Rheology of disordered particles
-suspensions, glassy and granular materials
YITP, Kyoto Univ.   2018/06/29

Stability-reversibility map of hard sphere glasses

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Fluctuation & Structure

科研費
KAKENHI

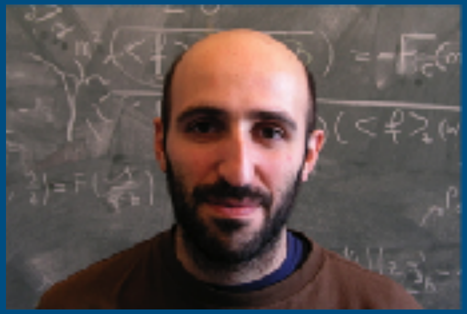
大阪大学
OSAKA UNIVERSITY

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

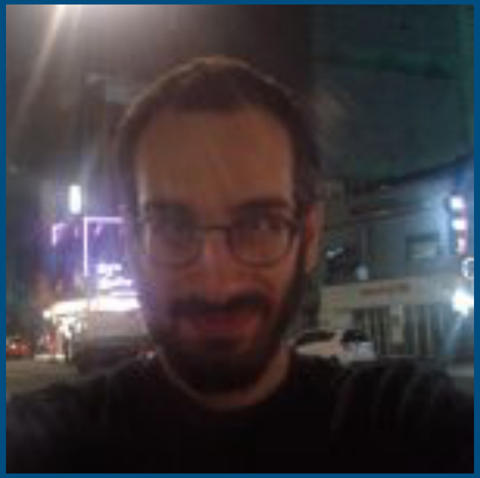
Collaborators

Yuliang Jin (ITP, CAS)

Francesco Zamponi (ENS Paris)

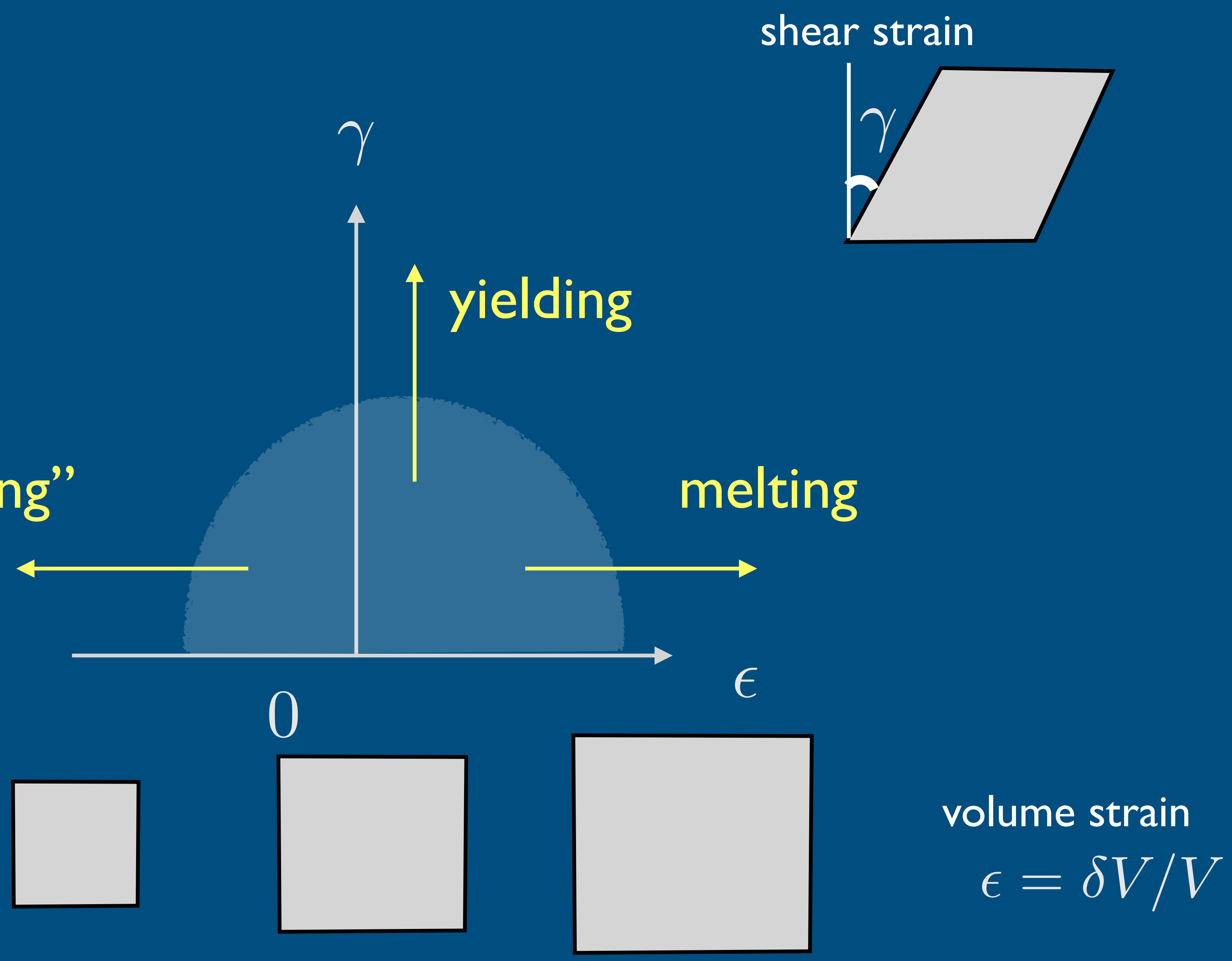


Pierfrancesco Urbani(CEA Saclay)



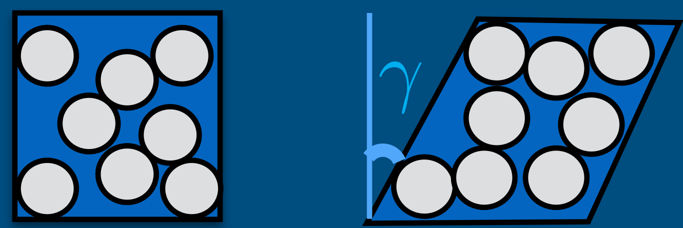
Stability map of a piece of solid

Stability against quasi-static deformations

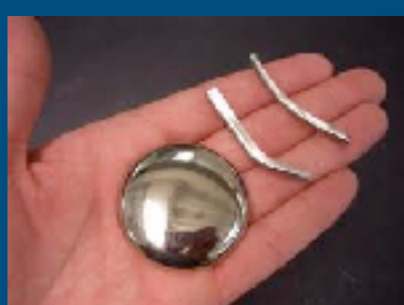


c.f. In the context of jamming… A. Liu and S. Nagel (1998)

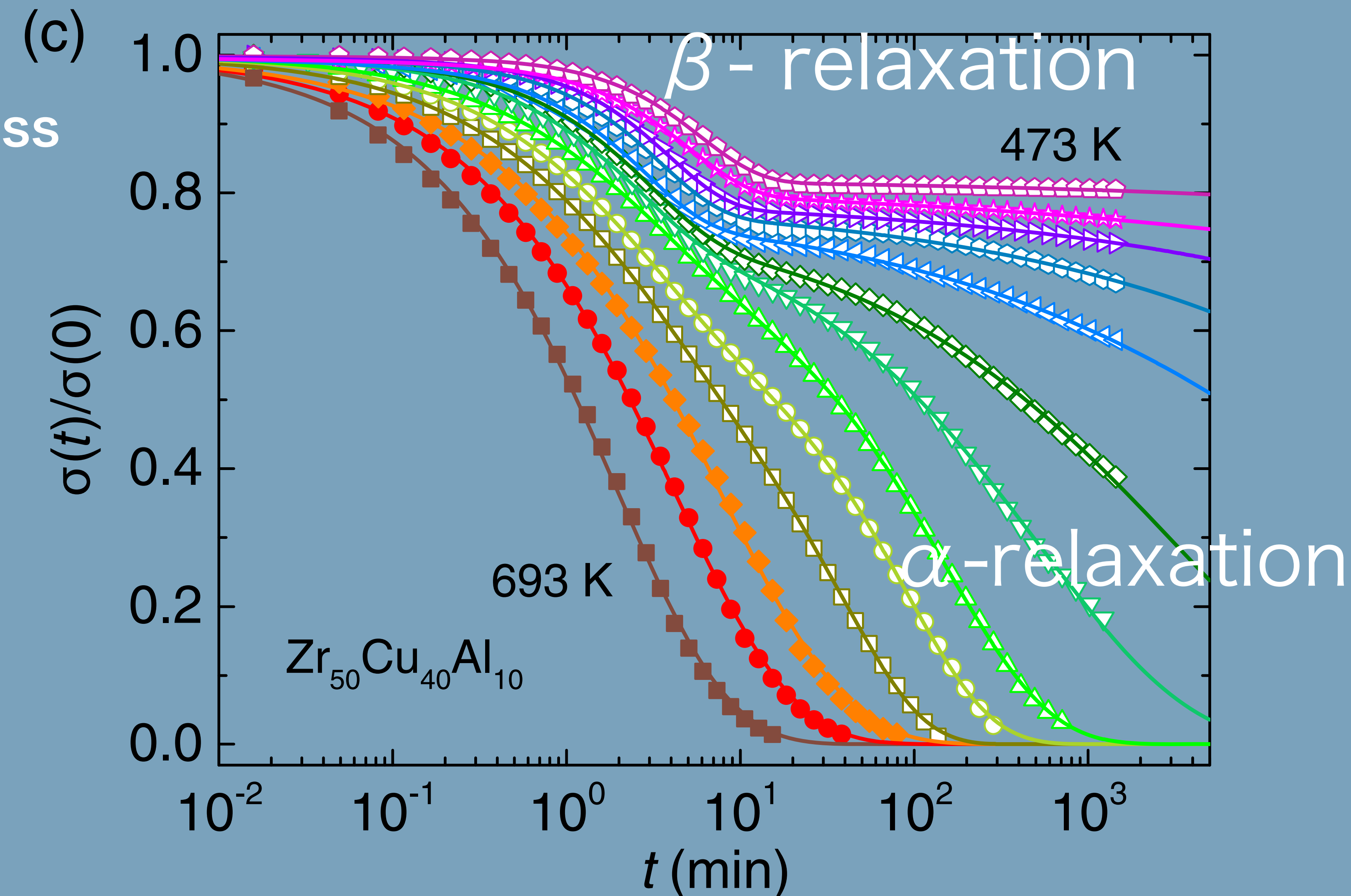
Liquid and glass : stress relaxation



shear stress

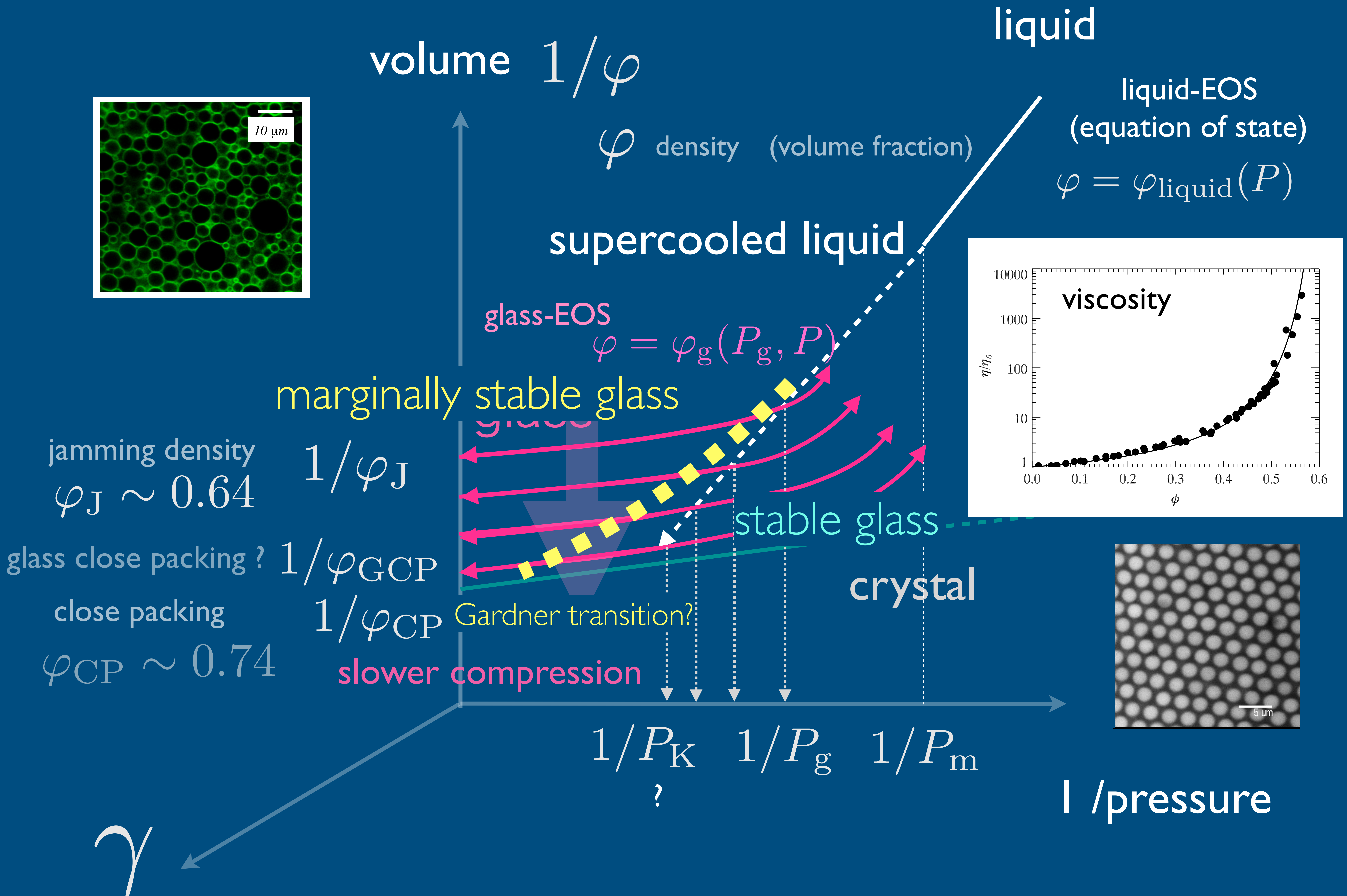


metallic glass



P. Luo, P. Wen, H. Y. Bai, B. Ruta and W. H. Wang,
PRL 118, 225901 (2017)

colloidal glass (hardsphere glass)



