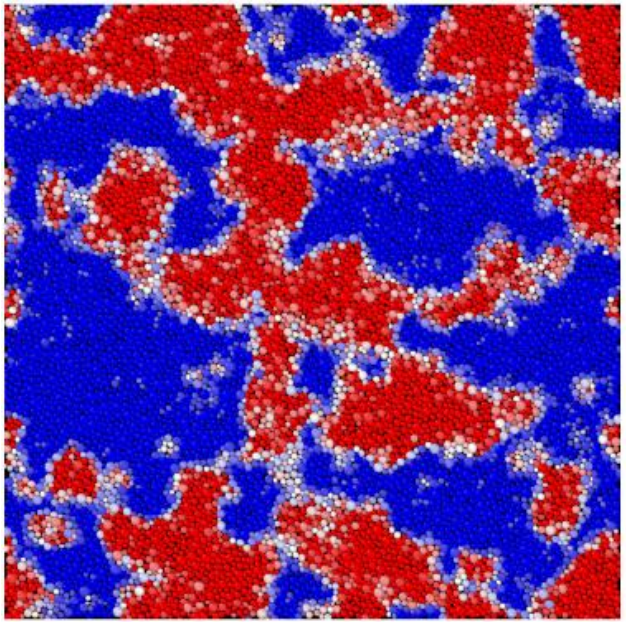
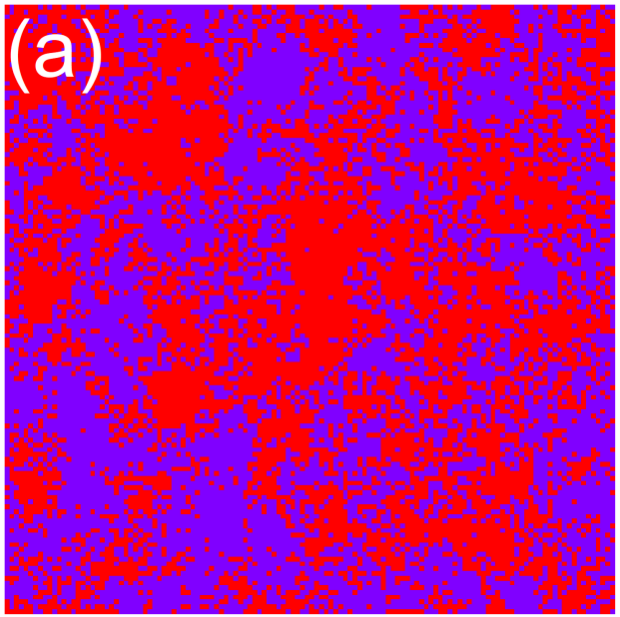
Elasticity, Facilitation and Dynamic Heterogeneity in Glass Forming liquids





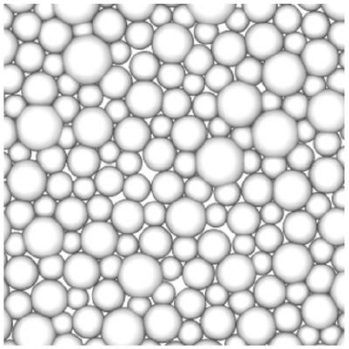
Misaki Ozawa

In collaboration with Giulio Biroli

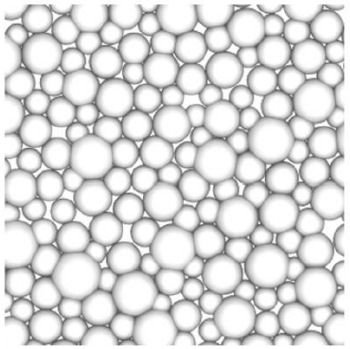
Ozawa and Biroli, arXiv:2209.08861, 2022

