Yielding

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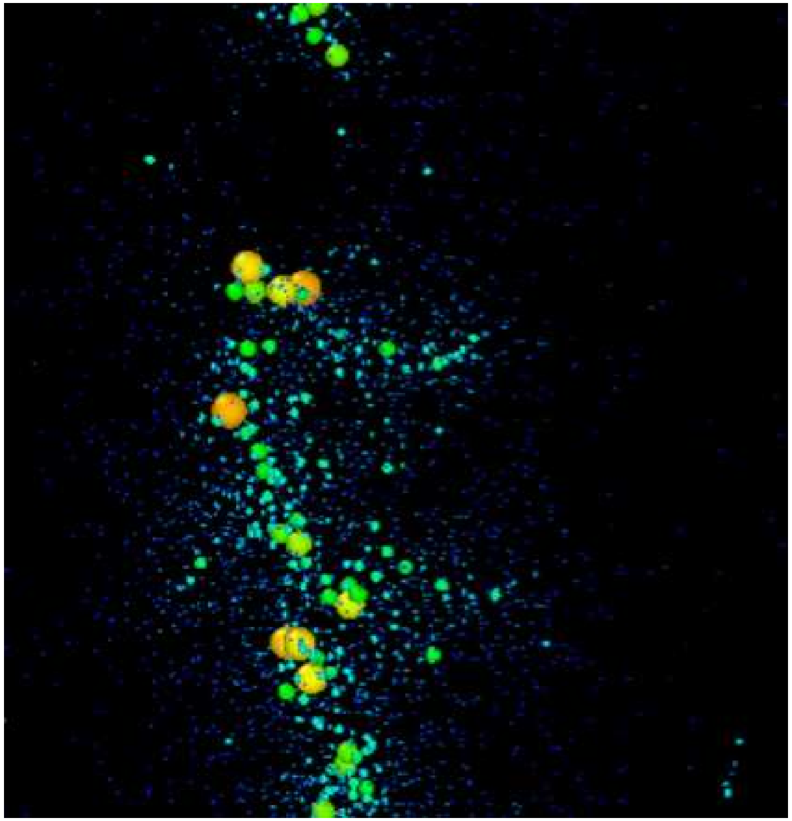
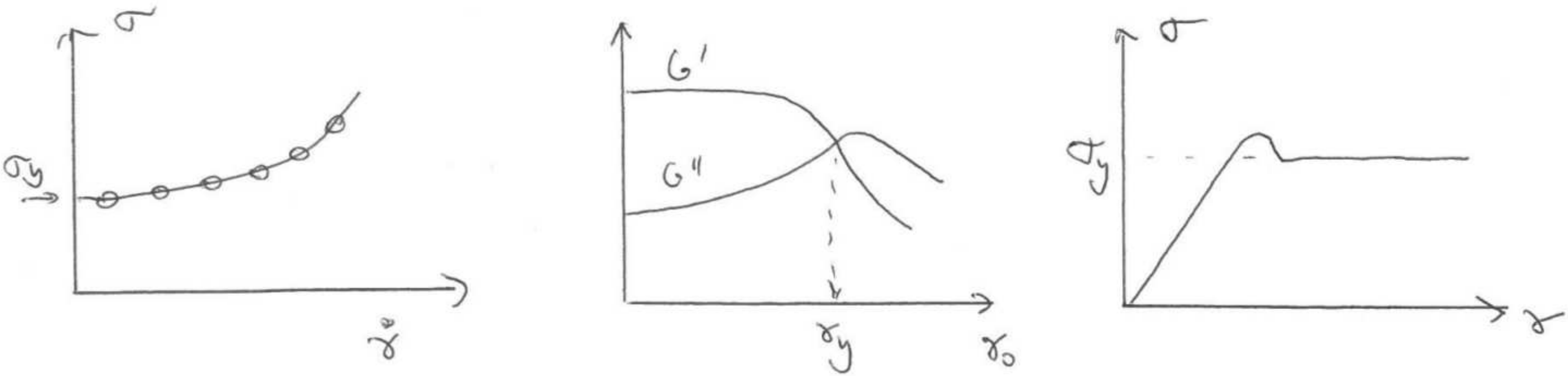
Coworkers

- On-going work with:

  D. Coslovich,
  T. Kawasaki,
  A. Ninarello,
  M. Ozawa.

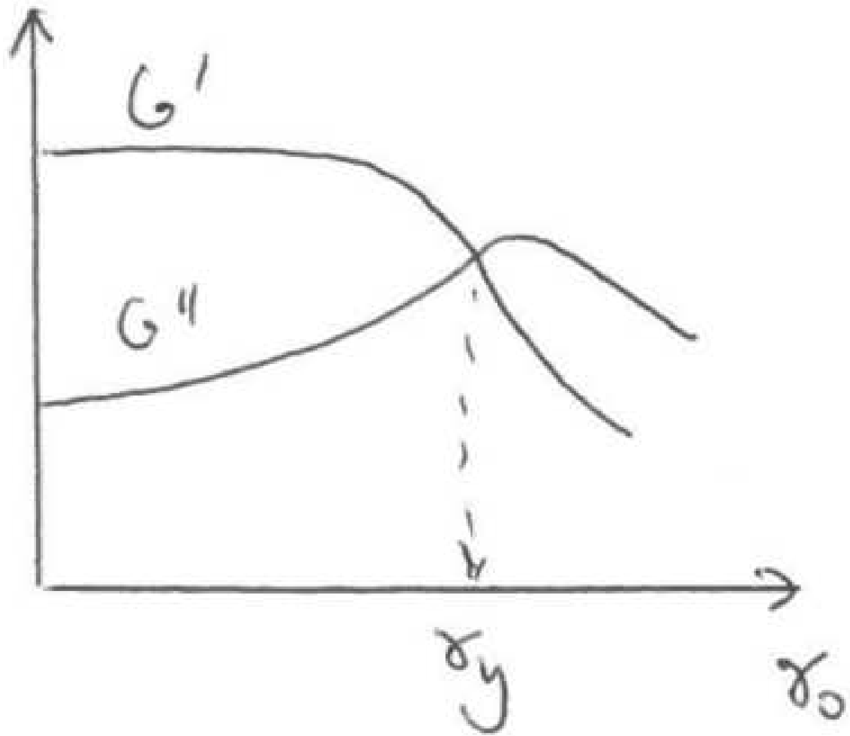


Yielding(s): Experimental review



[Bonn, Denn, Berthier, Divoux, and Manneville, Rev. Mod. Phys. ’17]

A critical yielding transition?



- Ideas from irreversibility transition and absorbing states.

[Nagamanasa *et al.* PRE '14, Regev *et al.* PRE '13, Fiocco *et al.* PRE '13]

- Discontinuous transition observed in confocal microscopy.

[Knowlton *et al.*, Soft Matter '14]

Oscillatory shear: Setup

- T. Kawasaki and L. Berthier, *Macroscopic yielding in jammed solids is accompanied by a non-equilibrium first-order transition in particle trajectories*, PRE 94, 022615 (2016).

- Overdamped athermal simulations of soft harmonic spheres above jamming: Shearing a simple jammed solid / glass at $T = 0$.

- Periodic boundary conditions: spatially homogeneous flow.

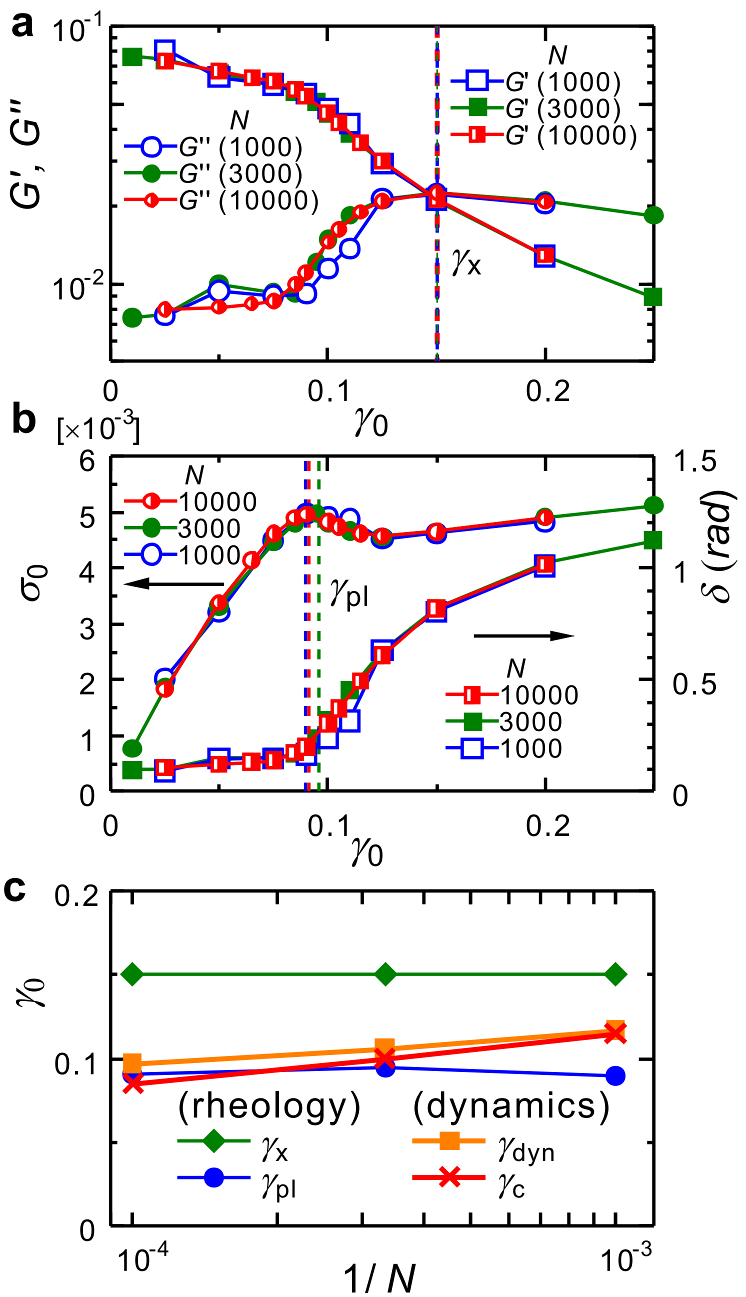
- Apply periodic deformation: $\gamma(t) = \gamma_0(1 - \cos(\omega t))$, with $\omega \ll \epsilon/(a^2\xi)$.