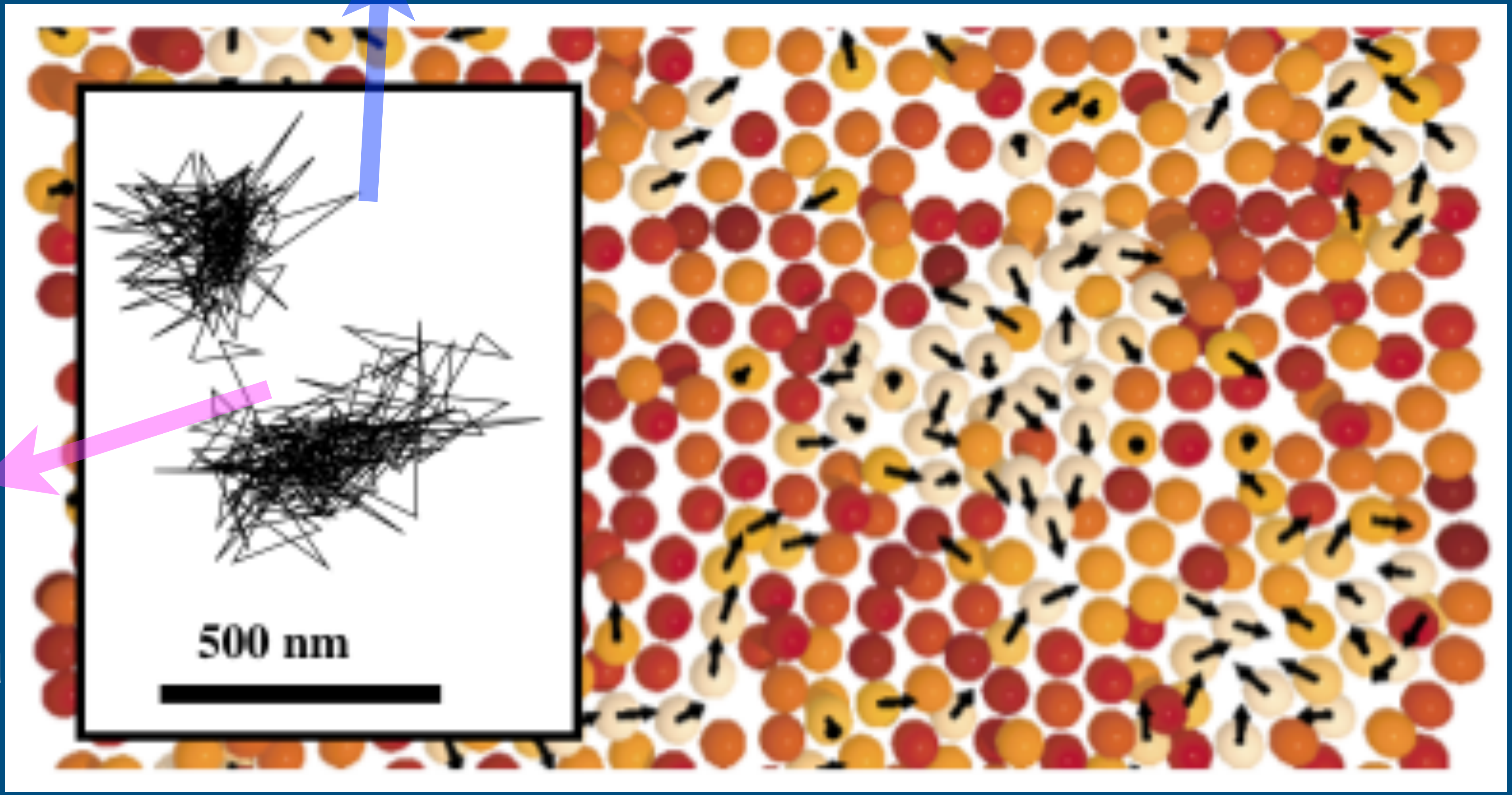
Colloidal glass

Vibrations within "cages"

β - relaxation

Structural relaxation

α-relaxation



Confocal scope image (E. Weeks and D. Weitz (2002))

Outline

1. Introduction

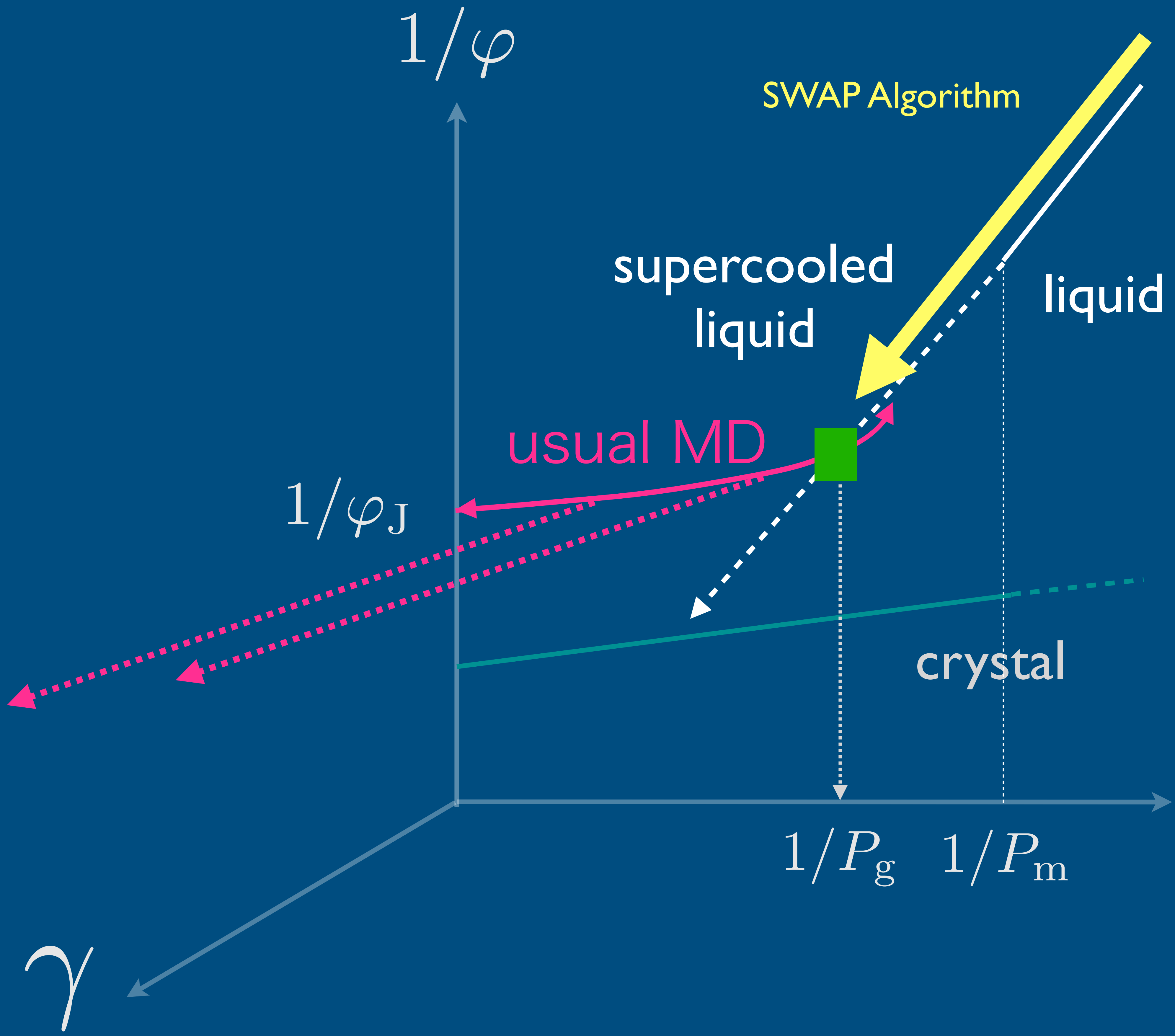
   One way to create a hard-sphere glass : swap then MD

   Theoretical results in large-d limit $d \to \infty$

2. 3D hard-sphere glass : MD simulation

3. Conclusions

One way to create a hard-sphere glass : swap then MD



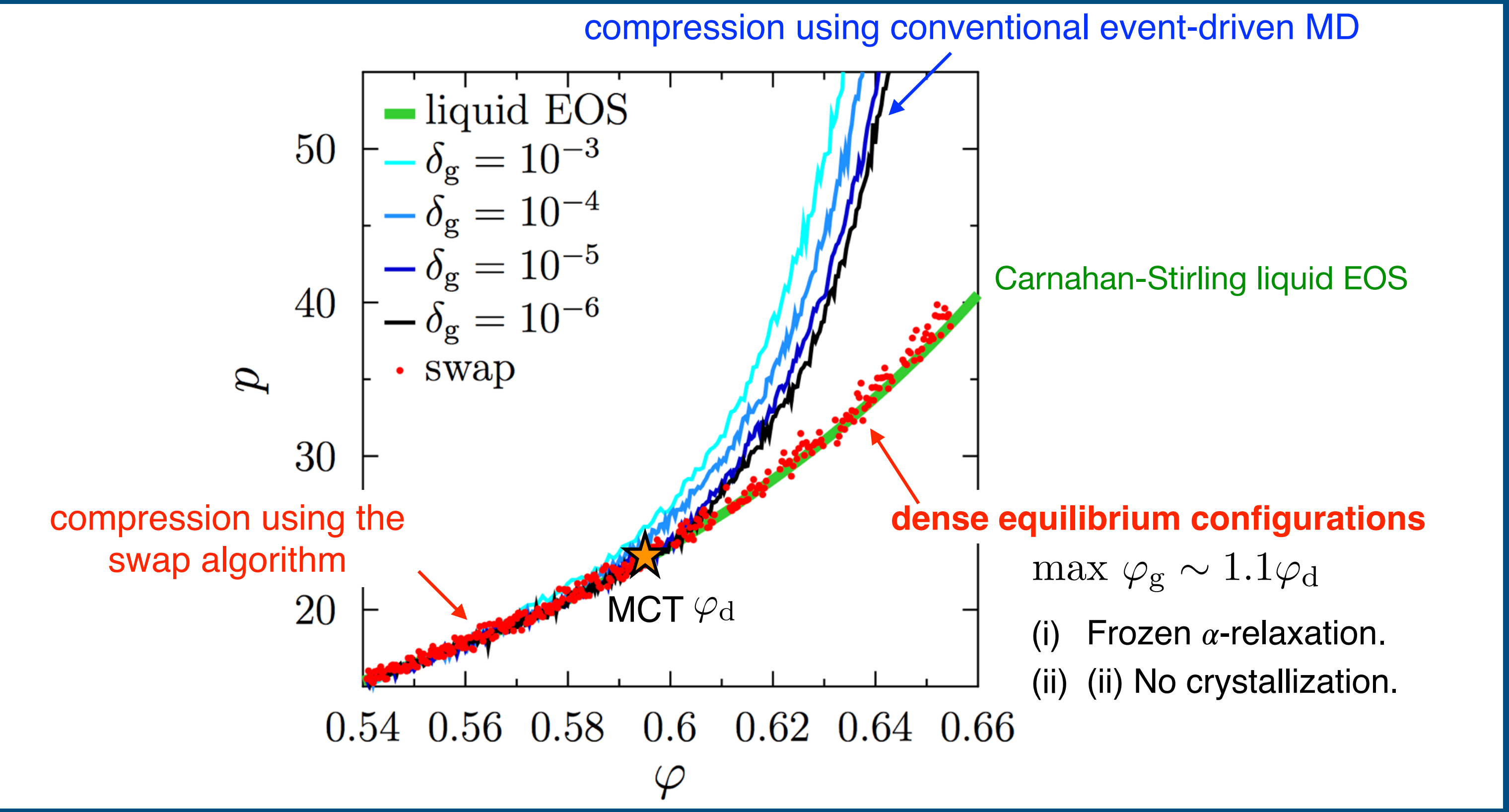
Preparation of dense equilibrium liquid via Swap Algorithm

Early works: Kranendonk-Frenkel (1991), Grigera-Parisi (2001)

Recent progress: Berthier et. al. (2016)

Polydisperse hard spheres $P(D) \sim D^{-3}, D_{\min} < D_{\min}/0.45$

our check



Exact theoretical results in large-d limit $d \to \infty$

liquid density functional theory + replica method

Kurchan-Parisi-Zamponi (2012), Kurchan-Parisi-Urbani-Zampoi (2013)

