Creep simulations with periodic boundary conditions using LAMMPS

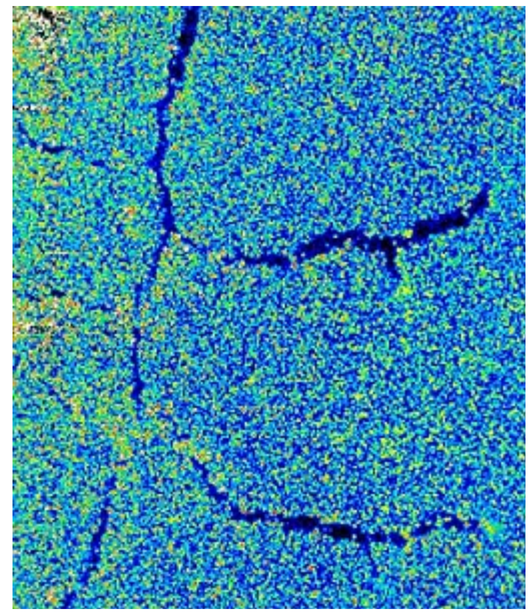
Raffaela Cabriolu, Jürgen Horbach, Pinaki Chaudhuri,
Kirsten Martens
LIPhy

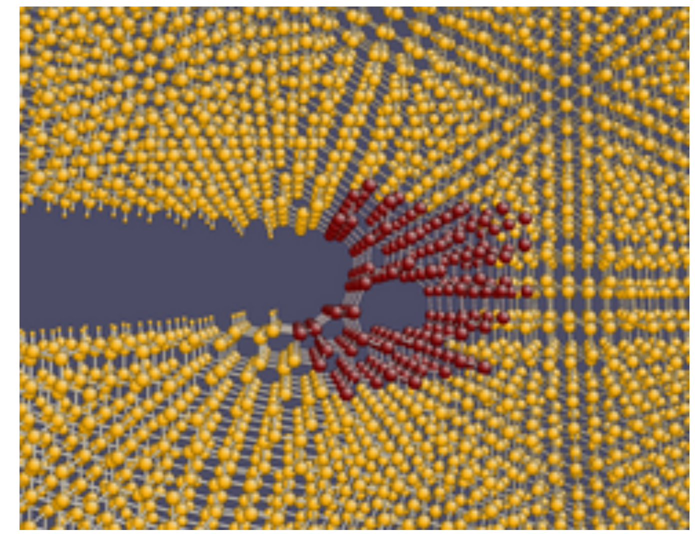
LAMMPS for molecular dynamics simulations : from development to applications

Lyon, June 26, 2018

Failure in soft materials under load

12th conference on sinkholes **Cracks in cornstarch, L2C** **Crack at atomistic level,**





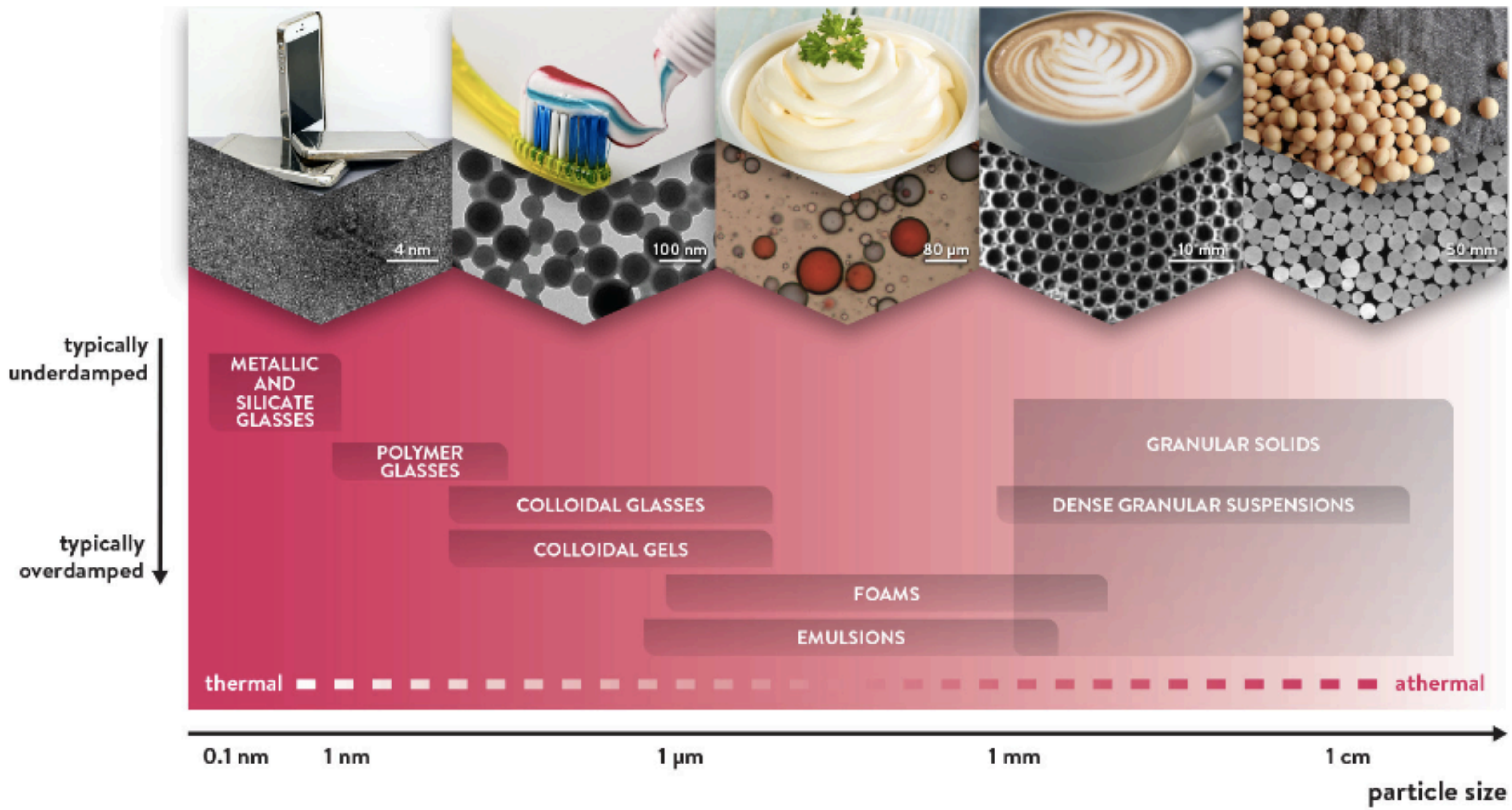
G. Csányi, U. Cambridge

Why? How?

Prediction possible?

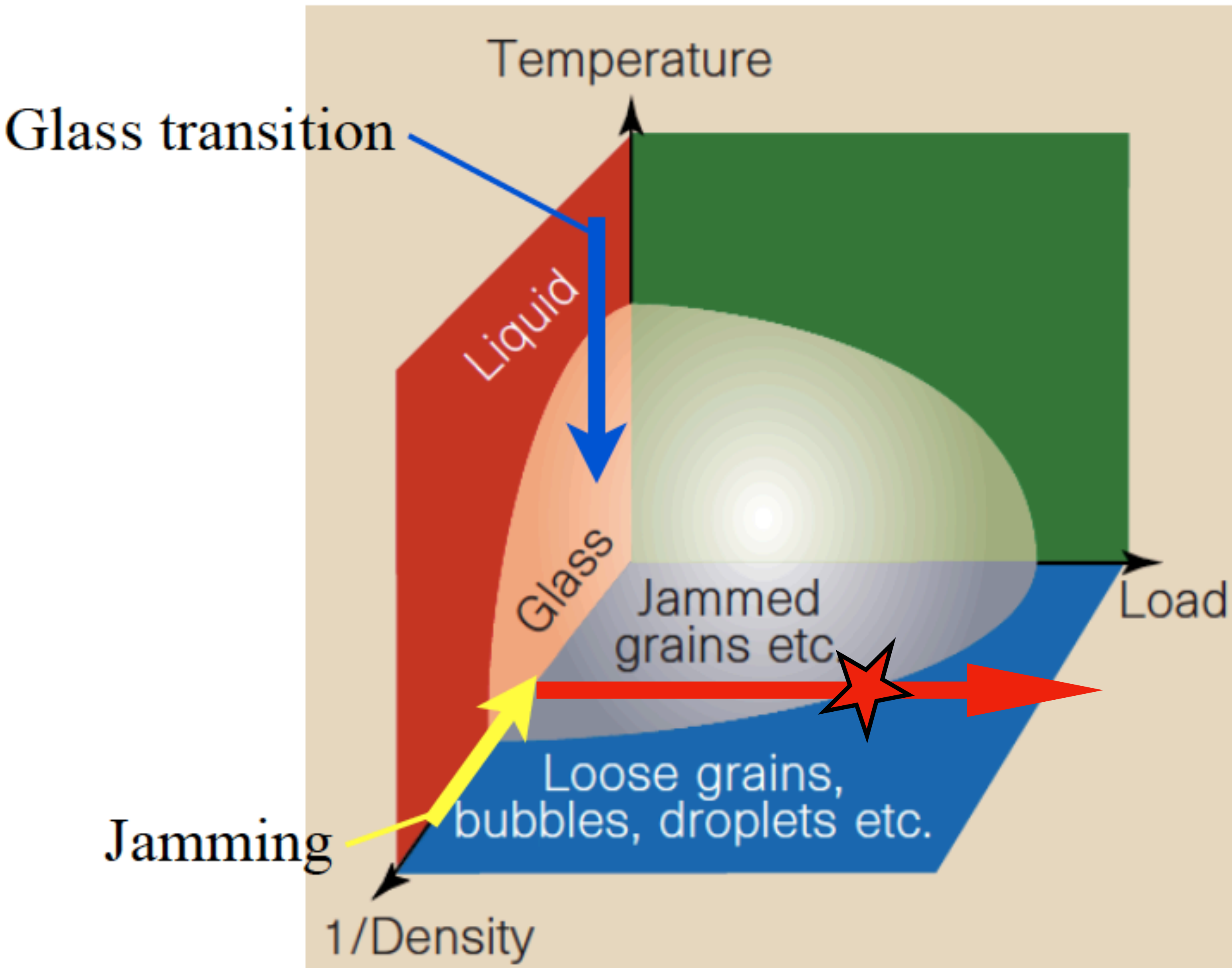
ANR - project FAPRES

Examples of glassy material



Nicolas, Ferrero, KM & Barrat, Rev. Mod. Phys. (2018)

