Oscillatory deformation of amorphous materials: a numerical investigation

Davide Fiocco

PhD private defense

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My thesis in a nutshell

Study the behavior of model **metallic glasses** under deformation, by means of atomistic computer simulations

Figure : Shear strain $\gamma = \tan\theta$ is varied between $-\gamma_{max}, \gamma_{max}$

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Figure : Shear strain $\gamma = \tan\theta$ is varied between $-\gamma_{max}, \gamma_{max}$

1. What happens in the deformed glass at a microscopic level?
2. Are there any similarities with other systems?

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Manufacturing of a metallic glass

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- Brittle failure ✗

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Input and benchmarks for mesoscopic descriptions (e.g. STZ)

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Examples of microscopic models

- Embedded Atom Potentials (EAM)
- Lennard-Jones mixtures (LJ)

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One can then unleash the arsenal of numerical integration methods

Simulating glasses with LJ binary mixtures

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Tuning of the LJ interaction potential

Parameters in the potential

$$\phi_{ij}(r) = 4\epsilon_{ij}\left(\left(\frac{\sigma_{ij}}{r}\right)^{12} - \left(\frac{\sigma_{ij}}{r}\right)^{6}\right)$$

are chosen so to make the system less prone to crystallization/phase separation

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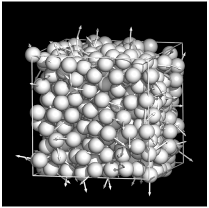

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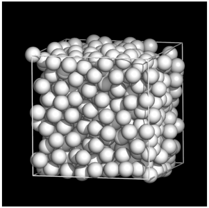

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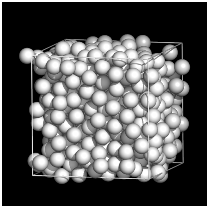
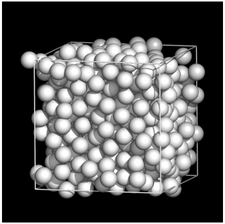


1. The system can be equilibrated at constant T with a Nosé-Hoover thermostat
2. Velocities are disregarded
   and configurations are energy minimized with a conjugate-gradient algorithm

Properties of undeformed samples

Energy minimization of configurations equilibrated at T yields *inherent structures* with *effective temperature* T



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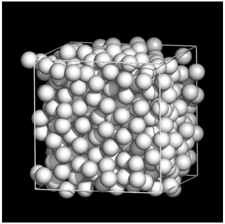

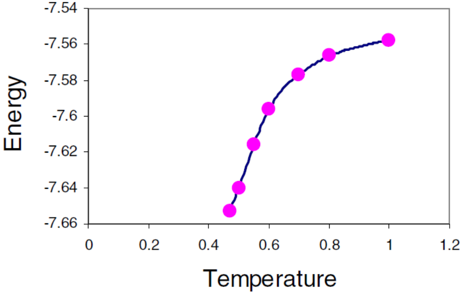

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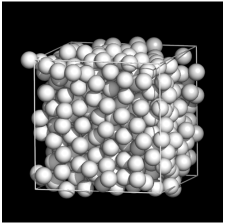
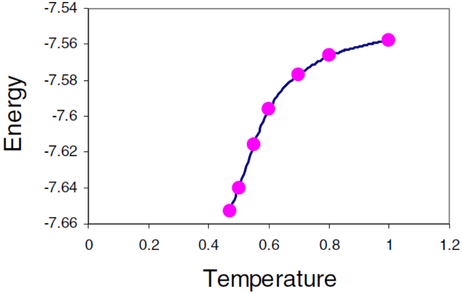


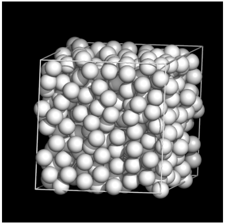


The properties of the inherent structures depend on the effective T

How to deform them?

Deformation

Deformation protocol: athermal quasi-static (AQS)



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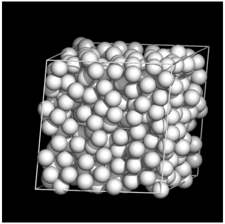

1. Affine transformation $+$
   update of the boundary conditions
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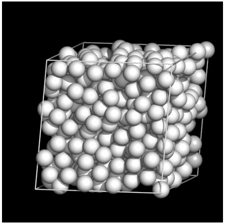

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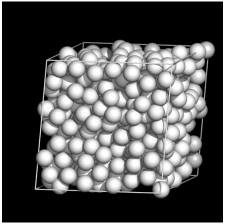

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   update of the boundary conditions
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- By iterating the steps, one can reach arbitrary strains

