Yielding of amorphous solids
(Simons workshop) @ENS,Paris
2017/10/27

Exploring complex free-energy landscape of the simplest glasses by rheology

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Fluctuation & Structure

科研費
KAKENHI

大阪大学
OSAKA UNIVERSITY

Synergy of Fluctuation and Structure :
Quest for Universal Laws in Non-Equilibrium Systems
2013-2017 Grant-in-Aid for Scientific Research on Innovative Areas, MEXT, Japan

10sec/0min

Collaborators

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Outline

Linear response of glasses under shear :theory

- First attempt - 3dim soft sphere (1RSB)

  HY and M. Mézard, Phys. Rev. Lett. 105, 015504 (2010).
  HY, J. Chem. Phys.136, 214108 (2012).

- Large-d hard sphere (1RSB/full RSB)

  HY and F. Zamponi, Phys. Rev. E 90, 022302 (2014).

3D hard sphere under shear (+ (de)compression) : simulation

- Linear responses in stable/marginal glasses

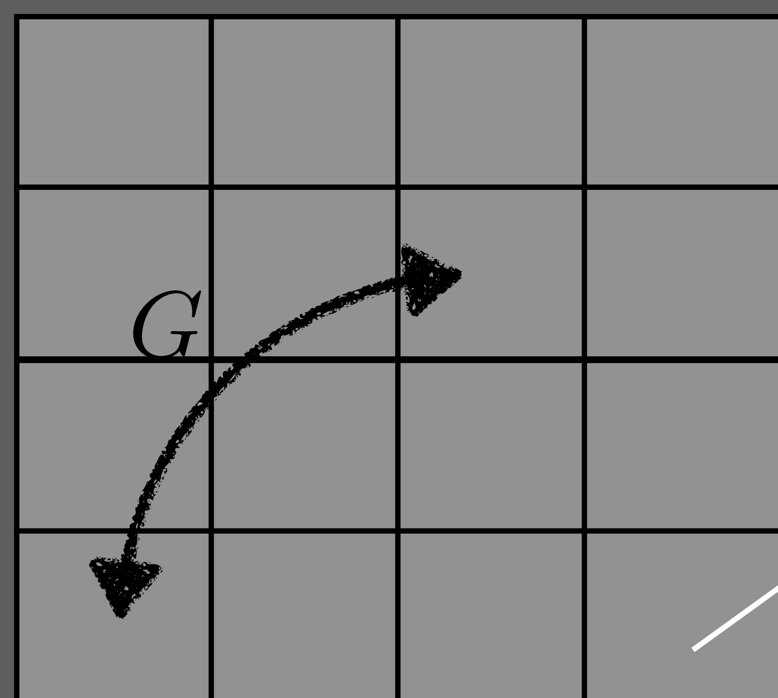
  Y. Jin and HY, Nature Communications 8, 14935 (2017).

- Non linear responses (shear jamming/yielding/plasticity)

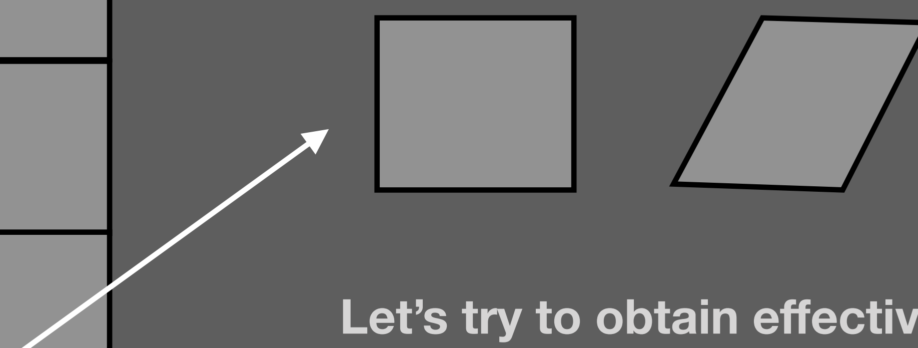
  Y. Jin, HY, P. Urbani and F. Zamponi, in preparation

P. Urbani's talk

Linear response of glasses under shear: theory



Replicated liquid theory=
1st principle computation
to extract effective
“Einstein model” for glasses



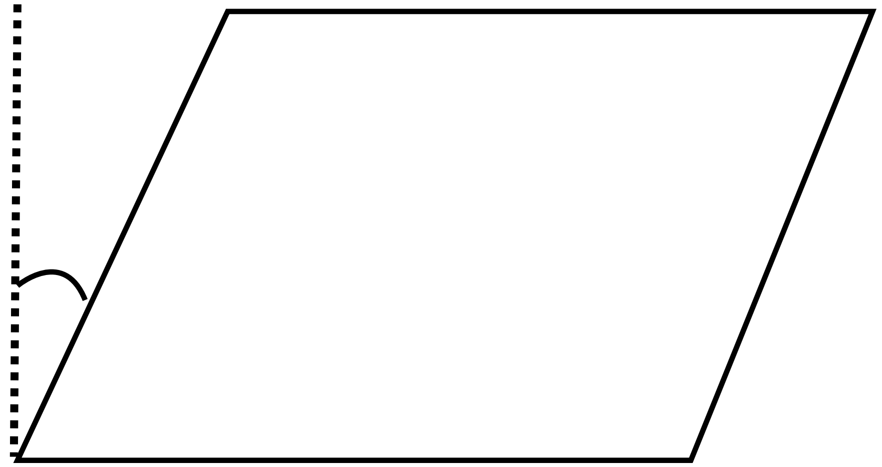
Let’s try to obtain effective
“Debye model” by computing
shearmoulous

“cells” in the elasto-plastic model

By “state following”
even non-linear responses
can be analyzed
P. Urbani’s talk

Shear modulus: a paradox and a lesson

Strain γ



$$f = F/N$$

$$f(\gamma) = f(0) + \gamma\sigma + \frac{\gamma^2}{2}\mu + \dots$$

stress

shear modulus or “rigidity”

「水は方円の器にしたがう」水随方円　荀子

Water conforms to the shape of its container.

liquid $\mu = 0$

solid $\mu > 0$

linear response, fluctuation

$\mu = 0$

thermodynamics

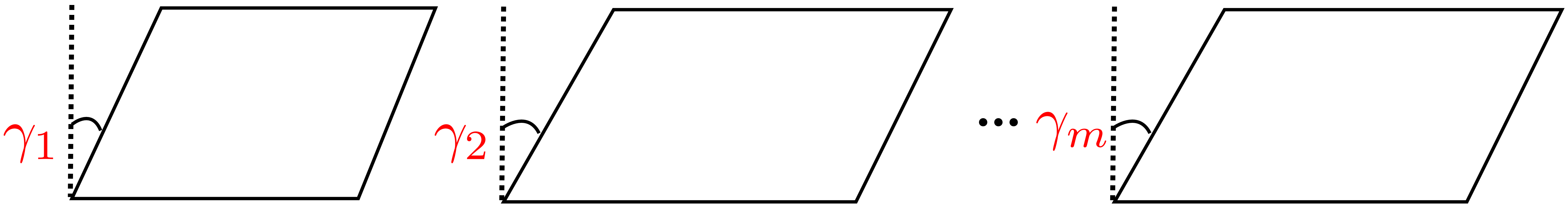
Shape of the container should not matter!

$$\lim_{N\to\infty} \lim_{\gamma\to 0} \neq \lim_{\gamma\to 0} \lim_{N\to\infty}$$

elasticity *must* emerge together with plasticity

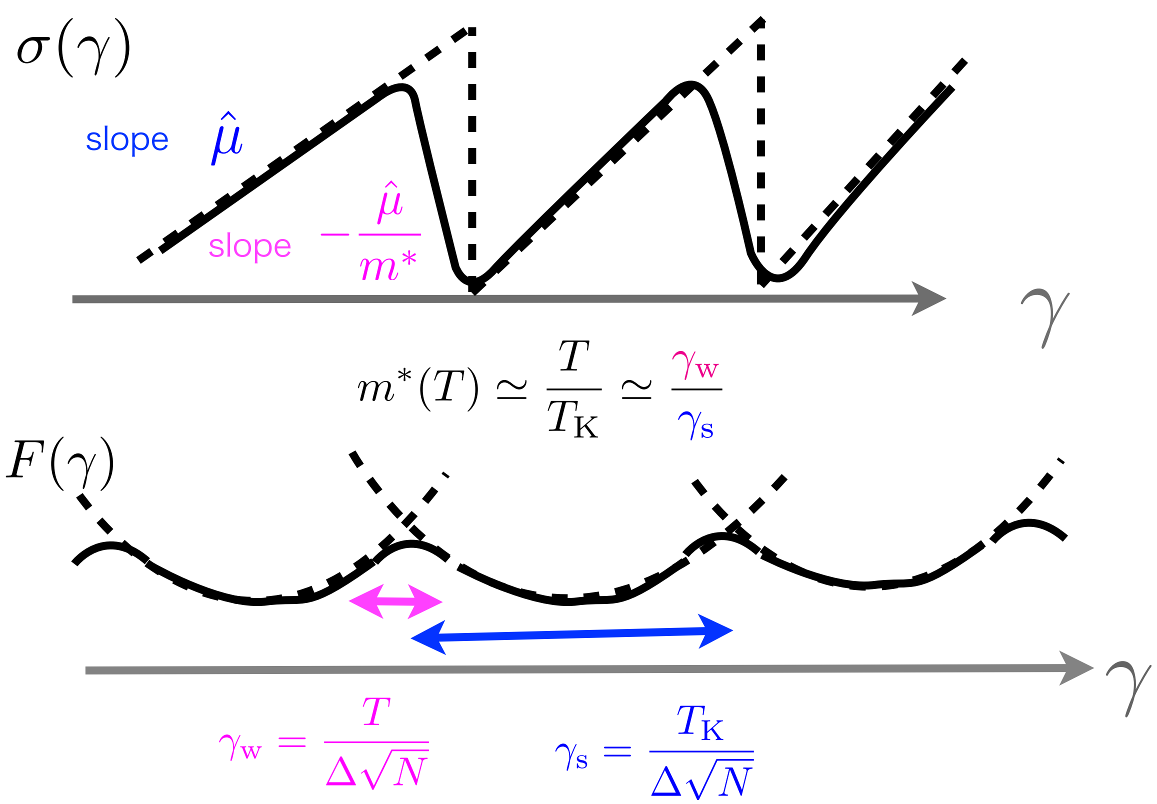
Linear response of replicated liquid & physical interpretation

HY and M. Mézard, Phys. Rev. Lett. 105, 015504 (2010). HY, J. Chem. Phys. 136, 214108 (2012).



Expansion of replicated liquid free-energy

$$F_m(\{\gamma_a\})/N = F_m(\{0\})/N + \sum_{a=1}^{m} \sigma_a \gamma_a + \frac{1}{2}\sum_{a,b}^{1,m} \mu_{ab}\gamma_a\gamma_b + \cdots$$



$$\mu_{ab} = \hat{\mu}\delta_{ab} - \frac{\hat{\mu}}{m^*}$$

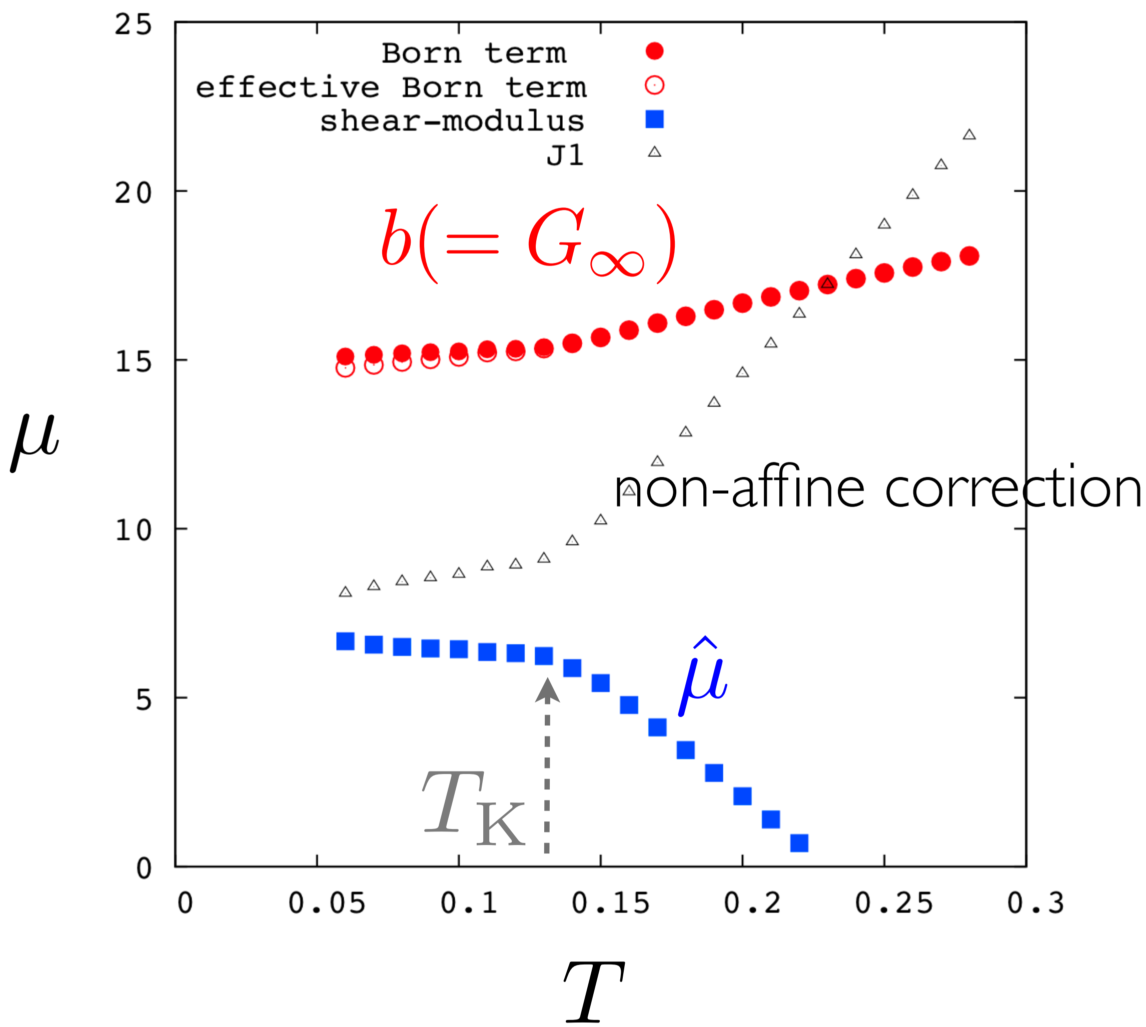
$$\overline{\mu} = \sum_{b=1}^{m^*} \mu_{ab} = 0$$

C.F.. step-wise magnetic response in spin-glasses : H. Y. and Tommaso Rizzo, Phys. Rev. B 77, 104429 (2008).

A model computation of the shear modulus

HY and M. Mézard, Phys. Rev. Lett. 105, 015504 (2010). HY, J. Chem. Phys. 136, 214108 (2012).

1st order cage expansion +HNC approx+Kirkwood approx



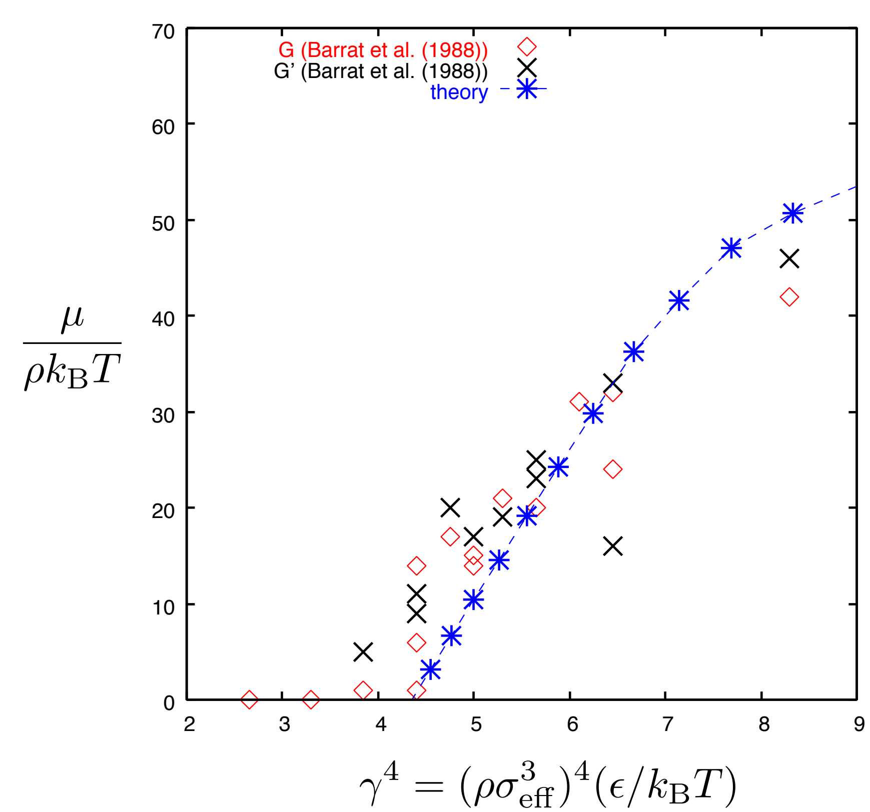
Binary mixture of soft-shere

$$\sigma_i = \sigma_A \quad \text{or} \quad \sigma_B$$

$$v(r_{ij}) = \left(\frac{\sigma_i + \sigma_j}{r_{ij}}\right)^{12}$$

Comparison with MD simulation

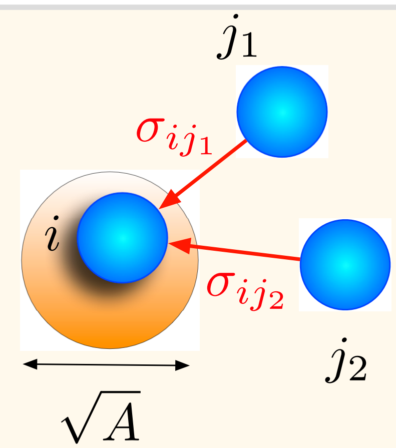
J. L. Barrat, J. -N. Roux, J.-P. Hansen and M. L. Klein, Europhys. Lett., 7 (1988) 707



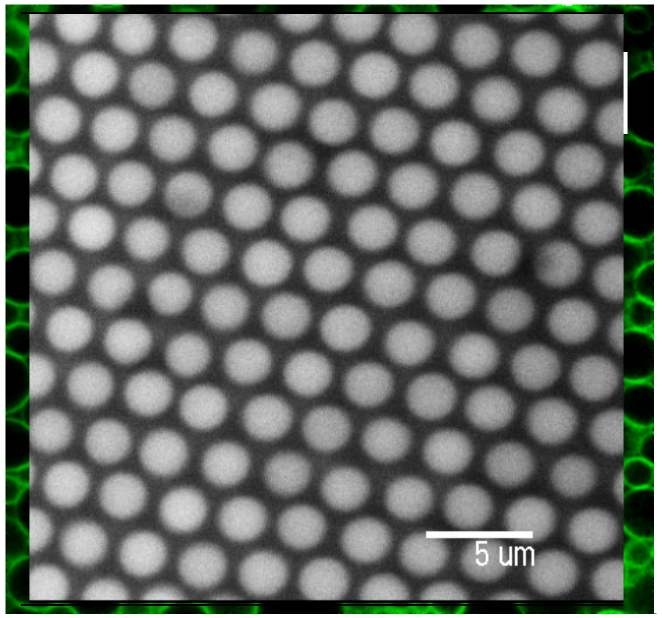
non-affine correction

$$\hat{\mu} = b_{\mathrm{eff}} - c\beta^* \frac{1}{N} \sum_{i=1}^{N} \langle (\Xi_i)^2 \rangle_* + ..$$

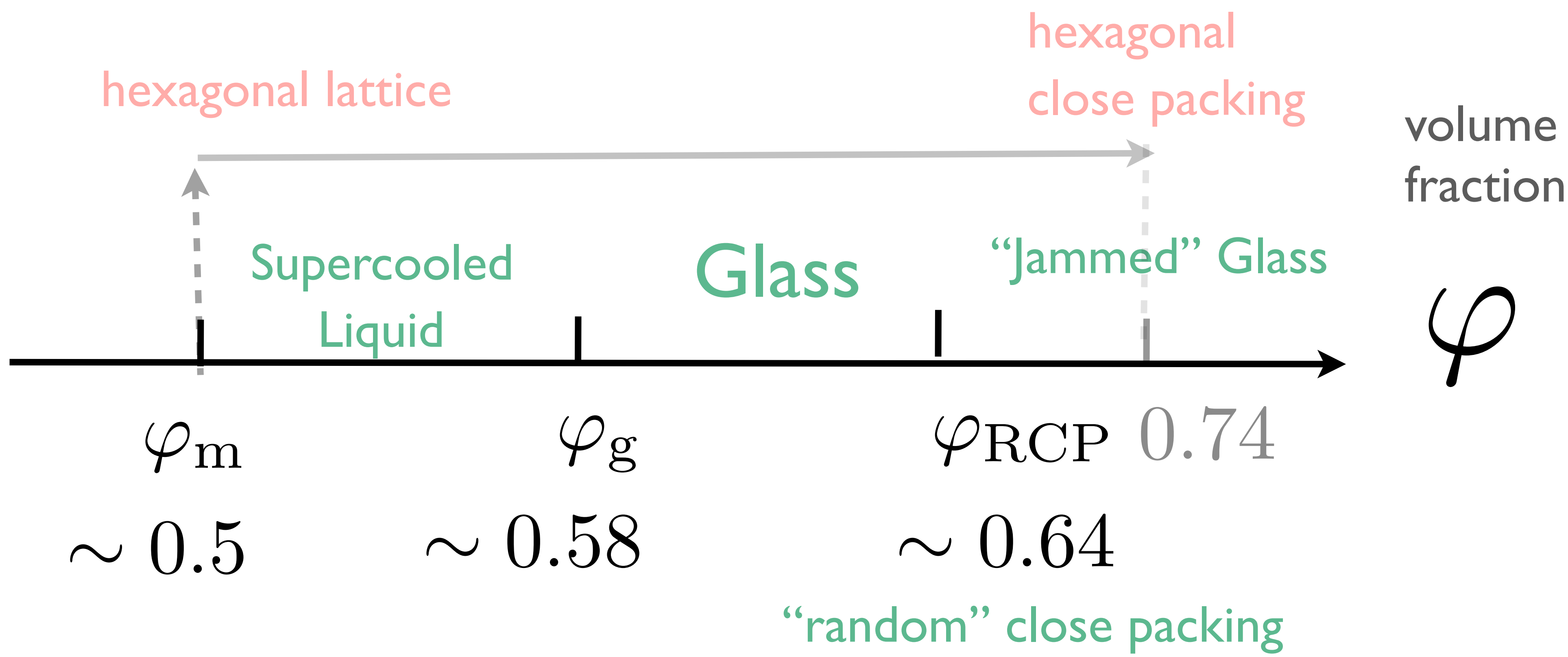
$$c = 2\frac{A}{m} = \frac{d}{\beta^* \frac{1}{N} \sum_{i<j} \langle \nabla^2 v(r_{ij}) \rangle_*}$$



Emulsions, colloids,...



