Particle dynamics close to jamming

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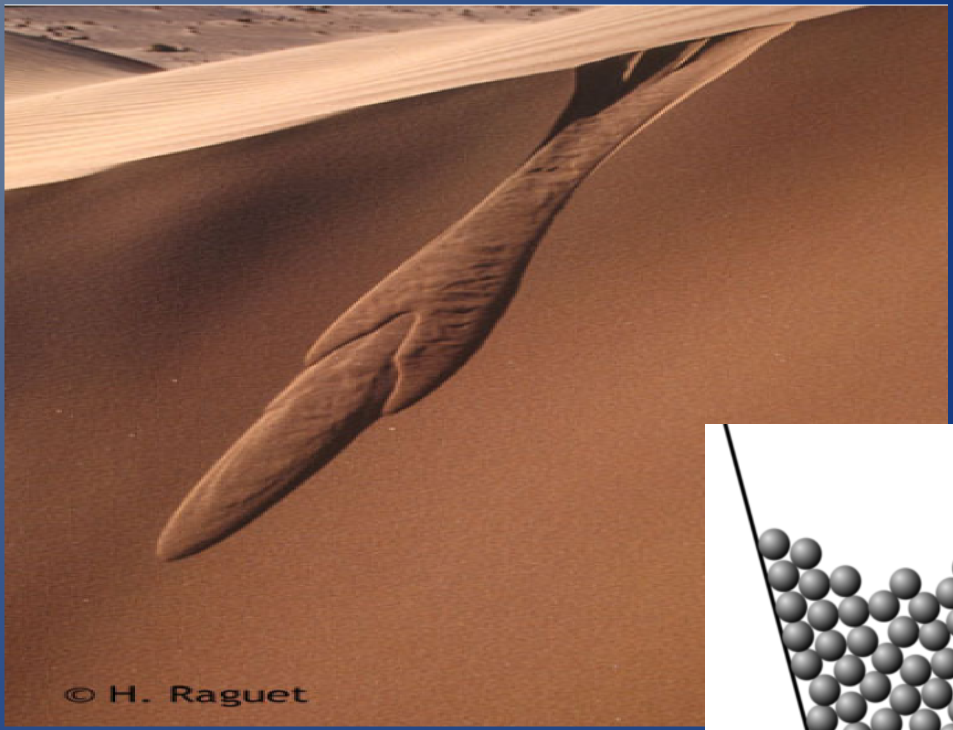
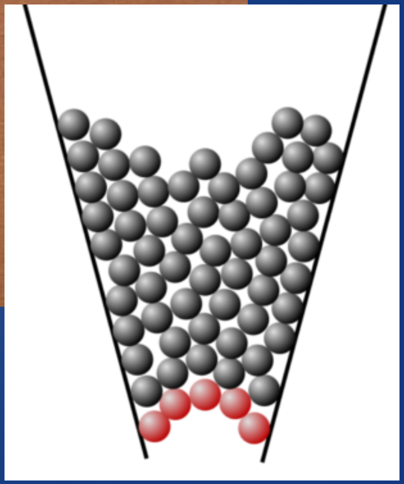
Jamming

- Transition between fluid and solid phase
- “blocked” state, “fragile”
- Yield-stress fluid





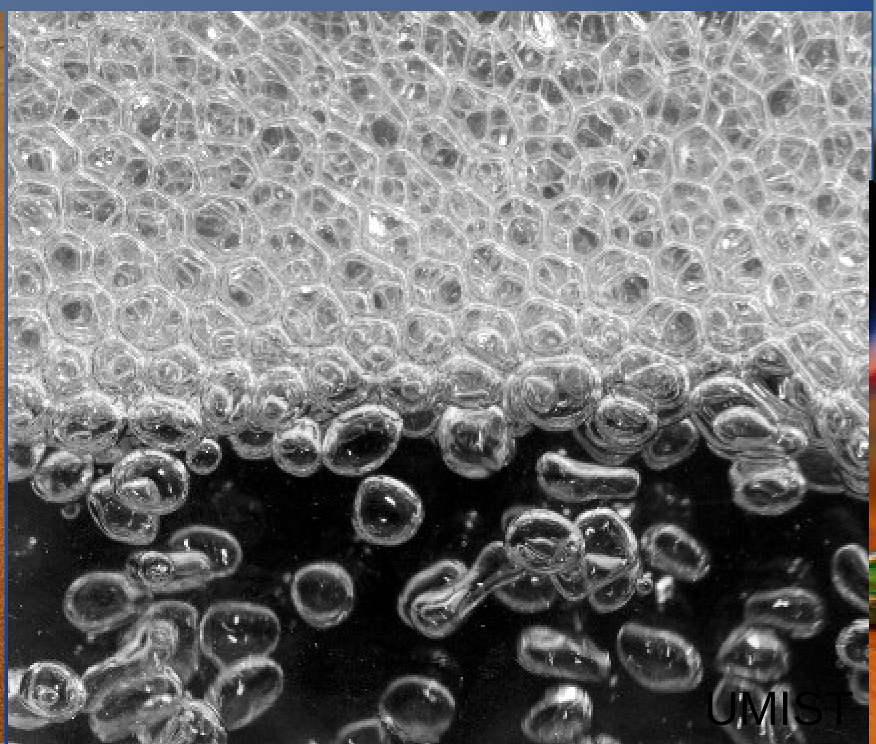
Soft, amorphous materials

Foam: shaving foam

Suspension: paint

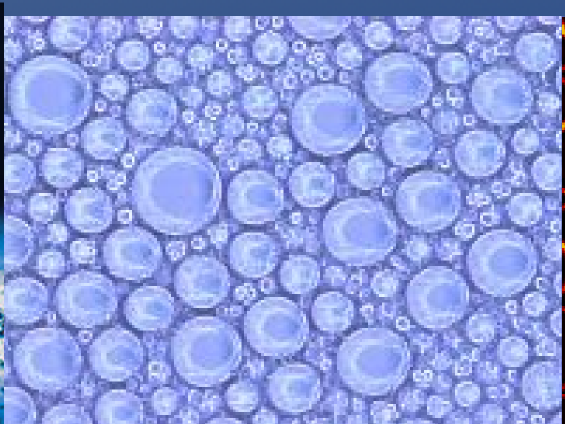
Granulate: sand, flour

Emulsion: mayonnaise

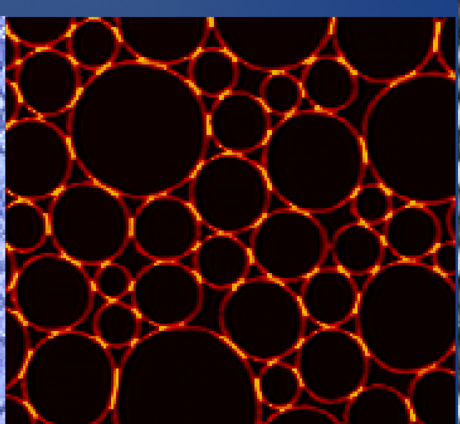


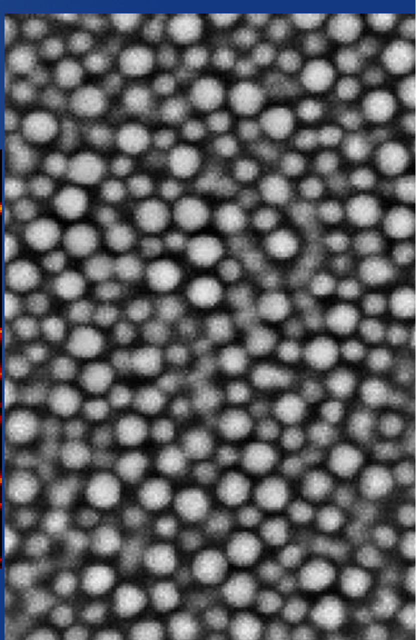
Variety of material properties

- Densly packed assembly of “particles”
  - Soft or hard
  - Dissipative mechanisms: hydrodynamics, friction, etc
- Diverse mechanical properties
- Different scientific communities: fundamental and applied science



Cox, Birmingham

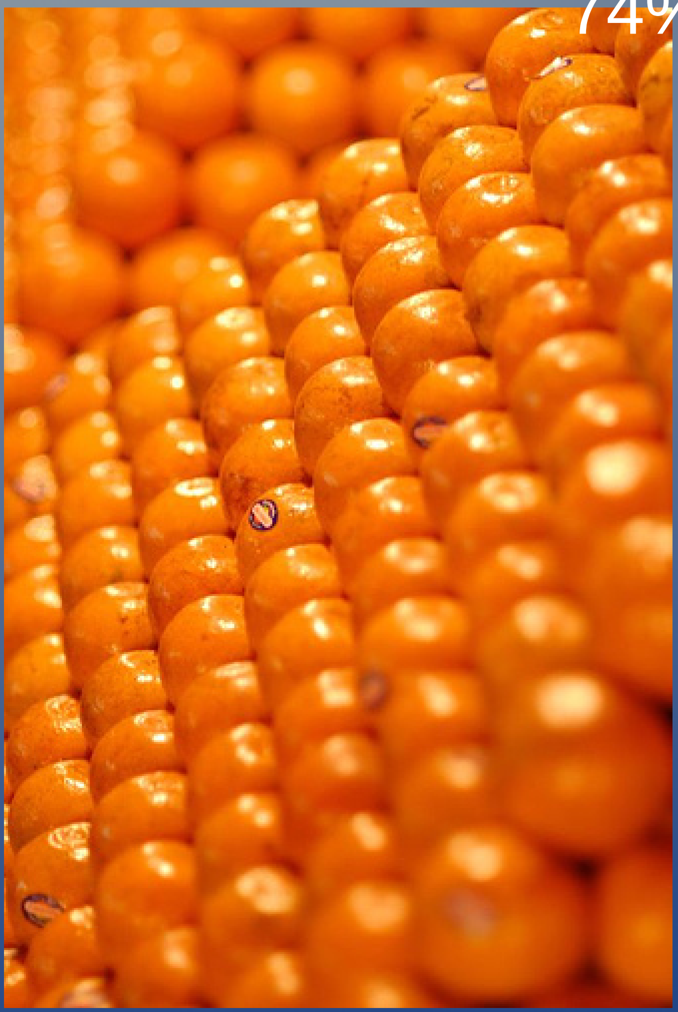




Weeks, Emory

Close packing

FCC
74%



Random Close Packing
64%

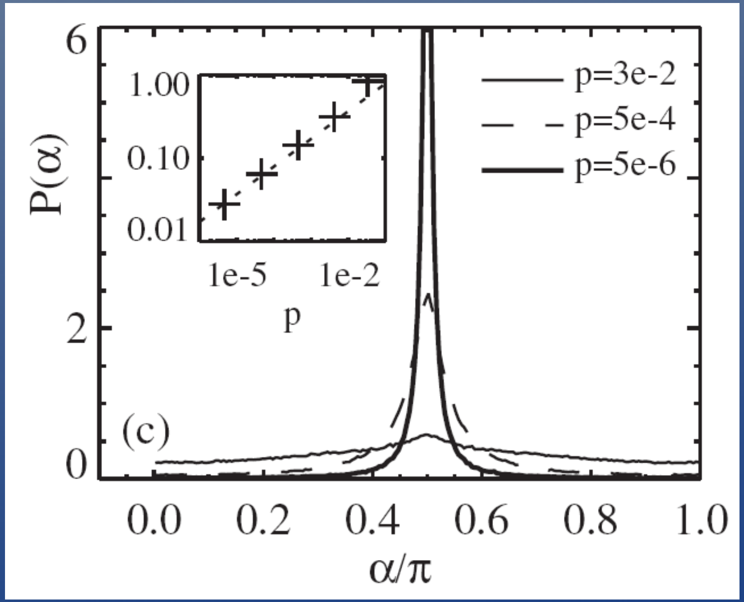
$\phi > \phi_{RCP}$: (Motion) only possible if particles deform