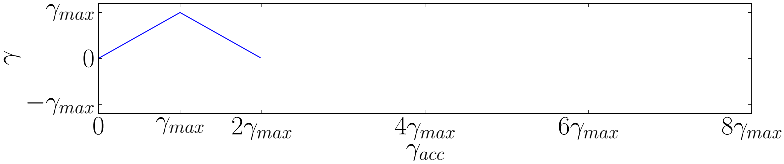
What is the effect of changing the strain?

in 3D space

in ($3N$D) configuration space

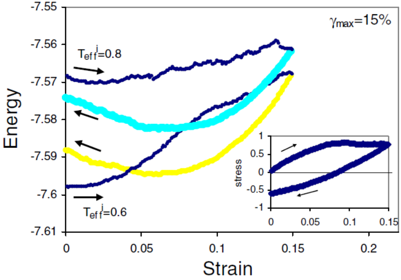
Oscillatory strain

Consider a triangle wave strain profile ranging in $[-\gamma_{max}, \gamma_{max}]$, and define $\gamma_{acc} = \sum |d\gamma|$



What is the effect of a single semicycle?

Straining the sample back and forth once[1]



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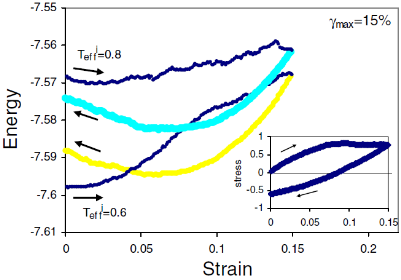

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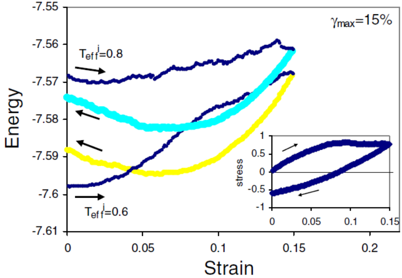

- Samples differing in their effective T change their energy
- The result (increase or decrease) depends on T (and γ_{max})

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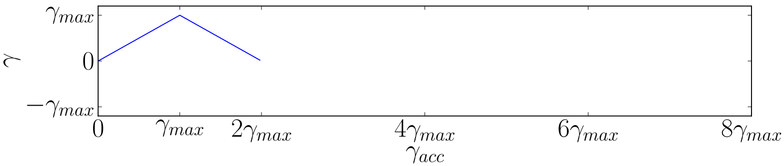

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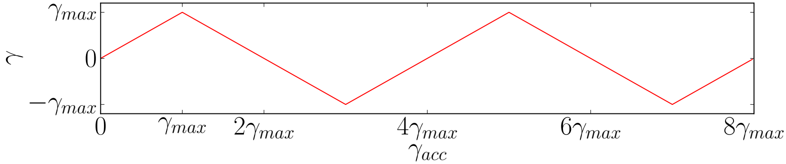

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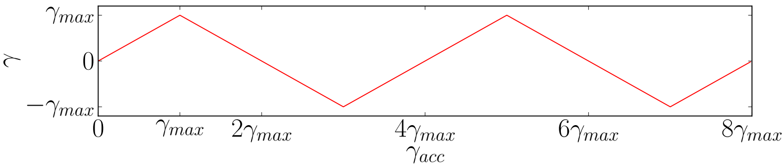

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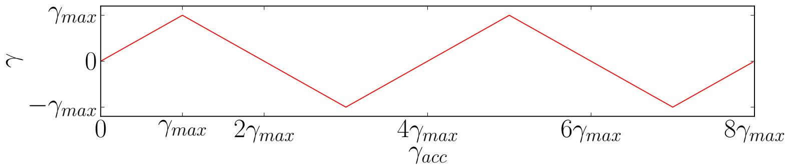

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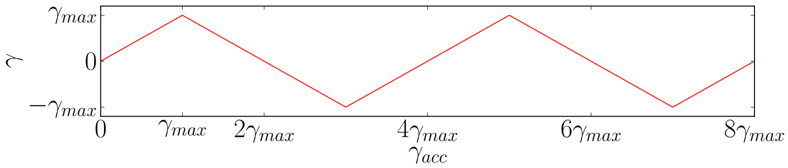

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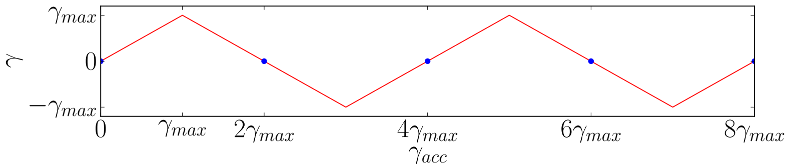

