization curve $\Delta m_{\max}$. At T=0 the thermal fluctuations are absent, but we need to average over many realizations of the disorder and measure sample-to-sample fluctuations





The sample-to-sample fluctuations scale as

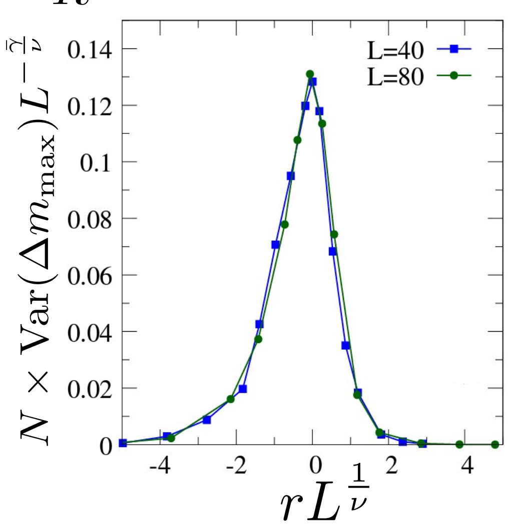
$$\chi_{\rm disc} = N\mathrm{Var}(\Delta m_{\max}) \sim L^{\bar{\gamma}/\nu}\Psi(rL^{1/\nu})$$

with $\Psi(\cdot)$ the scaling function and $\bar{\gamma}, \nu$ the scaling exponents and

$$r = \frac{R - R_c(L)}{R}$$

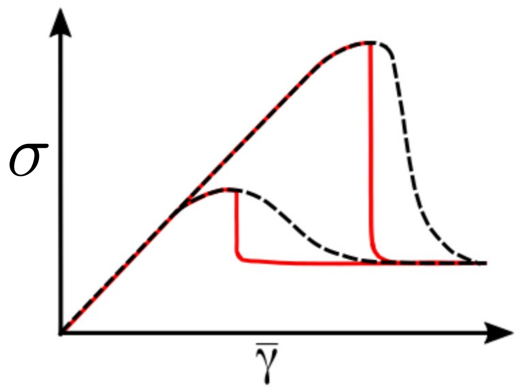
In 3D: $\bar{\gamma}/\nu \approx 2.95$ and $\nu \approx 1.3$

Tarjus et al., 2019



Questions

- How to properly characterize the existence and the properties of the yielding critical point? Need for large systems sizes and large number of samples! Hard to achieve in atomistic MD simulations.
- Linear stability analysis: continuous stress curves with overshoot are unstable and do not exist. Previous observation is due to small system sizes. Is yielding always brittle?



Fielding et al., 2020,2022

In order to answer these questions one needs larger system sizes to perform a careful finite-size scaling

The Elasto-Plastic model: basic ingredients

Microscopic scale ⟶ Mesoscopic scale

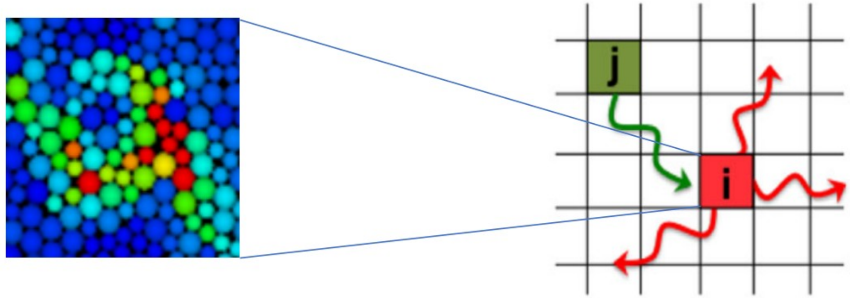
Many different versions of Elasto-Plastic Model (EPM) have been proposed.