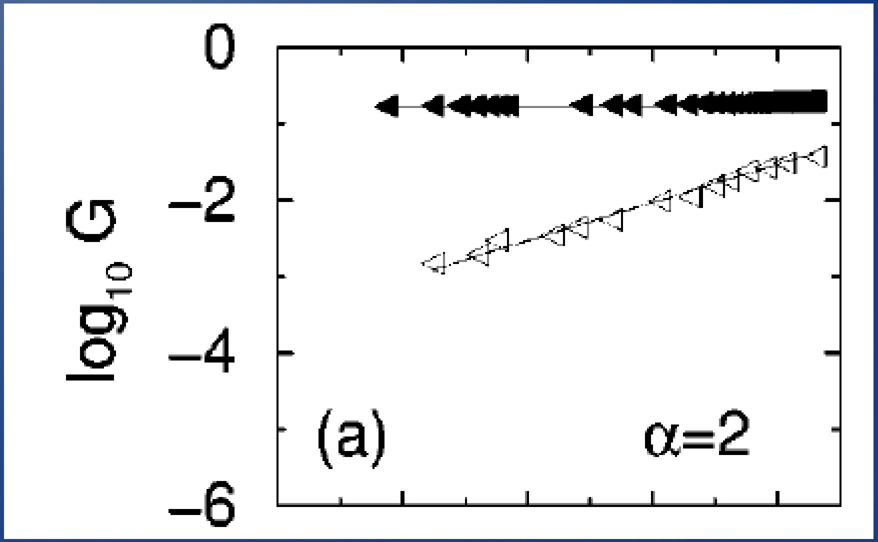
$\phi < \phi_{RCP}$: Motion possible, but:

"lack of space"

At around RCP

- Response to deformation “non-affine”
- Elastic moduli: G/B $\rightarrow$ 0 at ϕ_c
- Where does this come from ? – contact network

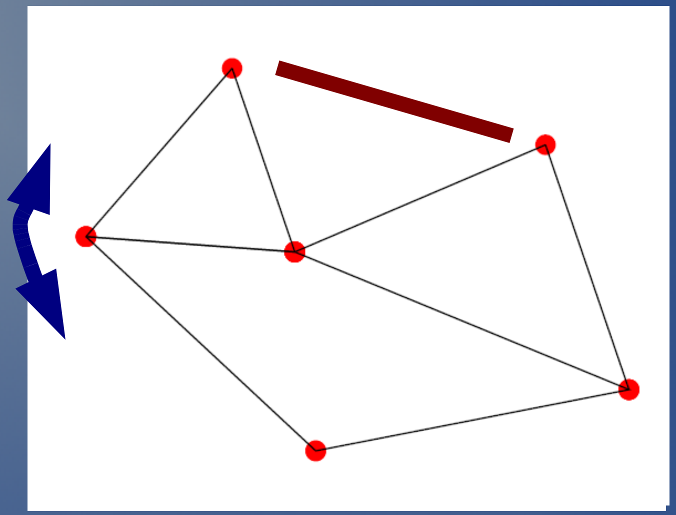




Ellenbroek et al. PRL (2006), O'Hern et al. PRE 68 (2003)

At jamming contact network is "isostatic"

"Just enough inter-particle contacts"



$z < z_{iso}$ floppy modes – zero energy modes

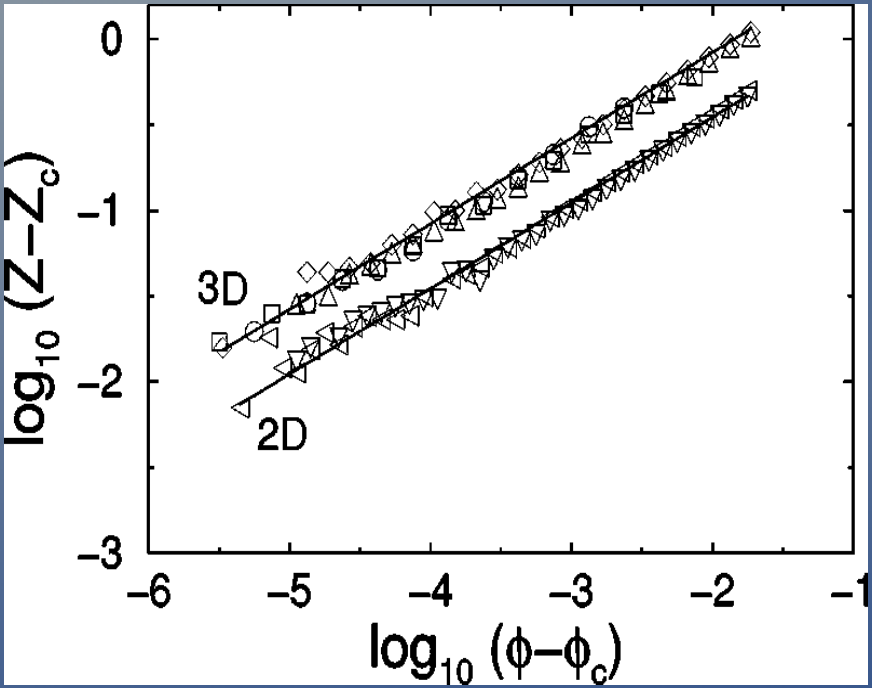
$z > z_{iso}$ elastic solid

$z = z_{iso}$ minimally rigid, isostatic

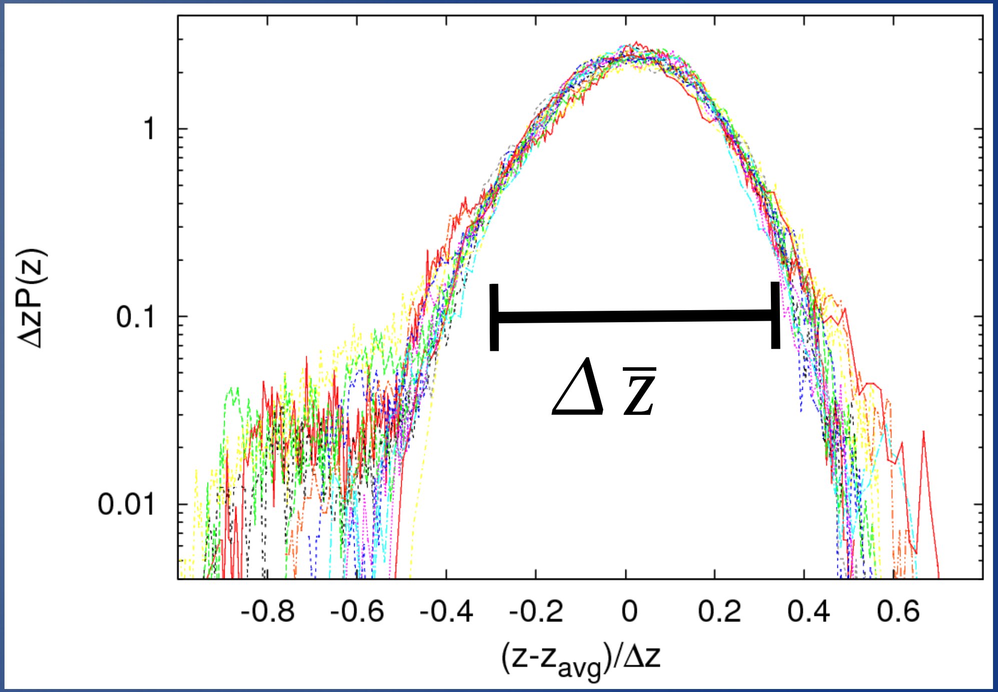
Maxwell counting: $z_{iso} = 2c/p = 2d$

Contacts

Average z



Pdf($\bar{z}$)



$$z - z_{iso} \sim (\phi - \phi_J)^{1/2}$$

Intensive Variable

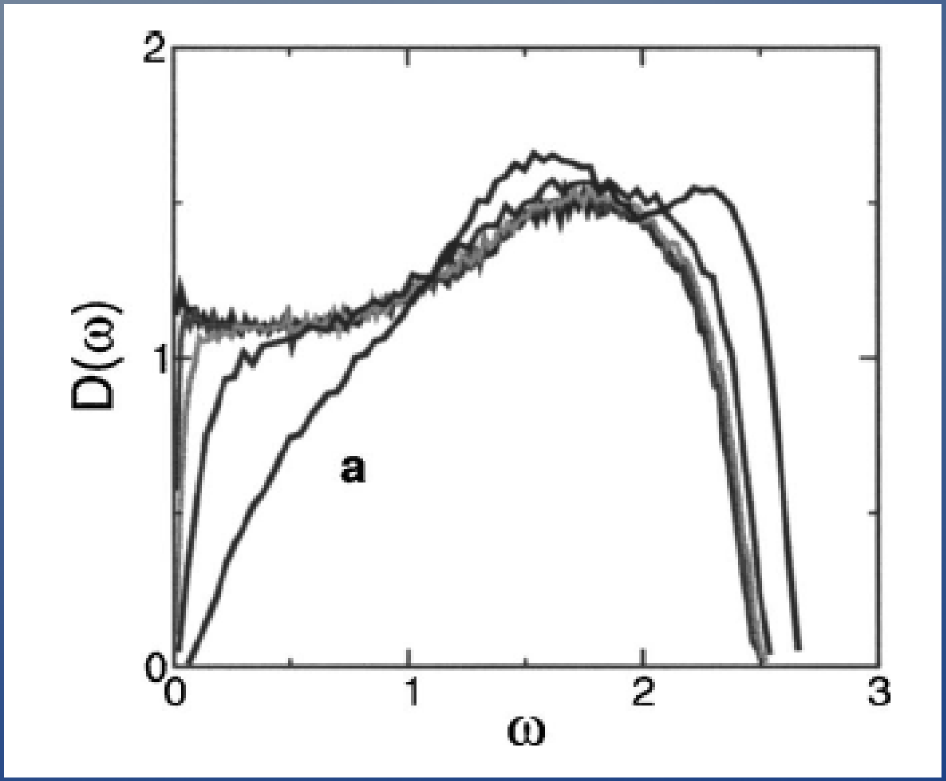
$$\bar{z} = \frac{1}{N}\sum_i z_i$$

$$N\,\Delta\bar{z}^2 \sim (\phi - \phi_J)^{-0.7}$$

O'Hern et al. PRE 68 (2003), CH, P. Chaudhuri, JL Barrat, Soft Matter (2010)

Vibrational density of states

- Many low frequency vibrations
- Frequency cut-off: $\omega_c \sim z - z_{iso}$



- What is important: distance to isostatic state

$$z - z_{iso}$$

rather than

$$\phi - \phi_c$$

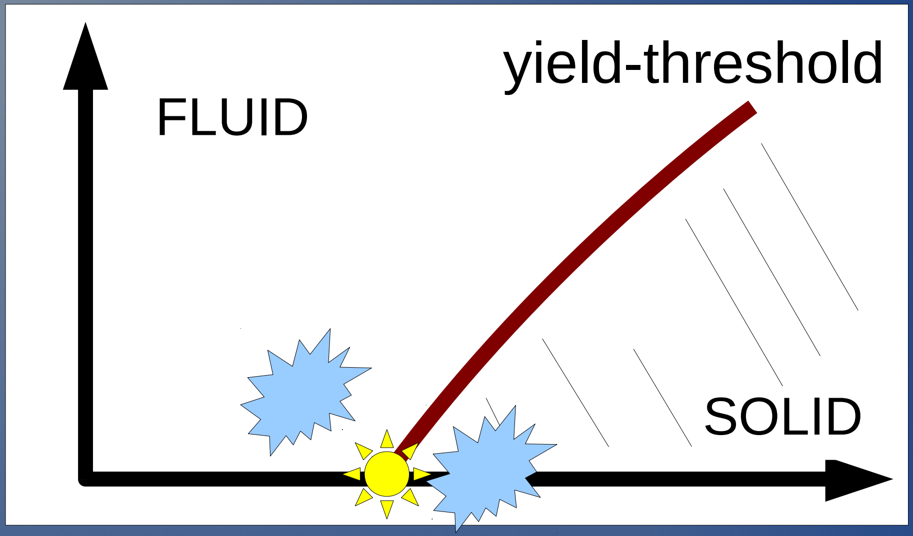
Wyart PRE 72 (2005)

Research Questions

What happens in fluid state ??