Simplified sketch



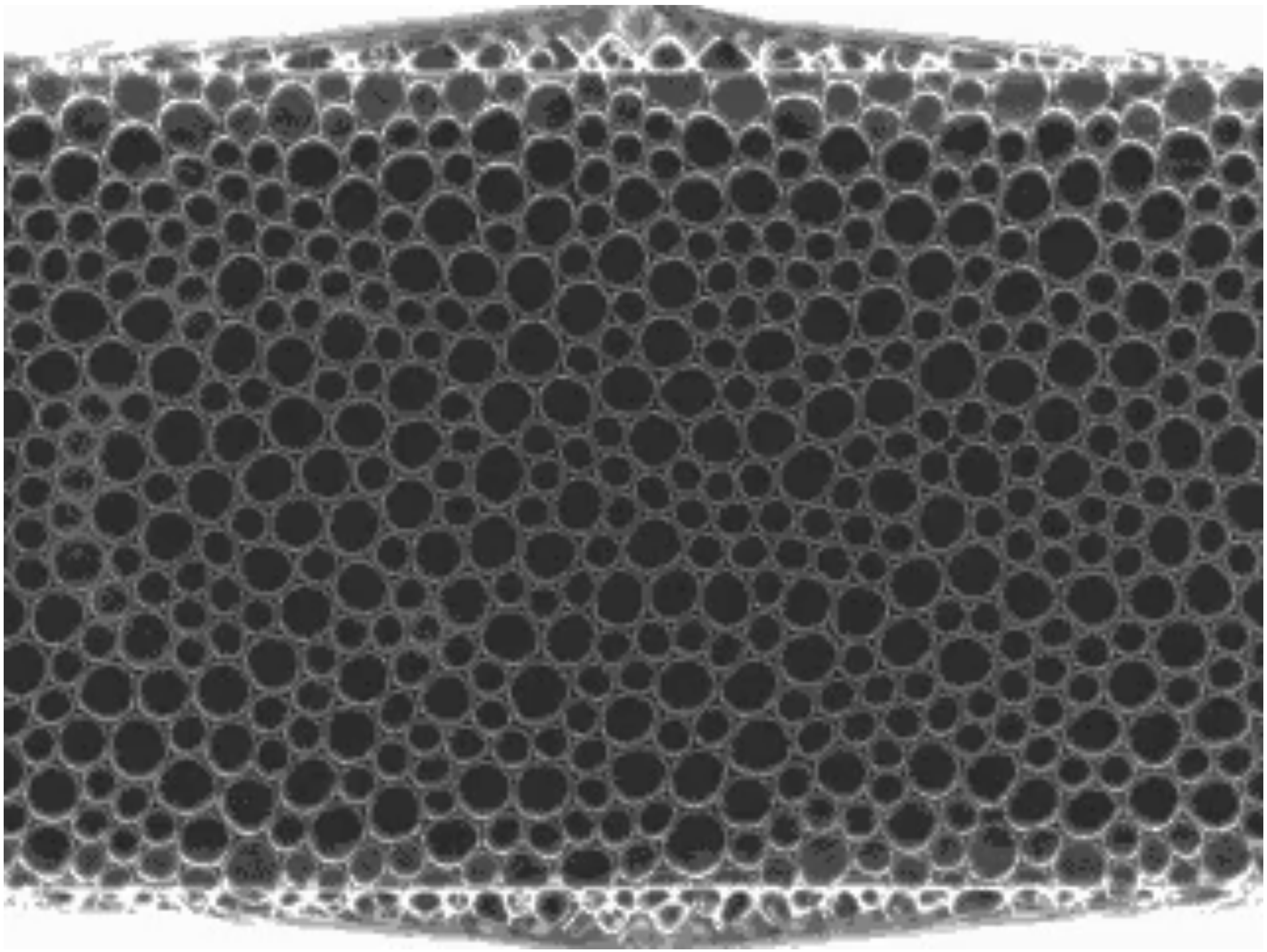
A.J.Liu & S.R.Nagel, 1998

Yielding transition

Elastic, plastic and viscous properties

Elasto-plastic dynamics

homepage: G. Katgert, & M. van Hecke



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Localized plastic events:
Ali Argon (1979)

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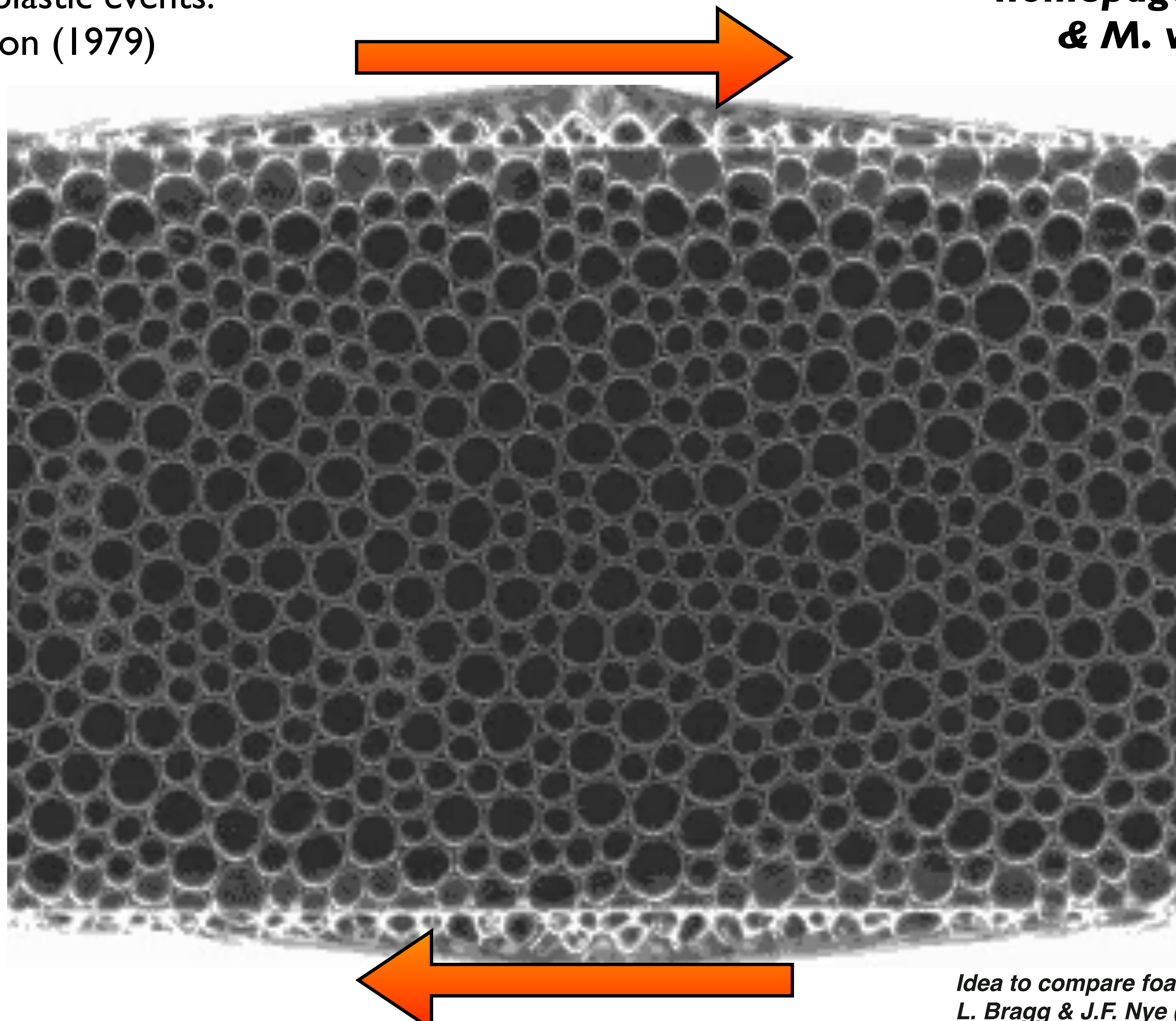

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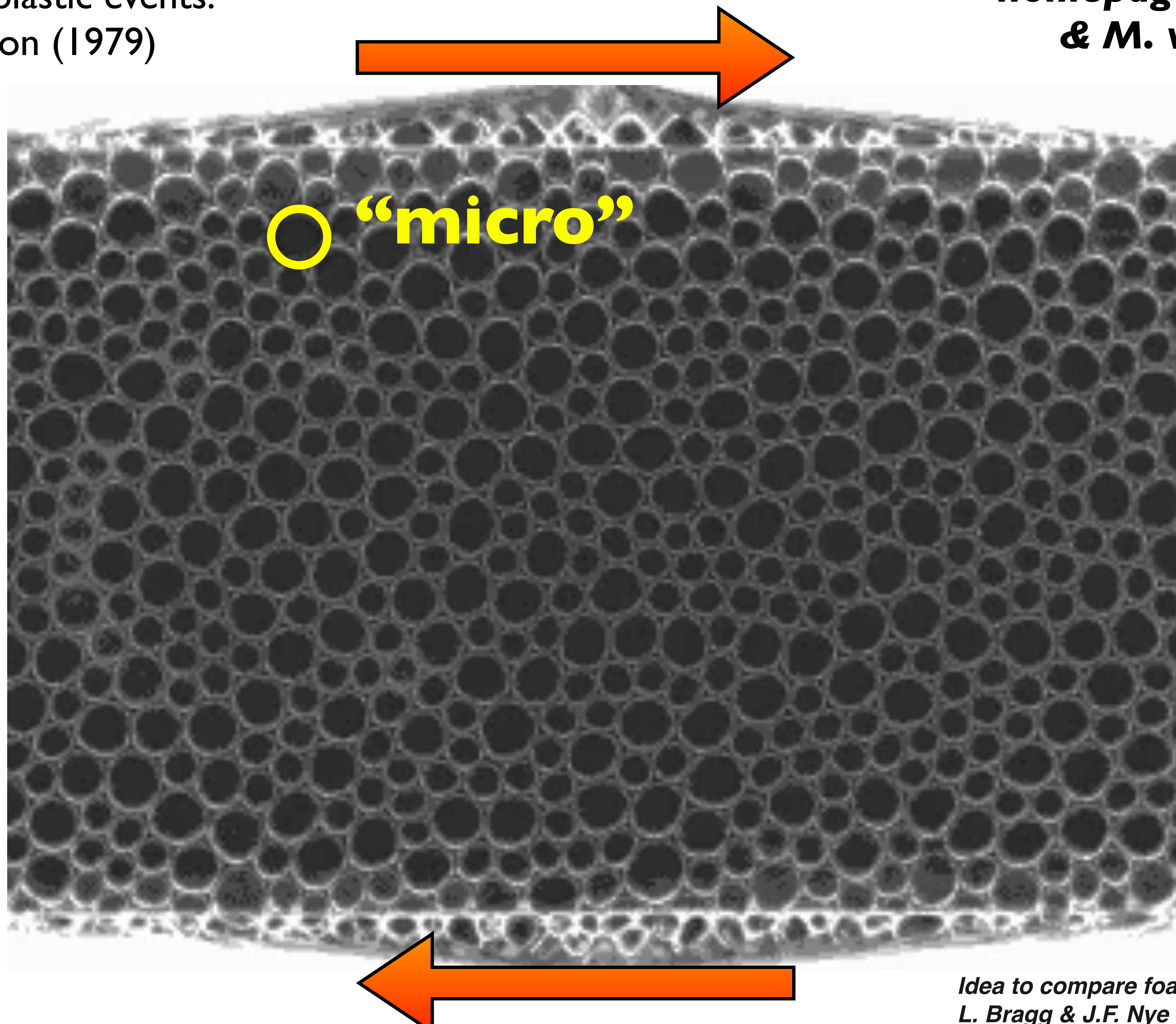

