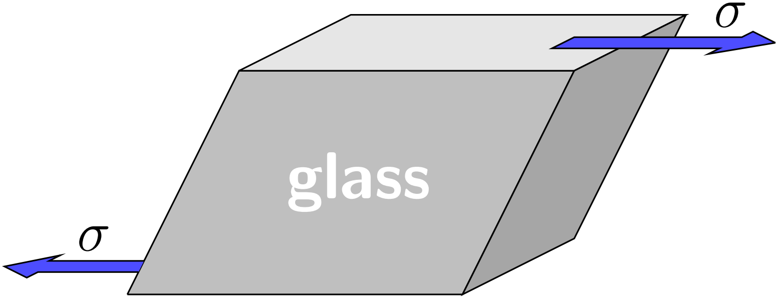
# Nonlinear plastic modes – micromechanics and statistics

Edan Lerner

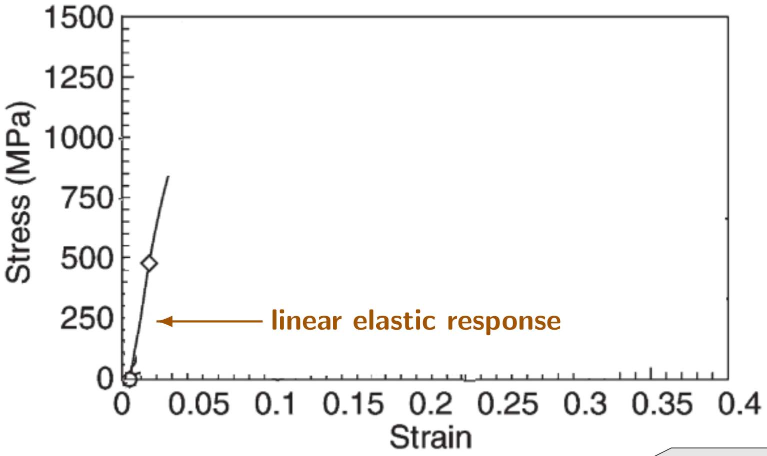
Institute for Theoretical Physics
University of Amsterdam

yielding of amorphous solids
ENS Paris
Oct 2017

**what happens when a glass is deformed?**

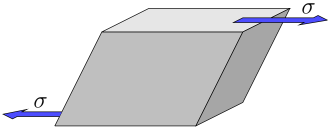


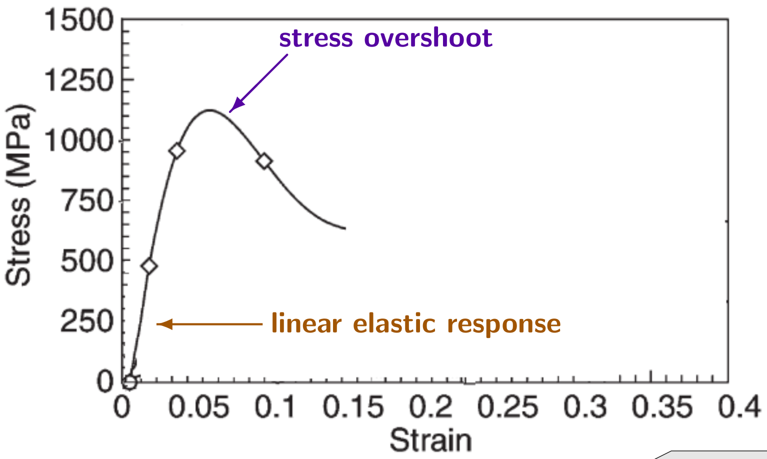
# elasto-plasticity – macroscopic response & yielding

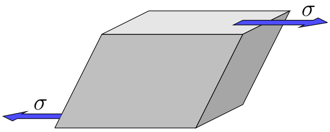



**'Vitreloy 1' (metallic glass)**

**J. Lu, G. Ravichandran, W. Johnson, Acta Materialia 51 (2003)**



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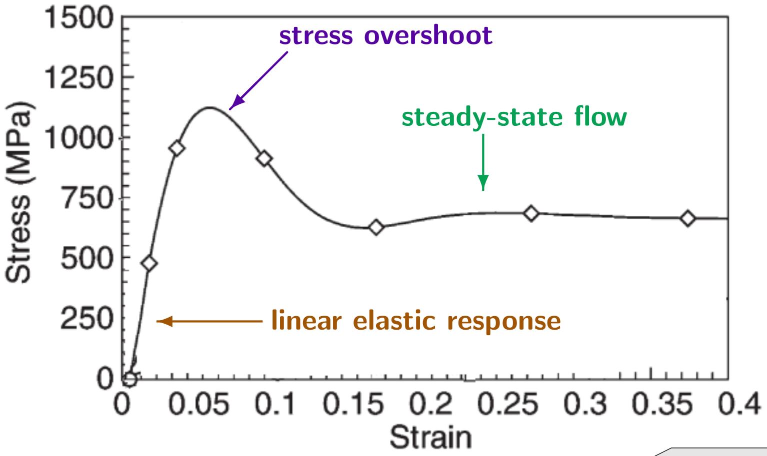


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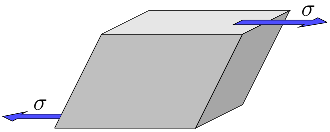


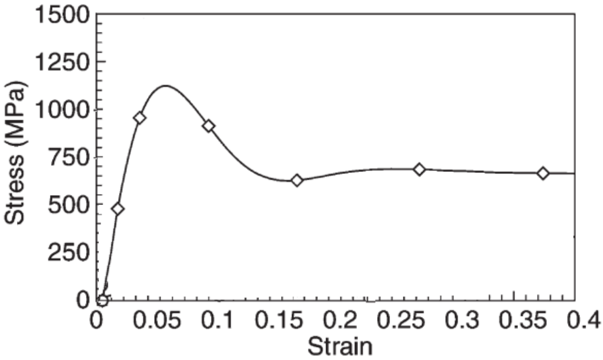

**J. Lu, G. Ravichandran, W. Johnson, Acta Materialia 51 (2003)**

# what do we want to find?

**goal: theory for**

$\boldsymbol{\sigma} \equiv$ stress
$\dot{\boldsymbol{\gamma}} \equiv$ deformation rate
$\boldsymbol{T} \equiv$ Temperature

$$\frac{d\sigma}{dt} = f(\sigma, \dot{\gamma}, T, \ldots)$$



## experiments, metallic glass

**J. Lu, G. Ravichandran, W. Johnson, Acta Materialia 51 (2003)**

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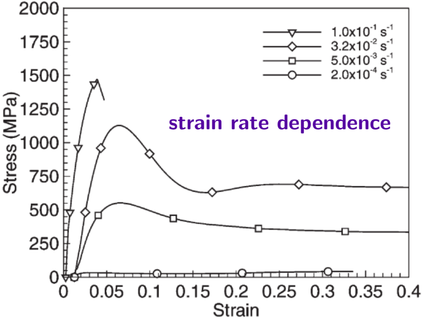


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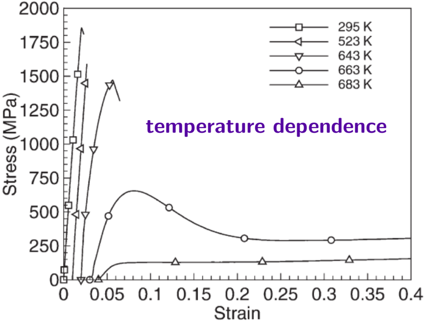
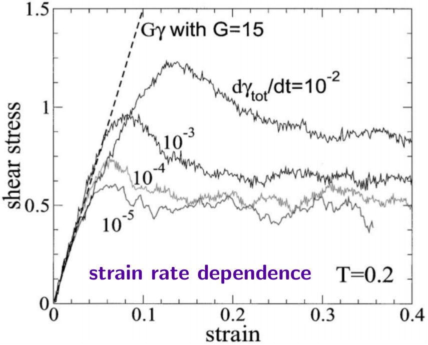


## simulations of model glasses

F. Varnik, L. Bocquet, and J.-L. Barrat, J. Chem. Phys. 120, 2788 (2004)

$$\frac{d\sigma}{dt} = f(\sigma, \dot{\gamma}, T, \ldots)$$

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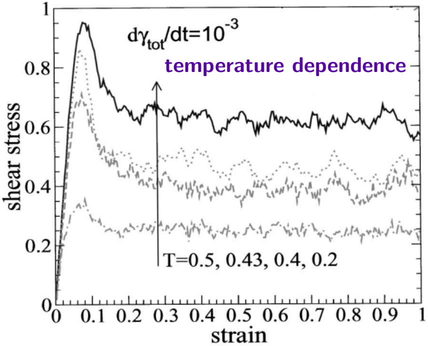
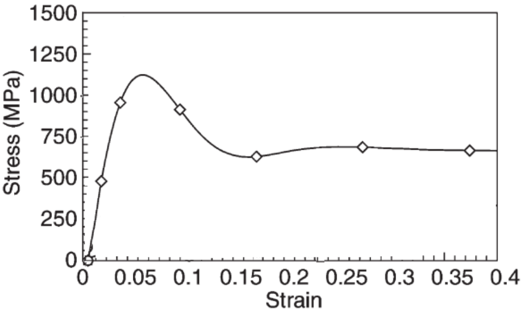


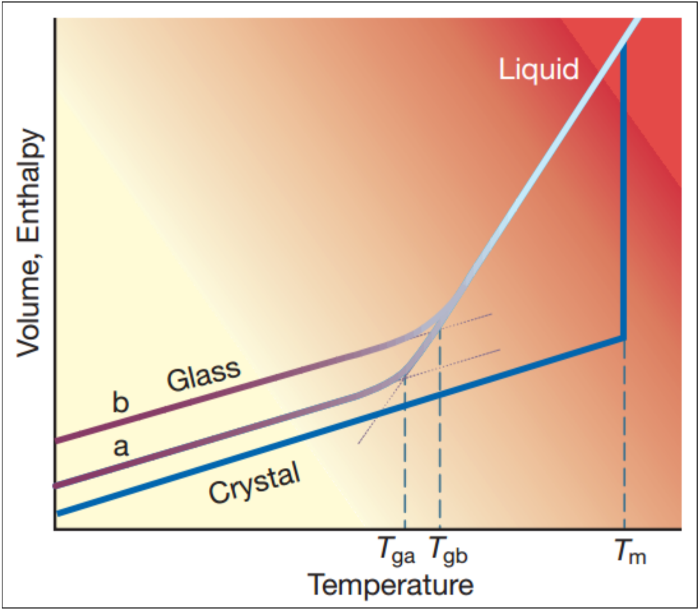
# this talk: **structural** order parameters

$$\frac{d\sigma}{dt} = f(\sigma, \dot{\gamma}, T, ???)$$

what should go here?