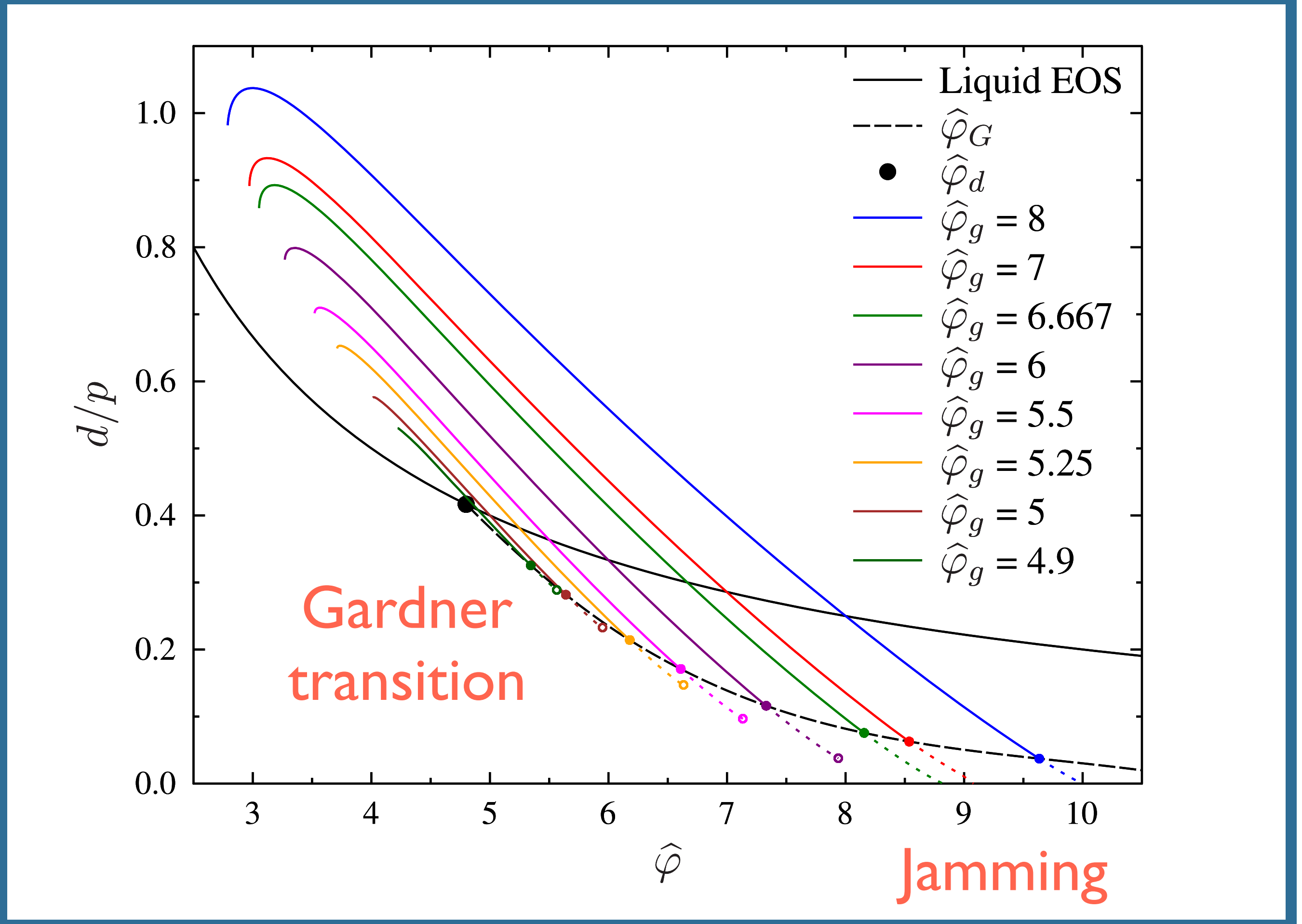
Charbonneau-Kurchan-Parisi-Urbani-Zamponi (2014)

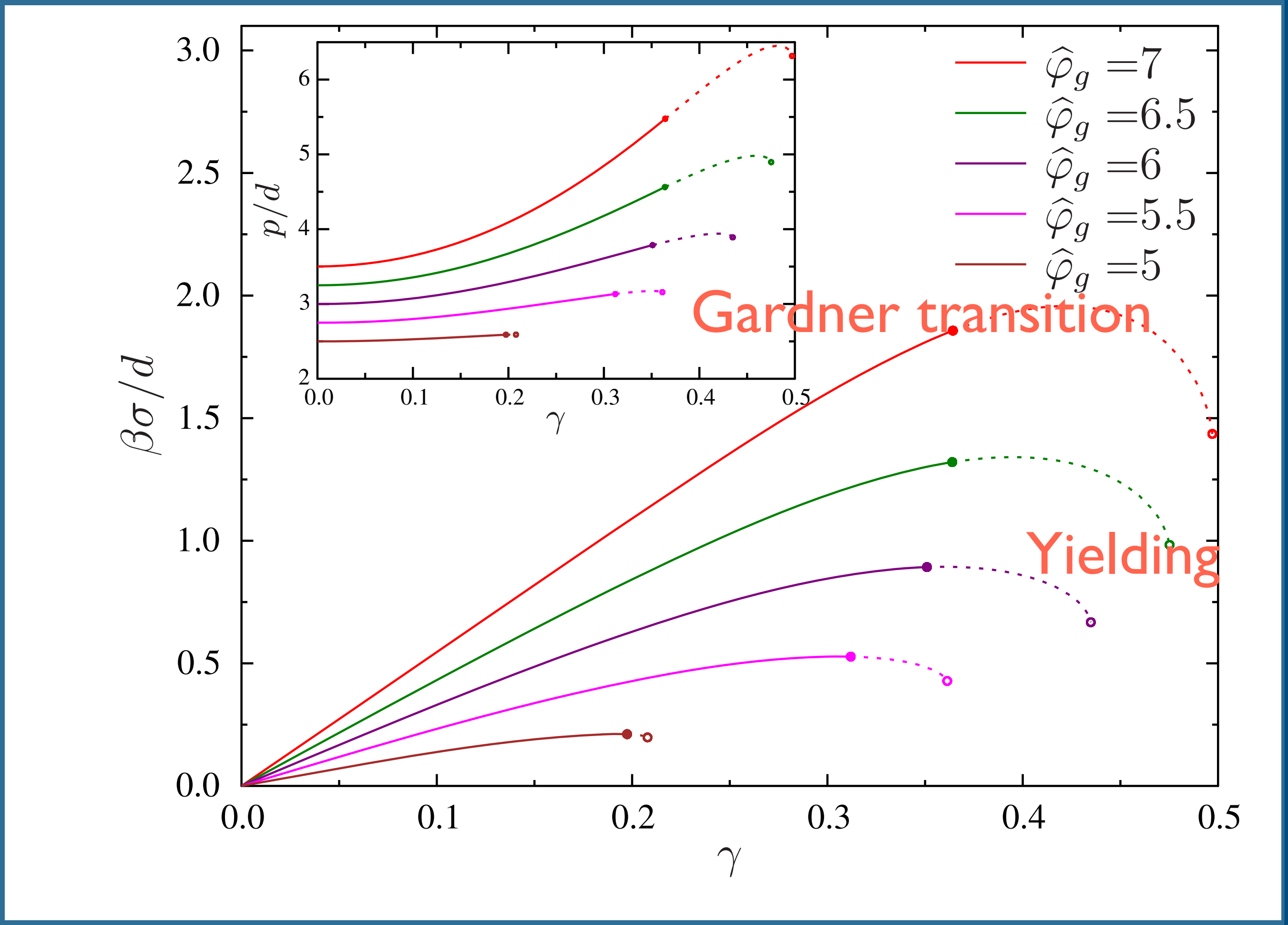
Dynamic glass transition
Static glass transition (Kauzmann transition)

Gardner transition
isostaticity and criticality at jamming

" Shear" Yoshino-Zamponi (2014)

"Glass state following" Rainone-Urbani-Yoshino-Zamponi (2015)





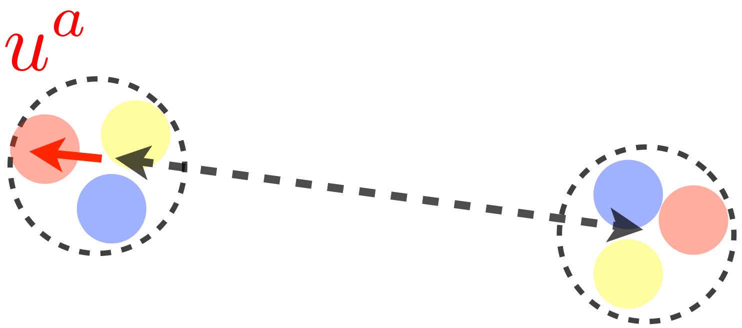
Rainone-Urbani (2015), Biroli-Urbani (2017), Urbani-Zamponi (2017)

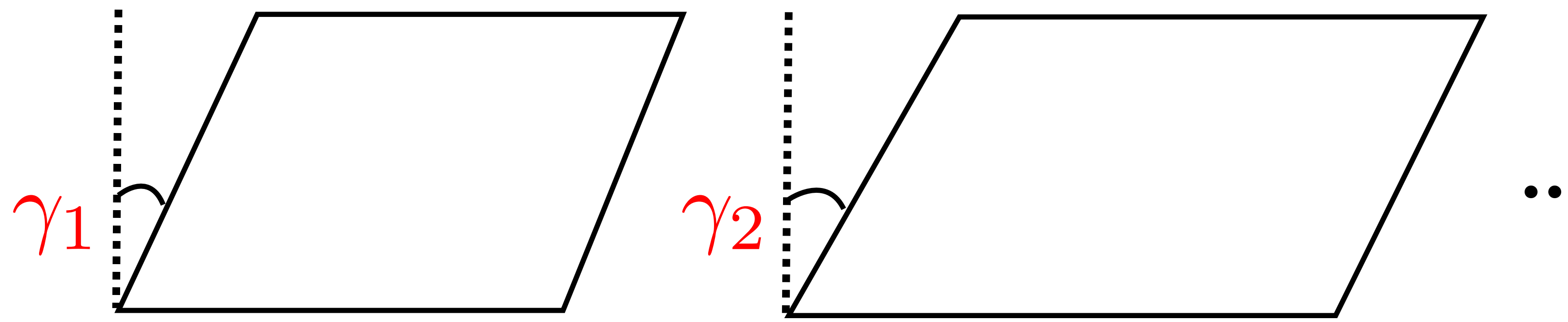
Replicated simple liquids in $d \to \infty$

Kurchan-Parisi-Zamponi (2012), Kurchan-Parisi-Urbani-Zampoi (2013)

Charbonneau-Kurchan-Parisi-Urbani-Zamponi (2014)

"Shear on replicated liquid" : HY and F. Zamponi, (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

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

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

1 step RSB

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

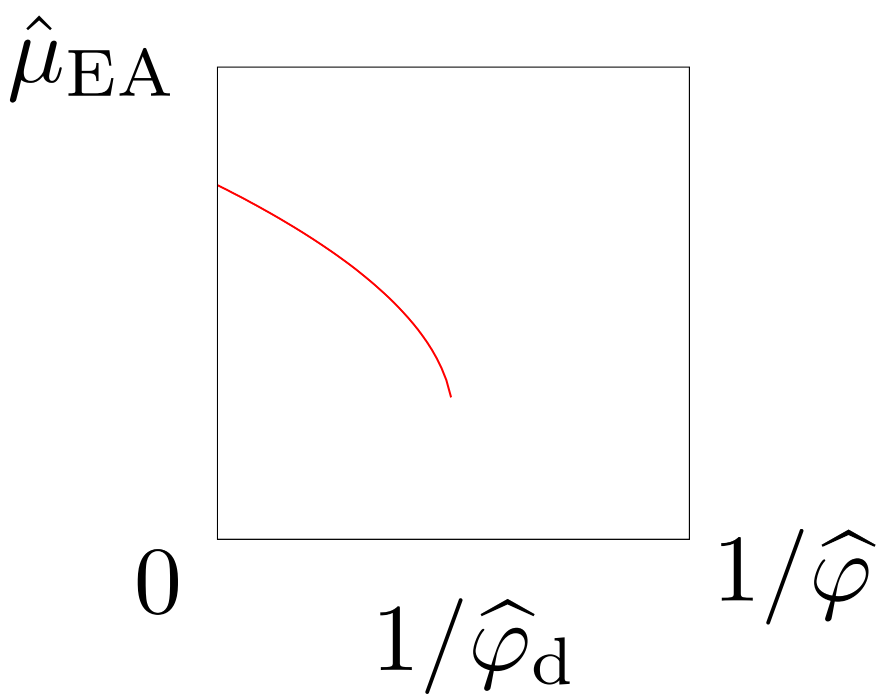
$$\beta\widehat{\mu}_{ab} = \beta\widehat{\mu}_{\rm EA}\left(\delta_{ab} - \frac{1}{m}\right)$$

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

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).