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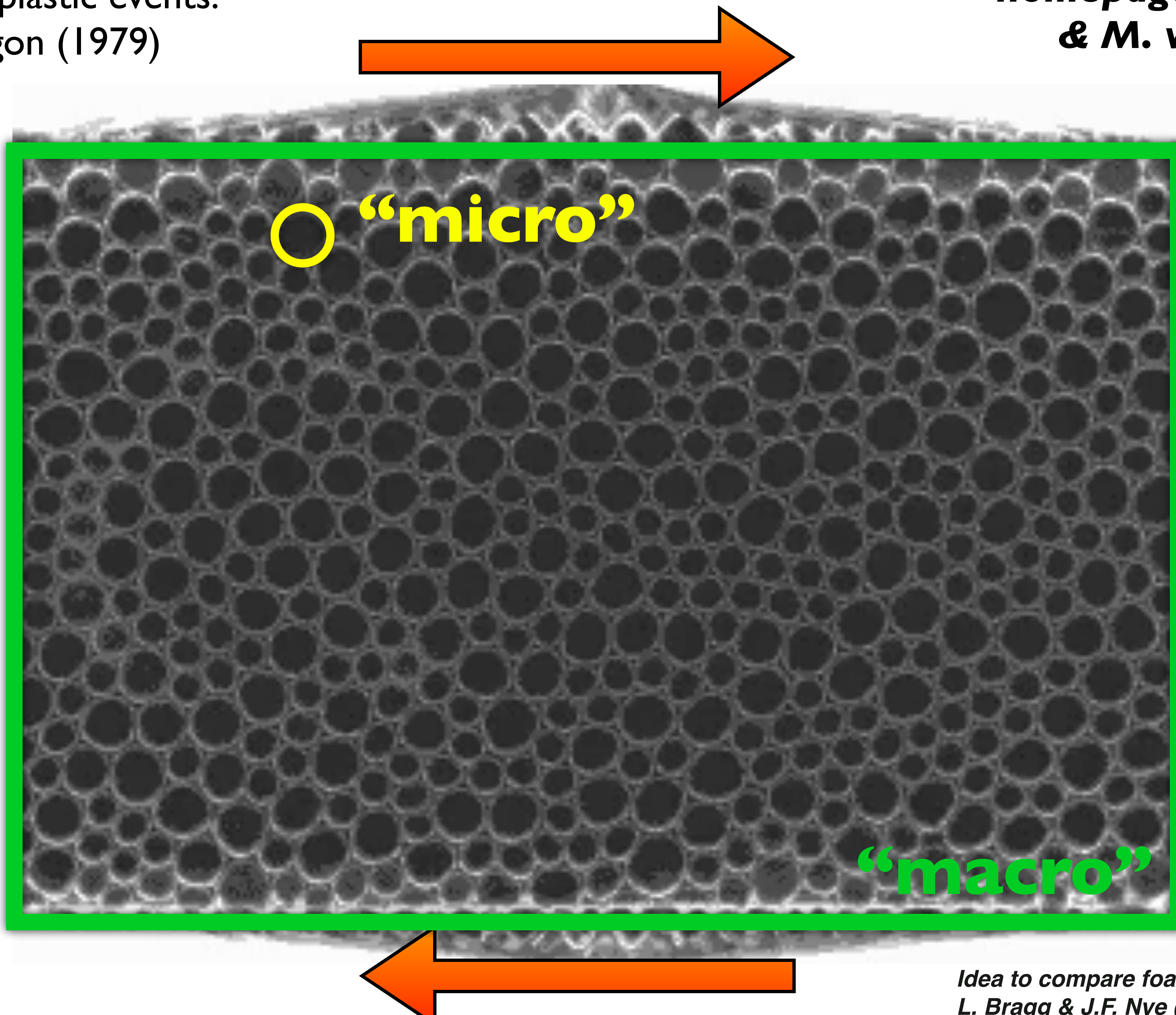

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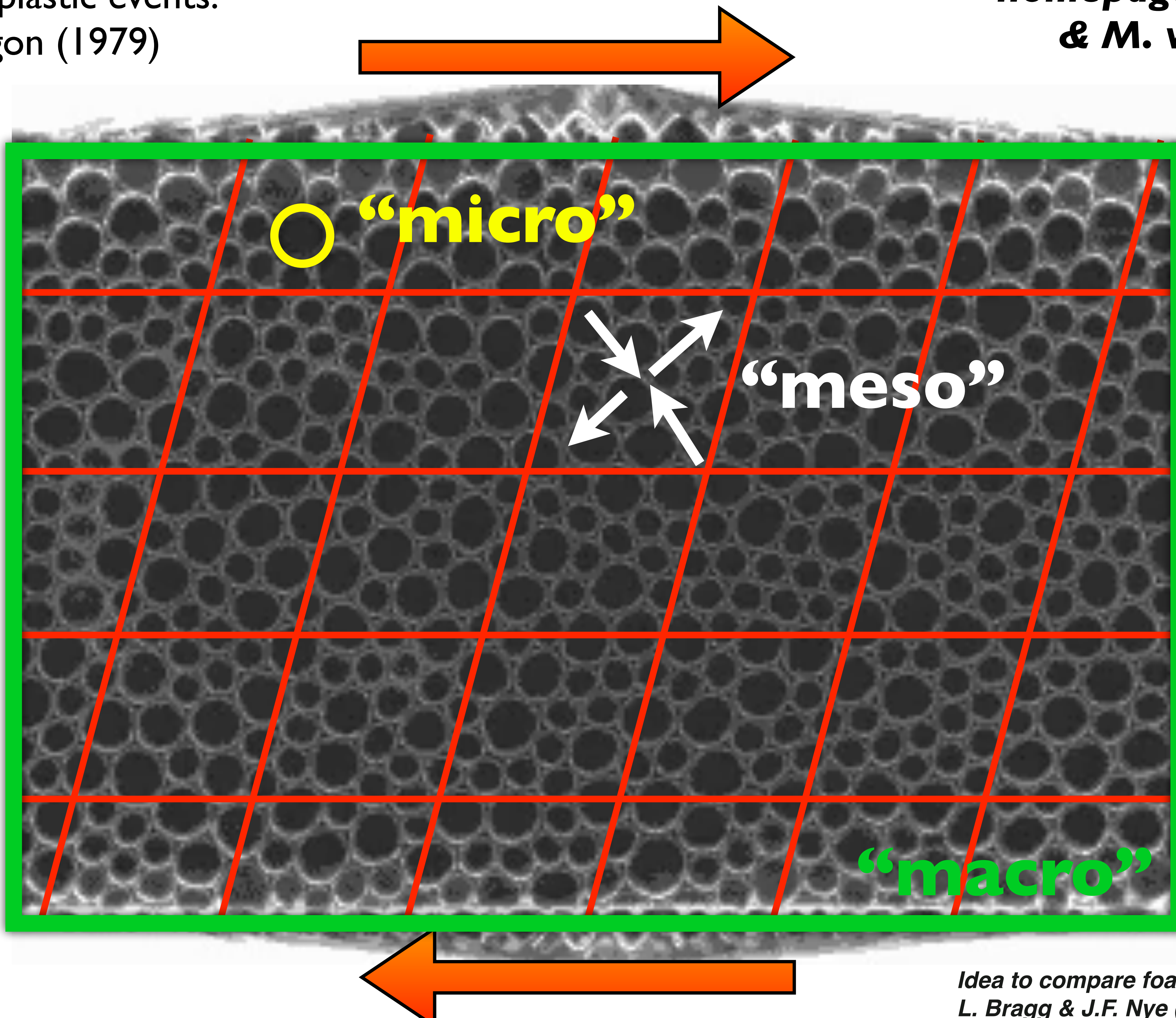

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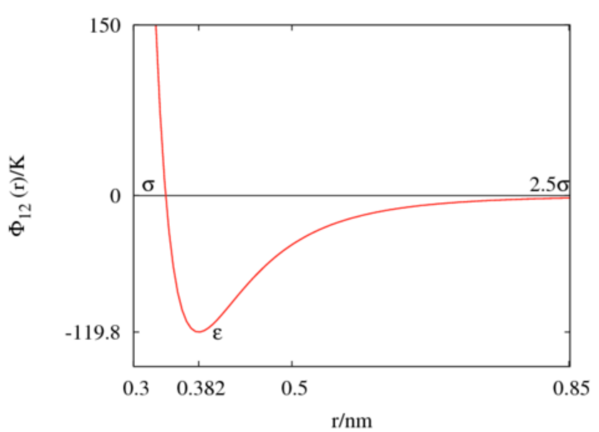
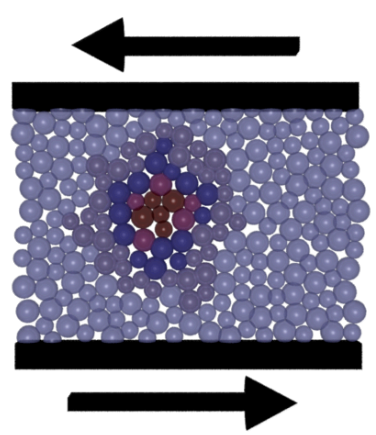
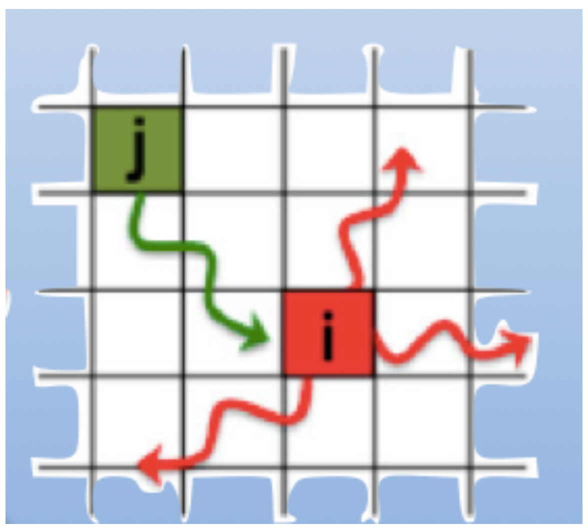
The different scales

Micro	Meso	Macro
Particle simulations:	**Lattice models:**	**Mean-field considerations:**
Bidisperse Lennard-Jones (Kob-Andersen model)	Simplistic model for the critical dynamics (similar to Ising model)	Neglect correlations and write single site dynamics that are hopefully analytically solvable