Snapshots have no feature

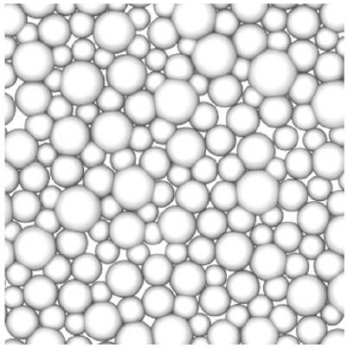
Glass

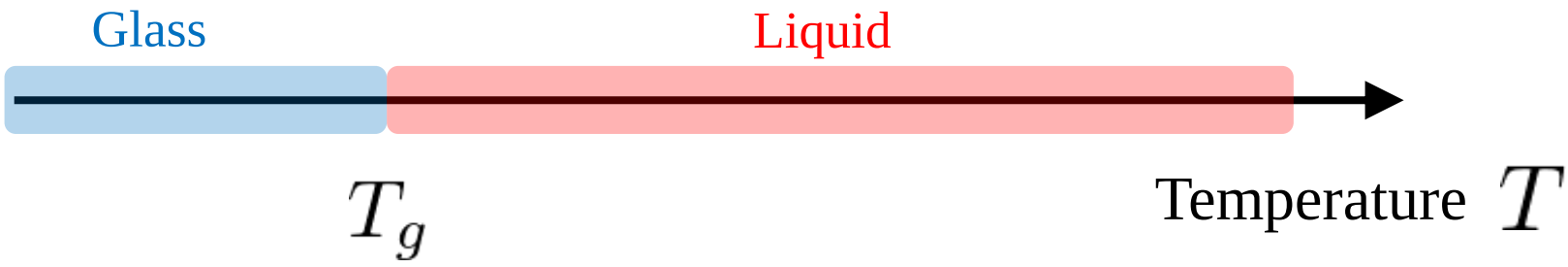


Low T liquid



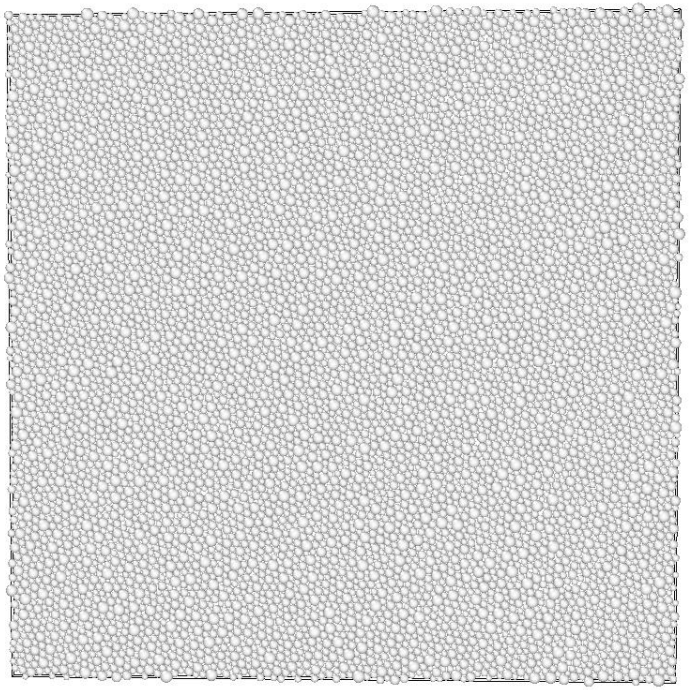
High T liquid





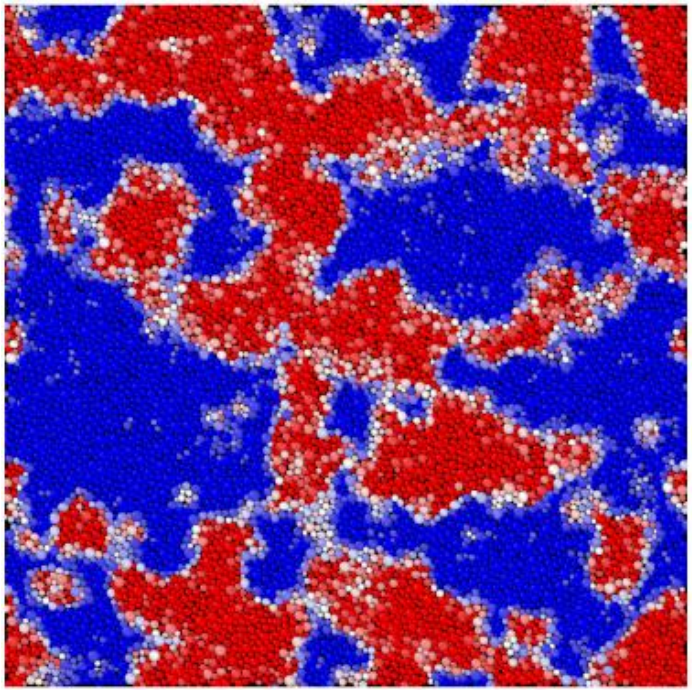
Dynamical heterogeneity

Snapshot



Low T liquid

Dynamics



Red: Mobile
Blue: Immobile

The mechanism of dynamical heterogeneity is unclear

Many theories and scenarios

- Thermodynamic scenarios

  Adam and Gibbs, JCP 1965

  Kirkpatrick, Thirumalai, and Wolyness, PRA 1989

  Bouchaud and Biroli, JCP 2004

- Dynamic facilitation

  Chandler and Garrahan, Annu. Rev. Phys. Chem. 2010

  Hedges, Jack, Garrahan, and Chandler, Science 2009

- Elasticity scenarios

  Dyre, RMP 2006

  Lemaitre, PRL 2014

- Geometrical considerations

  Tarjus, Kivelson, Nussinov, and Viot, J. Phys. Condens. Matter 2005

  Tanaka, Kawasaki, Shintani, and Watanabe, Nat. Mater 2010

- Etc..

The New York Times

The Nature of Glass Remains Anything but Clear

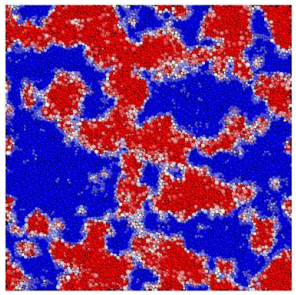
Different approaches

?