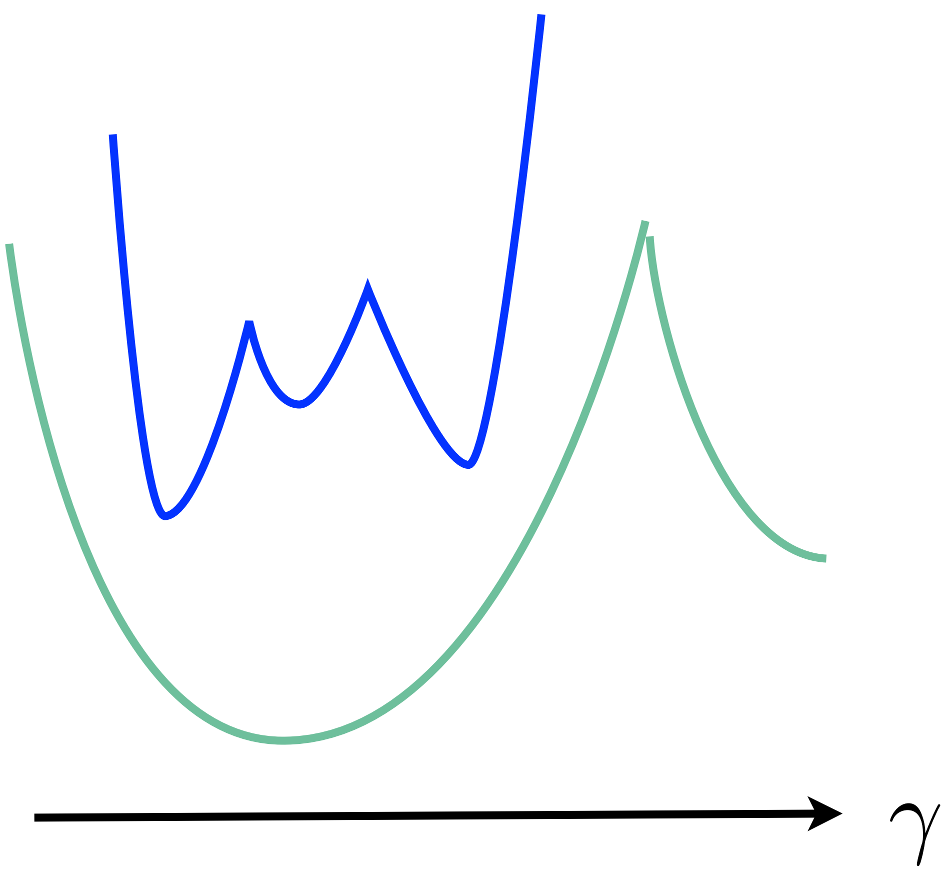
HY and F. Zamponi, Phys. Rev. E 90, 022302 (2014).

1+continuous RSB

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

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

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



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

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"

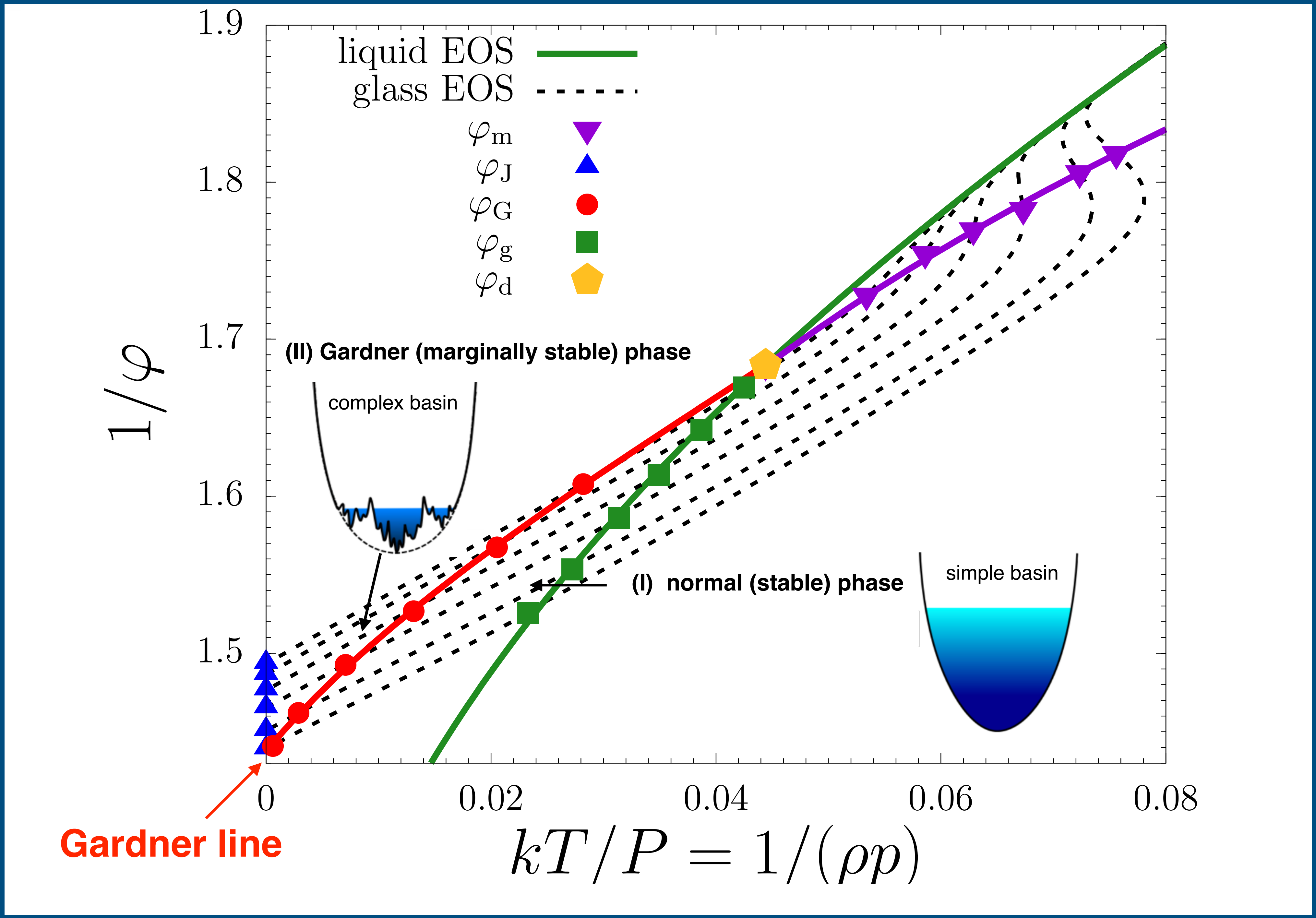
HY and F. Zamponi, Phys. Rev. E 90, 022302 (2014).

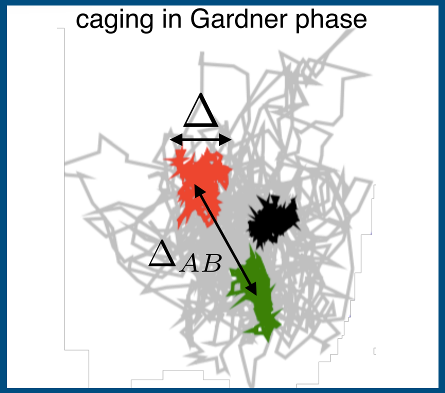
3D hard-sphere glass : MD simulation

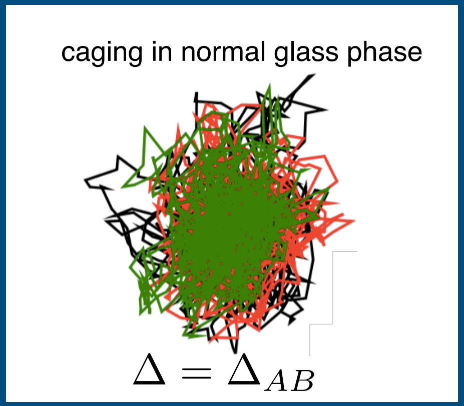
Y. Jin and HY, Nature Communications 8, 14935 (2017).

Y. Jin, P. Urbani, F. Zamponi and HY, arXiv: 1803.04597.

Y. Jin and HY, in preparation


liquid EOS
glass EOS
φ_m
φ_J
φ_G
φ_g
φ_d
(II) Gardner (marginally stable) phase
complex basin
(I) normal (stable) phase
simple basin
Gardner line
$1/\varphi$
$kT/P = 1/(\rho p)$
1.9
1.8
1.7
1.6
1.5
0
0.02
0.04
0.06
0.08

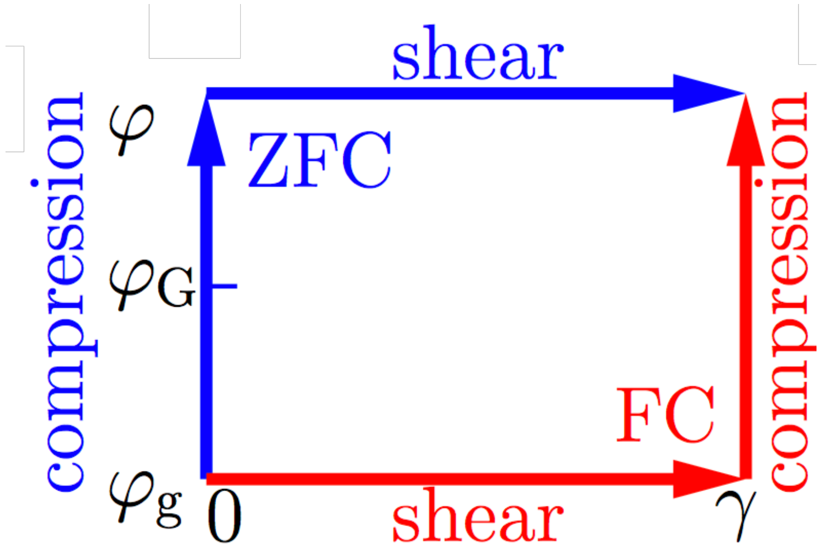

caging in Gardner phase
Δ
Δ_{AB}


caging in normal glass phase
$\Delta = \Delta_{AB}$

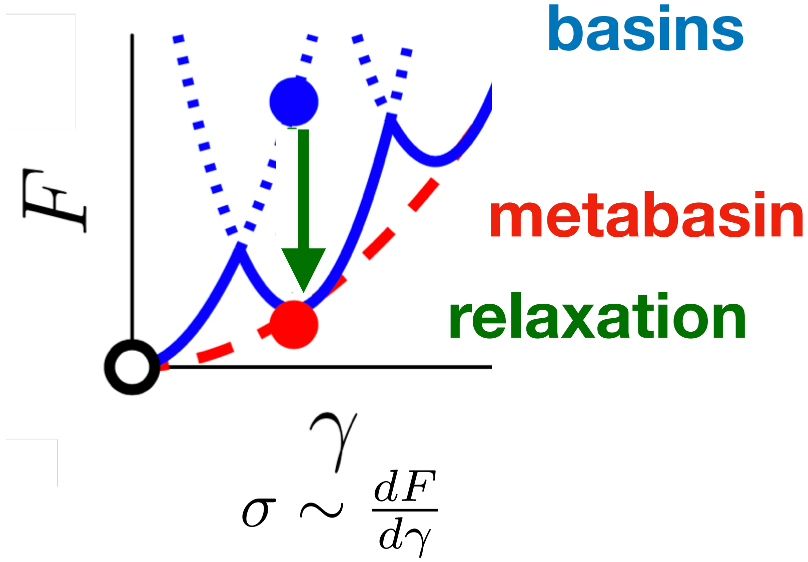
Consequence of Gardner transition on shear modulus — protocol dependence

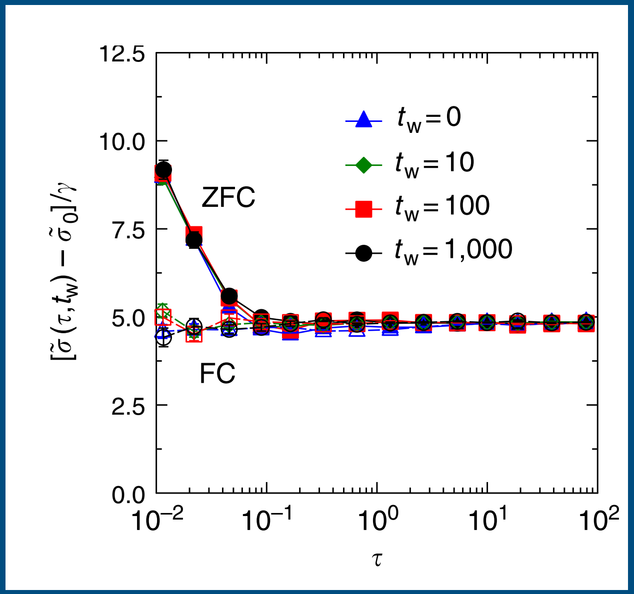
Hard sphere simulations:

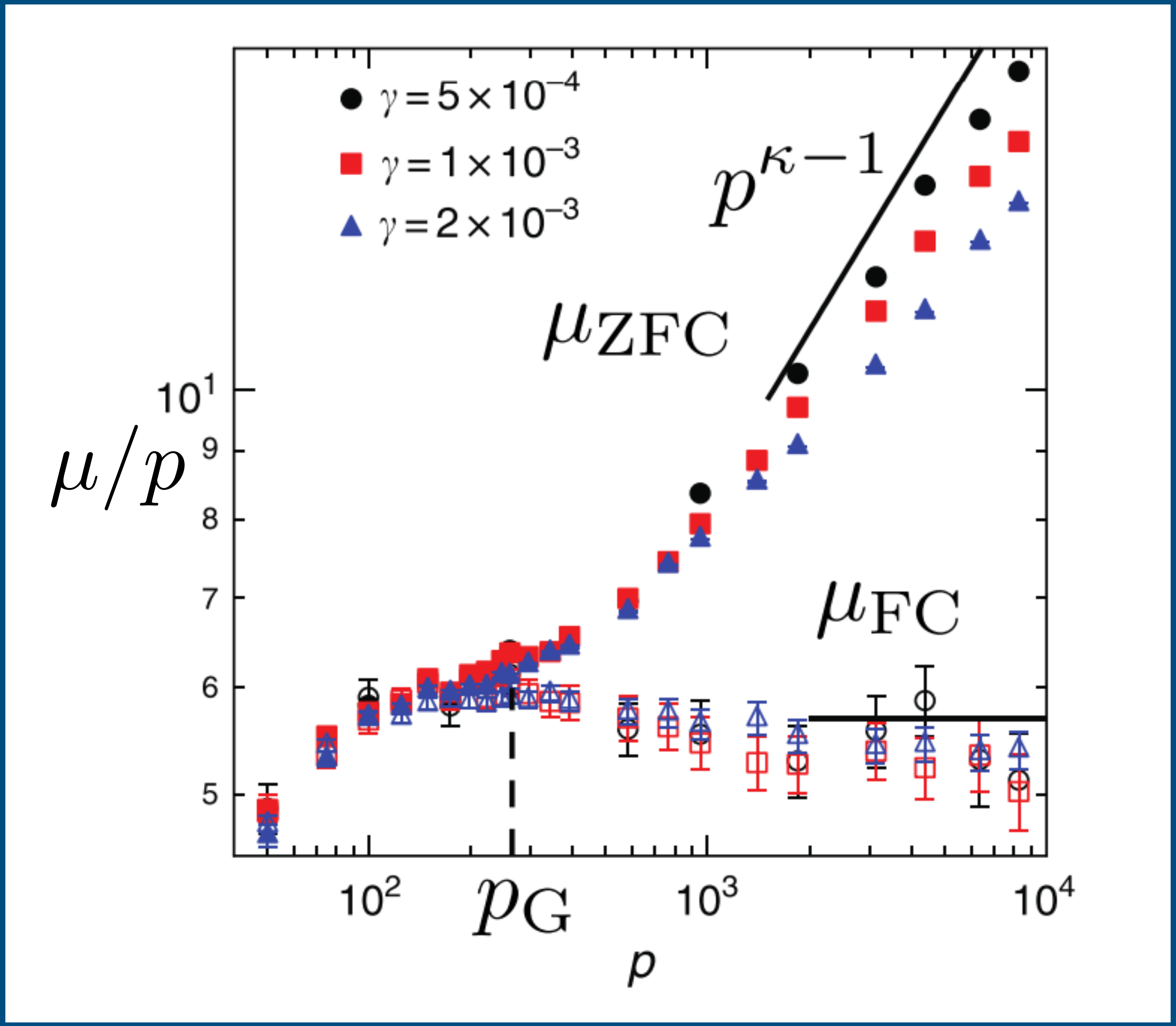
ZFC: zero field compression
FC: field compression

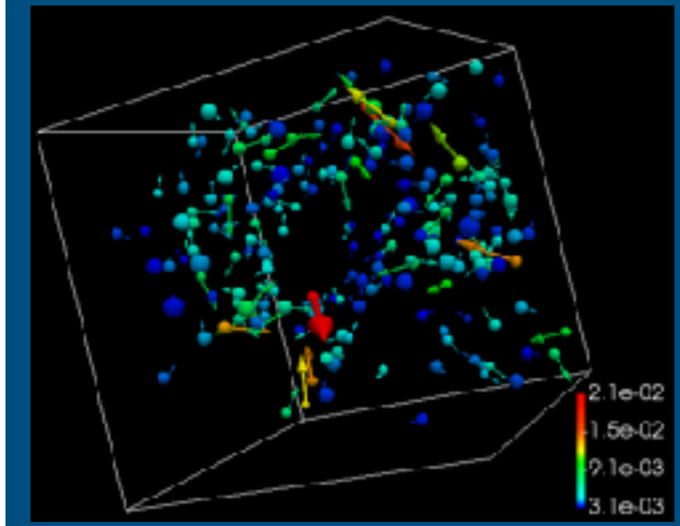


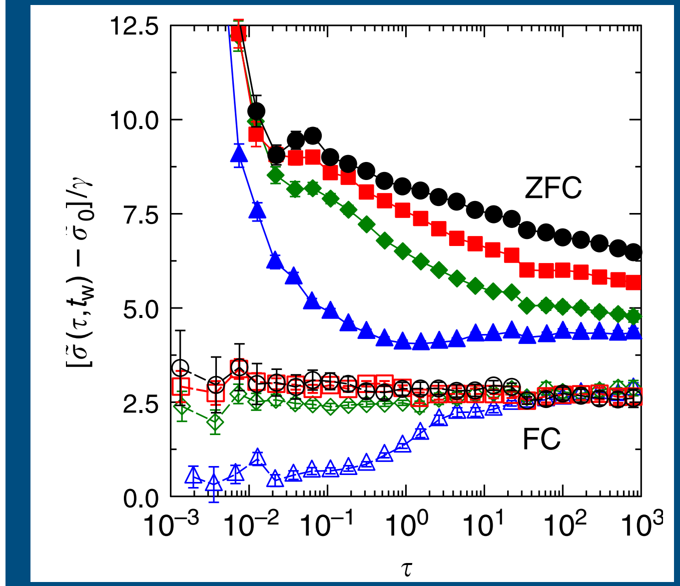
Gardner phase:











stable glass

marginally stable glass

Experiment (colloid)

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

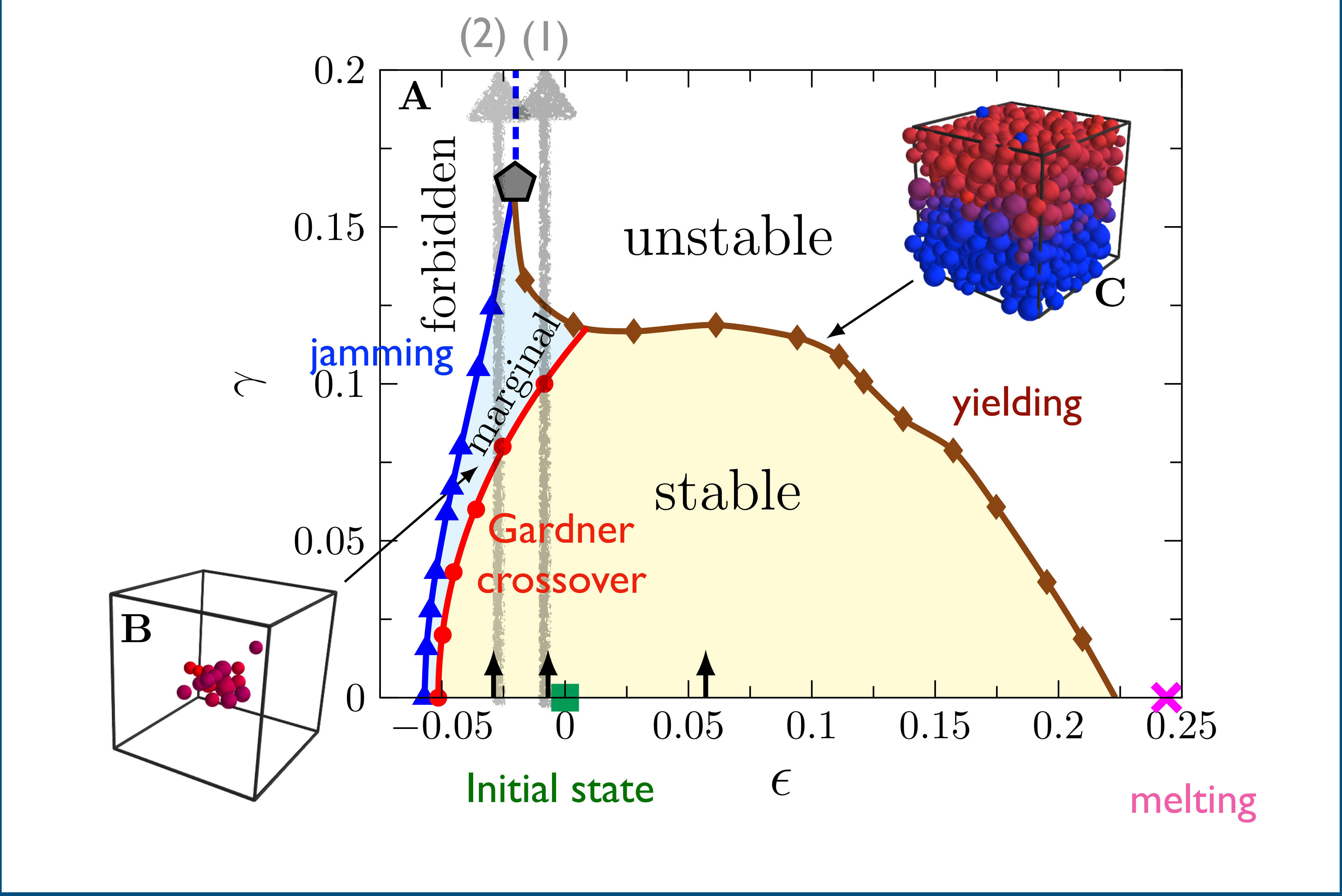
$$\mu \sim p$$

R. Zargar, E. DeGiuli and D. Born, EPL 116.6, 68004 (2017)

$$\mu \sim p^{1.3}$$

Stability-reversibility map

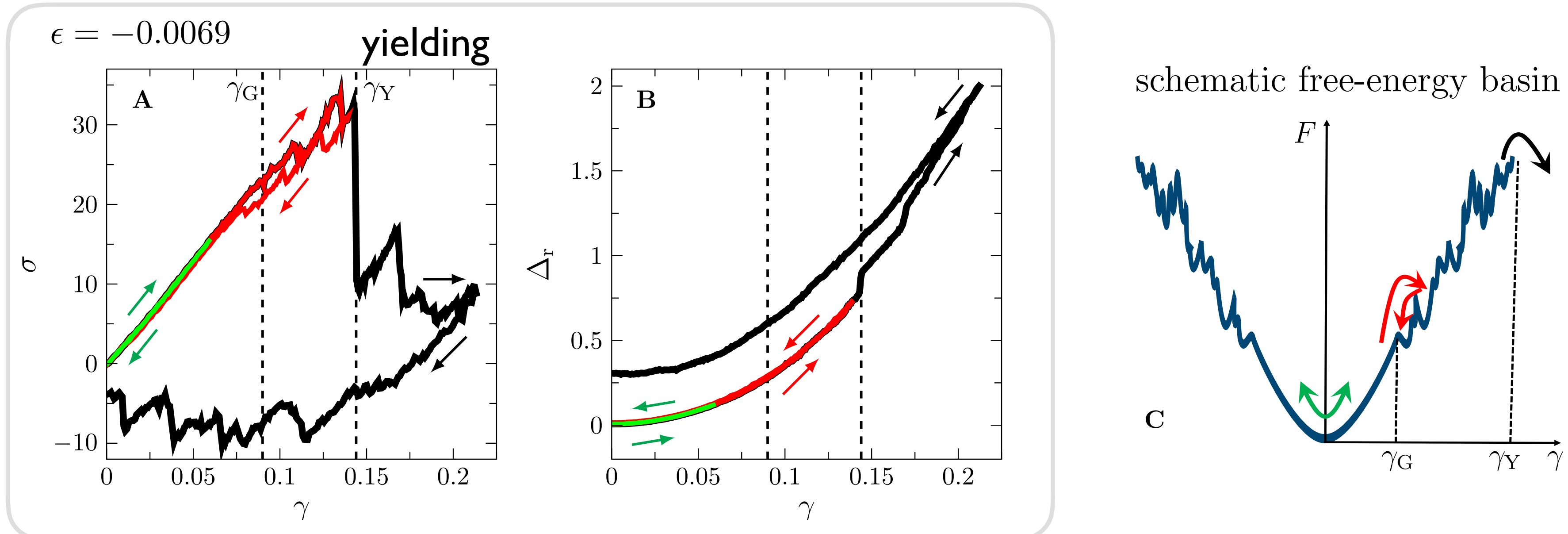
$\varphi_{\mathrm{g}} = 0.655$



Response to shear

(1)

yielding

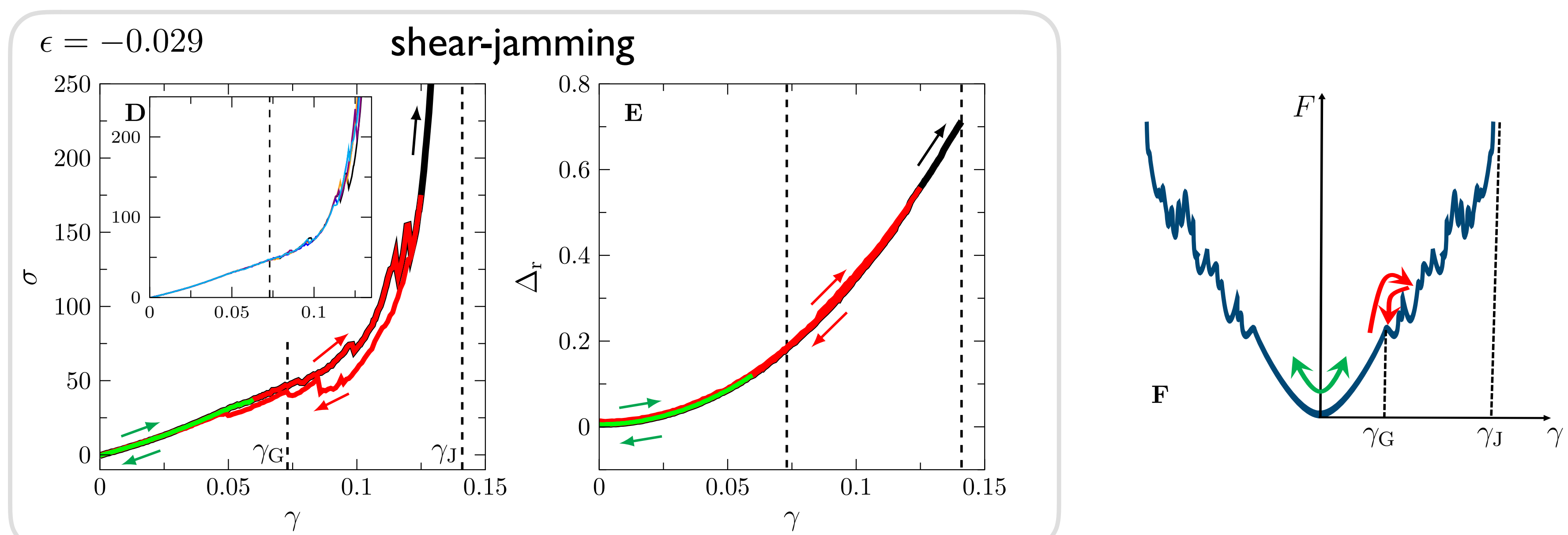


Elastic
(reversible)

partially plastic
(partially irreversible)