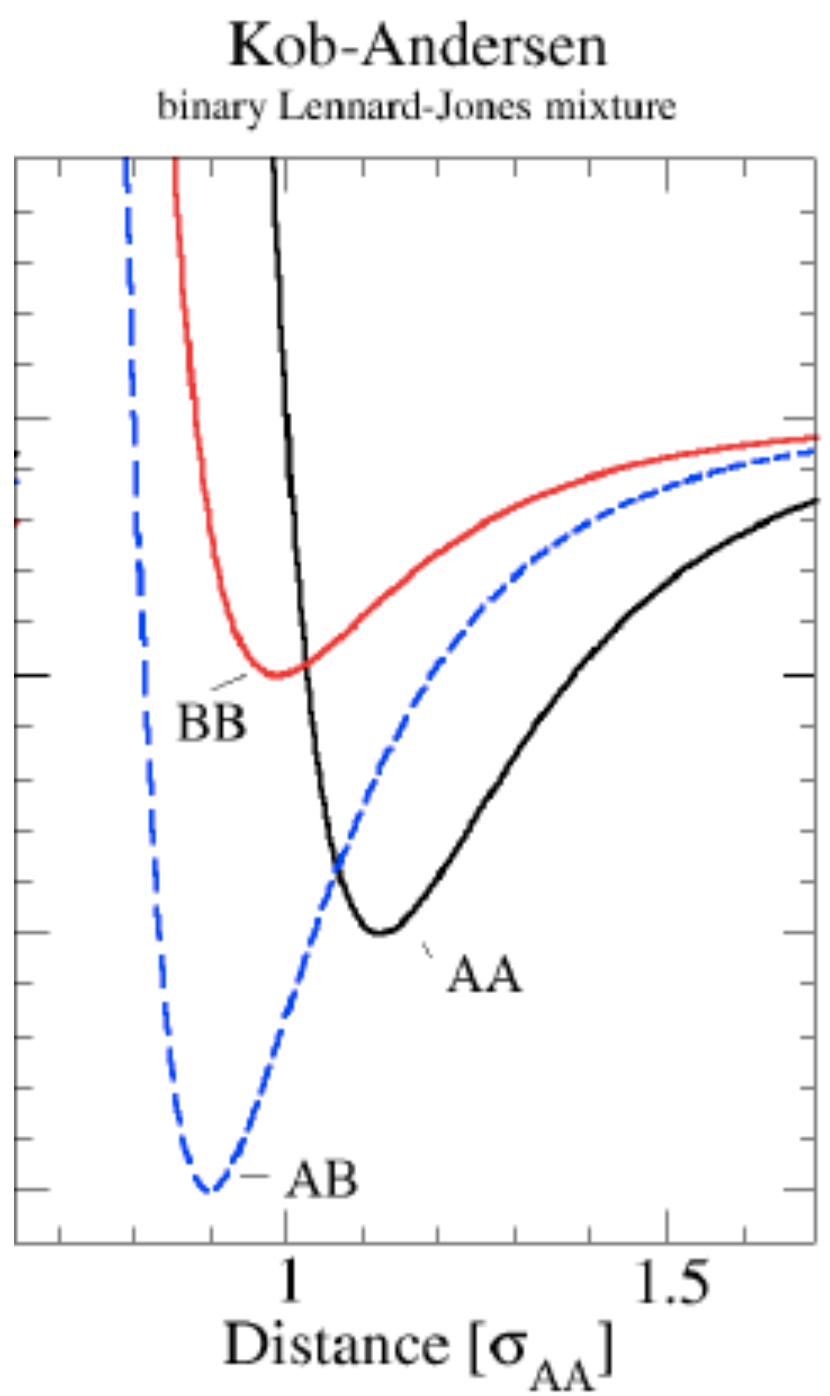




$$\partial_t P(\sigma_{xy}, t) = ?$$

Typical MD simulations

Potential

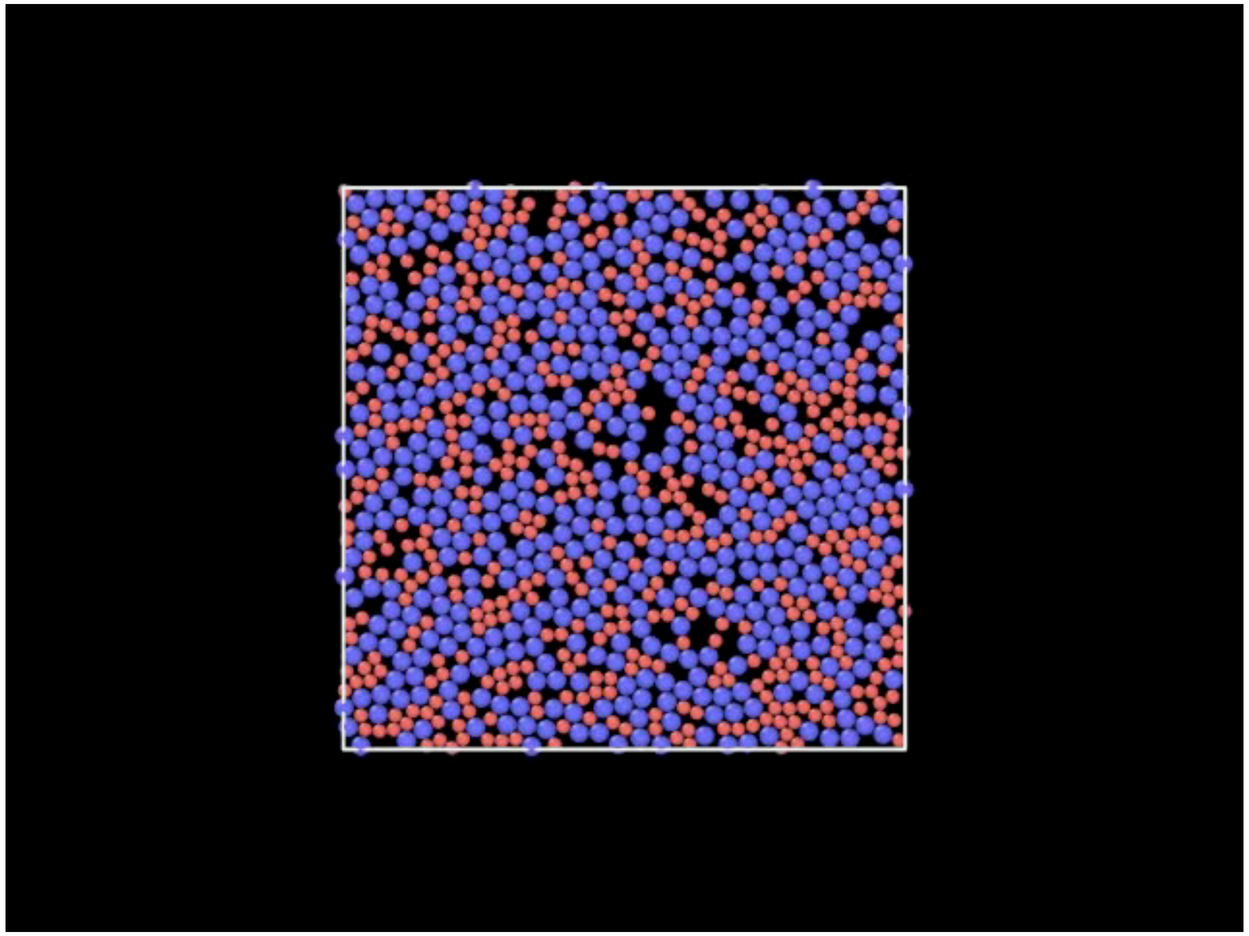


Langevin dynamics (friction with solvent):

$$\mathbf{F} = m\mathbf{a} = -\nabla V(\mathbf{r}) - \gamma m \mathbf{v} + \sqrt{2\gamma m k_b T}\mathbf{R}(t)$$

+ periodic boundary conditions

+ shear (e.g. by tilting the simulation box)



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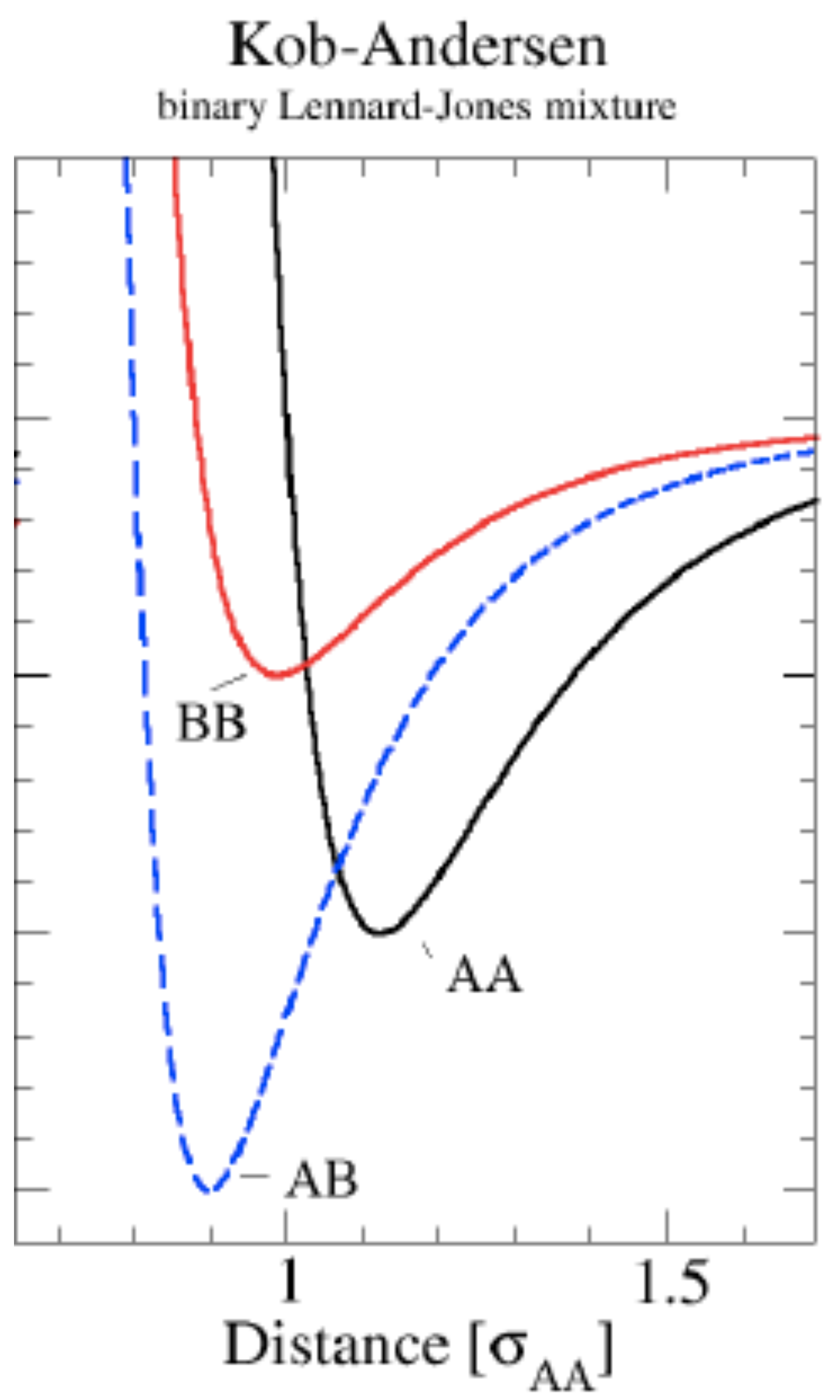