# structural order parameters? aging effects




**P. G. Debenedetti and F. H. Stillinger, Nature 2001**

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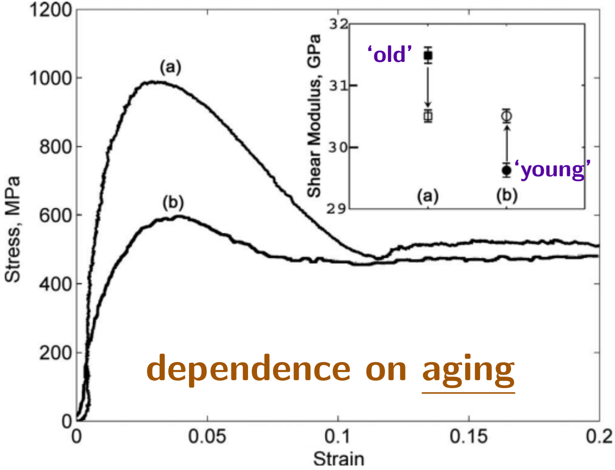

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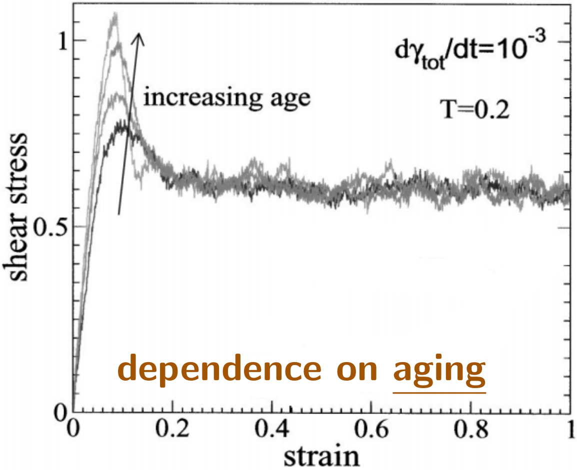
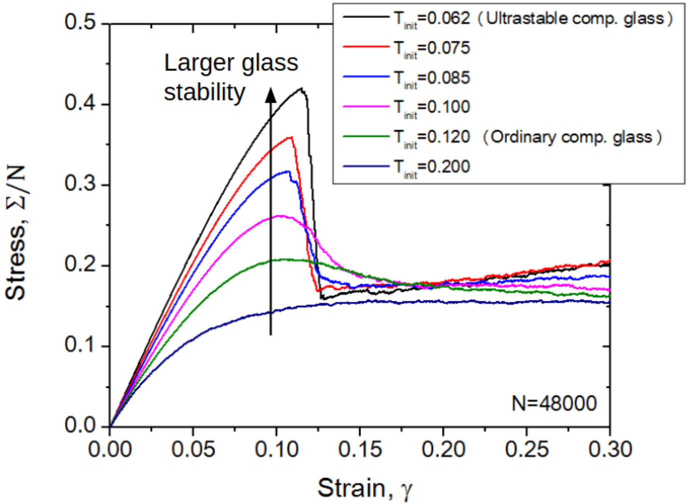


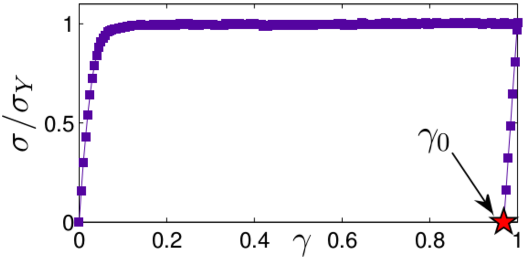

**dependence on aging**

# structural order parameters? aging effects



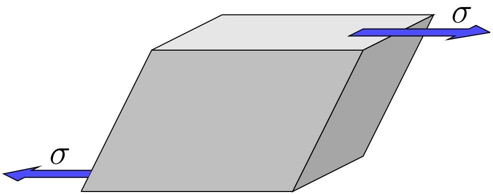

**many thanks to Misaki Ozawa!**

$$\frac{d\sigma}{dt} = f(\sigma, \dot{\gamma}, T, ???)$$



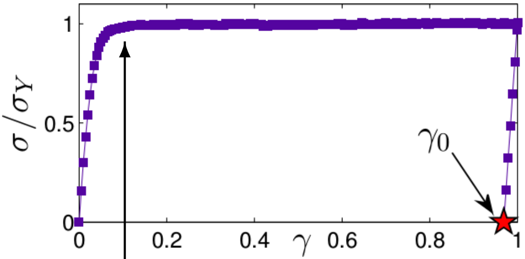

**simulations @**

$$T \to 0$$
$$\dot{\gamma} \to 0$$



# structural order parameters? anisotropy

$$\frac{d\sigma}{dt} = f(\sigma, \dot{\gamma}, T, ???)$$

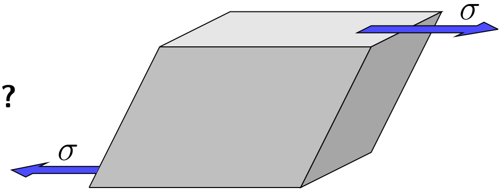



**simulations @**

$$T \to 0$$
$$\dot{\gamma} \to 0$$

**no stress overshoot**

**$\Rightarrow$ does structure evolve?**



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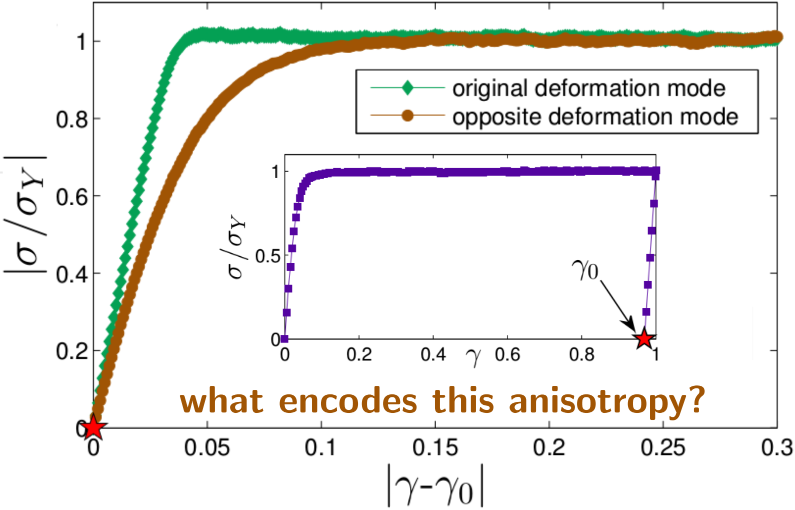
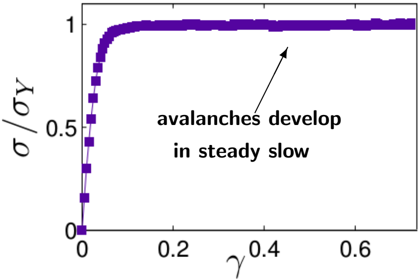


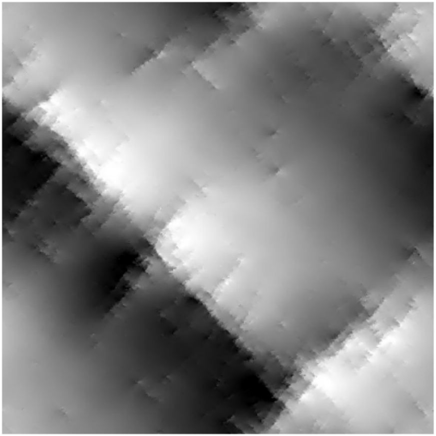

**what encodes this anisotropy?**

# structural order parameters? development of avalanches

$$\frac{d\sigma}{dt} = f(\sigma, \cancel{\dot{\gamma}}, \cancel{T}, ???)$$

$T = 0, \dot{\gamma} = 0$
**simulations**



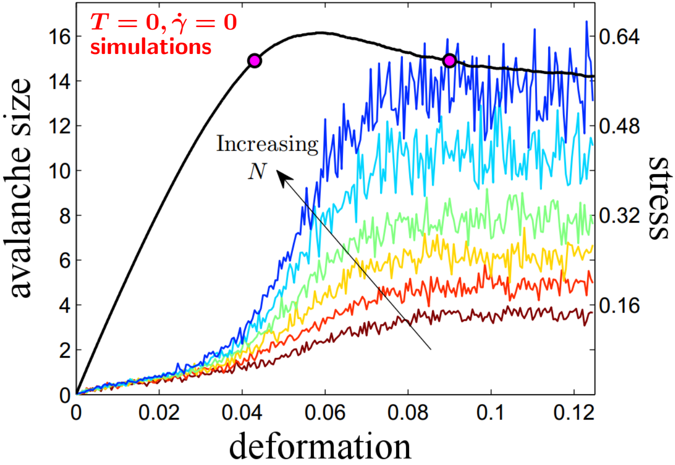



C.E. Maloney and M. O. Robbins, J. Phys.: Cond. Mat. (2008)

# structural order parameters? development of avalanches

$$\frac{d\sigma}{dt} = f(\sigma, \dot{\gamma}, T, ???)$$

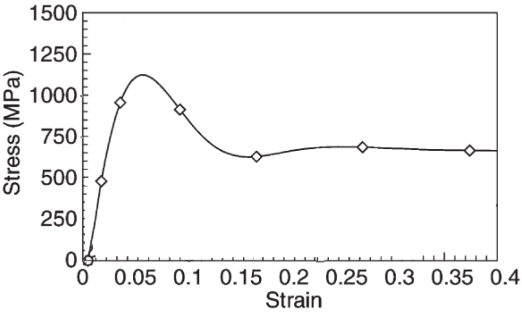
S. Karmakar, EL, and I. Procaccia, Phys. Rev. E 82, 055103(R) (2010).



# **structural** order parameters

$$\frac{d\sigma}{dt} = f(\sigma, \dot{\gamma}, T, ???)$$

what should go here?



# **structural** order parameters

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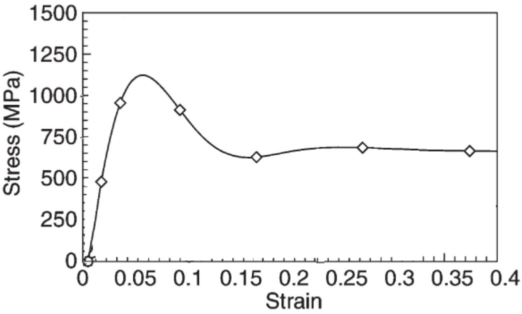
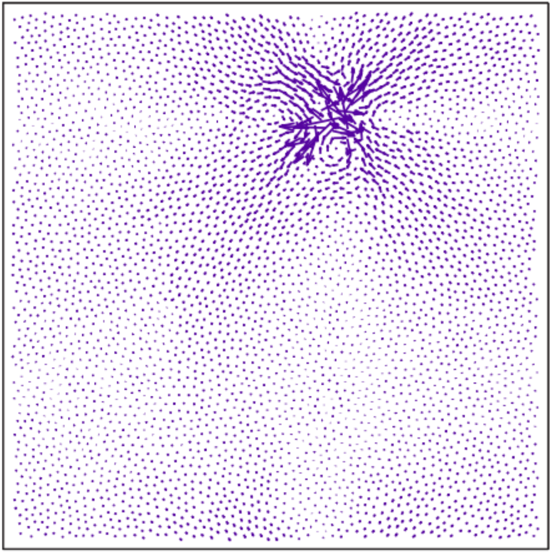
what should go here?

