Oscillatory Shear Deformation of Amorphous Solids: Transition from localized to ergodic behavior and memory effects

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Complexity in Mechanics
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Phys Rev Lett 112 025702 (2014)
JPCM (submitted, 2014)

Outline

- ✧ Deformation of amorphous solids: Motivation
- ✧ Our approach
- ✧ A model glass subjected to oscillatory shear
- ✧ A non-equilibrium phase transition
- ✧ Memory
- ✧ Summary

Deformation of Amorphous Solids

Some reasons and issues of interest (already discussed in this meeting):

The nature of elementary events of plastic deformation.

The yielding transition.

Fracture.

Avalanches.

Jamming and Rigidity in Granular Matter.

There are strange people who worry endlessly about how a liquid becomes a glass, but once they have a glass, they lose all interest!!

Michael Falk

KITP, 2010

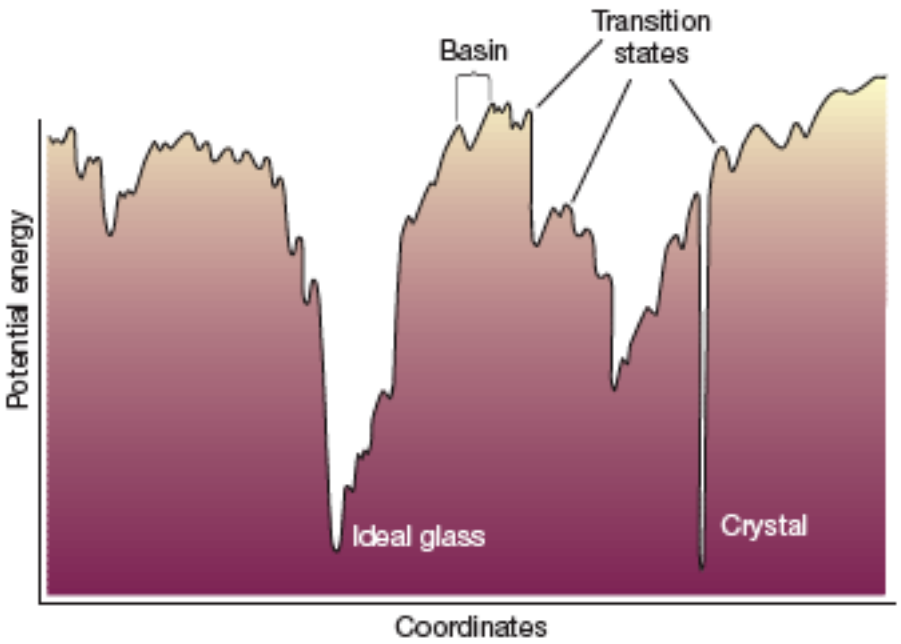
What we do: Approach and Questions

1. Energy landscape picture of configuration space. Probed by computer simulations of model glasses.
2. Mechanical response to affine, shear deformations studied by analyzing the modification of the landscape, and transitions between minima, through the AQS (Athermal Quasi Static) protocol.
3. Limitation: No information on the interplay between relaxation processes and instabilities triggered by deformation. But useful insights obtained.

Focus for this talk:

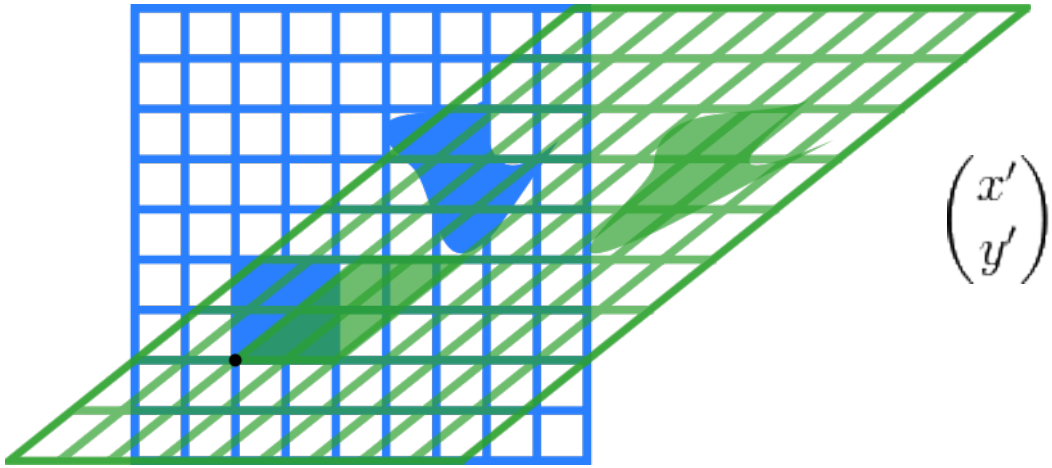
Role of cyclic shear deformations in triggering nonequilibrium transition to ergodic state.

Memory effects.