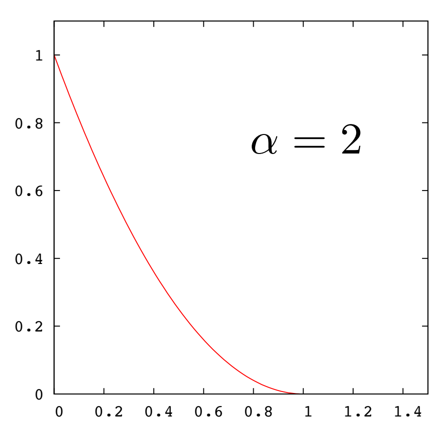
E. R. Weeks,
in "Statistical Physics of Complex Fluids",
Eds. S Maruyama & M Tokuyama
(Tohoku University Press, Sendai, Japan, 2007).



$$k_{\rm B}T_{\rm room}/\epsilon \sim 10^{-5}$$

Model

$v(r)/\epsilon$



r/D

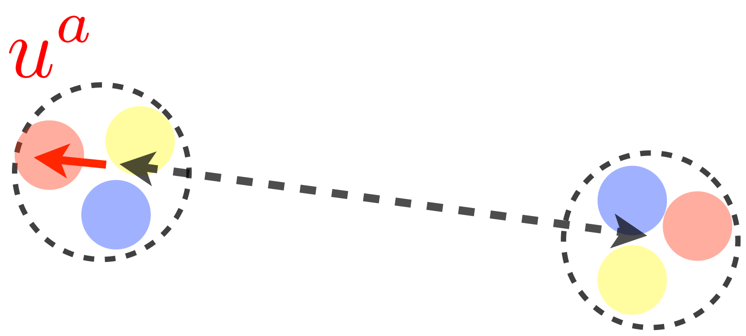
$$U = \sum_{\langle ij \rangle} v(r_{ij}) \qquad r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$$

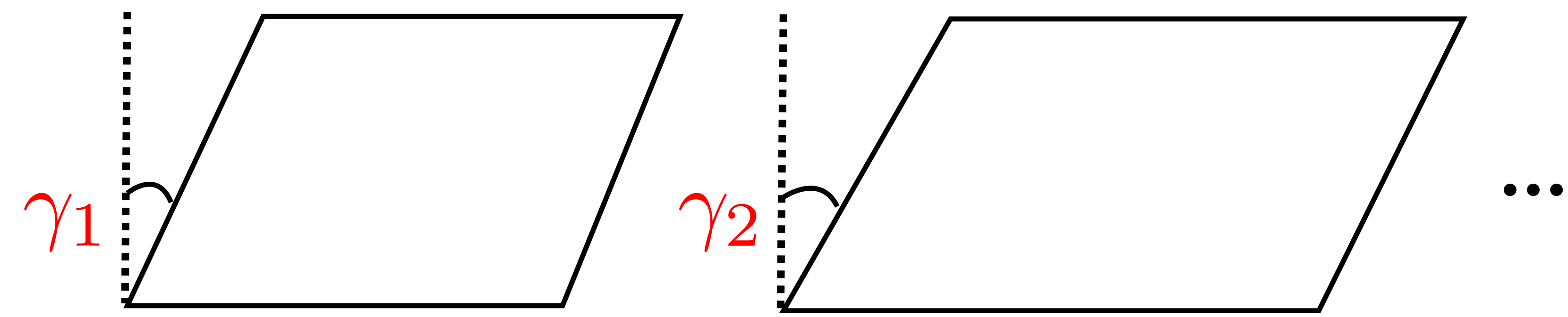
$$v(r) = \epsilon(1 - r/D)^\alpha \theta(1 - r/D)$$

I. J. Jorjadze, L-L. Pontani and J. Brujic, PRL **111**, 048302(2013).

Shear on hardspheres in large dimensional limit $\quad d \to \infty$

HY and F. Zamponi, Phys. Rev. E 90, 022302 (2014).





$$-\beta F(\{\gamma_a\}) = \int d\overline{x}\rho(\overline{x})[1-\log\rho(\overline{x})] + \frac{1}{2}\int d\overline{x}d\overline{y}\rho(\overline{x})\rho(\overline{y}) f_{\{\gamma_a\}}(\overline{x},\overline{y})$$

Replicated Mayer function (under shear)

$$f_{\{\gamma_a\}}(\overline{x},\overline{y}) = -1+\prod_{a=1}^{m} e^{-\beta v(|S(\gamma_a)(x_a-y_a)|)} \qquad S(\gamma)_{\mu\nu} = \delta_{\mu\nu}+\gamma\delta_{\nu,1}\delta_{\mu,2}$$

$$\boxed{\begin{aligned}-\beta F(\hat{\alpha},\{\gamma_a\})/N \quad &= 1-\log\rho + d\log m + \tfrac{d}{2}(m-1)\log(2\pi e D^2/d^2) + \tfrac{d}{2}\log\det(\hat{\alpha}^{m,m}) \\ &\quad - \tfrac{d}{2}\widehat{\varphi}\int\frac{d\lambda}{\sqrt{2\pi}}\mathcal{F}\left(\Delta_{ab}+\frac{\lambda^2}{2}(\gamma_a-\gamma_b)^2\right)\end{aligned}}$$

I step RSB

$$\widehat{\varphi}_{\rm d} < \widehat{\varphi} < \widehat{\varphi}_{\rm Gardner}$$

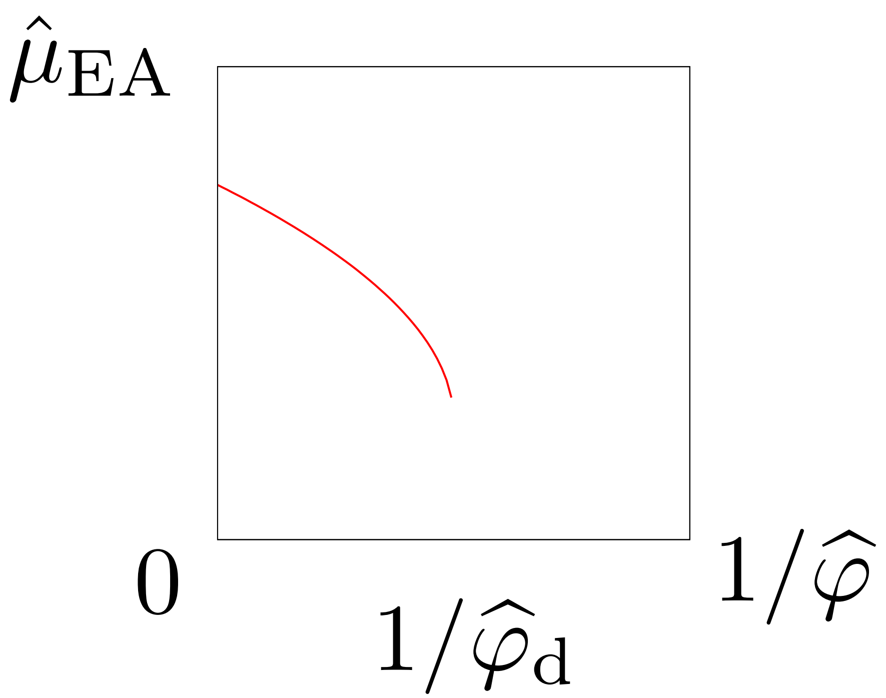
$$\beta\widehat{\mu}_{ab} = \beta\widehat{\mu}_{\rm EA}\left(\delta_{ab} - \frac{1}{m}\right)$$

$$\beta\hat{\mu}_{\rm EA} = \widehat{\Delta}_{\rm EA}^{-1} \qquad \widehat{\Delta}_{\rm EA} \sim \widehat{\Delta}_{d} - C(\widehat{\varphi} - \widehat{\varphi}_{d})^{1/2}$$

in agreement with MCT

W. Gotze, *Complex dynamics of glass-forming liquids: A mode-coupling theory*, vol. 143 (Oxford University Press, USA, *2009).*

G. Szamel and E. Flenner, PRL 107, 105505 (2011).



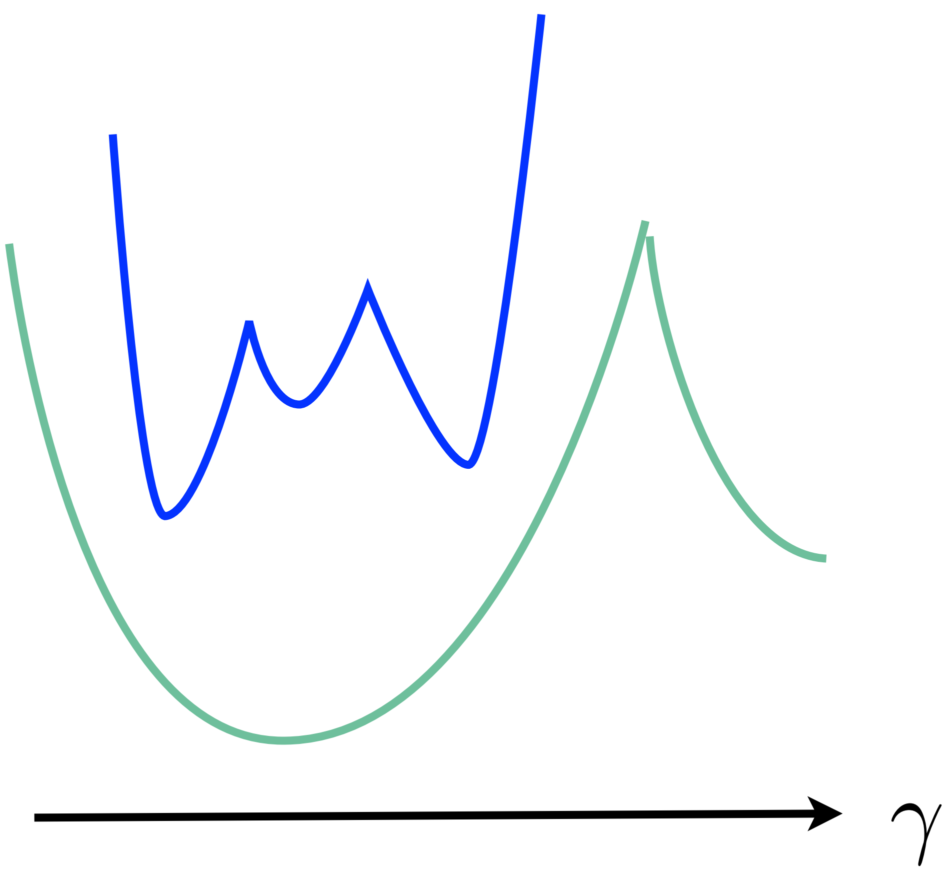
HY and F. Zamponi, Phys. Rev. E 90, 022302 (2014).

1+continuous RSB

$$\widehat{\varphi}_{\rm Gardner} < \widehat{\varphi} < \widehat{\varphi}_{\rm GCP}$$

$$\widehat{\varphi} \to \widehat{\varphi}_{\rm GCP}^{-} \qquad p \propto 1/m \to \infty$$

$$\gamma(y) \propto \gamma_\infty y^{-(\kappa-1)} \qquad \kappa = 1.41575$$



$$\beta \mu_{\rm EA} = 1/\Delta_{\rm EA} \propto m^{-\kappa} \propto p^{\kappa}$$

consistent with scaling argument + effective medium computation
E DeGiuli; E Lerner; C Brito; M Wyart, PNAS 111.48 (2014) 17054.

"rigidity of inherent structures"

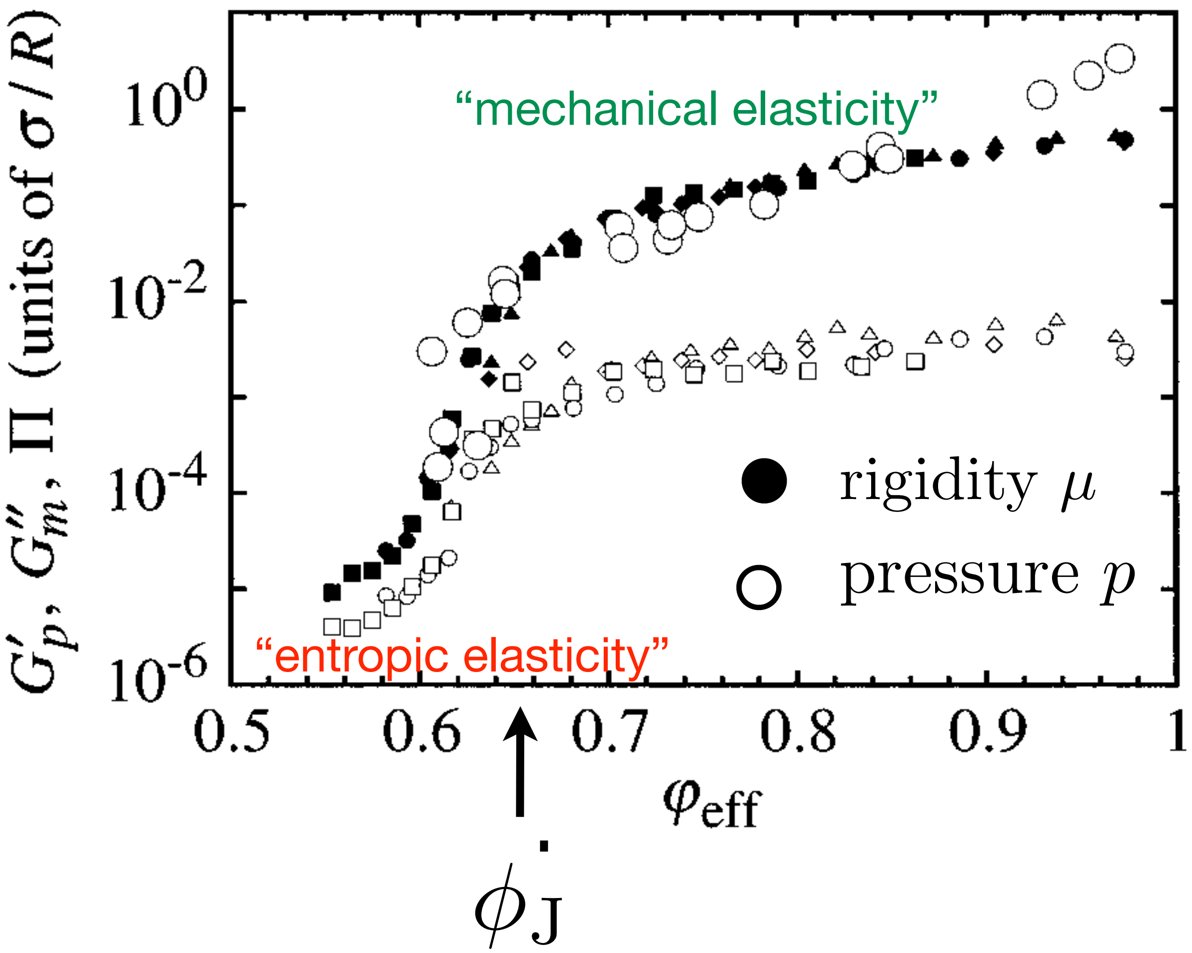
$$\beta \widehat{\mu}(1) = \frac{1}{m\gamma(1)} \propto p$$

"rigidity of metabasins"

HY and F. Zamponi, Phys. Rev. E 90, 022302 (2014).

Experiment: rigidity of emulsions

T. G. Mason, Martin-D Lacasse, Gary Grest, Dov Levine, J Bibette, D Weitz, Physical Review E 56, 3150 (1997)



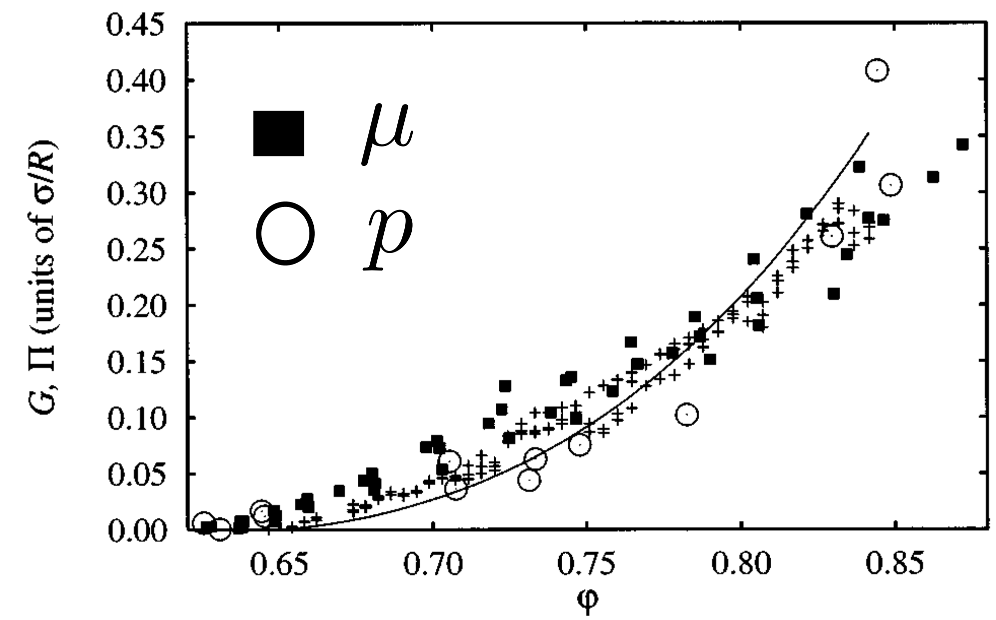


FIG. 1. The scaled shear modulus and osmotic pressure as a function of φ. The computed scaled static shear modulus $G/(\sigma/R)$ (+) and osmotic pressure $\Pi/(\sigma/R)$ (line), as obtained from the model presented in Sec. IV B 2, are compared with the experimental values of $G'_p(\varphi_{\rm eff})$ (■) and $\Pi(\varphi_{\rm eff})$ (○).

rigidity (shear-modulus) pressure

$$\mu \sim p$$

measurements at room temperature

$$k_{\rm B}T/\epsilon \sim 10^{-5}$$

1RSB also gives this scaling : H. Yoshino, AIP Conference Proceedings 1518, 244 (2013)

But "harmonic" response should give different scaling:
O'hern, Corey S., et al. Physical Review E 68.1 (2003): 011306.