- Measure the steady state shear stress: $\sigma(t) = \sigma_0 \cos(\omega t + \delta)$. Extract (σ_0, δ) to measure 'linear' response - even beyond linear regime.

- Equivalently: $G'(\omega) + iG''(\omega) = \sigma_0/\gamma_0 e^{i\delta}$ are the well-known experimental measurements of the linear response. Extract (G', G'').

- Access also microscopic structure (e.g. $g(r)$, $S(q)$) and dynamics (e.g. mean-squared displacement).

Macroscopic rheology



- Crossing of G' and G'' defines $\gamma_\times \approx 0.15$. Standard location of 'yielding' transition under oscillatory shear.

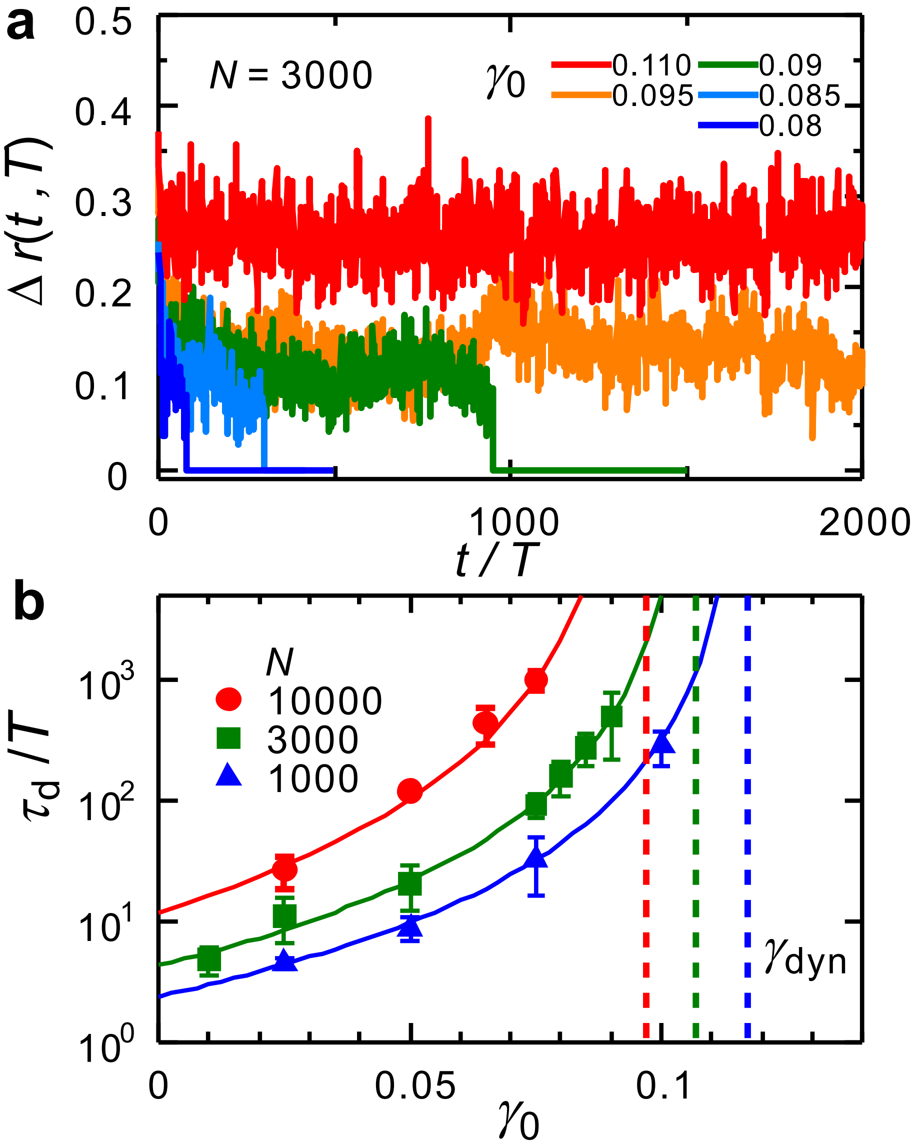
- Maximum of σ_0 defines $\gamma_{\rm pl} \approx 0.1$ ($\gamma_\times$ is invisible here).

- $\gamma_{\rm pl}$ also corresponds to onset of dissipation, when $\delta > 0$.

- We thus have at least 2 good definitions of 'the' yielding transition, which is ok if it's not a transition and just a crossover.

- Finite-size effects are small, which is ok.

Microscopic dynamics: Transition?



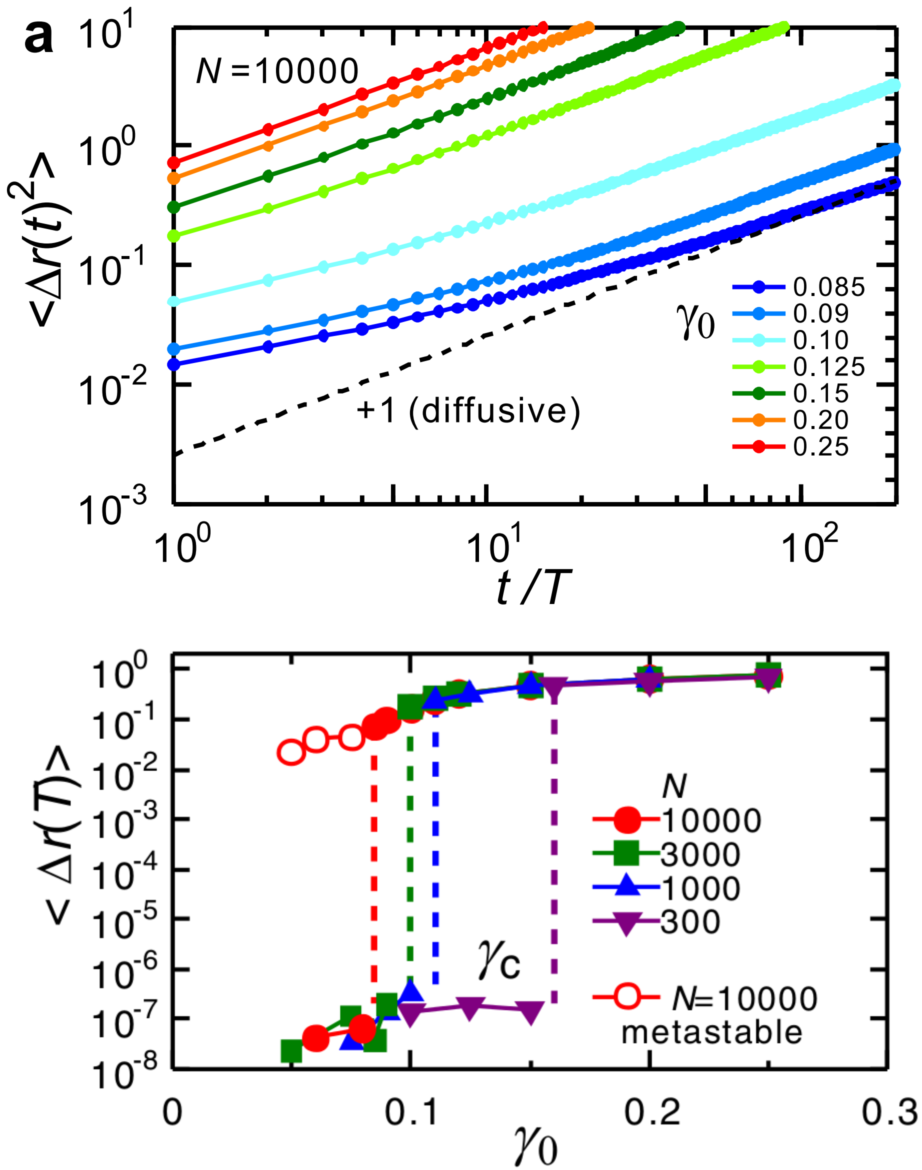
- Mean particle displacement after one cycle: $\Delta r(t, T = 2\pi/\omega)$.

- Starting from a random configuration at $t = 0$, $\Delta r(t, T)$ either vanishes when $\gamma_0 < \gamma_{\rm dyn}$ or fluctuates around well-defined average value otherwise.