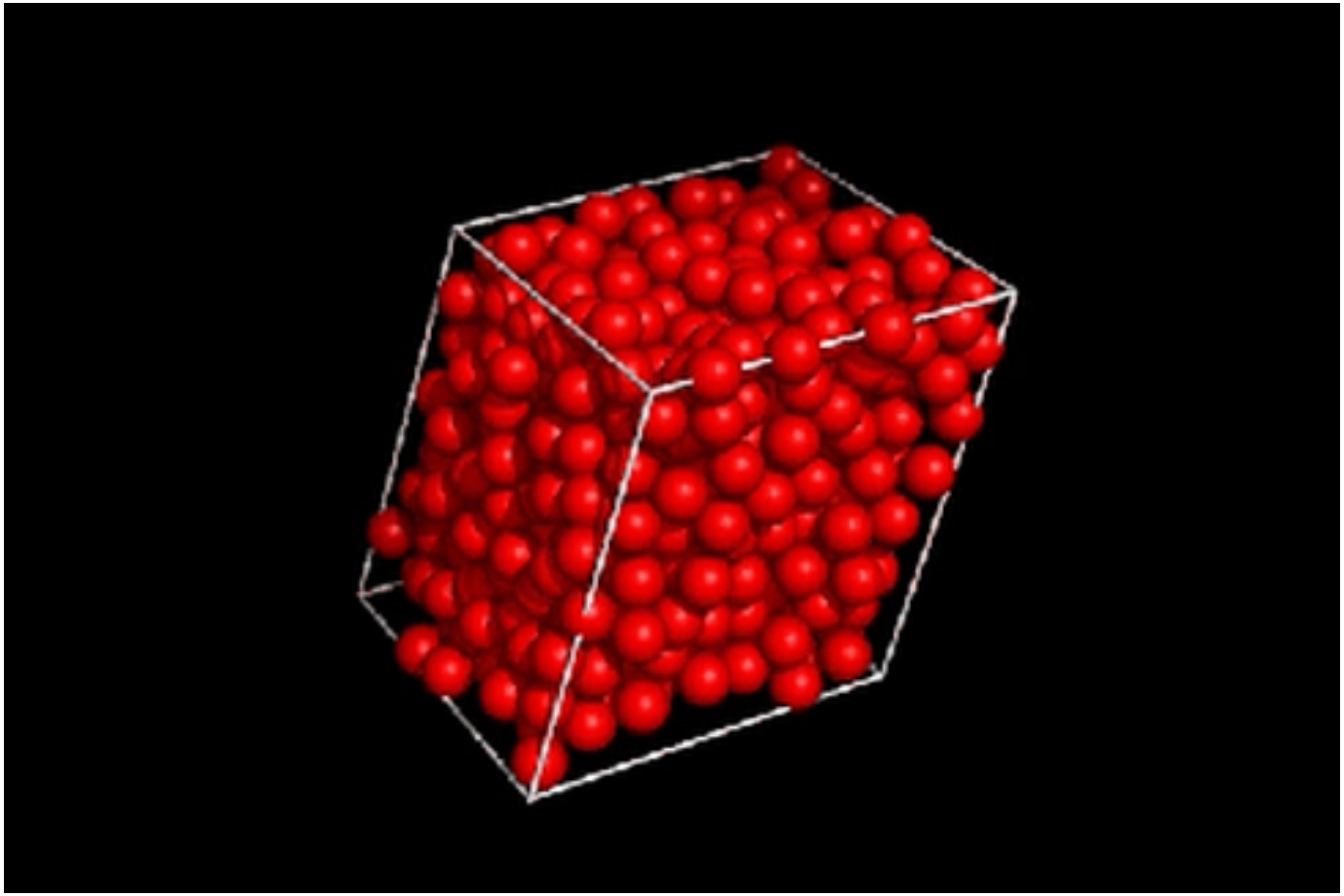
Athermal Quasi Static Deformation

1. Subject energy minimum structures to shear deformation.
2. Minimize the resulting deformed structure subject to suitable (Lees-Edwards) boundary conditions.
3. Deformation strain increased quasi-statically.
4. The procedure produces a sequence of configurations that are always energy minima.
5. Continuous change of energies interrupted by discontinuous change.
6. Discontinuous changes correspond to rearrangements.



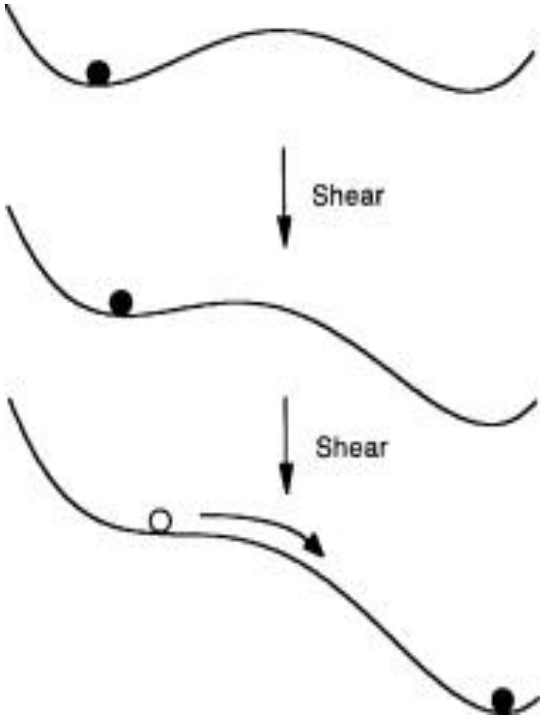
$$\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} 1 & \lambda \\ 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}.$$

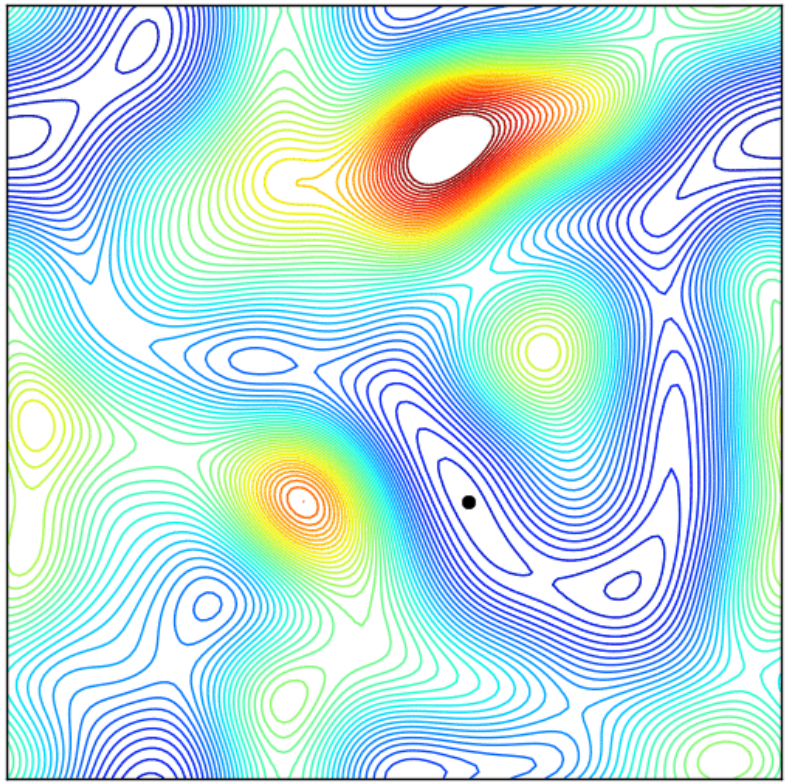
Athermal Quasi-Static simulations of deformation



Energy landscape picture: Schematic

Shear deformation modifies the potential energy landscape and destabilizes the system,
eventually leading to irreversible rearrangements



