Computer simulation studies of flow and deformation in sheared glassy systems

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Overview

- Homogeneously driven systems, effective temperature
  - Two time scale, two temperature scenario
  - Numerical study
- Shear banding and yield stress
- Elastic and plastic deformation of 2d systems

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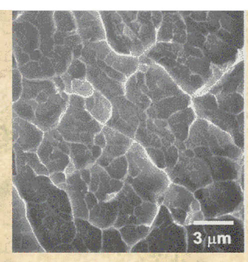
GLASSY SYSTEMS

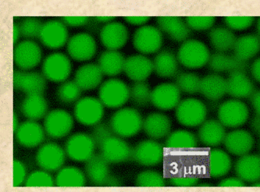
$$\tau_{micro} \ll \tau_{exp} \ll \tau_{relax}$$

Separation of time scales between microscopic time, experimental time (possibly computer time) and relaxation time.
The system is out of equilibrium on the experimental time scale.

- « hard » (usual) glasses (SiO2, metallic glasses) have a high shear modulus, ca 10GPa. Difficult to drive by external stress.
- « soft » glasses: complex liquids, foams, granular systems. Low modulus (10Mpa). Easy to shear.



Shear bands in a metallic glass



Colloidal glass (E. Weeks)

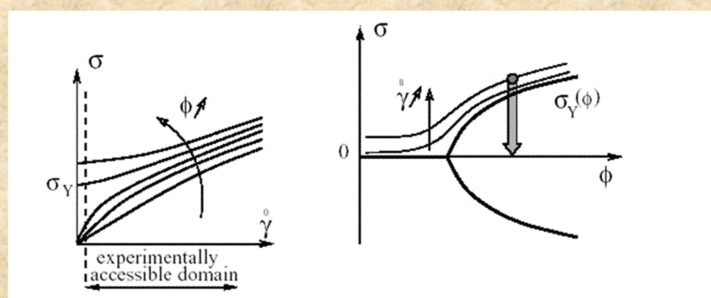
ALL these systems, when quenched below the « glass temperature » exhibit aging phenomena. Time translation invariance is lost

Driven glassy systems

- By driving the system through an external force (shear, stirring) one can recover time translation invariance (« rejuvenation »).
- Rheology for soft glassy materials
- Contact friction at the nanoscale (Robbins, Muser)

DEFINITIONS

(« soft glassy rheology » context)



-flow curve: σ versus $\dot{\gamma}$ (Couette flow)

-σ_Y: yield stress

-ϕ_c: packing fraction above which the yield stress is nonzero (jamming)

Many models

-mean field/mode-coupling type models (L. Berthier, JLB, J. Kurchan ; M. Fuchs, M. Cates) ; nonlinear integrodifferential equations

-soft glassy rheology (Sollich, Cates,Lequeux, Hébraud) ; partial differential equations

-rate and state descriptions (Argon Bulatov, Falk Langer, Lemaître..) ; coupled nonlinear ordinary differential equations

Either many assumptions or incomplete descriptions

More general concepts beyond specific models ?

Effective temperature (1)

An effective temperature T_{eff} can be defined from the fluctuation dissipation (FD) ratio (*see* ***Cugliandolo,Kurchan, Peliti,*** *Phys. Rev.* ***E55****, 3898, 1997*). Recall first equilibrium FD theorem (***Einstein*** 1905; ***Onsager*** 1931):

Correlation function

$$C_{OO'}(t) = \langle O(t+t_0)O'(t_0)\rangle - \langle O(t_0)\rangle\langle O'(t_0)\rangle$$

Response function: $R_{OO'}(t) = \frac{\delta\langle O(t+t_0)\rangle}{\delta h_{O'}(t_0)}$

Equilibrium FDT: $R_{OO'}(t) = -\frac{1}{T}\frac{\mathrm{d}C_{OO'}(t)}{\mathrm{d}t}$

Susceptibility: $\chi_{OO'}(t) = \int_0^t \mathrm{d}t'\, R_{OO'}(t') = \frac{1}{T}\big(C_{OO'}(0) - C_{OO'}(t)\big)$

$\Rightarrow$ χ versus C is a straight line with slope $1/T$ (associated with Gibbs phase space distribution $\exp(-H/T)$).

In particular Einstein's relation $D = \mu k_B T$ relates mobility and diffusion of tracers

Effective temperature (2)

Nonequilibrium system (stationary)

$$R_{OO'}(t) = -\frac{1}{T_{\mathrm{eff}}^{OO'}(C_{OO'})}\frac{\mathrm{d}C_{OO'}(t)}{\mathrm{d}t}$$

defines the effective "FDT" temperature for these observables.

$$\chi_{OO'}(t) = \int_0^t \mathrm{d}t'\left(-\frac{1}{T_{\mathrm{eff}}^{OO'}(C_{OO'})}\frac{\mathrm{d}C_{OO'}(t')}{\mathrm{d}t'}\right) = \int_{C_{OO'}(t)}^{C_{OO'}(0)} \frac{\mathrm{d}x}{T_{\mathrm{eff}}^{OO'}(x)}$$

In a class of nonequilibrium models (mean-field) T_{eff} has well defined properties that depend on the time scale of observation (***Cugliandolo,Kurchan, Peliti,*** *Phys. Rev.* ***E55****, 3898, 1997)* Different temperatures for different time scales

Could be general for nonequilibrium systems with two well separated time scales.

