Poorly connected soft solids: dynamical processes, shear localization and yielding in colloidal gels

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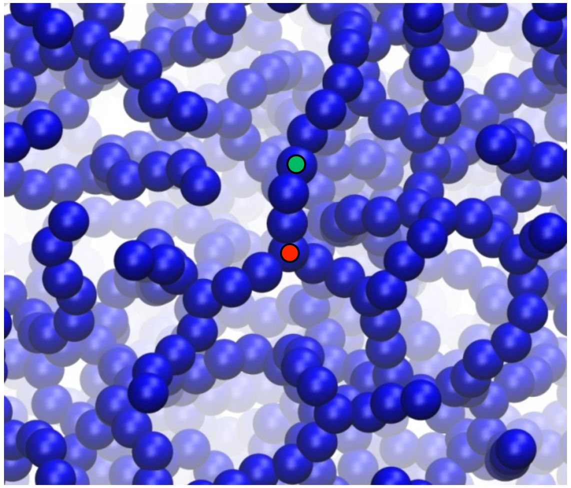
Outline

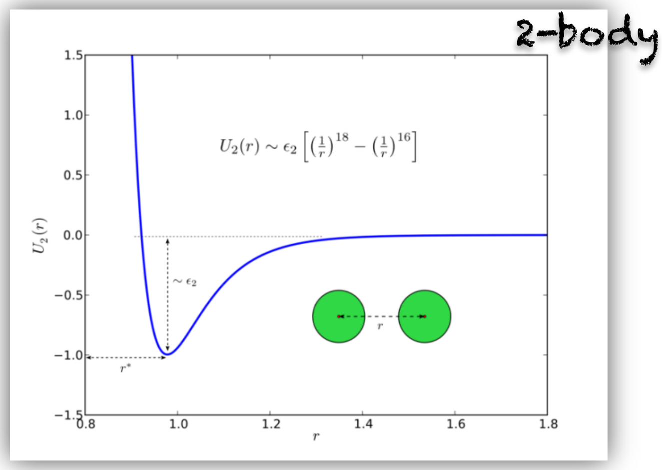
- Colloidal gels and model gels
- Dynamical processes for restructuring at rest.
- Athermal deformation and yielding.

A colloidal gel *in silico*

Jader Colombo, Asaph Widmer-Cooper and EDG, PRL 2013
Jader Colombo and EDG, Soft Matter 2014



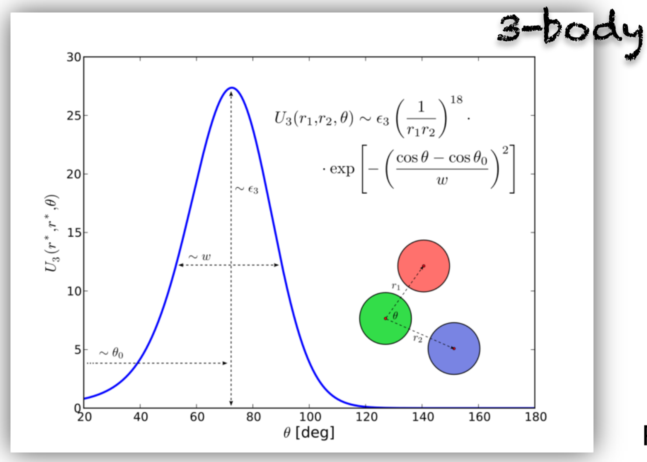
- 3-coordinated particle (cross-link)
- 2-coordinated particle (chain)



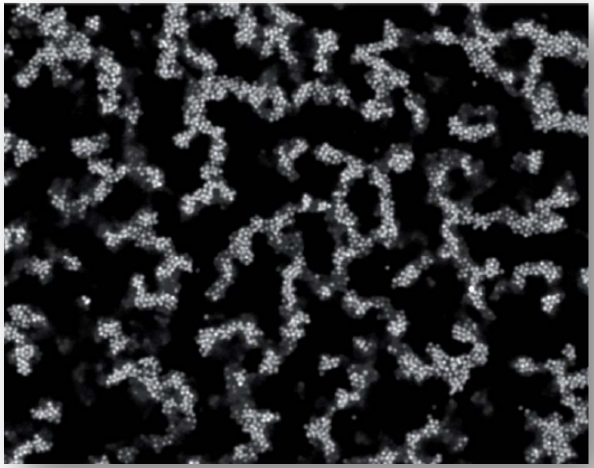
short-range attraction

+

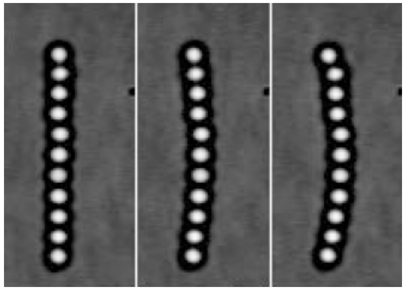
chains with bending stiffness



- Molecular Dynamics
- ~10^6 particles
- $\Phi = 0.1$
- periodic boundaries

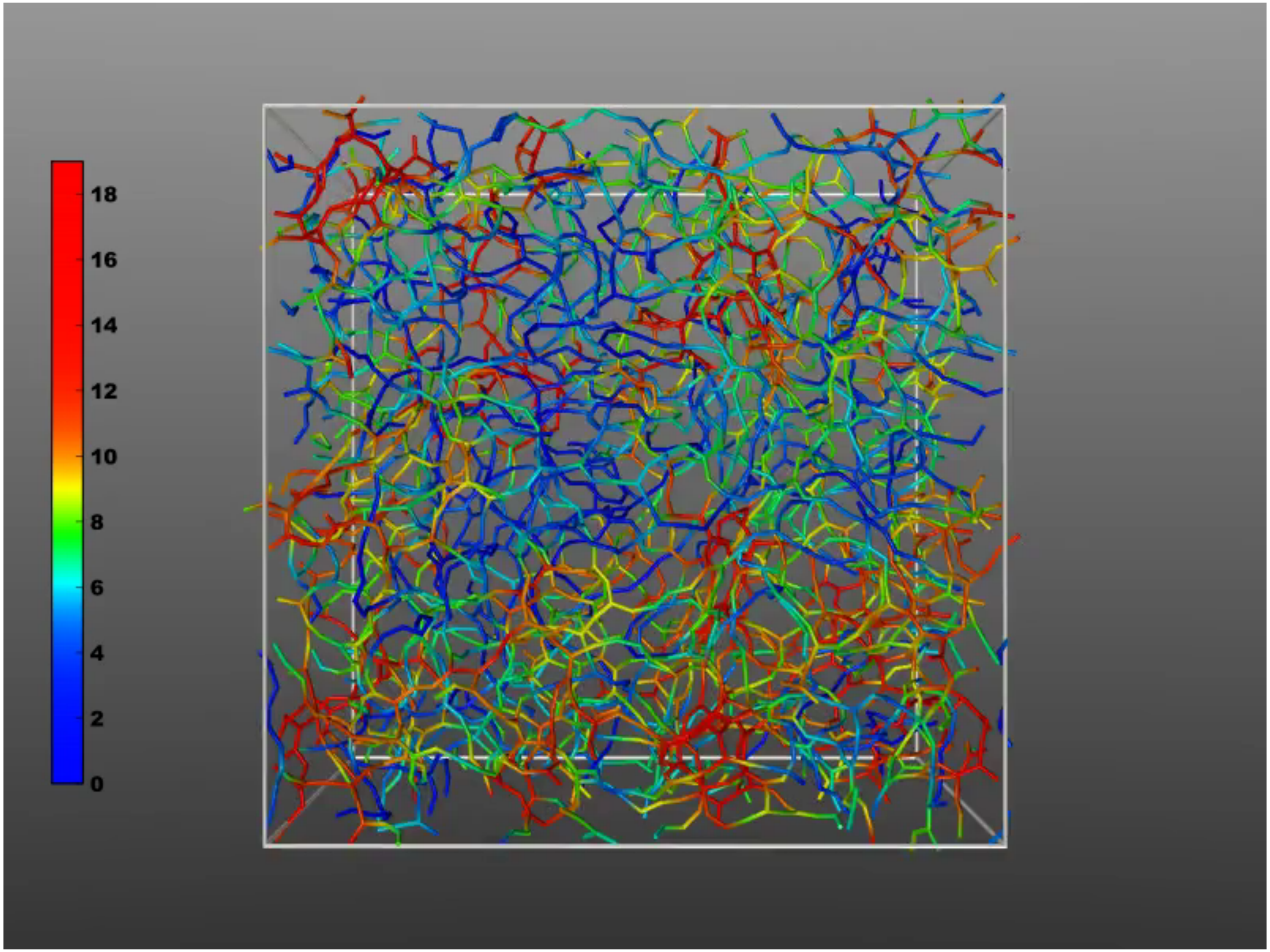


Lindström et al., *Soft Matter* **8**, 3657 (2012)