Driving amplitude

(T=0)



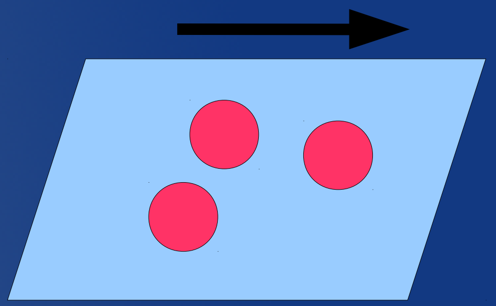
Particle volume fraction

Driving mechanisms: rattling, shear, air flow, ...

Dissipative mechanisms: friction, viscous, ...

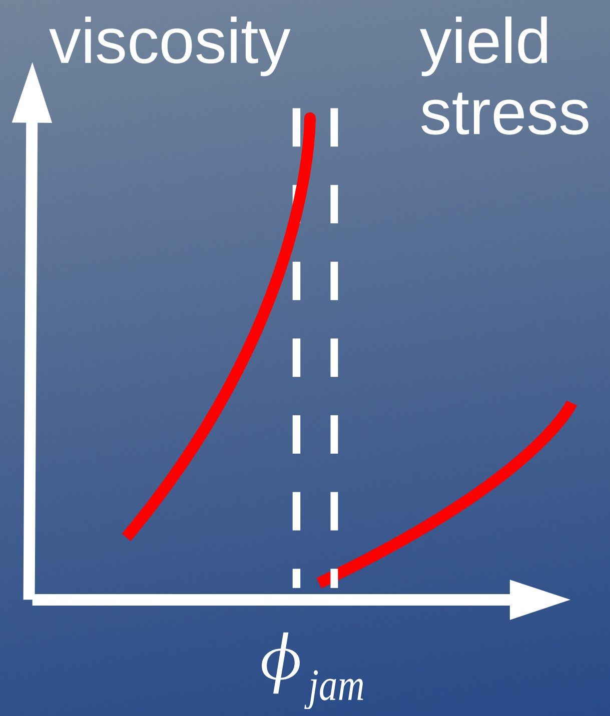
Anything universal ? Role of particle contacts ?

Two driving mechanisms



Steady shear flow:

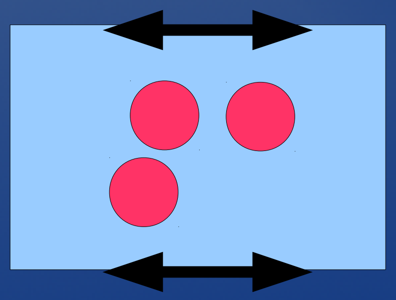
How and why does the viscosity diverge ?



Rattling:

Glassy vs Jamming dynamics

“Melt a glass by freezing”

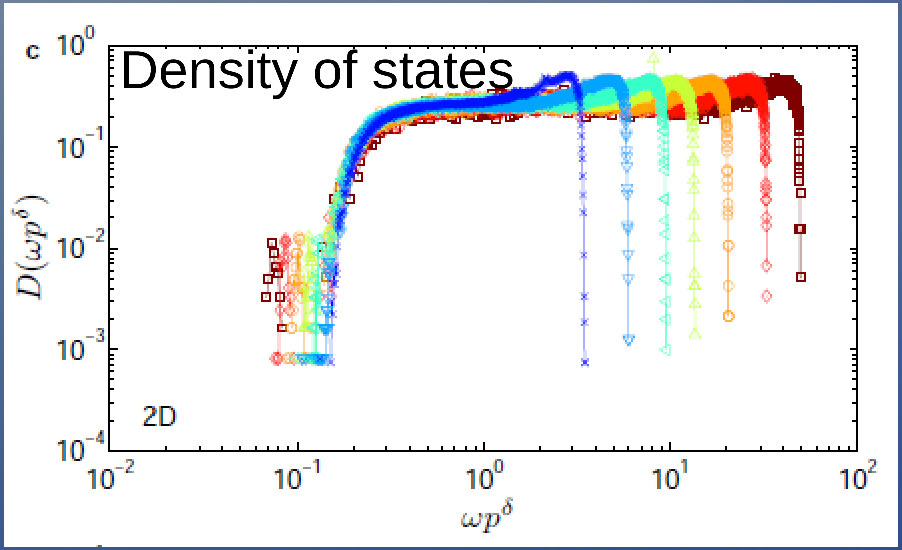


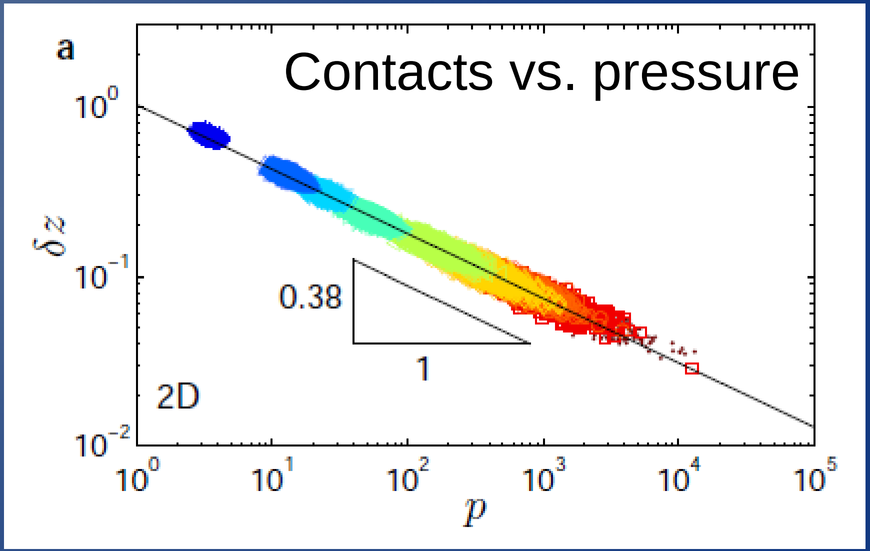
Shear flow $\phi<\phi_c$

Divergence of viscosity at ϕ_c

Role of contacts ?

- Shear flow of near-isostatic contact network
- Breaking/rewiring of contacts z

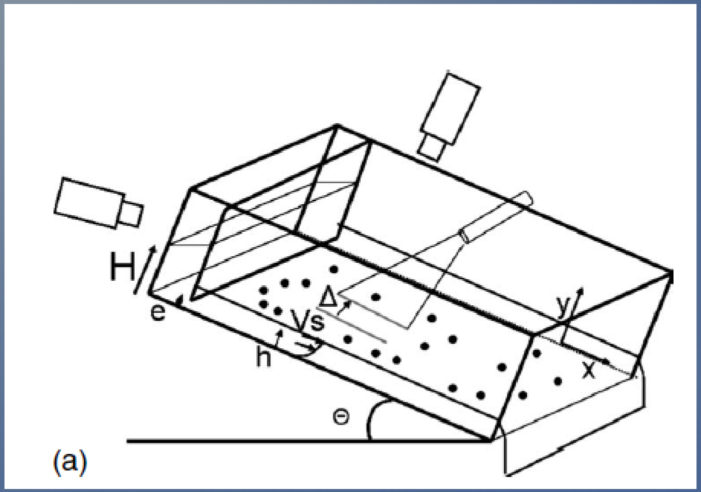


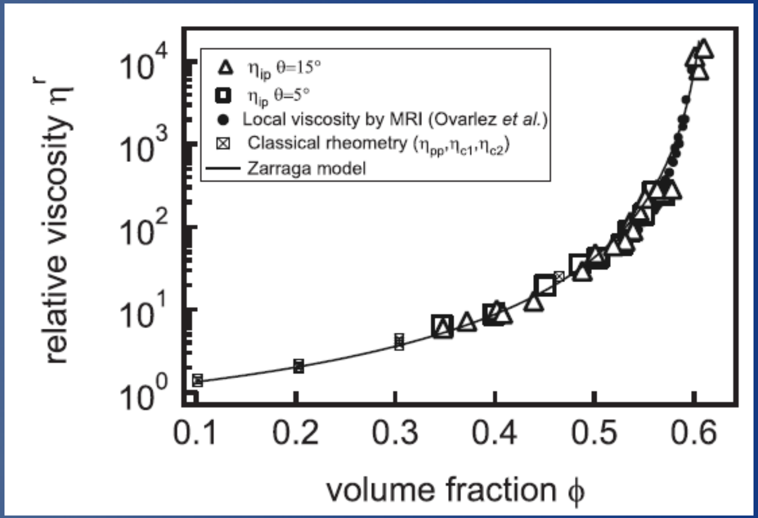


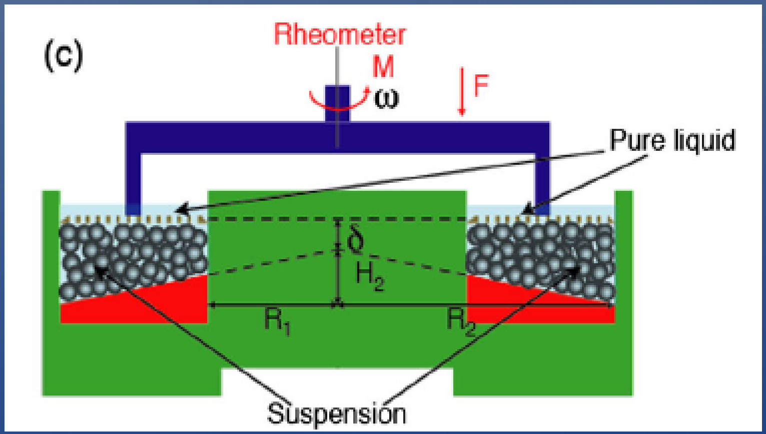
Connection to rheology of particle-based system ?

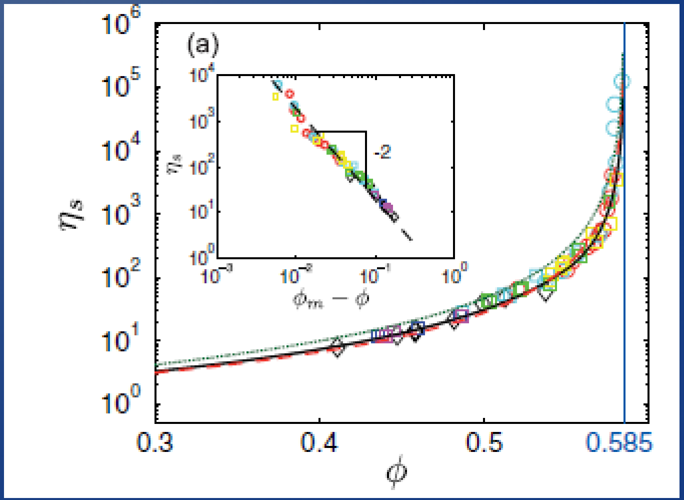
M. Wyart arXiv (2011)

Experiments: granular suspension









C. Bonnoit et al. J Rheol. (2010), Boyer et al PRL (2011)

Viscous dissipation in small gaps

$$h \sim (\phi - \phi_c)$$

- Dissipation volume

$$V_0 \sim h d^2$$

- Local strainrate

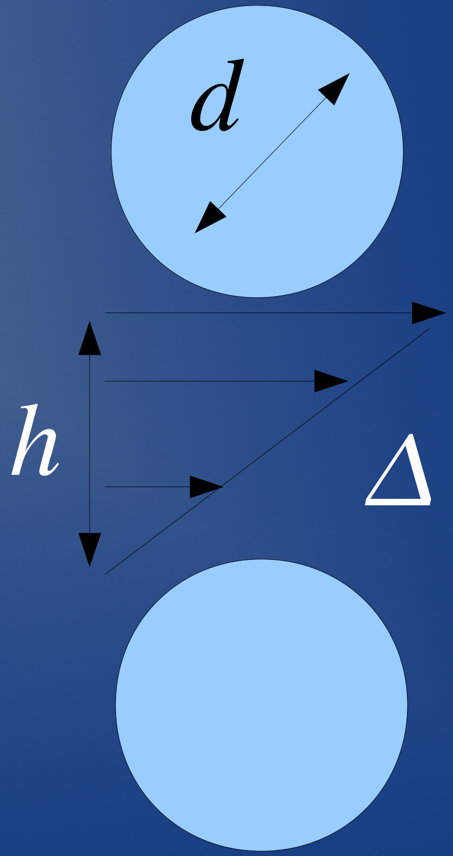
$$\dot{\gamma}_0 = \Delta v / h$$

- Dissipated energy

$$\eta_0 \dot{\gamma}_0^{\,2} V_0$$

- Viscosity $\eta \sim \eta_0 h^{-1}$

  Experiments: -2 ... -3



$$\Delta v \sim \dot{\gamma} d$$

e.g. Mills/Snabre EPJE (2009)