Main ingredients:

- Stress (scalar or tensorial) assigned at each of the total N sites
- Elastic behavior of the block under external deformation
- Local condition for the onset of plasticity
- Stress redistribution to the rest of the system
- Local condition for the return to elasticity

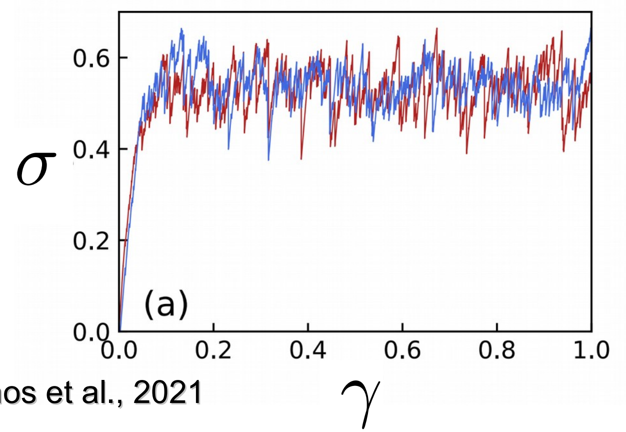
Some examples:

Nicolas et al., 2018
Jagla et al., 2007
Baret et al., 2002



Bocquet et al., 2009

Realistic results (compared to MD) if well calibrated



Castellanos et al., 2021

The Elasto-Plastic model: our version

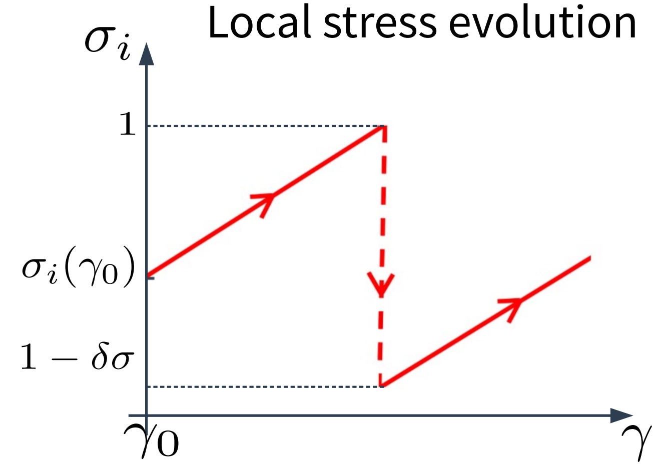
We are interested in critical properties, that should be universal. Focus on few ingredients

- Elastic behavior: $\gamma \to \gamma + \delta\gamma \longrightarrow \sigma_i \to \sigma_i + \mu\delta\gamma$ $(\mu = 1)$
- Block becomes unstable when
$$\sigma_i > \sigma_i^{\mathrm{th}} = 1$$
- If unstable, local stress drops as
$$\sigma_i \to \sigma_i - \delta\sigma$$
with $\delta\sigma$ from an exponential distribution with mean value 1
- Stress drop at site i redistributed to the whole system as
$$\sigma_j \to \sigma_j + G_{i,j}\delta\sigma_i$$
- Initial distribution of stress:
$$P_0(\sigma_i) = \frac{(1-\sigma_i^2)}{\mathcal{N}} e^{-\sigma_i^2/(2R^2)}, \quad \sigma_i \in [-1, 1]$$

- small R ⟶ well annealed, stable glass
- large R ⟶ poorly annealed

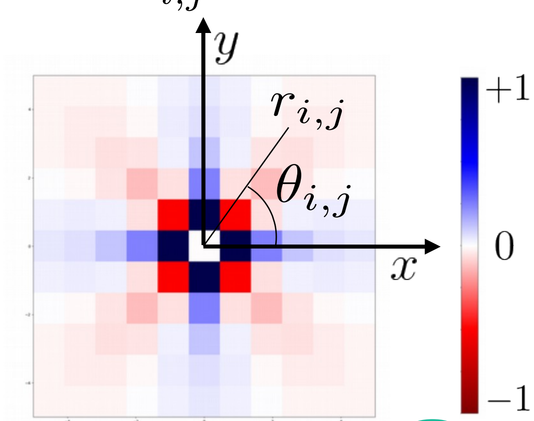
Model is strain-driven with the AQS protocol