**what actually is $p(x)$ from elasto-plastic models?**



**what is plasticity on the micro-scale?**

## what is plasticity on the micro-scale?

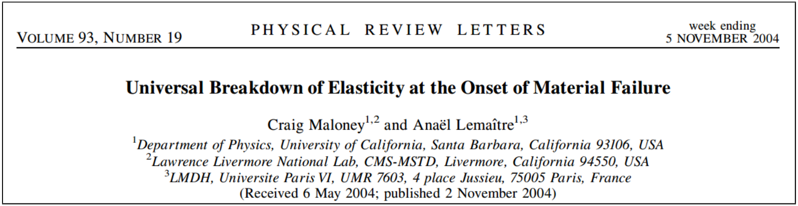


**'shear-transformation'**

**or**

**'shear-transformation-zone'**

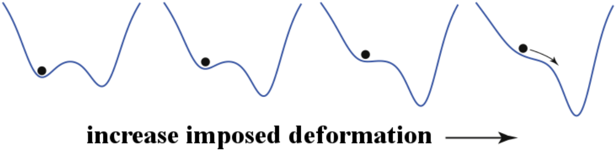
## how are plastic instabilities triggered?

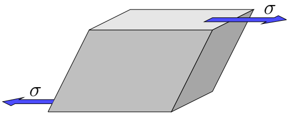

VOLUME 93, NUMBER 19 PHYSICAL REVIEW LETTERS week ending 5 NOVEMBER 2004

**Universal Breakdown of Elasticity at the Onset of Material Failure**

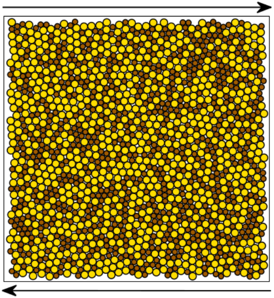
Craig Maloney[1,2] and Anaël Lemaître[1,3]
[1]*Department of Physics, University of California, Santa Barbara, California 93106, USA*
[2]*Lawrence Livermore National Lab, CMS-MSTD, Livermore, California 94550, USA*
[3]*LMDH, Universite Paris VI, UMR 7603, 4 place Jussieu, 75005 Paris, France*
(Received 6 May 2004; published 2 November 2004)

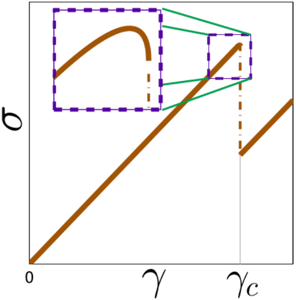
**'energy landscape' picture:**



# micromechanics of plastic instabilities





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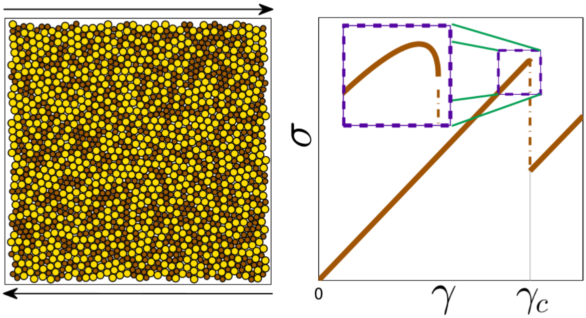


**consider linear stability**

$$\mathcal{M}_{jk} \equiv \frac{\partial^2 U}{\partial \vec{x}_j \partial \vec{x}_k}$$

**dynamical matrix / hessian**

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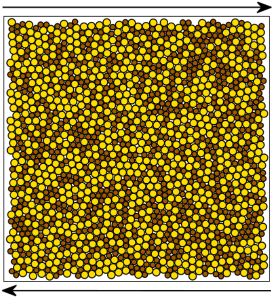

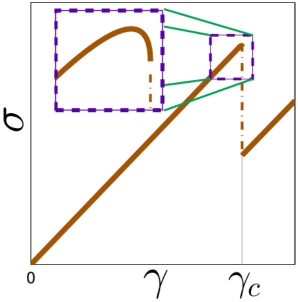


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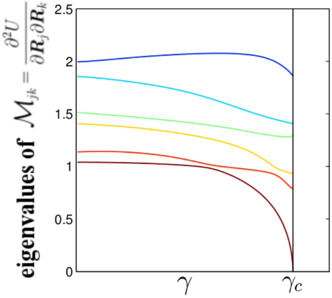

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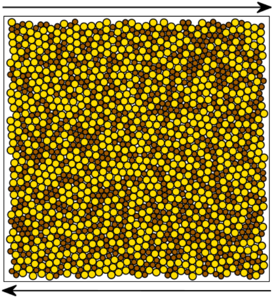
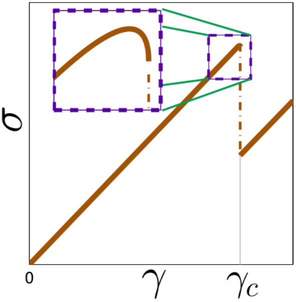
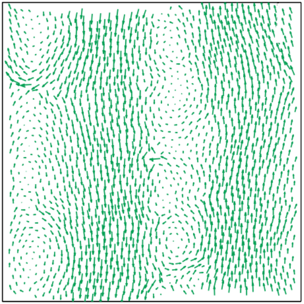
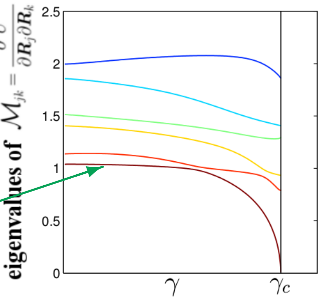
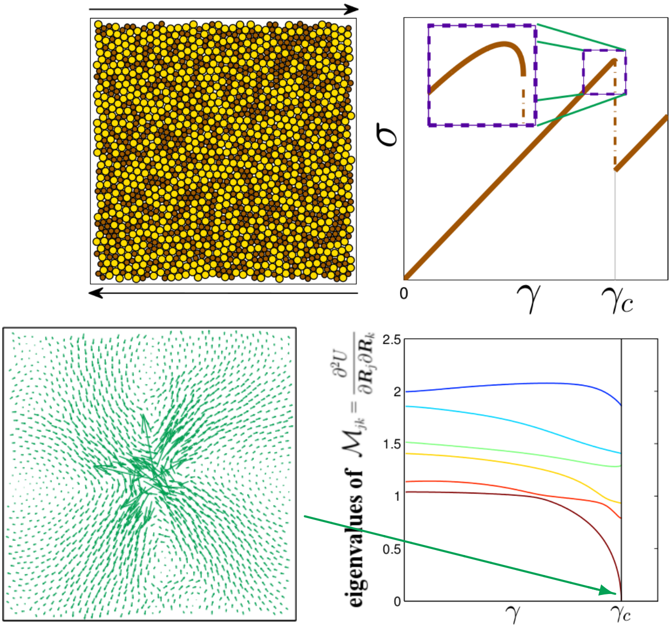






# micromechanics of plastic instabilities



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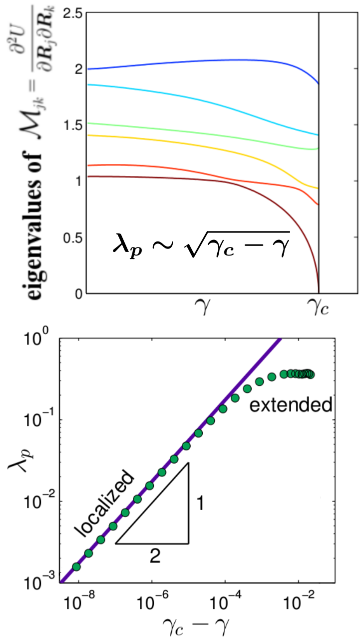

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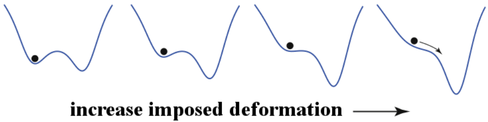


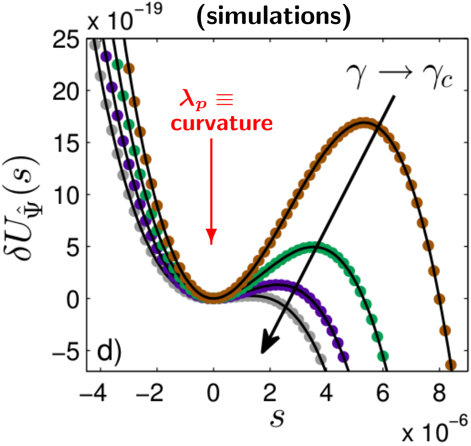


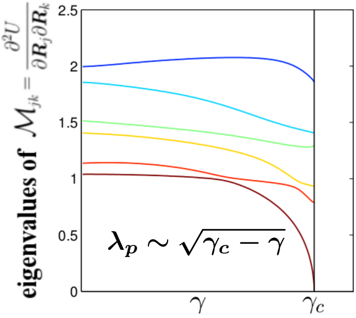


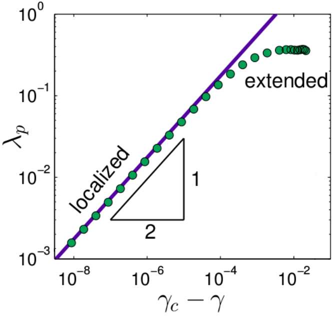

# predicting plastic instabilities using normal modes

**observation: 'linear' (normal) modes are indicative of plastic instabilities.**

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**proposition: use normal modes to detect 'soft spots'**

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epl A Letters Journal Exploring the Frontiers of Physics
April 2010
EPL, **90** (2010) 16004 www.epljournal.org
doi: 10.1209/0295-5075/90/16004

**Vibrational modes as a predictor for plasticity in a model glass**

A. Tanguy[(a)], B. Mantisi and M. Tsamados

*Université de Lyon - F-69622, Lyon, France, EU and*
*CNRS, UMR5586, Laboratoire de Physique de la Matière Condensée et des Nanostructures, Université Lyon 1*
*F-69622, Villeurbanne Cedex, France, EU*

PRL **107,** 108302 (2011) PHYSICAL REVIEW LETTERS week ending 2 SEPTEMBER 2011

**Vibrational Modes Identify Soft Spots in a Sheared Disordered Packing**

M. L. Manning*
*Princeton Center for Theoretical Science, Princeton, New Jersey 08544, USA*
*Department of Physics, Syracuse University, Syracuse, New York 13244, USA*

A. J. Liu
*Department of Physics, University of Pennsylvania, Philadelphia, Pennsylvania 19130, USA*
(Received 21 December 2010; published 31 August 2011)

PHYSICAL REVIEW E **89**, 042304 (2014)

**Predicting plasticity with soft vibrational modes: From dislocations to glasses**

Jörg Rottler,[1] Samuel S. Schoenholz,[2] and Andrea J. Liu[2]
[1]*Department of Physics and Astronomy, University of British Columbia, 6224 Agricultural Road, Vancouver, British Columbia, Canada V6T 1Z4*
[2]*Department of Physics, University of Pennsylvania, Philadelphia, Pennsylvania 19130, USA*
(Received 19 December 2013; revised manuscript received 26 February 2014; published 14 April 2014)