- Timescale to reach (nearly) reversible state diverges as $\gamma_0 \to \gamma_{\rm dyn}^-$: power law with pronounced finite size effects. [Seen by Foffi, Sastry, Reichhardt...]

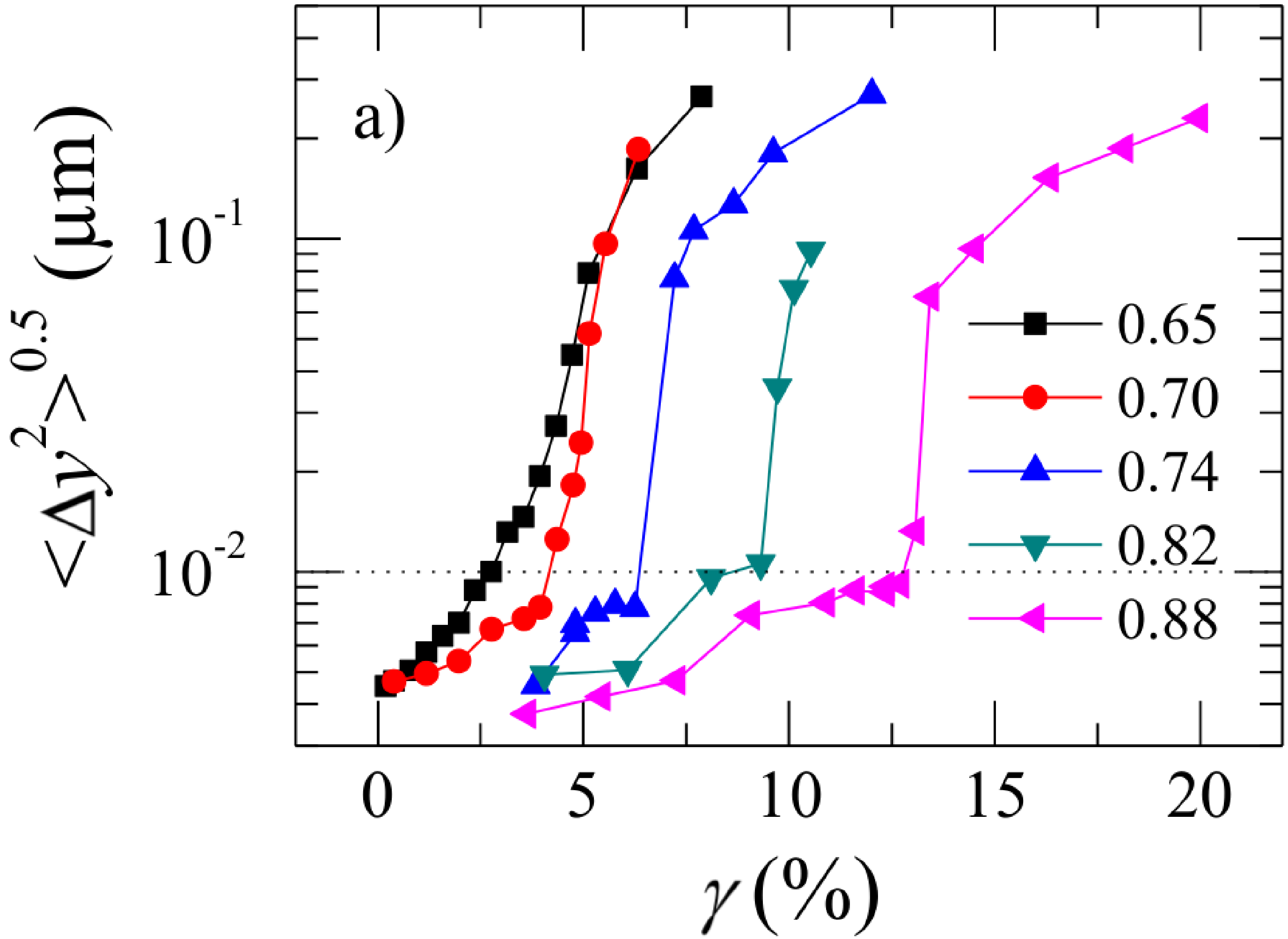
- Empirically, we find that $\gamma_{\rm dyn} \approx 0.1$ when N gets larger: Critical point?

First-order dynamic transition



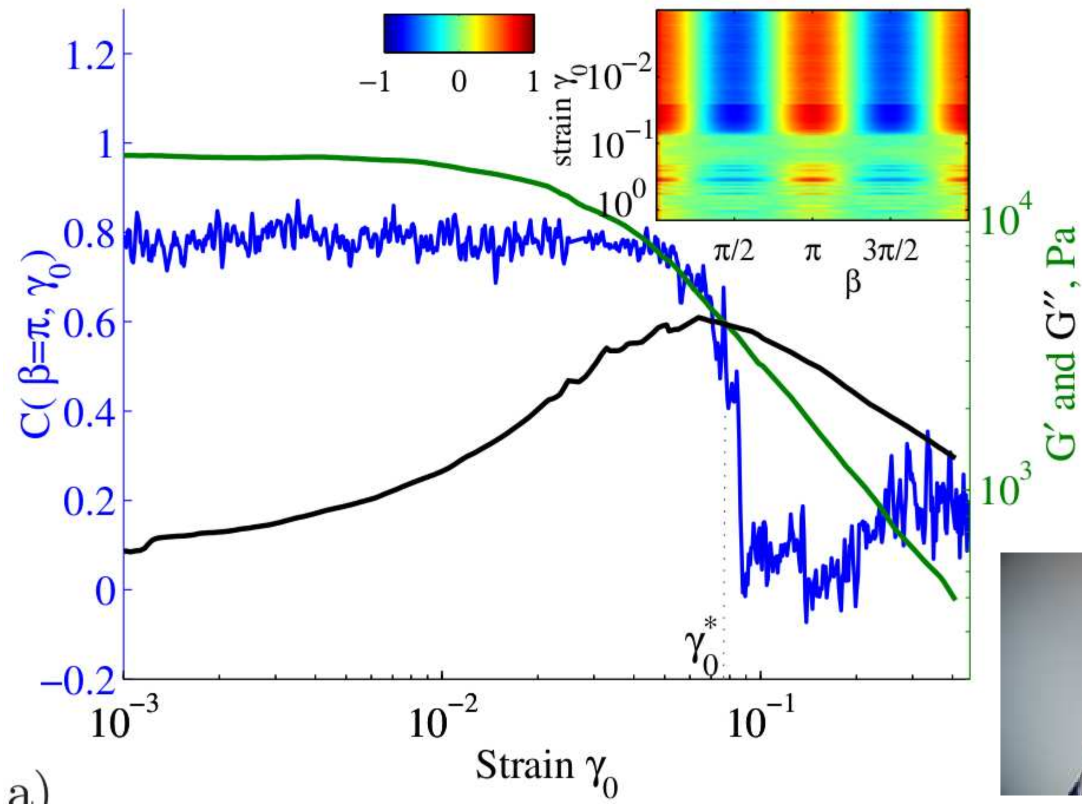
- Dynamics in steady-state regime for $\gamma_0 > \gamma_c$ is diffusive.
- Modest decrease of diffusion constant as $\gamma_0 \to \gamma_c^+$.
- Discontinuous jump to zero at γ_c.
- Transition in microscopic dynamics appears first-order.
- Consistent with 'metastable' dynamics seen in transient regime.
- Empirically, we find $\gamma_c \approx \gamma_{\rm dyn} \approx 0.1$ when N gets larger.

1 - Cipelletti's experiment



• Sharp (discontinuous?) increase of mean displacement per cycle at yielding unrelated to crossing of G' and G''. [Knowlton et al., Soft Matter '14]