Simulated system

- 2d
- Two particle types
  - diameter a, 1.4a
- Lee-Edwards bc
- Control parameters
  - Particle volume fraction ϕ
  - Strainrate $\dot{\gamma}$
- Observables
  - Shear stress σ
  - Particle trajectories

Dissipative MD Simulations

- Repulsive contact interactions

$$E = k\left(r - r_c\right)^2 \qquad r \leq r_c$$

- Dissipation

$$F_{diss} = -\zeta\left(v - v_{flow}\right)$$

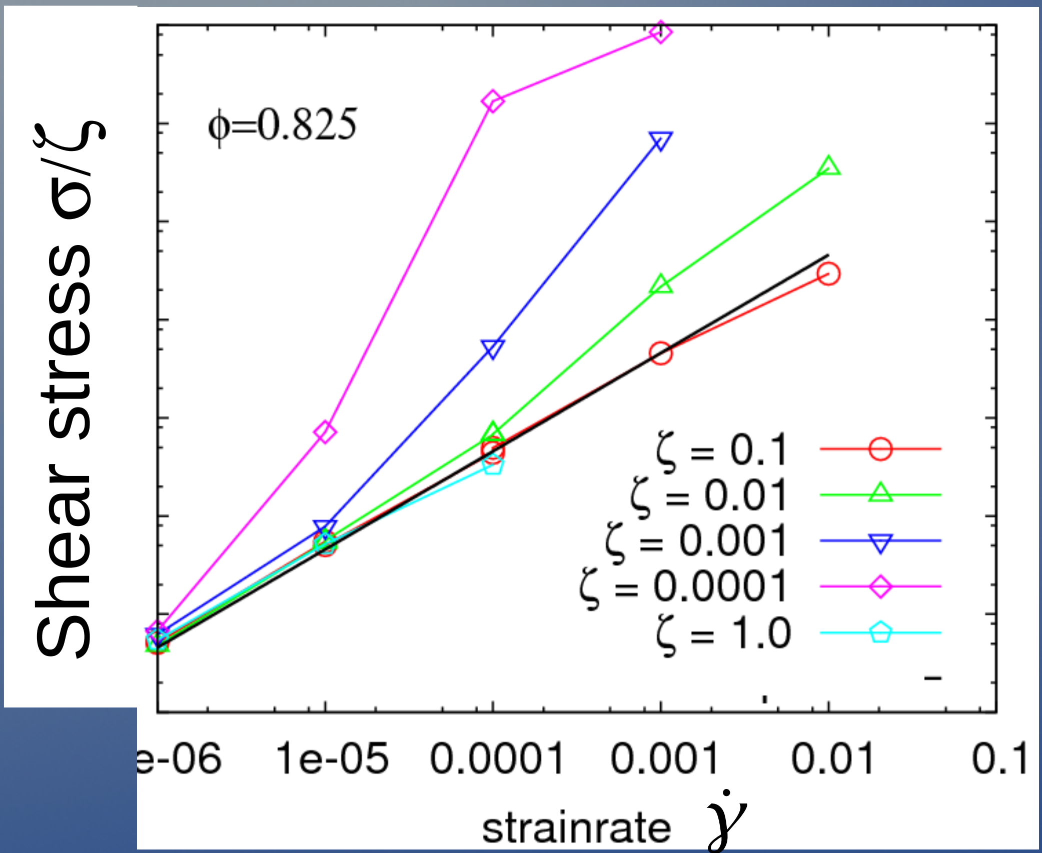
$$v_{flow}(x, y) = \hat{e}_x \, y \, \dot{\gamma}$$

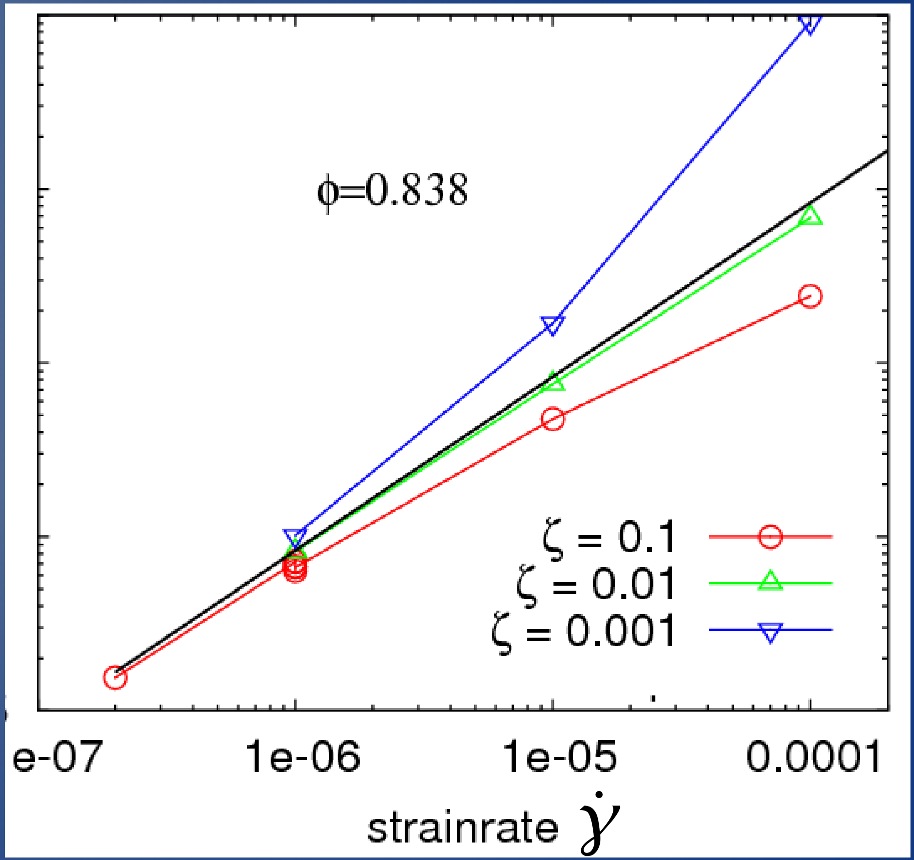
- Inertial forces: mass *m*

- No friction, temperature, no “hydrodynamics”