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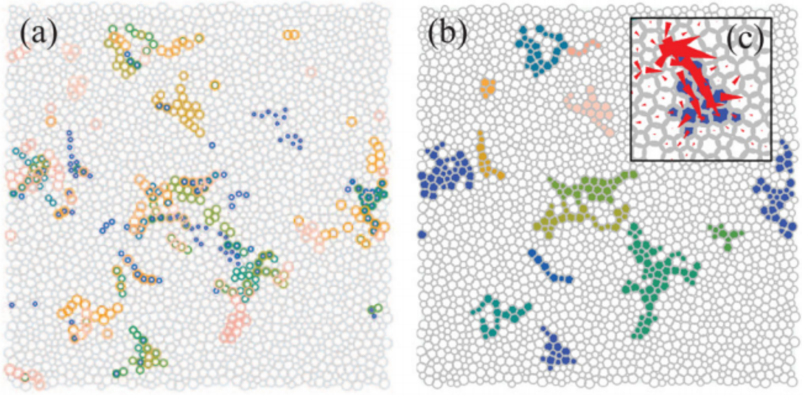
**problems:**

# predicting plastic instabilities using normal modes

**observation**: **'linear' (normal) modes are indicative of plastic instabilities.**

**proposition**: **use normal modes to detect 'soft spots'**

**problems:** **1) no quantitative information**




**(Manning and Liu, PRL 2011)**

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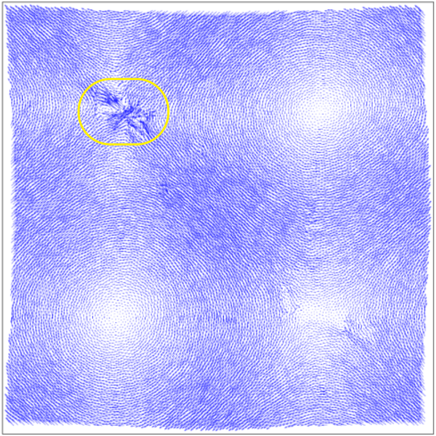
**problems:** **2) hybridizations with plane waves**



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**problems:** **2) hybridizations with plane waves**

compare lowest energy
plane wave freq. $\omega^2 \sim 1/L^2$
with $\lambda_p \sim \sqrt{\gamma_c - \gamma}$

$\Rightarrow \quad \gamma_c - \gamma \sim L^{-4}$
dehybridization strain scale

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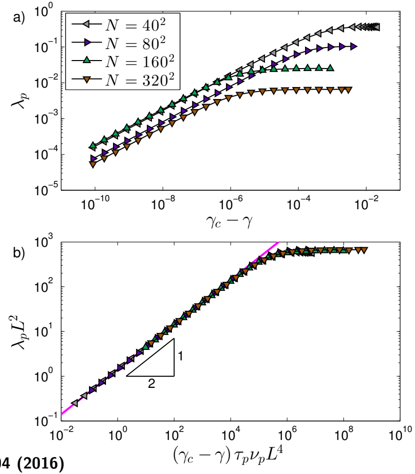


EL, Phys. Rev. E 93, 053004 (2016)

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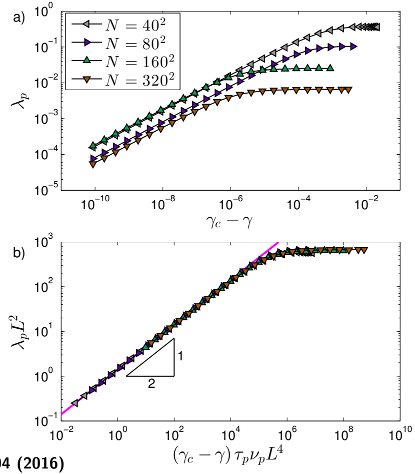
**problematic as $L$ increases...**




**EL, Phys. Rev. E 93, 053004 (2016)**

# predicting plastic instabilities – can we do better?

**is there a way to define and detect plastic modes far from instability strains, deep in the hybridized regime?**

**yes**

**probably**

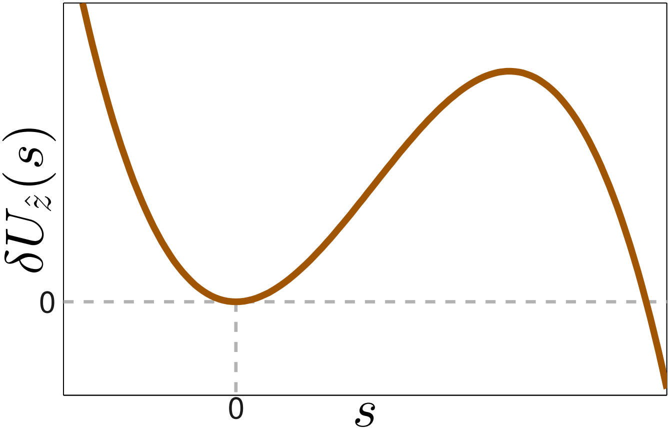
**(TBD...)**

**is there a way to <u>define</u> and <u>detect</u> plastic modes far from instability strains, deep in the hybridized regime?**

# the barrier function – definition

**consider the energy variation upon displacing particles' coordinates $\vec{x}$ according to $\delta\vec{x} = s\hat{z}$**

$$\delta U_{\hat{z}}(s) \simeq \frac{1}{2}\kappa_{\hat{z}} s^2 + \frac{1}{6}\tau_{\hat{z}} s^3$$



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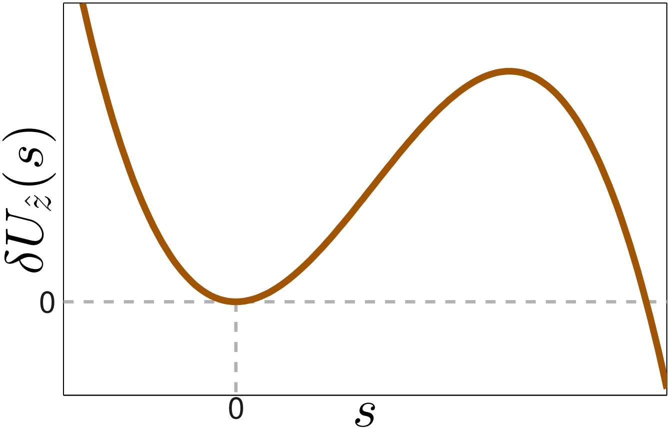

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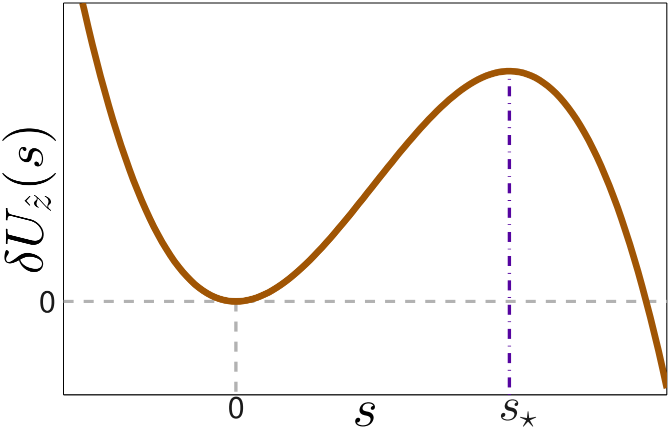

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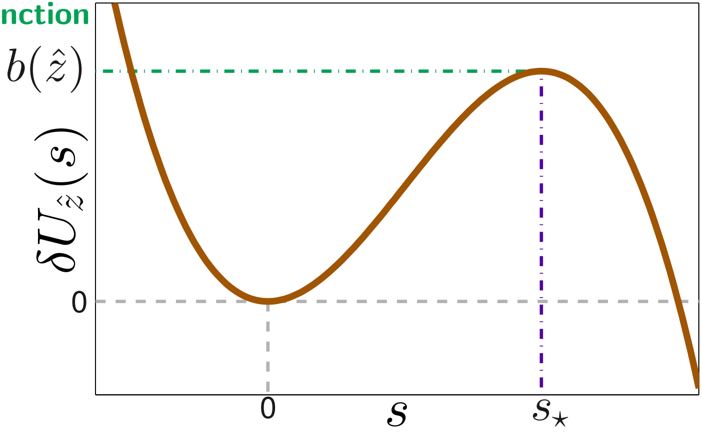

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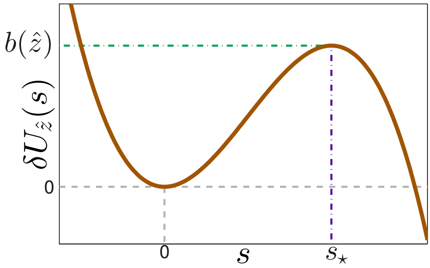

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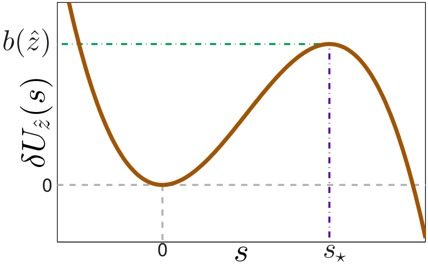
shorthand notations:

$$\mathcal{M} \equiv \frac{\partial^2 U}{\partial\vec{x}\partial\vec{x}} \quad \text{'dynamical matrix'}$$

$$U''' \equiv \frac{\partial^3 U}{\partial\vec{x}\partial\vec{x}\partial\vec{x}} \quad \text{'cubic tensor'}$$



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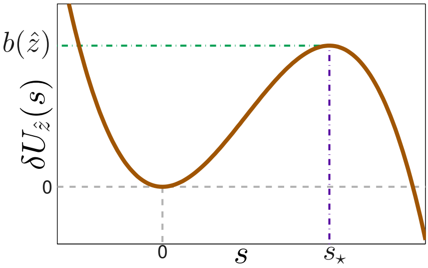
only a function of **inherent state information**, and the direction $\hat{z}$



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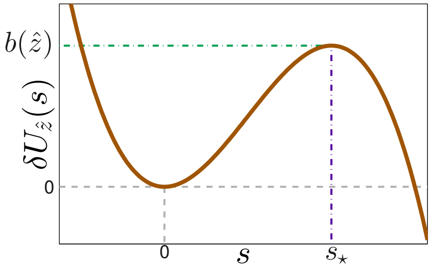
**directions $\hat{z}$ which take the system over low saddle points will have small $b(\hat{z})$'s**



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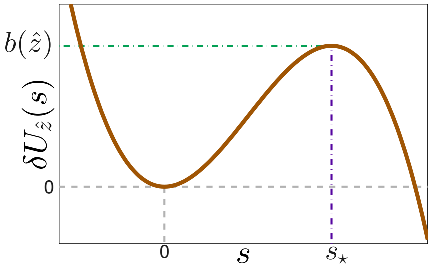
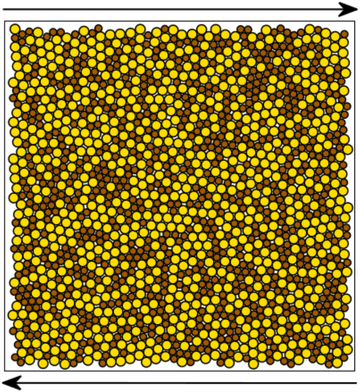
**directions $\hat{z}$ which take the system over low saddle points will have small $b(\hat{z})$'s**