Pantina, Furst, *PRL* **94**, 138301 (2005)

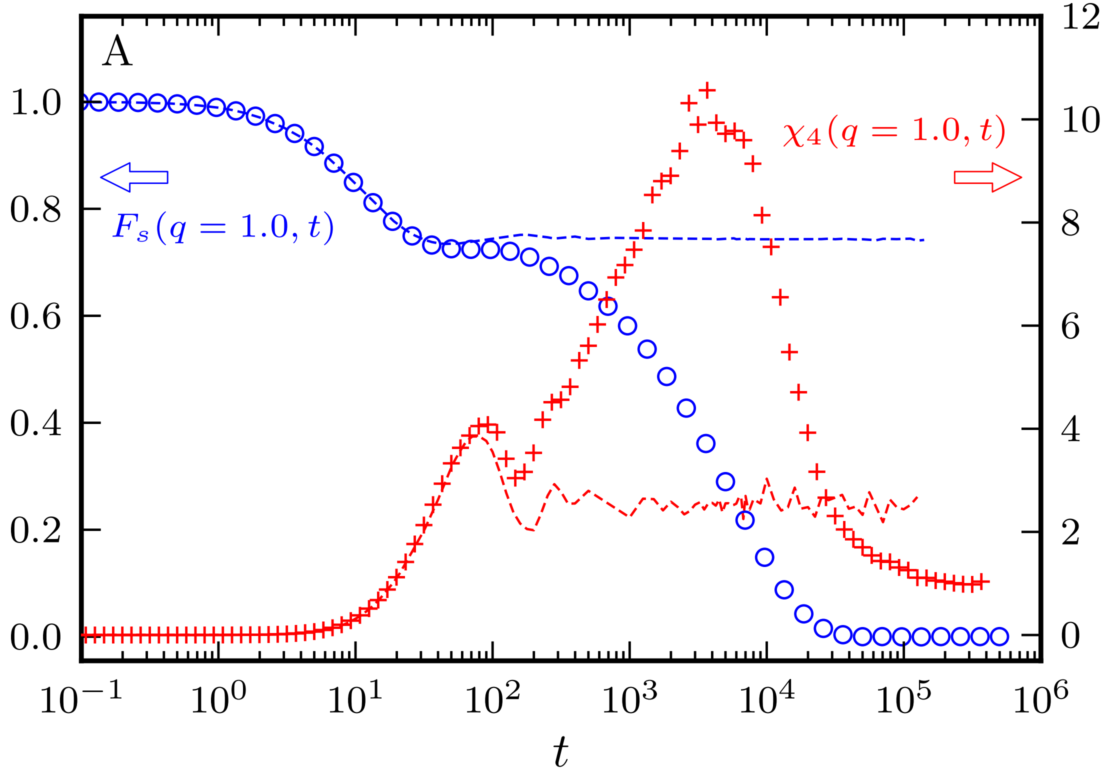
Local density of nodes



J. Colombo, A. Widmer-Cooper and EDG, PRL 2013

Cooperative dynamics

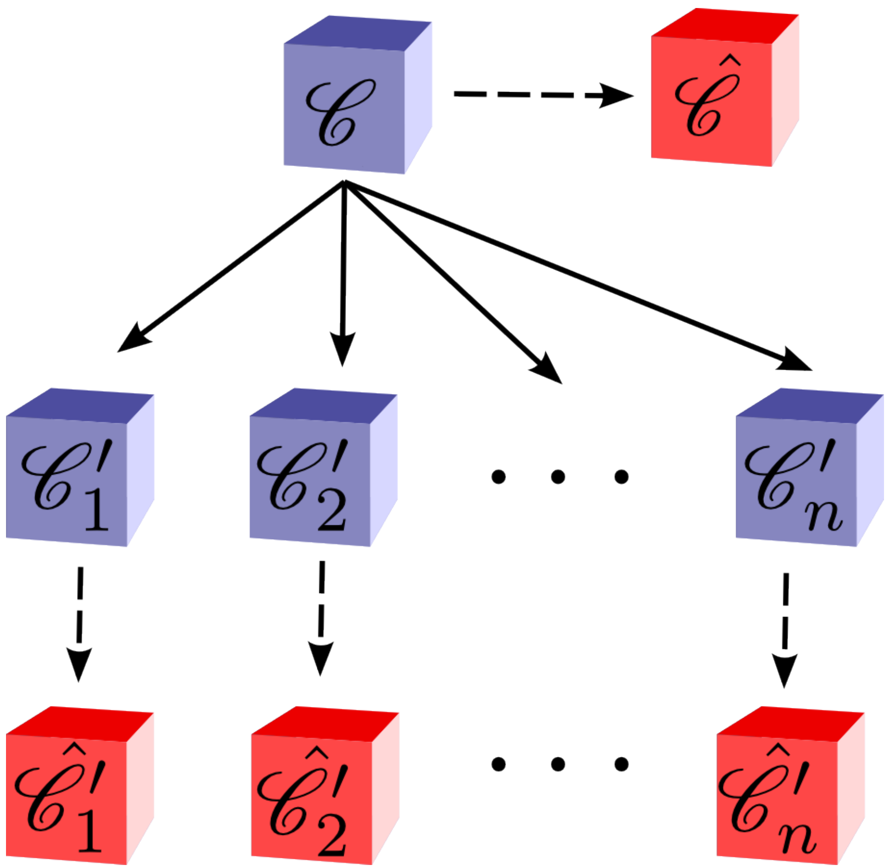
$$\Phi_s(q,t+t_0) = \frac{1}{N}\sum_{j=1}^{N} e^{i\mathbf{q}\cdot[\mathbf{r}_j(t+t_0)-\mathbf{r}_j(t_0)]} \qquad F_s(q,t) = \langle \Phi_s(q,t+t_0)\rangle_{t_0}$$



$$\chi_4(t) = N\left[\langle|\Phi_s(q,t+t_0)|^2\rangle_{t_0} - \langle\Phi_s(q,t+t_0)\rangle_{t_0}^2\right]$$

J. Colombo, A. Widmer-Cooper and EDG, PRL 2013
J. Colombo and EDG, Soft Matter 2014

Iso-configurational analysis for gels



For the same initial configuration, draw momenta from Maxwell-Boltzmann and evolve for a prescribed τ^*

Filter vibrations: constrain bonds and compute average position of every particle during a sufficiently long run