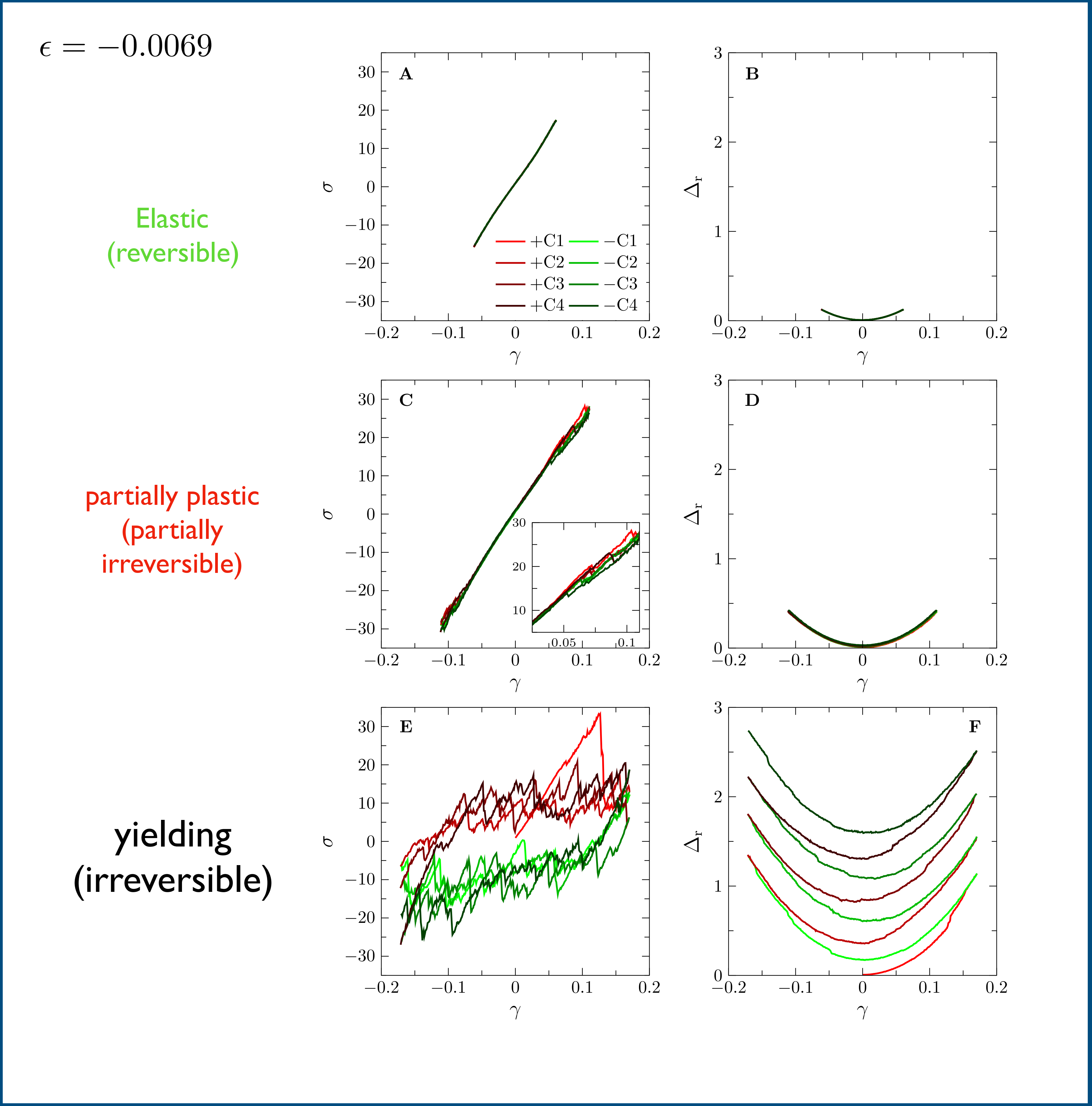
(2)

shear-jamming



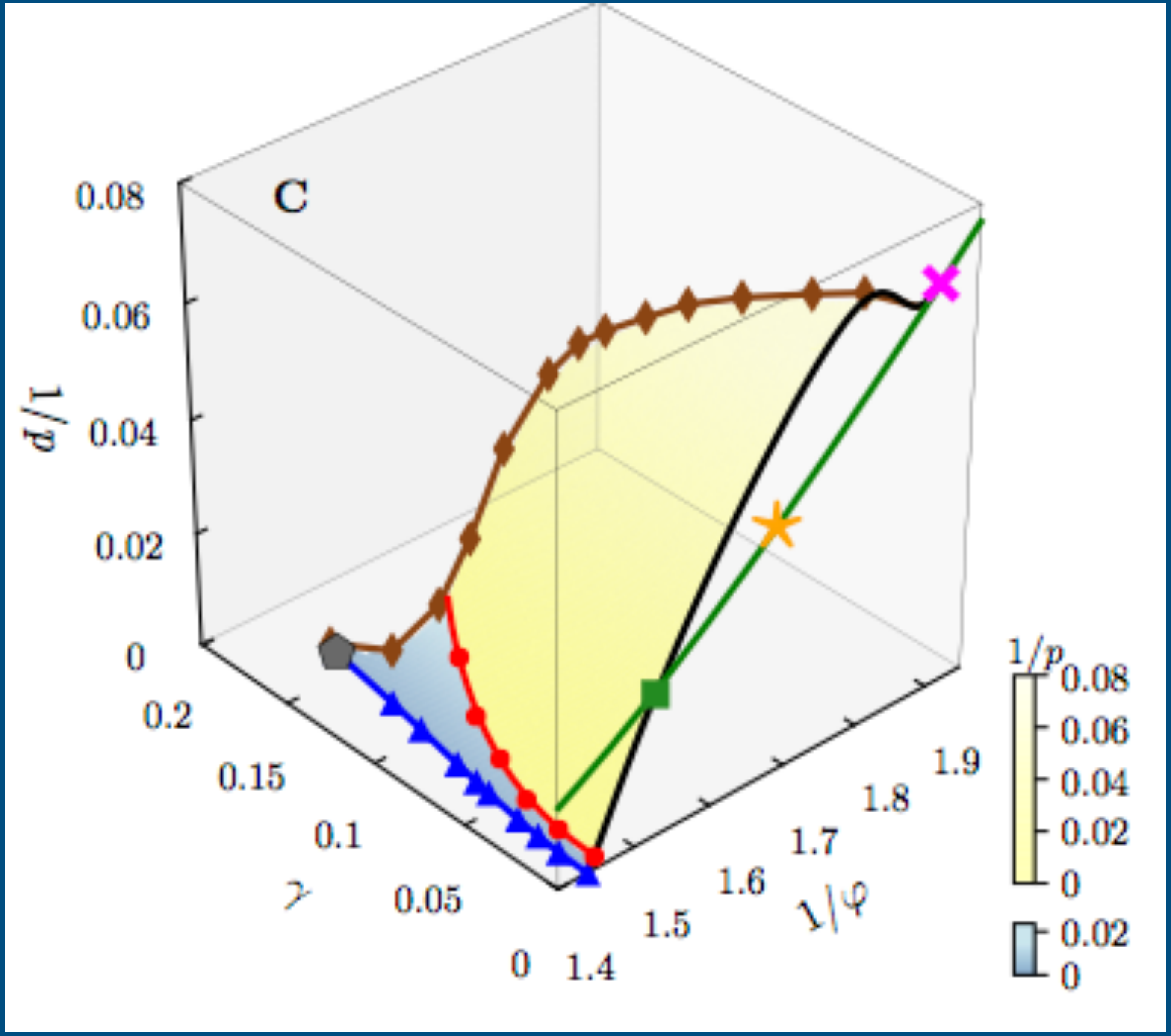
$\varphi_g = 0.655$

More cycles…


$\epsilon = -0.0069$
Elastic
(reversible)
partially plastic
(partially
irreversible)
yielding
(irreversible)
A
B
C
D
E
F
σ
Δ_r
γ
+C1
+C2
+C3
+C4
−C1
−C2
−C3
−C4

Glass equation of sates

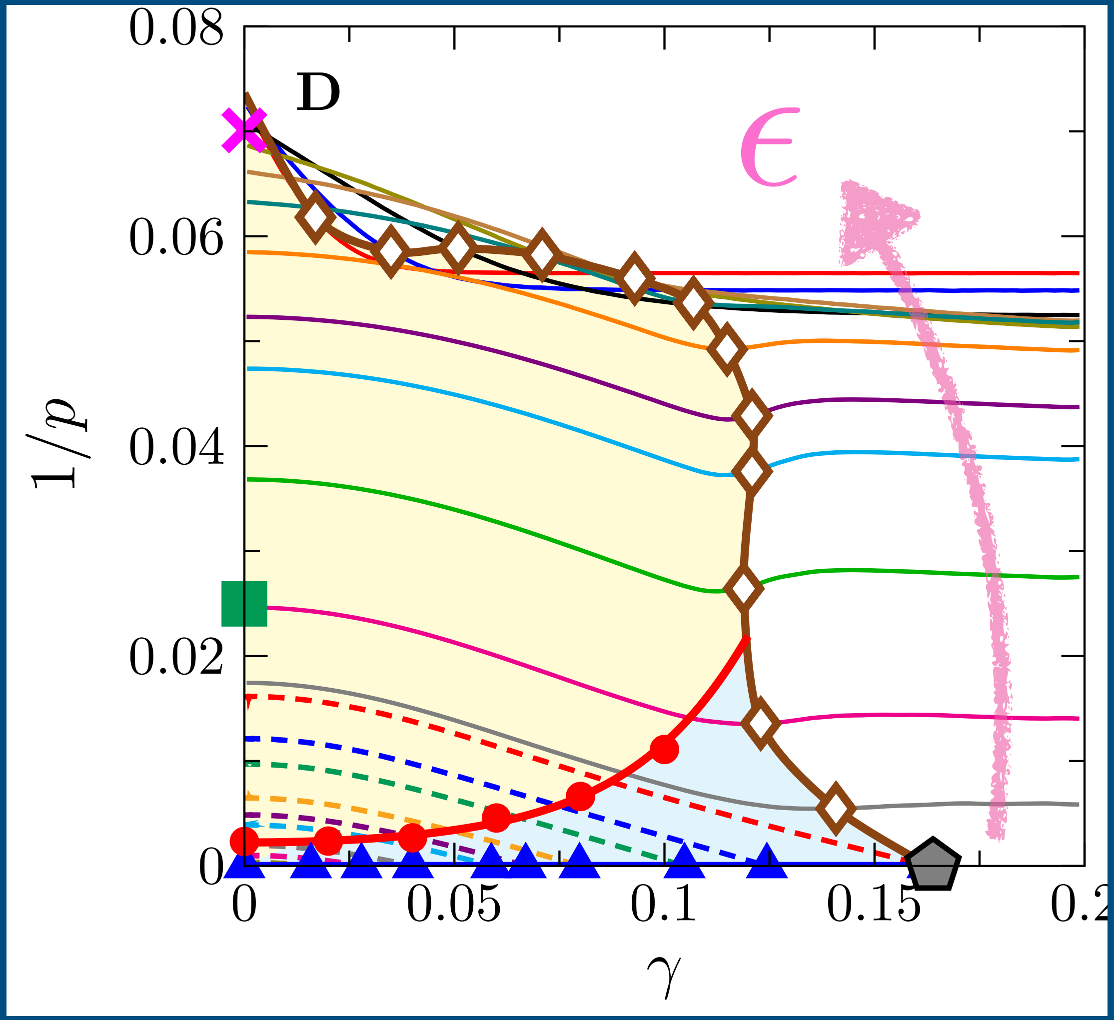
$$p = p_{\rm glass}(\varphi_{\rm g}; \gamma, \epsilon)$$