Effective temperature (3)

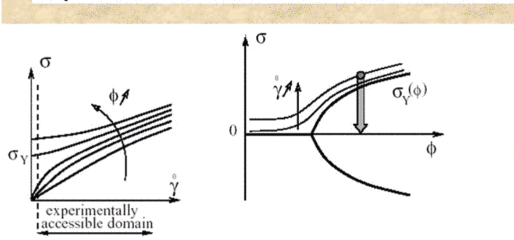
Mean field model predictions (two time scales model)

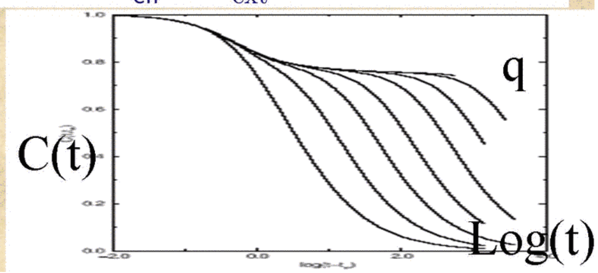
- Below ϕ_c: $T_{\text{eff}} = T_{\text{ext}}$ in the Newtonian regime ; $T_{\text{eff}} > T_{\text{ext}}$ in the shear thinning regime.
- Above ϕ_c: $T_{\text{eff}} \neq T_{\text{ext}}$ even in the small drive limit.
- T_{eff} predicted to be independent of the observable.

- T_{eff} predicted to be a step function of the correlation C

Short time scales, $C > q$: the system is at equilibrium with the external bath, $T_{\text{eff}} = T_{\text{ext}}$.

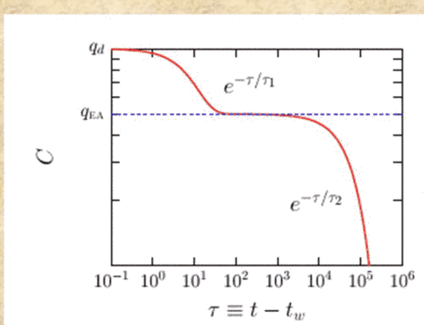
Long time scales $C < q$: system explores phase space with out of equilibrium distribution associated with $T_{\text{eff}} > T_{\text{ext}}$

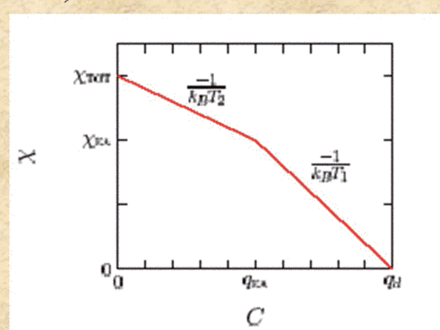




Effective temperature (4)

Toy model : brownian harmonic oscillator coupled to mixed bath: high T+ high friction, low T + low friction (see L. Cugliandolo, les Houches lecture notes cond-mat0210312)





Response-correlation plot is a combination of 2 straight lines, with 2 temperatures associated with different time scales

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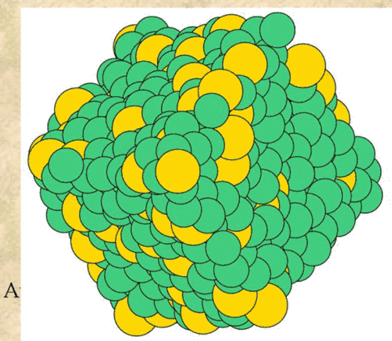
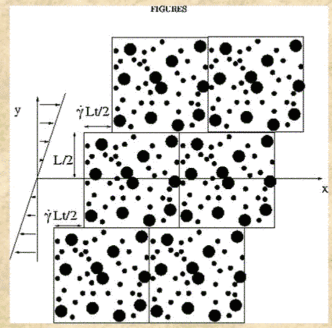
Driving a « real » glassy system; a numerical experiment

The model: Lennard-Jones mixture, originally model for metallic glasses.

Periodic boundary conditions



Homogeneous Couette flow, thermostatted



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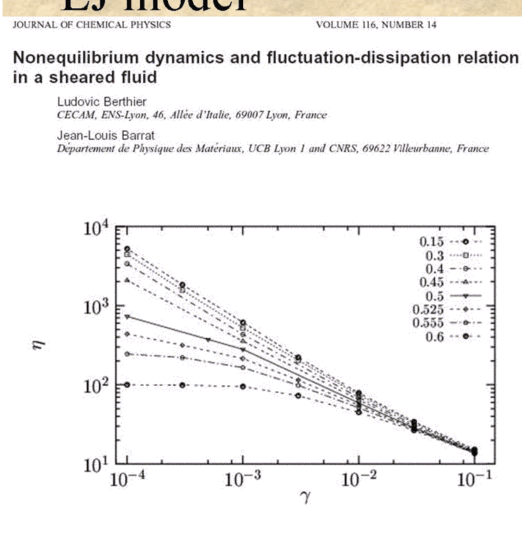
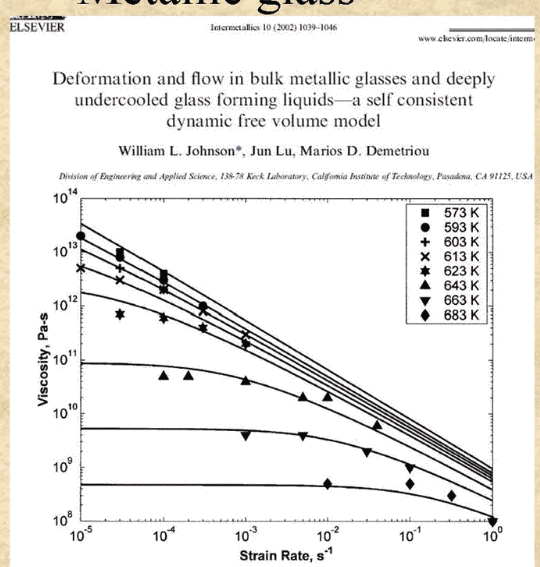
Flow behaviour: viscosity vs strain rate: shear thinning