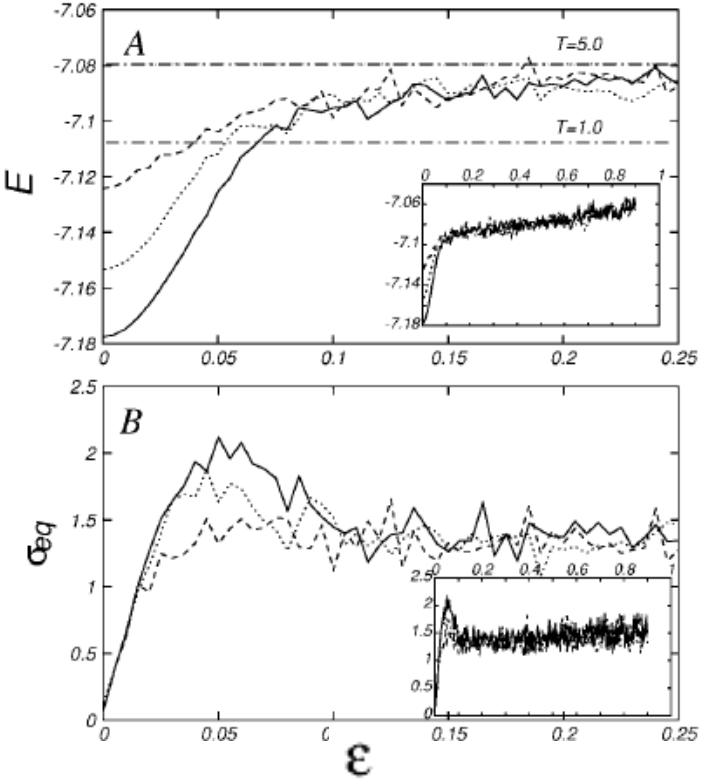


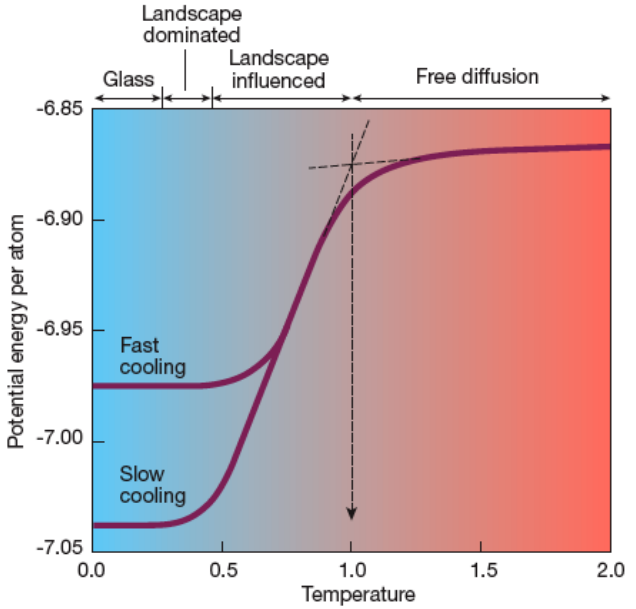
How does such deformation modify the properties of the glasses?

Mechanical deformation leads to *rejuvenation*..?

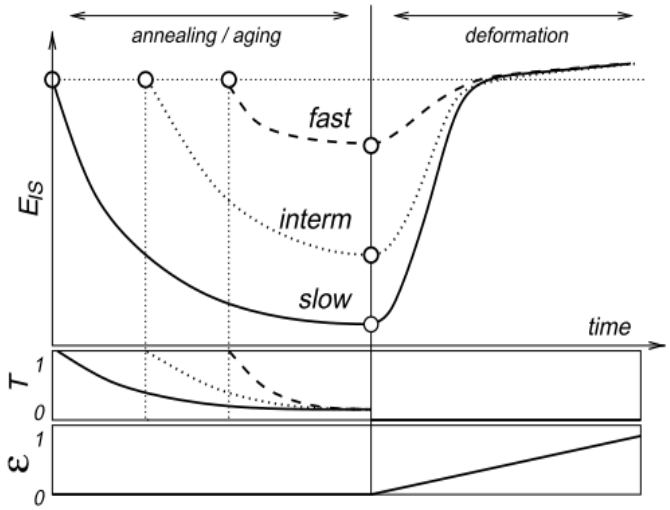
Observations from previous simulations:

1. Deeper energy minima are sampled at lower temperatures.
2. Upon shearing, the energy of the minima rises to those at very high temperatures.
3. Deformation induced ‘rejuvenation’ (as opposed to aging; with caveats).





Sastry, et al Nature 1998

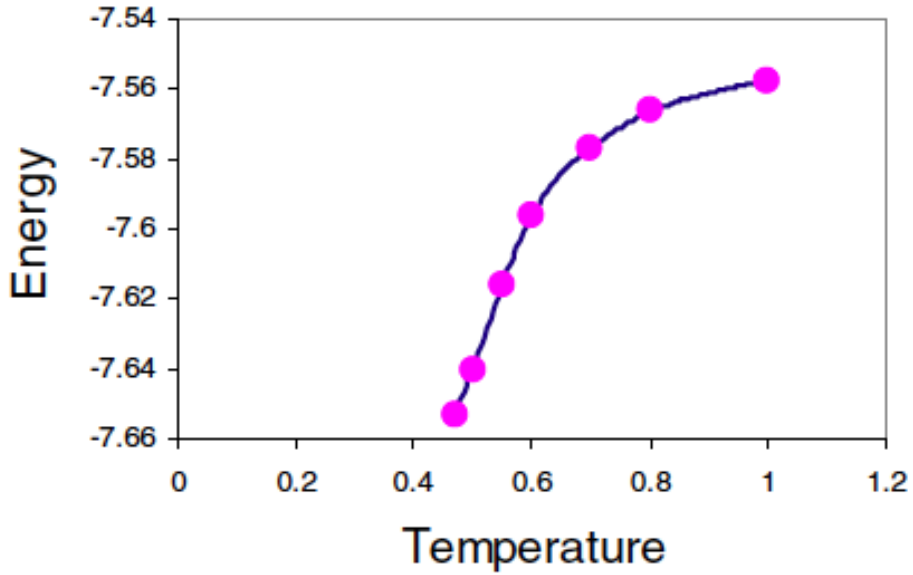


Utz, Debenedetti and Stillinger and Utz, 2000

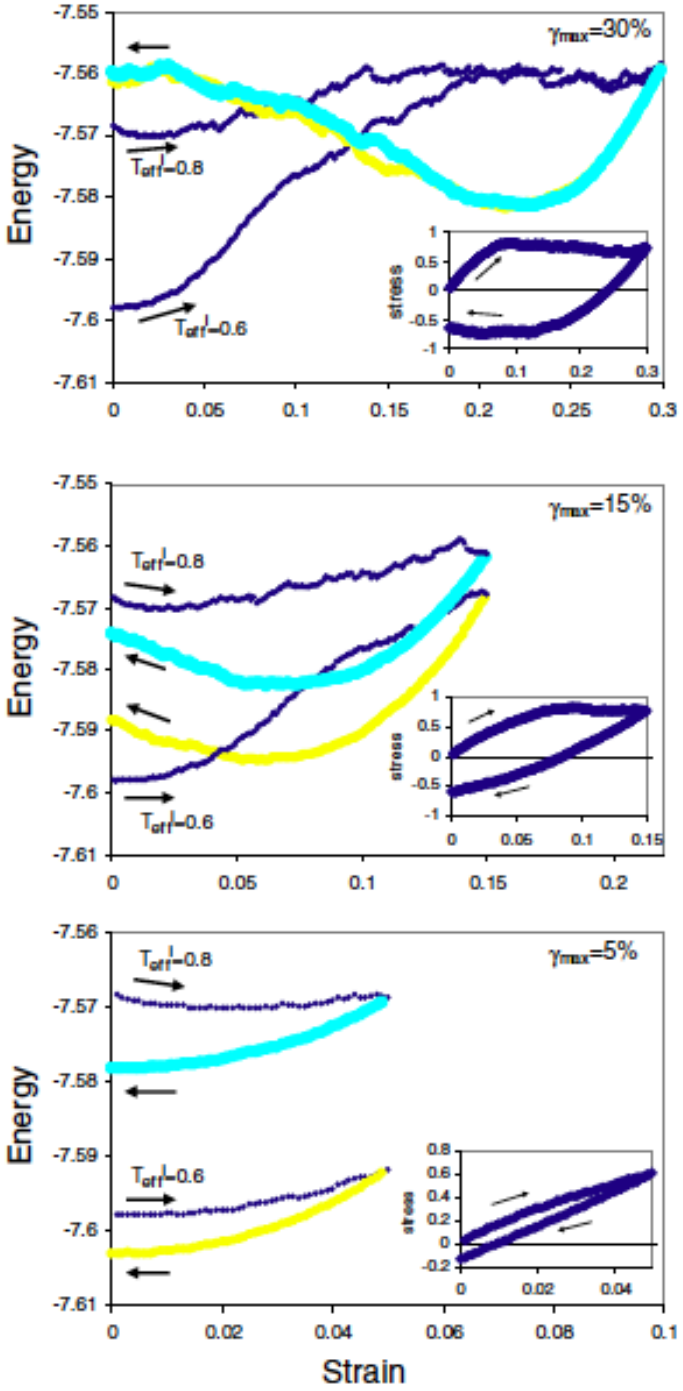
Somewhat more complicated picture when a forward and back cycle of strain is applied:

The nature of change (aging or rejuvenation) depends on amplitude of strain and the initial state..