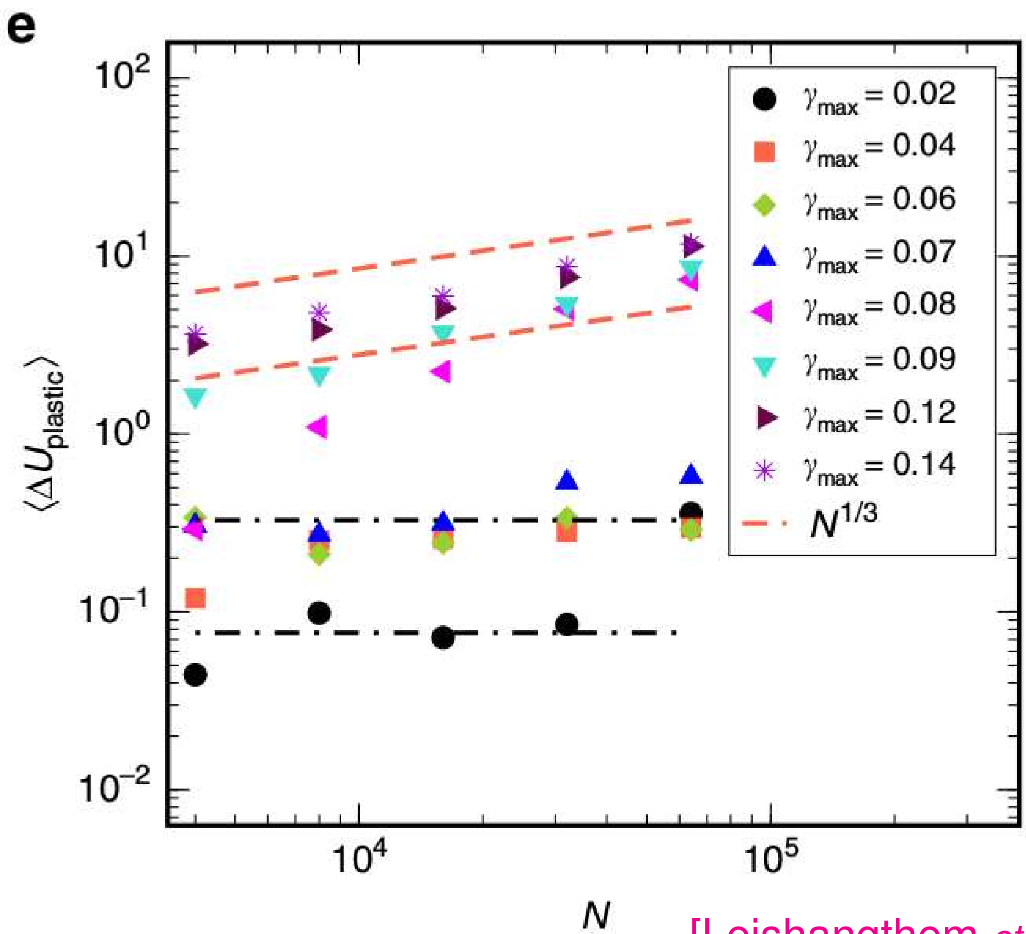
2 - Schall's experiment



• $C(\beta)$ measures tiny (about 1 %) anisotropy in $S(q)$ in diffraction plane. Sudden change from anisotropic (deformed elastic glass) to isotropic (plastic flow) right where G' and G'' cross. [Denisov *et al.*, Sci. Rep. '15]

• We see nothing at all in $S(q)$, and our interpretation is totally different.

3 - Sastry's simulations

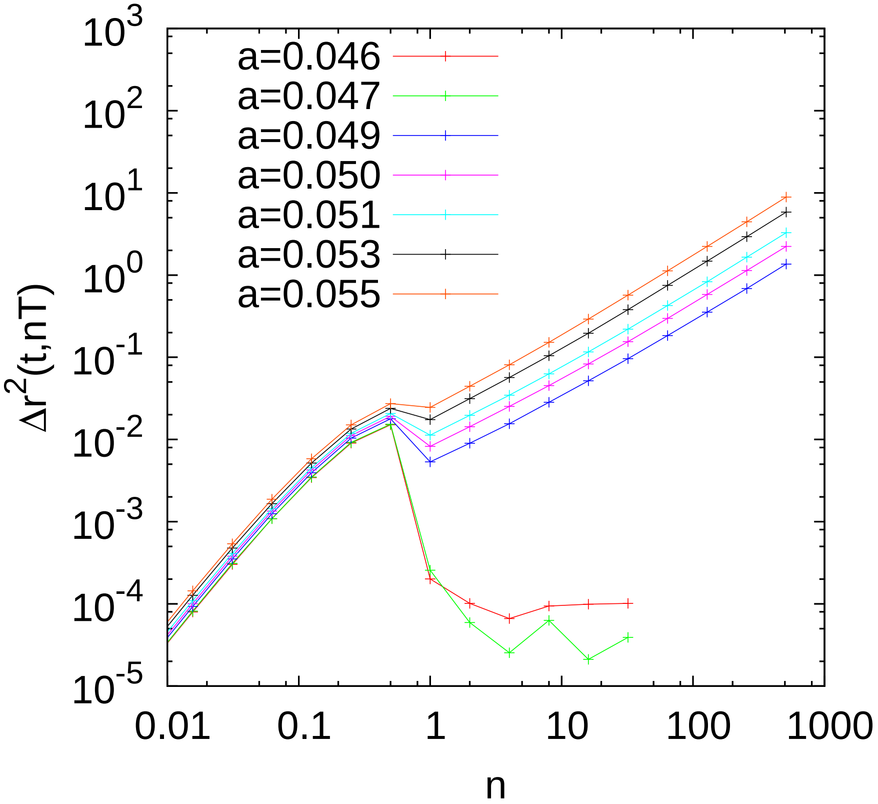


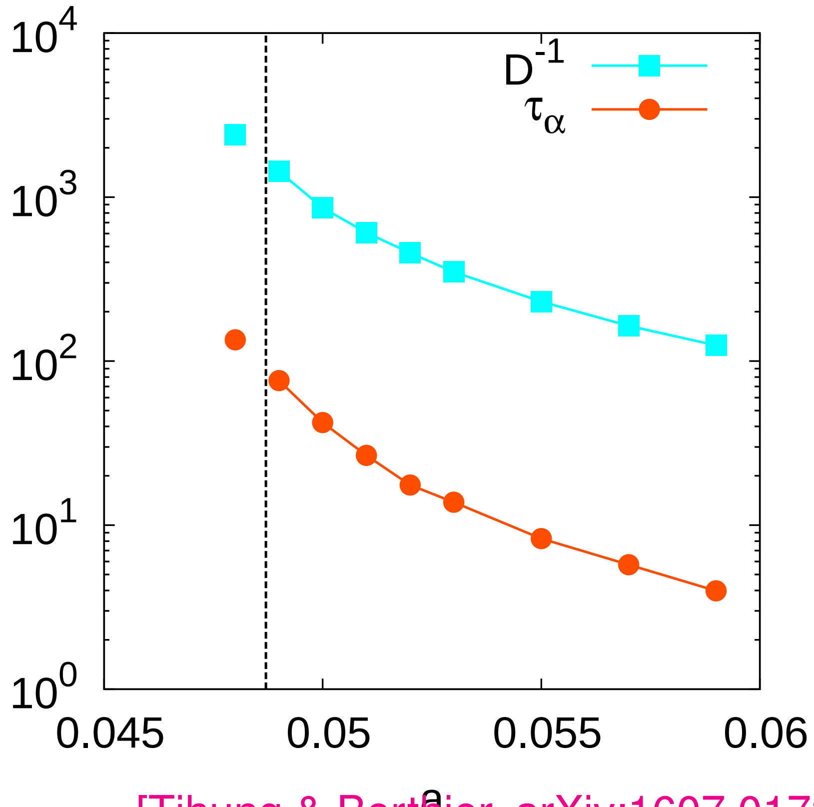
[Leishangthem *et al.*, Nature Comm. '15]

- Different scaling above and below the transition, which seems to confirm the discontinuous nature of the transition. See also [Regev *et al.*, Nature Comm. '15] for opposite conclusions!

4 - Periodic volume fluctuations

• Abrupt emergence of diffusive motion; dynamical first-order transition in actively-deforming particles. [Small versus large amplitude.]

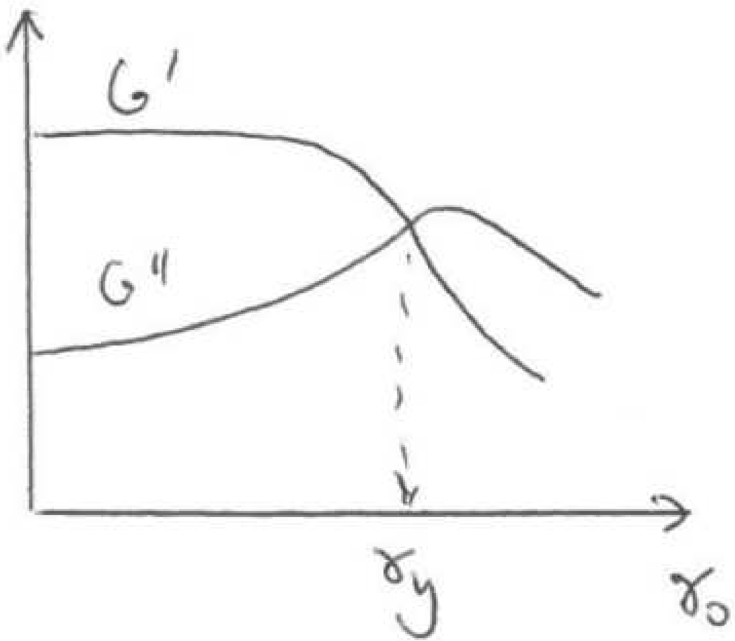


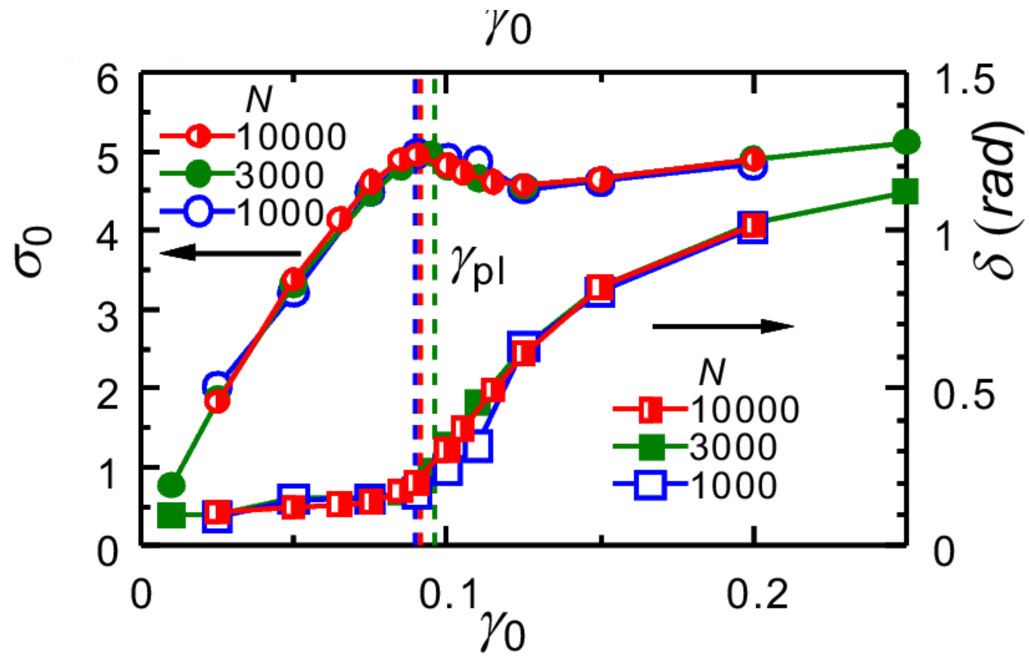


[Tjhung & Berthier, arXiv:1607.01734]

• Qualitatively similar to periodic global deformation. Only difference is forcing at small rather than large scale–physics strikingly similar.