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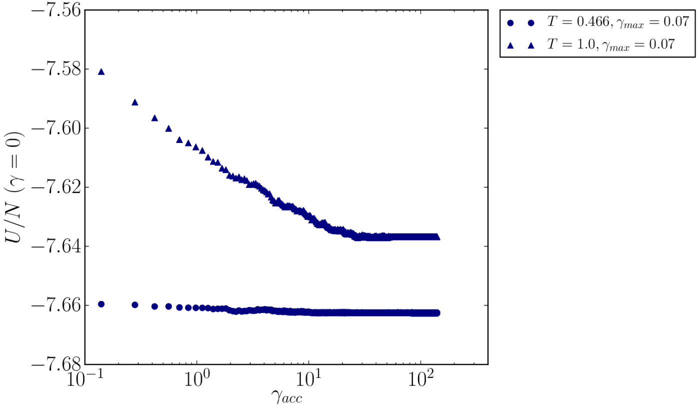

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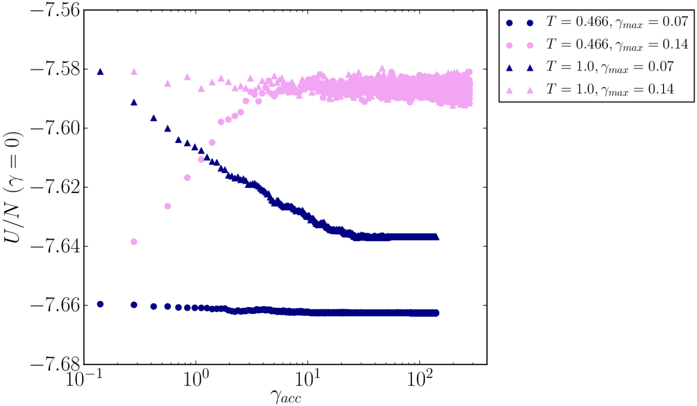

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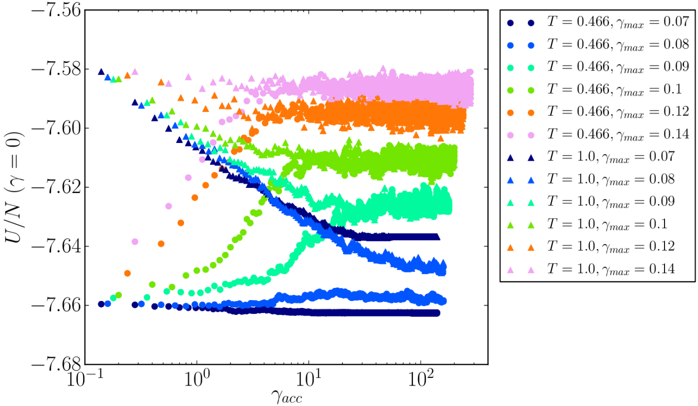

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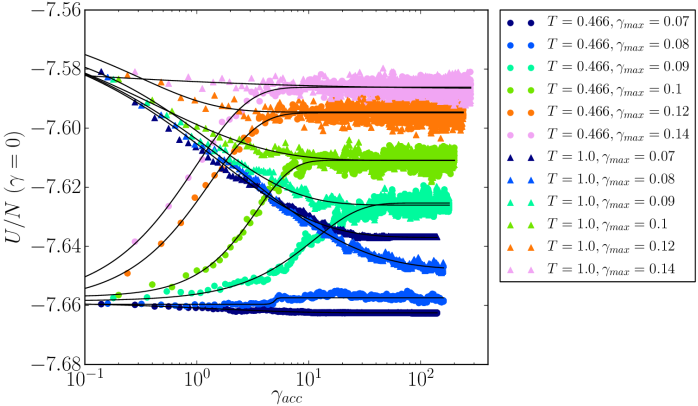

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  - Low γ_{max}: fixed values of U_∞, dependence from T
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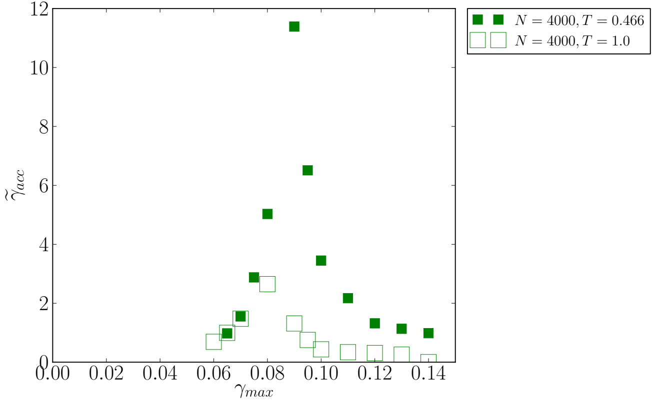
- Energy profiles are described by stretched exponentials

$$U = (U_0 - U_\infty)e^{-(\gamma_{acc}/\widetilde{\gamma}_{acc})^\alpha} + U_\infty$$

Values of $\widetilde{\gamma}_{acc}$ from the energy fits

$\widetilde{\gamma}_{acc}$ marks the onset of a "steady state"