LJ model



Metallic glass



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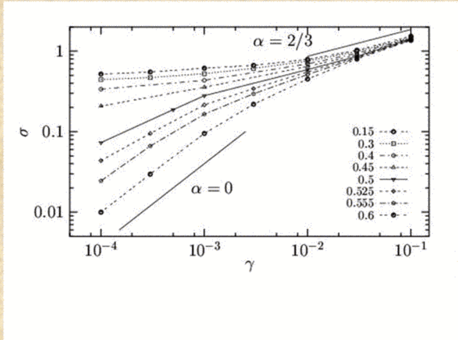
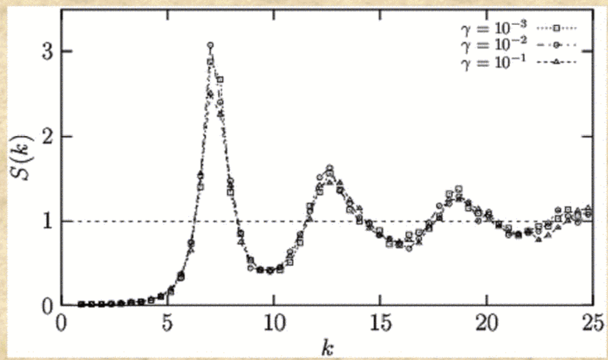


Flow curve:

High T: newtonian, then shear thinning

Low T: $\sigma = \sigma_0 + A\dot{\gamma}^{\alpha}$



Structure essentially constant under shear

Effective temperature

Observables:

$O(t) = \frac{1}{N_A}\sum_{j=1}^{N_A} \varepsilon_j \exp\left(i\boldsymbol{k}\cdot\boldsymbol{r_j}(t)\right)$

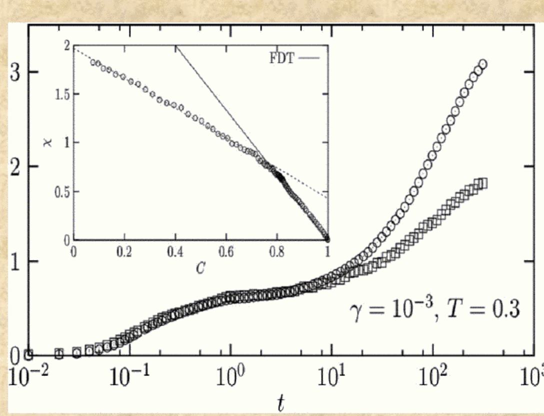
$O'(t) = 2\sum_{j=1}^{N_A} \varepsilon_j \cos\left(\boldsymbol{k}\cdot\boldsymbol{r_j}(t)\right)$

where $\varepsilon_j = \pm 1$ **random variable.**

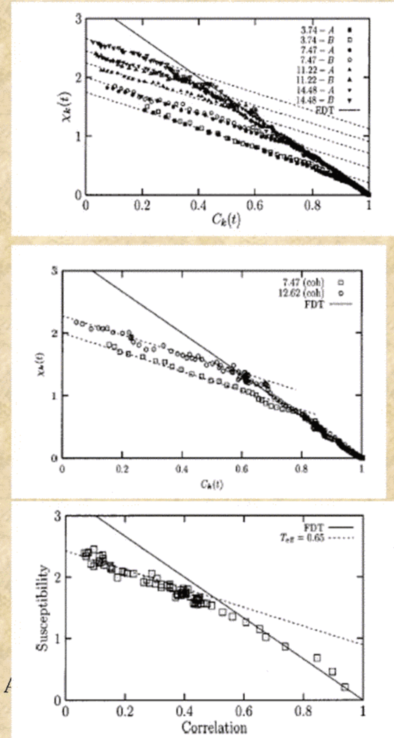
$C_{\boldsymbol{k}}(t) = \overline{C_{OO'}(t)}$

External field to compute $\chi_{OO'}$

$\boldsymbol{F_j}(\boldsymbol{k},t) = -\frac{\partial}{\partial \boldsymbol{r_j}}\left(- h_{O'}O'(t)\right)$



Other observables

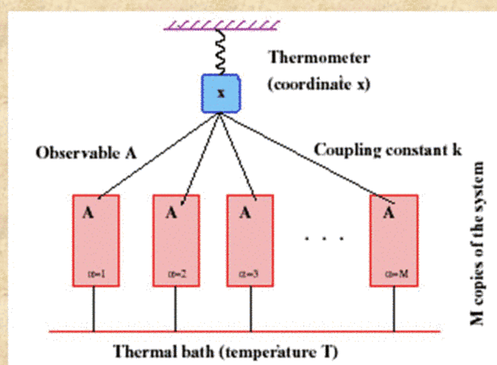


Various wavevectors incoherent

Various wavevectors coherent

Stress response

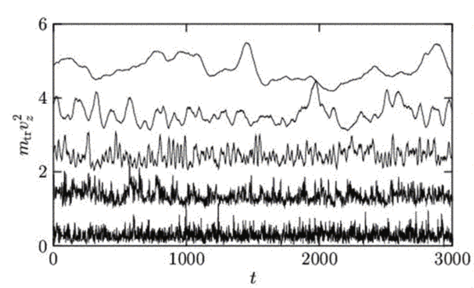
A « practical » measurement of T_{eff}



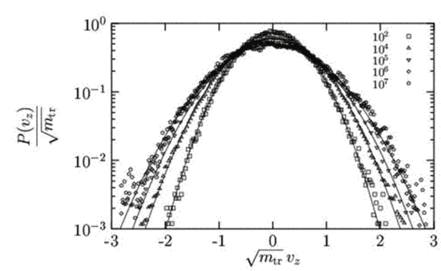
Cugliandolo, Kurchan, Peliti, Phys. Rev. B 1997