Local stress evolution



Eshelby kernel

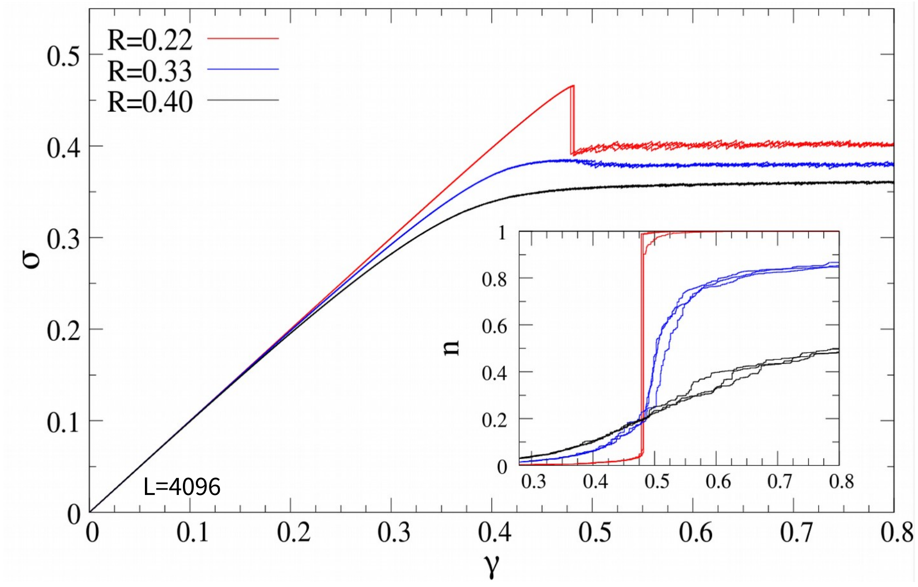
$$G_{i,j} \propto \frac{\cos(4\theta_{i,j})}{r_{i,j}^2}, \; G_{i,i} = -1$$