Flow curve

$\phi_c = 0.843$

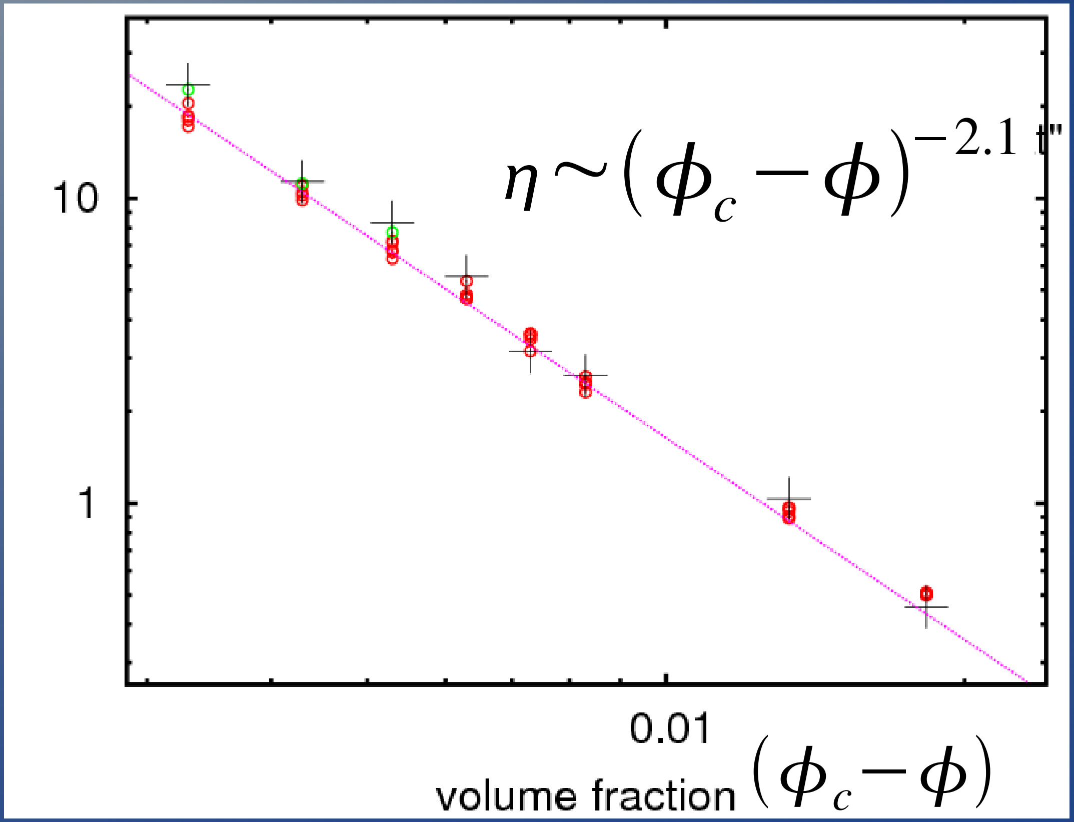




Newtonian – shear thickening – shear thinning

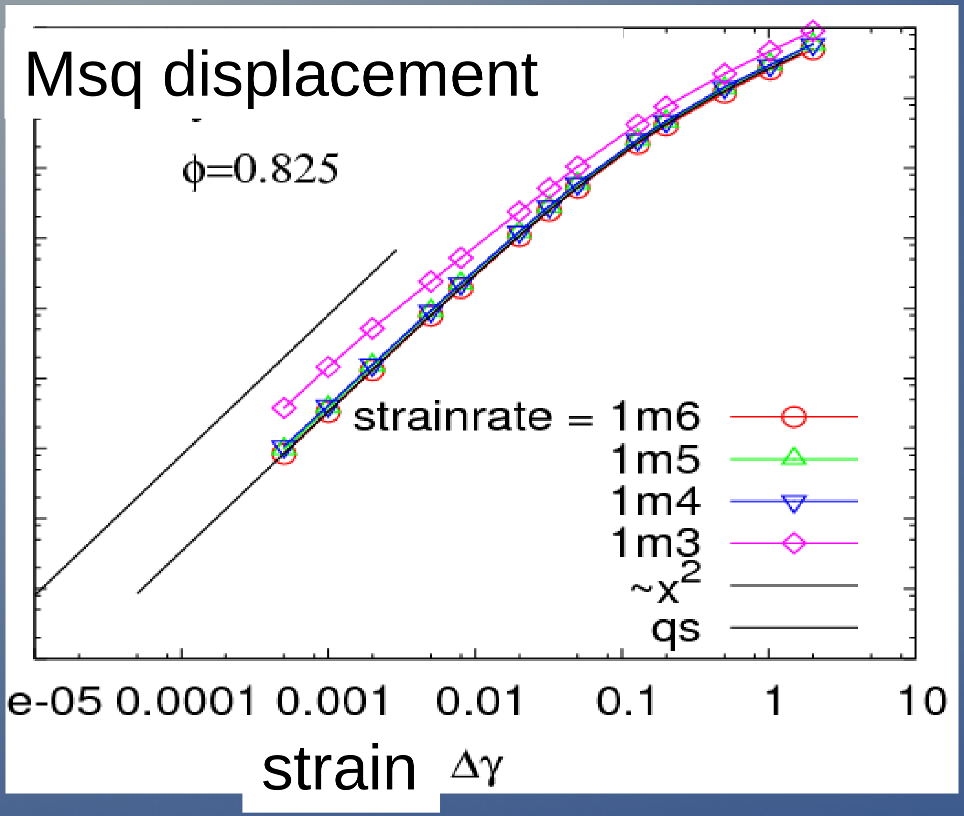
Newtonian regime

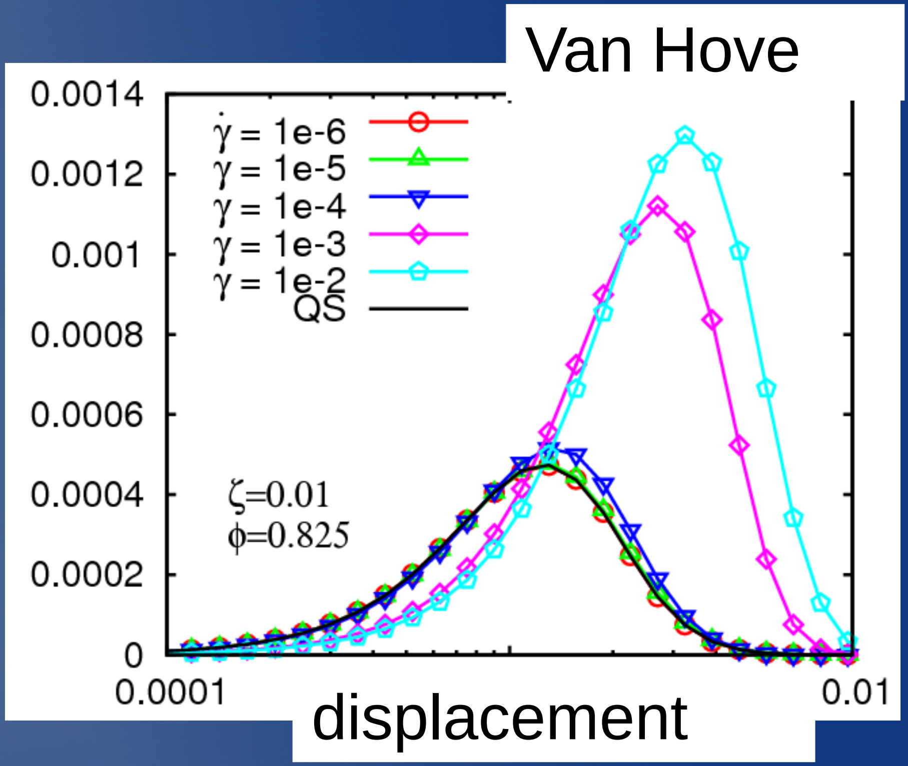
viscosity $\eta = \sigma / \dot{\gamma}$



Also see P. Olsson and S. Teitel PRL (2007), PRE (2011)

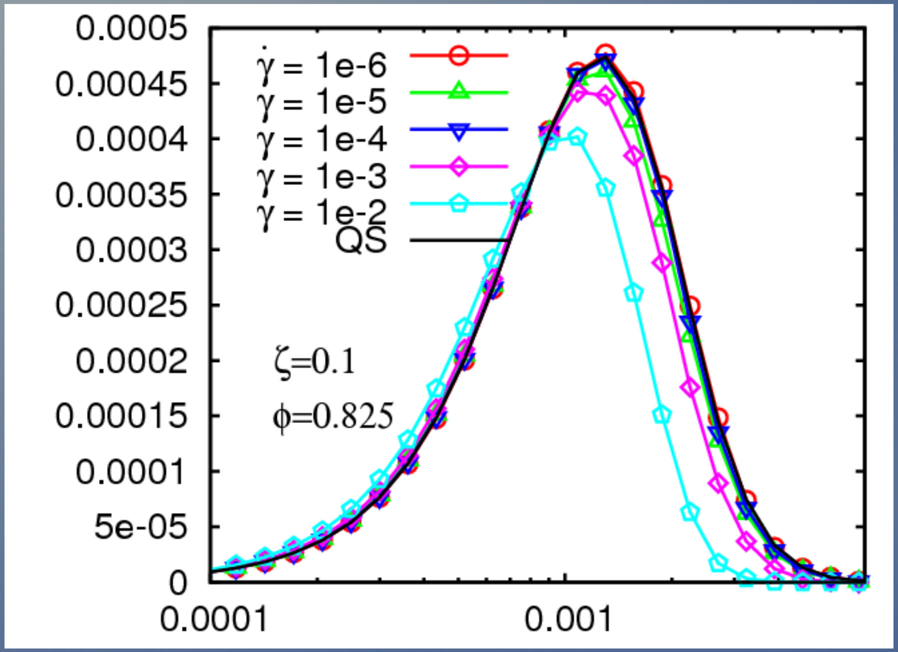
Particle dynamics

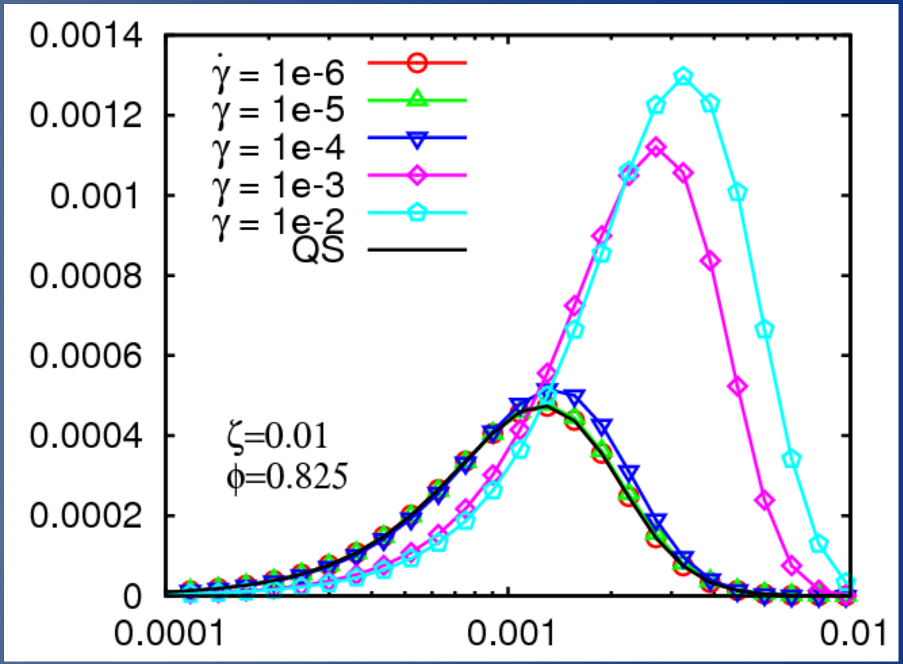


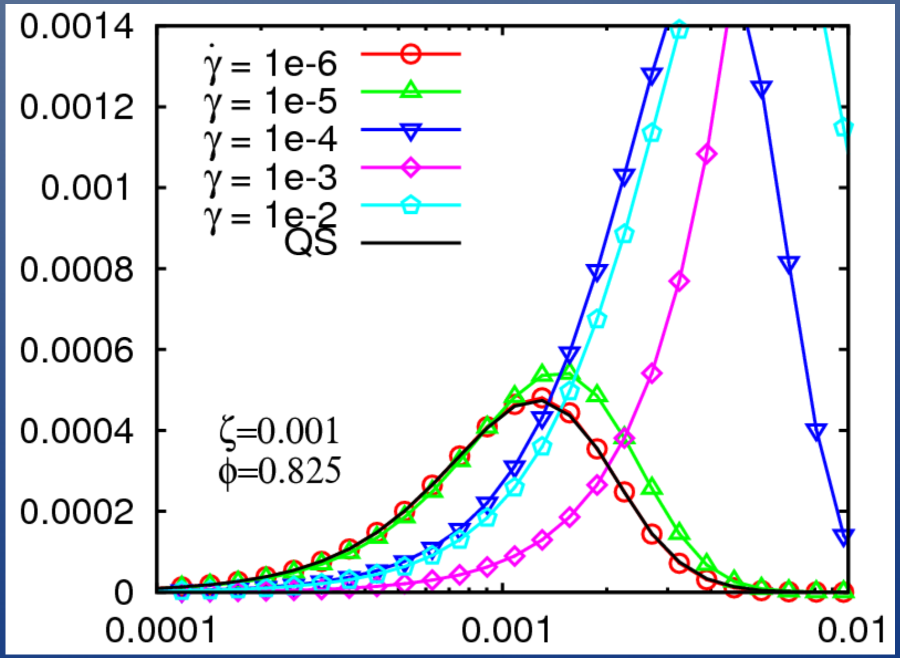


- In Newtonian regime: trajectories strainrate independent
- Identical trajectories from quasistatic simulations (energy minimization, $\dot{\gamma} \to 0$)
- Newtonian = Quasistatic

Role of dissipative coefficient ζ







- In Newtonian regime: trajectories independent of dissipative coefficient ζ

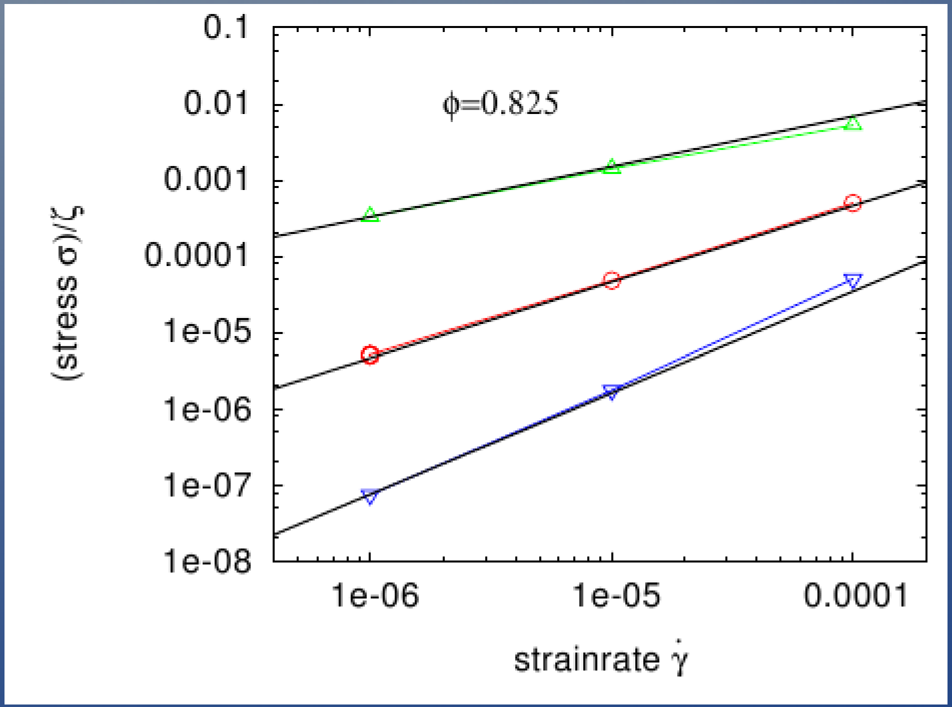
$$F_{diss} = -\zeta(v - v_{flow})$$

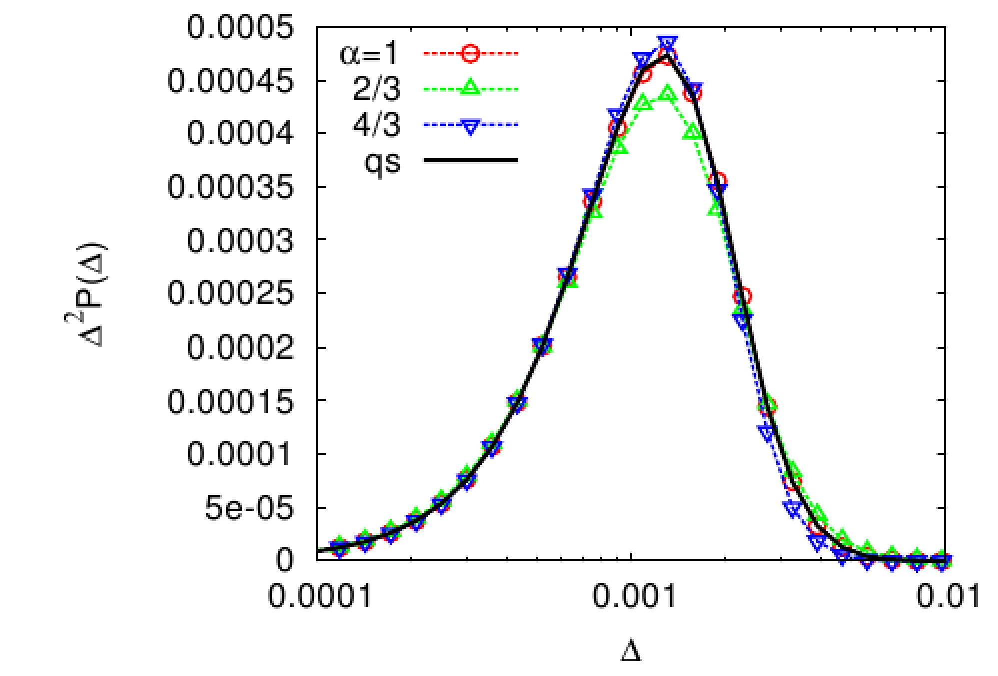
- One and the same QS limit

Modified dissipation law

$$\vec{F}^{\mathrm{visc}}(\vec{v}_i) = -\zeta \delta\vec{v}\,|\delta\vec{v}|^{\alpha-1}$$