E DeGiuli; E Lerner; C Brito; M Wyart, PNAS 111.48 (2014) 17054.

Scaling for hard-sphere colloidal glasses near jamming

Rojman Zargar[1], Eric DeGiuli[2] and Daniel Bonn[1]

[1] *Van der Waals-Zeeman Institute, Institute of Physics, University of Amsterdam 1098 XH Amsterdam, The Netherlands*
[2] *Institute of Physics, École Polytechnique Fédérale de Lausanne (EPFL) - CH-1015 Lausanne, Switzerland*

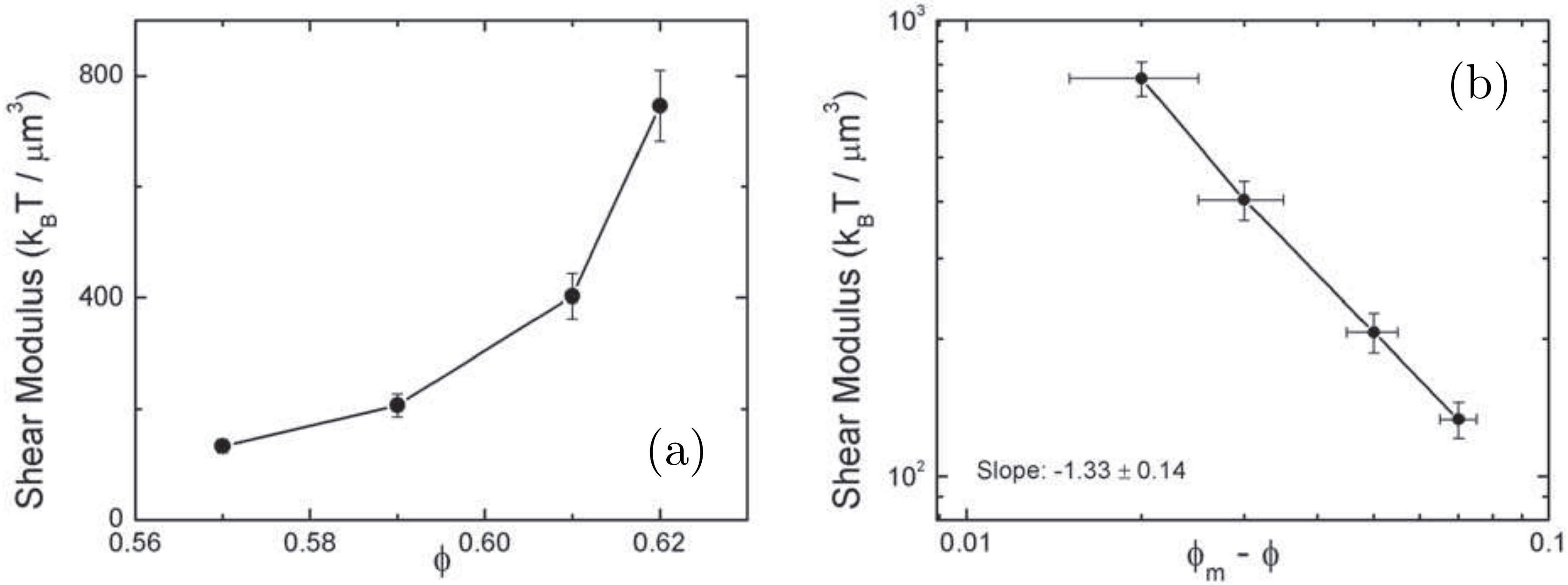
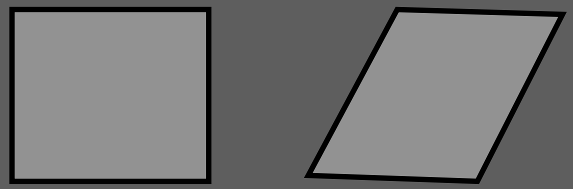


Fig. 4: Shear modulus μ *vs.* (a) volume fraction ϕ, and (b) distance from jamming, $\phi_m - \phi$.

Summary



- **1st principle computation of shear-modulus via replicated liquid theory in 3D** is possible. It should be tested in various systems.

- **Shearmodulus of inherent structure/metabasin** is different show different scaling approaching jamming.

3D hard sphere under shear (+ (de)compression) : simulation

- Linear response

  “Infinitesimal” shear strain

- Non-linear response

  Finite shear strain

Preparation of equilibrium configurations

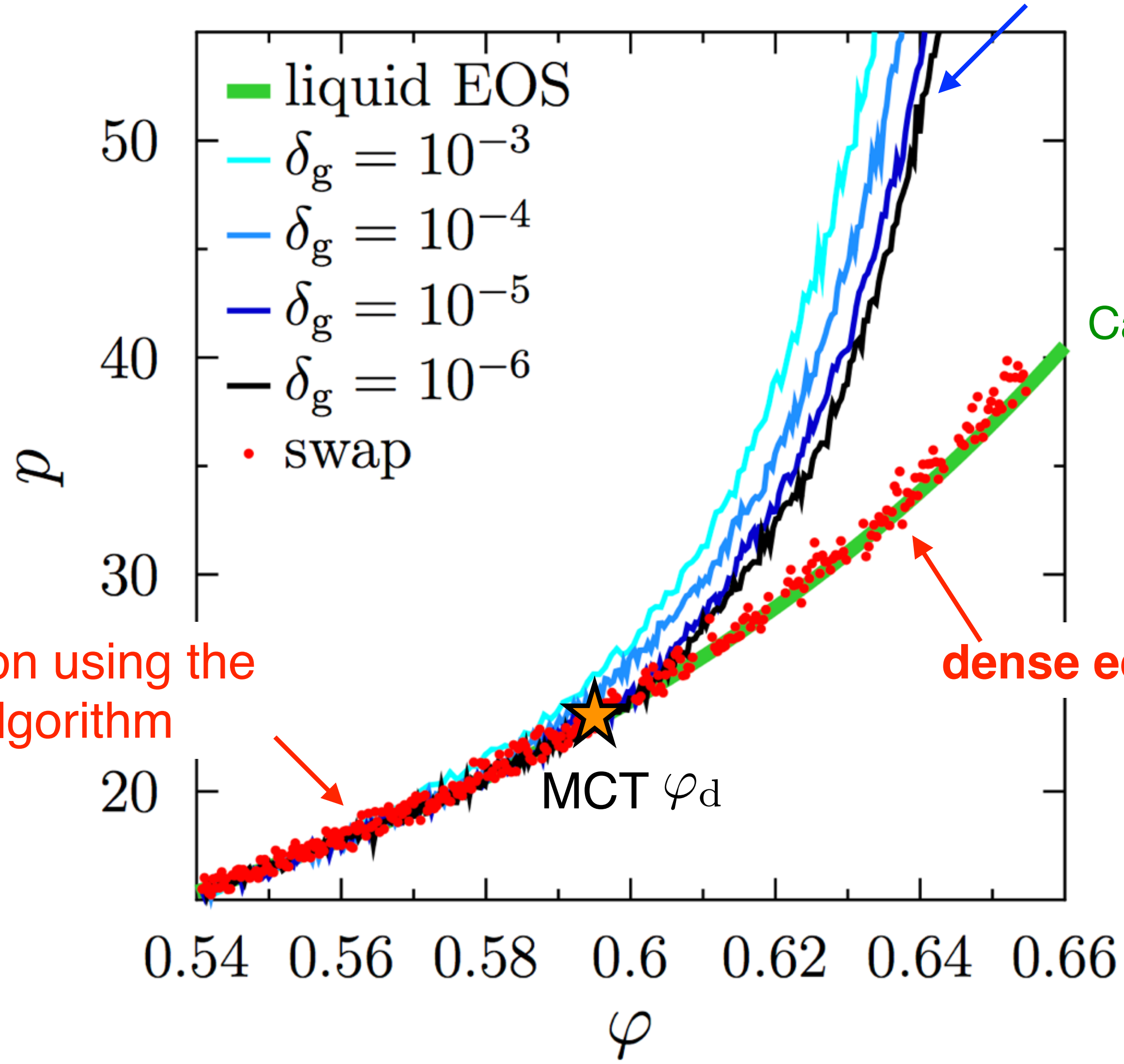
System: polydisperse hard spheres $P(D) \sim D^{-3}, D_{\min} < D < D_{\min}/0.45$ (polydispersity ~ 23%)

Swap algorithm: MC swap moves + conventional MC/MD

Grigera & Parisi, PRE (2001); Berthier, et al., PRL (2016)

L. Berthier's talk

compression using conventional event-driven MD



Carnahan-Stirling liquid EOS

compression using the swap algorithm

dense equilibrium configurations

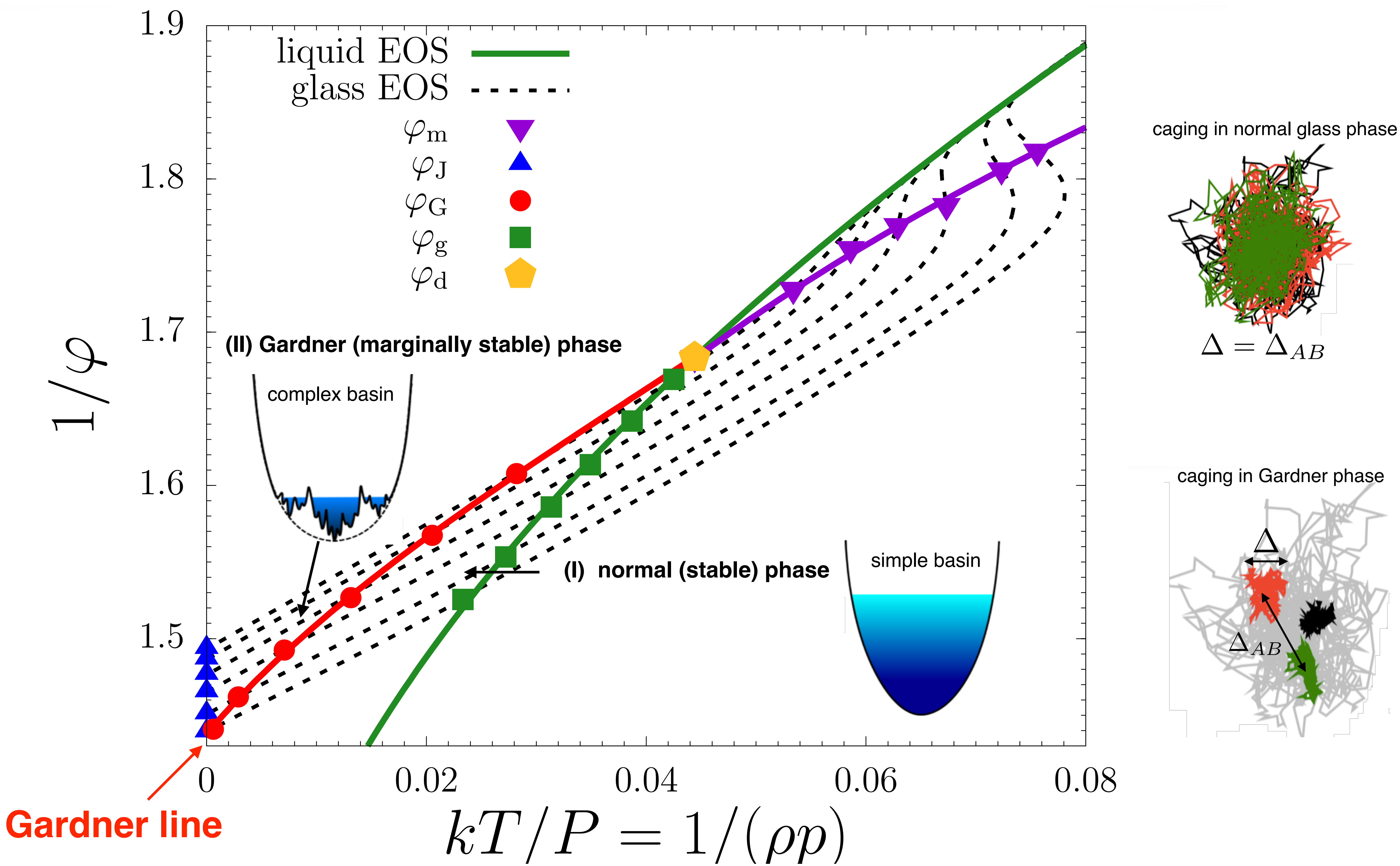
$\max \varphi_g \sim 1.1\varphi_d$

(i) Frozen α-relaxation.

(ii) (ii) No crystallization.

Ultra-stable glasses in experiments: (1) very old nature glasses; (2) vapour deposition.

Zhao, et al., Nat. Commun. (2016). Yu, et al., PRL (2015).



Experiment:

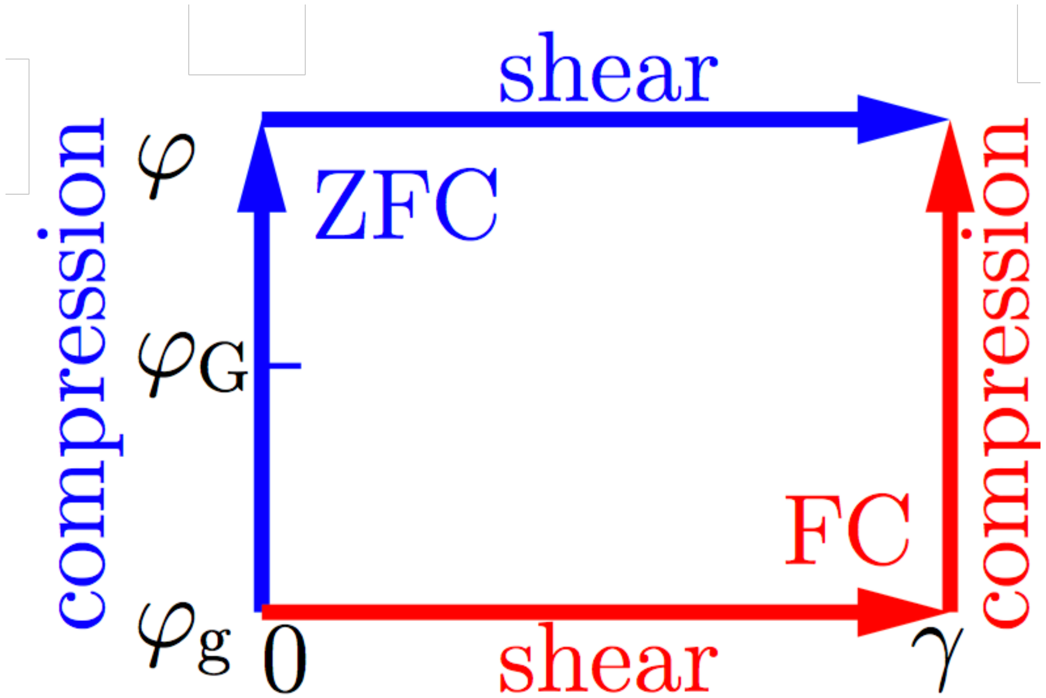
Experimental evidence of the Gardner phase in a granular glass, Seguin & Dauchot, PRL (2016).

Consequence of Gardner transition on shear modulus — protocol dependence

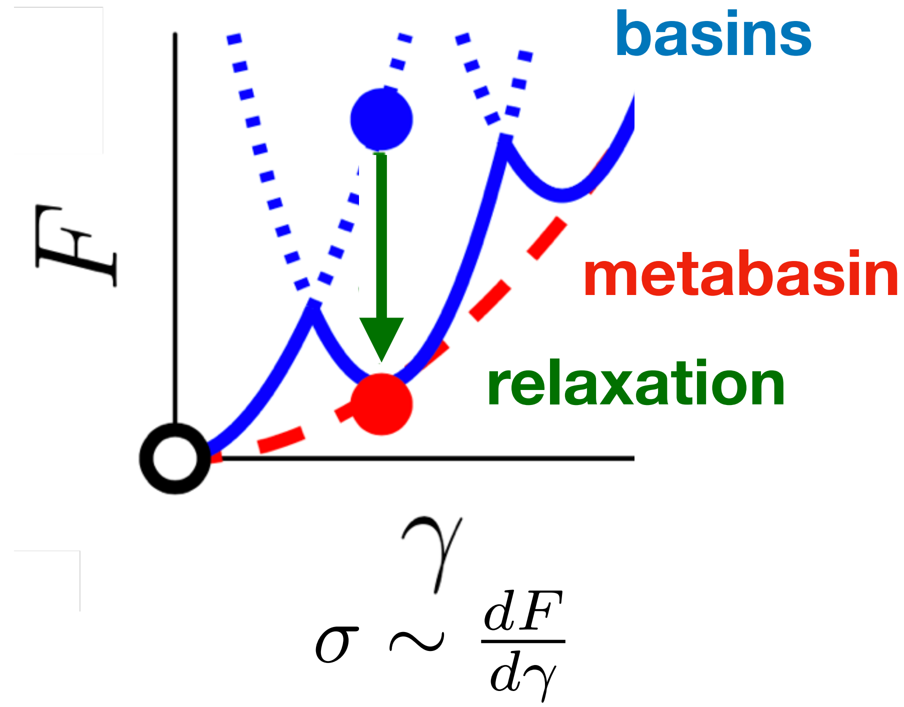
Hard sphere simulations:

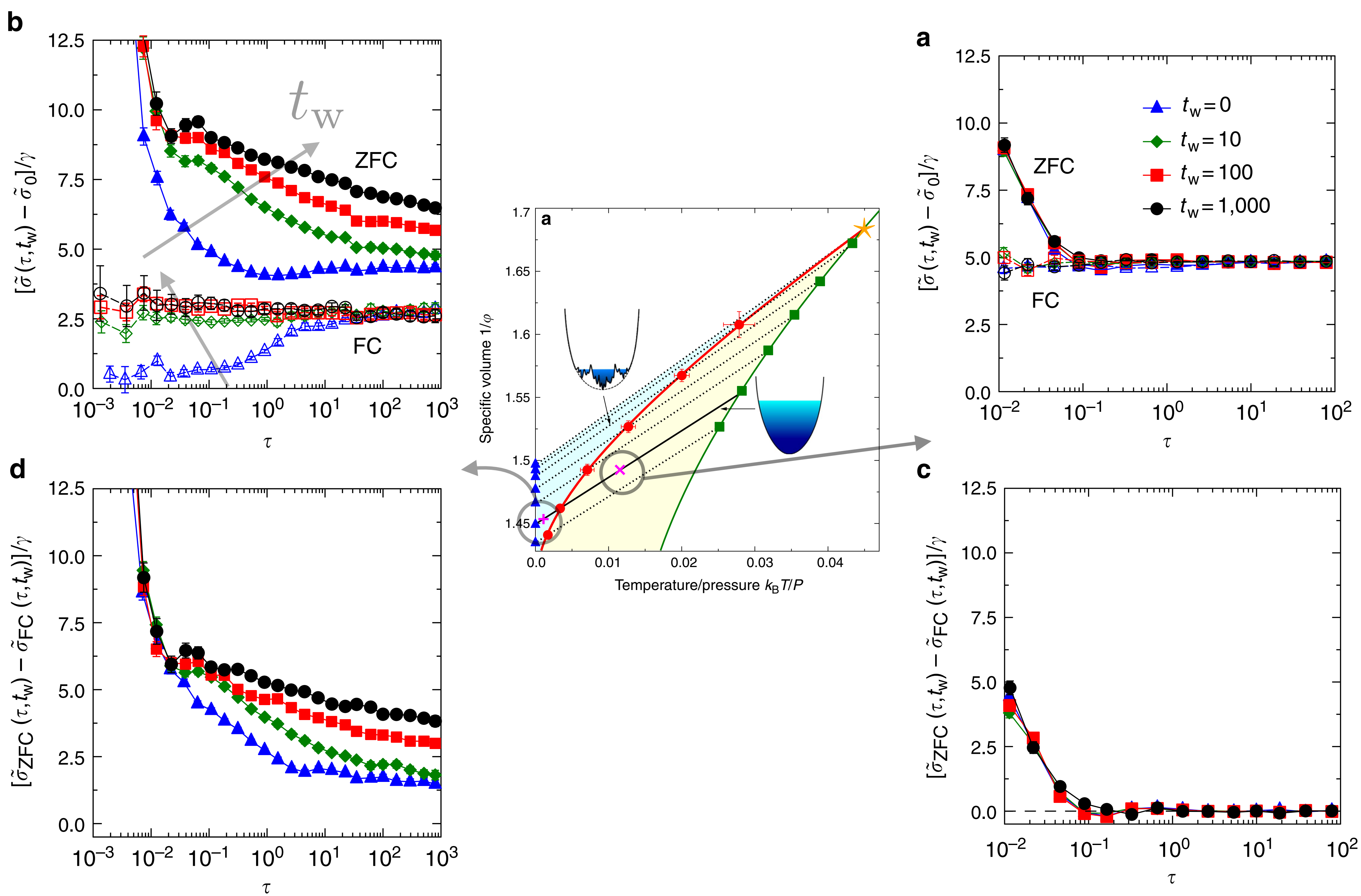
ZFC: zero field compression

FC: field compression



Gardner phase:





b
ZFC
FC
t_w
$[\tilde{\sigma}(\tau,t_w)-\tilde{\sigma}_0]/\gamma$
τ
a
$t_w = 0$
$t_w = 10$
$t_w = 100$
$t_w = 1{,}000$
Specific volume $1/\varphi$
Temperature/pressure $k_B T/P$
c
d
$[\tilde{\sigma}_{ZFC}(\tau,t_w)-\tilde{\sigma}_{FC}(\tau,t_w)]/\gamma$