What happens if this cycle is repeated?



Lacks and Osborne, PRL 2004.



Oscillatory Shear

Application of steady shear takes the system away from its initial structure.

Does this change if one applies oscillatory shear?

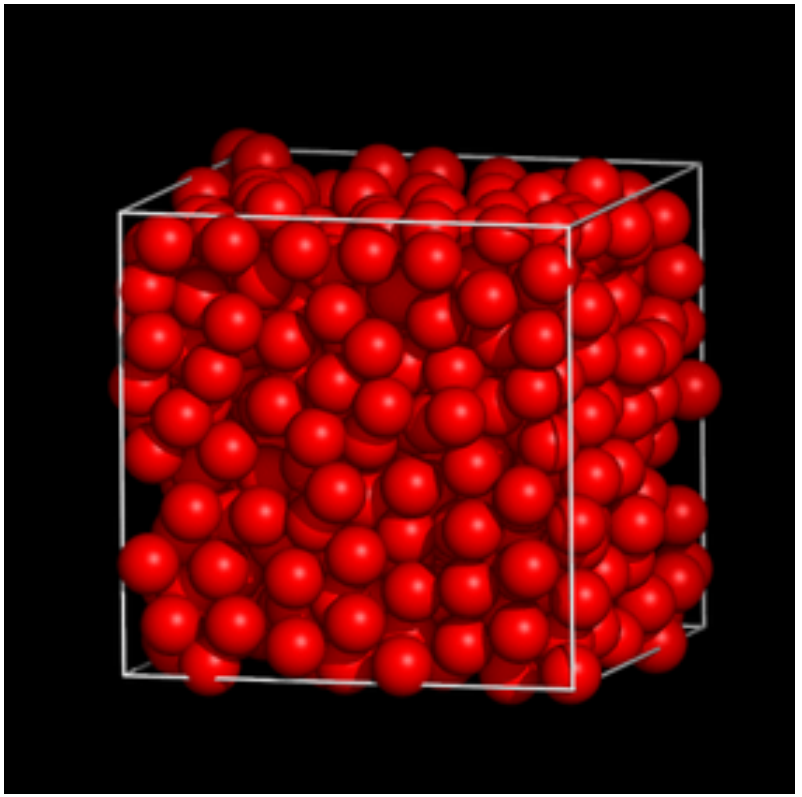
For small amplitude, the system should remain localized near its initial structure.

For large amplitude, the system approaches the behavior for steady shear.

How does the transition occur from being localized in configuration space to evolution to higher energy structures ?

Amplitude of oscillatory strain is the control parameter.

Simulations of oscillatory strained binary Lennard-Jones (LJ) solids



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

Kob-Andersen LJ potential avoids crystallization, can be seen as a simple model for metallic glass.

Different system sizes: 500, 4000, 32000.

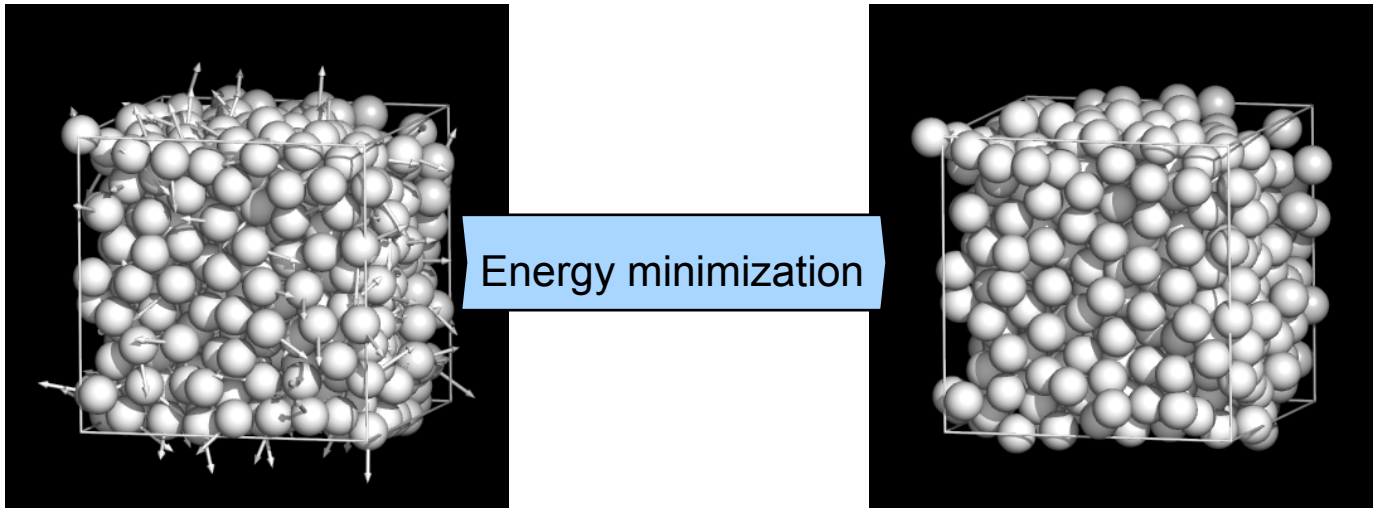
Two starting temperatures: 1.00 and 0.466

Simulations of oscillatory strained Lennard-Jones solids

Preparation of the sample:

1.Equilibrate samples at a given T (using NVT MD).

2.Strip off velocities and quench configuration via CG potential energy minimization.