Solid that flows

Dyre, RMP 2006

Lemaitre, PRL 2014



Viscous fluid

Majority of theories

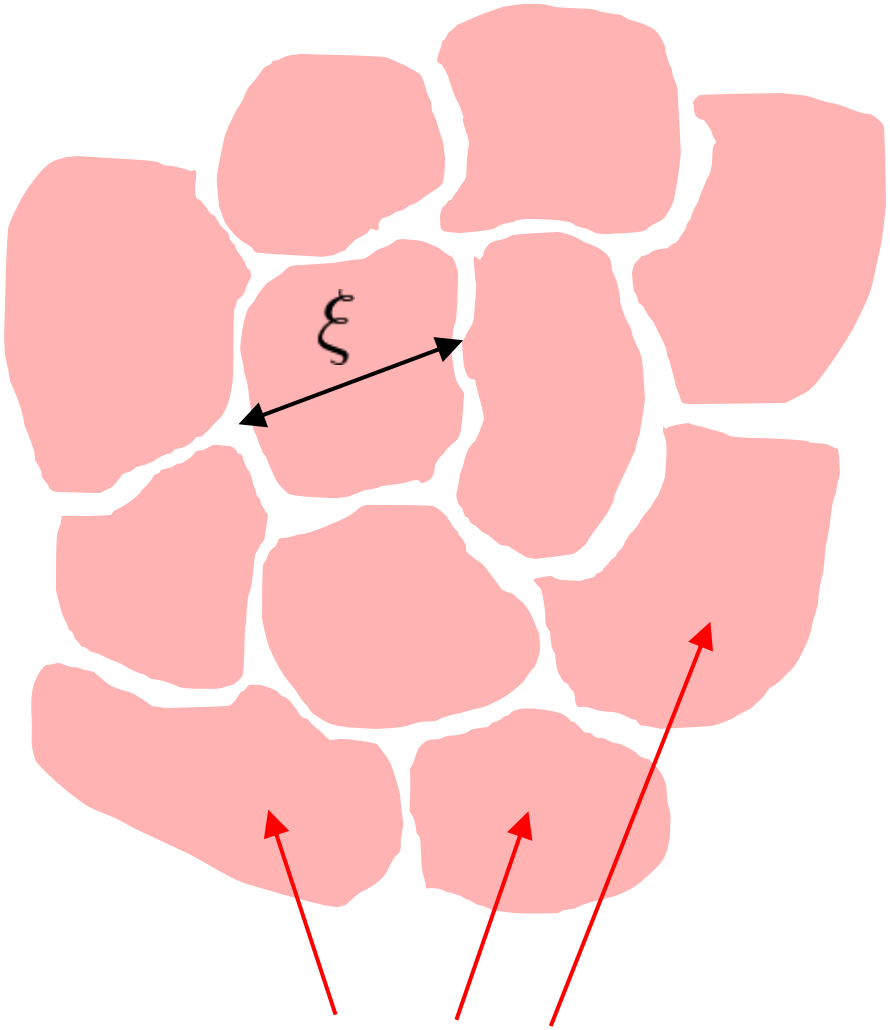
Glass

Liquid

T_g

Temperature T

Thermodynamic scenario



Relaxation time

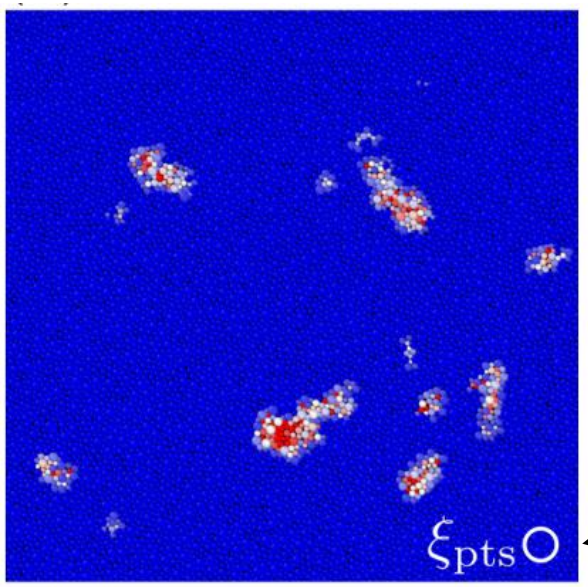
$$\tau_\alpha \sim e^{\frac{\xi^\psi}{T}}$$