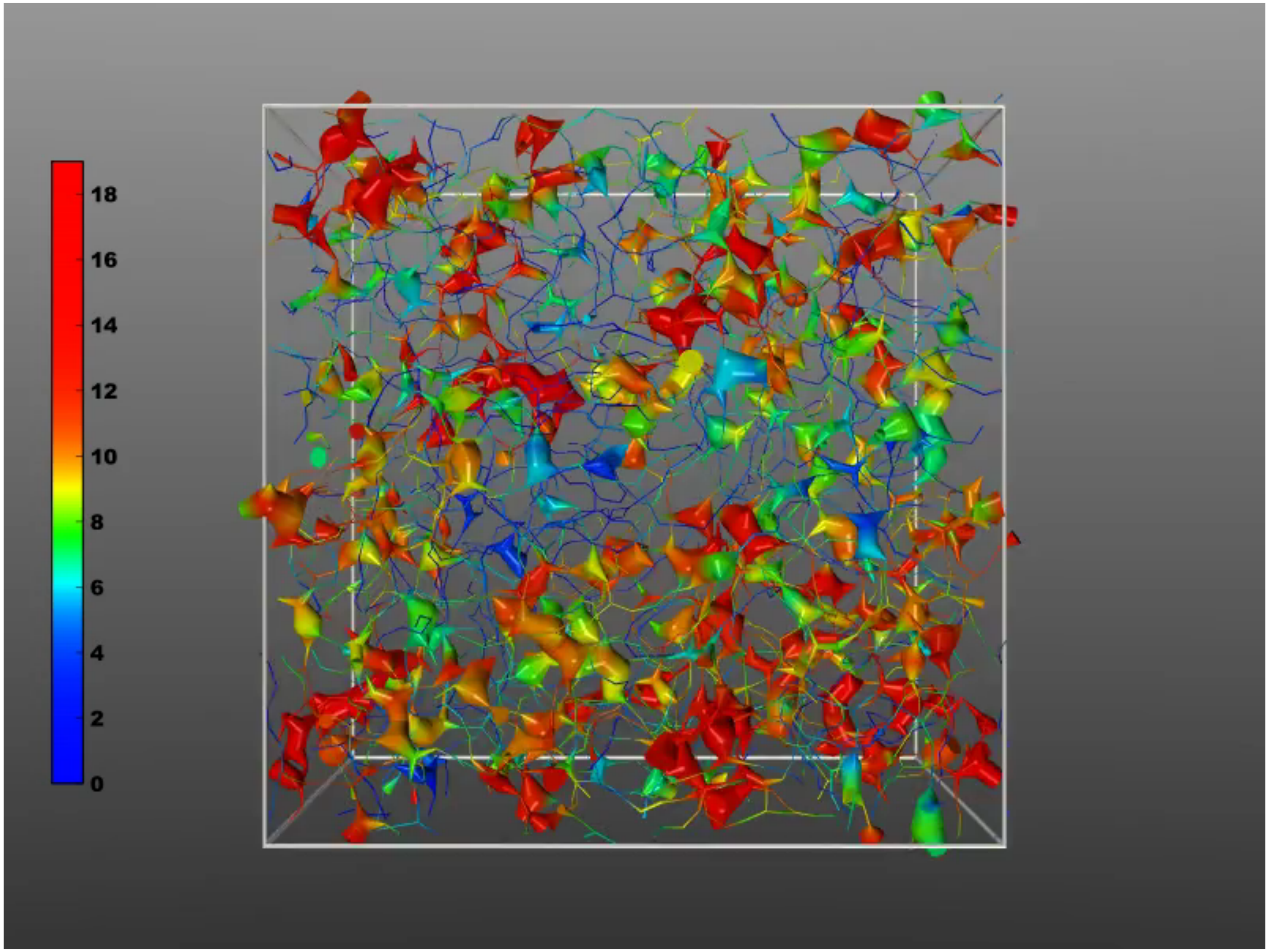
$$p_i = \langle (\mathbf{r}'_i - \mathbf{r}_i)^2 \rangle_{\mathscr{C}'}$$

propensity for displacement

$$b_i = \langle n_i \rangle_{\mathscr{C}'}$$

propensity for breaking

Bond-breaking events



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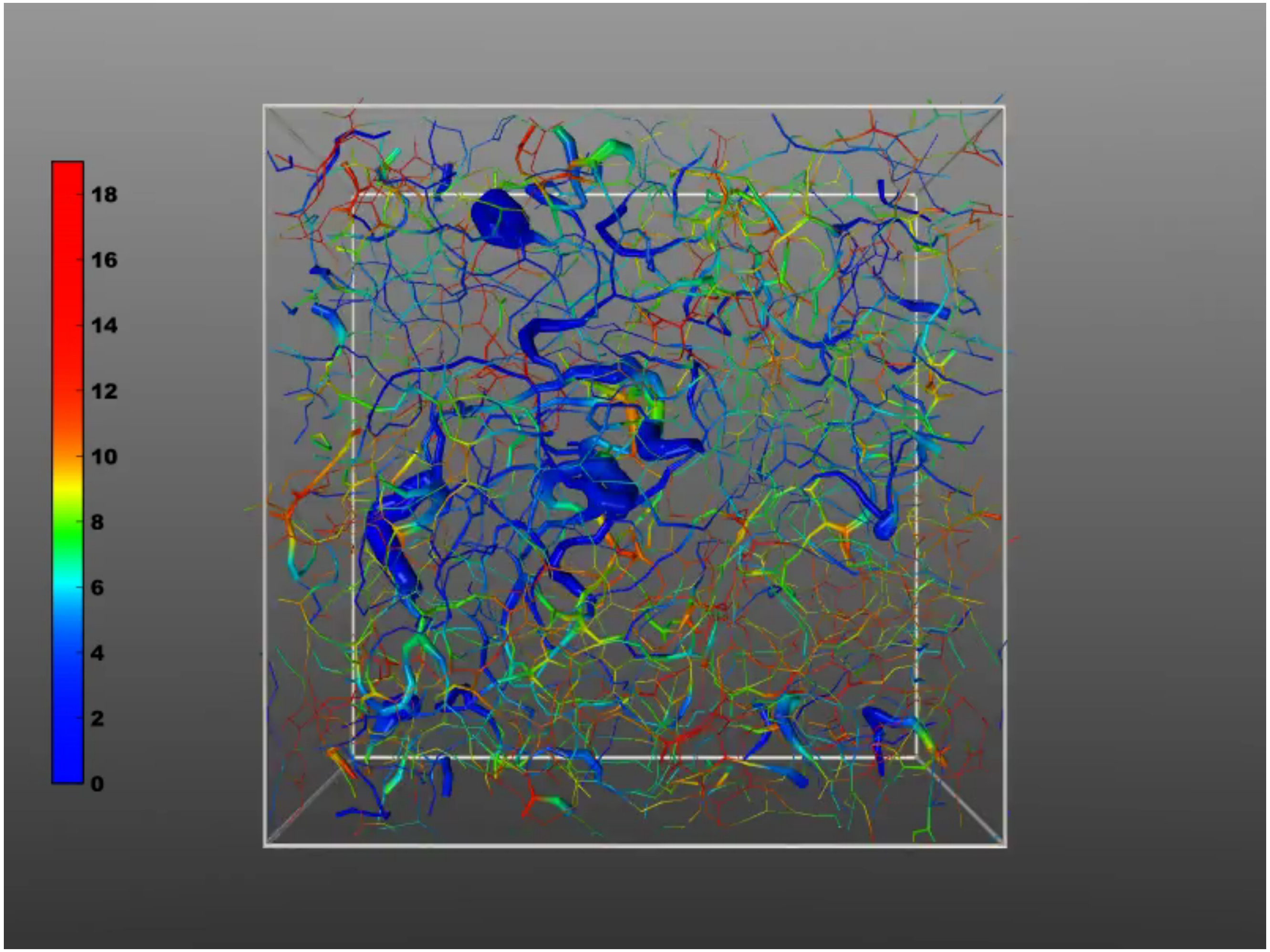
Consequences of bond-breaking



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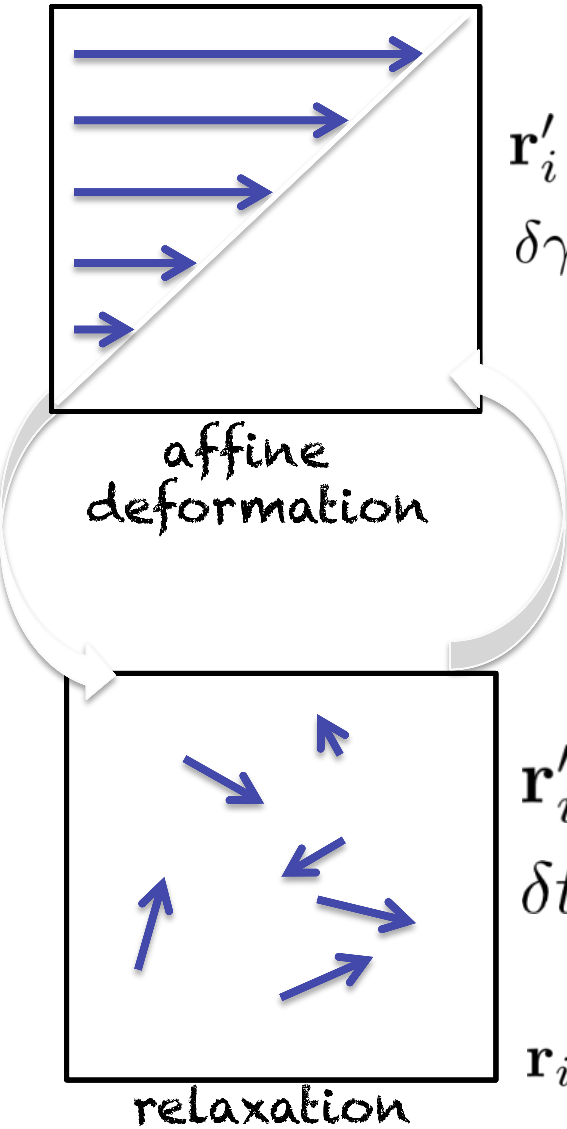
Athermal, incremental strain