- $\widetilde{\gamma}_{acc}$ peaks for some intermediate value

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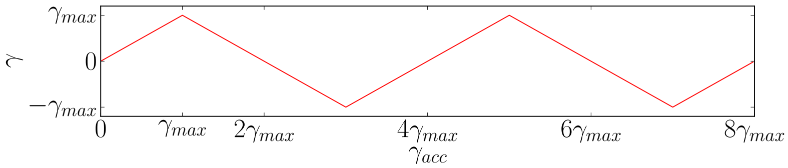

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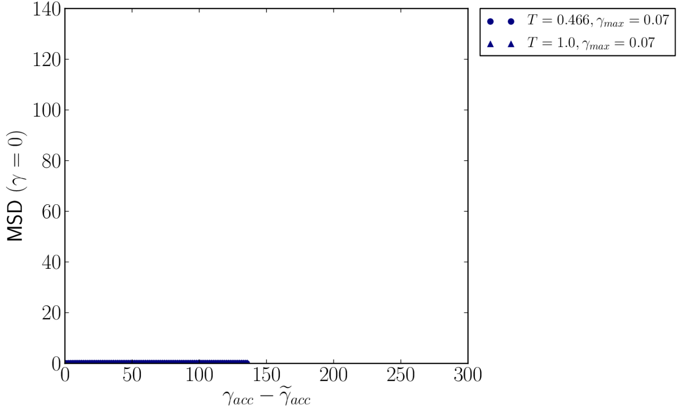
MSD in the asymptotic state

The MSD measured from samples encountered for $\gamma_{acc} > \widetilde{\gamma}_{acc}$



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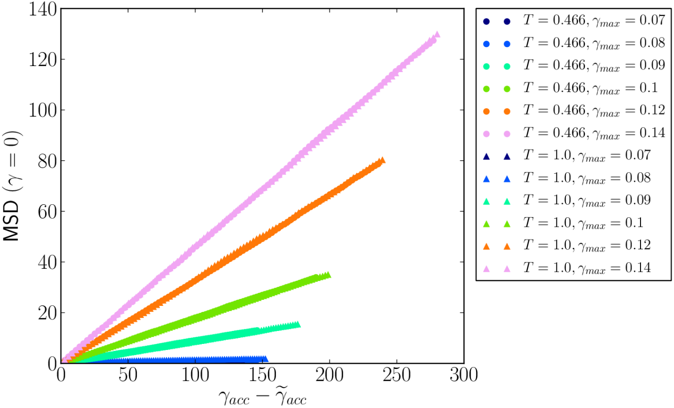

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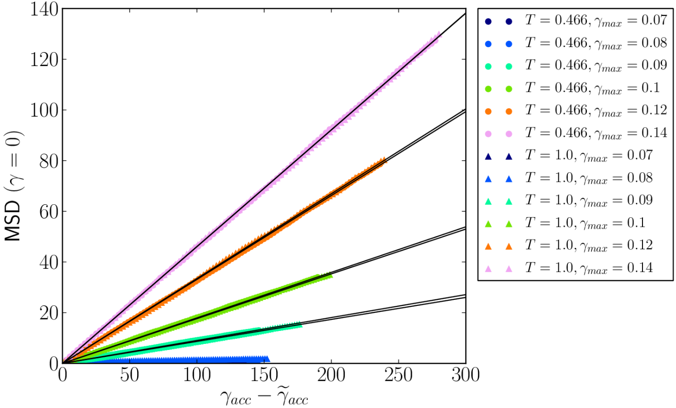
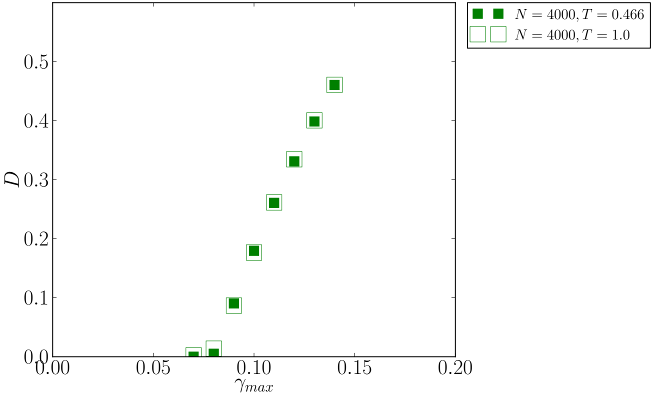


- Two regimes:
  - Low γ_{max}: samples do not move at all (absorbing)
  - High γ_{max}: samples diffuse
- The trends can be fit with: $\text{MSD} = D(\gamma_{acc} - \widetilde{\gamma}_{acc})$