Protocol-dependent shear modulus

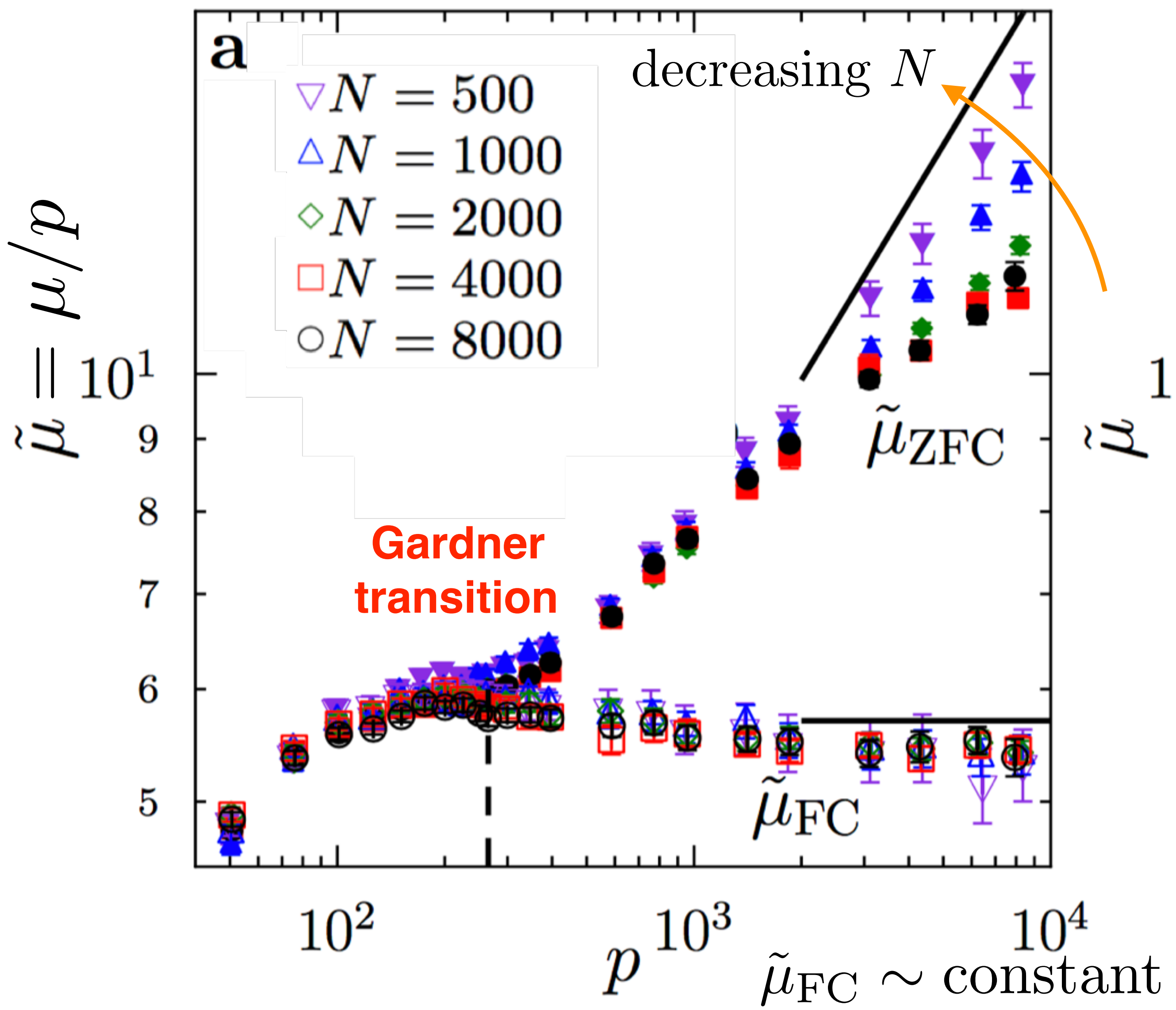
(a) system-size dependence

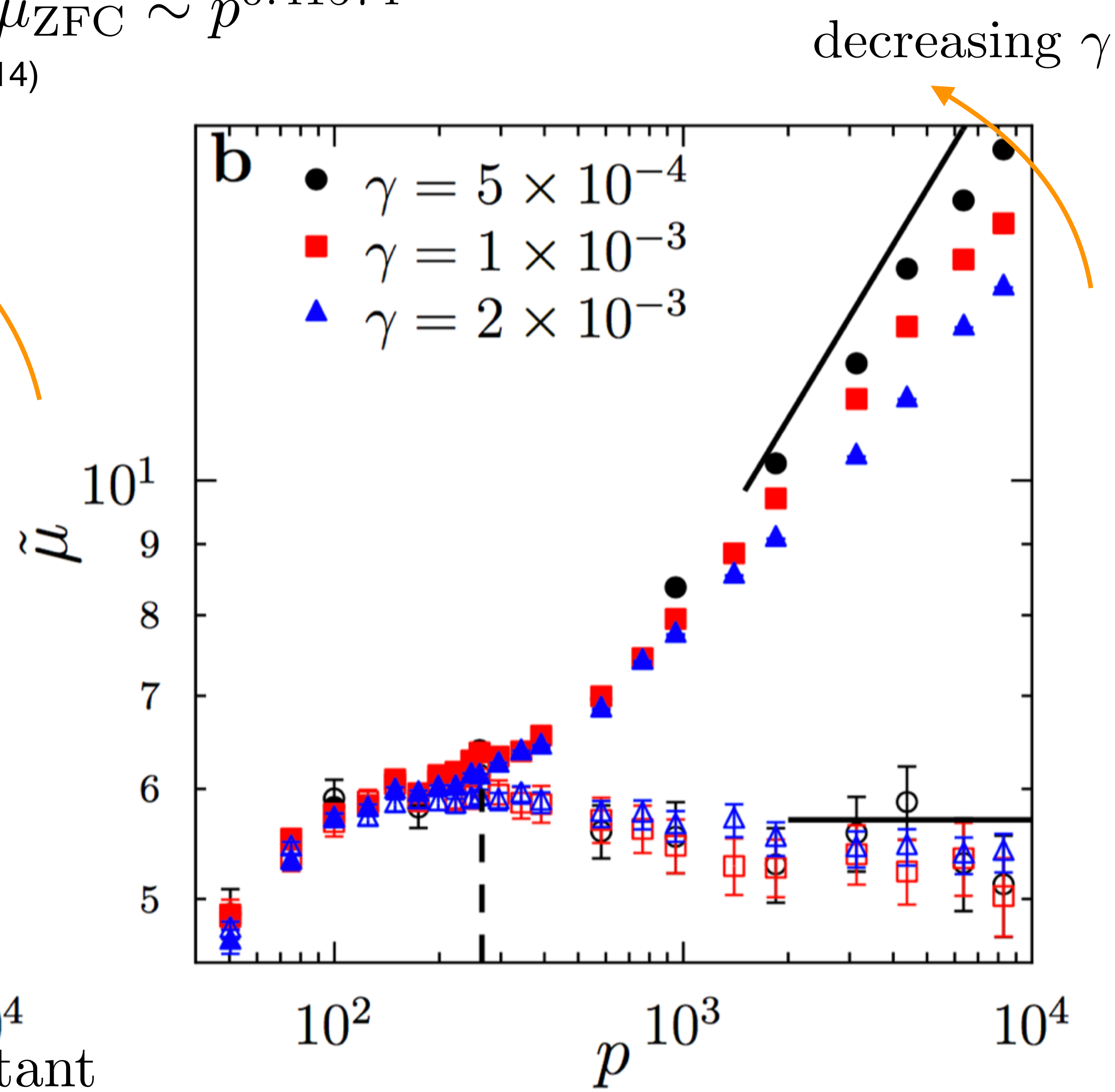
(b) strain dependence

$\gamma = 2 \times 10^{-3}$

mean-field theory: $\tilde{\mu}_{\mathrm{ZFC}} \sim p^{0.41574}$

Yoshino and Zamponi, PRE (2014)





3D hard sphere under shear (+ (de)compression) : simulation

- Linear response

  "Infinitesimal" shear strain

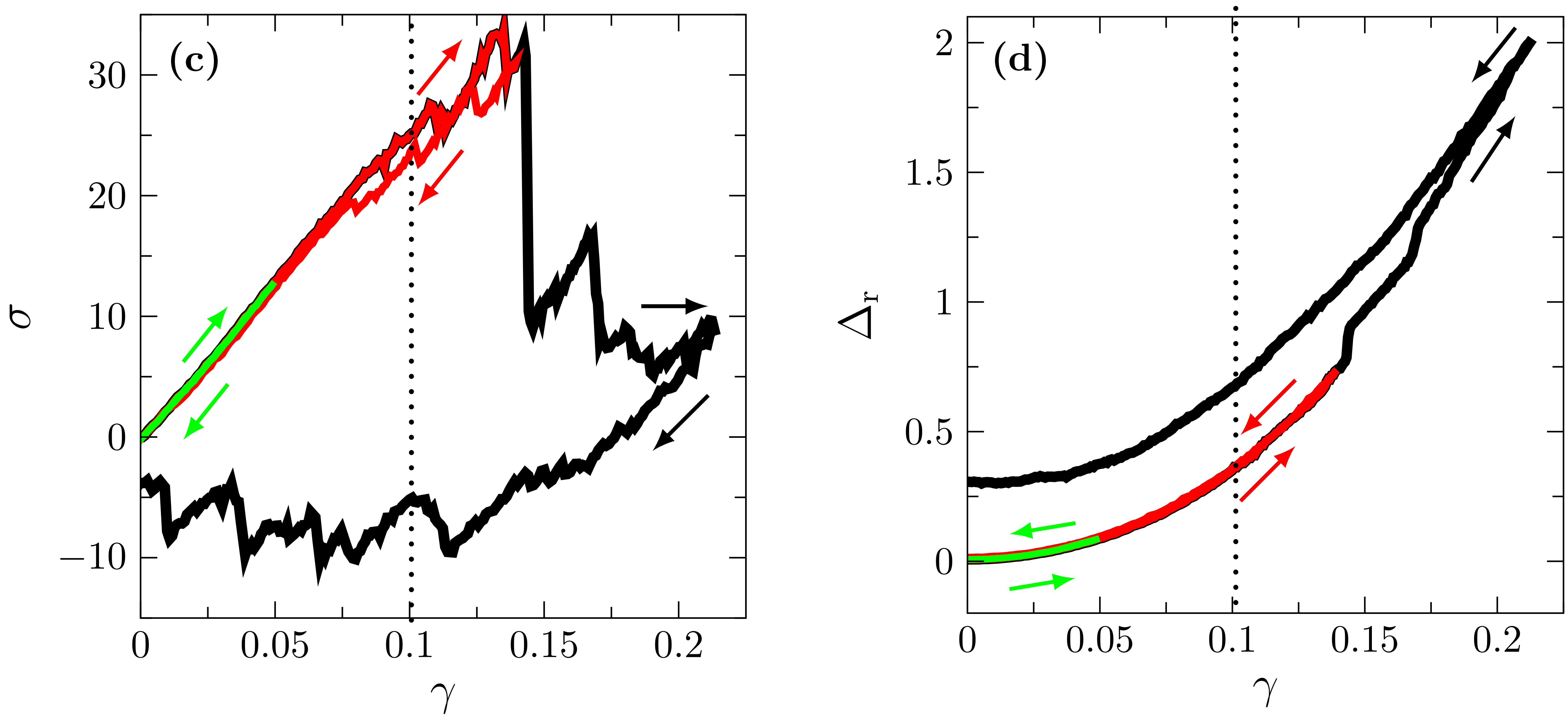
- Non-linear response

  Finite shear strain

Reversibility to HOME (the reference liquid state)

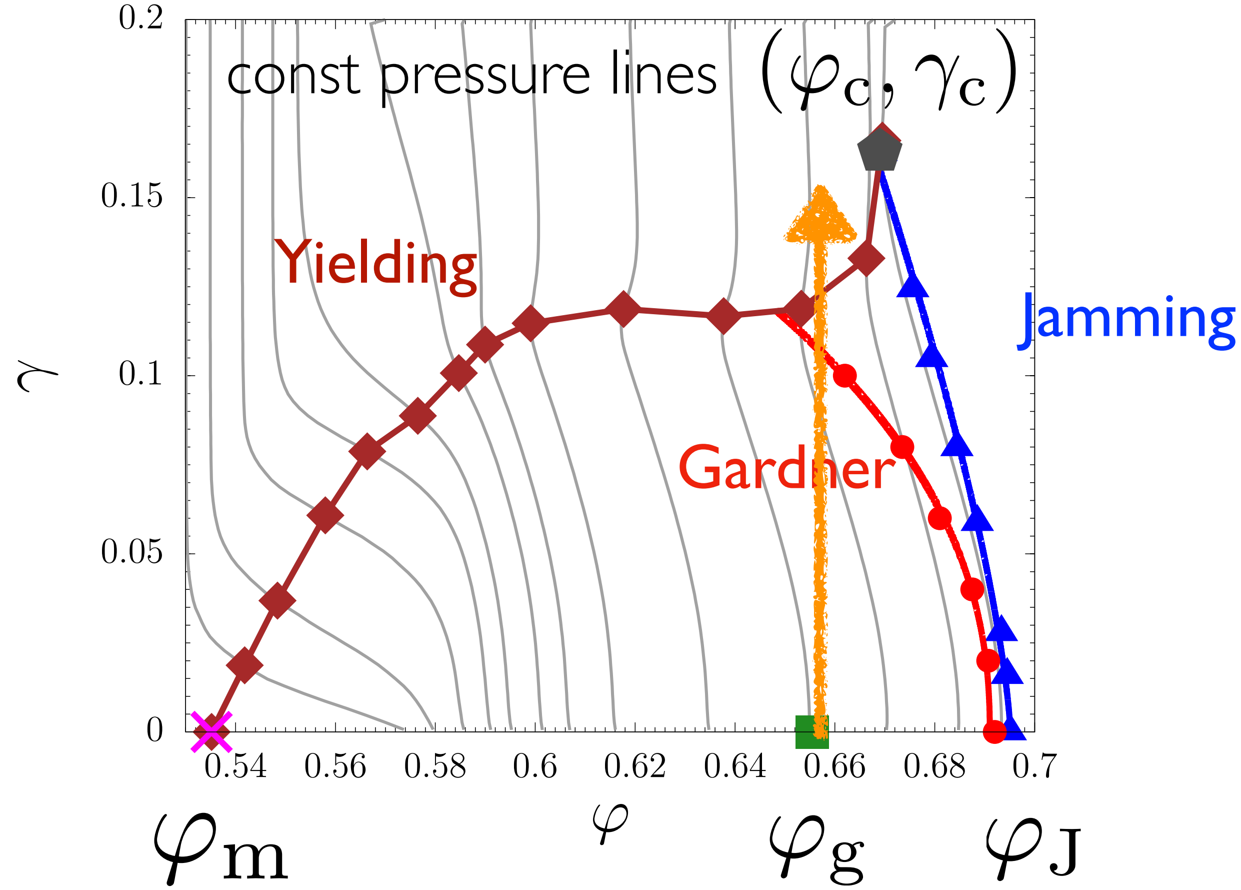
$\varphi_g = 0.655$ $\varphi = 0.66$ $\gamma_G = 0.1$

MSD to the initial state



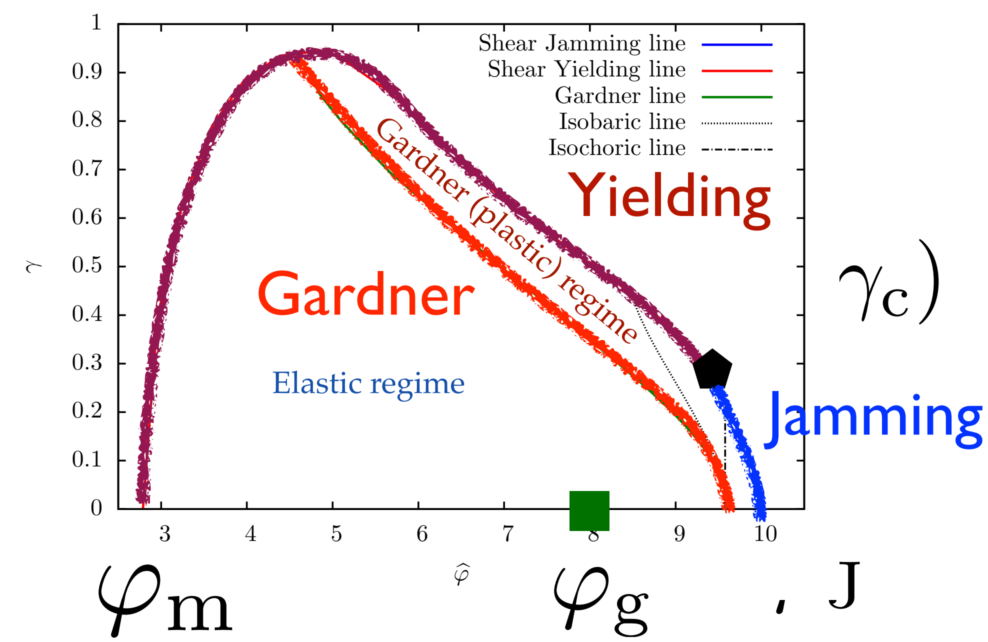
See also oscillatory shear simulations: Kawasaki, Takeshi, and Ludovic Berthier. Physical Review E 94.2 (2016): 022615.
Leishangthem, Premkumar, Anshul DS Parmar, and Srikanth Sastry. Nature Communications 8 (2017): 14653.