Tracer particles = Numerical thermometers

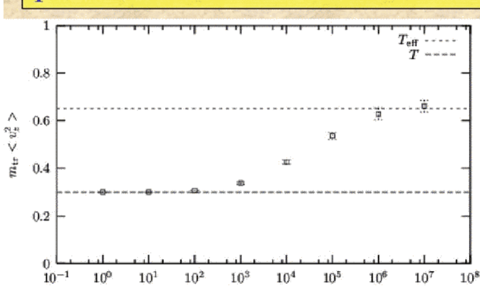
- Heavy tracer particles (same as other particles – only the mass is different)
- Typical vibrational frequency $\omega_E(tracer) = \omega_E(solvent)\sqrt{m/M_{tracer}}$
- If $\omega_E(tracer)\tau_{relax} \ll 1$ the particle will be sensitive only to slow fluctuations (low pass filter)



Velocity fluctuations of a tracer particle



Tracer velocity distribution function: Maxellian with effective temperature

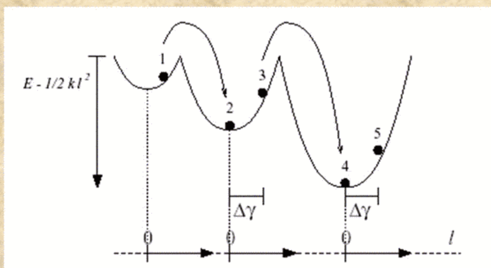


Effective temperature of the tracer (from kinetic energy)

Open questions

Role in activated processes ? Link with « x » parameters in soft glassy rheology models ?

Sollich P., Lequeux, F., Hebraud P. and Cates M. E., "Rheology of Soft Glassy Materials", Phys. Rev. Lett. 78 (1987) 2020–2023.



l strain variable, increases with time for system trapped in a given minimum

$$E \to E - kl^2/2$$

$$\tau = \tau_0 \exp\left[(E - kl^2/2)/x\right]$$

$$\dot{P}(E,l,t) = -\dot{\gamma}\partial P/\partial l - \Gamma_0 e^{-(E-kl^2/2)/x} P(E,l,t) + \Gamma(t)\rho(E)\delta(l)$$

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Experimental measurement ?

Experimental measurement of an effective temperature for jammed granular materials

Chaoming Song, Ping Wang, and Hernán A. Makse*

Levich Institute and Physics Department, City College of New York, New York, NY 10031

Song, Wang, Makse, PNAS 2005, granular system

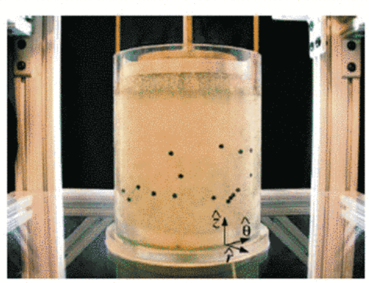
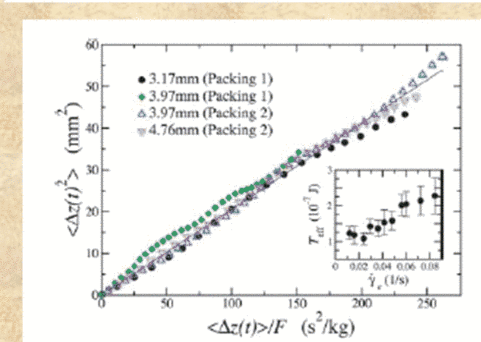


Fig. 1. Experimental setup. Transparent acrylic grains and black tracers in a refractive index and density-matched solution are confined between the inner cylinder of radius 50.8 mm and the outer cylinder of radius 66.7 mm.

Simultaneous measurement of **tracer** diffusion and mobility

$$\langle [z(t+t_0) - z(t_0)]^2 \rangle = 2T_{\text{eff}} \frac{\langle z(t+t_0) - z(t_0) \rangle}{F}.$$



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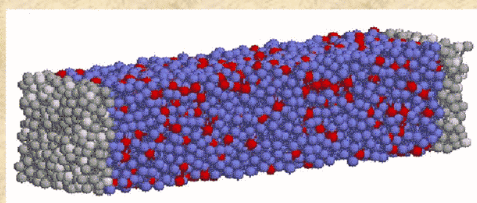
Boundary driven system: shear banding, and yield stress



-Previous results obtained with forced homogeneous flow (SLLOD equations)

-Different situation: moving rough walls identical to the flowing material (no slip). Planar Couette flow.

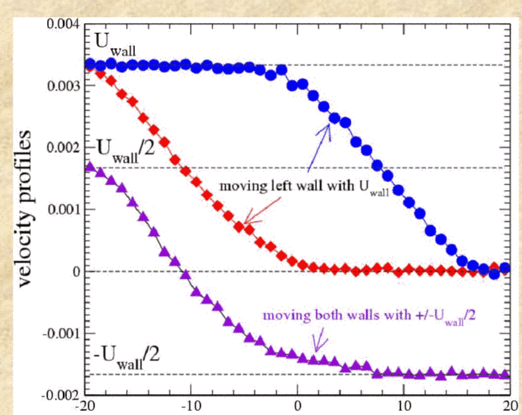
-Homogeneous flow is obtained only above some critical shear rate ; for small shear rate, shear band formation

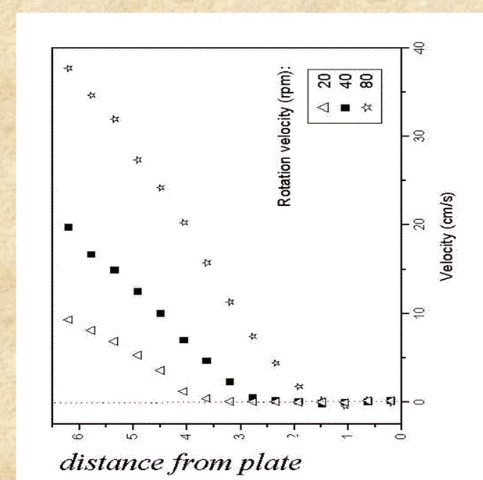
Shear band velocity profile:

Simulation

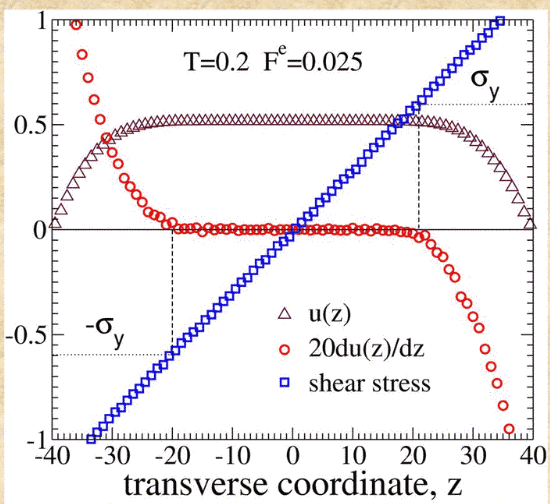
MRI imaging of velocity profiles in bentonite (clay)

(Coussot et al, PRL 2001)

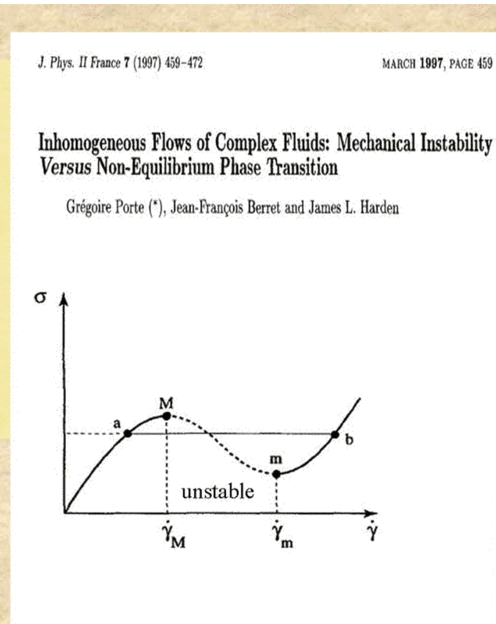




Poiseuille flow



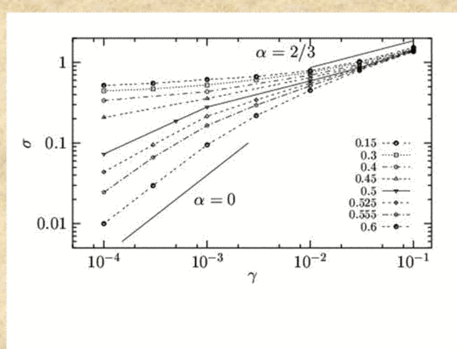
Shear bands are well known to form in systems with non monotonic flow curves (e.g. giant wormlike micelles) associated with coupling of flow with nematic order parameter


J. Phys. II France 7 (1997) 459–472 MARCH 1997, PAGE 459

Inhomogeneous Flows of Complex Fluids: Mechanical Instability Versus Non-Equilibrium Phase Transition

Grégoire Porte (*), Jean-François Berret and James L. Harden

Here flow curve is monotonic !



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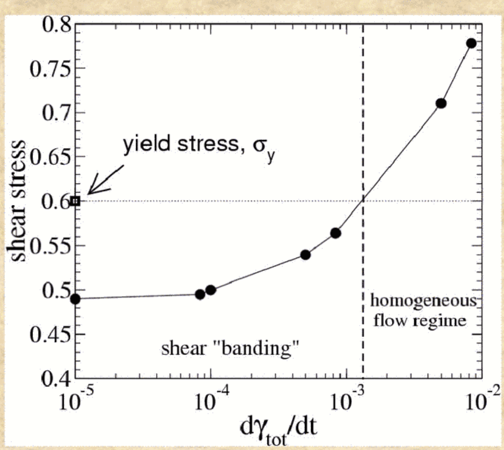
Flow curve with a finite yield stress

$\sigma_Y > \lim_{\dot\gamma \to 0} \sigma_{homogeneous}(\dot\gamma)$



Full curve: homogeneous flow data.

Shear band selection is an unsolved problem

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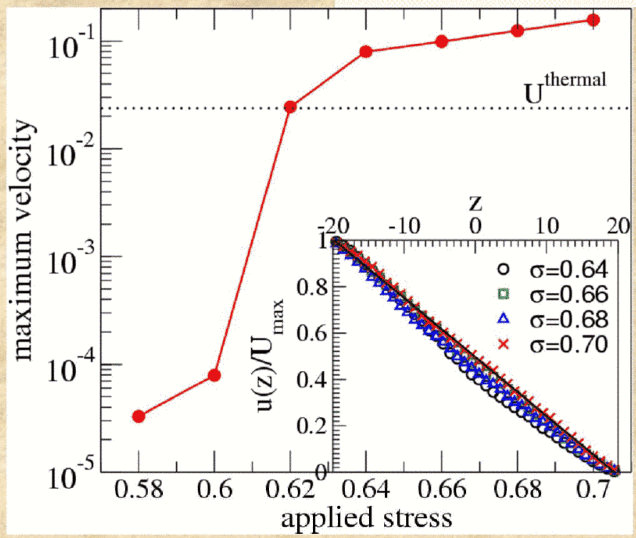
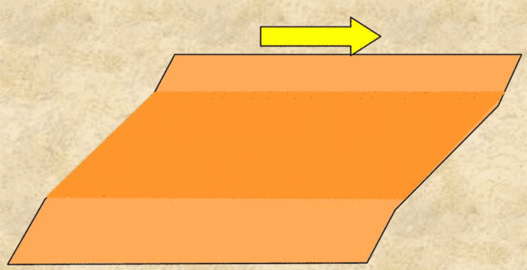
Definition of yield stress ? Apply an external stress (time scale τ_{exp}) and measure wall displacement $\Delta x = \Delta x_{el} + Vt$