Values of D extracted from the MSD



- A transition at a value γ_c

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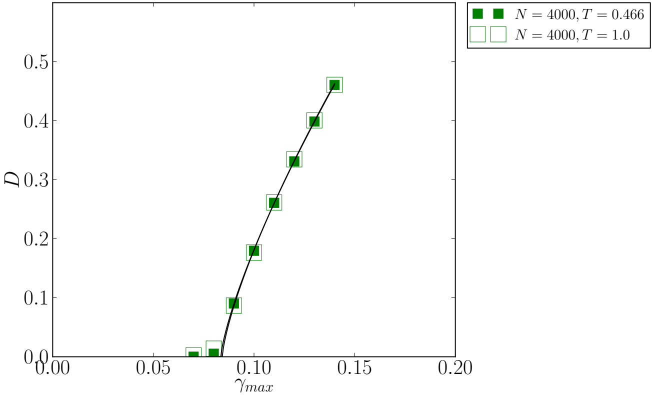

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- $D \propto (\gamma_{max} - \gamma_c)^{\beta}$?

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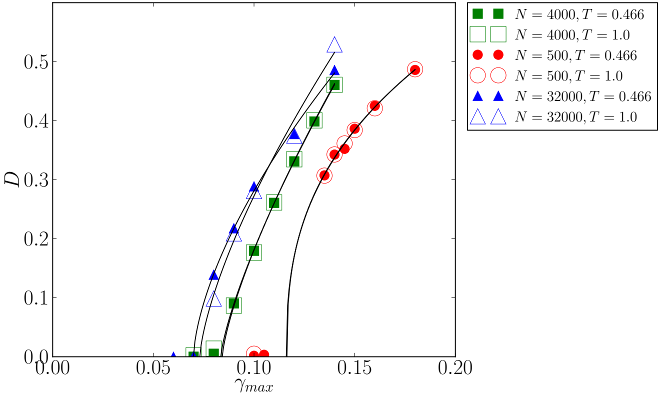

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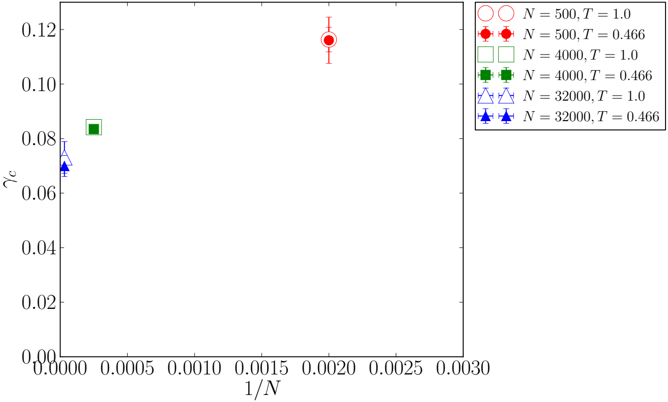
Scaling of γ_c



The putative γ_c seems not to be vanishing for $N \to \infty$

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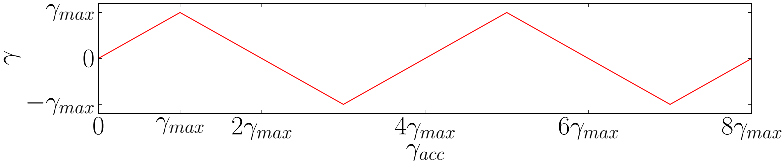

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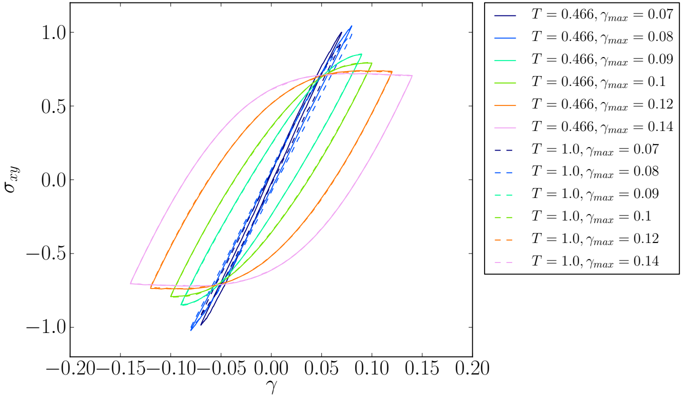