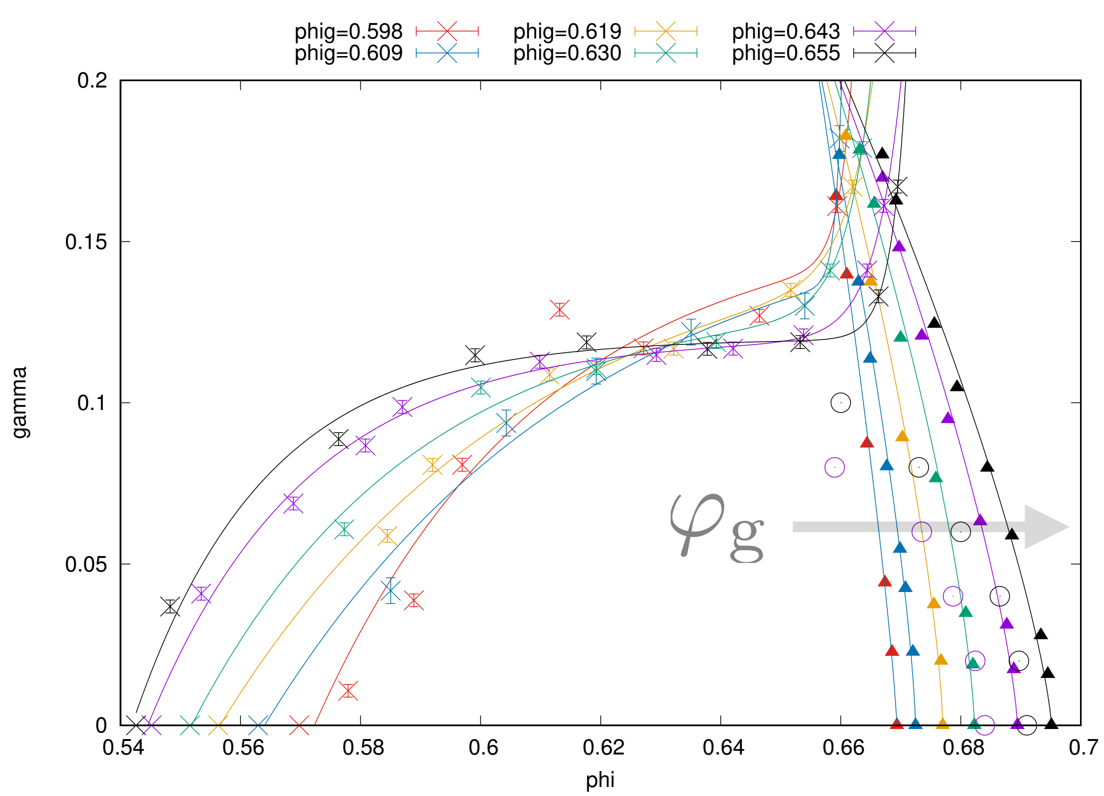
Glass equation of state with shear-strain axis

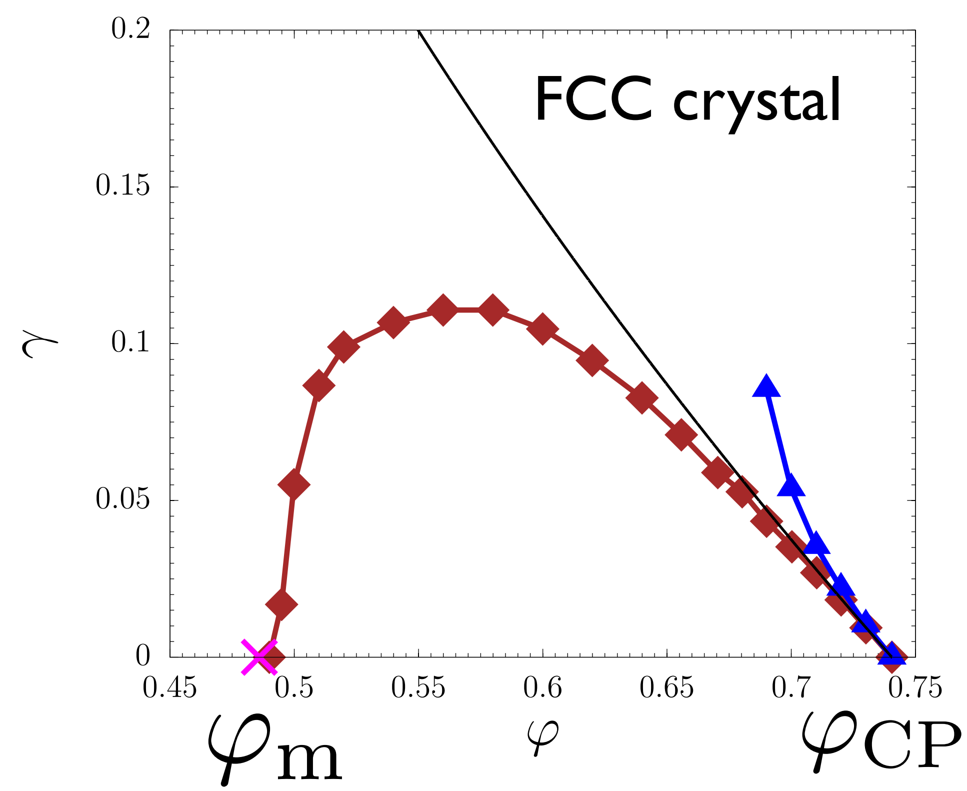


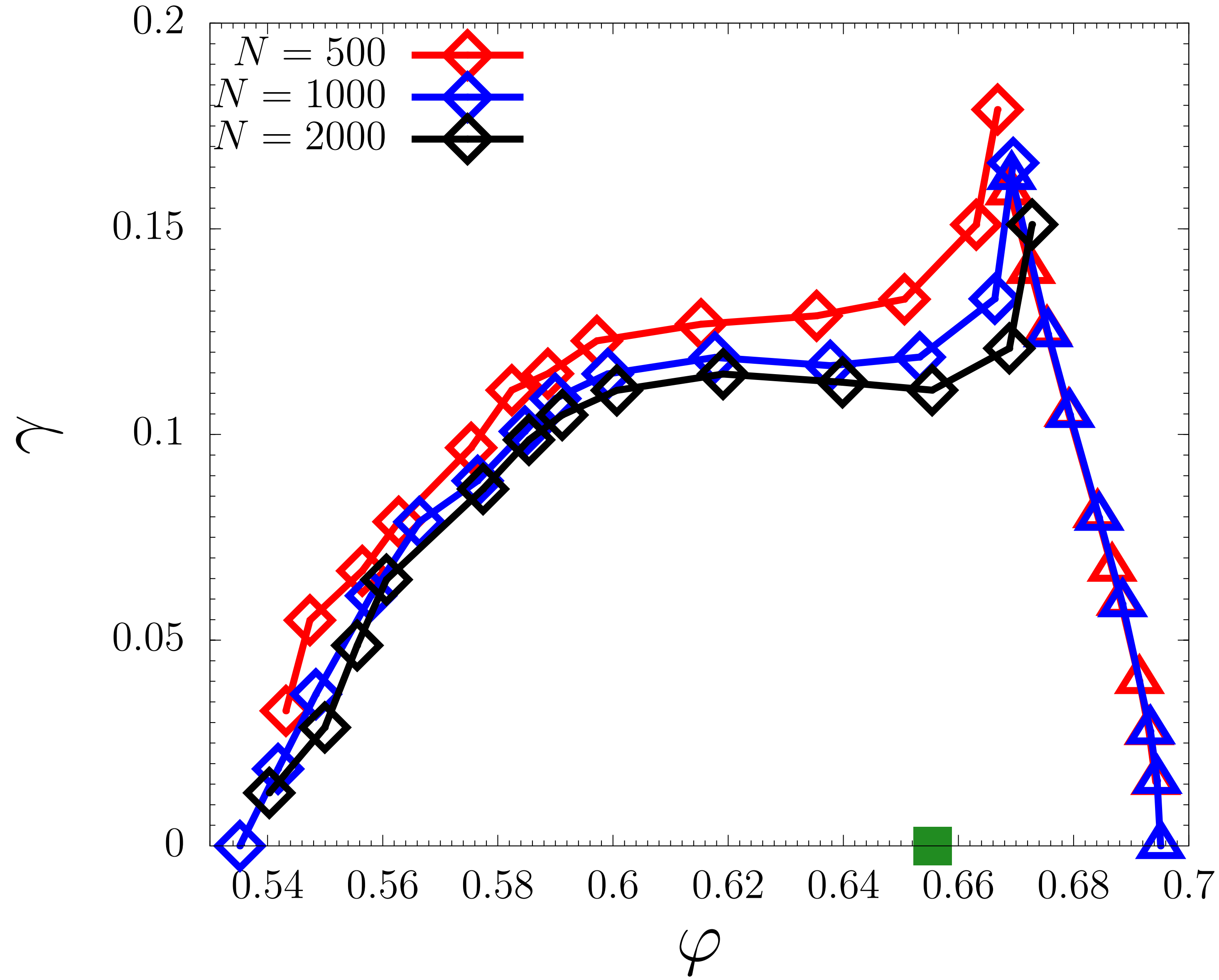
Large-d theory (1RSB)

Urbani,Zamponi, Phys. Rev. Let 118(3),038001 (2017)+ A. Altieri



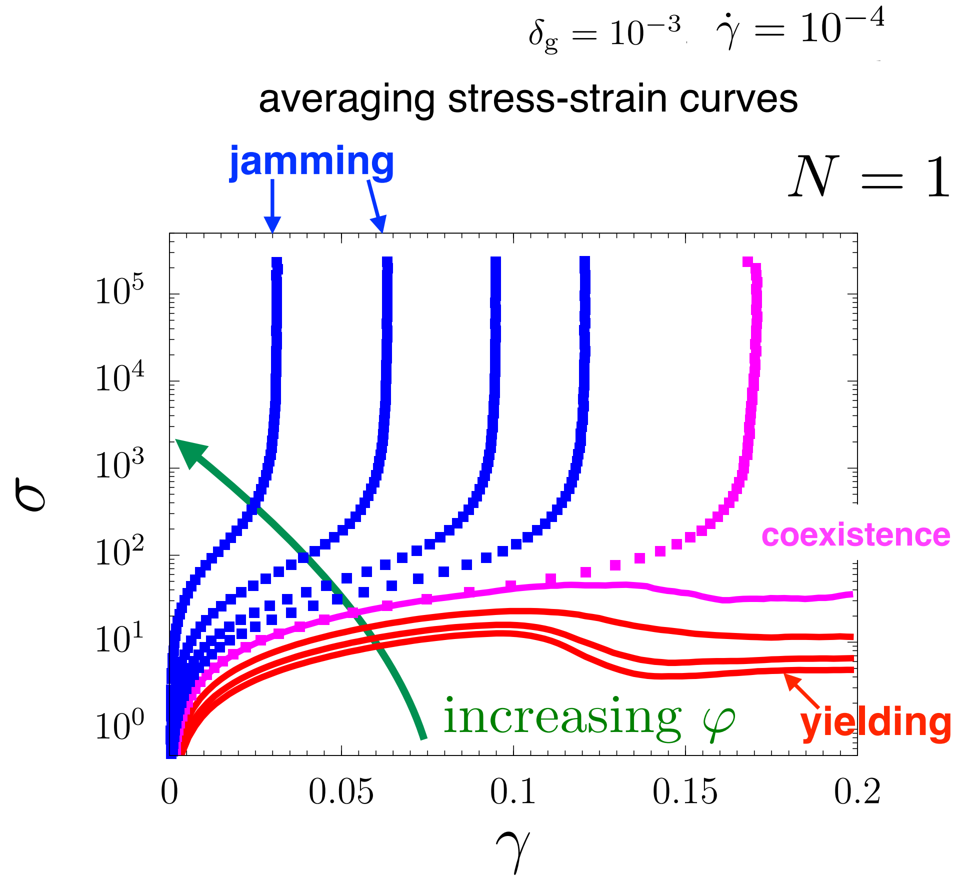




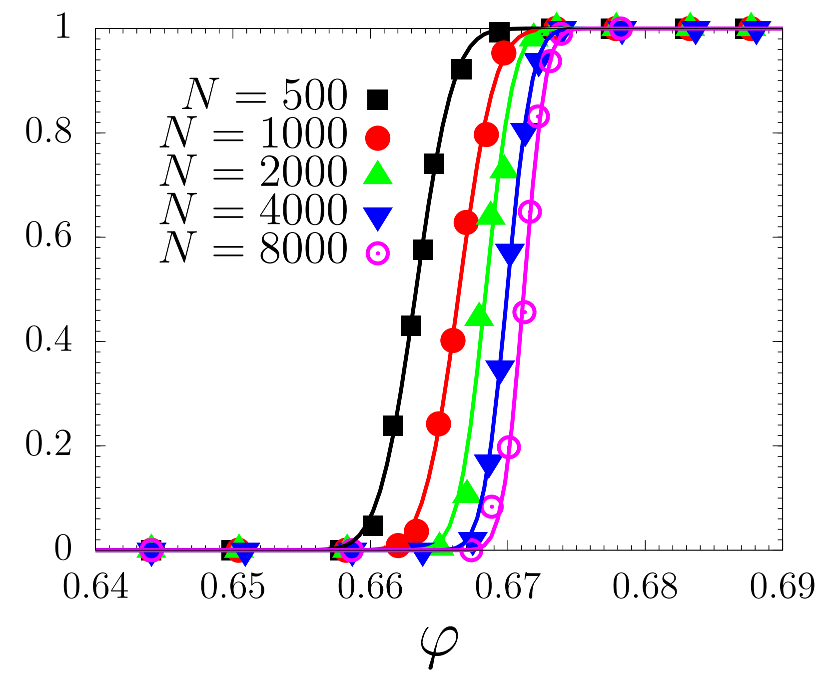


$N = 500$
$N = 1000$
$N = 2000$
0.2
0.15
0.1
0.05
0
γ
0.54
0.56
0.58
0.6
0.62
0.64
0.66
0.68
0.7
φ

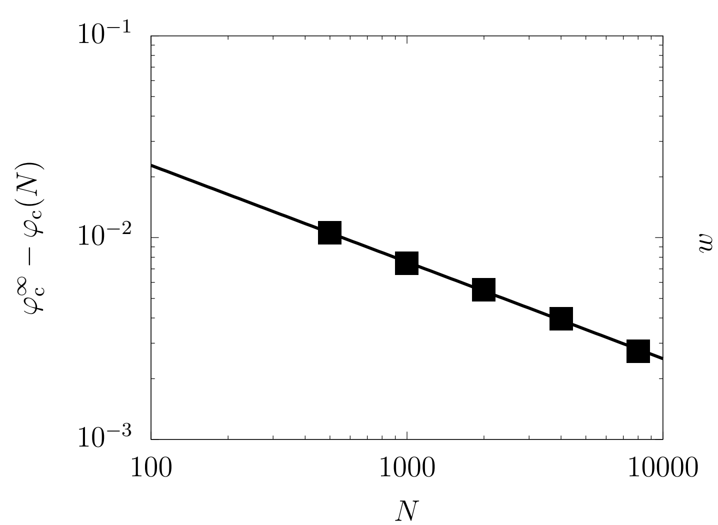
Critical point between jamming/yielding φ_c

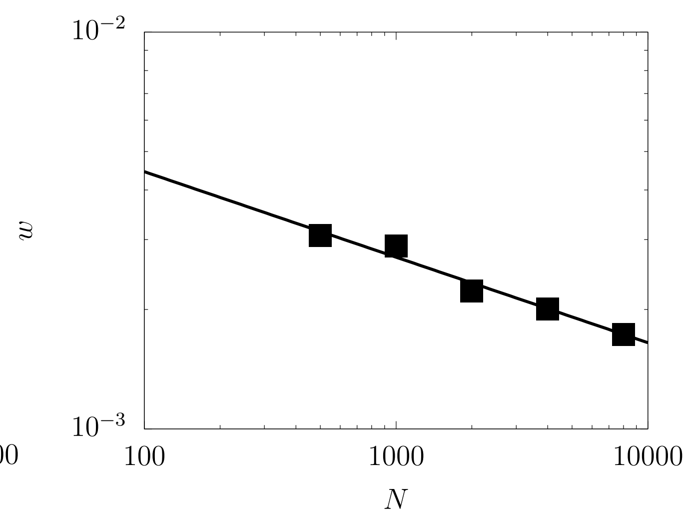


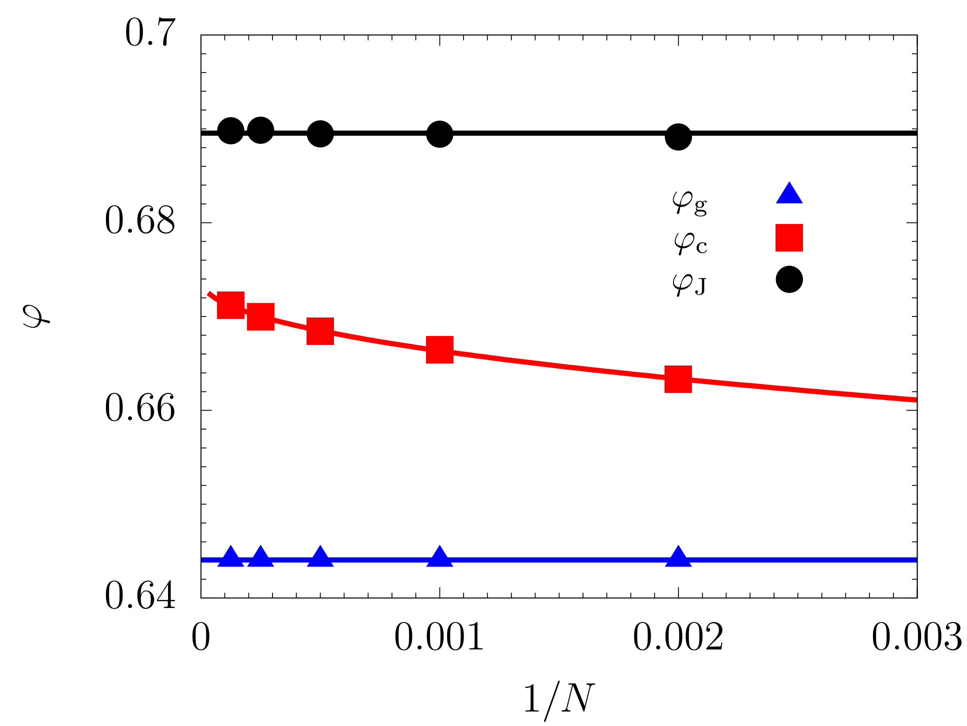
fraction of jamming



$$f_{\mathrm{jamming}}(\varphi) = 1 + \mathrm{erf}[(\varphi - \varphi_c(N)/w(N)]/2$$