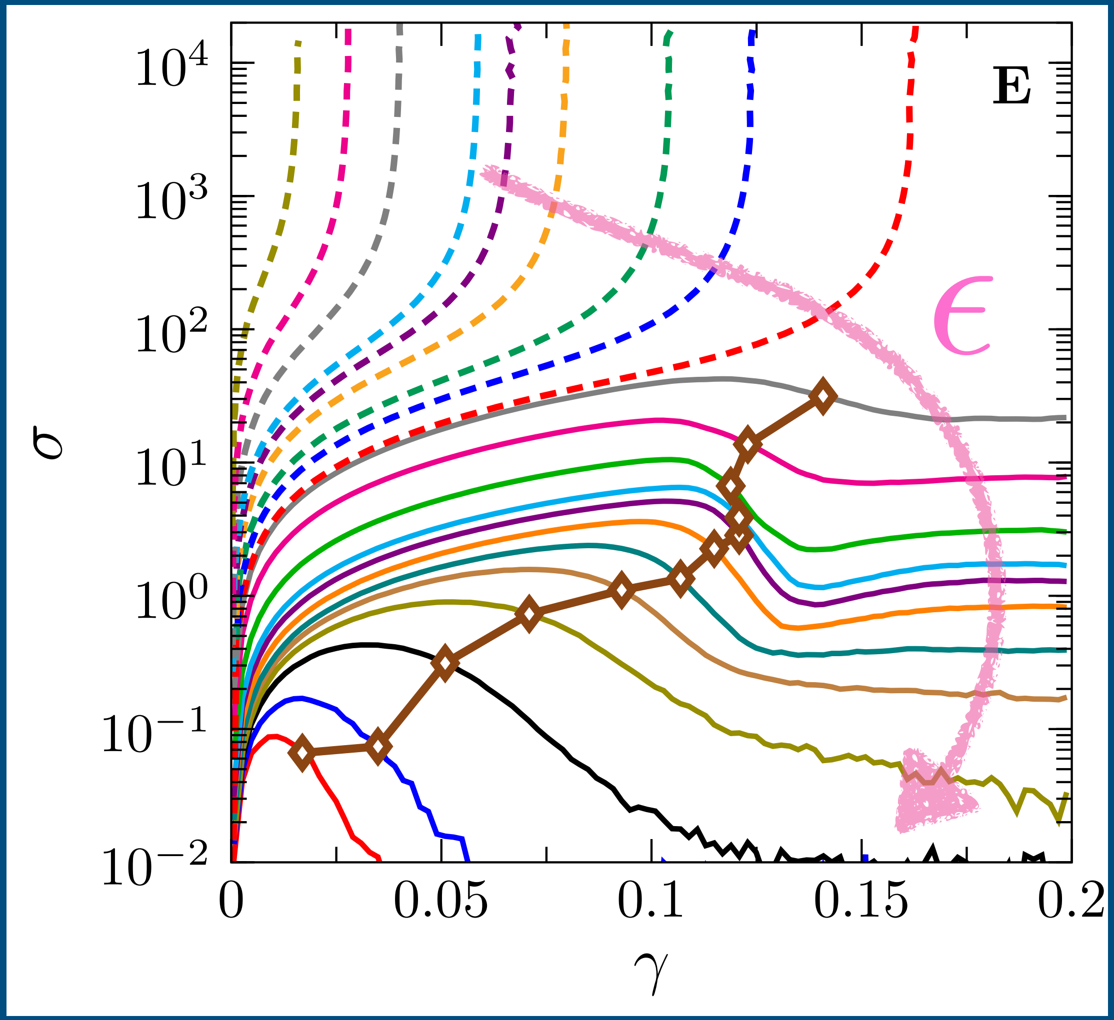


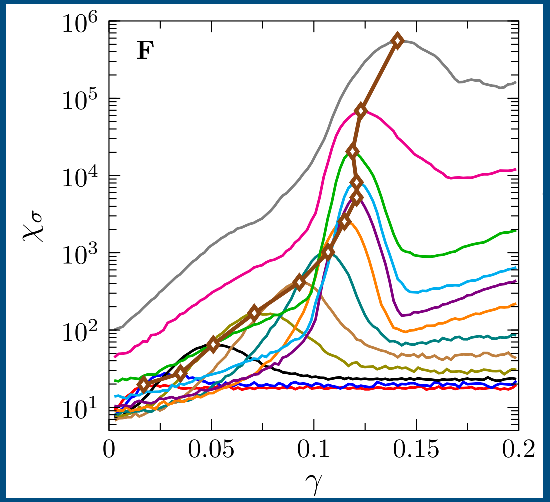
$$\varphi_{\rm g} = 0.655$$

Glass equation of sates

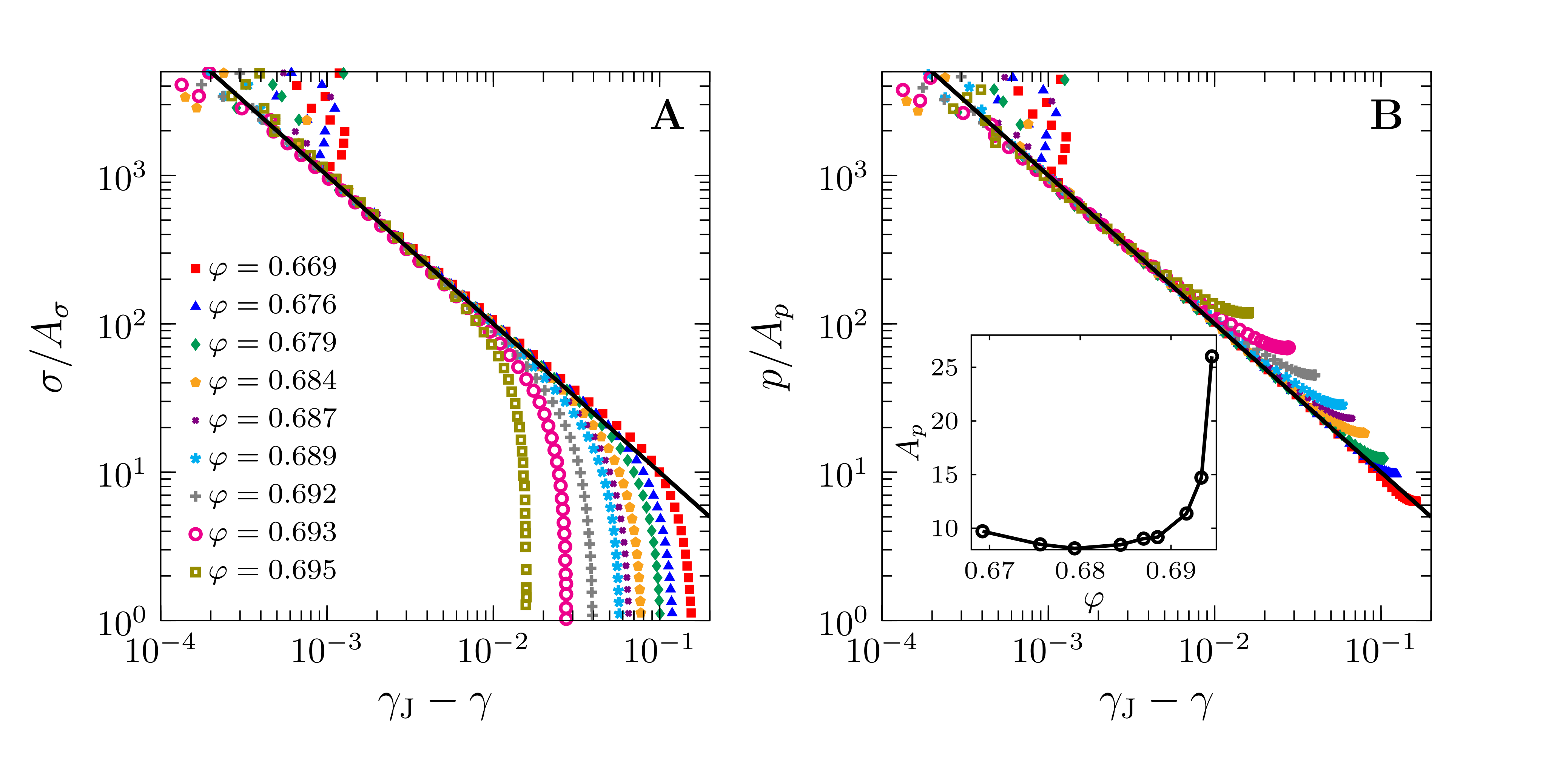
$$p = p_{\mathrm{glass}}(\varphi_{\mathrm{g}}; \gamma, \epsilon) \qquad \sigma = \sigma_{\mathrm{glass}}(\varphi_{\mathrm{g}}; \gamma, \epsilon)$$







Shear-jamming

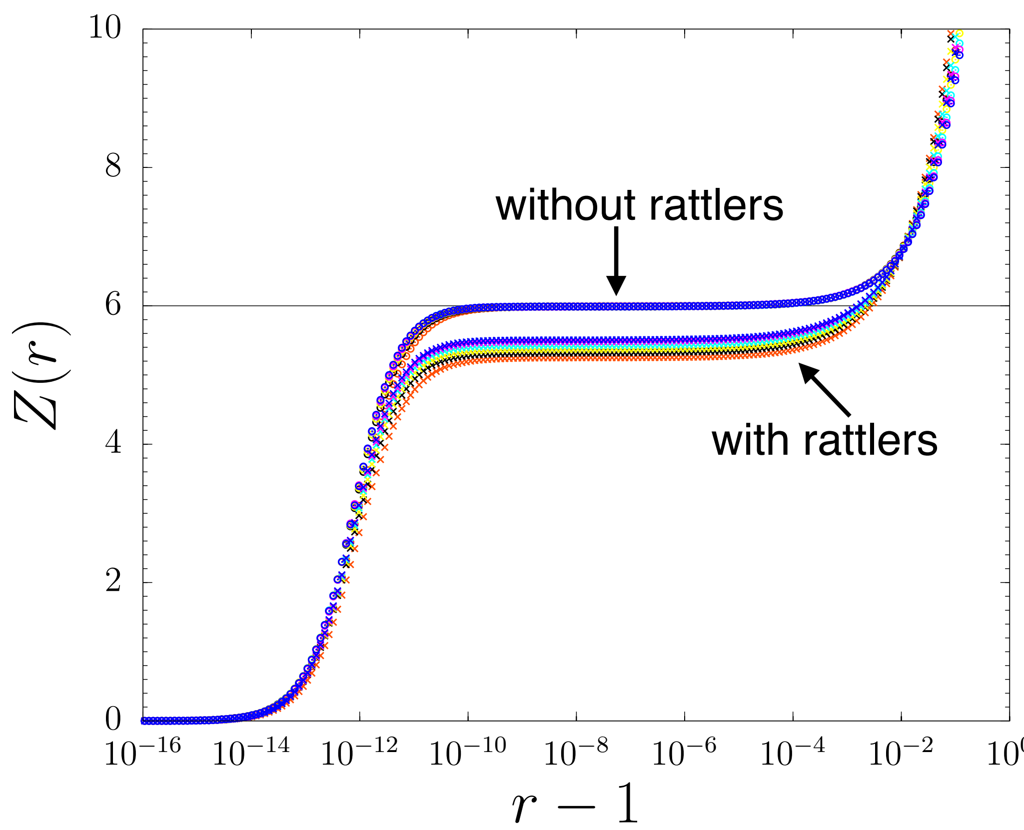


$$\sigma \propto (\gamma_J(\varphi) - \gamma)^{-1}$$

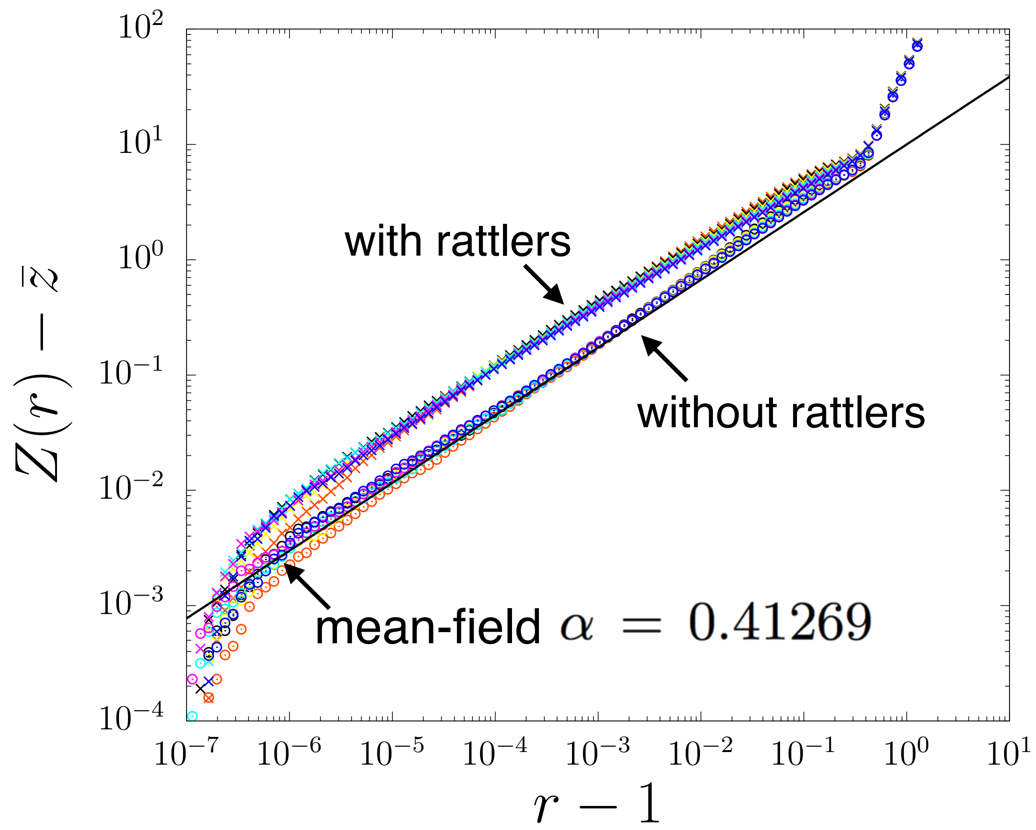
$$p \propto (\gamma_J(\varphi) - \gamma)^{-1}$$