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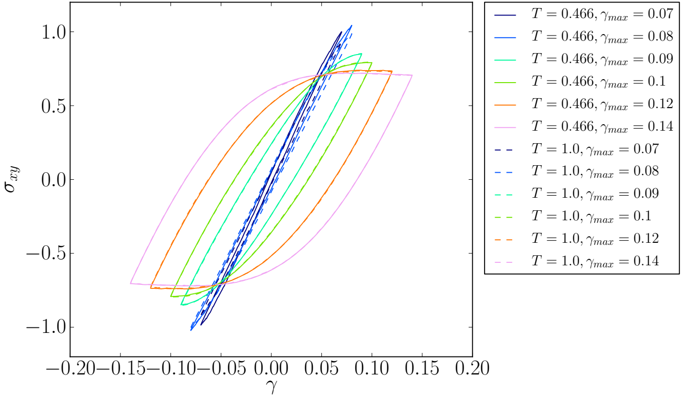
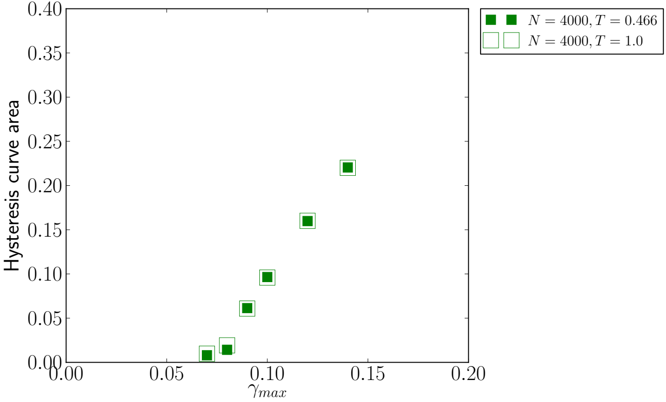


- Two regimes:
  - Low γ_{max}: narrow curves
  - High γ_{max}: broad curves

Area of the hysteresis curves



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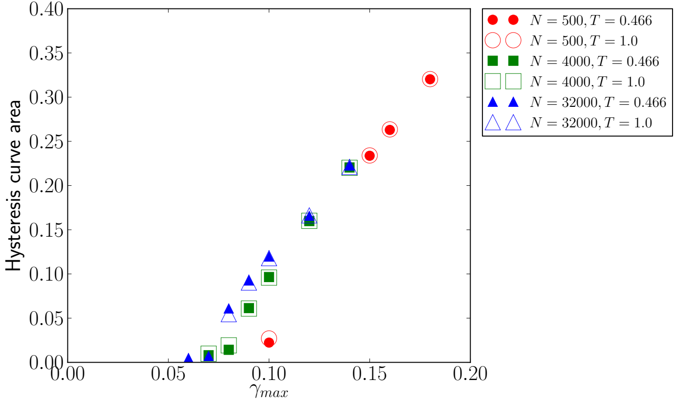

The onset of dissipation is compatible with γ_c

A comparison: suspensions and their behavior[2]

- Particles suspended in a viscous medium

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- *Active* particles collide with others during a cycle and don't come back to the initial position

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A comparison: suspensions and their behavior[2]

- Particles suspended in a viscous medium
- *Active* particles collide with others during a cycle and don't come back to the initial position
- After some cycles the number of active particles doesn't change anymore

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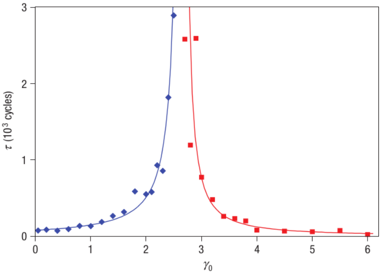
Suspensions and their behavior[3]: a comparison



- The number of cycles needed to reach the steady fraction of active particles resembles $\widetilde{\gamma}_{acc}$ in LJ

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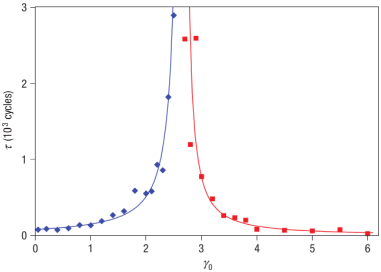

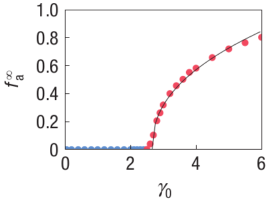

- The number of cycles needed to reach the steady fraction of active particles resembles $\widetilde{\gamma}_{acc}$ in LJ
- The asymptotic fraction of active particles as a function of γ_{max} resembles D in LJ

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Partial summary: existence of a transition

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- The scenario is qualitatively similar to that of suspensions

Pushing the analogy further: memory phenomena[4]

Training at γ_1 Reading at different γ_r

Encoding and reading of memory

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Encoding and reading of memory

- Samples are *trained* by N_{cyc} cycles of amplitude γ_1
- Trained samples are *read* with one cycle of amplitude γ_r: the number of active particles is measured as a function of γ_r

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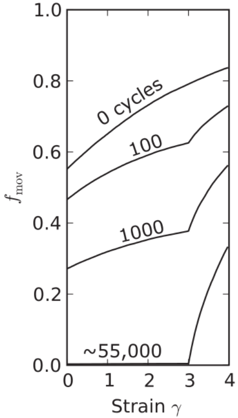
Memory phenomena in suspensions (continued)