$$m \frac{d^2 \mathbf{r}_i}{dt^2} = -\xi \frac{d\mathbf{r}_i}{dt} - \nabla_{\mathbf{r}_i} U$$

$$\mathbf{r}_i' = \Gamma_{\delta\gamma} \mathbf{r}_i$$

$$\delta\gamma = 10^{-2}$$

$$\mathbf{r}_i'' = \mathscr{T}_{\delta t} \mathbf{r}_i'$$

$$\delta t$$

$$\mathbf{r}_{i,n} = (\mathscr{T}_{\delta t} \Gamma_{\delta\gamma})^n \, \mathbf{r}_{i,0}$$

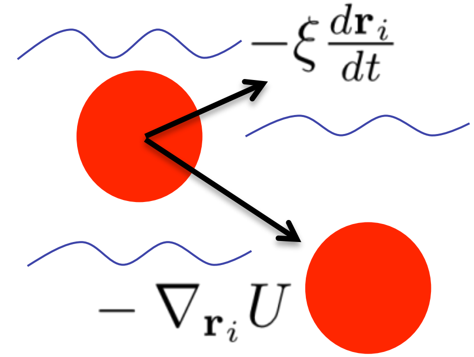
$$n = 100$$

$$\tau_0 = \xi \sigma^2 / \epsilon$$

$$\dot{\gamma}_1 = 2 \cdot 10^{-5} \, \tau_0^{-1}$$

$$\dot{\gamma}_2 = 10^{-4} \, \tau_0^{-1}$$

$$\dot{\gamma}_3 = 10^{-3} \, \tau_0^{-1}$$



Aqueous colloidal suspension:

$\sigma \approx 100$ nm

$\epsilon \approx 10 \, k_B T$

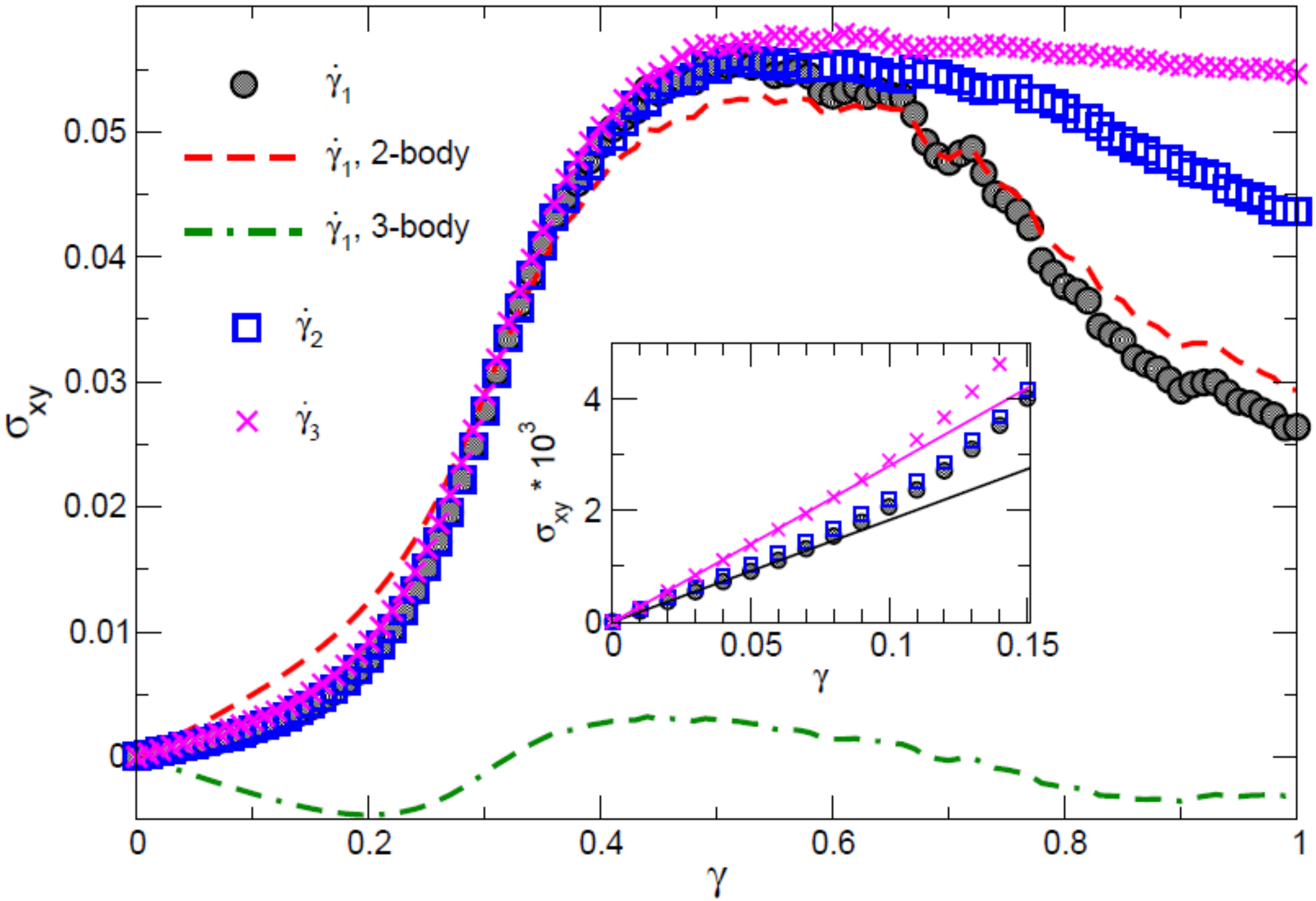
$\tau_0 \approx 10^{-4}$ s

$\dot{\gamma}_1 \approx 0.2 s^{-1}$

$\dot{\gamma}_2 \approx 1.0 s^{-1}$

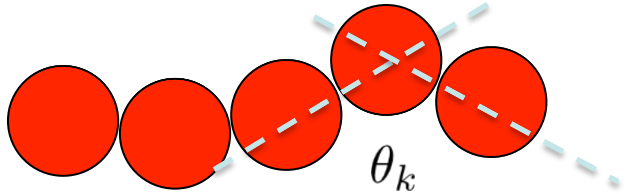
$\dot{\gamma}_3 \approx 10 s^{-1}$

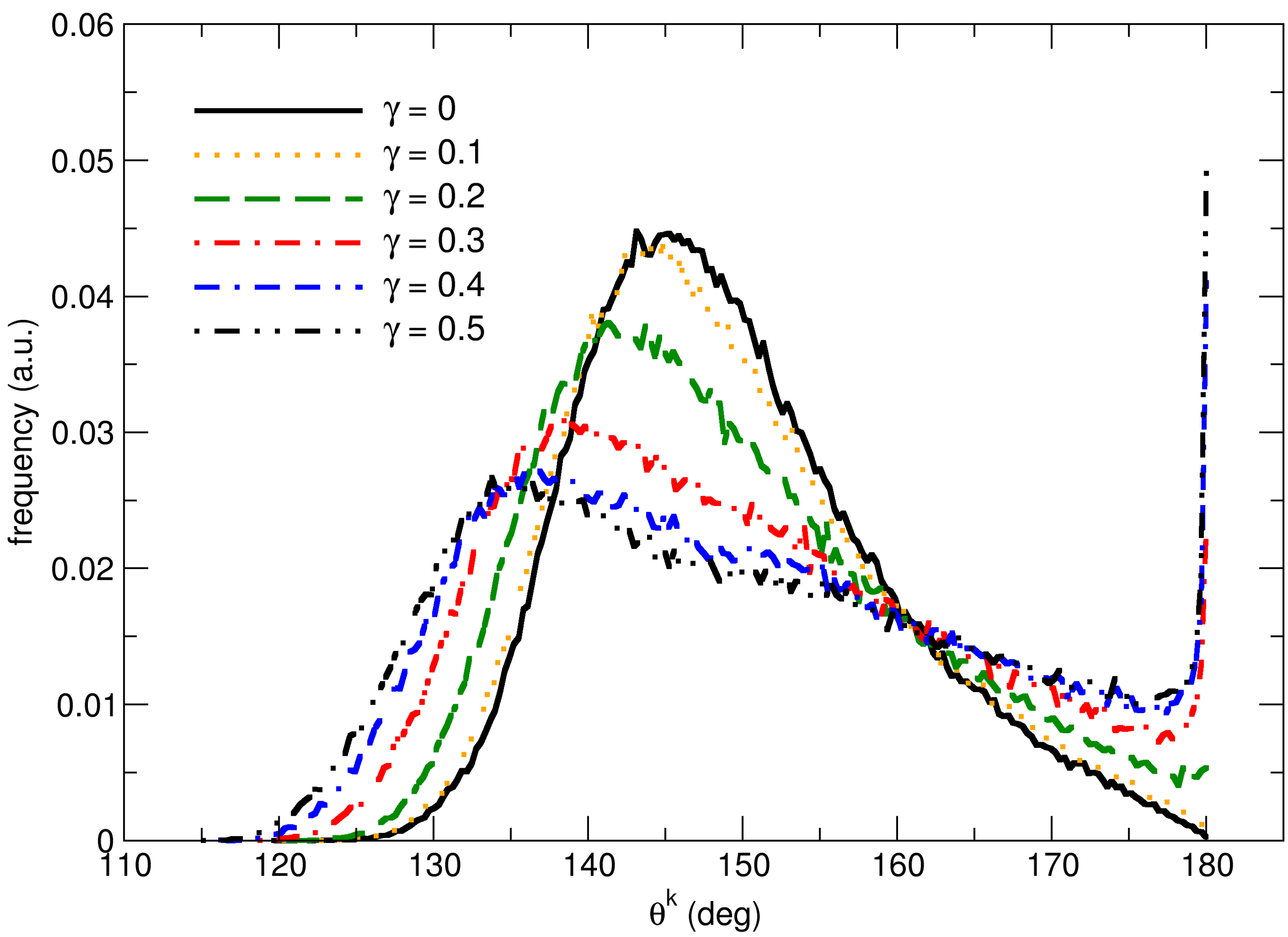
Load curves



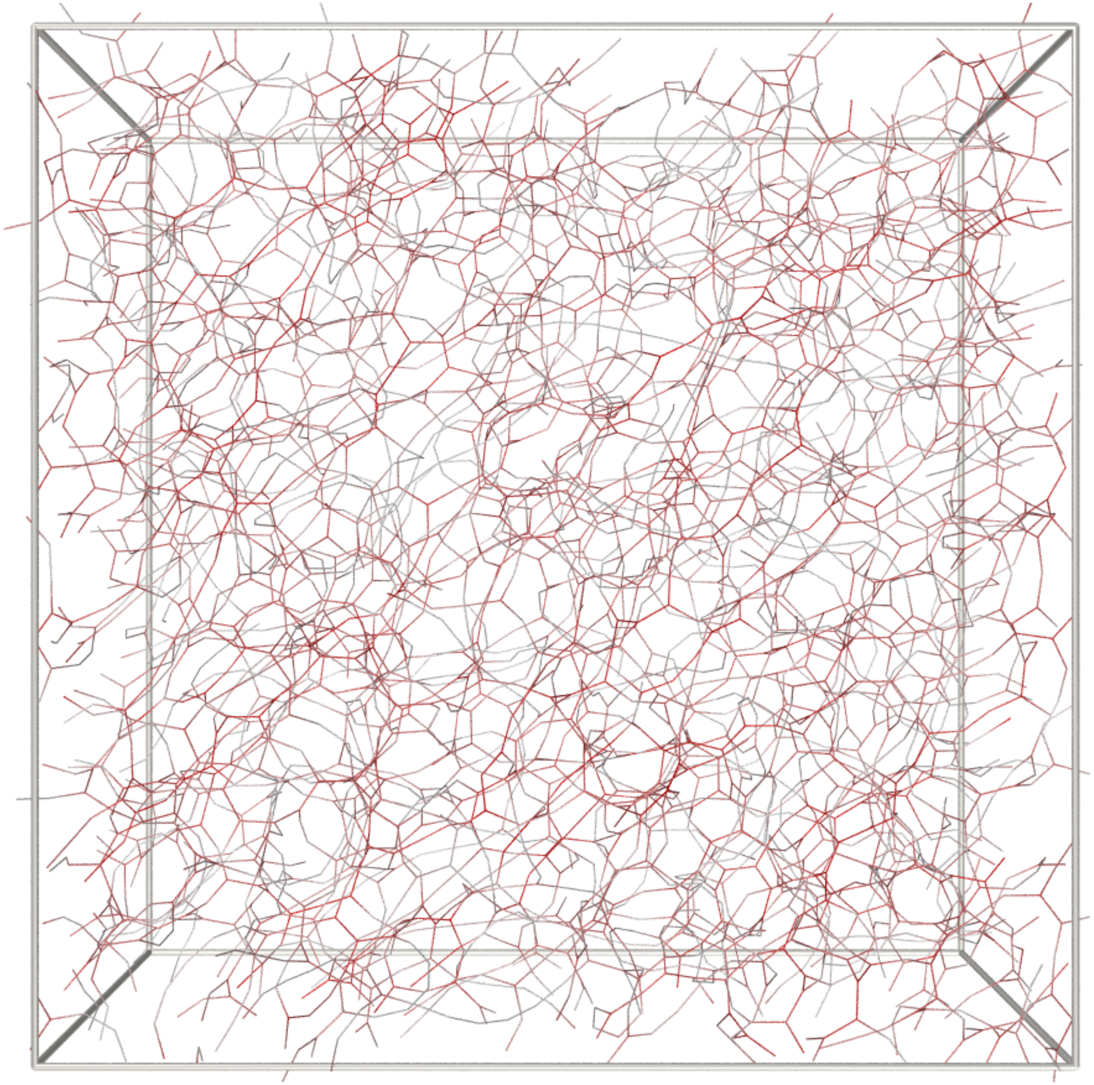
$\dot{\gamma}_1$
$\dot{\gamma}_1$, 2-body
$\dot{\gamma}_1$, 3-body
$\dot{\gamma}_2$
$\dot{\gamma}_3$
σ_{xy}
γ
0
0.01
0.02
0.03
0.04
0.05
0
0.2
0.4
0.6
0.8
1
$\sigma_{xy} * 10^3$
0
2
4
0
0.05
0.1
0.15
γ