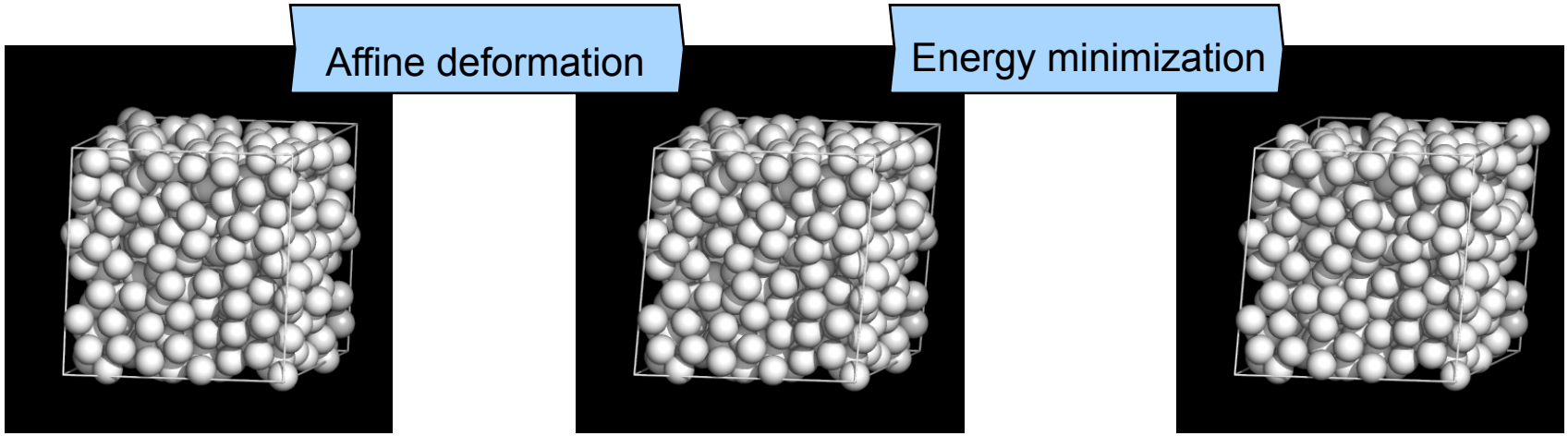


By construction, we thus put the system in a local minimum of the energy landscape.

Simulations of oscillatory strained Lennard-Jones solids (continued)

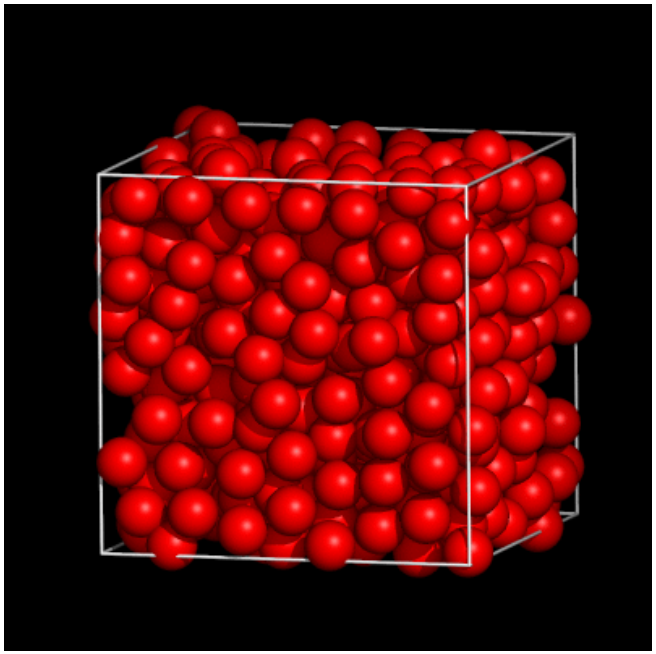
Deformation of the sample:

1. Increment strain by $d\gamma$ with an affine transformation
2. Minimize the potential energy according to suitable Lees-Edwards boundary conditions



Behaviour we focus on

Increase γ in steps of $d\gamma$ up to γ_{max} and decrease to $-\gamma_{max}$ and increase back to $\gamma = 0$.



Record the γ =0 configurations and label them with the *accumulated* strain γ_{acc}, i.e. the sum of all the $|d\gamma|$ imposed on the system.

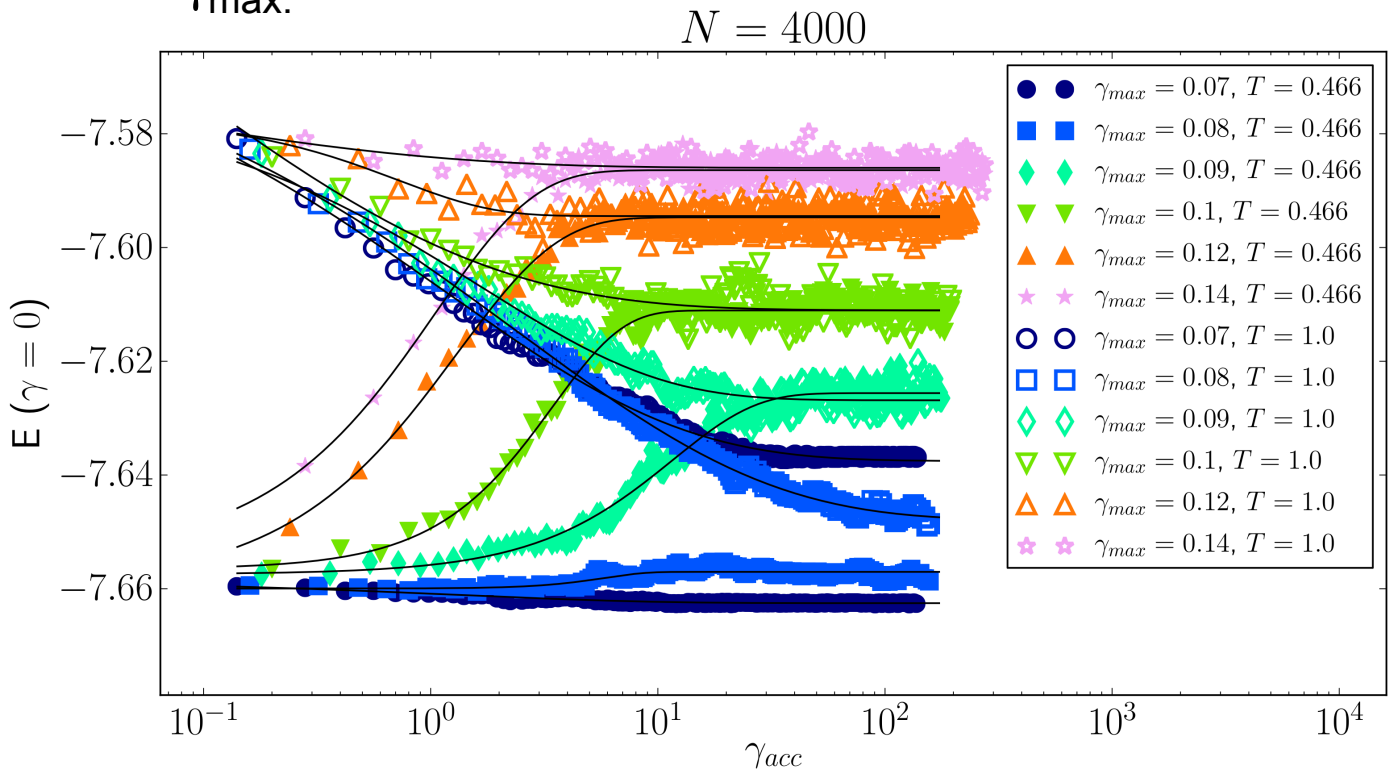
Do this for different samples for different system sizes

Measure (for all the γ =0 encountered configurations)

Average energy per particle
Particle displacements

Potential energy vs accumulated strain

The potential energy per particle reaches a plateau that (a) depends on γ_{max} **only** at large values of γ_{max}. (b) depends on γ_{max} and initial state for small γ_{max}.