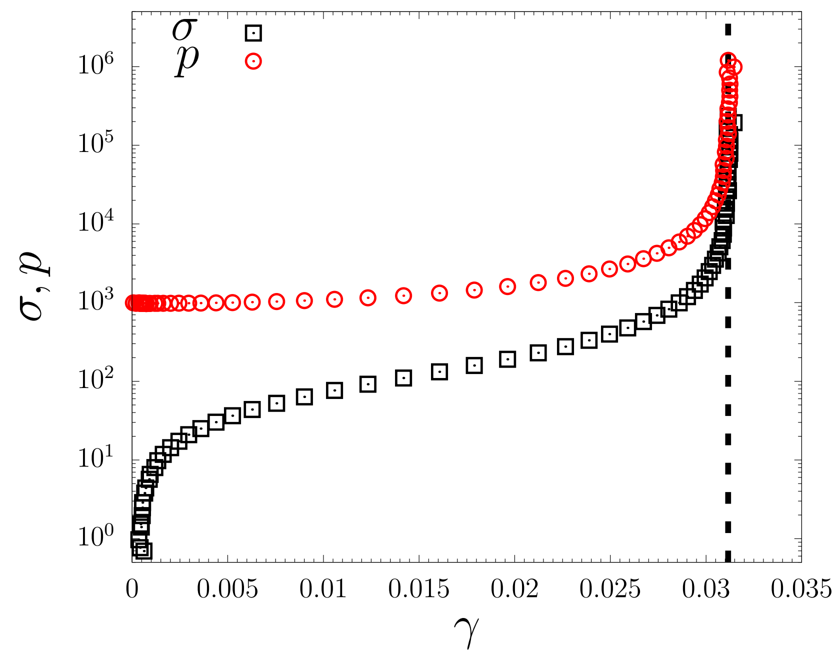
Jamming under shear

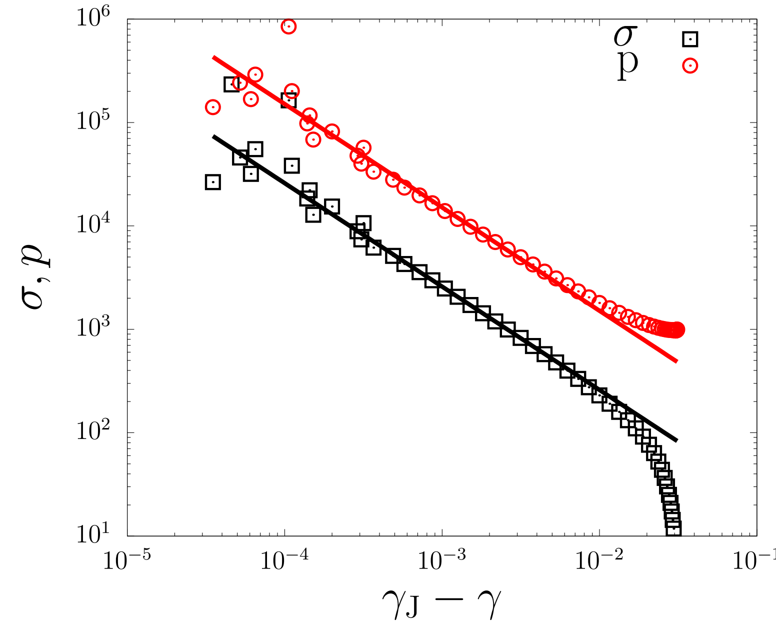
free-volume theory:

$$\sigma \sim (\gamma_\mathrm{J} - \gamma)^{-1}$$

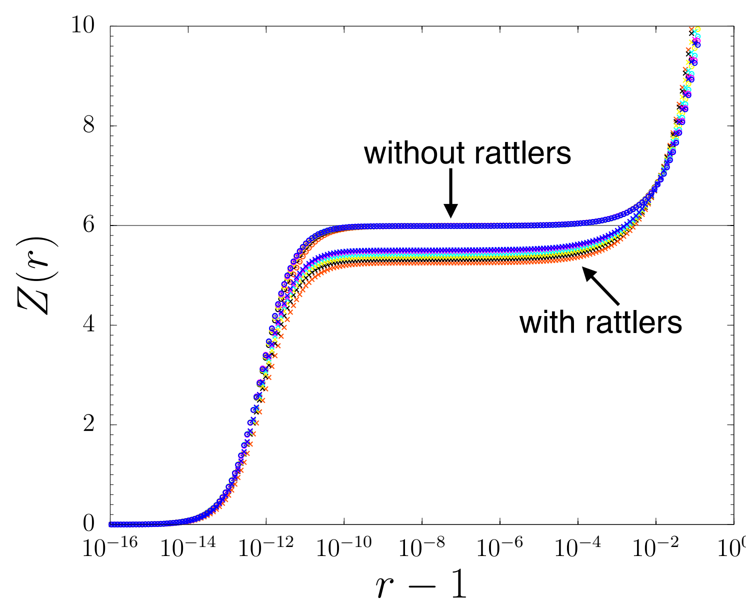
$$p \sim (\gamma_\mathrm{J} - \gamma)^{-1}$$

jamming γ_J





shear-jammed packings are **isostatic**

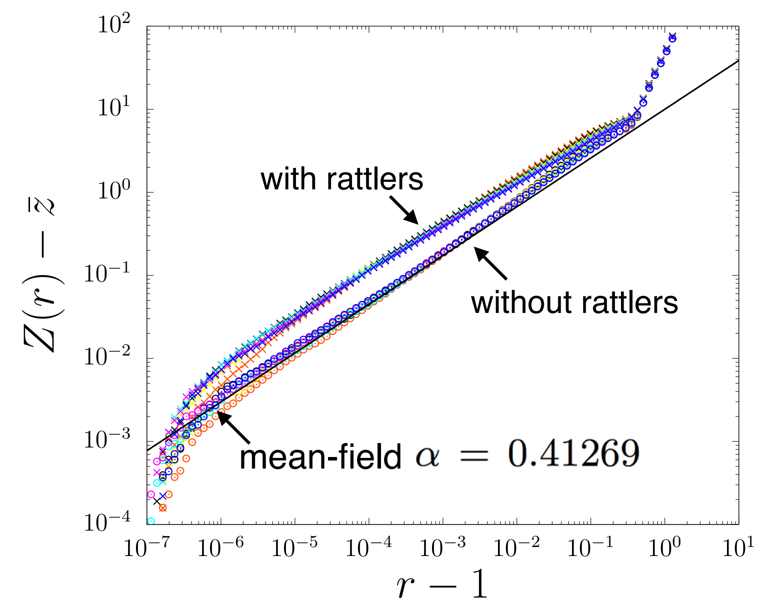


cumulative correlation function

$$Z(r) = \rho S_{d-1} \int_0^r ds s^{d-1} g(s)$$

pair correlation function

shear-jammed and compression-jammed packings belong to **the same universality class**



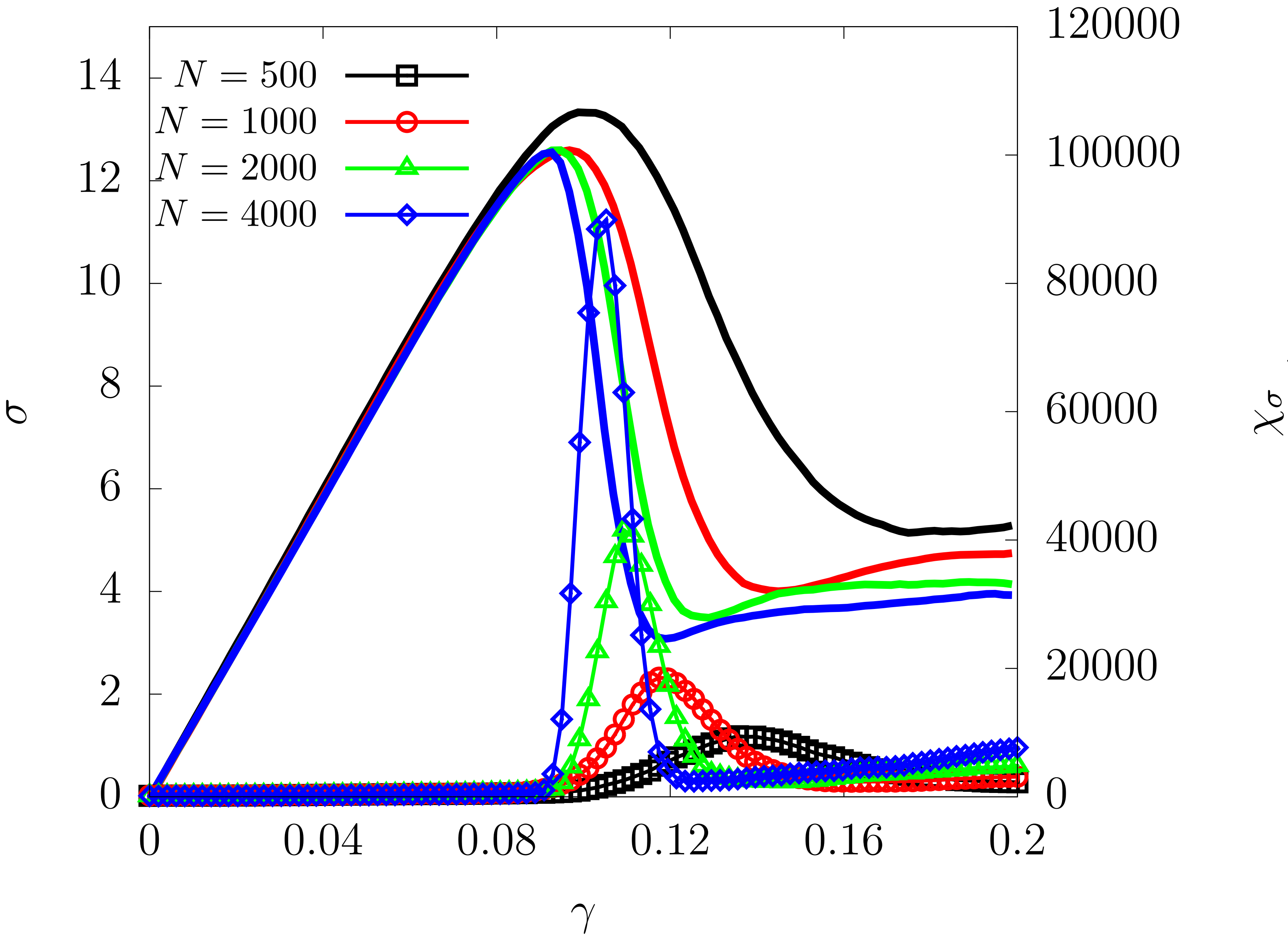
$$Z(r) - \bar{z} \propto (r-1)^{1-\alpha}$$

plateau value

Yielding under shear

$\varphi_{\mathrm{g}} = 0.644$

$\varphi = 0.644$



path-to-path fluctuation of stress

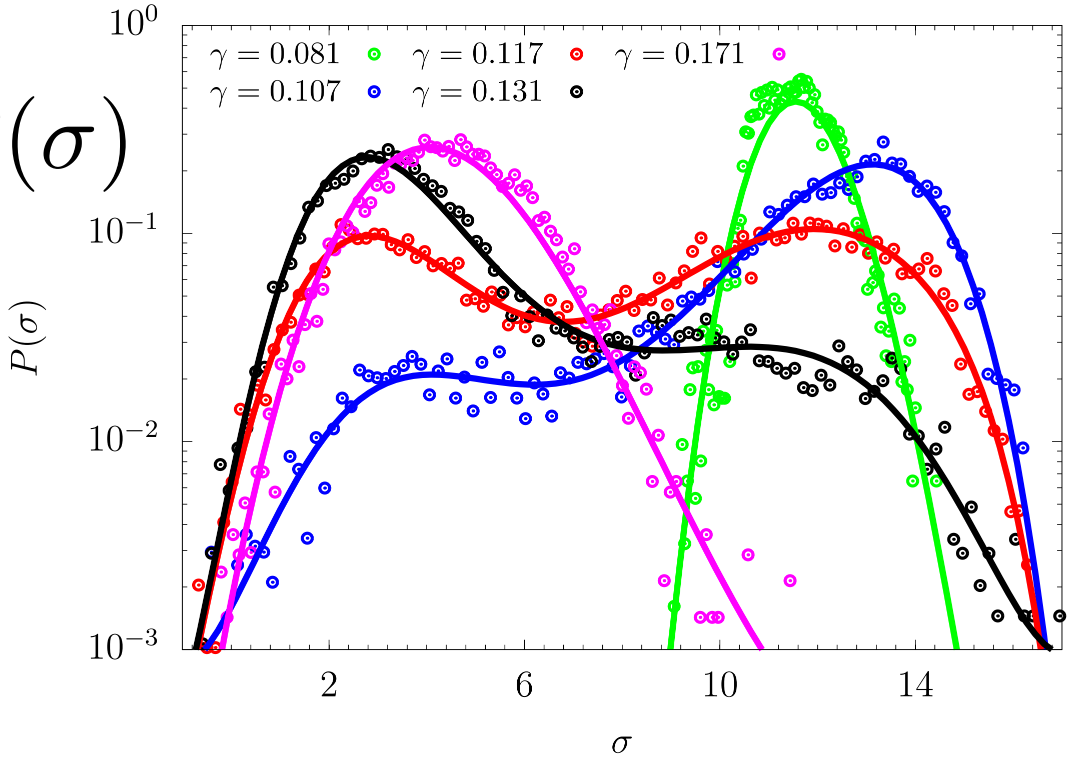
$$\chi_\sigma = N[\langle\sigma^2\rangle - \langle\sigma\rangle^2]$$

see also Jaiswal, P. K., Procaccia, I., Rainone, C., & Singh, M. (2016). Mechanical yield in amorphous solids: A first-order phase transition. Physical review letters, 116(8), 085501; Parisi, G., Procaccia, I., Rainone, C., & Singh, M. (2017). Shear bands as manifestation of a criticality in yielding amorphous solids. Proceedings of the National Academy of Sciences, 114(22), 5577-5582.

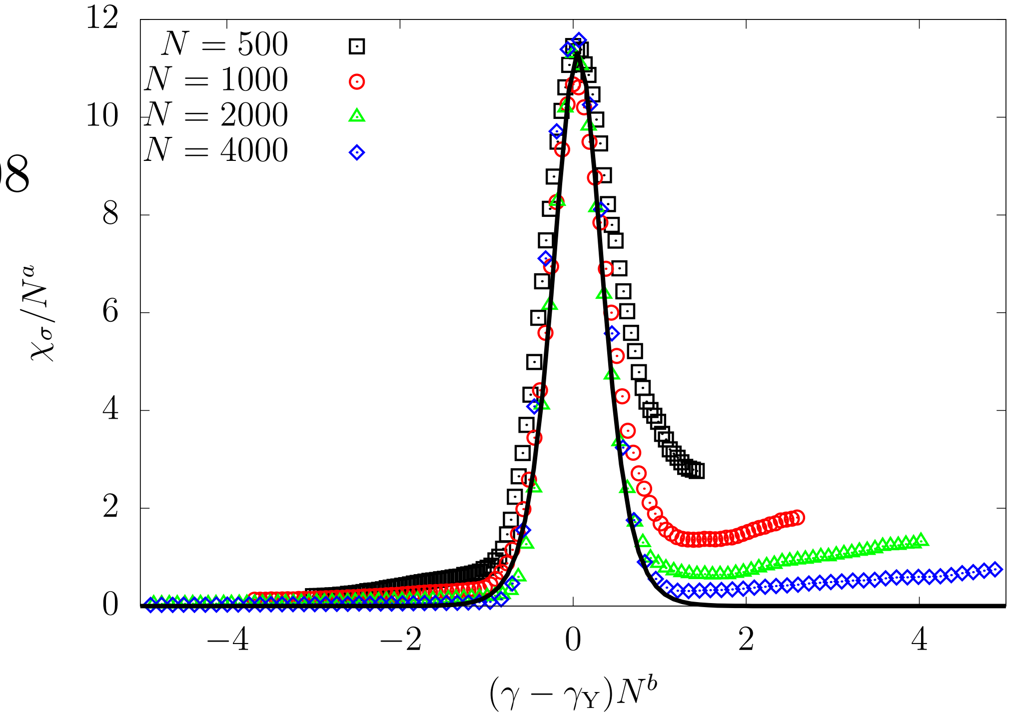
✱ Path-to-path fluctuation of stress

“liquid peak” “glass peak”

$P(\sigma)$



$a = 1.08$



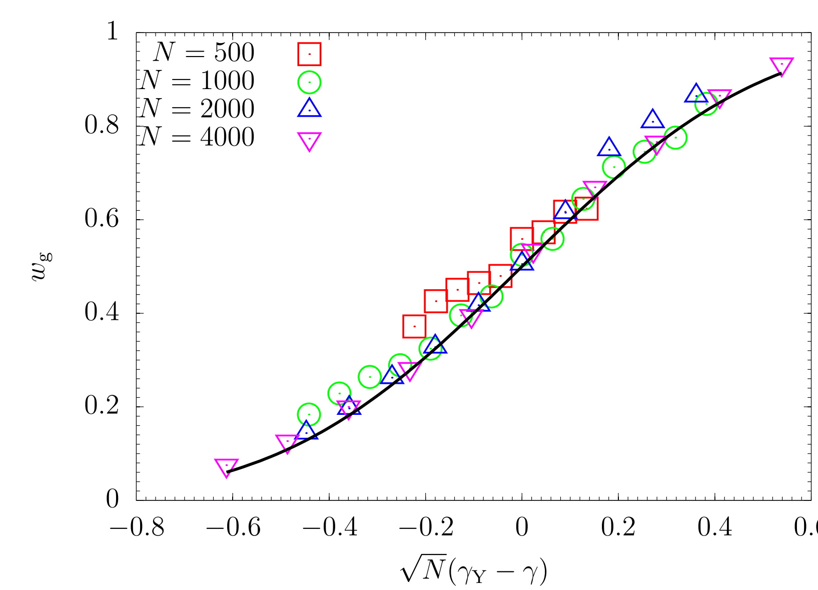
$b = 0.5$

$$P(\sigma) = (1 - w_{\mathrm{g}})\frac{e^{-\frac{(\sigma-\sigma_{\mathrm{l}})^2}{2N\delta_{\mathrm{l}}}}}{\sqrt{2\pi N\delta_{\mathrm{l}}}} + w_{\mathrm{g}}\frac{e^{-\frac{(\sigma-\sigma_{\mathrm{g}})^2}{2N\delta_{\mathrm{g}}}}}{\sqrt{2\pi N\delta_{\mathrm{g}}}}.$$

$$\chi_\sigma/N \sim F_\chi[\sqrt{N}(\gamma_{\mathrm{Y}} - \gamma)])$$

Fraction of paths not yielded at a given strain assuming Gaussian dist. of the yield stress

$$w_{\mathrm{g}} = \int_\gamma^\infty d\gamma_{\mathrm{Y}}^{\mathrm{ind}}\frac{e^{-\frac{N\left(\gamma_{\mathrm{Y}}^{\mathrm{ind}}-\gamma_{\mathrm{Y}}\right)^2}{2\delta_{\mathrm{Y}}}}}{\sqrt{2\pi\delta_{\mathrm{Y}}/N}} = \int_{\frac{\sqrt{N}(\gamma-\gamma_{\mathrm{Y}})}{\sqrt{\delta_{\mathrm{Y}}}}}^\infty dx\frac{e^{-\frac{x^2}{2}}}{\sqrt{2\pi}} = \frac{1}{2} + \frac{1}{2}\mathrm{erf}\left(\frac{\sqrt{N}(\gamma_{\mathrm{Y}}-\gamma)}{\sqrt{\delta_{\mathrm{Y}}}}\right).$$

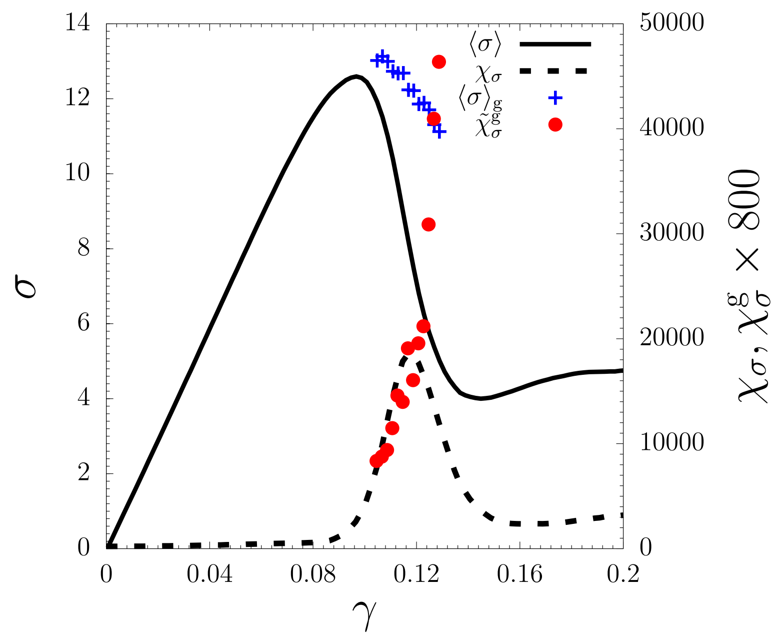


Note: 1st order transition $\quad w \propto \exp(-N\beta\Delta f)$

Spinodal like behavior of the glass peak

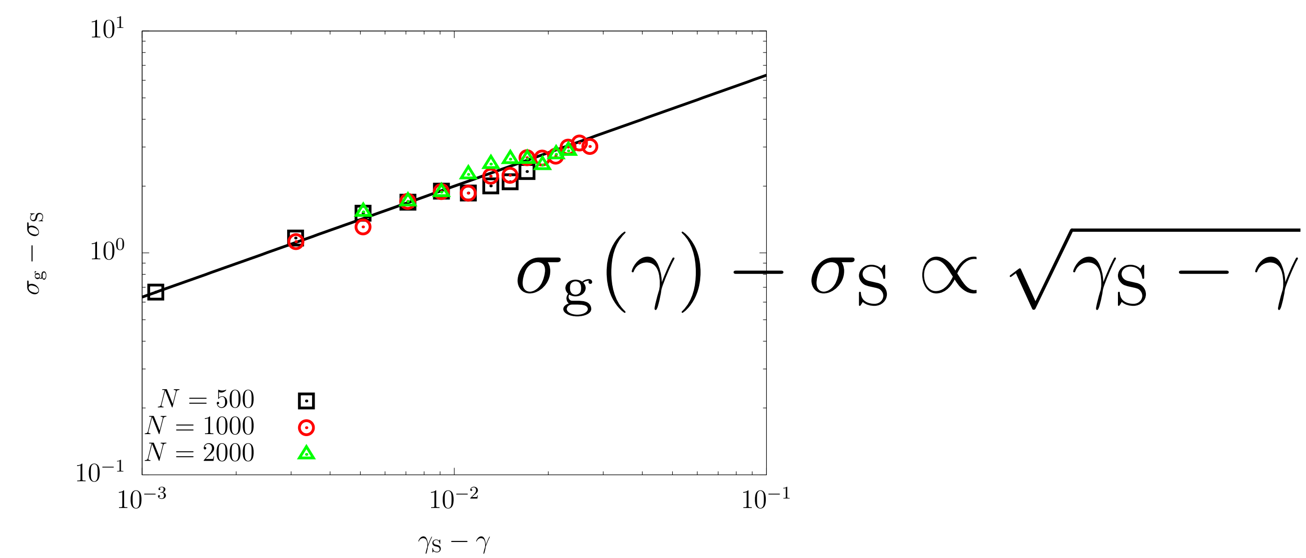
Closer look at the glass peak reveals some indication of a mean-field like behavior

$$\tilde{\chi}_\sigma^{\mathrm{g}} = N\left(\langle\sigma^2\rangle_{\mathrm{g}} - \langle\sigma\rangle_{\mathrm{g}}^2\right)/\langle\sigma\rangle_{\mathrm{g}}^2 = N^2\delta_{\mathrm{g}}/\sigma_{\mathrm{g}}^2$$