Shear-jamming

shear-jammed packings are **isostatic**



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



cumulative correlation function

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

pair correlation function

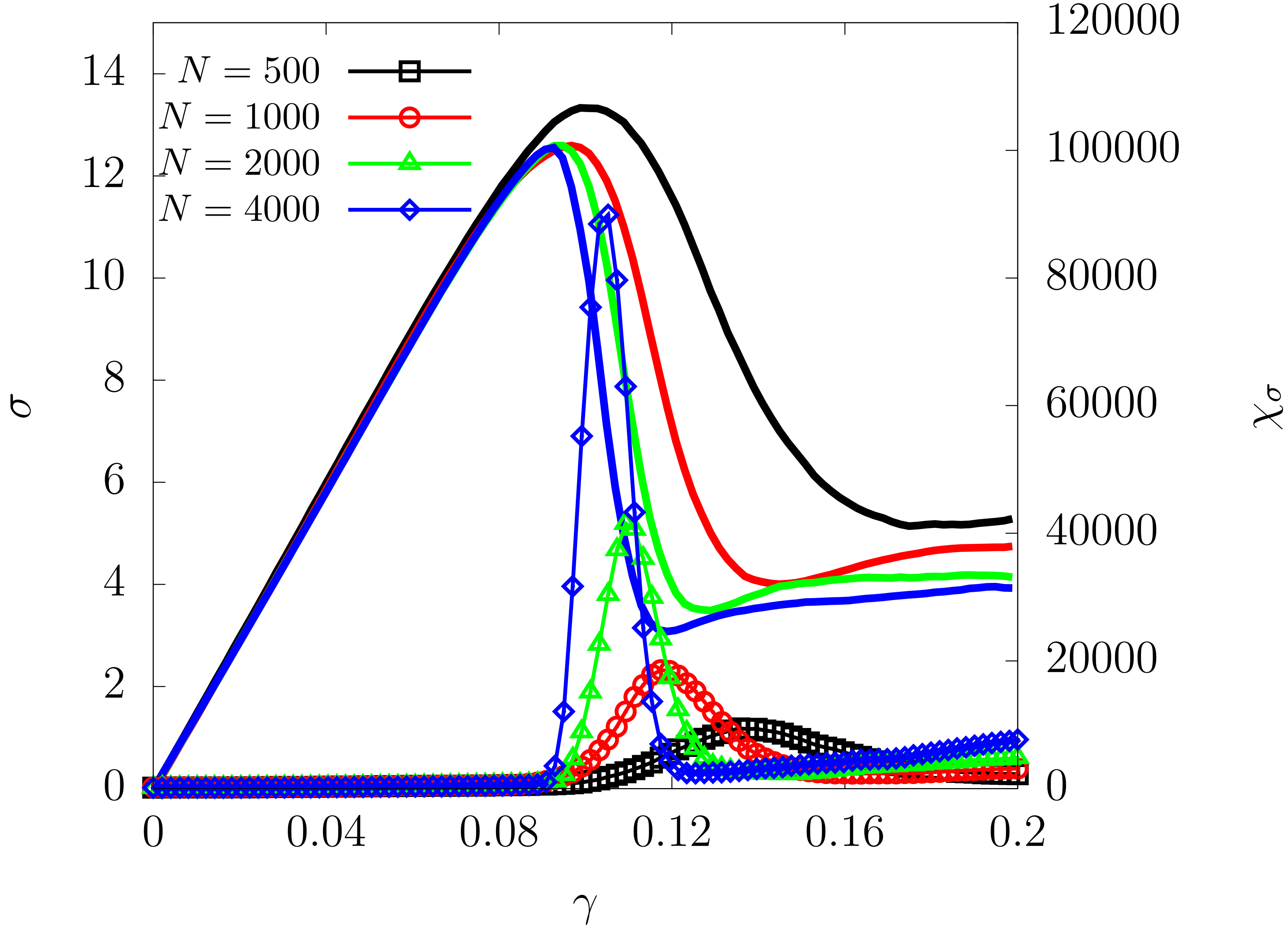
$$Z(r) - \bar{z} \propto (r-1)^{1-\alpha}$$

plateau value

Yielding

$\varphi_g = 0.644$

$\varphi = 0.644$

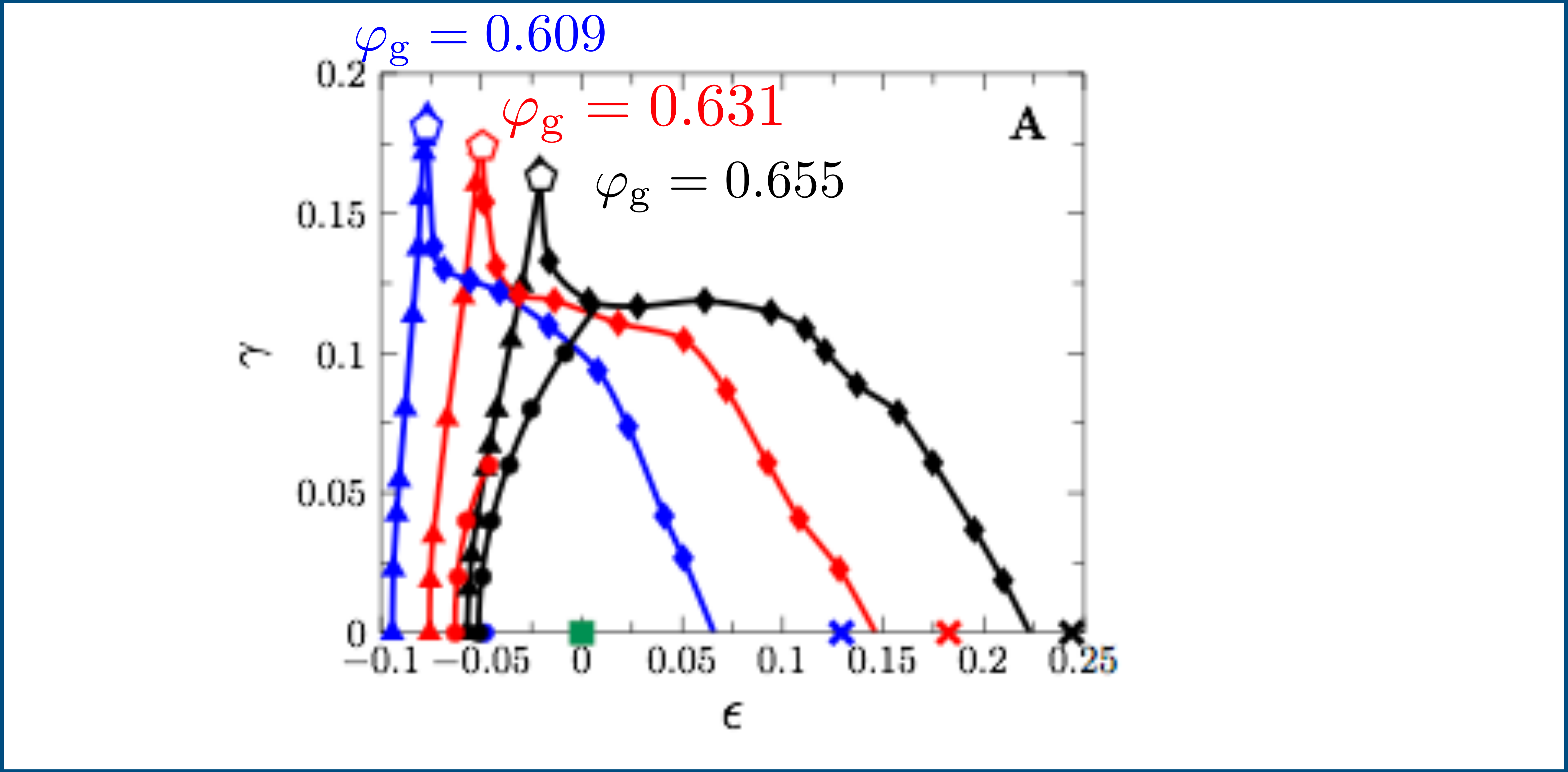


path-to-path fluctuation of stress

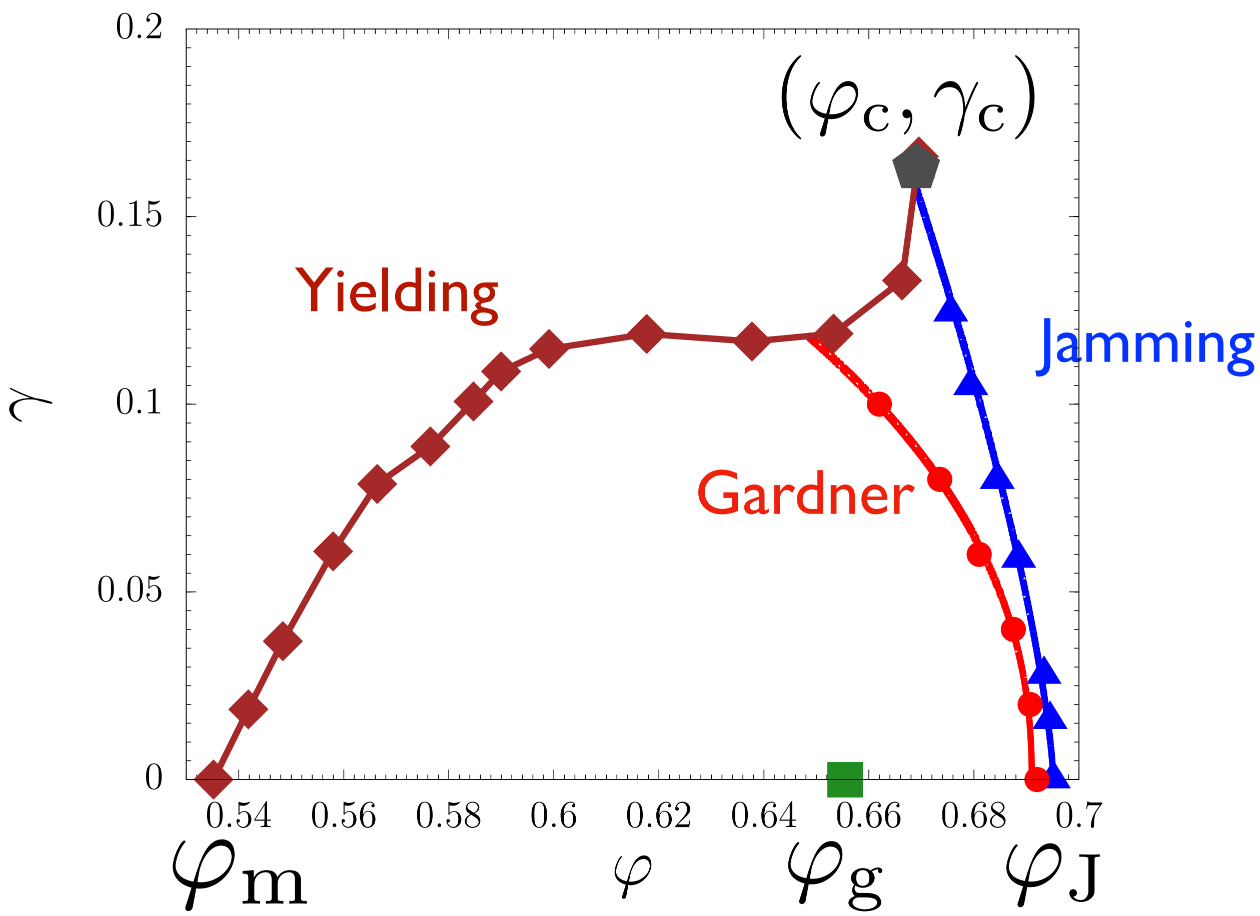
$$\chi_\sigma = N[\langle\sigma^2\rangle - \langle\sigma\rangle^2]$$

see also
Jaiswal, P. K., Procaccia, I., Rainone, C., & Singh, M. (2016). PRL 116(8), 085501;
Parisi, G., Procaccia, I., Rainone, C., & Singh, M., PNAS, 114(22), 5577-5582 (2017),
M. Ozawa, L. Berthier, G. Biroli, A. Rosso, G. Tarjus, PNAS, 115, 6656 (2018).

Dependence on φ_g

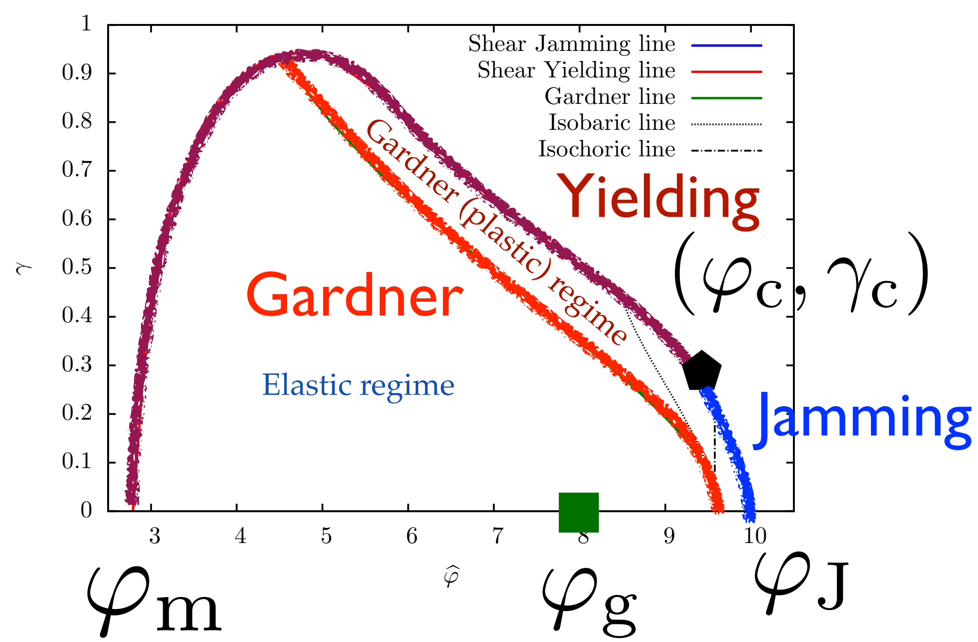


Stability-Reversibility map: comparison with theory



Large-d theory (1RSB level)

Urbani, Zamponi, Phys. Rev. Lett 118(3), 038001 (2017)



Conclusions

3D hard-sphere glass under shear/(de)compression

Swap + MD simulation

1. "Gardner phase": emergence of internal relaxation process deep inside the glass phase

2. Stability-reversibility map & glass-EOS

3. Shear-jamming : isostatic, universal criticality

4. Yielding: discontinuous