Summary



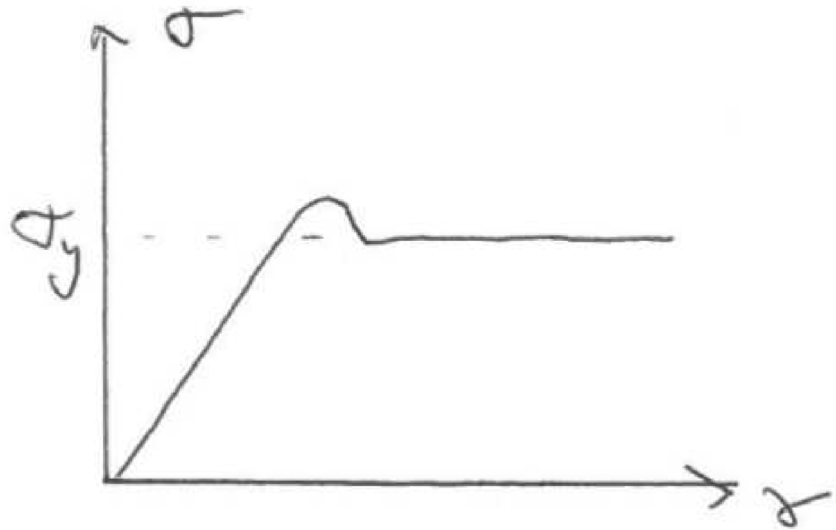


- Right set of variables should be used.

- Two phases are truly distinct: unyielded phase remembers initial conditions (e.g. very stable), steady state is automatically critical (i.e. threshold and marginal).

- Transition is bound to be discontinuous in character, with nothing interesting on the left side. Not really 'the' yielding transition...

A critical yielding transition?



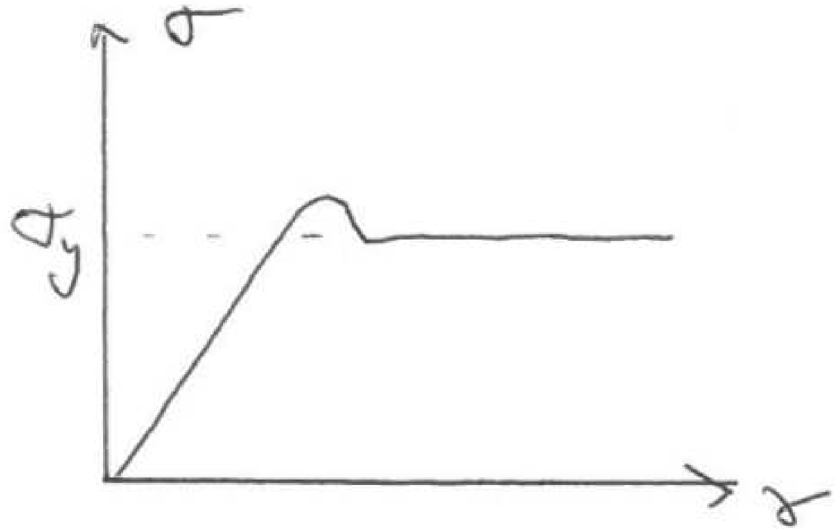
- Percolation ideas: empirical description.

[Horbach and Chaudhuri '17, Gosh *et al.* '17]

- Scale free spinodal: 'mean-field' description. First-order or/and critical?

[Zamponi and Urbani '17, Procaccia *et al.* '16, Procaccia *et al.* '17]

Elastic branch?



• Elastic branch is critical everywhere.
[Lin *et al.*, PRL '15]

• Elastic branch is not critical [everybody else?, Hentschel *et al.*, PRE '15], only becomes critical when $\gamma \to \gamma_Y$ [Procaccia *et al.* '17]

• Elastic branch becomes critical at Gardner point.
[Urbani & Zamponi '17, Jin & Yoshino]

‘Well-known’ facts

- Yielding transition is not seen directly through rheological observables (local dynamics, overlaps...).

- A lot of work for second order criticality and exponents in steady state, or equivalently for $\dot{\gamma} \to 0$.

- Shear bands are observed by accumulation of large number of discrete events, at large deformation.

- Behaviour is ‘universal’: foams, emulsions, glasses, chocolate, etc.

Computer simulations

- Usually limited to short time scales and small systems.

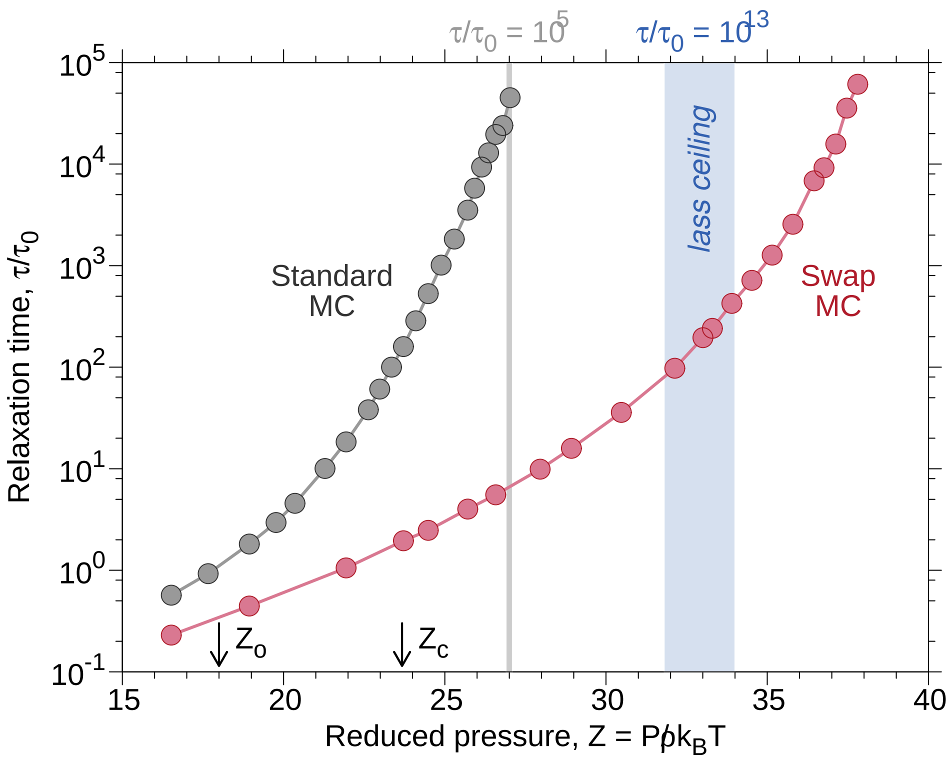
- Athermal quasi-static simulations solve one of two timescales problem: deformation rate becomes effectively slow enough.

- Ordinary computer simulations still face the preparation timescale problem. Cooling rate is about 8 orders of magnitude too fast.

- Thus, computer simulations may not be relevant for real glasses. Only useful for colloidal and granular materials. (Experiments on colloids may not be relevant for real glasses either.)

- Glass stability is typically not seriously taken into account in coarse-grained models & theories. Exception: mean-field!

Swap Monte Carlo



[Ninarello, Berthier, Coslovich, PRX ’17]

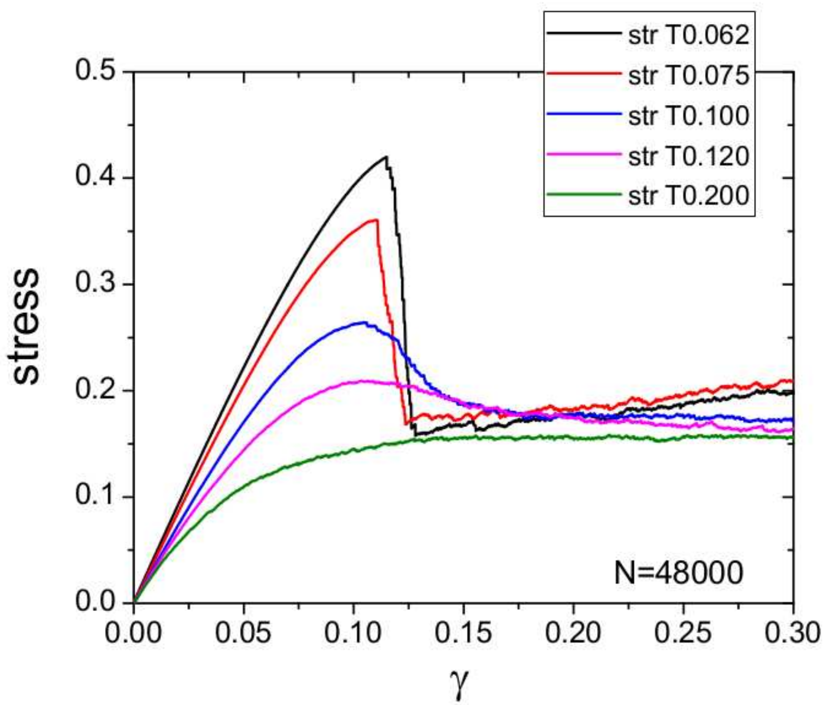
- Simple method solves the second timescale problem: we thermalise glasses below T_g.