Adam and Gibbs, JCP 1965

Kirkpatrick, Thirumalai, and Wolyness, PRA 1989

Bouchaud and Biroli, JCP 2004

Early time stage

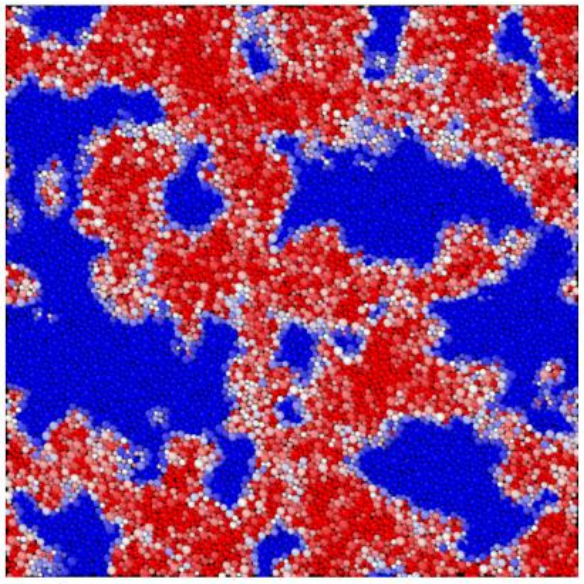


Red: Mobile

Blue: Immobile

Cooperative rearranging region

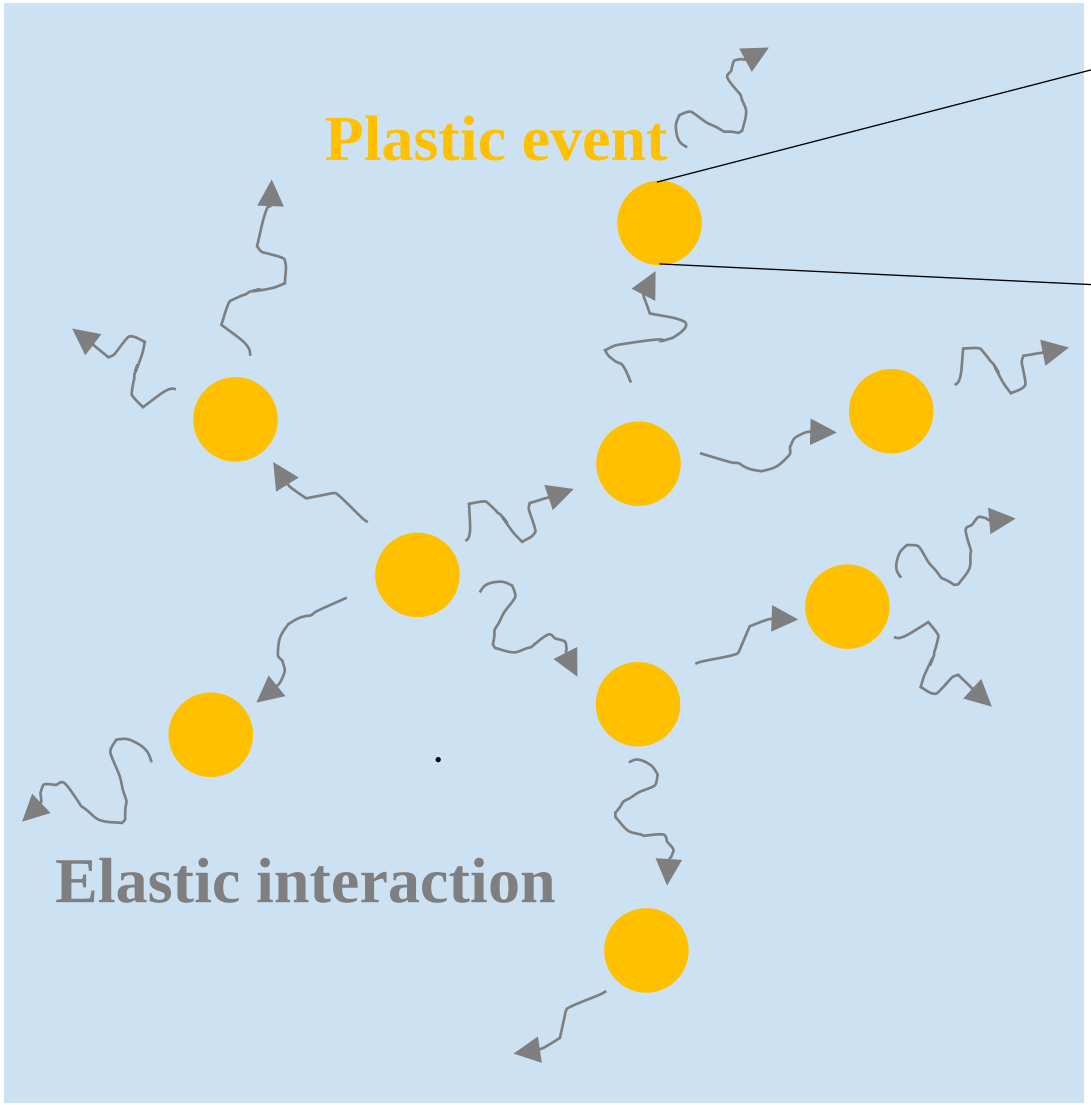
Later time stage

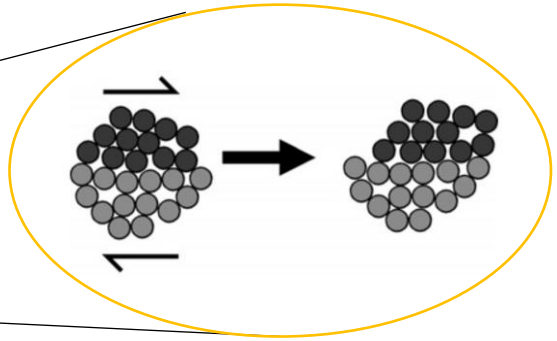


Guiselin, Scalliet, and Berthier, Nat. Phys. 2022

Scalliet, Guiselin, and Berthier, PRX. 2022

Cooperative rearranging region is too small compared with dynamical heterogeneity