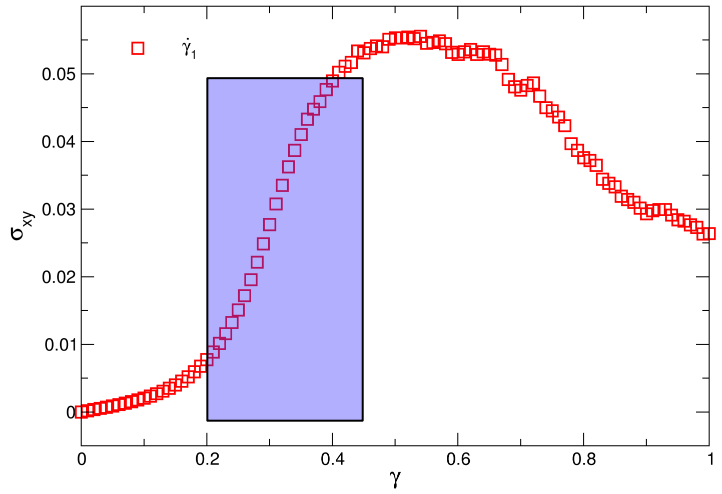
Stretching of the chains

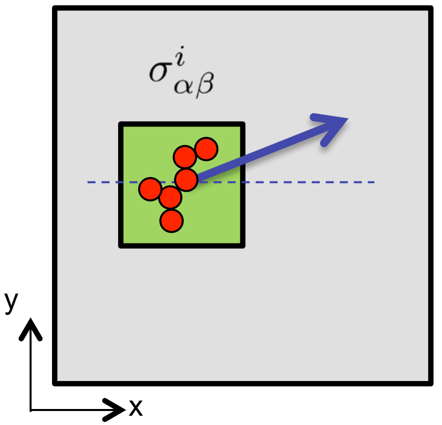




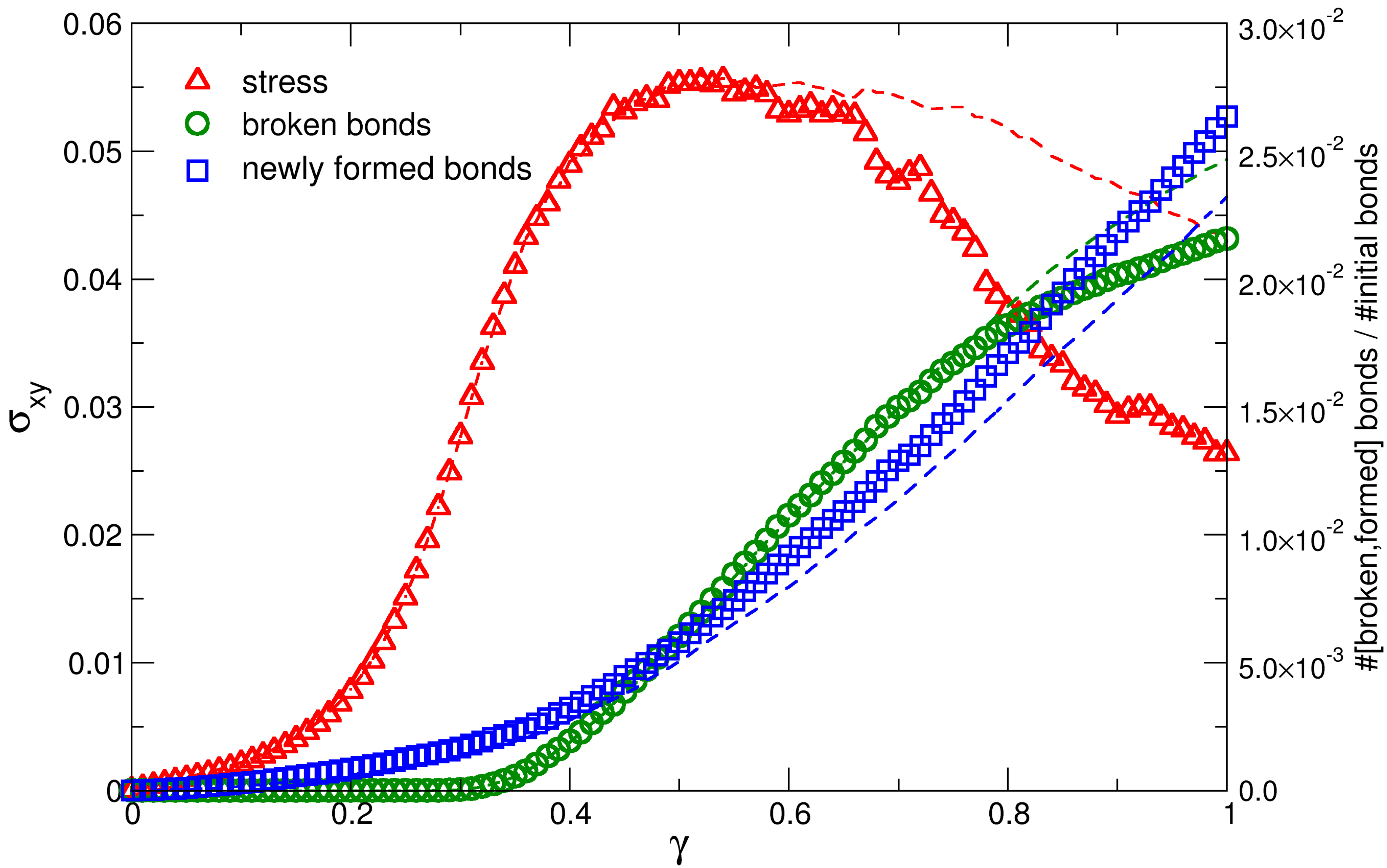
Stress localization



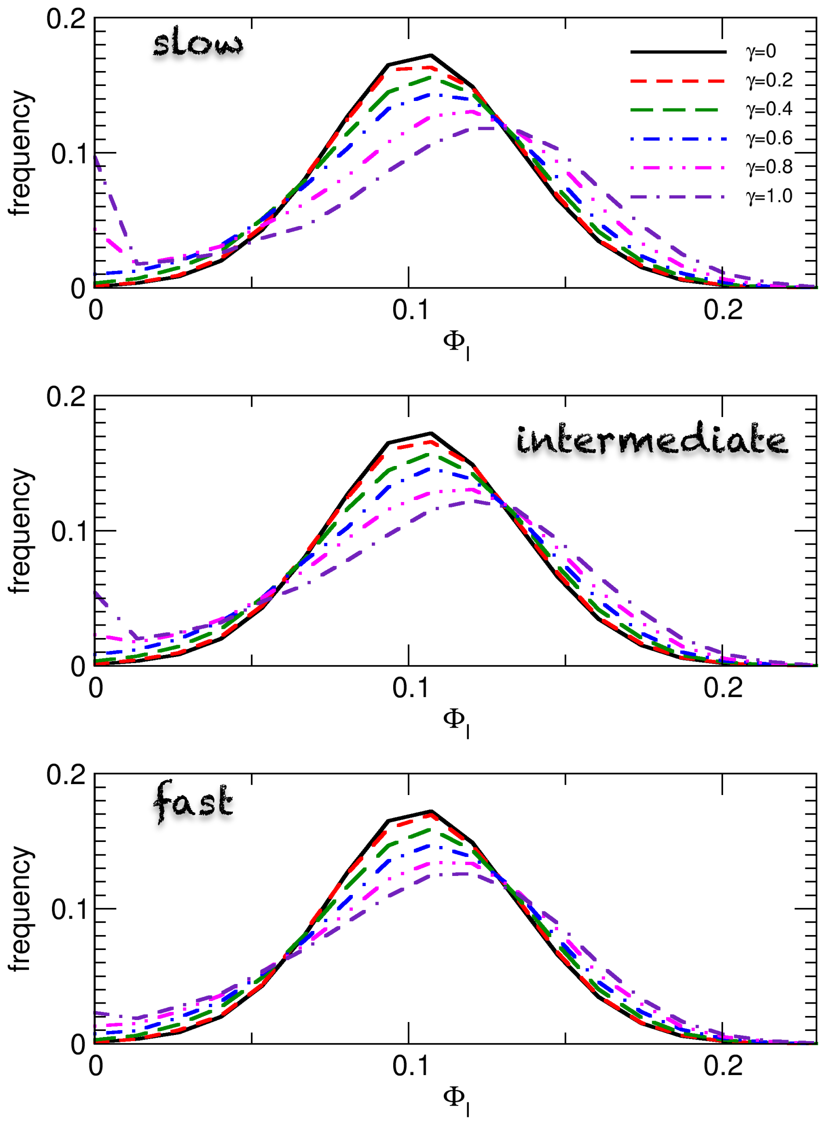


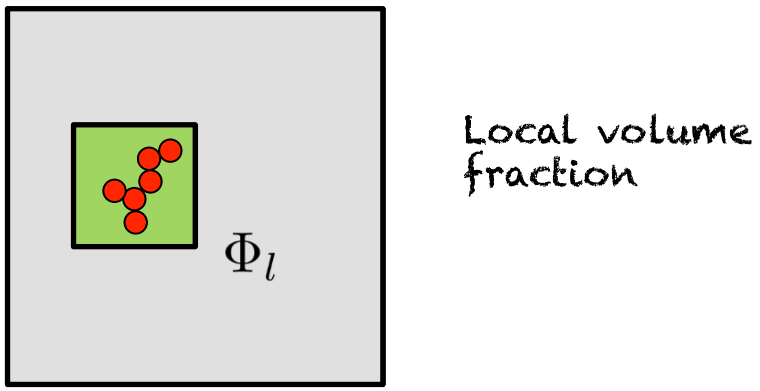


Bonds breaking & new bonds