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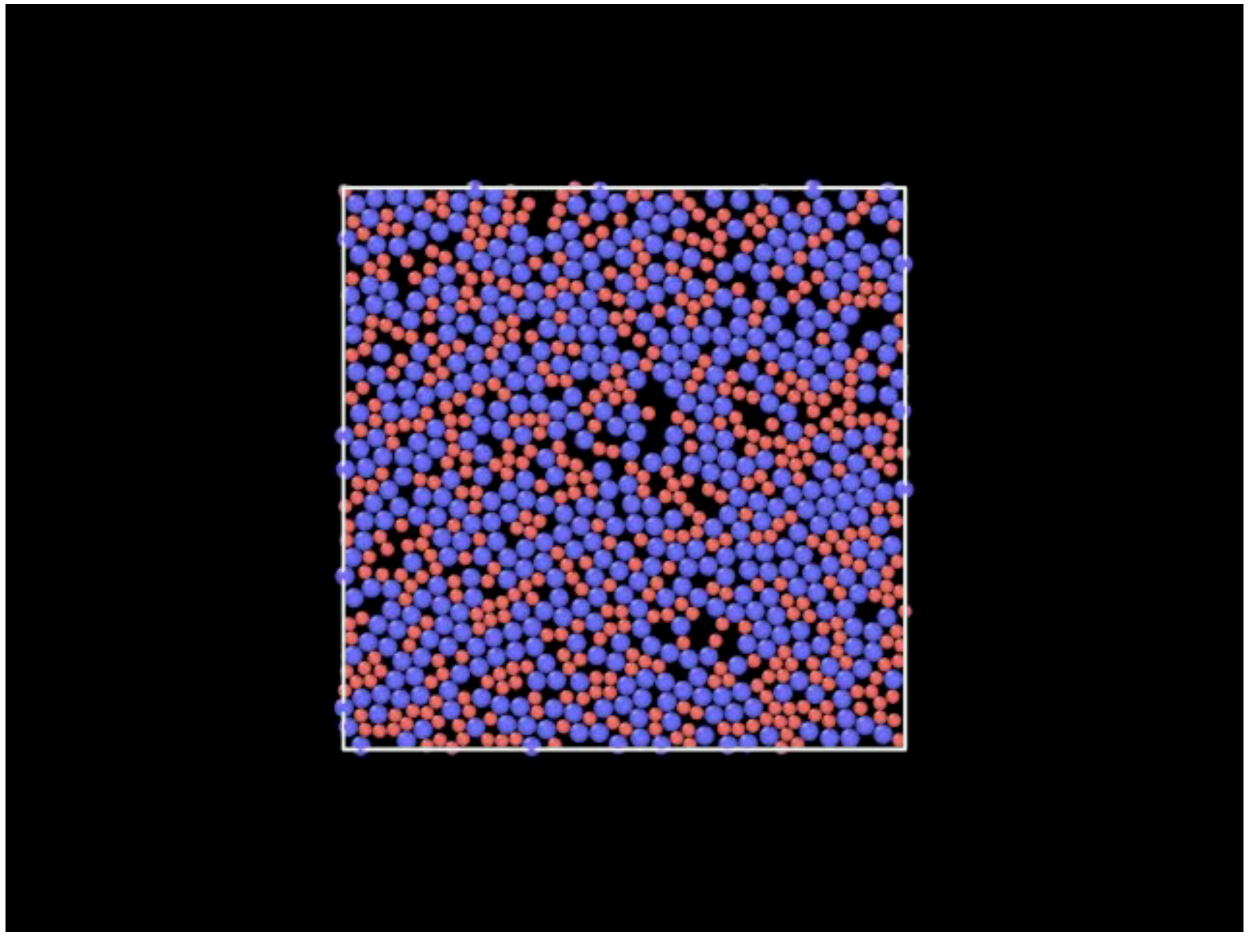
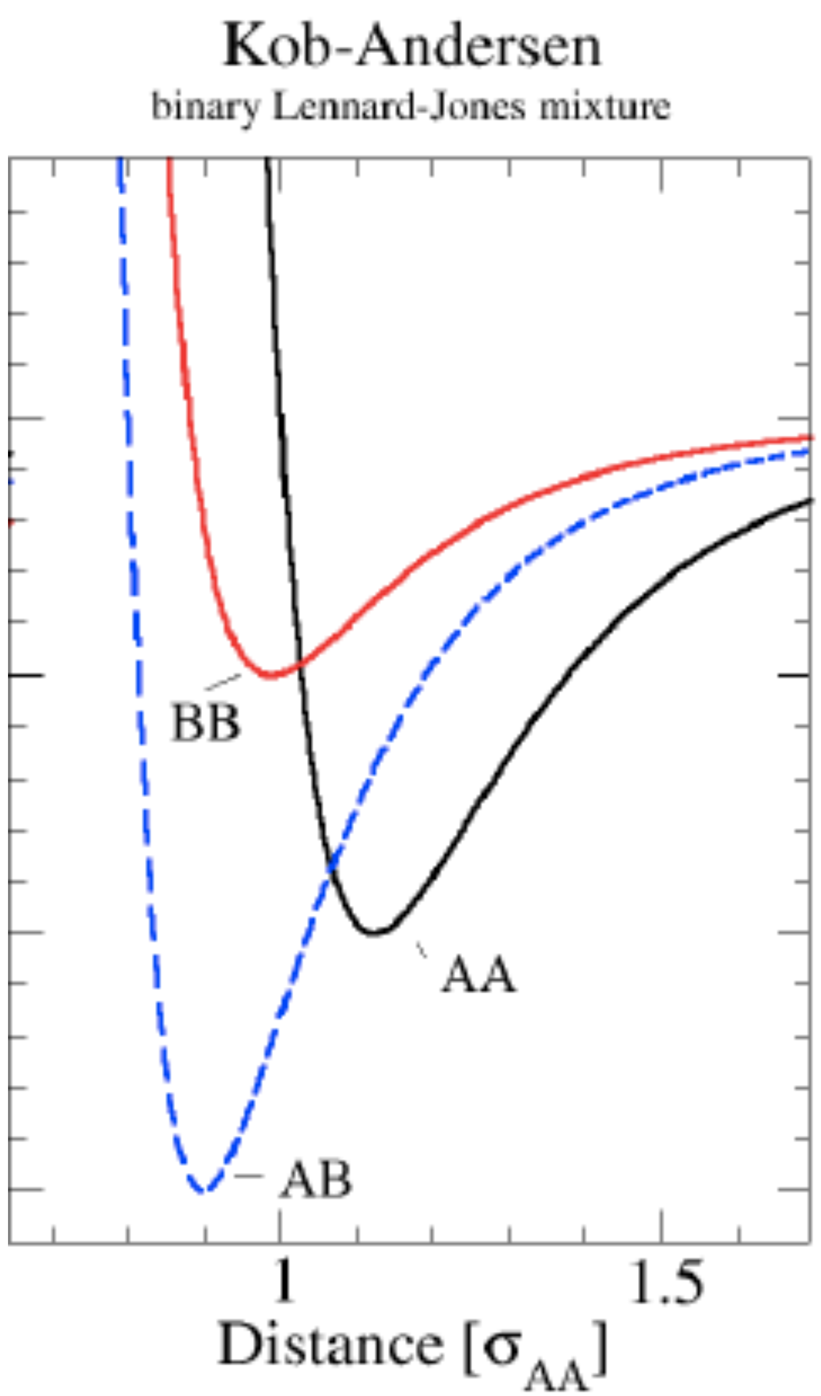
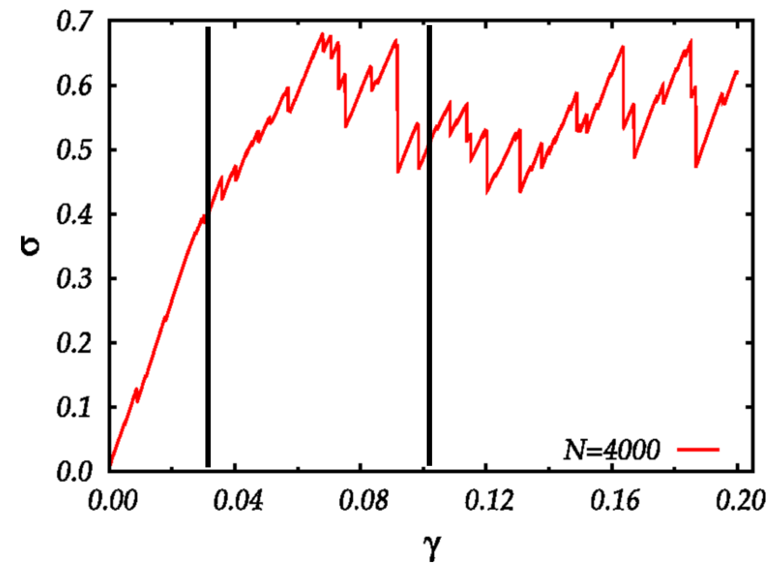