Well defined result in the quasistatic limit

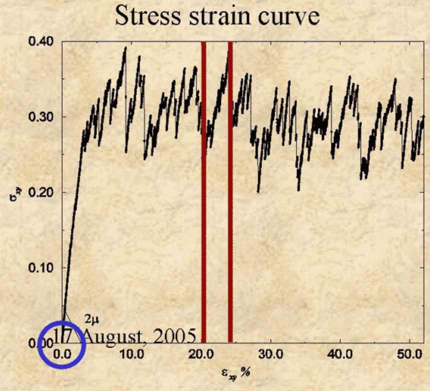
$\tau_{micro} \ll \tau_{exp} \ll \tau_{relax}$

QUASI STATIC DEFORMATION IN A 2D SYSTEM

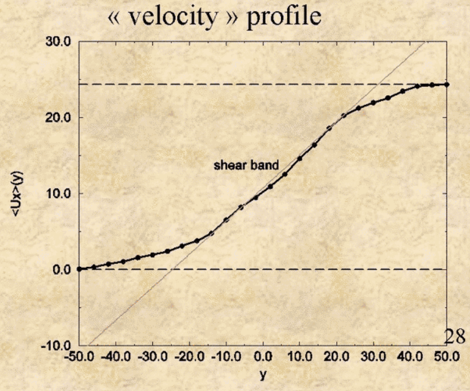


Polydisperse LJ system, quench to T=0, quasistatic shear (minimization after each deformation step 0.0001 strain increments)

Stress strain curve



« velocity » profile



ELASTIC RESPONSE AT VERY SMALL STRAIN

Elastic constants for a system of particles interacting through a pair potential ϕ(r)

$$C_{\alpha\beta\gamma\delta} = \frac{\partial t_{\alpha\beta}}{\partial \epsilon_{\gamma\delta}} = 2nk_BT(\delta_{\alpha\gamma}\delta_{\beta\delta} + \delta_{\alpha\delta}\delta_{\beta\gamma})$$ **Kinetic term**

$$-\frac{V_0}{k_BT}\left[\langle \widehat{T}_{\alpha\beta}\widehat{T}_{\gamma\delta}\rangle - \langle \widehat{T}_{\alpha\beta}\rangle\langle \widehat{T}_{\gamma\delta}\rangle\right]$$ **Fluctuation term**

$$+C^{Born}_{\alpha\beta\gamma\delta}$$ **Born term**

$\hat{T}_{\alpha\beta}$ microscopic stress tensor (Irving-Kirkwood)

$$C^{Born}_{\alpha\beta\gamma\delta} = \frac{1}{V_0}\langle \sum_{ij} R_{ij,\alpha}R_{ij,\beta}R_{ij,\gamma}R_{ij,\delta}\left(\frac{\phi"(R_{ij})}{R_{ij}^2} - \frac{\phi'(R_{ij})}{R_{ij}^3}\right)\rangle$$

Born term corresponds to the change in energy under a purely affine deformation (see e.g. Ashcroft and Mermin. Solid state physics)

Fluctuation term ?

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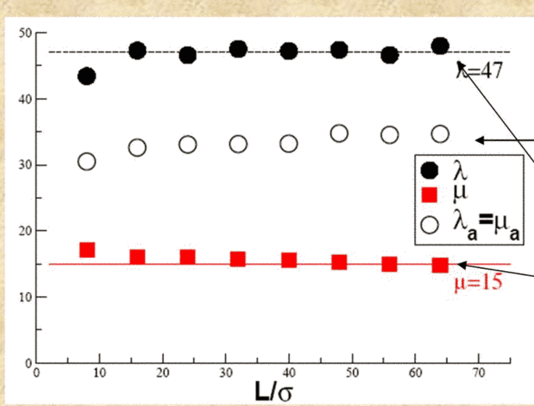
Elastic constants of a model (Lennard-Jones polydisperse mixture) amorphous system at low temperature, vs system size



Born term only (affine deformation at all scales)

Actual result with non affine deformation (fluctuations or relaxation term)

λ, μ Lamé coeffients
$\mu = G$ shear modulus
$\lambda + \mu = B$ bulk modulus

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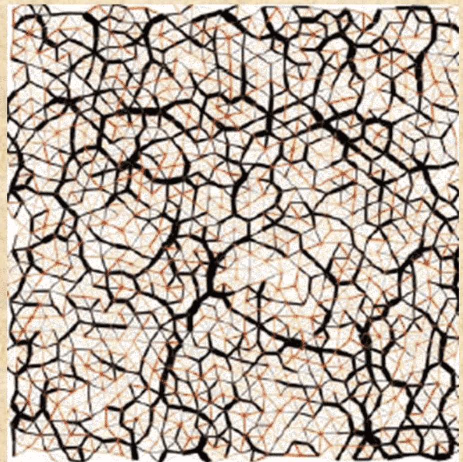
System: 2d, amorphous – similar results in 3d

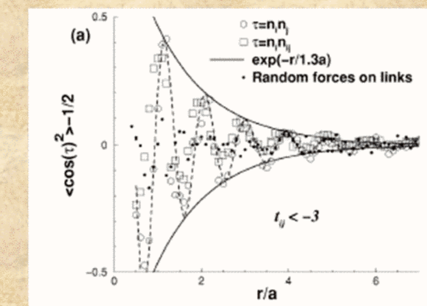


Equilibrium configuration at zero temperature – zero pressure

Vertices: particles

Black lines: repulsive force

Red lines: attractive forces



Force chains ? Nothing obvious in correlation functions

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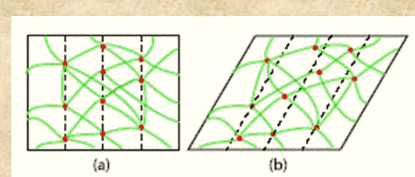
Born term innacurate →