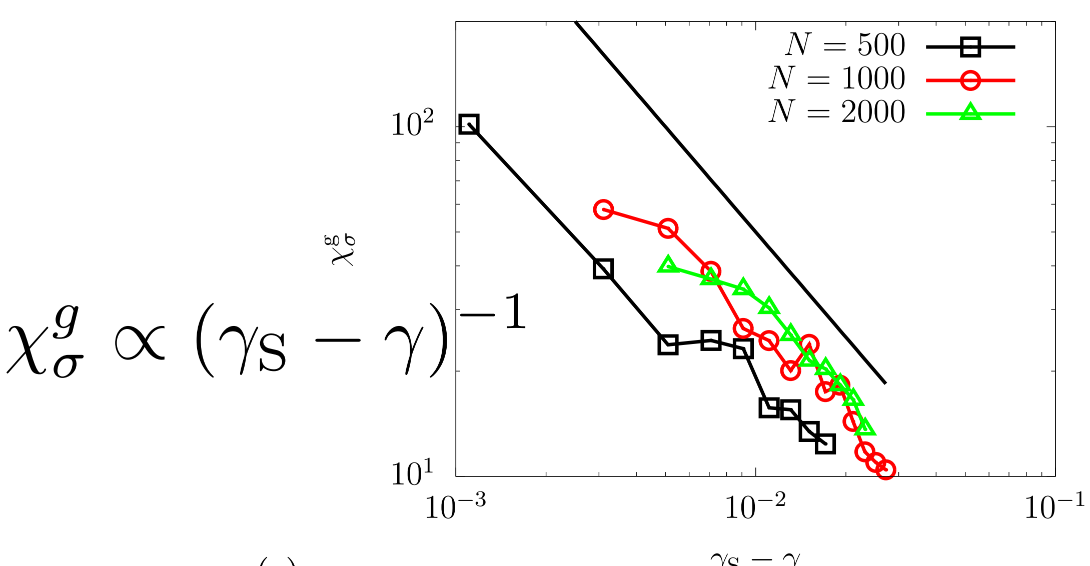


(a)

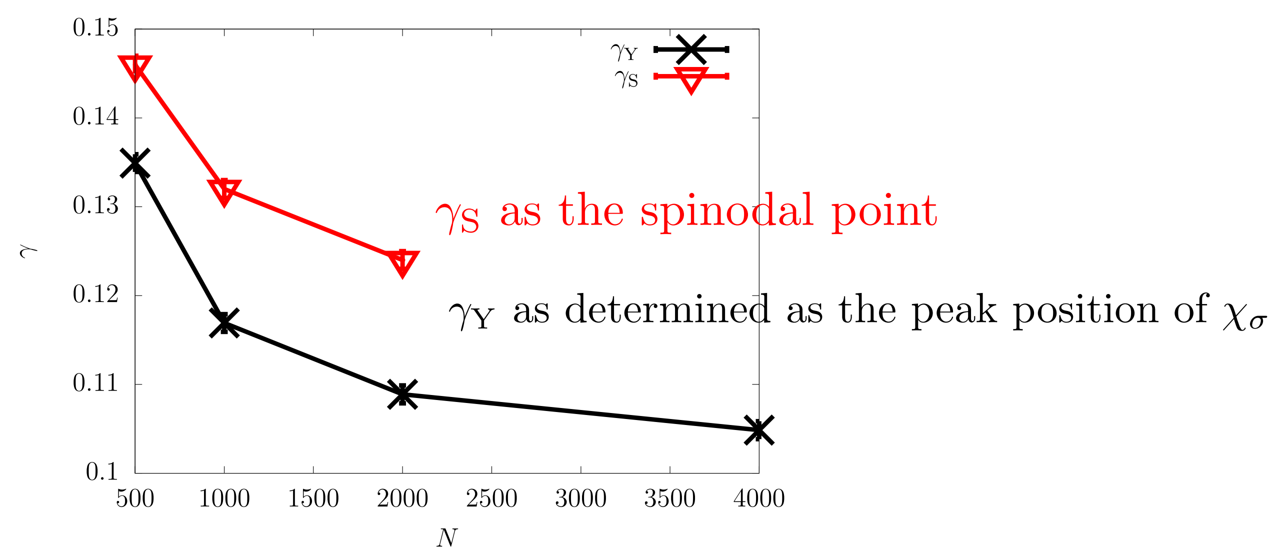
Stress at the glass peak



(b)

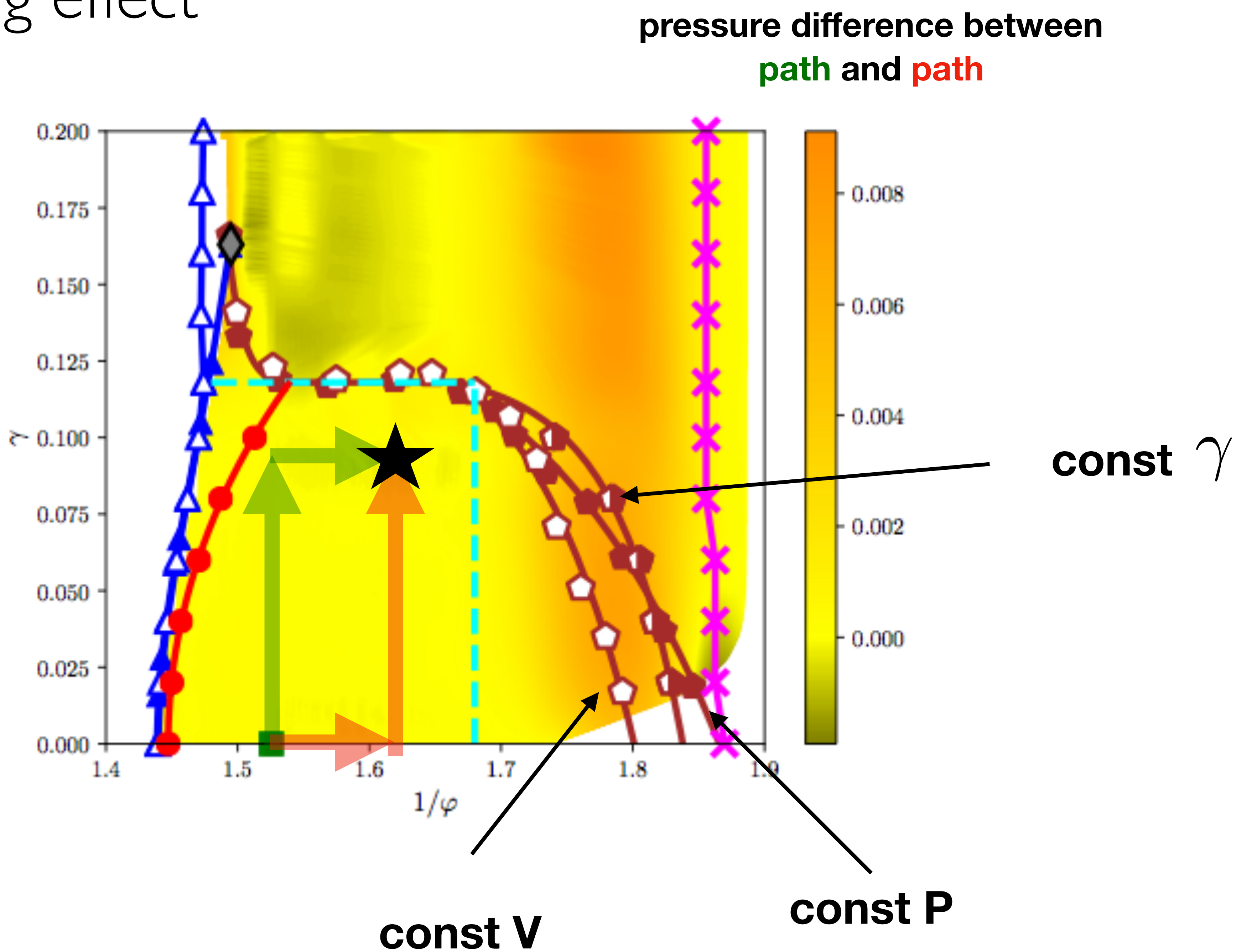


(c)



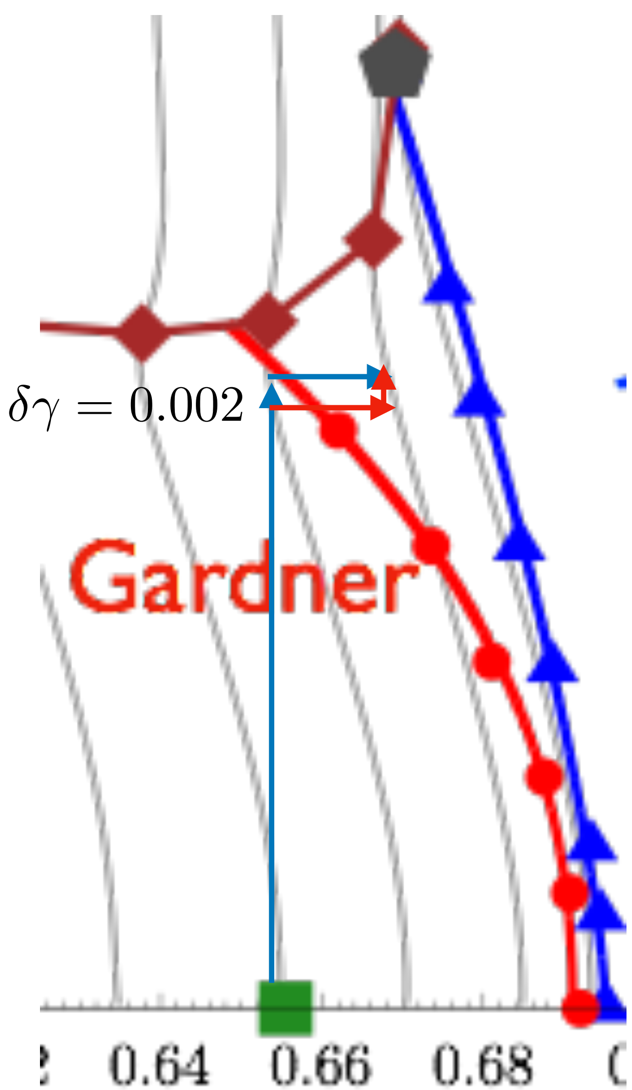
(d)

Melting effect

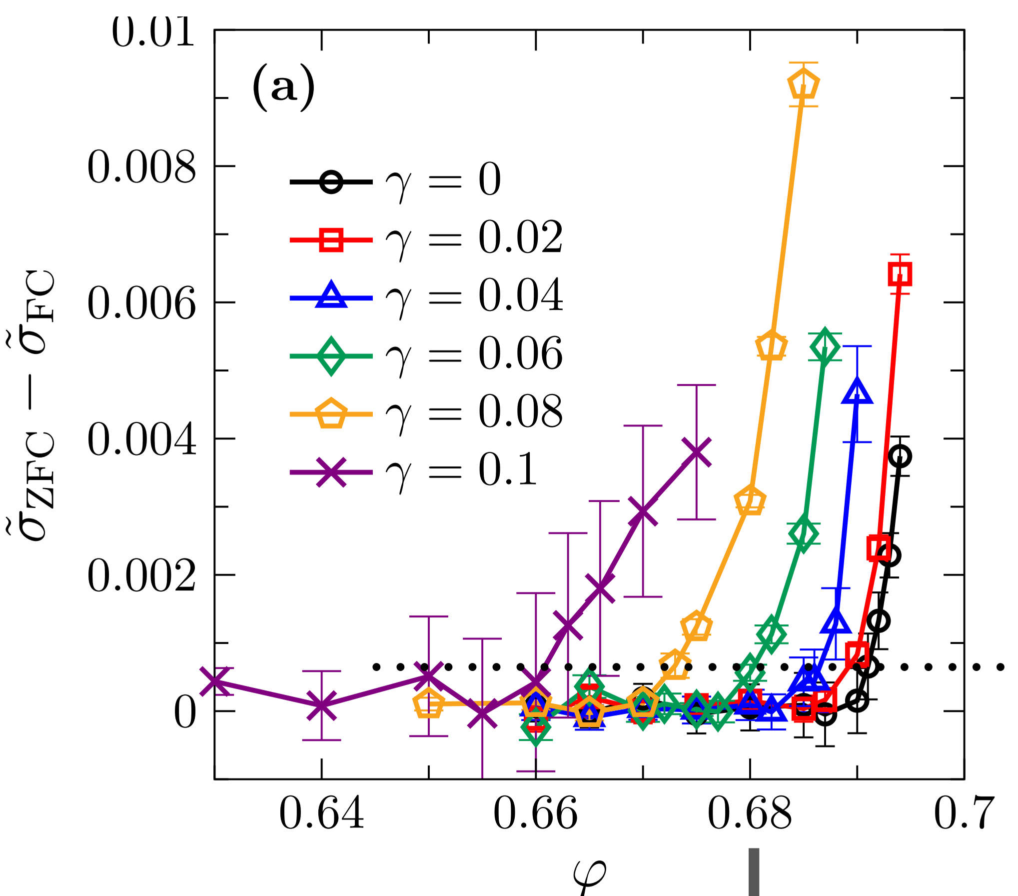


See also Fullerton, Christopher J., and Ludovic Berthier. “Density controls the kinetic stability of ultrastable glasses." EPL (Europhysics Letters) 119.3 (2017): 36003.

Gardner transition under shear

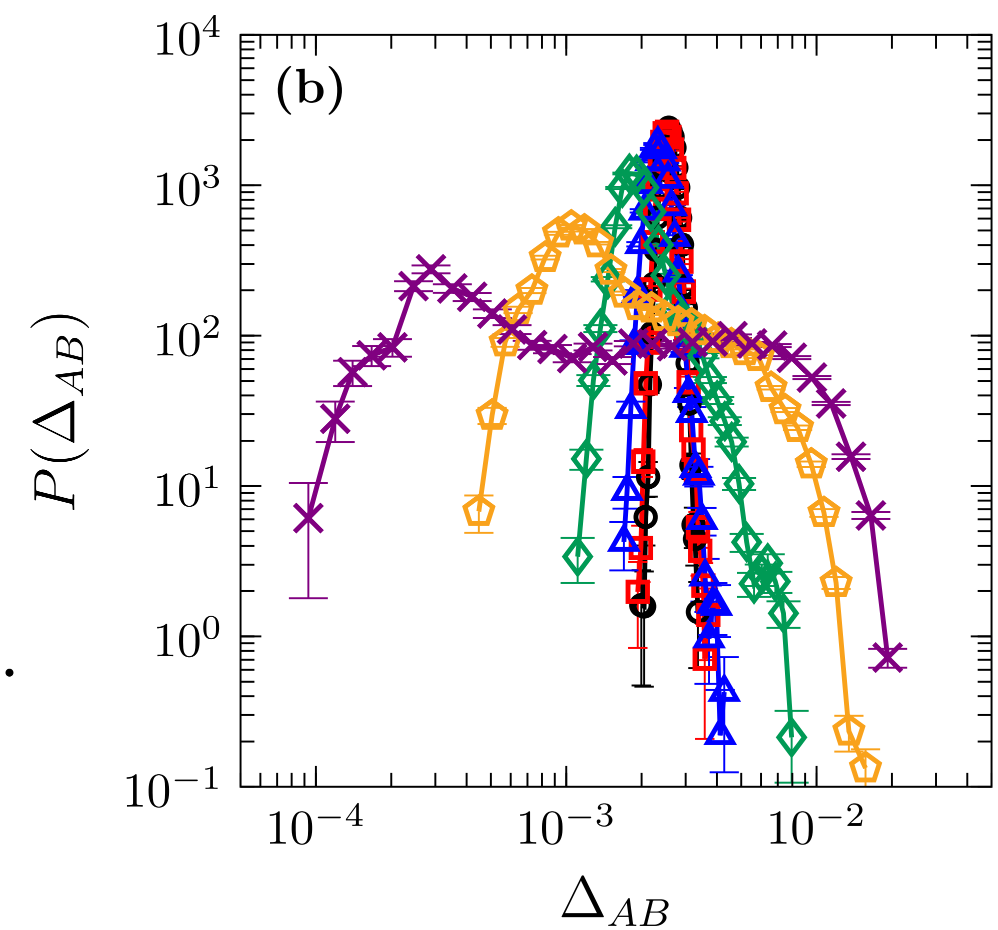


"Anomaly" in the shear-modulus



Broadening of the distribution of the glass order parameter

$\varphi = 0.68$

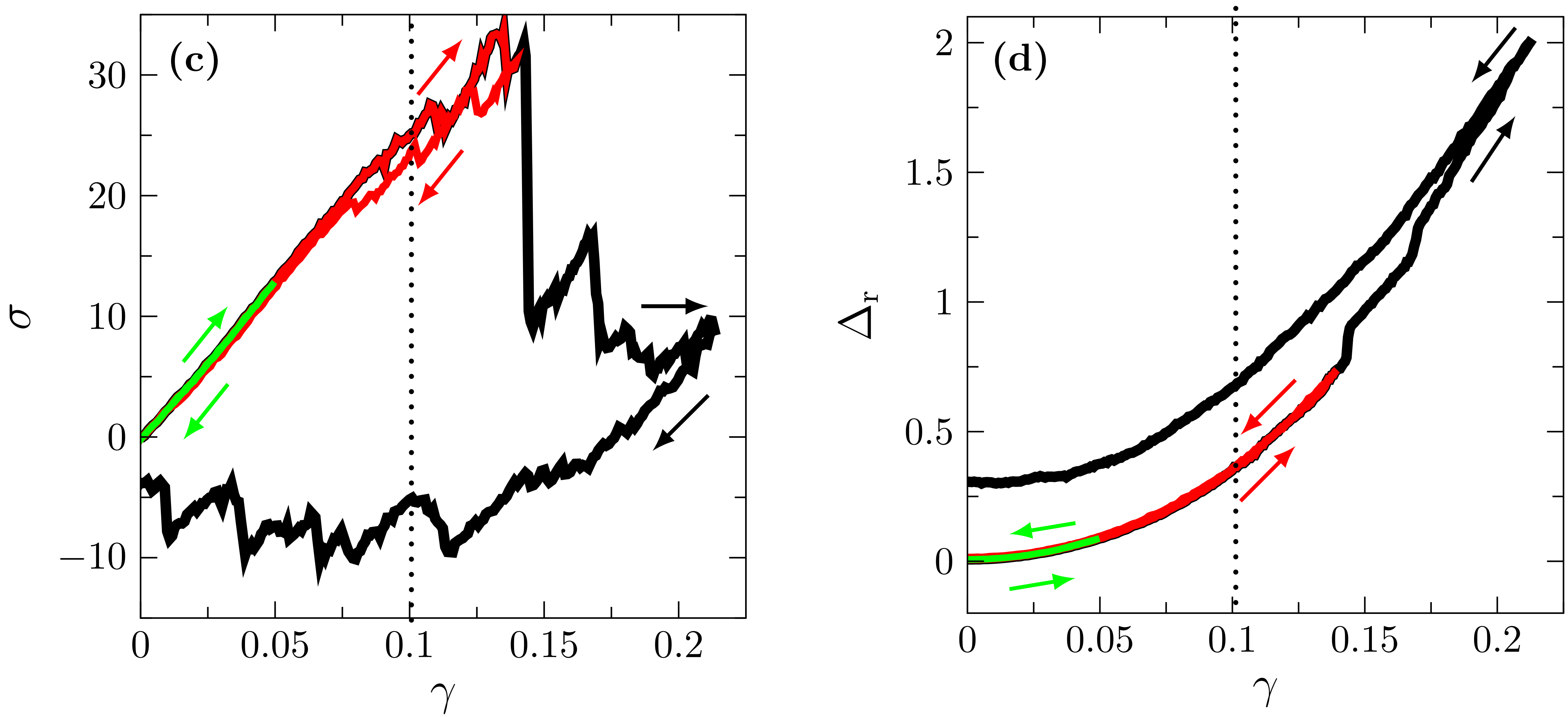


$$\gamma_{\mathrm{G}}(\varphi = 0.68) \sim 0.06$$

Reversibility to HOME (the reference liquid state)