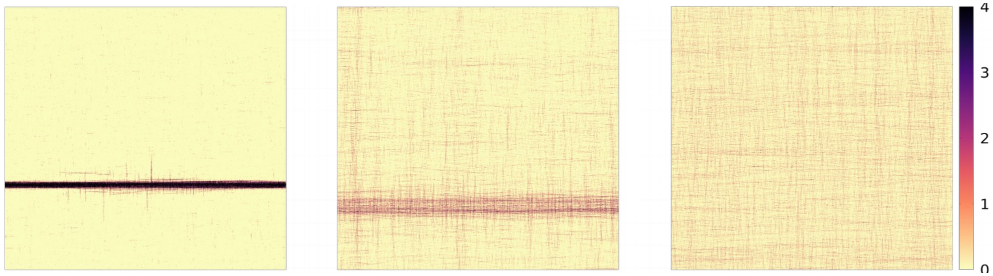


Eshelby, 1957
Picard et al., 2004

Stress-vs-strain curves

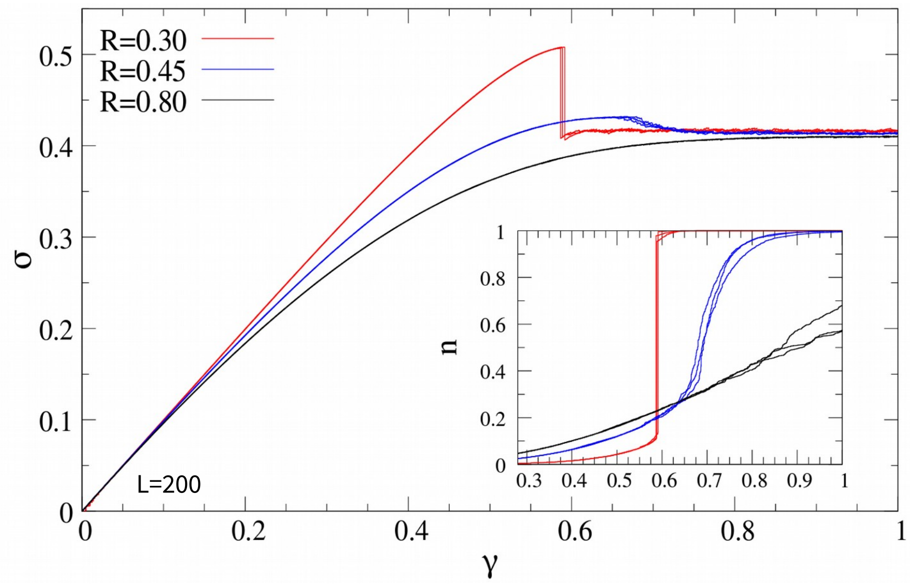
2D

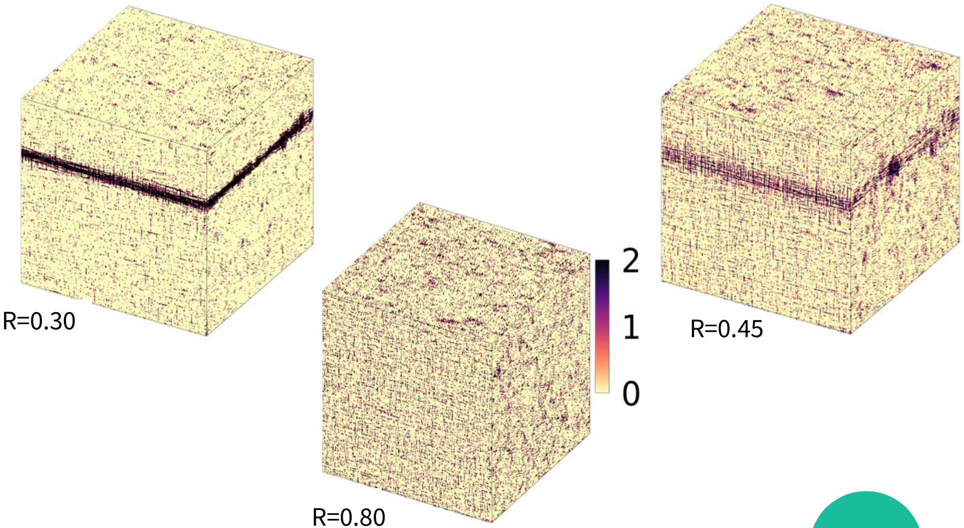




R=0.22 R=0.33 R=0.40

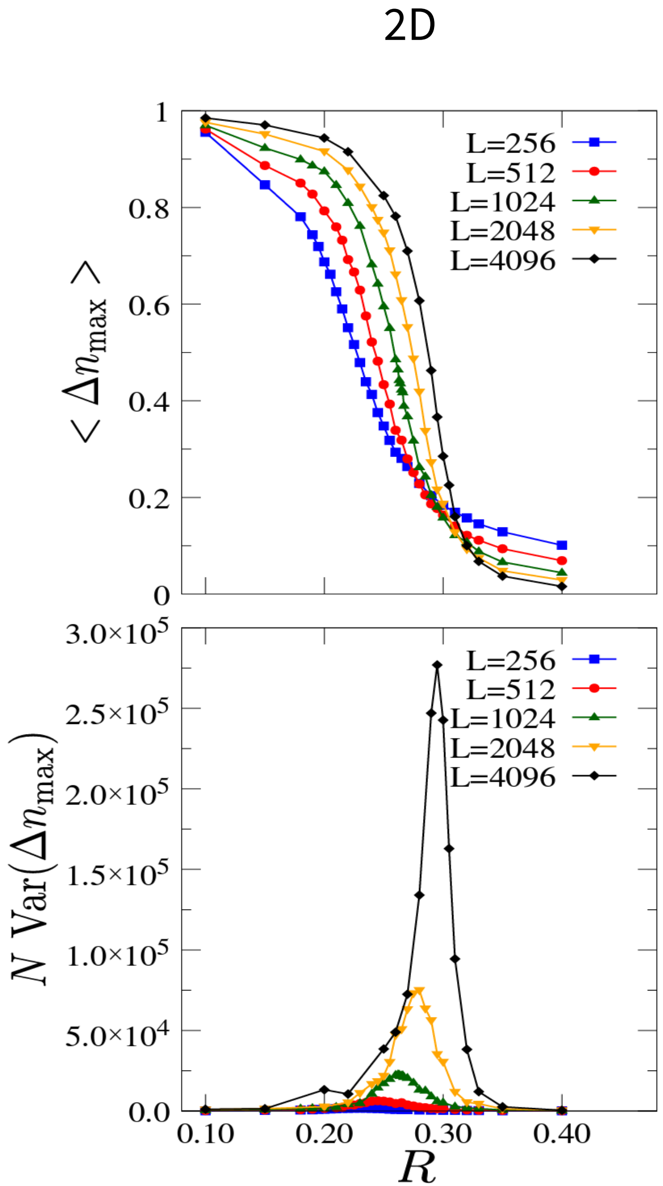