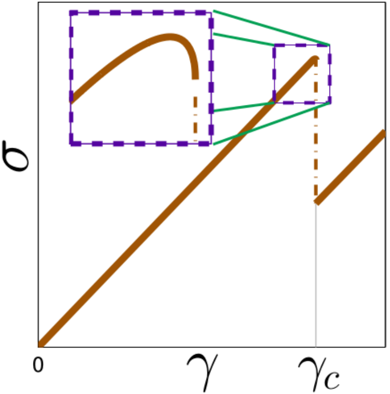
**$\Rightarrow$ find directions with small $b(\hat{z})$ by minimizing $b(\hat{z})$ over directions $\hat{z}$**



# finding small $b(\hat{z})$'s

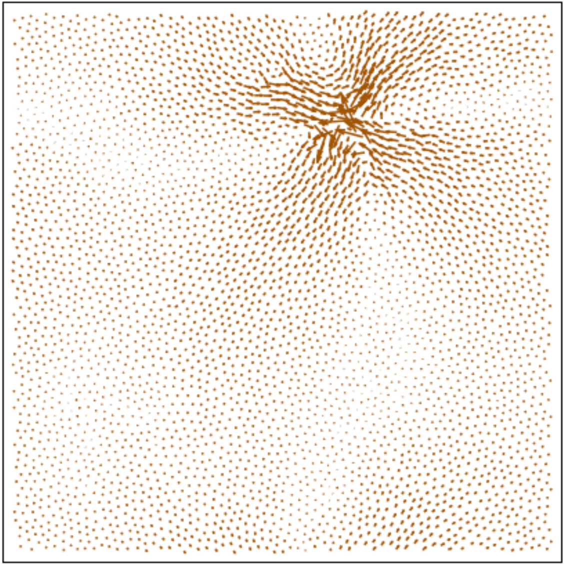
**setup:**

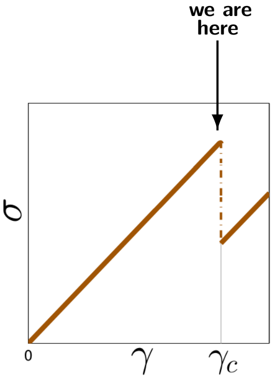




# finding small $b(\hat{z})$'s

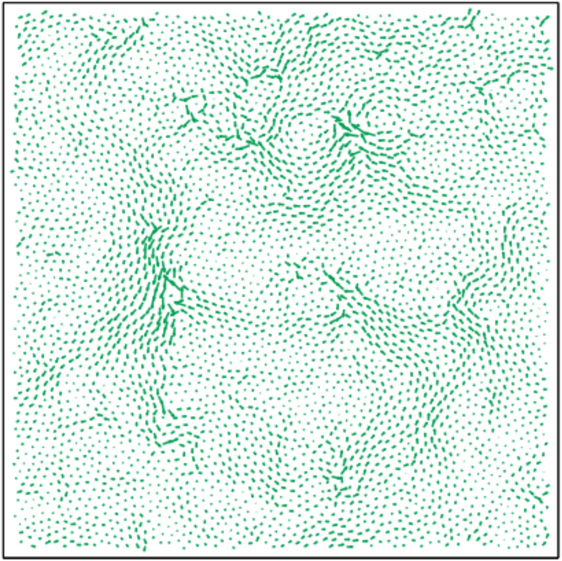
destabilizing **linear** mode $\hat{\Psi}_p$, $\gamma \to \gamma_c$

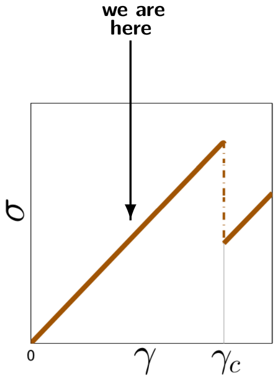




# finding small $b(\hat{z})$'s

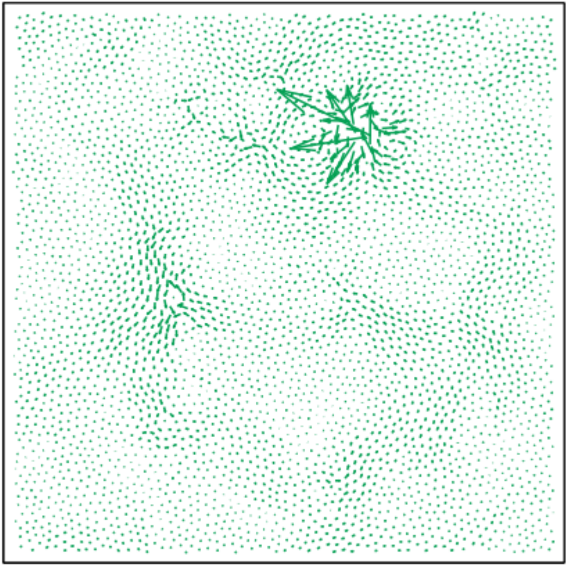
linear response to shear, $\gamma_c - \gamma \sim 10^{-2}$, use as initial guess $\hat{z}_{\text{ini}}$

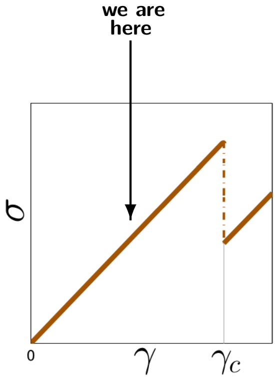




# finding small $b(\hat{z})$'s

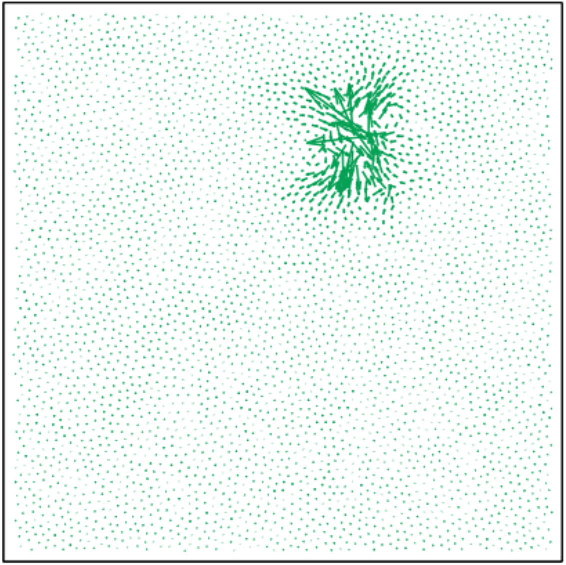
minimize $b(\hat{z})$, after 12 iterations, $\gamma_c - \gamma \sim 10^{-2}$

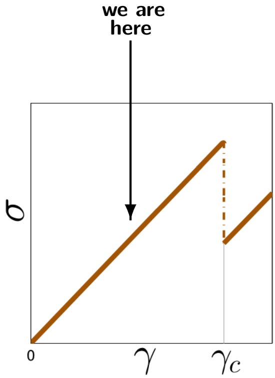




# finding small $b(\hat{z})$'s

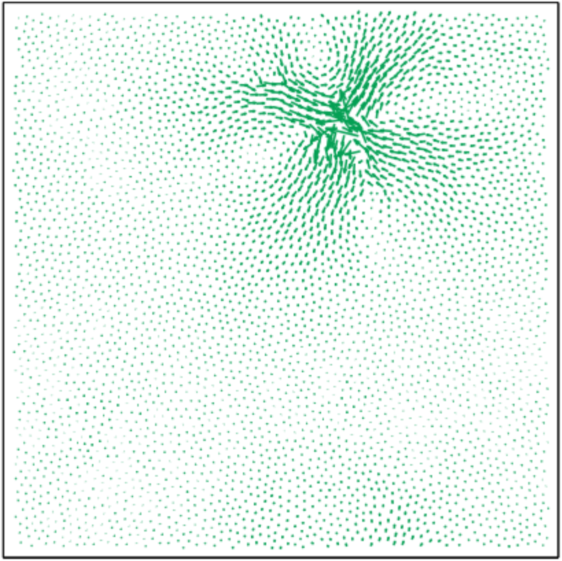
minimize $b(\hat{z})$, after 24 iterations, $\gamma_c - \gamma \sim 10^{-2}$

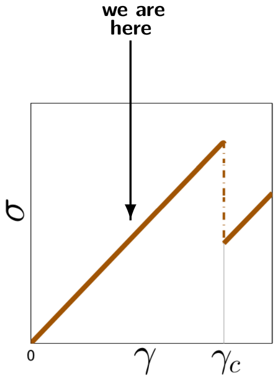




# finding small $b(\hat{z})$'s

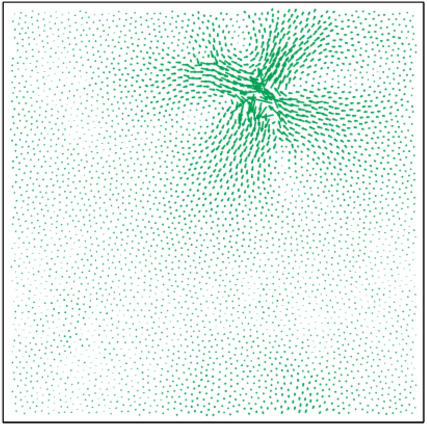
minimization converged, $\gamma_c - \gamma \sim 10^{-2}$



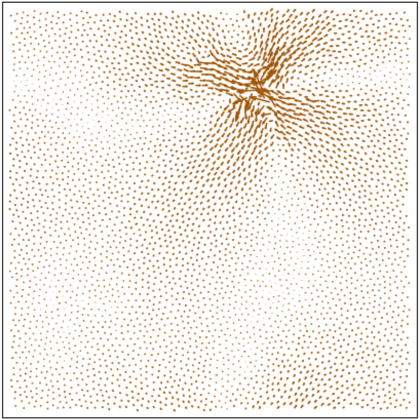


# finding small $b(\hat{z})$'s

direction $\hat{z}$ that **minimizes** $\boldsymbol{b(\hat{z})}$
$\boldsymbol{\gamma_c - \gamma \sim 10^{-2}}$



destabilizing **linear** mode $\boldsymbol{\hat{\Psi}_p}$
$\boldsymbol{\gamma_c - \gamma \sim 10^{-7}}$