Macroscopic response

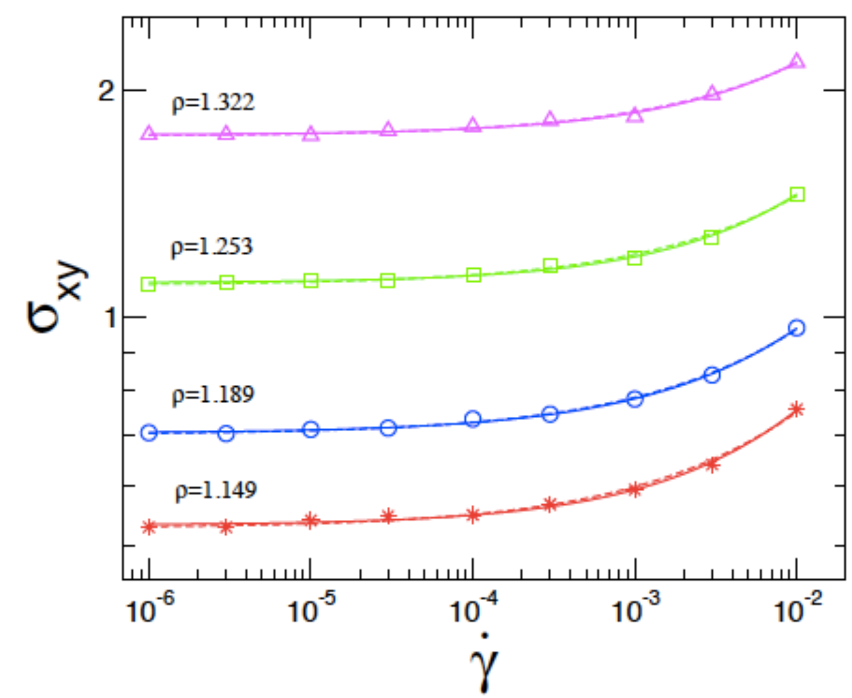
Potential



Stress-strain curve



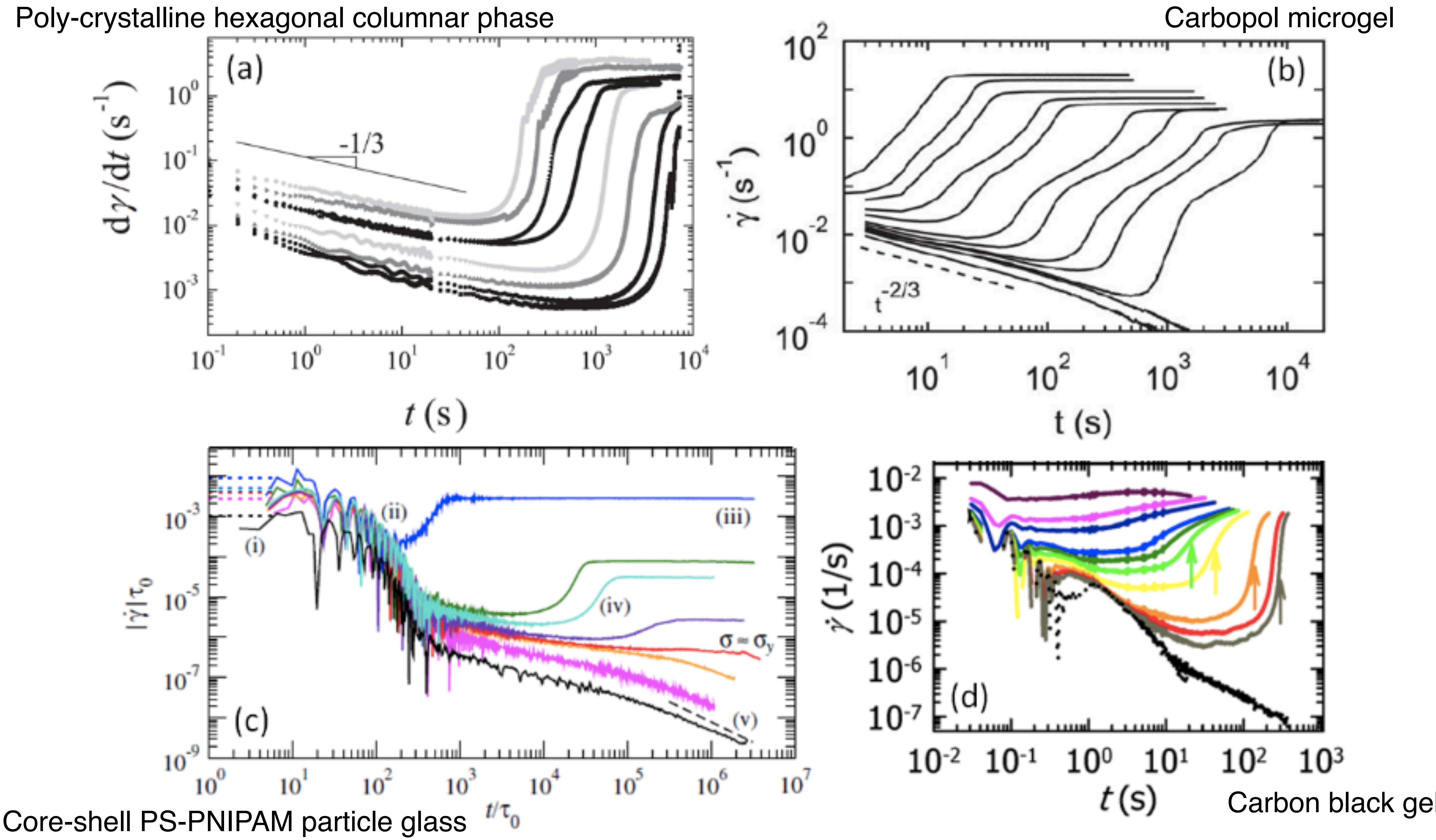
Steady state flow curve



Puosi, Olivier, KM, Soft Matter (2015)

Creep dynamics

Strain rate response to a sudden applied external stress



Bonn et al. Rev. Mod. Phys. 2017

Model details

Three dimensional glass-forming 50:50 colloidal binary mixture:

$$U_{1,2}(r) = \varepsilon_{1,2} d_{1,2} \frac{exp(-k_{1,2}(r-d_{1,2}))}{r} \quad 1,2 \in \{a,b\} \qquad \text{(Yukawa)}$$

DPD equations of motion:

$$\dot{\mathbf{r}}_i = \frac{\mathbf{p}_i}{m_i}; \qquad \dot{\mathbf{p}}_i = \sum_{j(\neq i)}^{N} [\mathbf{F}_{i,j} + \mathbf{F}^D_{i,j} + \mathbf{F}^R_{i,j}] \, ,$$

$$\mathbf{F}_{i,j} = -\nabla(U_{i,j}) \quad \text{(Particle interactions)}$$

$$\mathbf{F}^D_{i,j} = -\xi w^2(r_{i,j})(\hat{\mathbf{r}}_{i,j} \cdot \mathbf{v}_{i,j})\hat{\mathbf{r}}_{i,j} \quad \text{(DPD term for dissipation)}$$

$$\mathbf{F}^R_{i,j} = \sqrt{2k_B T \xi} w(r_{i,j}) \theta_{ij} \hat{\mathbf{r}}_{i,j} \quad \text{(Random force obeying FDR)}$$

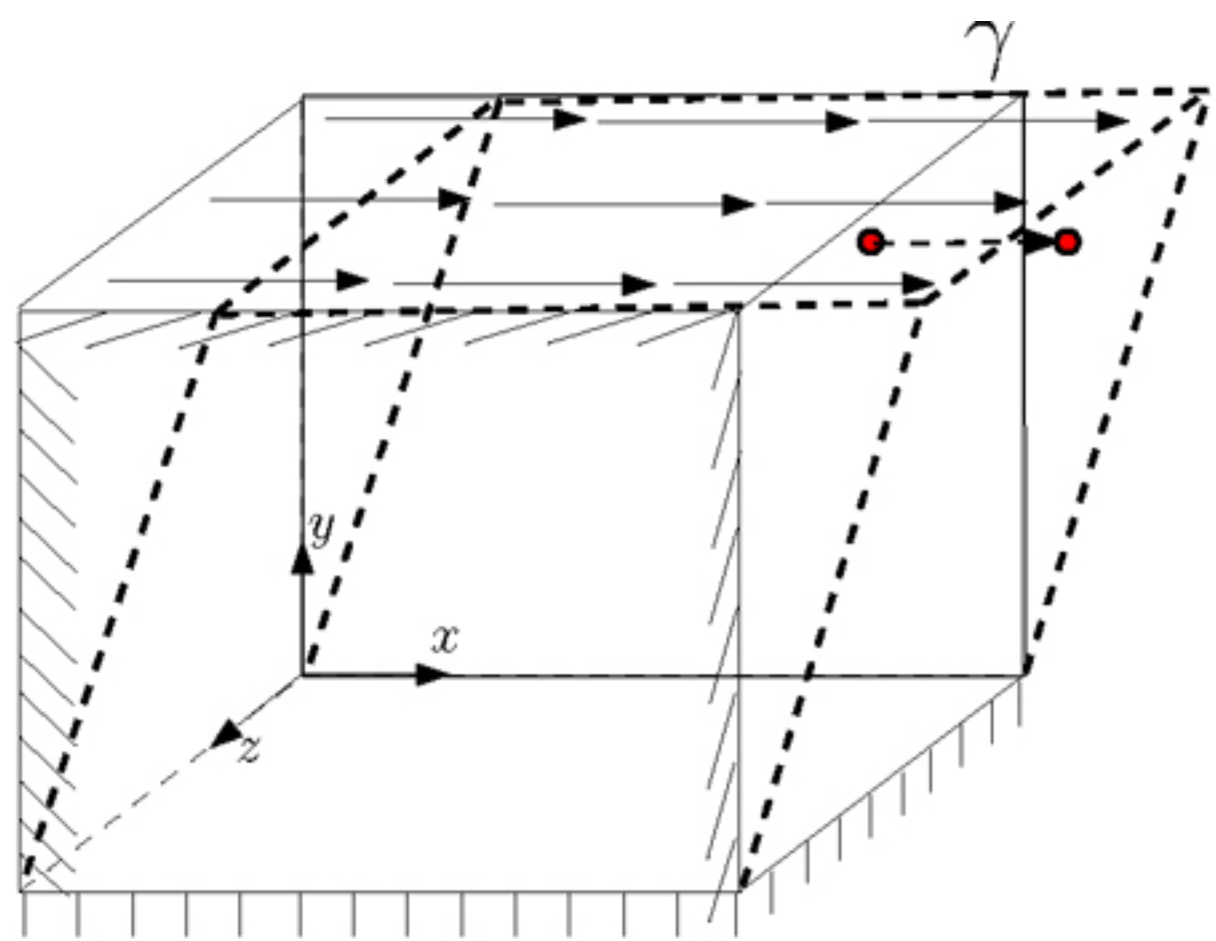
Large density and low temperature (glassy regime):

$$\phi > \phi_J \quad T < T_g$$

Model details

Big question: How to implement correctly the bulk creep dynamics?

Impose a constant shear loading at fixed volume?



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Impose shear stress through walls:
(Horbach, Chaudhuri, PRE 2013)
Approach ok, but how to distinguish bulk dynamics and wall effects?