Modified Newtonian" regime $\sigma = \hat{\eta}\dot{\gamma}^{\alpha}$

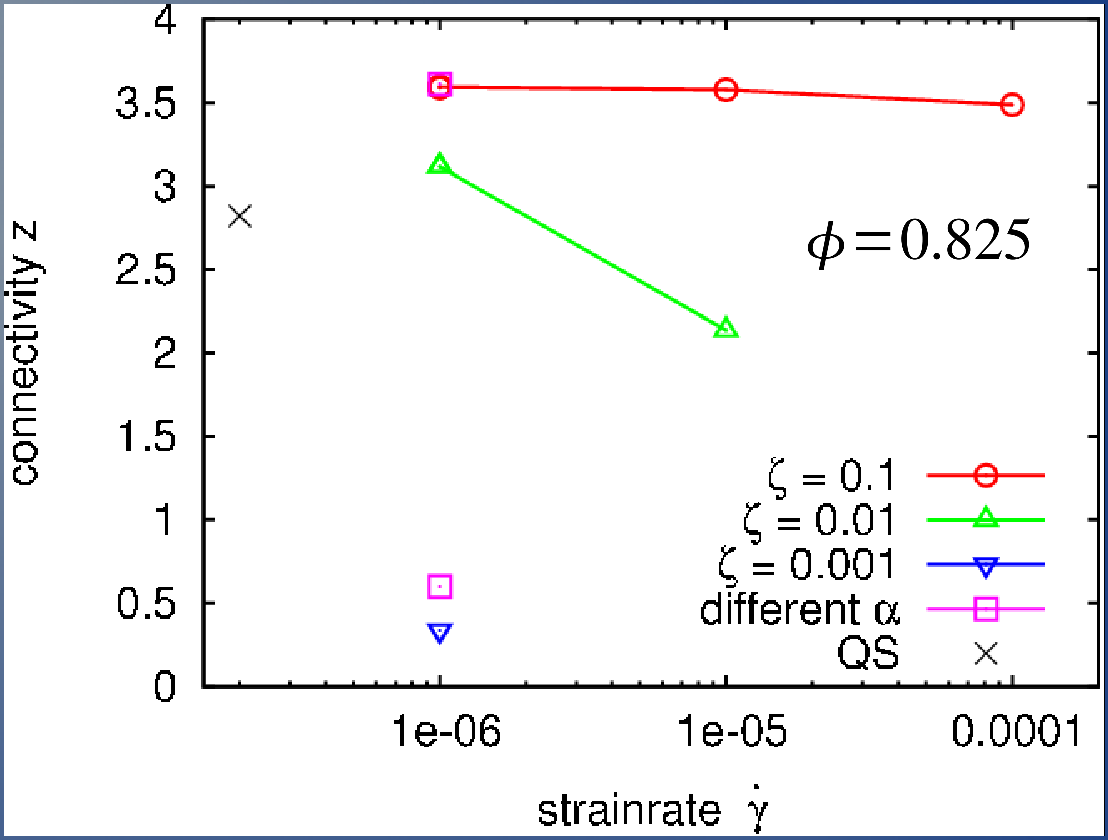




In "Newtonian" regime: trajectories independent of exponent α

Andreotti, Barrat, CH arXiv (2011)

Contacts *z*



- In "Newtonian" regime: contacts z not well defined
- Identical trajectories (and therefore viscosities) with widely varying contact numbers
- No predictive power

“Lack of space”

$\delta\phi = 0.023$

$\delta\phi = 0.003$

Velocity fluctuations $\delta v \sim (\phi_c - \phi)^{-1.1}$

- Fragile: small cause ... large effect

CH, Berthier, Barrat EPL (2010)

$(\phi_c = 0.843)$

Lubrication

- Dissipation volume

$$V_0 \sim h d^2$$

- Local strainrate

$$\dot{\gamma}_0 = \Delta v / h$$

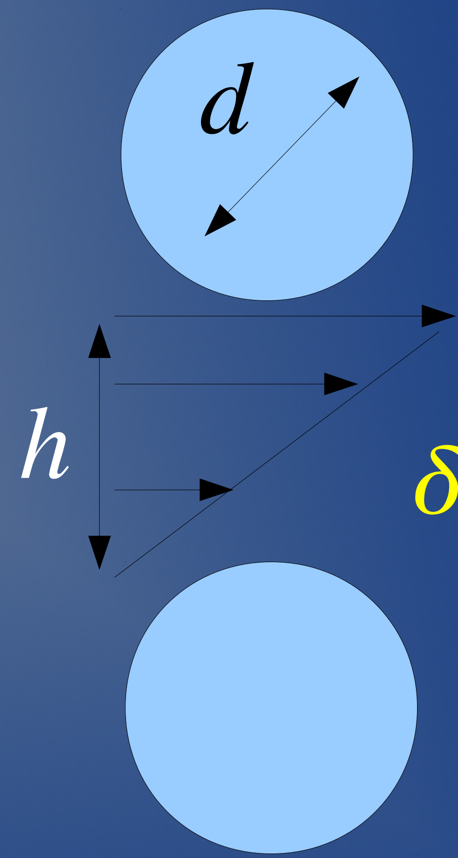
- Dissipated energy

$$\eta_0 \dot{\gamma}_0^{\,2} V_0$$

- Viscosity

$$\eta \sim \eta_0 h^{-1}$$

$$\eta \sim \eta_0 \, \delta\phi^{-(2x+1)}$$



$$\delta v \sim \dot{\gamma} d$$

$$\delta v \sim \delta\phi^{-x} \dot{\gamma} d$$

$$h \sim (\phi - \phi_c)$$

Conclusions: Shear

- Particle trajectories approach unique quasistatic limit in Newtonian flow regime
- Connectivity z is NOT unique in this regime

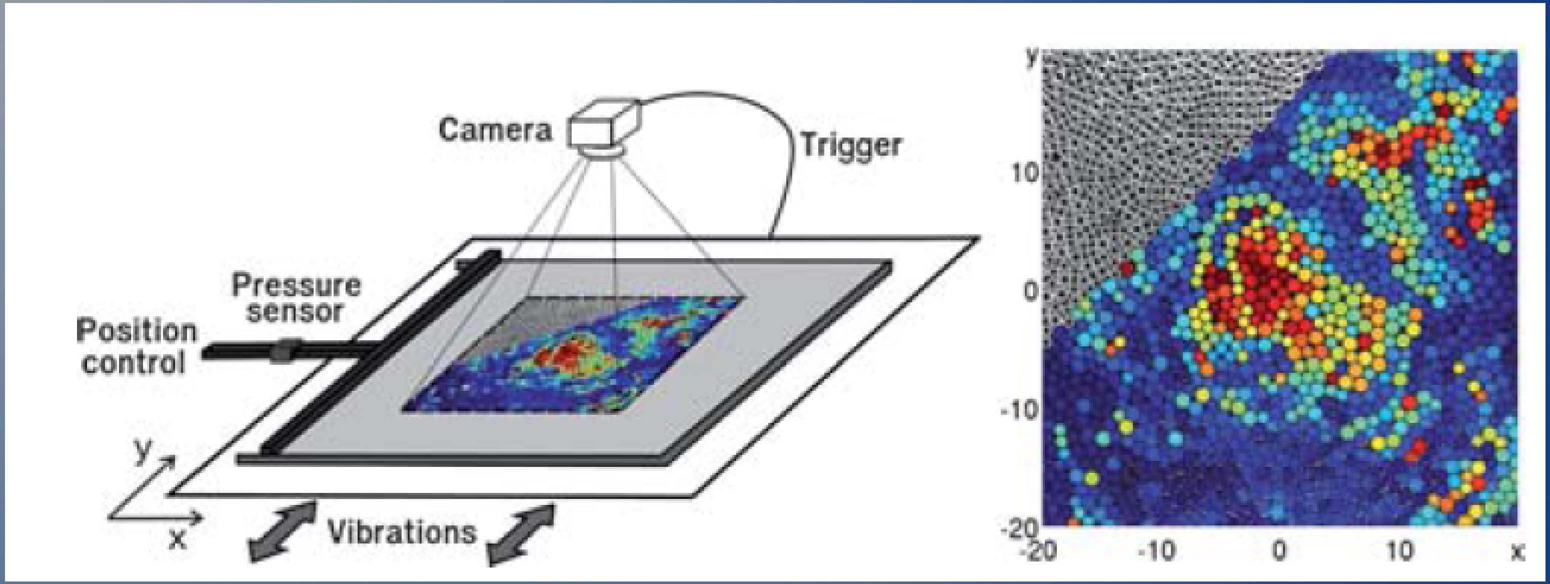
  → Isostatic point not relevant for flow properties
- Rather: “lack of space” leads to singular velocity fluctuations
- Additional contribution to divergence of viscosity

$\phi - \phi_{RCP}$ $z - z_{iso}$

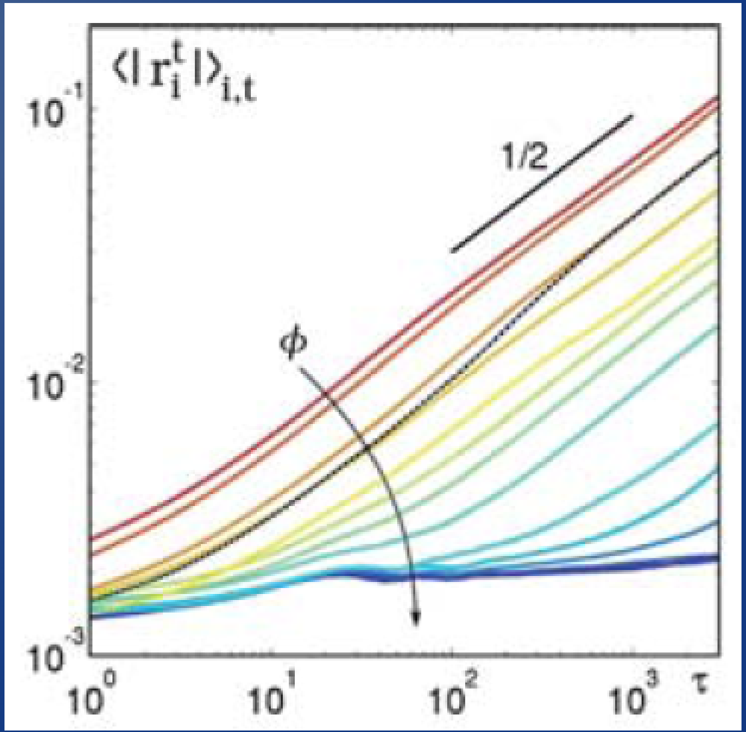
Rattling

“melt a glass by freezing” ??

Motivation



- Dynamics on small lengthscales
- Close to jamming: superdiffusion
- Role of friction: exploration of sub-cage structure ??