3D

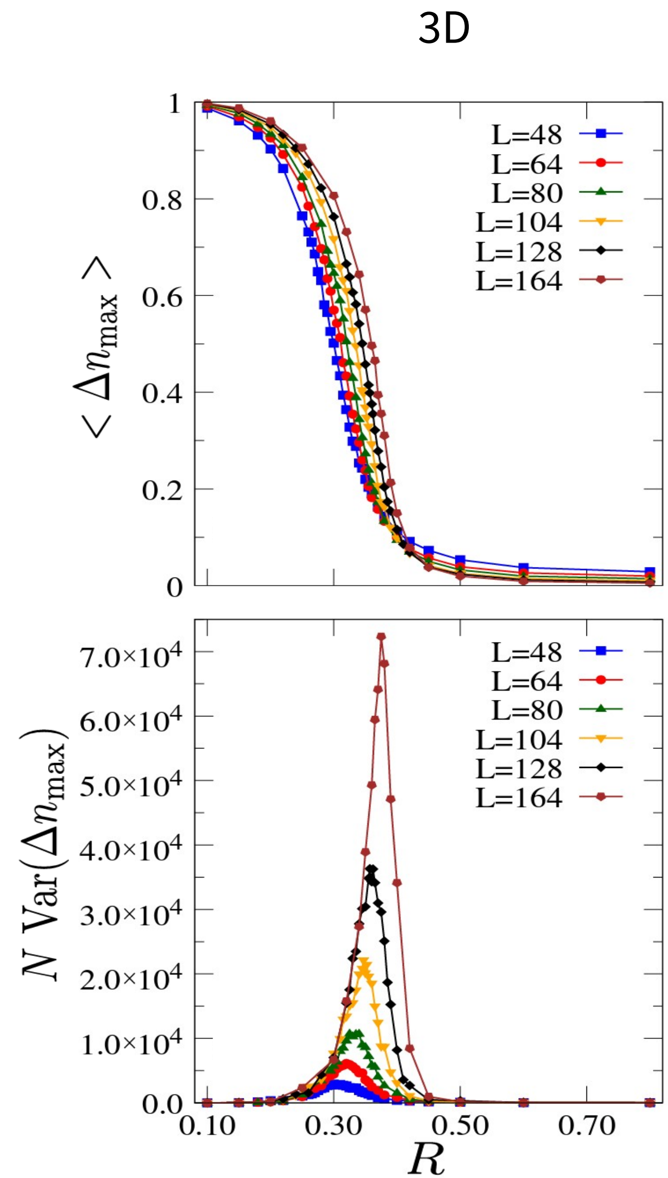




R=0.30 R=0.80 R=0.45

Characterizing the critical point





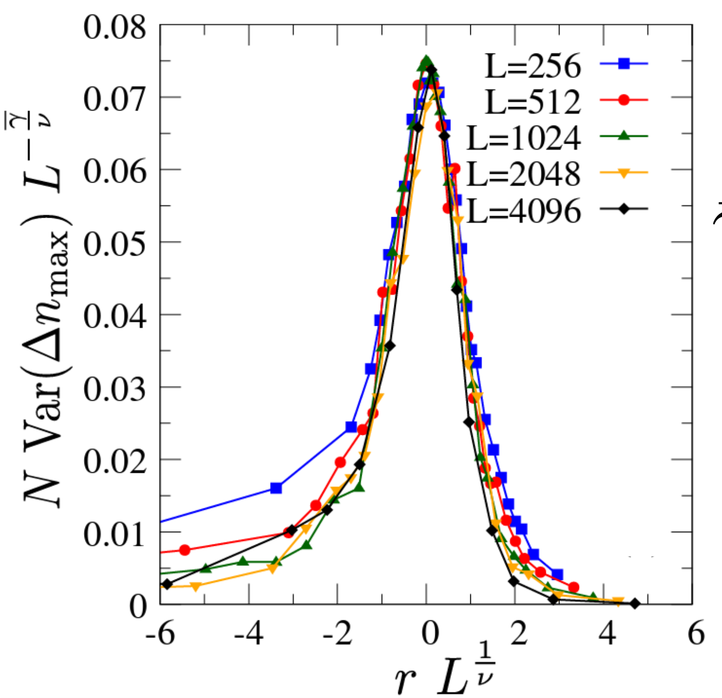
Finite-size analysis of the critical point

Using the same scaling ansatz of the RFIM:

$$\chi_{\text{disc}} = N\text{Var}(\Delta n_{\max}) \sim L^{\bar{\gamma}/\nu}\Psi(rL^{1/\nu})$$

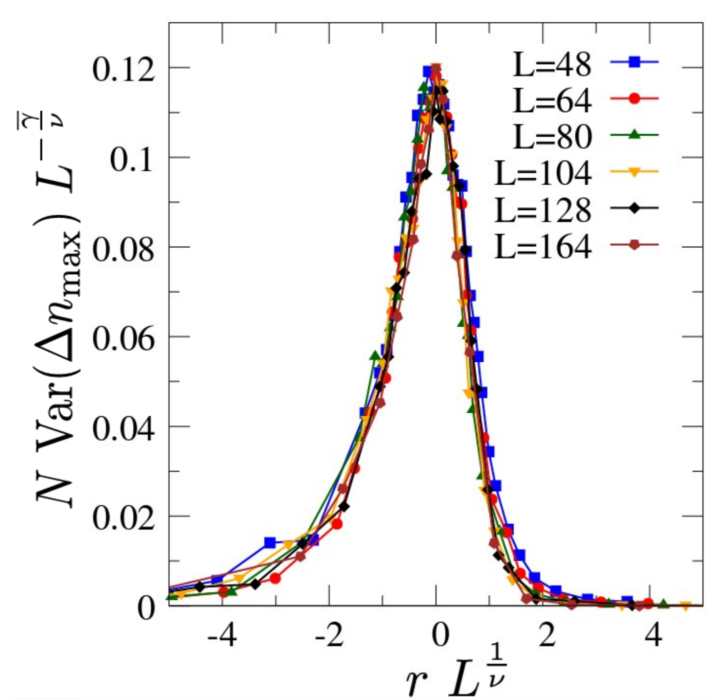
with $\Psi(\cdot)$ the scaling function and $\bar{\gamma}, \nu$ the scaling exponents and $r = \dfrac{R - R_c(L)}{R}$