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SLLOD equation of motions:
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No: Transient dynamics is very heterogeneous (formation of transient shear bands…)

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Our proposition:

Adapt usual shear rate controlled protocol with periodic boundary conditions, using a feedback protocol (similar to experiments):

Evolution of time dependent shear rate:

$$\frac{d\dot{\gamma}(t)}{dt} = B[\sigma_0 - \sigma_{xy}(t)]$$

Target stress (σ_0) — *Bulk stress* ($\sigma_{xy}(t)$)

Cabriolu, Horbach, Chaudhuri & KM, to be published

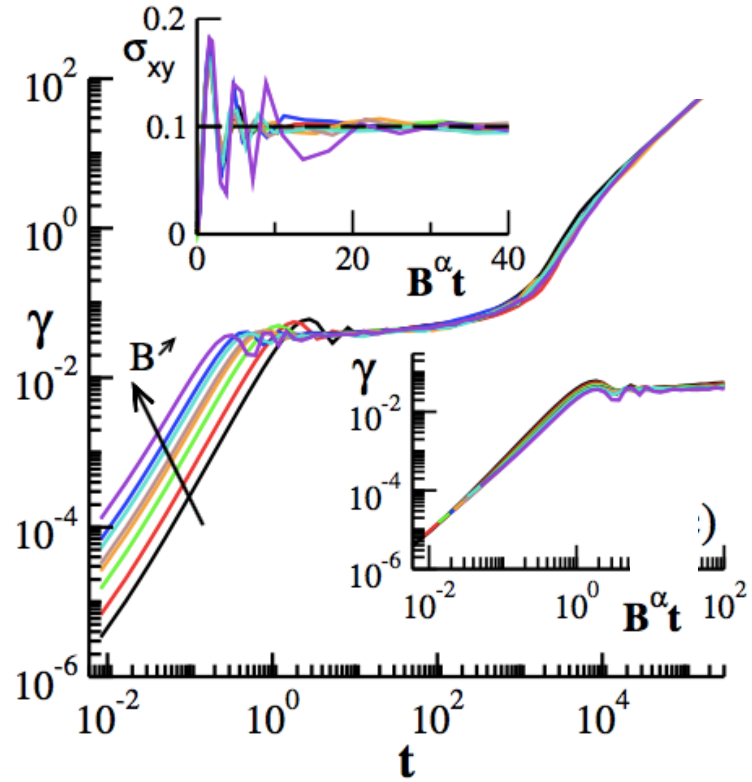
LAMMPS implementation

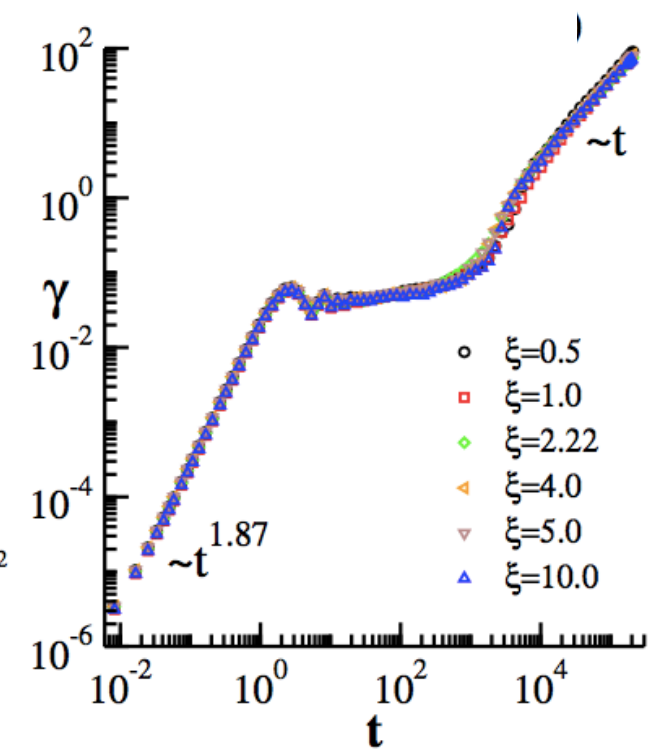
```
...

variable        sigmaxy equal -pxy
variable        sigma0 equal 0.09
variable        damp equal 1.0
variable        dt equal 0.0083
variable        Ly equal 30

change_box      all triclinic

fix             1 all nve
fix             2 all deform 1 xy variable v_deltatild v_rate remap x

variable        deltatild equal f_oldrate*${dt}+f_oldtild
variable        rate equal f_oldrate+${damp}*(${sigma0}-v_sigmaxy)*${dt}*${Ly}

fix             oldtild all ave/time 1 1 1 v_deltatild
fix             oldrate all ave/time 1 1 1 v_rate

...
```

Cabriolu, Horbach, Chaudhuri & KM, to be published

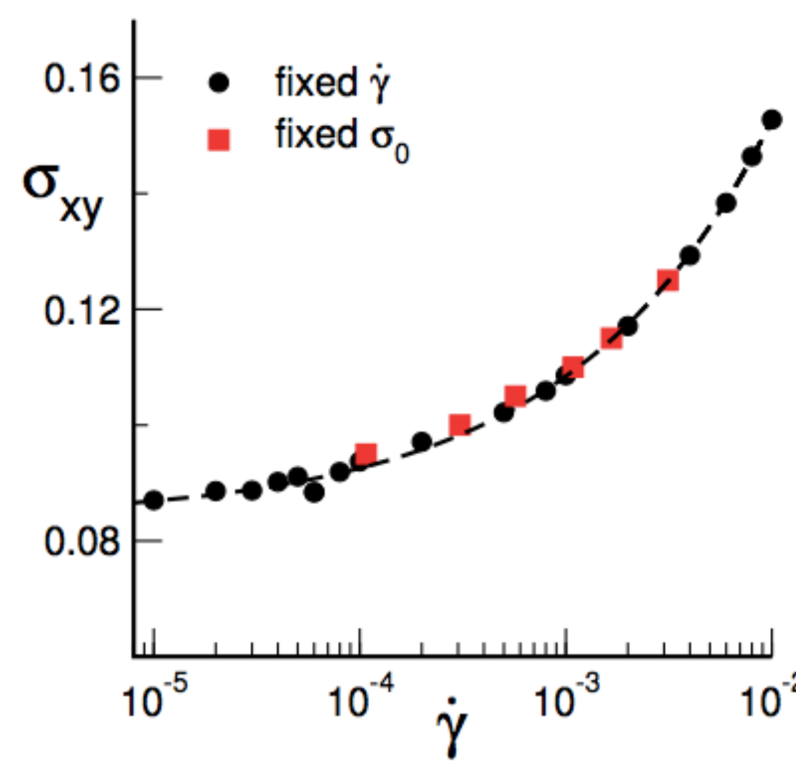
Testing the feedback protocol

1) Test robustness of the protocol:
with respect to damping factor in the feedback protocol and to viscous friction





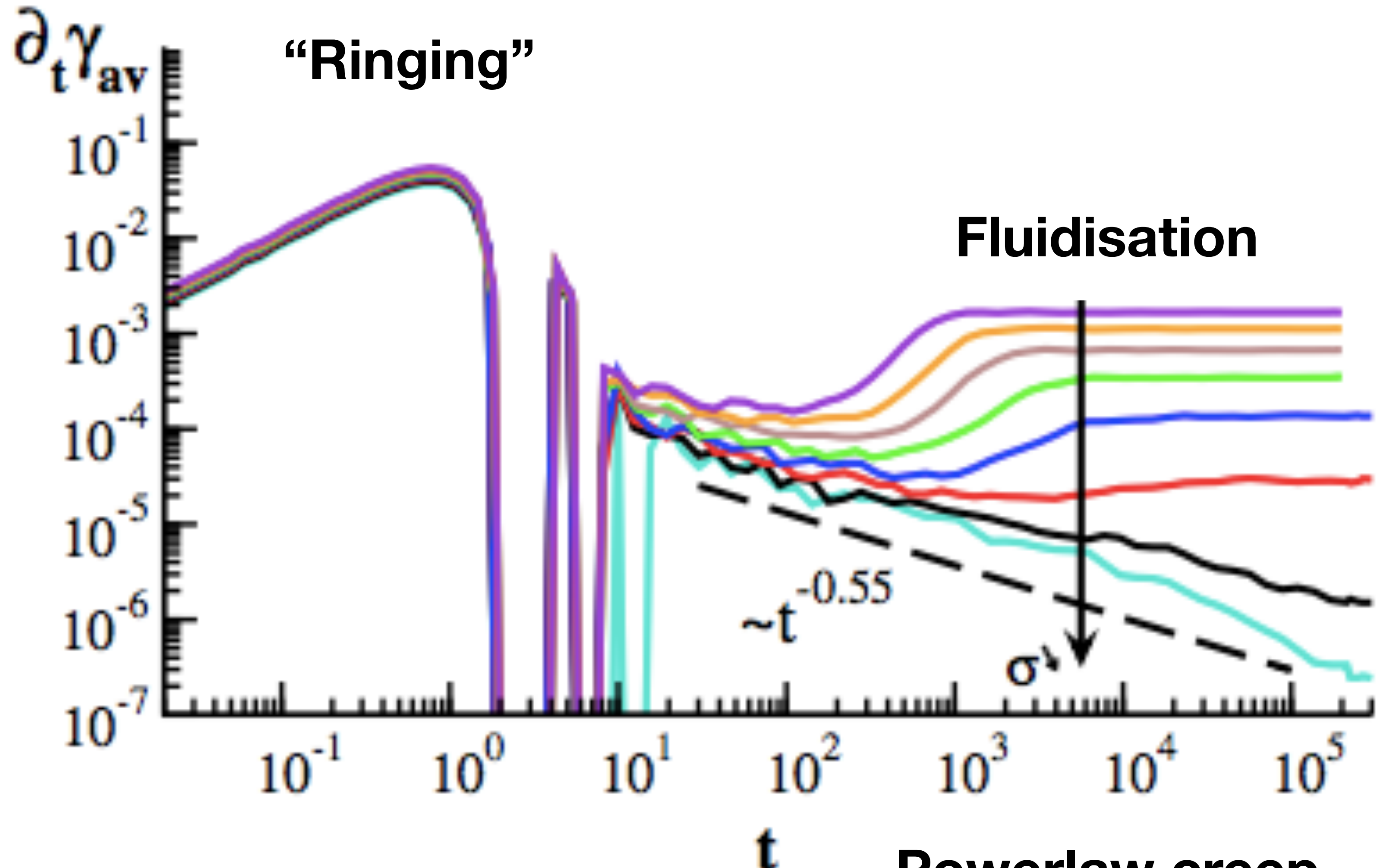
2) Compare flow-curves:
fixed shear rate vs fixed shear stress protocol