Lechenault EPL (2008), Soft Matter (2010)

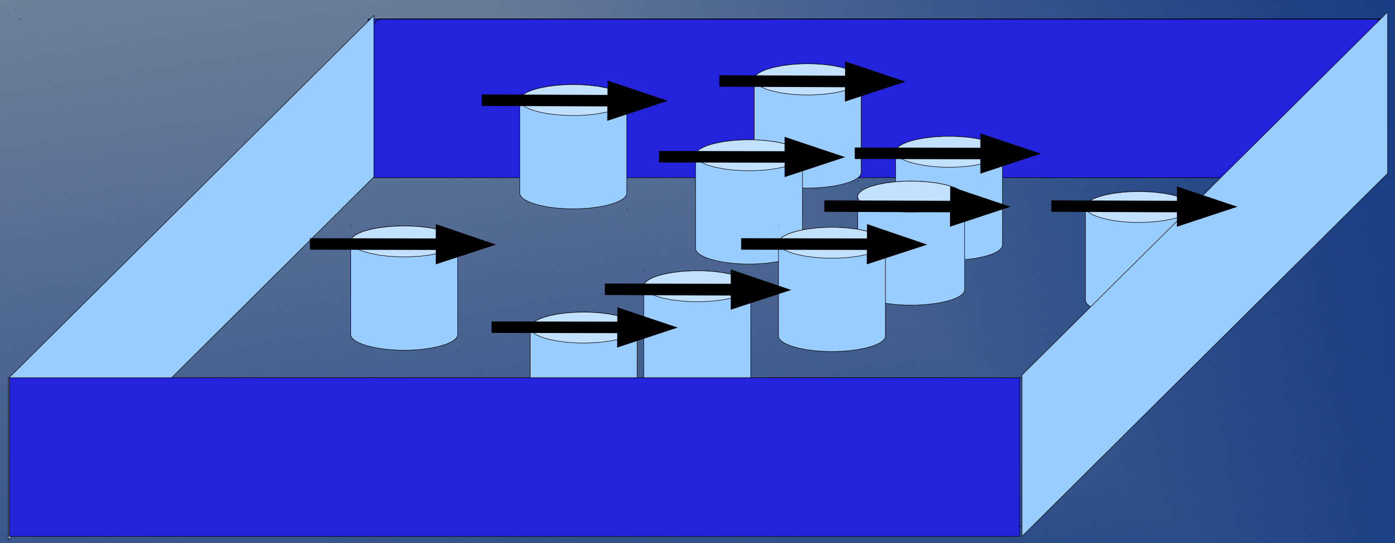
Simulated system

- 2d
- Polydisperse:
  - diameter [a,1.4a]
  - mass [m,1.4^3m]
- Walls on all four sides
- Friction: $F_t \leqslant \mu F_n$
  - Frictional bottom plate
  - Interparticle friction: tangential forces

Driving

Bottom plate stationary

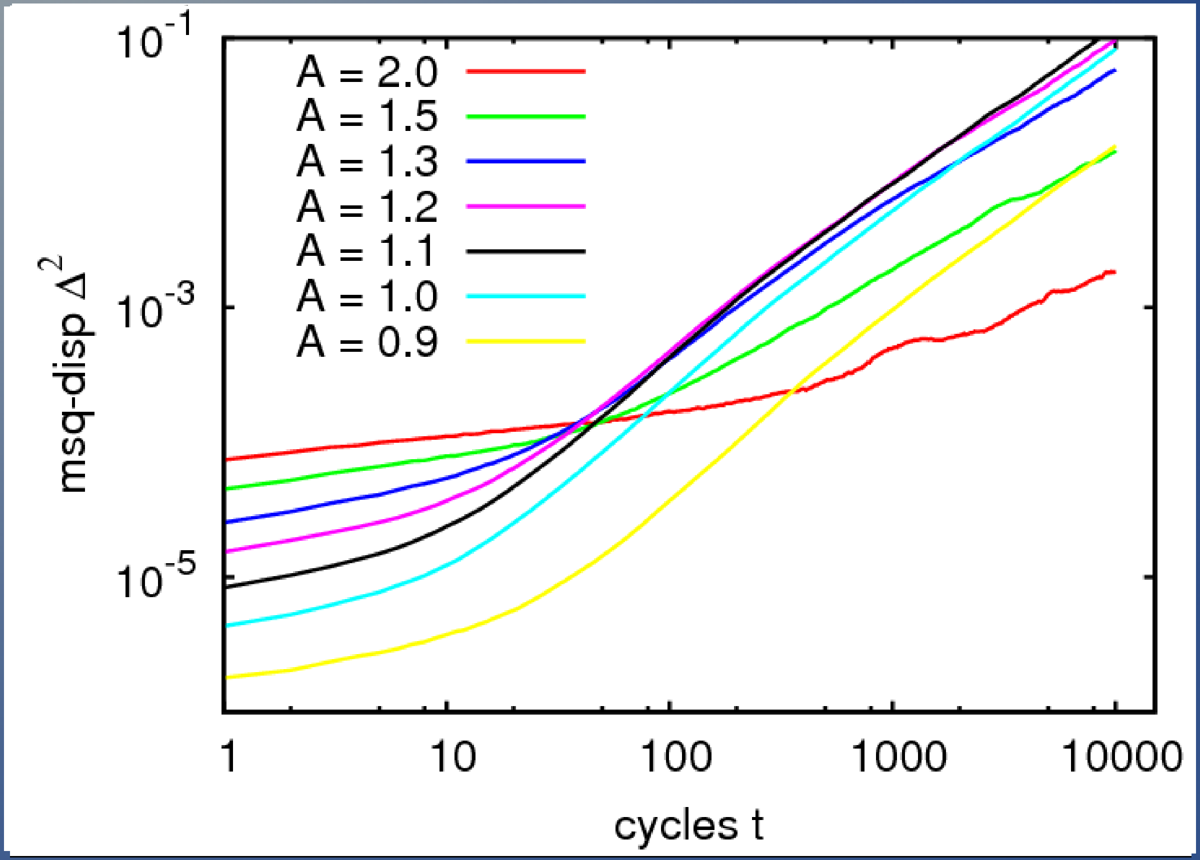
Periodic forcing of particles $F = A\, sin(\omega t)$