2D



$\bar{\gamma}/\nu \approx 1.82$
$\nu \approx 2.9$

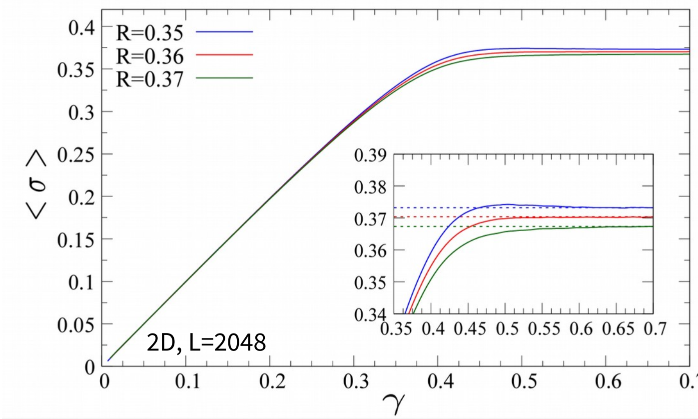
3D



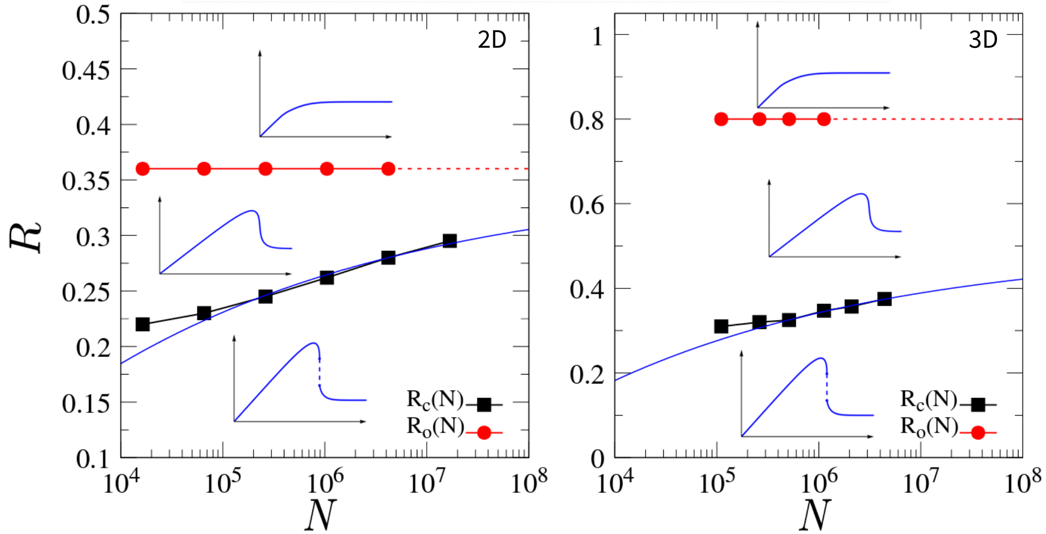
$\bar{\gamma}/\nu \approx 2.61$
$\nu \approx 2.2$

Bounding the location of the critical point

The critical point shifts towards larger R as the system size increases. What happens at the thermodynamic limit?



Above some value R_o the system does not show an overshoot anymore



The value of R_o stays unchanged as the system size increases. The critical point is bounded by this value.

Conclusion

- From finite-size scaling analysis over a large range of system sizes and number of samples (thanks to the mesoscale modeling) we have obtained strong evidence for the existence of a critical point between brittle and ductile yielding and first characterization of the associated scaling behavior.

- The putative linear instability, which should already be operative for the system sizes that we consider does not seem to destroy the existence of a critical point. The instability is possibly pinned when disorder is strong enough.