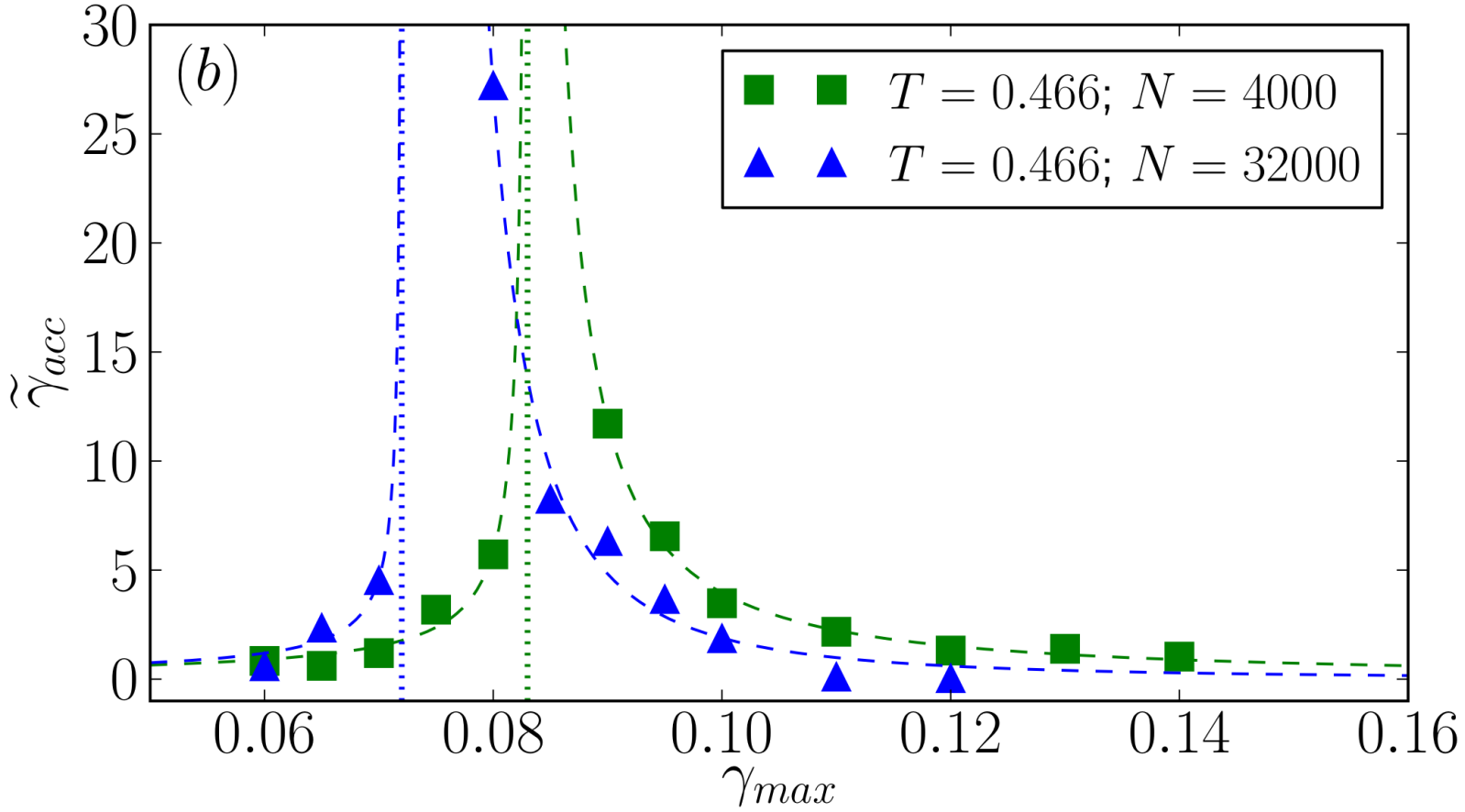


Aging/rejuvenation depends on strain amplitude and initial annealing on the glasses.

Change in behavior across a critical strain amplitude γ_c

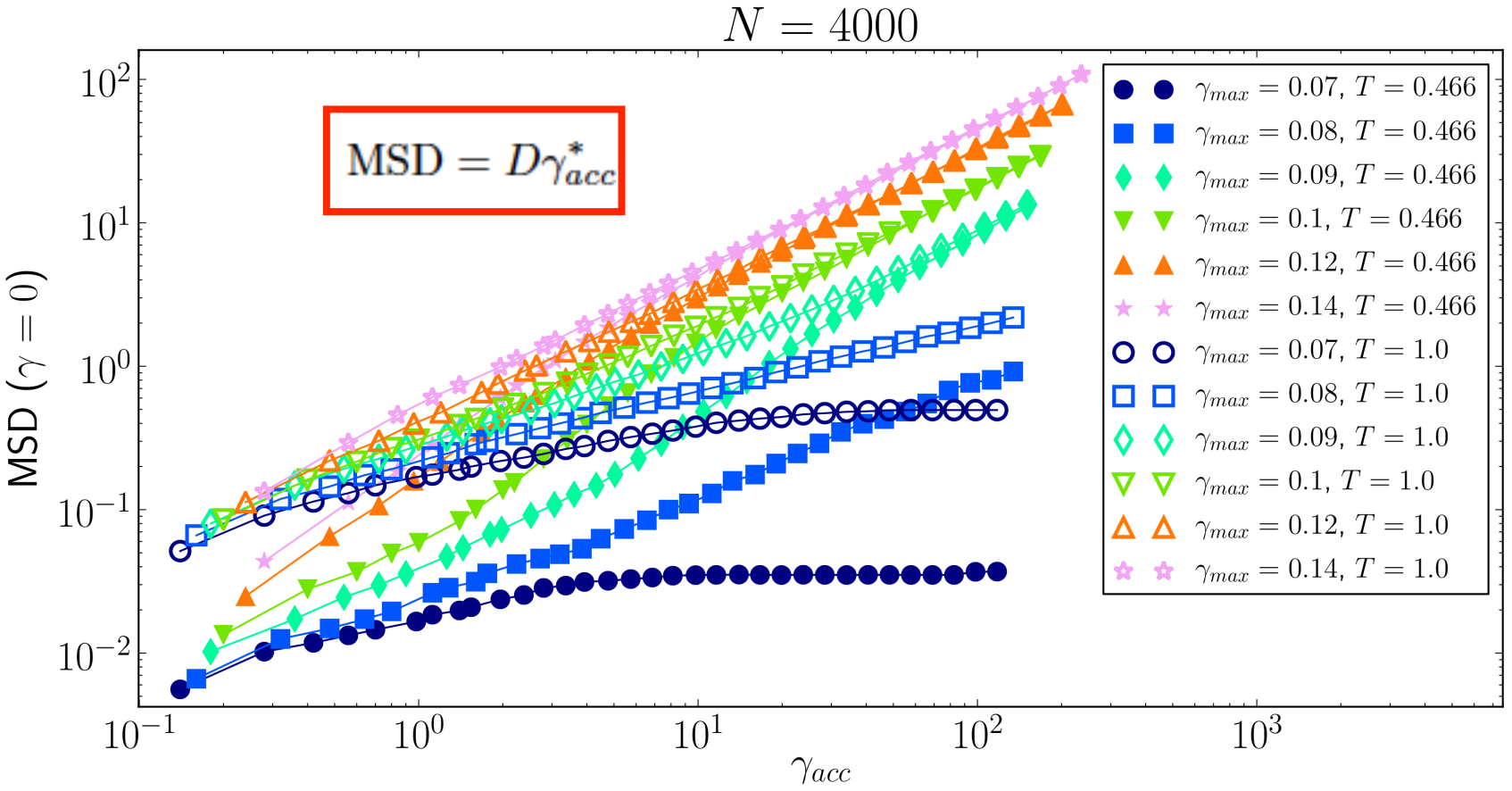
Relaxation to the steady state becomes more sluggish as γ_c is approached.