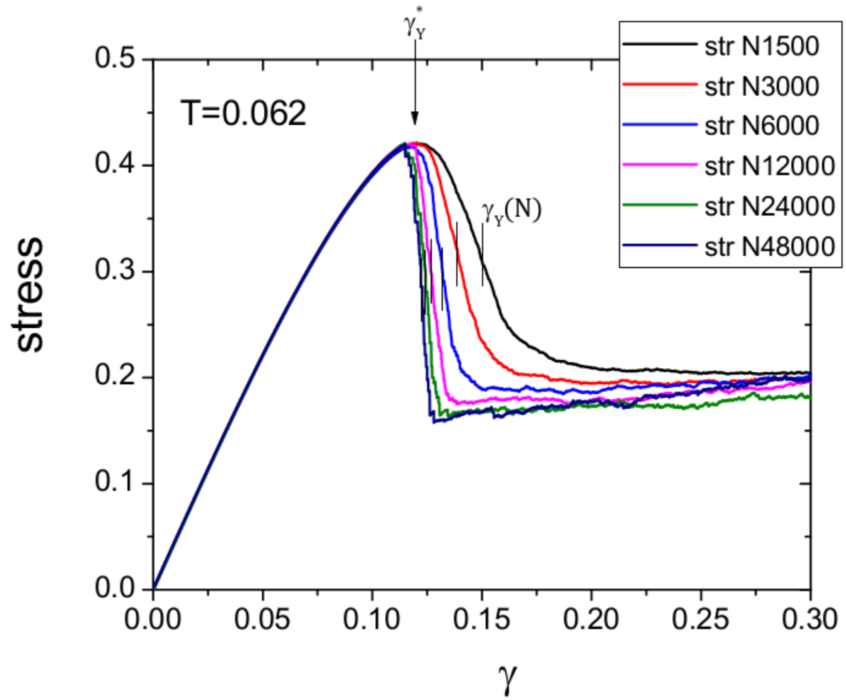
- Several models thermalised below T_g (13 decades): we gain more than 11 decades.

- Physics: Slow diffusion in diameter space facilitates particle diffusion in real space.

- We can now study the mechanical response of glass configurations that are experimentally relevant: ‘Well-annealed’ glasses...

Yielding transition exists





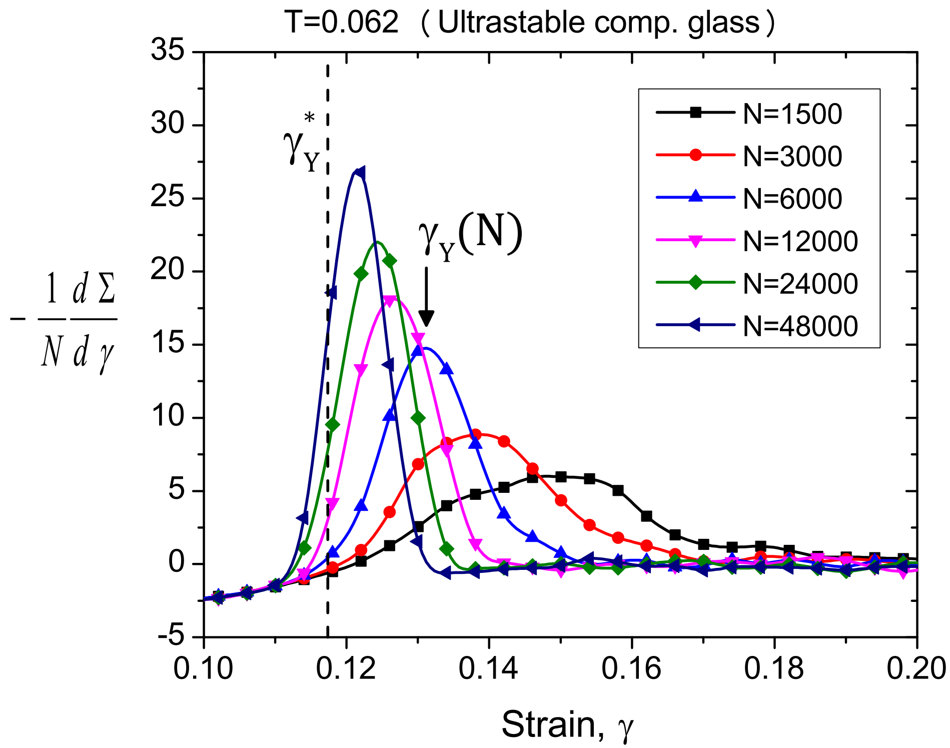
- For low 'enough' T, the transition becomes easily observable from macroscopic rheological observables.

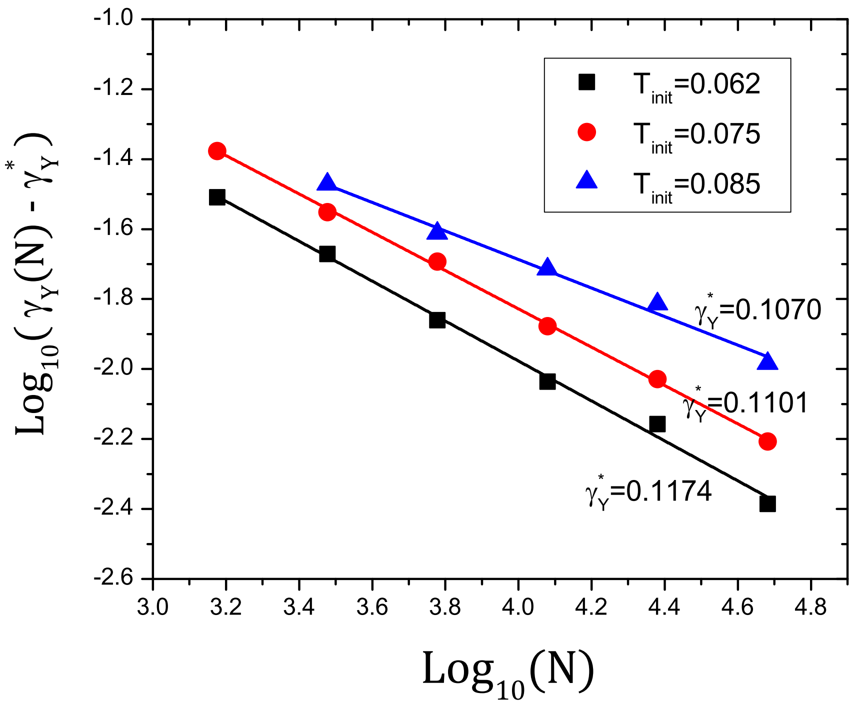
- Becomes sharper as $N \to \infty$: A bona fide phase transition.

- No need for complicated microscopic observables. Glass stability changes the physics qualitatively.

Finite size scaling

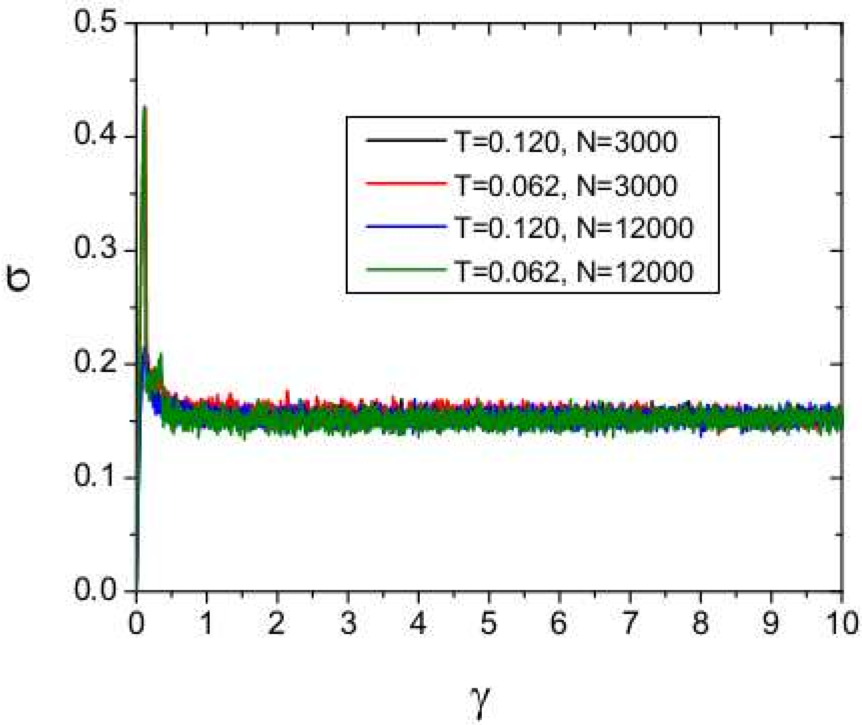
- Convergence with system size appears under control.