Plastic events induced by
- Thermal fluctuation
- Elastic interaction

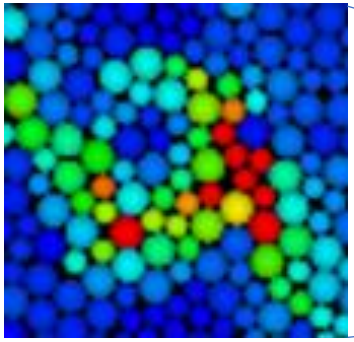
Chacko, Landes, Biroli, Dauchot, Liu, and Reichman PRL 2021

Lerbinger, Barbot, Vandembroucq, and Patinet, PRL 2022

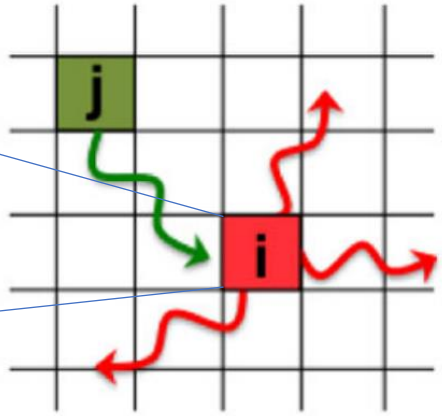
Cascade of events: Facilitation

Chandler and Garrahan, Annu. Rev. Phys. Chem. 2010

Molecular simulation



Elastoplastic model



Bocquet, Colin, Ajdari, PRL 2009

Many variations

Nicolas, Ferrero, Martens, and Barrat, RMP 2018

Bulatov and Argon, Mod. Sim. 1994

Baret, Vandembroucq, and Roux, PRL 2002

Onuki, PRE 2003

Jagla, PRE 2007

Lin, Lerner, Rosso, and Wyart PNAS 2014

1) Local dynamics condition for local stress σ_i

i) $\sigma_i \leq \sigma^{\mathrm{th}}$: Elastic (immobile)

ii) $\sigma_i > \sigma^{\mathrm{th}}$: Plastic (mobile) with a stress drop $\sigma_i \rightarrow \sigma_i - \delta\sigma_i$

iii) Thermal fluctuation: Elastic → Plastic with probability $e^{-E(\sigma_i)/T}$