Cabriolu, Horbach, Chaudhuri & KM, to be published

Results on creep

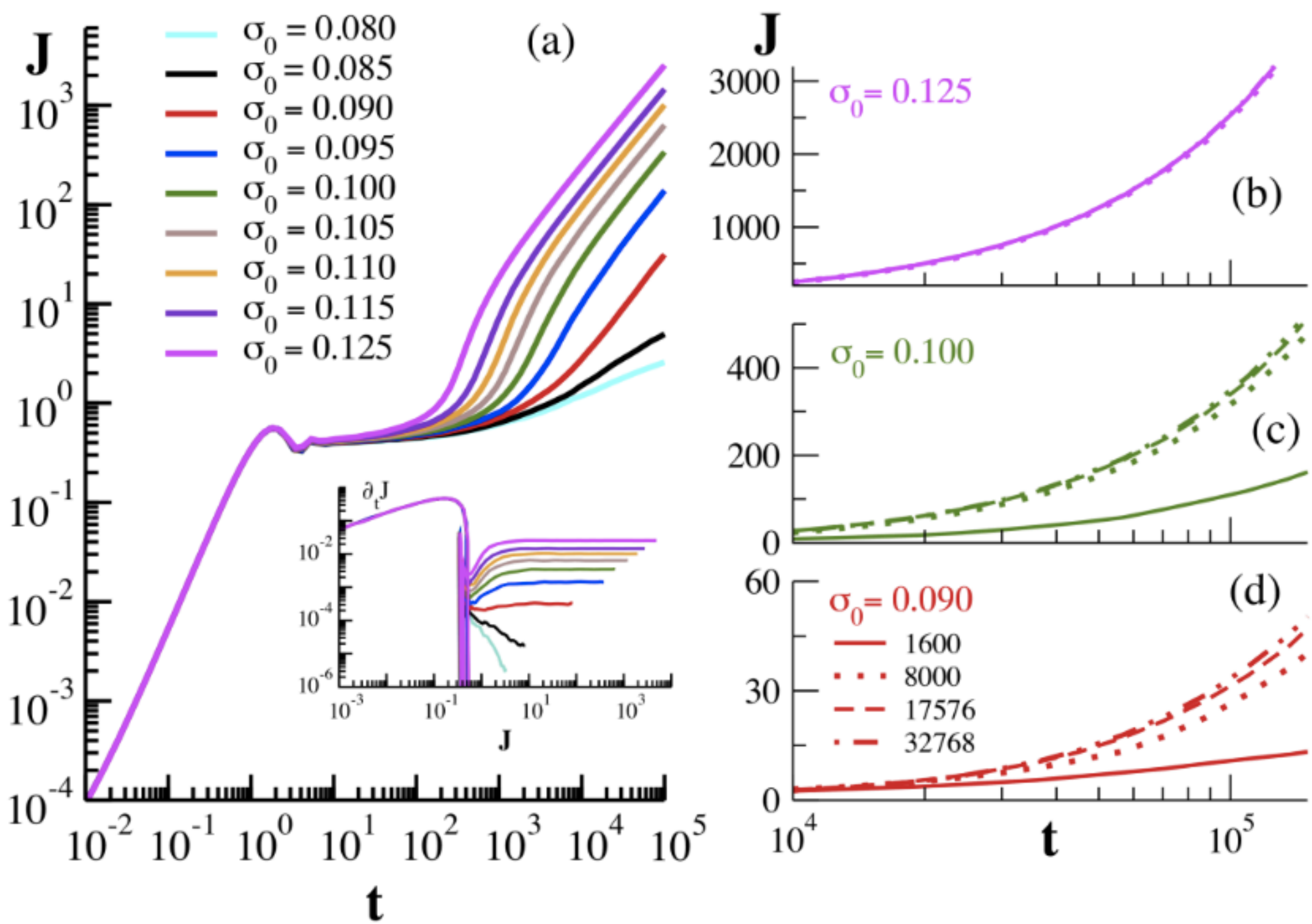
Typical creep curves (averaged over 80 samples):



Cabriolu, Horbach, Chaudhuri & KM, to be published

Results on creep

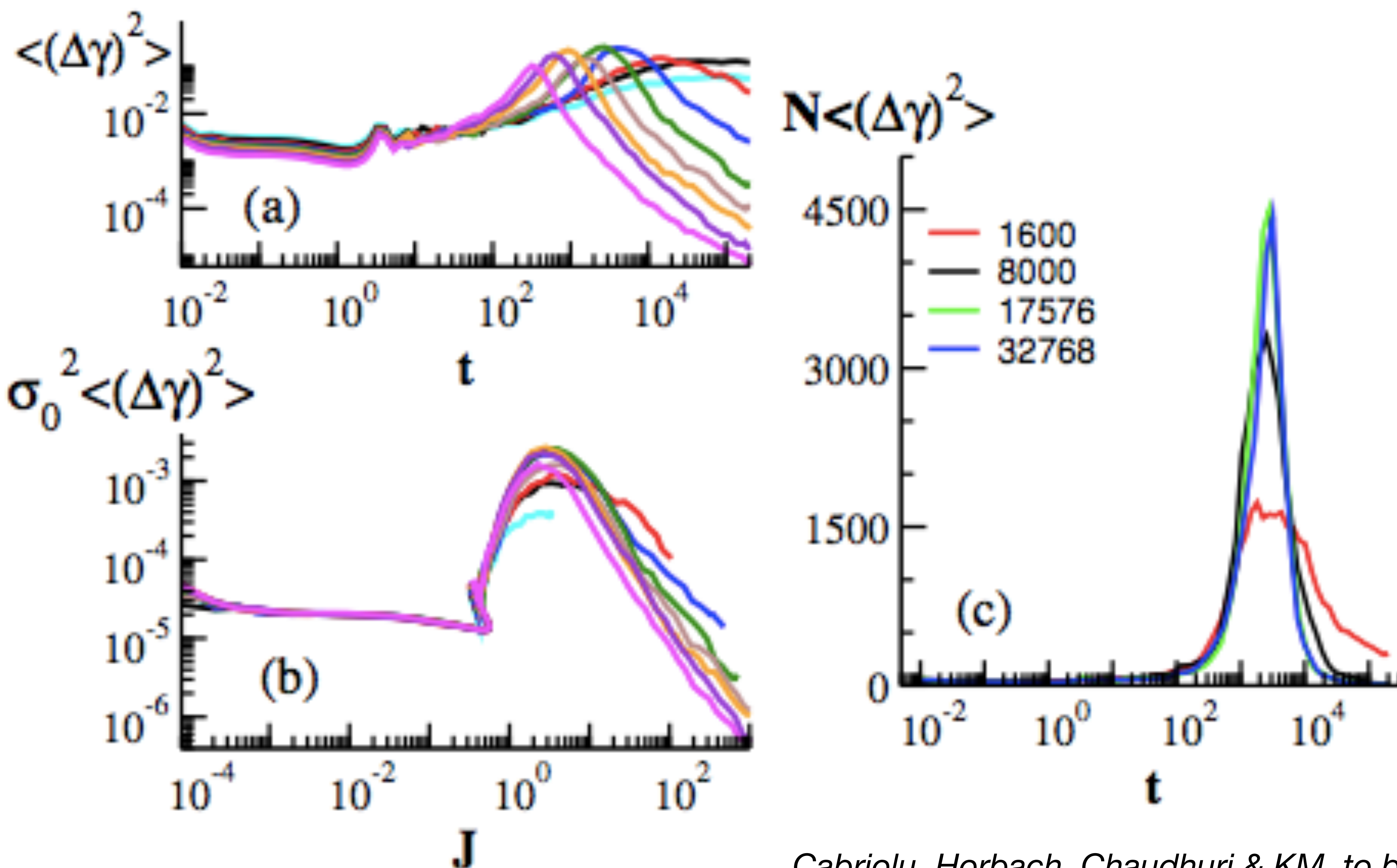
Compliance curves reveal onset of plasticity and finite size effects



Cabriolu, Horbach, Chaudhuri & KM, to be published

Results on creep

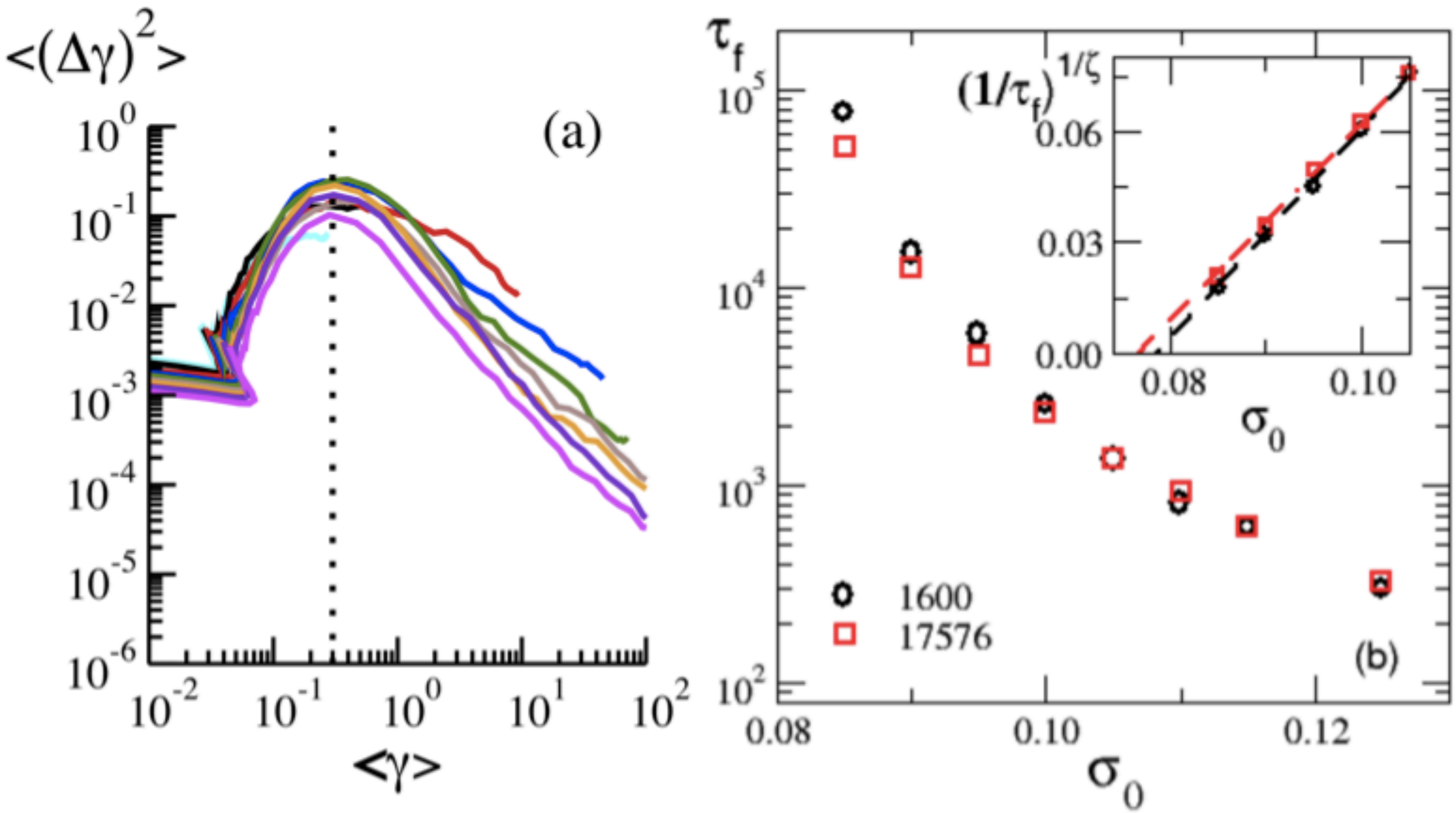
Fluctuations in strain reveal onset plasticity and finite size effects



Cabriolu, Horbach, Chaudhuri & KM, to be published

Results on creep

Fluctuations in strain reveal onset fluidisation and finite size effects



Cabriolu, Horbach, Chaudhuri & KM, to be published

Conclusions

- New technique to impose a shear stress at fixed volume with periodic boundary conditions

- Study of onset of plasticity and finite size effects in without any wall effects

- Observation of precursors of fluidisation in the strain fluctuations