Snapshots after $t_k = k \cdot 2\pi / \omega$

Vary the amplitude A

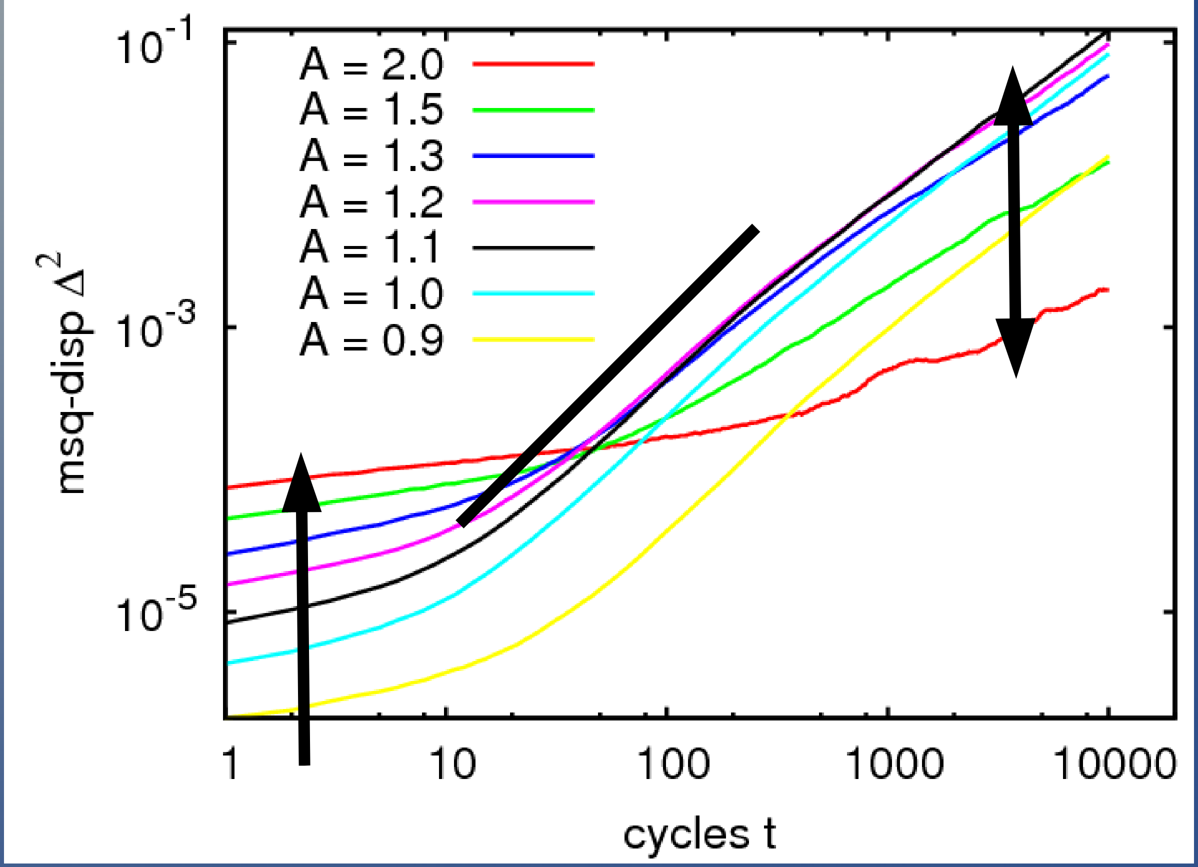
Particle dynamics: msq-disp



No interparticle friction

$\phi = 0.835$

Particle dynamics: msq-disp

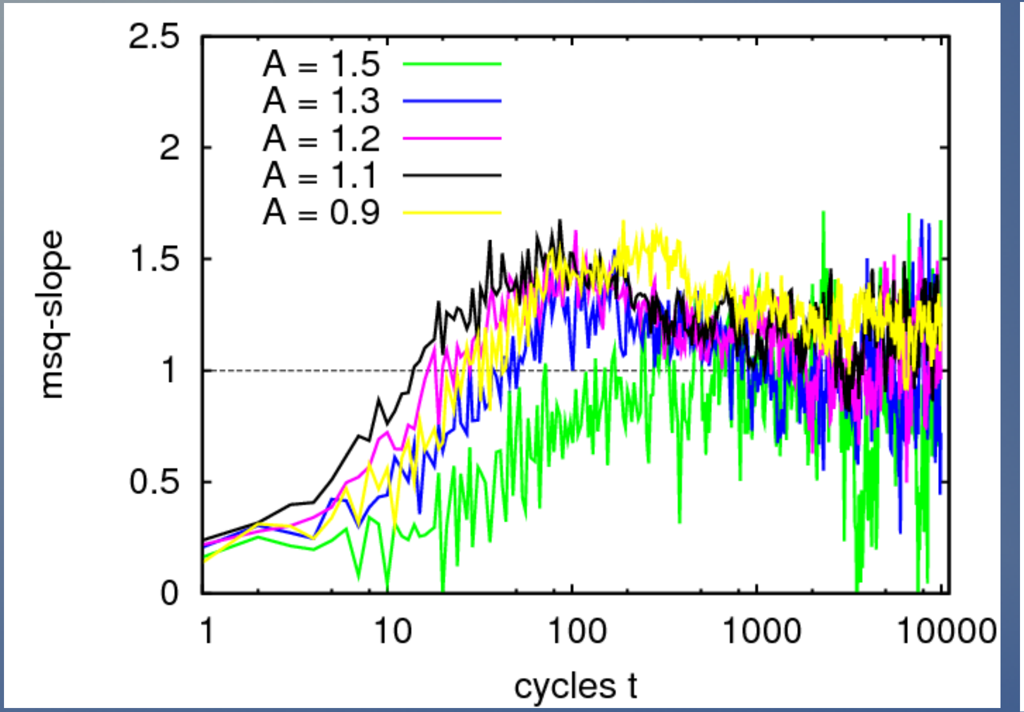


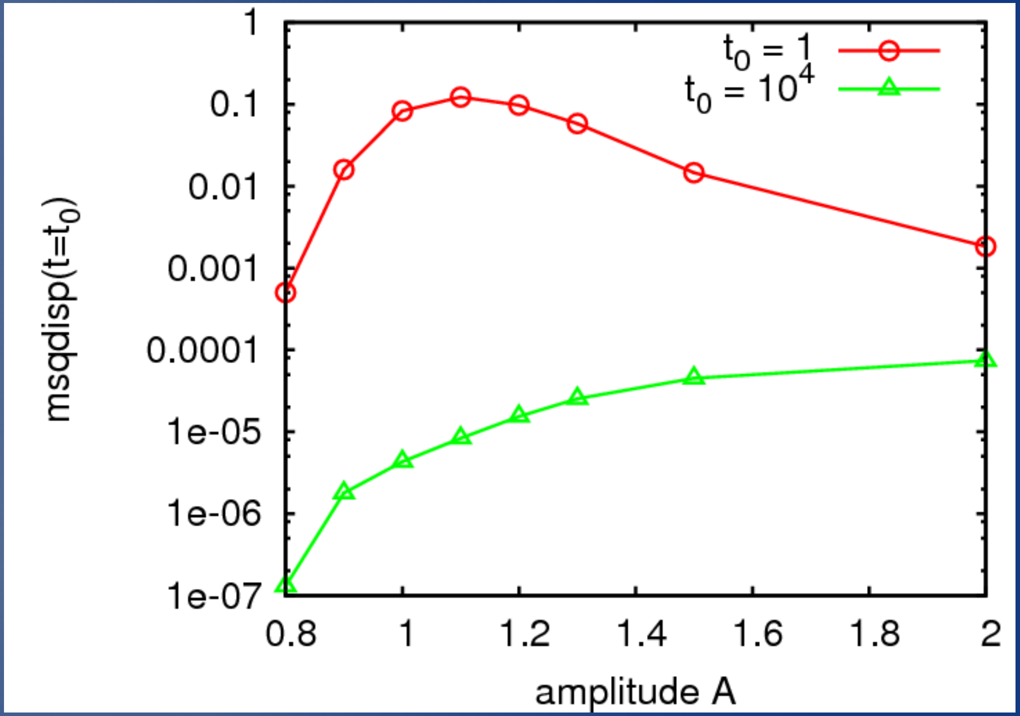
No interparticle friction

$\phi = 0.835$

- Short times: activity decreases with driving
- Long times: diffusion constant nonmonotonic
- Intermediate times: superdiffusion

Anomalous diffusion

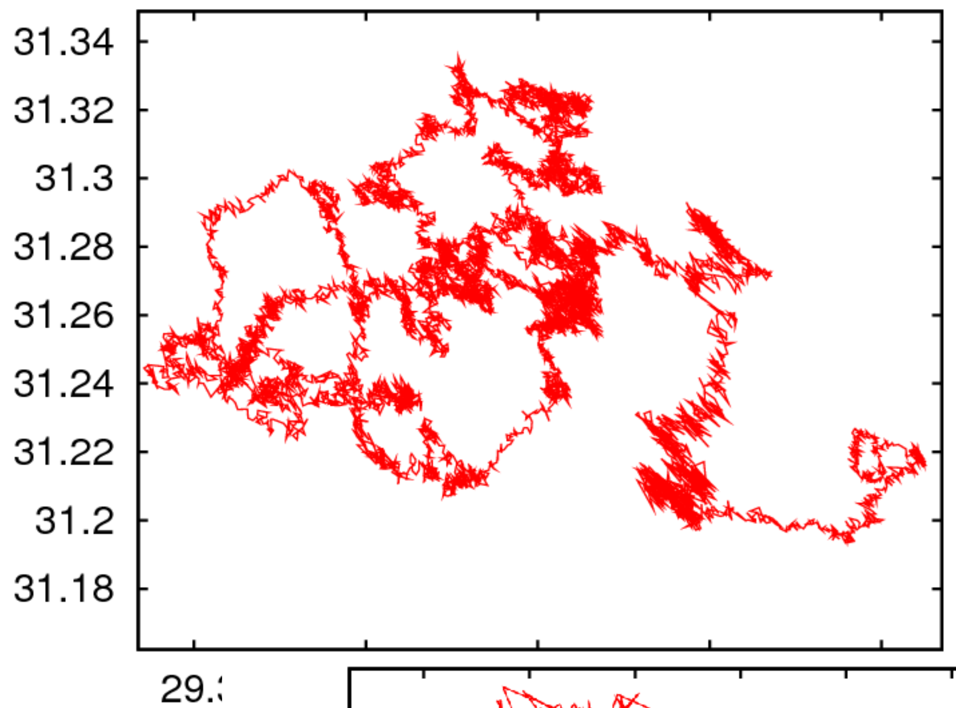


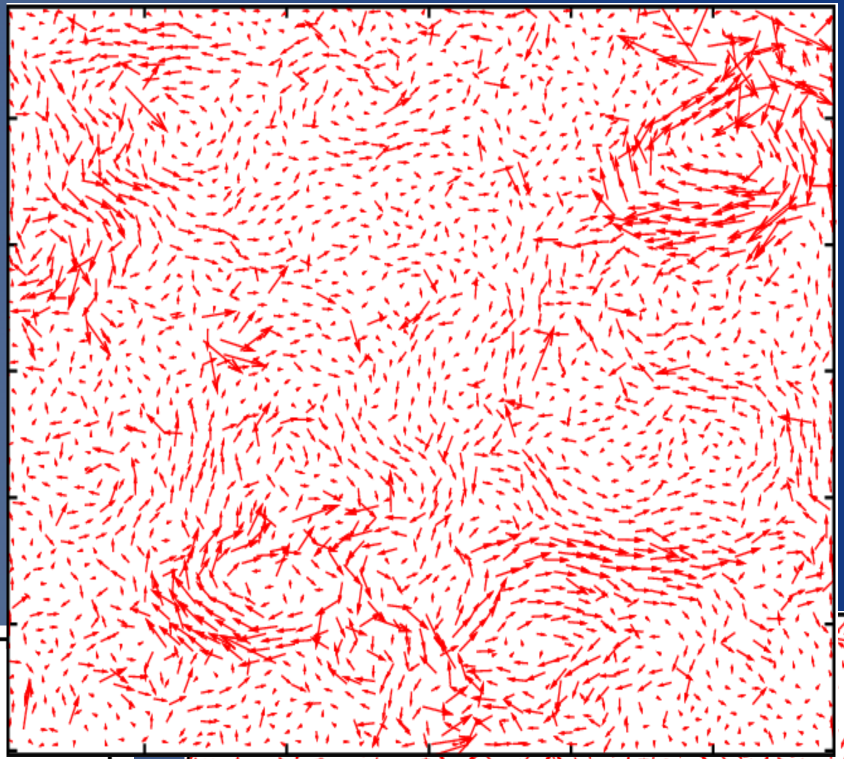


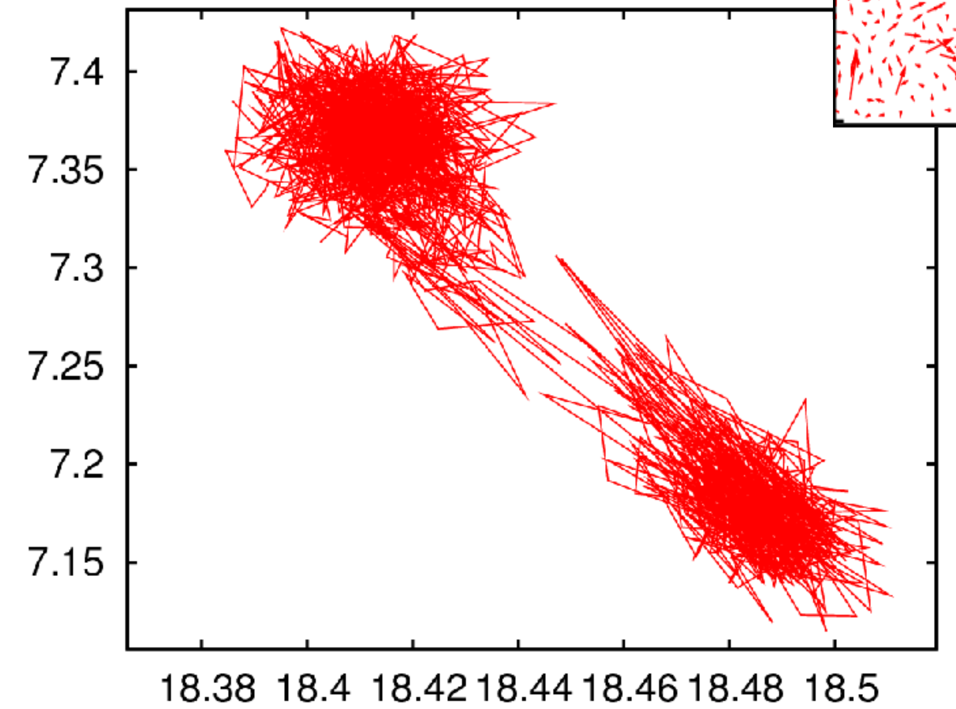
- Superdiffusion t < 1000 cycles
- Diffusivity maximum: A_c=1.1

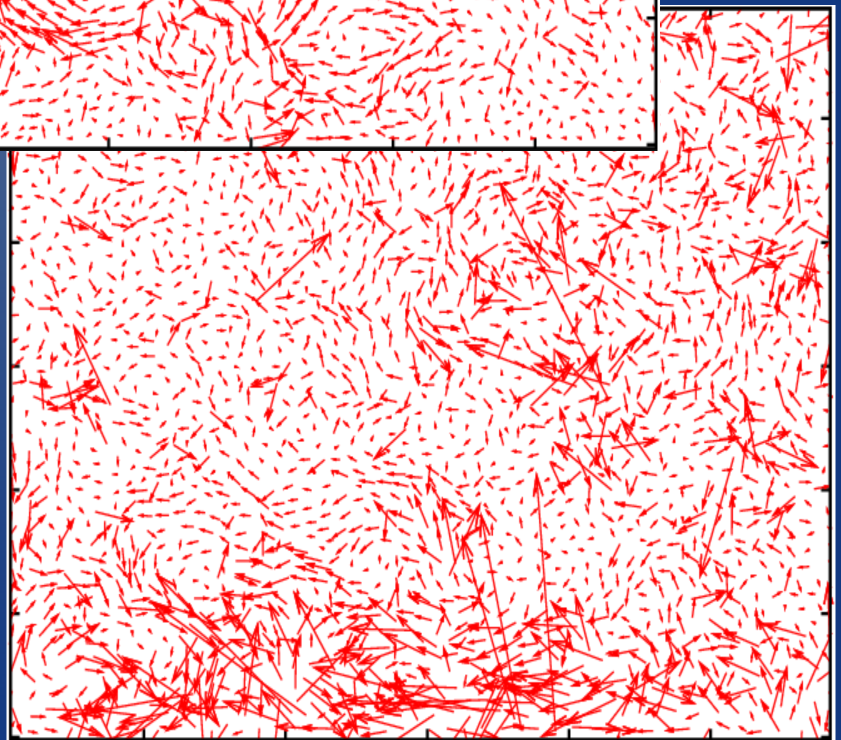
Trajectories

$A=A_c$









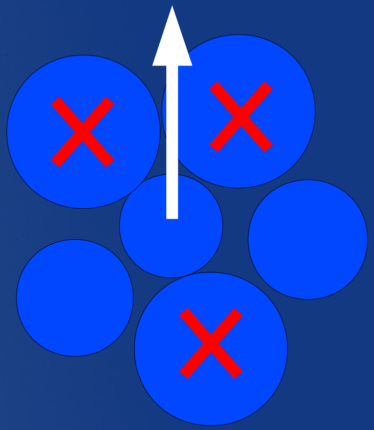
$A>A_c$

Role of friction: bottom plate

- Driving force $F_{drive} \sim A$

  vs. friction $F_{friction} \leqslant \mu m_i g$
  - Mobility threshold:

$$A_i > \mu m_i g$$



- At A_c: heavy particles immobilized
  - pushed around by light particles
  - Matrix of heavy particles evolves slowly
  - Memory effect, which leads to superdiffusion

- At $A > A_c$: glassy phase, vibrations erase memory

- Always hammer at the same place
- Make sure the hole is still there

Conclusion
Experiment – Simulation

Experiment:

- Superdiffusion
  - at phic

Simulation:

- Superdiffusion
  - Range of phi; no strong variation

Role of friction: helps fixating displacement steps

Experiment:

- Levy flight
- Spatial but no temporal correlations
- “hard-spheres”

Simulation:

- Exponential tails
- Spatio-temporal correlations
- Particles are much softer !

Lechenault EPL (2008), Soft Matter (2010)