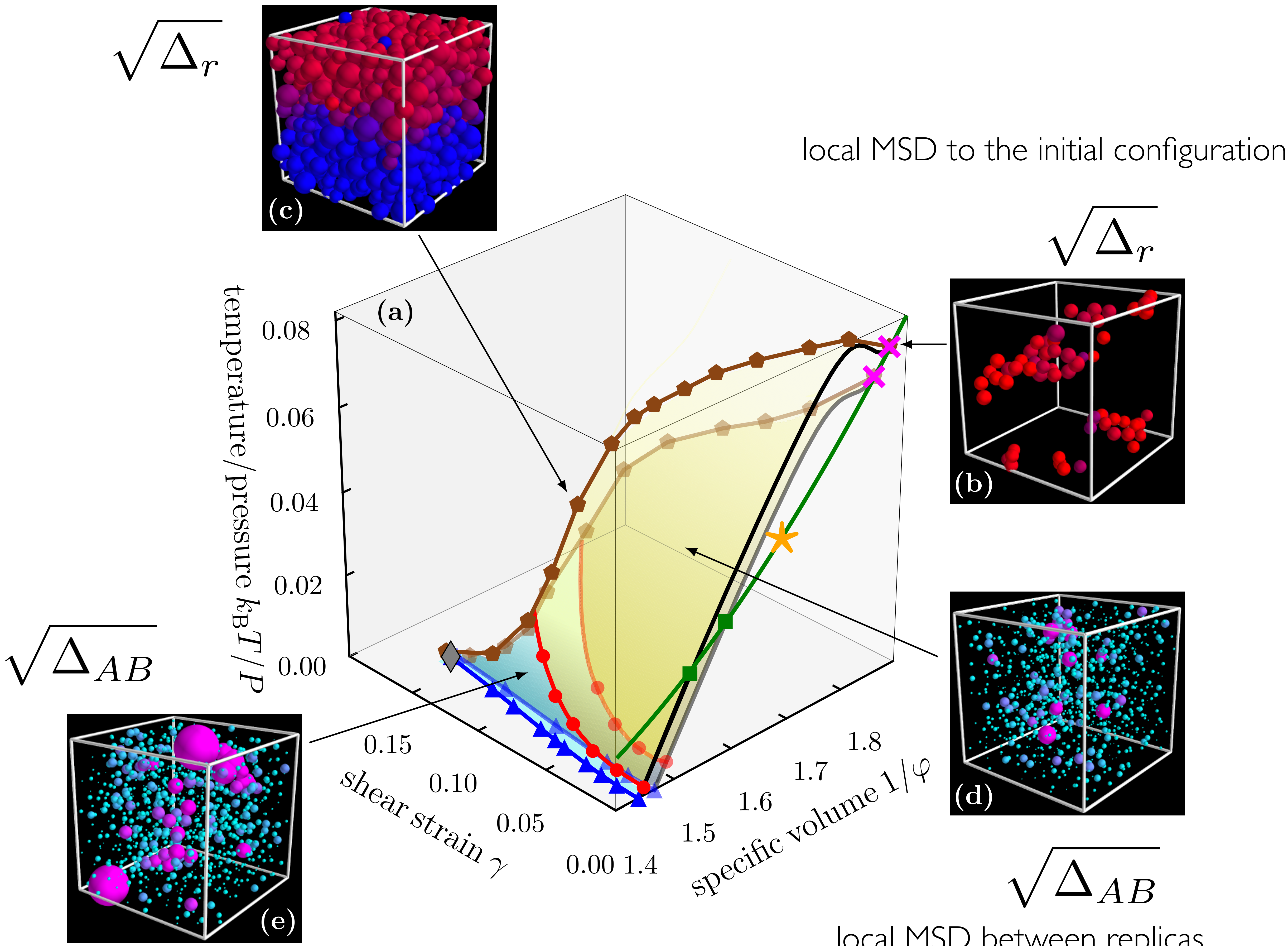
$\varphi_{\mathrm{g}} = 0.655$ $\quad \varphi = 0.66$ $\quad \gamma_{\mathrm{G}} = 0.1$

MSD to the initial state



See also oscillatory shear simulations: Kawasaki, Takeshi, and Ludovic Berthier. Physical Review E 94.2 (2016): 022615.
Leishangthem, Premkumar, Anshul DS Parmar, and Srikanth Sastry. Nature Communications 8 (2017): 14653.

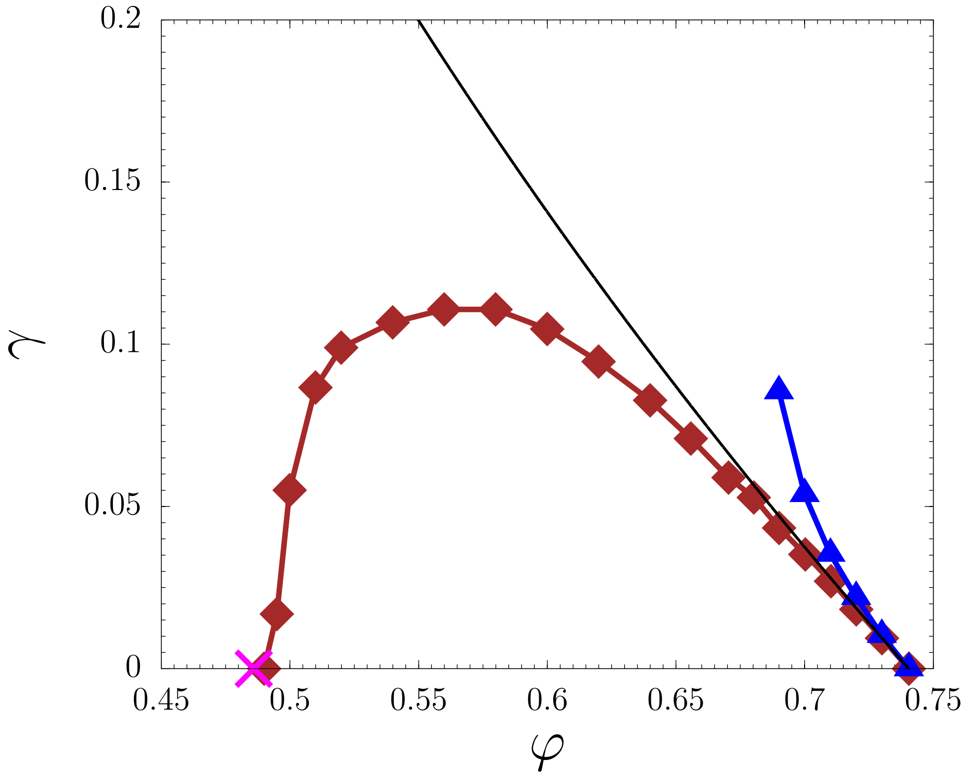
Extended glass equation of state with shear-strain axis

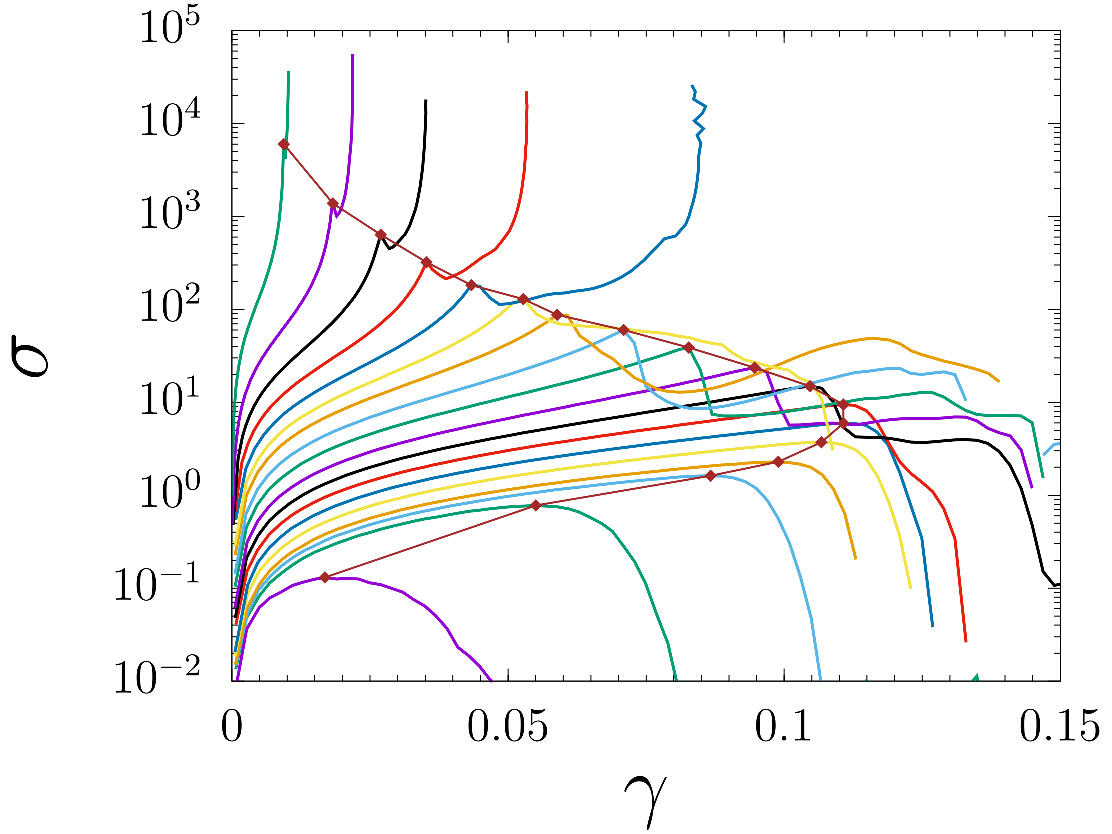


Summary

- **Shearmodulus of inherent structure/metabasin** emerge entering the marginal glass *(Gardner) phase*. We detected them via FC/ZFC protocols. The scaling of the shear modulus's agree well with large-d theory. Experiments should be interesting.
- **Shear jamming line:** the isostaticity holds and the criticality is universal.
- **Yielding :** is a discontinuous irreversible transition with Gaussian fluctuation of the yield strain. Glass peak disappear reaching a spinodal as in the large-d theory.
- **Shear jamming vs yielding :** a critical point exist as in the large-d theory.
- **Melting effect :** matters for the decompressed glasses.
- **Marginal glass appears to be stronger than stable glass**… full RSB computation should be interesting.

FCC Crystal under shear with constant volume





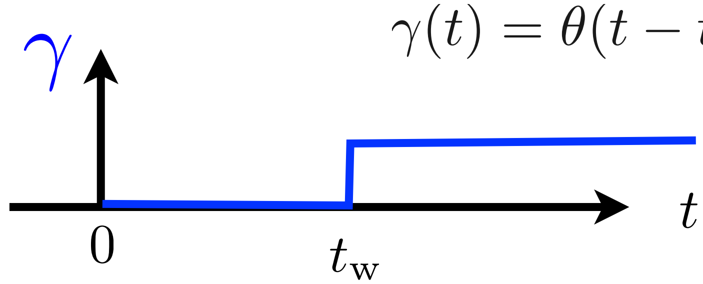
MD simulation :3D softsphere

S. Okamura and HY, arXiv:1306.2777 (not yet published)

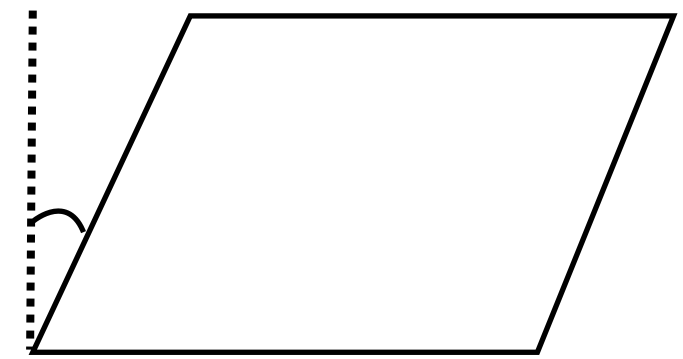
shear strain

$\gamma(t) = \theta(t - t_{\rm w})\delta\gamma$

quench $t = 0$



Aging



Initial configuration

$T/\epsilon = 10^{-3}$

Equilibrium state (liquid)

response function

$$\mu(t, t_{\rm w}) = \frac{\delta\langle\sigma(t; t_{\rm w})\rangle}{\delta\gamma}$$

autocorrelation function

$$C_\sigma(t, t_{\rm w}) = \langle\sigma(t)\sigma(t_{\rm w})\rangle$$

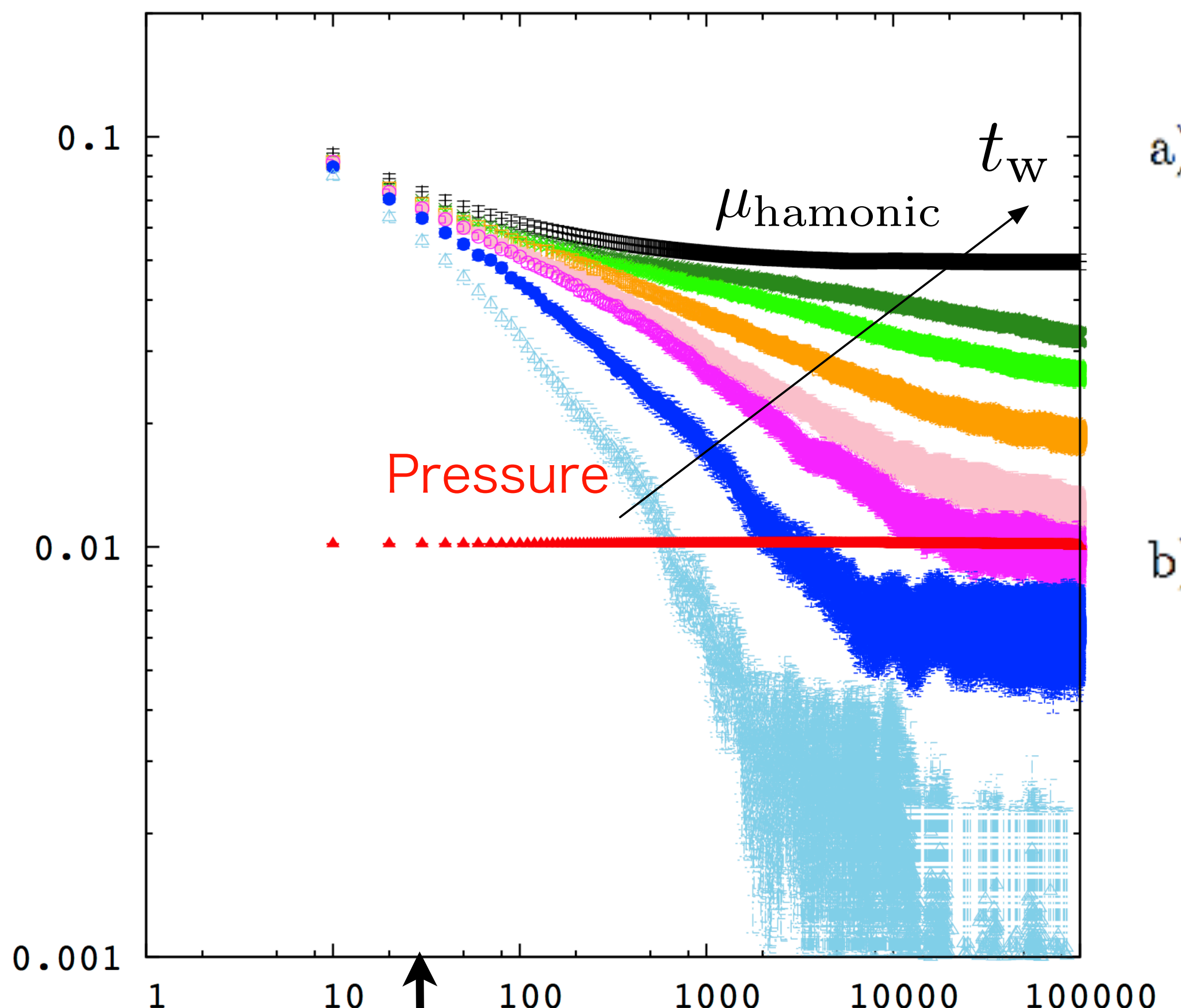
temperature	$k_{\rm B}T/\epsilon = 10^{-5}$	Langevin simulation	
shear-strain	$\gamma = 2.5 \times 10^{-3}$	Lee-Edwards boundary condition	
volume fraction	$\varphi = 0.65 - 0.67$		
# of particles	$N = 800, 1600$	time scale	$O(t/t_0) = 10^5$

# of sample (initial condition/ Langevin noise)

$\#$ of samples : 4096

$$\varphi = 0.67 \quad k_{\mathrm{B}}T/\epsilon = 10^{-5}$$

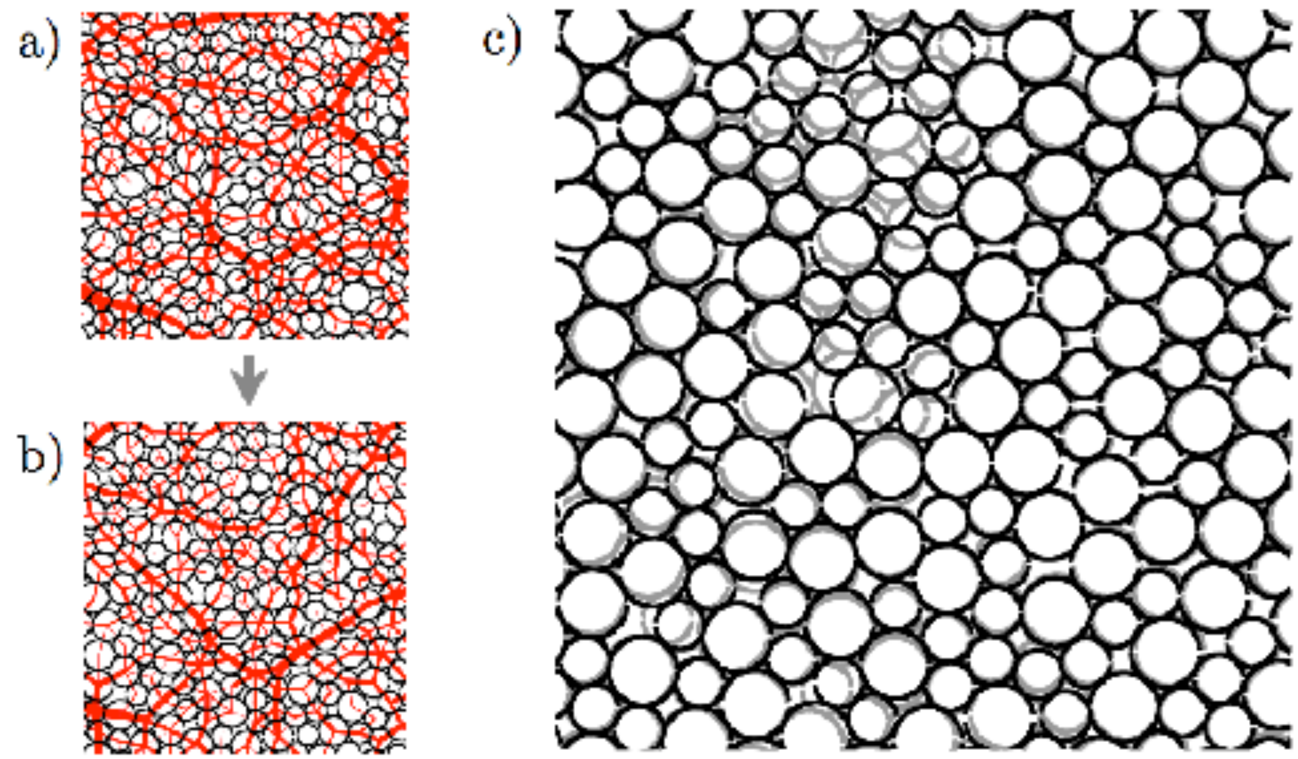
$\sigma(\tau; t_{\mathrm{w}})/\gamma$



τ

$$t^* = 2\pi/\omega^* = (\varphi = 0.67)$$

$t_{\mathrm{w}} = 3 \times 10^2, 10^3, 3 \times 10^3, 5 \times 10^3, 10^4, 3 \times 10^4, 10^5$



Stress does not decay fully down to zero... Metabasin?