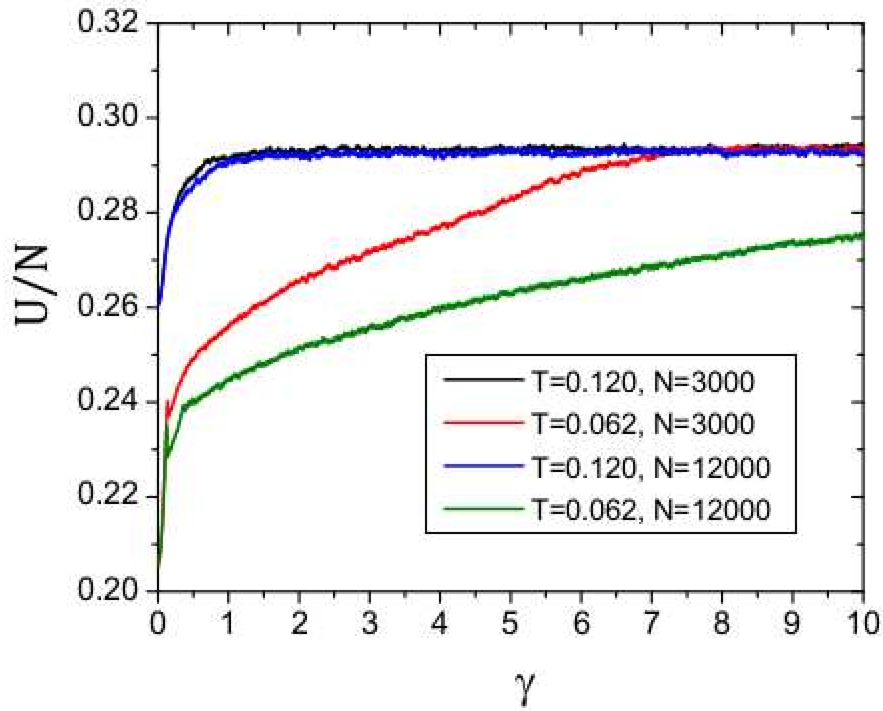




- Yielding is not a phase transition if T is too large. Previous simulations?
- There is a “critical” temperature below which discontinuity appears. We need to study that transition in more detail... In progress.

Steady state does not exist



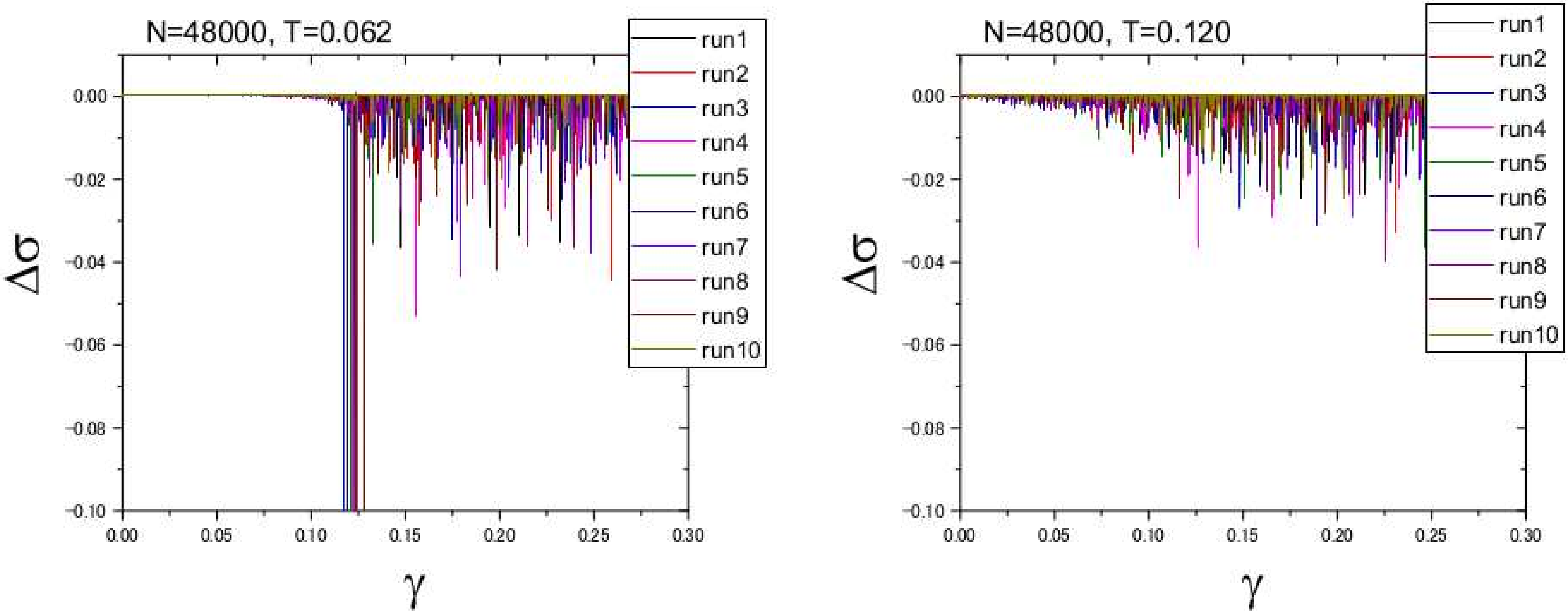


- The shear stress seems to converge.

- The energy never does. A steady state never exists in realistic glasses.

Relevance of the heavily discussed 'marginal' critical point for real (hard) glasses?

Elastic branch

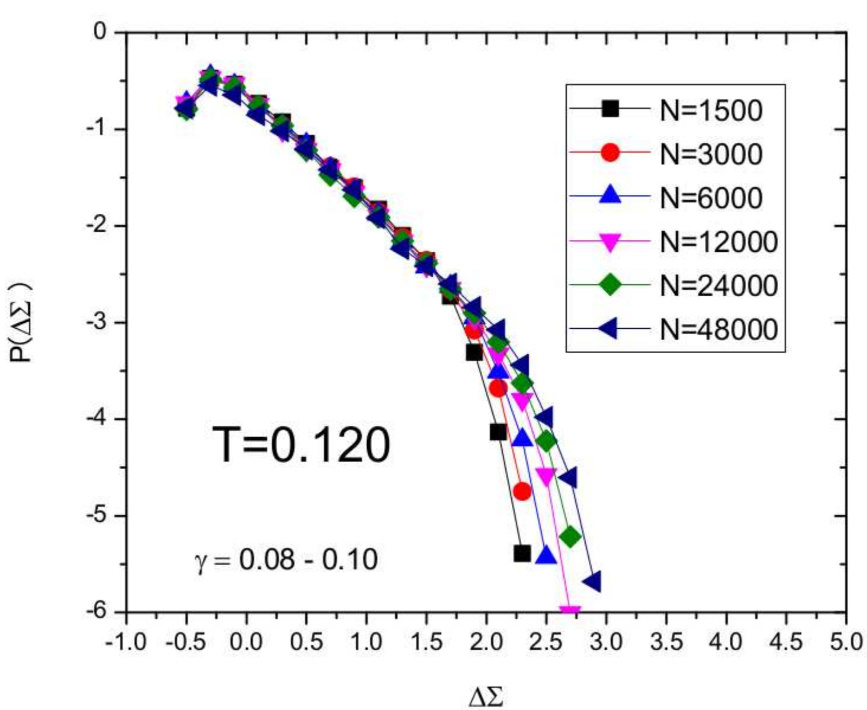


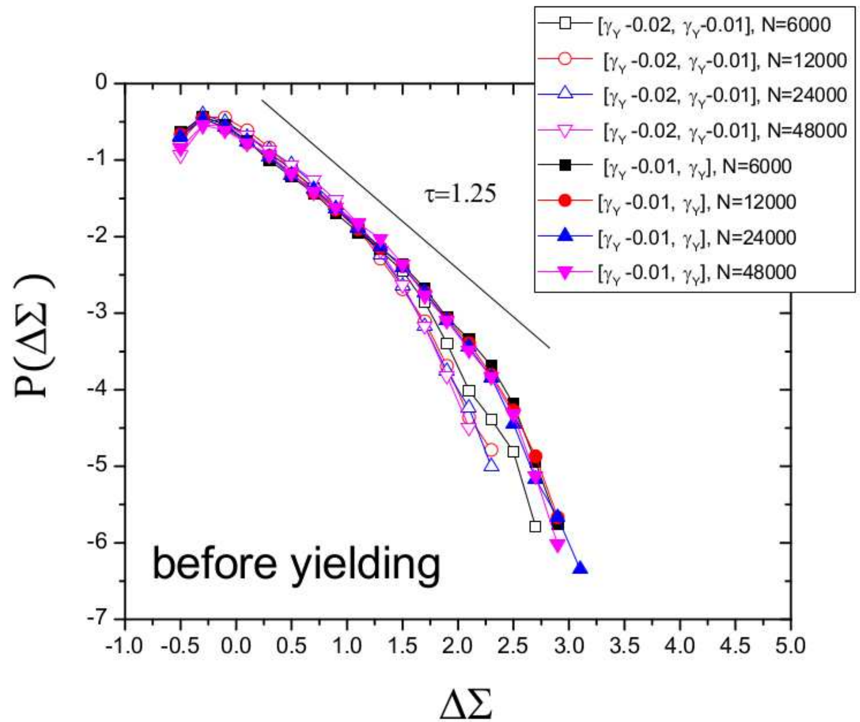
- Stress and energy drops along the elastic branch apparently disappear at low T.