- Trainings produce samples which bear a trace of γ_1 when read

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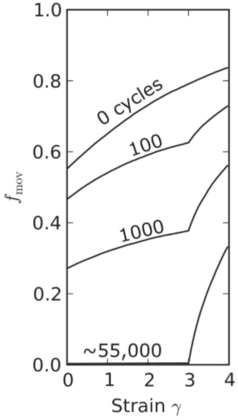

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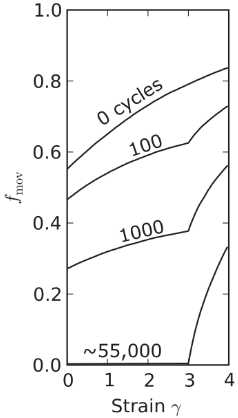

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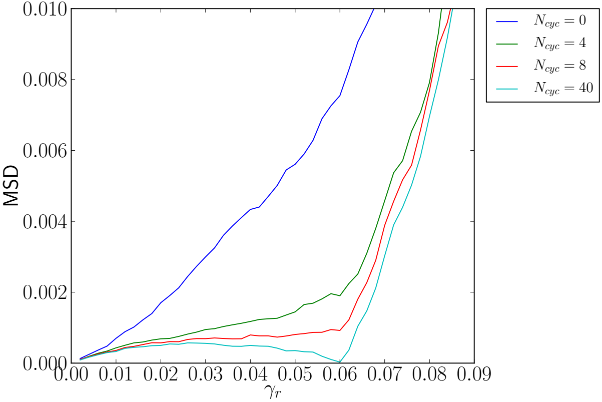
What happens if one applies the same protocol to a LJ sample?

Single memory in LJ samples

Take the MSD of particles of trained samples read with γ_r:



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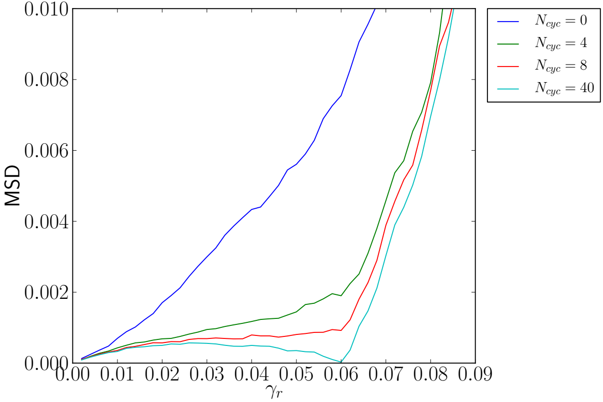

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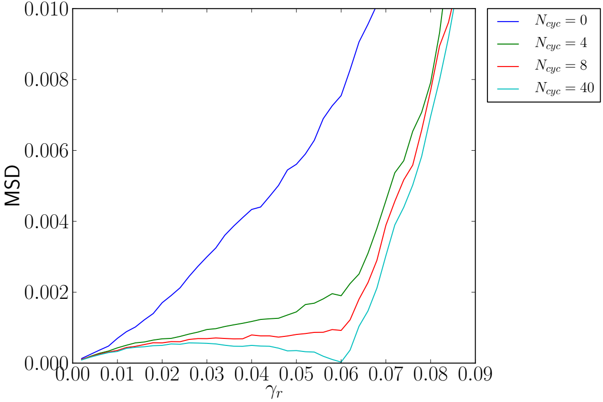

- The behavior agrees qualitatively with that of suspensions
- The "bump": MSD $\neq 0$ if $\gamma_r < \gamma_1$, even for long trainings

Why the bump?

$\gamma_r < \gamma_1$ $\gamma_r = \gamma_1$ $\gamma_r > \gamma_1$

- A sample trained at γ_1 returns into the original state after a reading cycle $\gamma_r = \gamma_1$, via a sequence of rearrangements

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- A sample trained at γ_1 returns into the original state after a reading cycle $\gamma_r = \gamma_1$, via a sequence of rearrangements
- If the amplitude $\gamma_r \neq \gamma_1$, the sequence is altered!

Partial summary: memory phenomena

- Memory can be encoded and read in LJ samples by means of oscillatory deformation
- There are qualitative differences with memory of suspensions

Can our results be generalized?

All the behavior above depends on the dynamics of the LJ system

in 3D space

in ($3N$D) configuration space

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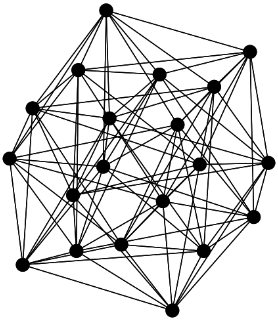
Is such behavior found in other systems with a deformable energy landscape?