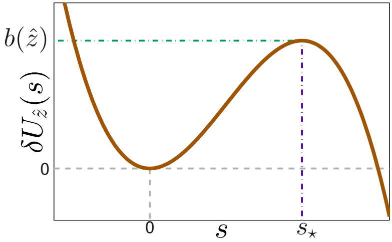


# nonlinear plastic modes – definition

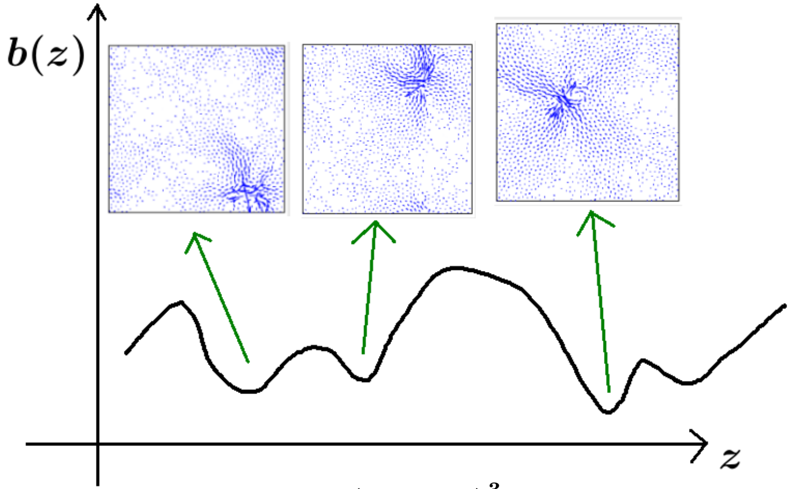
**nonlinear plastic modes** are collective displacement directions $\hat{\pi}$ for which the barrier function $b(\hat{z})$ displays a **local minimum**

$$\left.\frac{\partial b}{\partial \vec{z}}\right|_{\hat{\pi}} = 0, \quad \left.\frac{\partial^2 b}{\partial \vec{z} \partial \vec{z}}\right|_{\hat{\pi}} > 0$$

$$b(\hat{z}) \equiv \frac{2}{3} \frac{(\mathcal{M} : \hat{z}\hat{z})^3}{(U''' \vdots \hat{z}\hat{z}\hat{z})^2}$$



# nonlinear plastic modes – illustration

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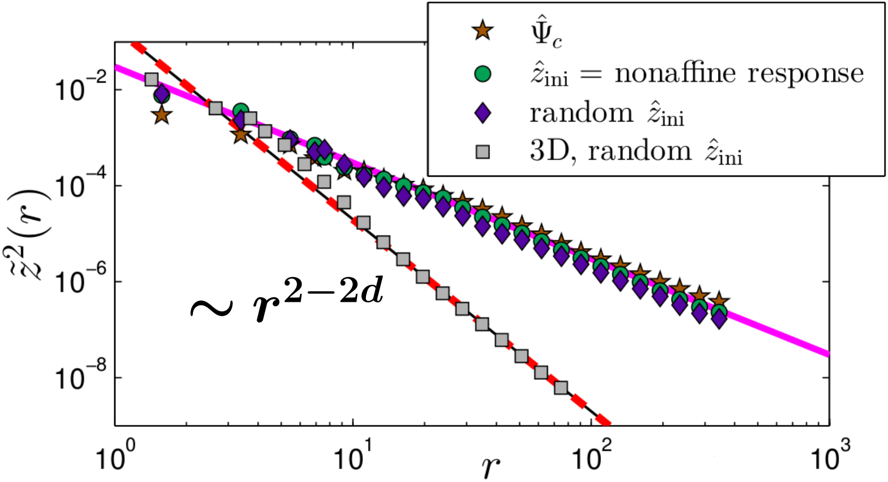
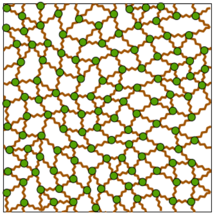
**nonlinear plastic modes decay like the response to local perturbation** $|\hat{\pi}| \sim r^{1-d}$

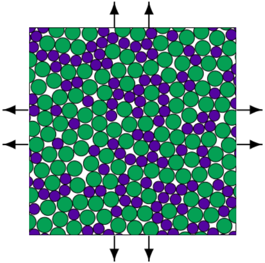


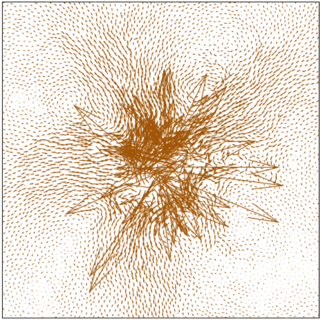
# nonlinear plastic modes – spatial structure

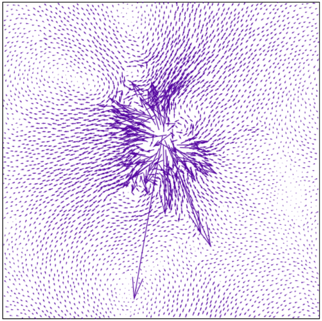
**no internal stresses**



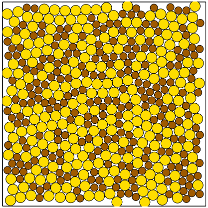
**glass under tension**





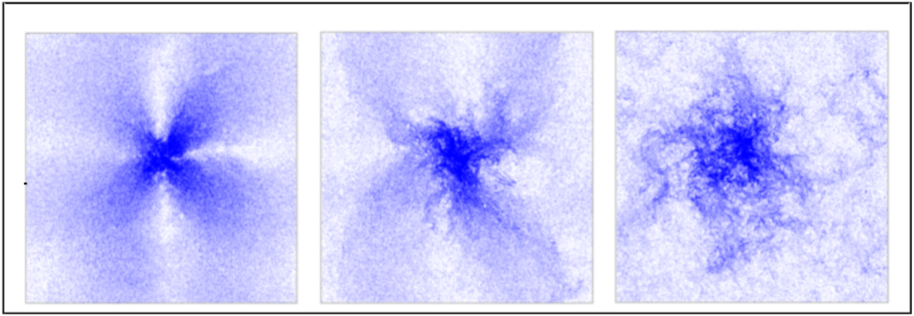


# nonlinear plastic modes – core size



packings of harmonic discs

'unjamming'



$p = 10^{-1}$ $p = 10^{-3}$ $p = 10^{-5}$

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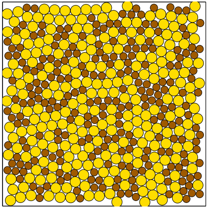
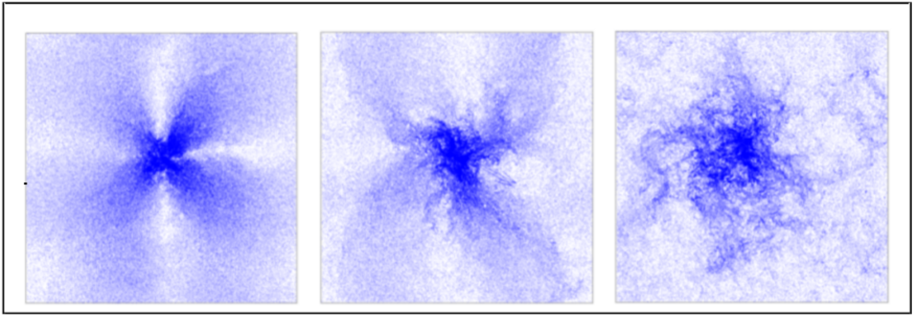


packings of harmonic discs

$$\ell_c \sim \frac{1}{\sqrt{z - z_c}} \sim p^{-1/4}?$$

'unjamming'



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$$\left.\frac{\partial b}{\partial \vec{z}}\right|_{\hat{\pi}} = 0, \quad \left.\frac{\partial^2 b}{\partial \vec{z} \partial \vec{z}}\right|_{\hat{\pi}} > 0$$

why are nonlinear plastic modes the **natural micromechanical objects** to consider in plasticity studies?

# nonlinear plastic modes – deformation dynamics

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$$(\star) \qquad \boldsymbol{\mathcal{M}} \cdot \hat{\boldsymbol{\pi}} = \frac{\boldsymbol{\kappa}_{\hat{\pi}}}{\boldsymbol{\tau}_{\hat{\pi}}} \boldsymbol{U}''' : \hat{\boldsymbol{\pi}}\hat{\boldsymbol{\pi}}$$

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**how do the stiffnesses $\boldsymbol{\kappa}_{\hat{\pi}}$ depend on deformation?**

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**how do the stiffnesses $\kappa_{\hat{\pi}}$ depend on deformation?**

$$\frac{d\kappa_{\hat{\pi}}}{d\gamma} \simeq \frac{d\boldsymbol{\mathcal{M}}}{d\gamma} : \hat{\pi}\hat{\pi} = -U''' \vdots \hat{\pi}\hat{\pi} \left( \boldsymbol{\mathcal{M}}^{-1} \cdot \frac{\partial^2 U}{\partial \vec{x} \partial \gamma} \right)$$

**following $(\star)$:**
$$= -\frac{\tau_{\hat{\pi}} \hat{\pi} \cdot \boldsymbol{\mathcal{M}} \cdot \boldsymbol{\mathcal{M}}^{-1} \cdot \frac{\partial^2 U}{\partial \vec{x} \partial \gamma}}{\kappa_{\hat{\pi}}}$$

$$= -\frac{\tau_{\hat{\pi}} \nu_{\hat{\pi}}}{\kappa_{\hat{\pi}}},$$

$\tau_{\hat{\pi}} \equiv \frac{\partial^3 U}{\partial \vec{x} \partial \vec{x} \partial \vec{x}} \vdots \hat{\pi}\hat{\pi}\hat{\pi}$ asymmetry

$\nu_{\hat{\pi}} \equiv \hat{\pi} \cdot \frac{\partial^2 U}{\partial \vec{x} \partial \gamma}$ shear coupling

# nonlinear plastic modes – deformation dynamics

**we found a simple form for** $$\frac{d\boldsymbol{\kappa}_{\hat{\pi}}}{d\boldsymbol{\gamma}} \simeq -\frac{\boldsymbol{\tau}_{\hat{\pi}}\boldsymbol{\nu}_{\hat{\pi}}}{\boldsymbol{\kappa}_{\hat{\pi}}}$$

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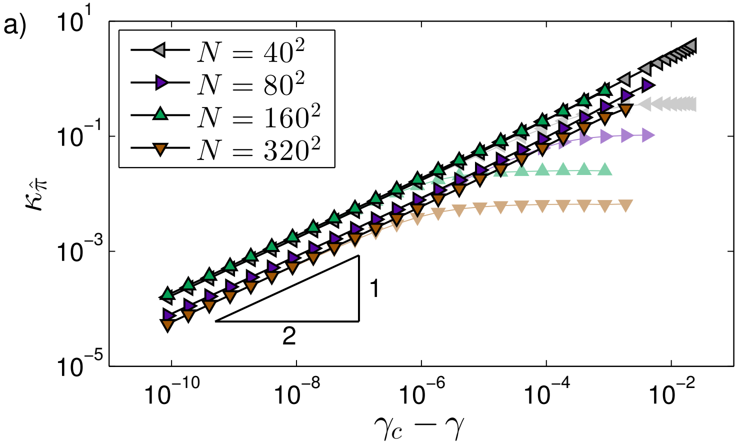