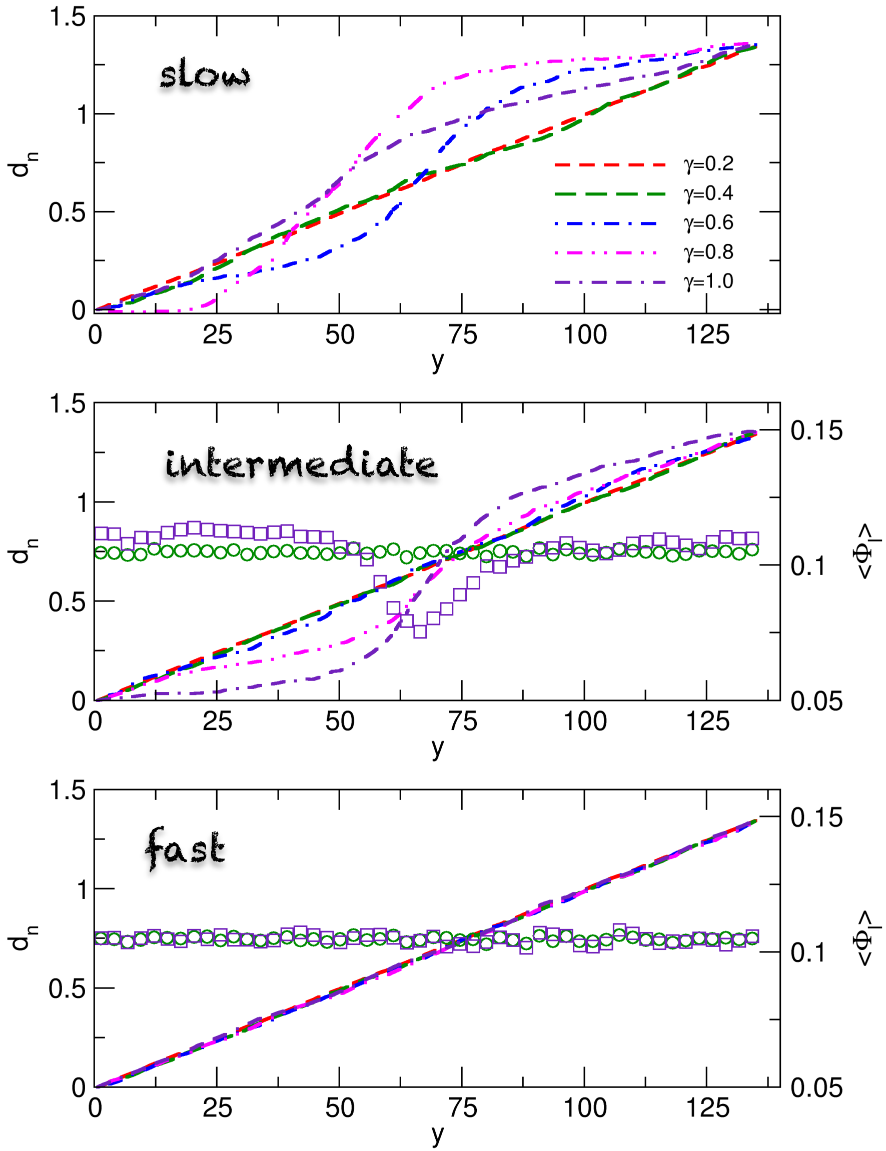
Density fluctuations

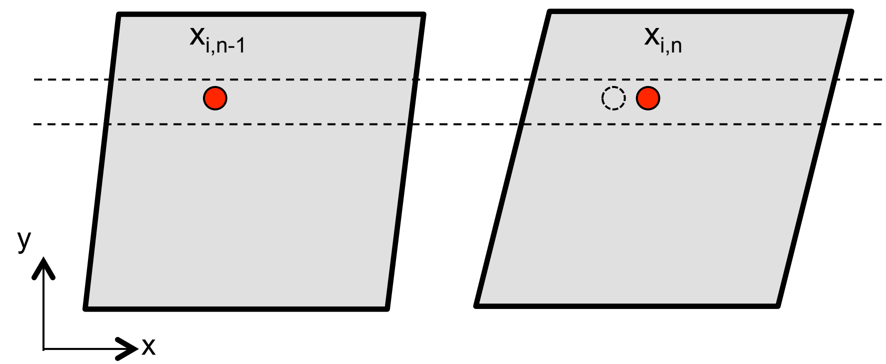




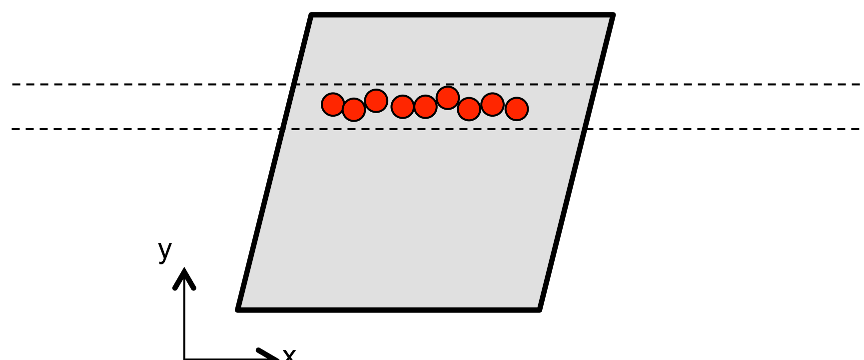
- Formation of excess bonds under shear favors a densification in certain regions
- A region from which particles are depleted starts to develop