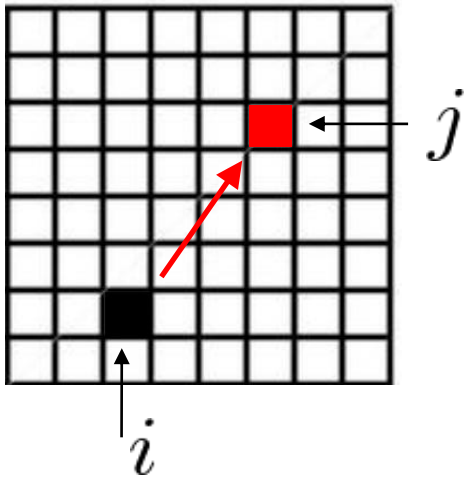
Ferrero, Martens, and Barrat, PRL 2014

Popovic, de Geus, Ji, and Wyart, PRE 2021

Lerbinger, Barbot, Vandembroucq, and Patinet, PRL 2022

$$E(\sigma_i) = (\sigma^{\mathrm{th}} - \sigma_i)^{3/2}$$

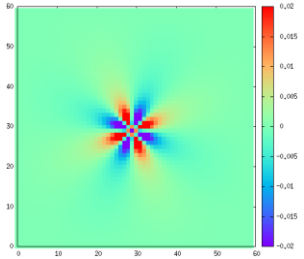
2) Elastic interaction



$$\sigma_j \rightarrow \sigma_j + g(\mathbf{r}_{ij})\delta\sigma_i$$

$$g(\mathbf{r}_{ij}) = \frac{\cos(4\theta)}{r_{ij}^2}$$

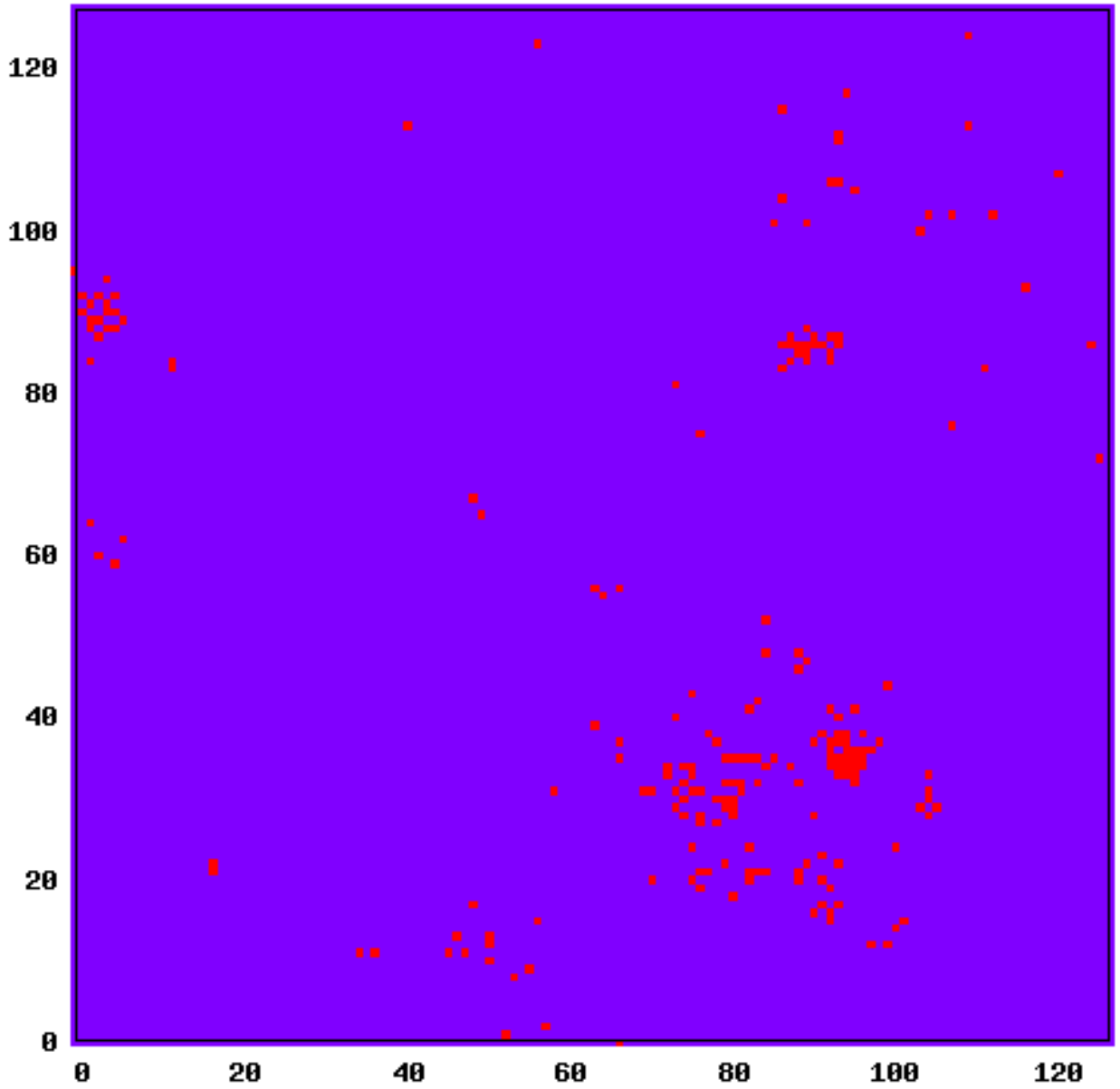
Random rotation of Eshelby kernel



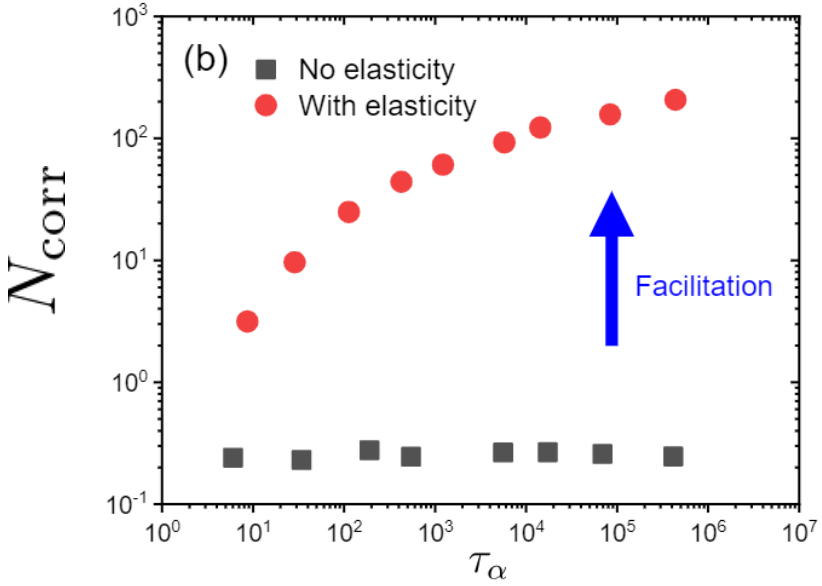
Picard, Ajdari, Lequeux, and Bocquet, EPJE 2004

3) Repeat 1) - 2)

Movie

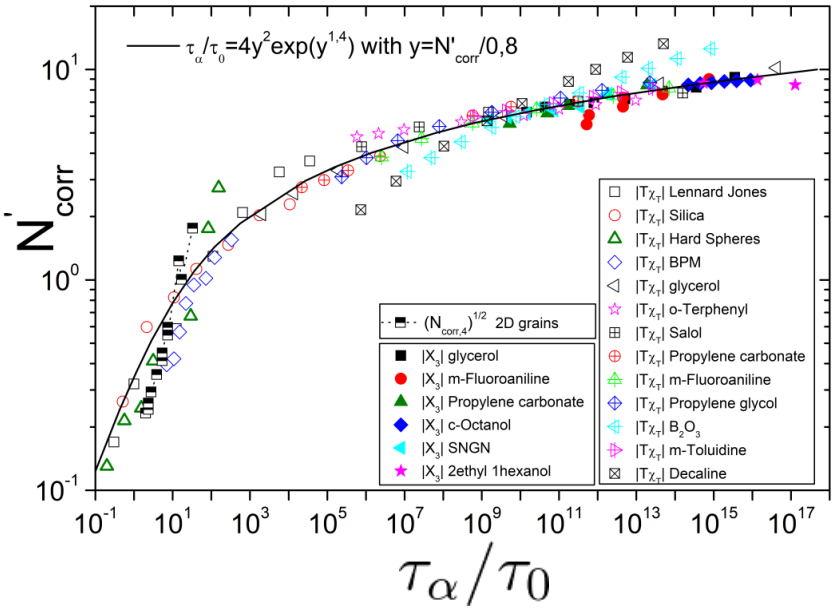


Elastoplastic model



Elasticity-induced facilitation

Experiments



Dalle-Ferrier, Thibierege, Alba-Simionesco, Berthier, Biroli, Bouchaud, Ladieu, L'Hote, and Tarjus, PRE 2007

Dauchot, Ladieu, and Royall, arXiv 2022

N_{corr} : Size of dynamically correlated region

Mean-field theory

Hébraud and Lequeux, PRL 1998

Agoritsas, Bertin, Martens, and Barrat, EPJE 2015

$$\frac{\partial P(\sigma,t)}{\partial t} = \alpha\Gamma(t)\frac{\partial^2 P(\sigma,t)}{\partial \sigma^2} - \nu(\sigma,\sigma_c)P(\sigma,t) + \Gamma(t)y(\sigma)$$

Magnitude of elastic interaction

$$\alpha = \frac{1}{2}\sum_{j\neq i}\left(g(\mathbf{r}_{ij})\delta\sigma_j\right)^2$$

Bocquet, Colin, Ajdari, PRL 2009

$$\tau_\alpha \simeq \Gamma^{-1} \simeq \tau_0 e^{\frac{E}{T}}$$