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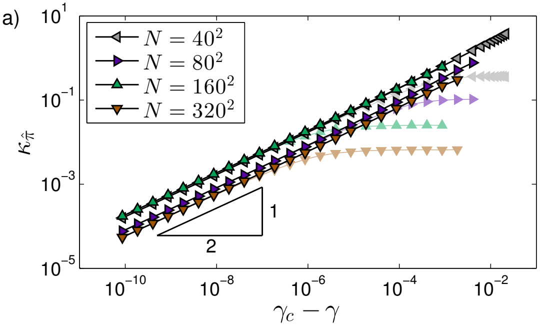
**important points:**

1) deformation dynamics only weakly coupled to other modes
2) $N$-independent range of validity, in stark contrast with linear modes



# nonlinear plastic modes – deformation dynamics

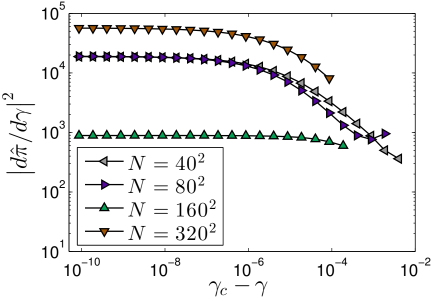
linear modes' variations are **singular**, plastic modes' are **regular**:

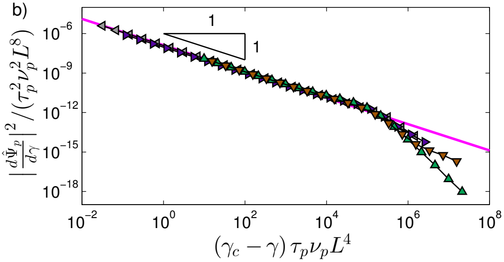
**nonlinear plastic modes**

$$\left|\frac{d\hat{\pi}}{d\gamma}\right| \sim \text{const.}$$

**linear destabilizing mode**

$$\left|\frac{d\hat{\Psi}_p}{d\gamma}\right| \sim \frac{L^2}{\sqrt{\gamma_c - \gamma}}$$




EL, *Micromechanics of nonlinear plastic modes*, Phys. Rev. E 93, 053004 (2016)

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**linear destabilizing mode**

$$\left|\frac{d\hat{\Psi}_p}{d\gamma}\right| \sim \frac{L^2}{\sqrt{\gamma_c - \gamma}}$$

**this is odd since both stiffnesses follow same EOM**

$$\frac{d\kappa}{d\gamma} \sim \frac{1}{\kappa}$$

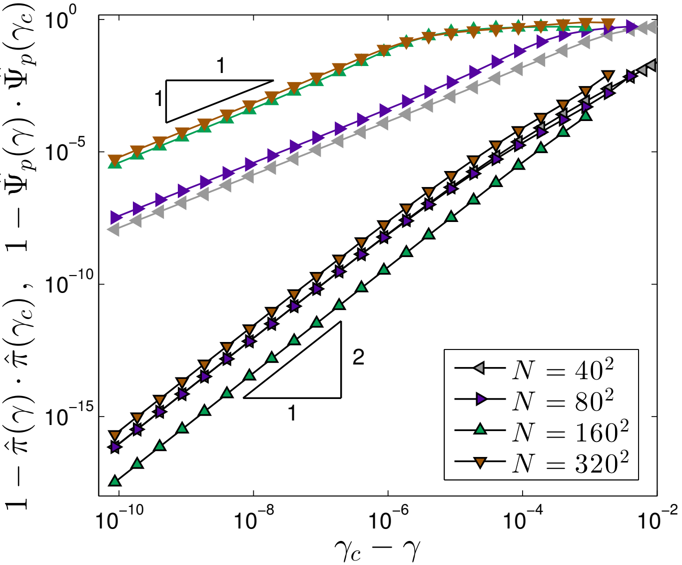
$$(\kappa \equiv \mathcal{M} : \hat{\pi}\hat{\pi})$$

$$\frac{d\lambda_p}{d\gamma} \sim \frac{1}{\lambda_p}$$

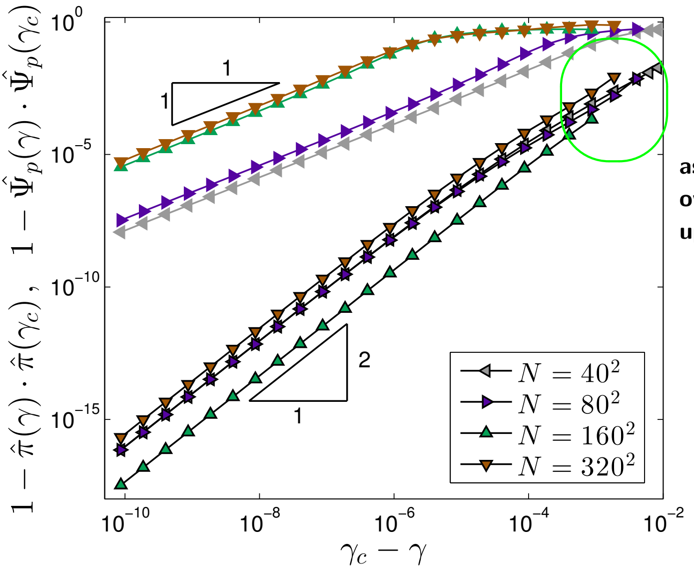
$$\left(\lambda_p \equiv \mathcal{M} : \hat{\Psi}_p\hat{\Psi}_p\right)$$

EL, *Micromechanics of nonlinear plastic modes*, Phys. Rev. E 93, 053004 (2016)

# predictiveness of nonlinear plastic modes

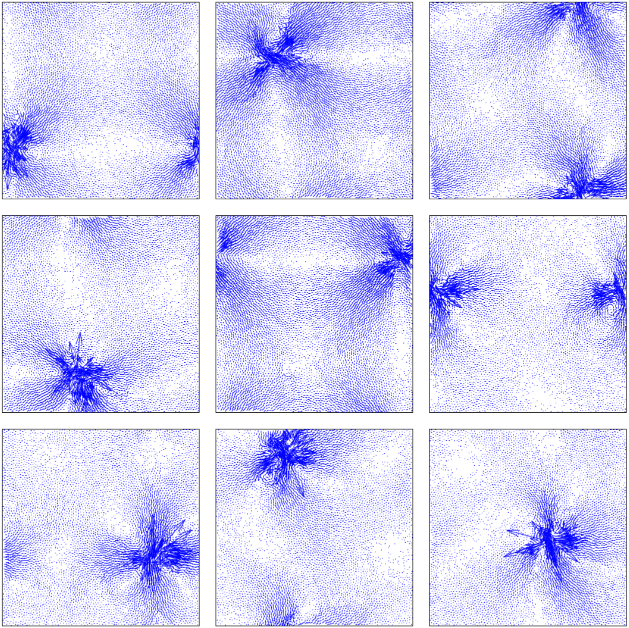


# predictiveness of nonlinear plastic modes




**as soon as detected, overlap with instability up to more than 99%!**

# TBD: detecting the **field** of nonlinear plastic modes



**modes detected in a single sample**

**in progress...**

# statistics of nonlinear plastic modes

what attributes of NPM's should we care about?

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<u>recall:</u> NPM's are characterized by:

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(recall that $\kappa = \sqrt{2\tau\nu}\sqrt{\gamma_c - \gamma}$, and $\frac{d\kappa}{d\gamma} = -\frac{\tau\nu}{\kappa}$)

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assume $\tau$ and $\nu$ have non-interesting distributions, **focus on stiffnesses $\kappa$**

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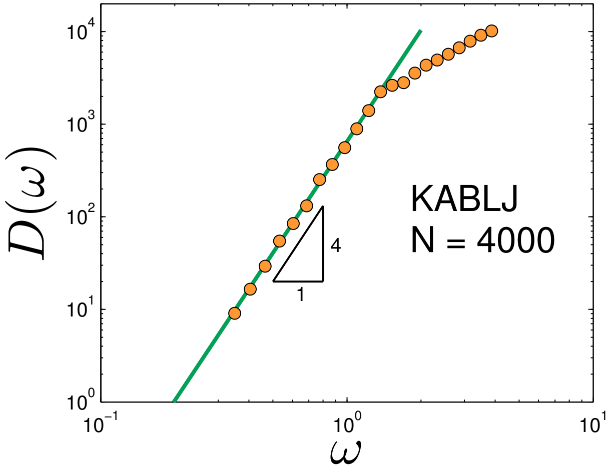
# how are NPM stiffnesses $\kappa$ distributed?

it was recently observed that a **universal** distribution $D(\omega) \sim \omega^4$ of quasi-localized **glassy modes** appears at low frequencies




EL, Düring, & Bouchbinder, PRL 2016

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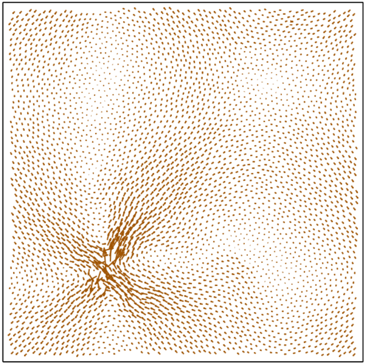
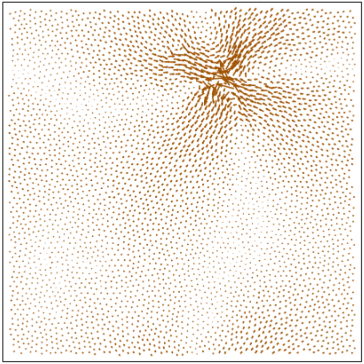
**harmonic** glassy mode
in **undeformed** sample



plastic instability
upon imposing **shear**



# how are NPM stiffnesses $\kappa$ distributed?

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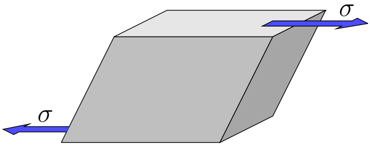


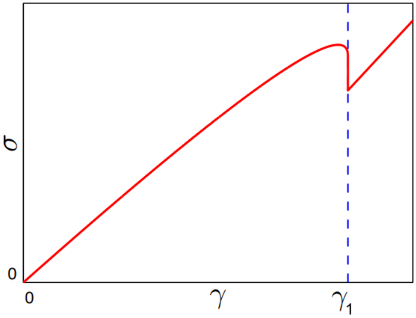

# extent of first elastic branch

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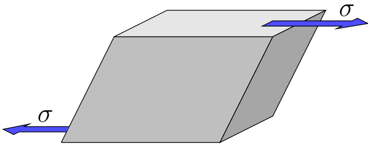
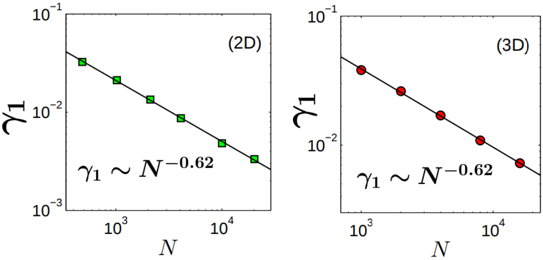
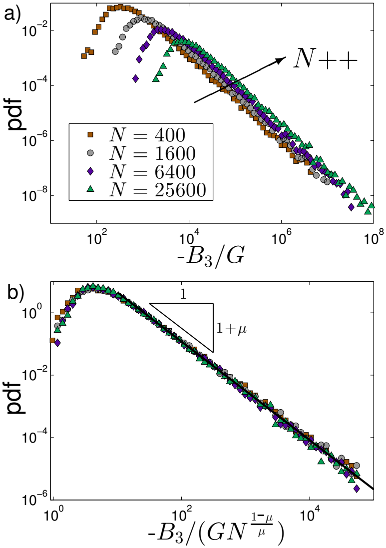