-Large fluctuation term (finite T)

-Large fraction of the elastic energy stored in a <u>nonaffine deformation field</u> (zero T)

Deform the sample (rescale all coordinates $X \to X(1+\epsilon)$)
Minimize energy $X(1+\epsilon) \to X'$
Substract affine deformation
$\to$ non affine deformation field $\delta X = X' - X(1+\epsilon)$



Contribution from nonaffine field (relaxation) at zero temperature is equivalent to fluctuation term in elastic constants

Lutsko 1994: take derivatives w.r.t. strain at mechanical equilibrium (zero force on all particles)

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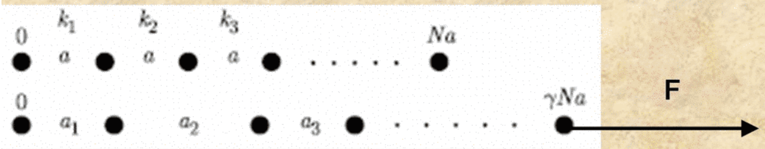
One dimensional example



$$\delta_p = a_p - a = F/k_p$$

$$u_p = F \times \sum_{i=1}^{p} k_i^{-1}$$

$$u_p^{NA} = F \times \sum_{i=1}^{p} (k_i^{-1} - < k^{-1} >)$$

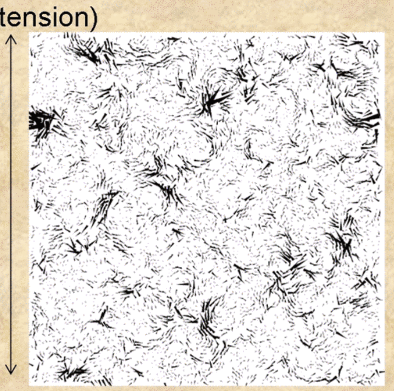
$$< (u_p^{NA})^2 > \sim p < (\delta k^{-1})^2 >$$

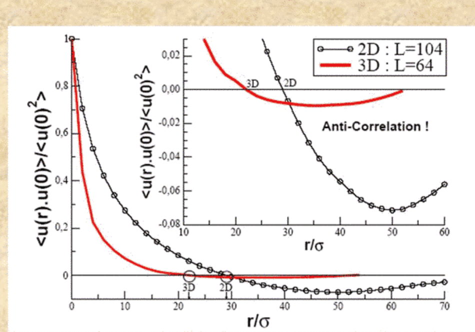
Divergence : 1 d effect or more general ??

(see DiDonna Lubensky 2005)

2d, 3d situation (from simulation)

Snapshot of nonaffine displacement (uniaxial extension)



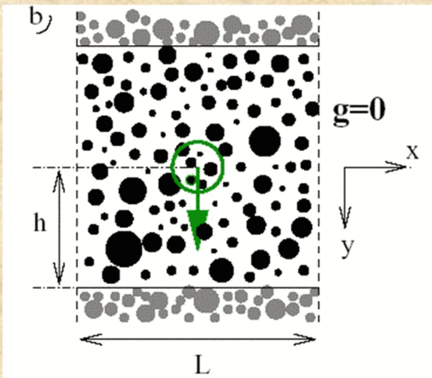


Large length scale $\xi = 30 - 50$ atomic sizes revealed by correlations of nonaffine field

→ continuum elasticity not applicable for L < ξ

Elastic response to a point force:

- Granular systems
- Nanoindentation

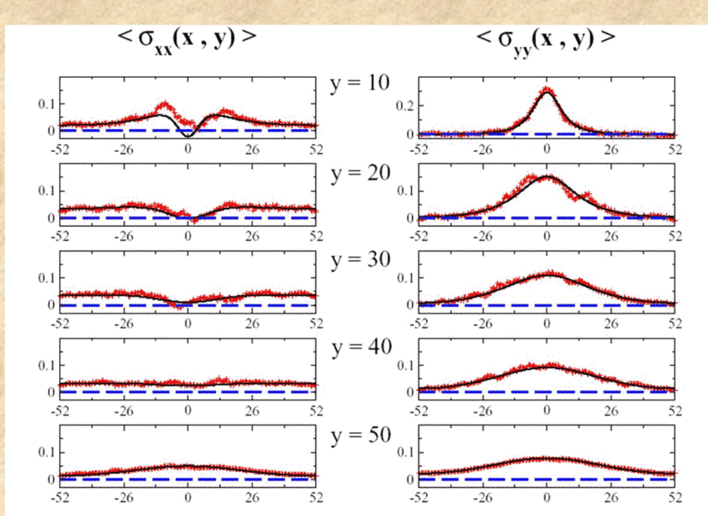


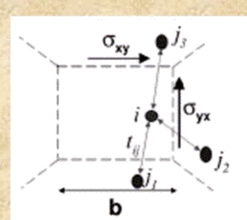
Small force applied to a few particles (source region, diameter 4a).

Fixed walls or compensation force on all particles.

Displacements, forces and incremental stresses computed in the elastic limit.