- The nature of shear transformation zones / soft spots changes dramatically. Amplitude of energy drops divided by 100!

- Abrupt change of critical exponents at yielding, see [Hentschel *et al.*, PRE '15]

No marginal stability





- Distributions of stress and energy drops show no sign of criticality upon approaching yielding. No spinodal criticality, no percolation.

- Apparence of criticality might be due to poor thermalisation (simulation) or incorrect modelling (elasto-plastic models).

- Real glasses are not marginally stable.

[Scalliet, Berthier, Zamponi, PRL ’17]

Shear bands

• Yielding at high temperature is gradual.

• Yielding at low T is brutal, one way or the other.

• No percolation.

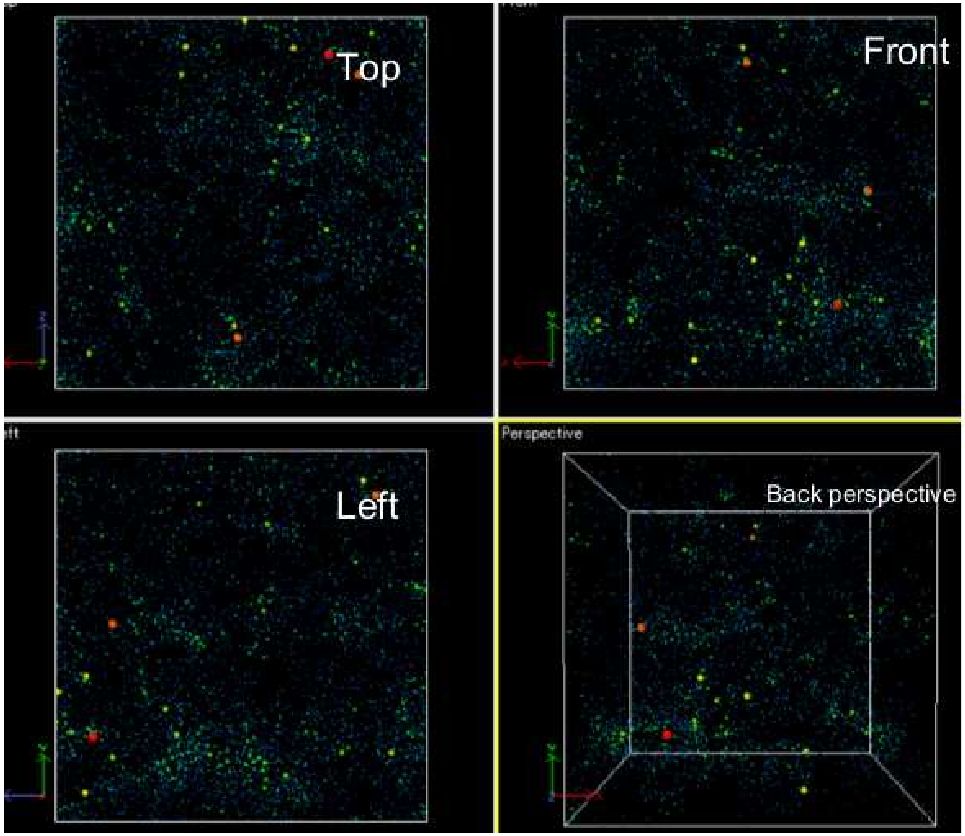
• Multiple breakings can occur in the same sample. Looks like metallic glasses...

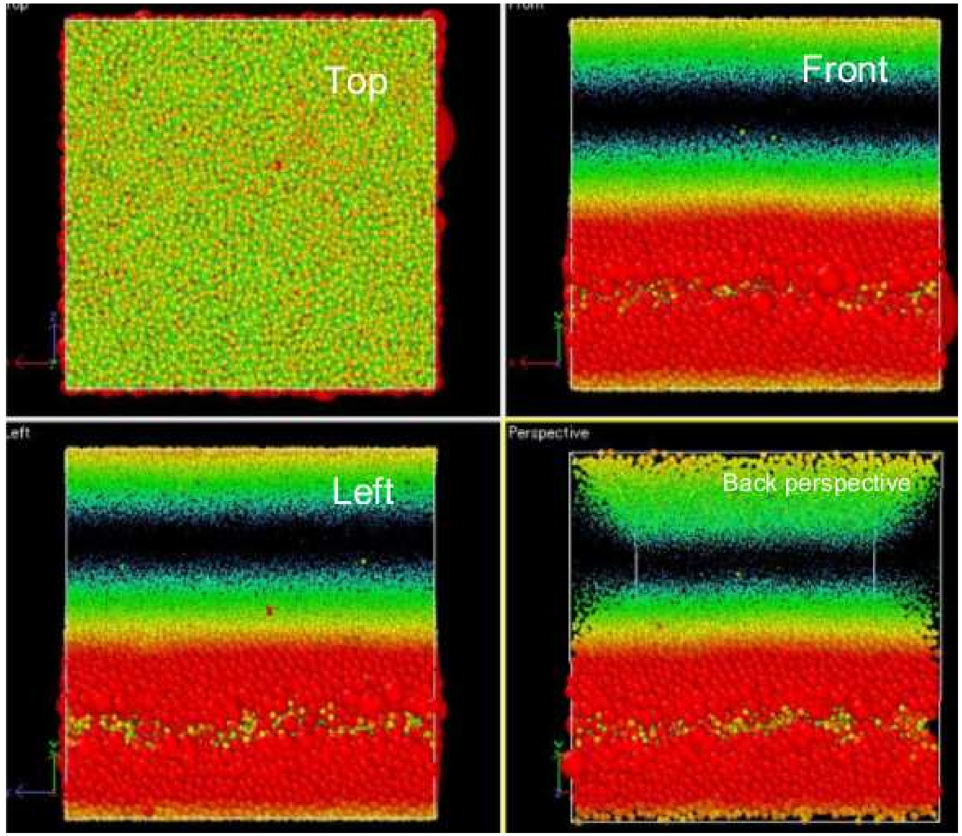
• The shear-band occurs within a single energy minimization, not through an accumulation of small events over large deformation.

• Anatomy of a single shear band.

Predictability?

- Non-affine displacement at $t-1$ (left) and at t (right).

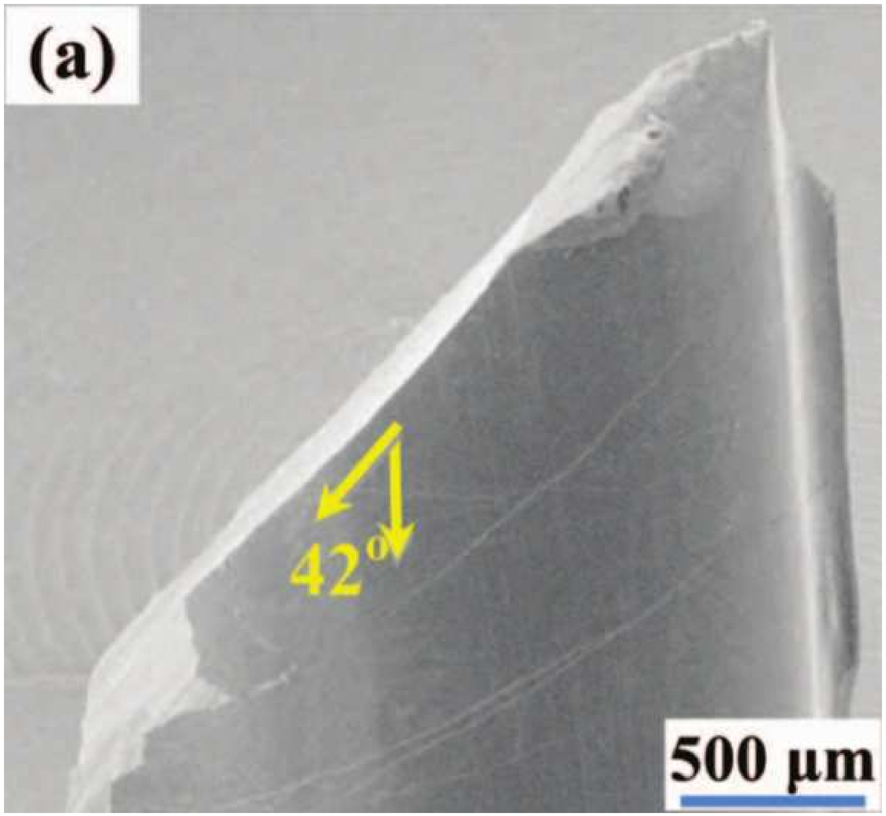




- Beuh.

Conclusion

- Discontinuous yielding under oscillatory shear, not sure it's useful after all.



- Sharp yielding transition exists for stable enough systems.

- Not critical, no diverging length-scale, no percolation.

- Our simulations seem appropriate for realistic glasses.