Hentschel, Karmakar, EL, & Procaccia, PRE 2011

# finite-size scaling of nonlinear elasticity

a similar discrepancy appears for nonlinear elastic moduli




$$B_3 \equiv \frac{d^3\sigma}{d\gamma^3}$$

we find $\mu \approx 0.57$,

whereas $D(\omega) \sim \omega^4$

implies $\mu = 1/2$

Hentschel, Karmakar, EL, & Procaccia, PRE 2011

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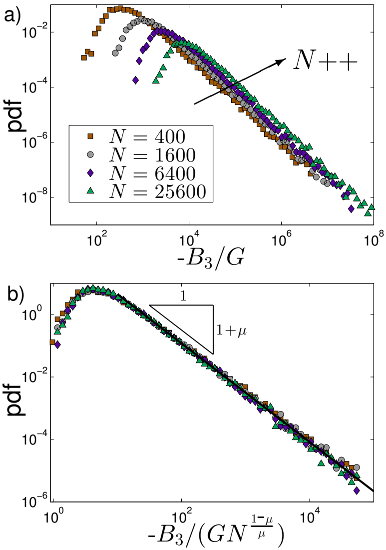


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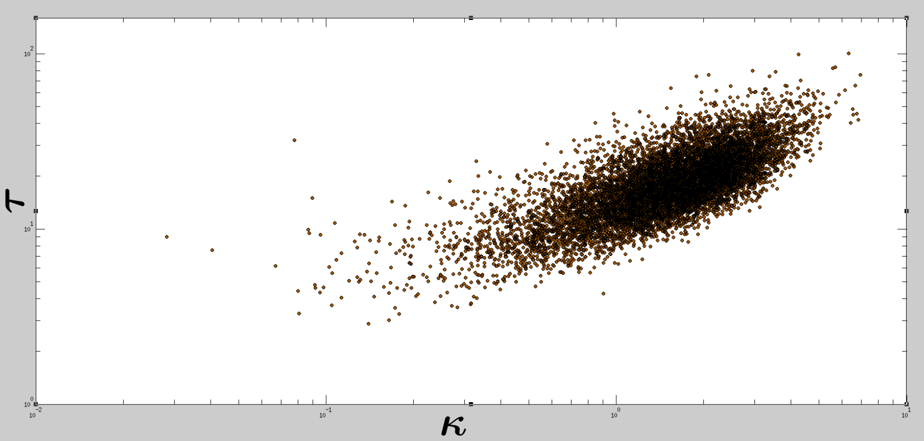
**asymmetries should depend on stiffnesses**

Hentschel, Karmakar, EL, & Procaccia, PRE 2011

# dependence of asymmetries on stiffnesses

data measured for low-energy NPMs in 3D with $N = 2000$



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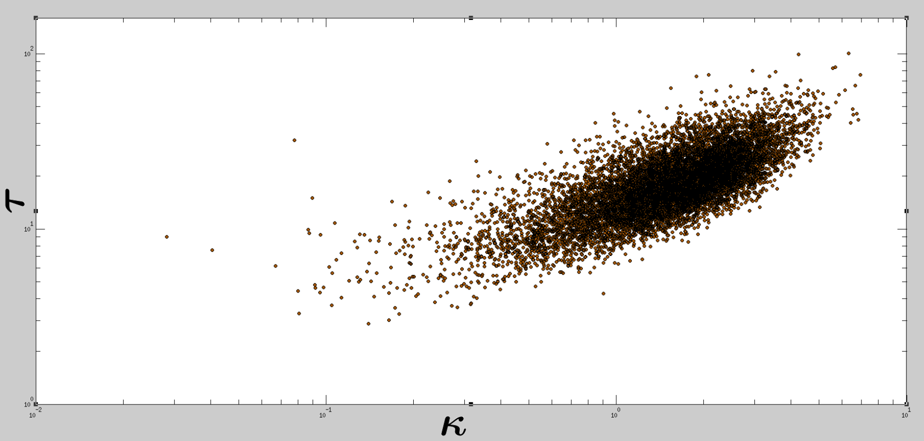
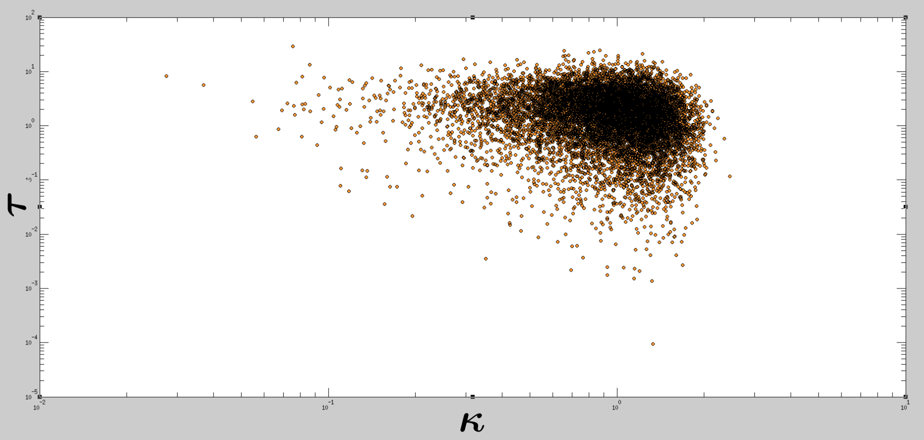



does this trend persist to $\boldsymbol{\kappa} \to \mathbf{0}$?

# dependence of asymmetries on stiffnesses

data measured for low-energy **harmonic modes** in 3D with $N = 2000$

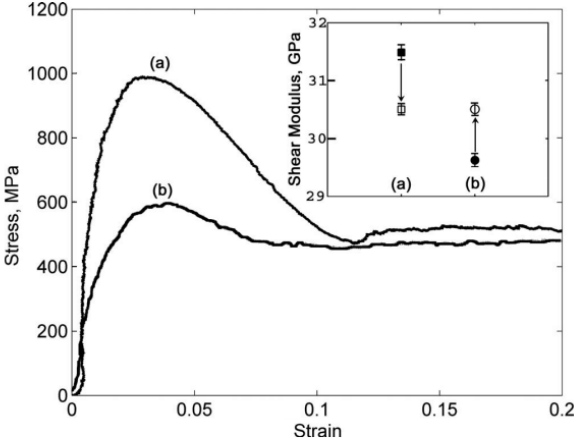



asymmetries appear to be **stiffness independent** for harmonic modes, but **not** for plastic modes

# summary: nonlinear plastic modes

- understanding elasto-plasticity and yielding requires the proper identification of the relevant structural state variables

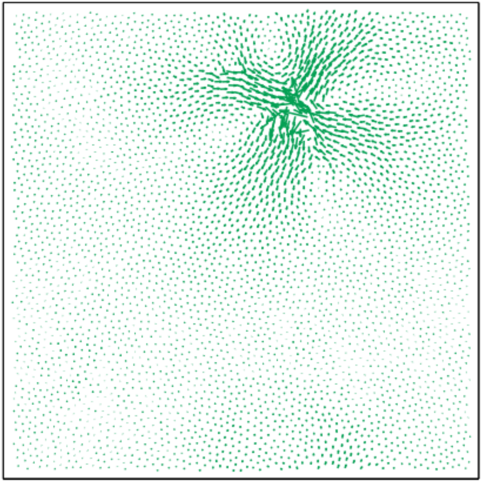
J. Lu, G. Ravichandran, W. Johnson, Acta Materialia 51 (2003)



# summary: nonlinear plastic modes

- NPMs offer a robust **micromechanical** definition of plasticity carriers, based solely on **inherent state information**

$$\left.\frac{\partial b}{\partial \vec{z}}\right|_{\hat{\pi}} = 0$$



# summary: nonlinear plastic modes

- deformation dynamics of NPMs: $N$-independent,
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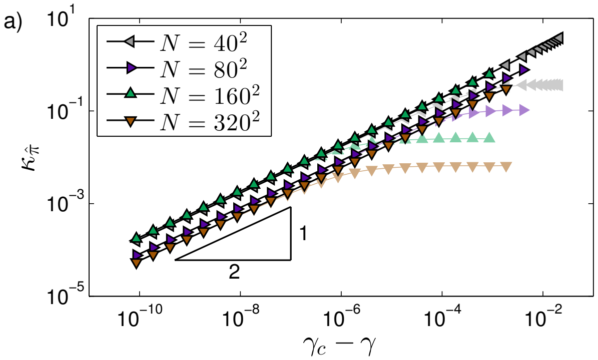
$$\frac{d\kappa}{d\gamma} \simeq -\frac{\tau\,\nu}{\kappa}$$



# summary: nonlinear plastic modes

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asymmetry — deformation coupling

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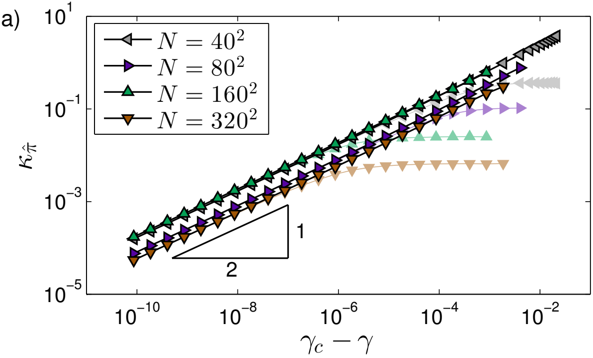
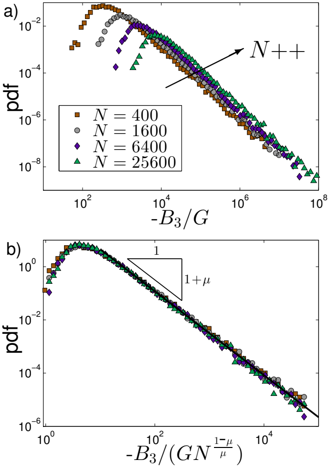
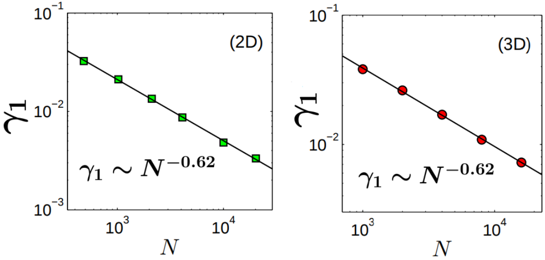


# summary: nonlinear plastic modes

- still something left to understand regarding the statistics of NPMs, and the stiffness-dependence of asymmetries & deformation coupling



Ph.D. & postDoc positions available!

e.lerner@uva.nl

thanks for your attention! questions?

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