Average response obeys classical elasticity



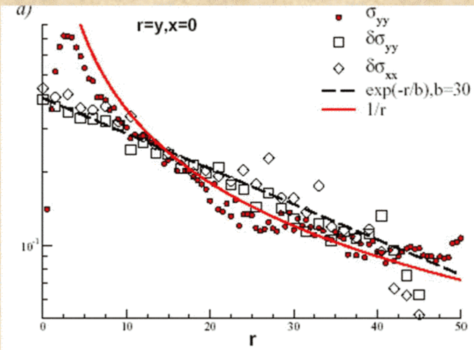


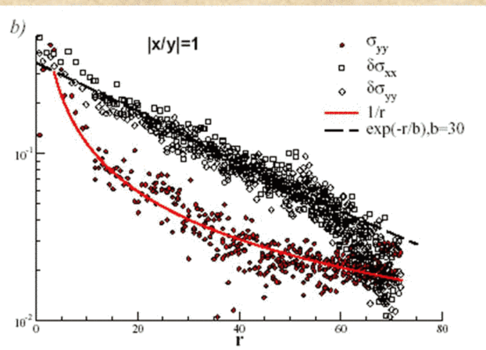
Local stress calculation for a cell of size b

simulation

Continuum prediction

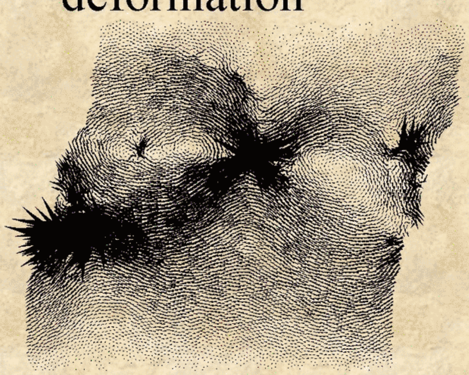
Large fluctuations between different realizations for distances smaller than 50 particle sizes

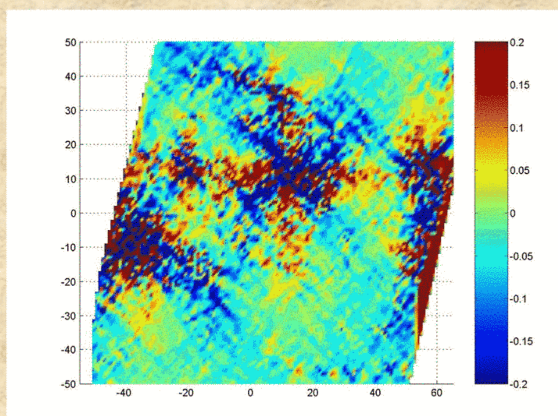




Material elastically inhomogeneous, even for perfectly uniform density (important also for vibrational spectrum in glasses)

Onset of plastic deformation

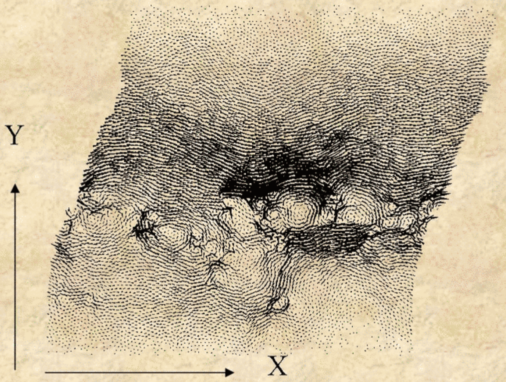


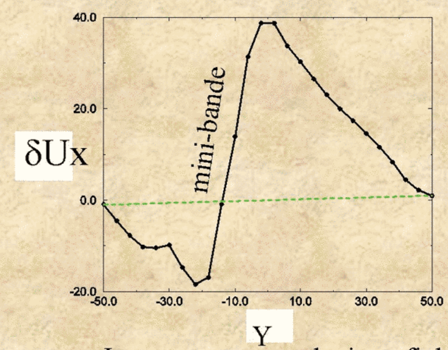


$\Delta\sigma$ xy

Localized, quadrupolar event
(see also similar observations by Maloney, Lemaitre PRL 2004).

L=104.0,N=10000,shear conf23-n2029





Instantaneous « velocity » field

Simultaneous alignement of events to form a « mini shear band » or « cracks »

L=104.0,N=10000,shear conf23-n2339

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Open question: how to link with « mesoscopic » modelling ?

STZ model
(Shear Transformation Zones)
M.L. Falk et J.S. Langer (1998):

$$\dot{n}_\pm = R_\mp n_\mp - R_\pm n_\pm - C_1(\sigma_s \dot{\epsilon}_s^{(in)}) n_\pm + C_2(\sigma_s \dot{\epsilon}_s^{(in)}).$$

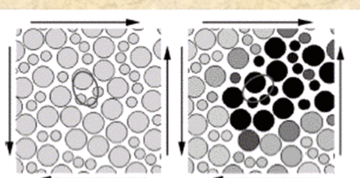

FIG. 8. Closeup picture of a shear transformation zone before and after undergoing transformation. Molecules after transformation are shaded according to their values of D^2_{min} using the same gray scale as in Fig. 7. The direction of the externally applied shear stress is shown by the arrows. The ovals are included solely as guides for the eye.

Elastic redistribution of local plastic events

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Picard, Bocquet Lequeux, Ajdari
Eur. Phys. J. E **15**, 371-381 (2004)
Baret,Vandembroucq, Roux
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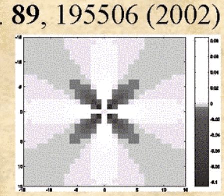

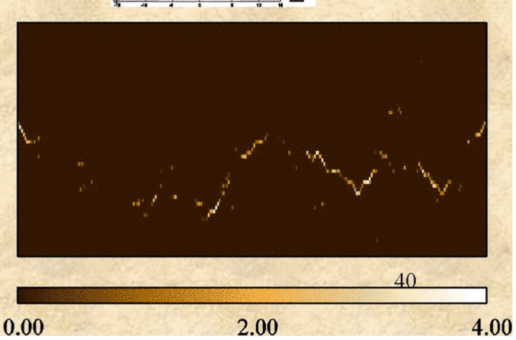

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