Shear localization





$$d_n(y) = \frac{1}{M}\sum_{|y_{i,n}-y|<\Delta/2}(x_{i,n} - x_{i,n-1})$$



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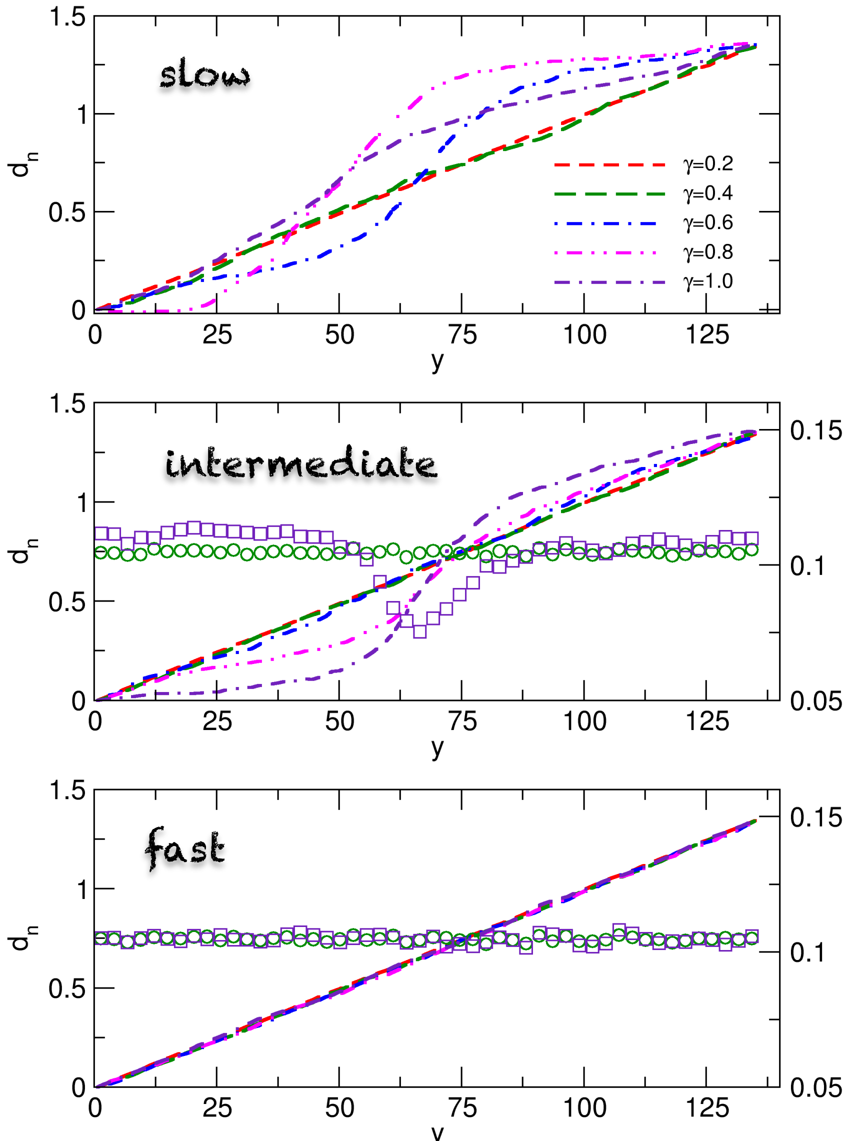
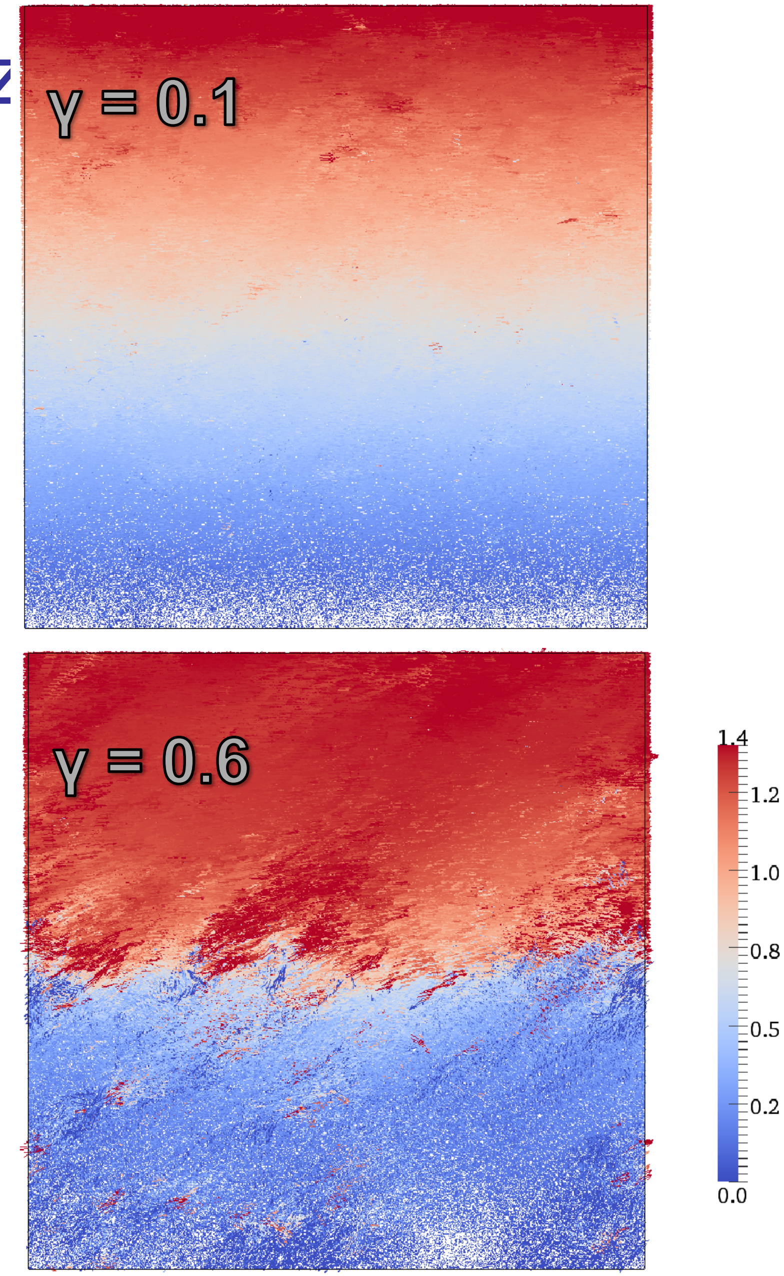
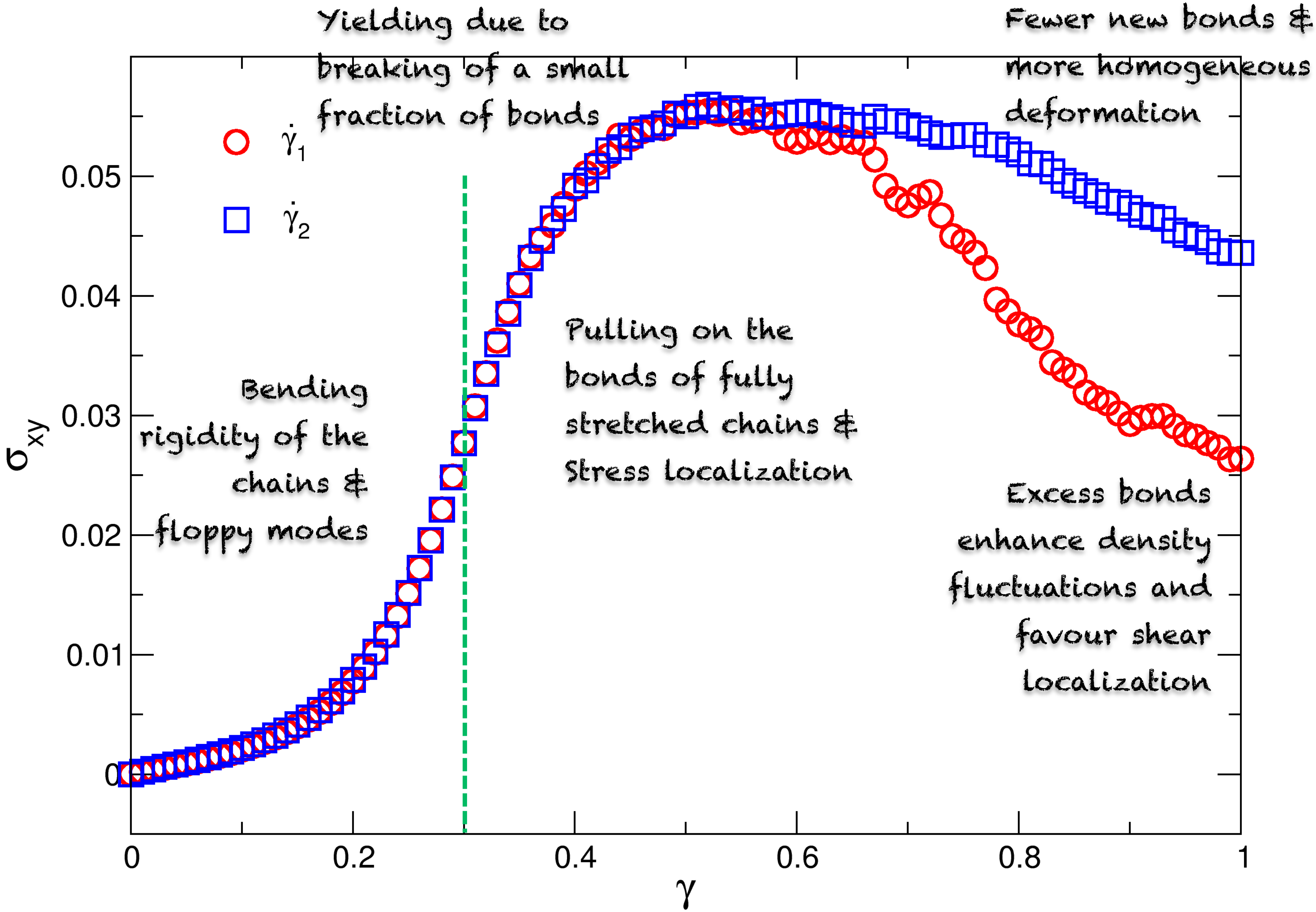
Shear localiz





See Divoux, Gibaud and Manneville experiments

Summary



Yielding due to breaking of a small fraction of bonds
Fewer new bonds & more homogeneous deformation
$\dot{\gamma}_1$
$\dot{\gamma}_2$
Bending rigidity of the chains & floppy modes
Pulling on the bonds of fully stretched chains & Stress localization
Excess bonds enhance density fluctuations and favour shear localization
0.05
0.04
0.03
0.02
0.01
0
σ_{xy}
0
0.2
0.4
0.6
0.8
1
γ

References

J. Colombo and EDG
Journal of Rheology 2014
Soft Matter 2014
J. Colombo, A. Widmer-Cooper and EDG, PRL 2013