[Estimate of γ_c in a moment..]



Mean squared displacement vs accumulated strain

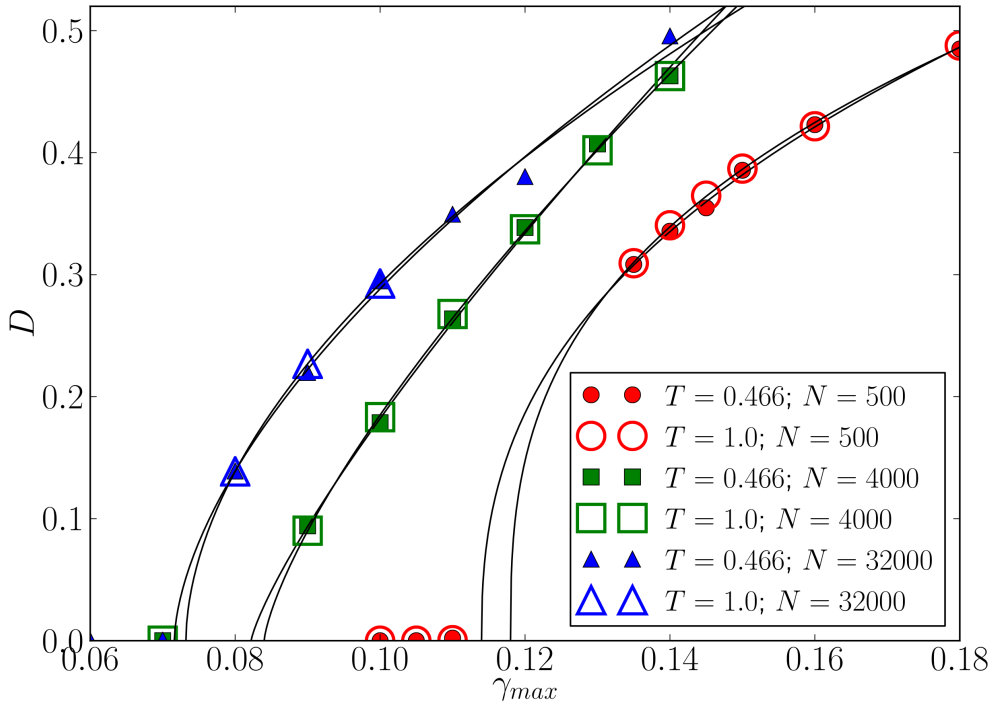
Depending on γ_{max} systems are:
(a) Freely diffusing or (b) Localized (MSD saturates).
In the diffusive regime, asymptotic slopes depend only on γ_{max}.



Vanishing of the Diffusion Coefficient

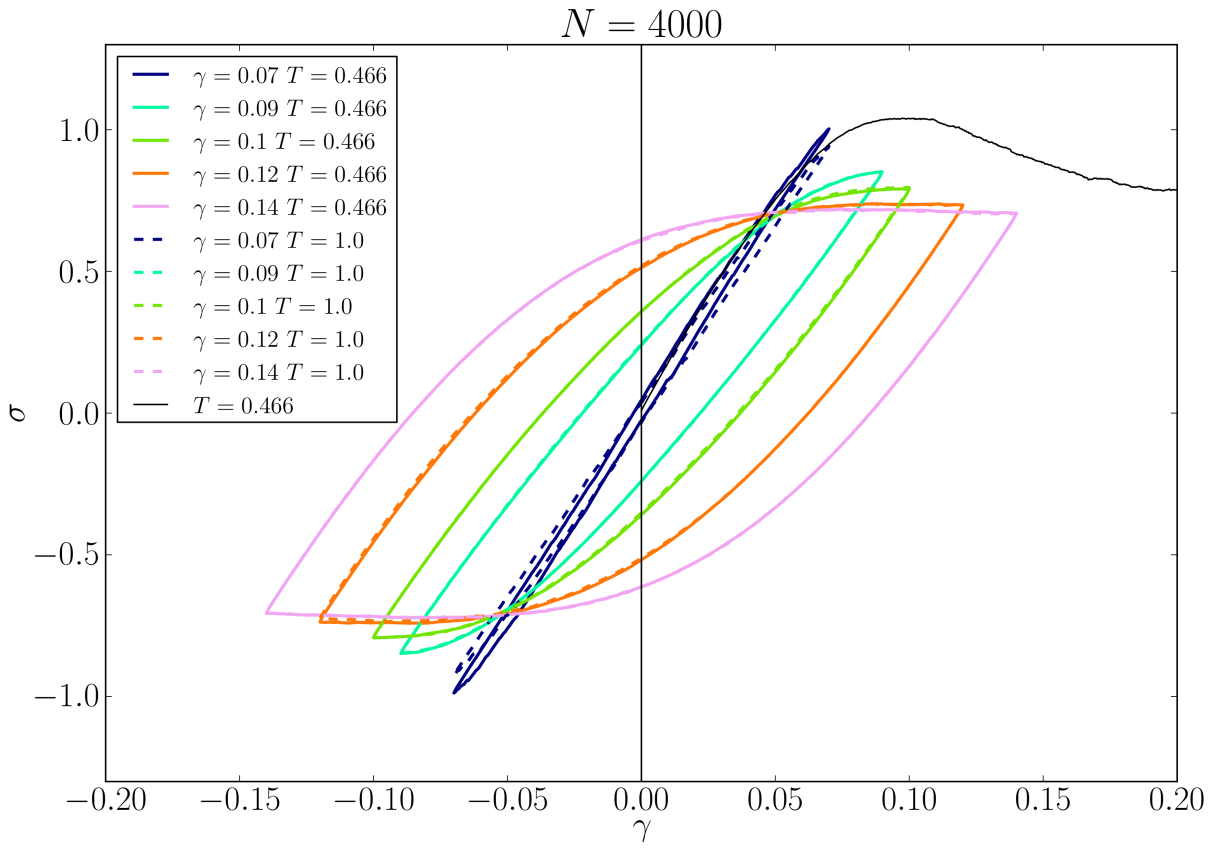
The diffusion coefficient vanishes at a finite value of γ_{max}.

Critical γ_{max} a function of system size… but approach finite value asymptotically.