NK model

A discrete energy landscape depending on a parameter γ



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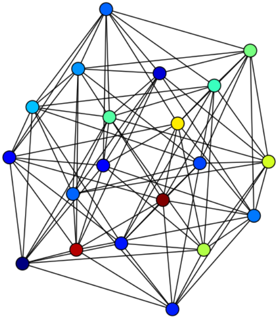

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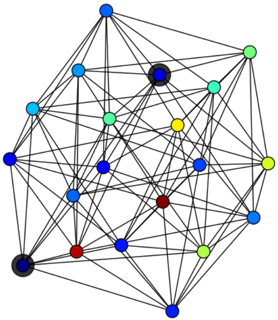

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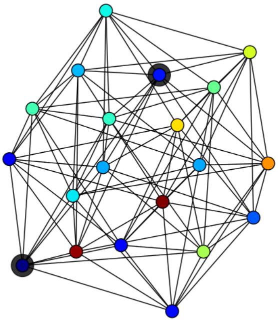

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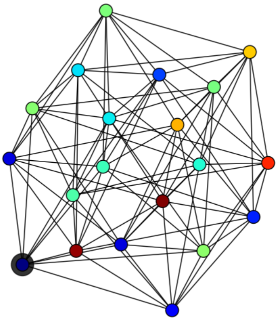

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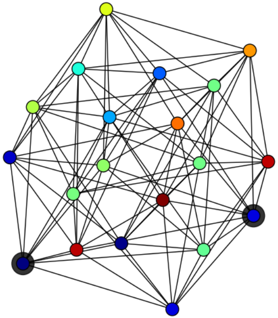

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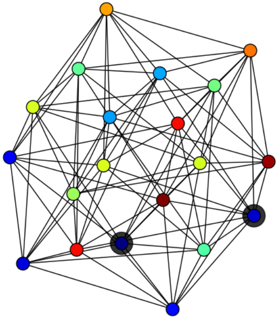

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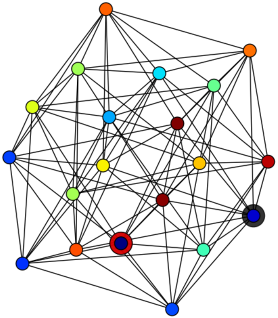

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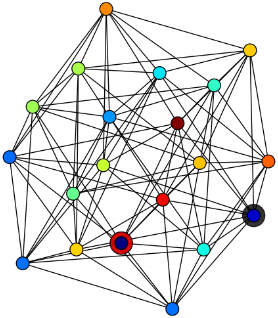

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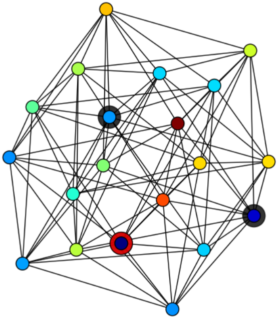

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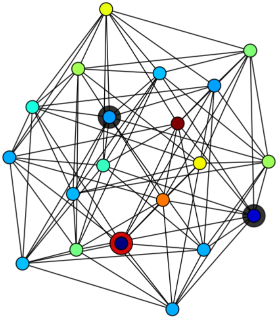

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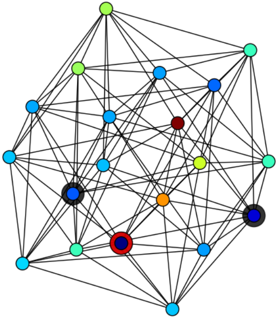

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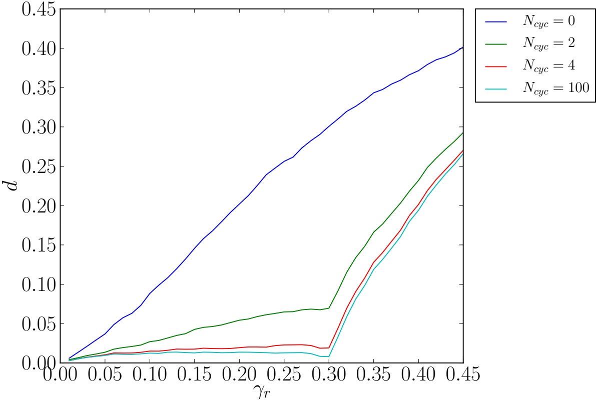
Information from the NK model

The energy behavior, diffusion and memory effects can be studied as γ is varied in an oscillatory way

Example: single memory in NK samples

Take the Hamming distance of trained samples read with amplitude γ_r:



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- Quantitative characterization of the transition at γ_c, assessment of size effects
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- Link with other physical systems

Thank you!

Thank you!

and to
G. Foffi, and S. Sastry (TIFR Hyderabad)