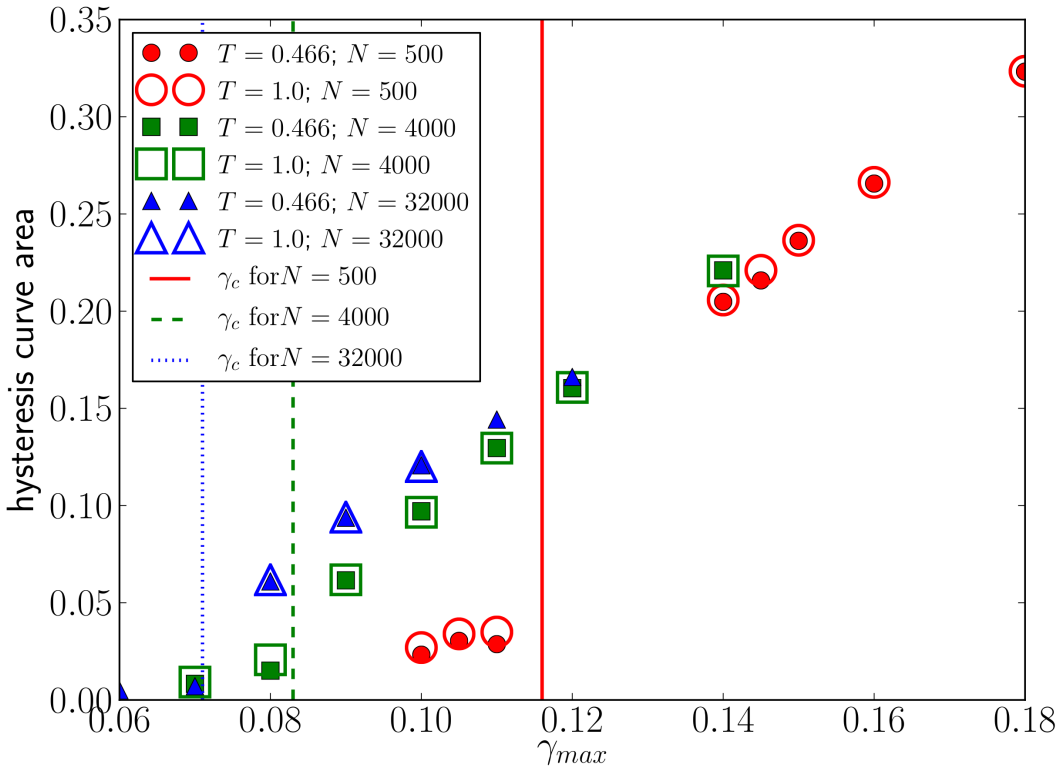
Energy Dissipation

In the non-diffusive regime, stress-strain curves show nearly non-dissipative behavior but display hysteresis in the diffusive regime.



Energy Dissipation

The onset of energy dissipation close to estimated critical strain!

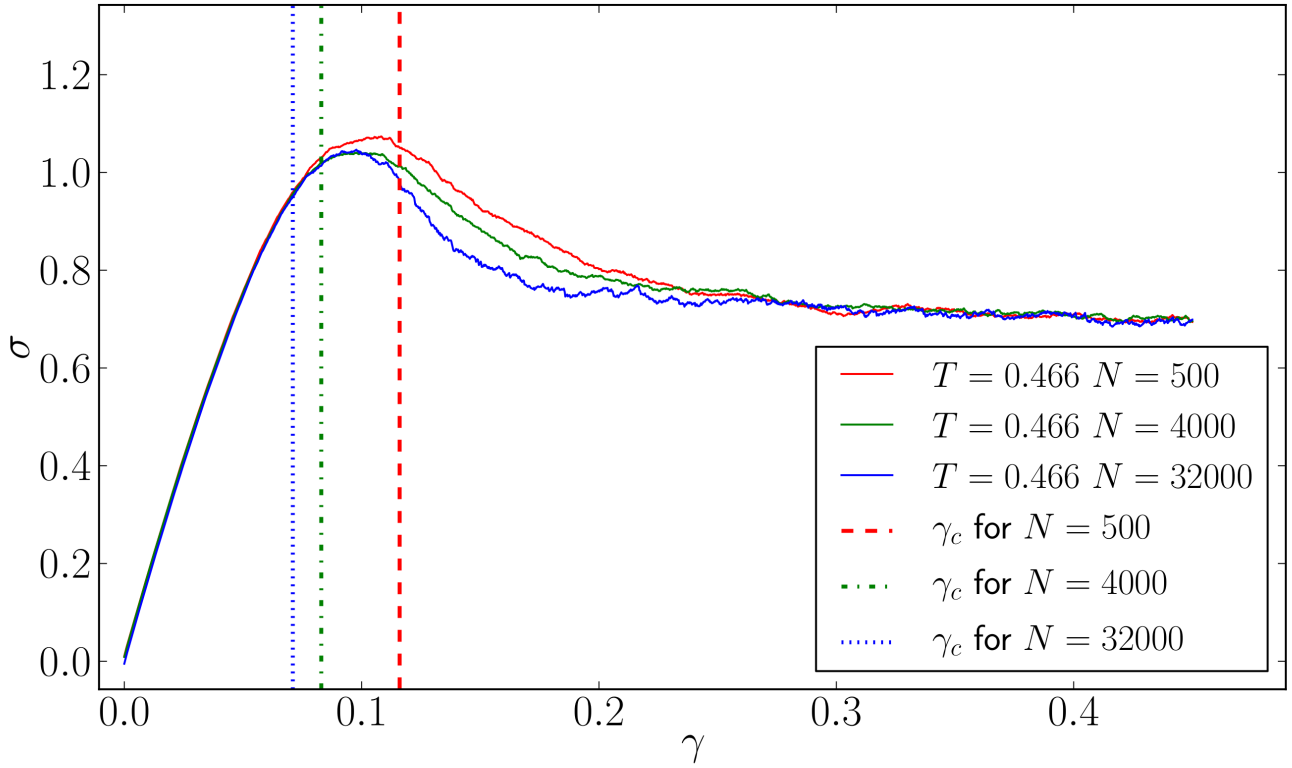


Critical *vs.* Yield Strain

Critical strain is roughly equal to the yield strain.

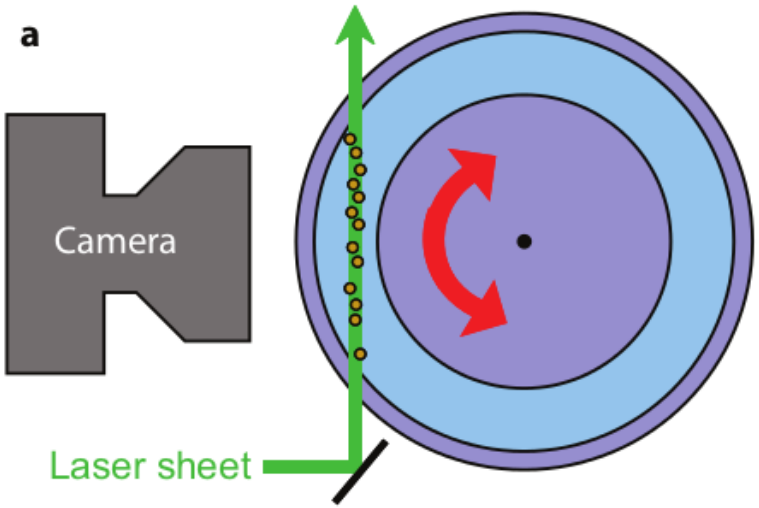
The yield strain is not strongly dependent on system size is but the critical strain is.

Critical strain values for the larger systems are lower than the yield strain.



Non-equilibrium phase transitions

The behavior seen in our system is similar to that observed in experiments dealing with colloids immersed in a viscous fluid subject to oscillatory deformation.

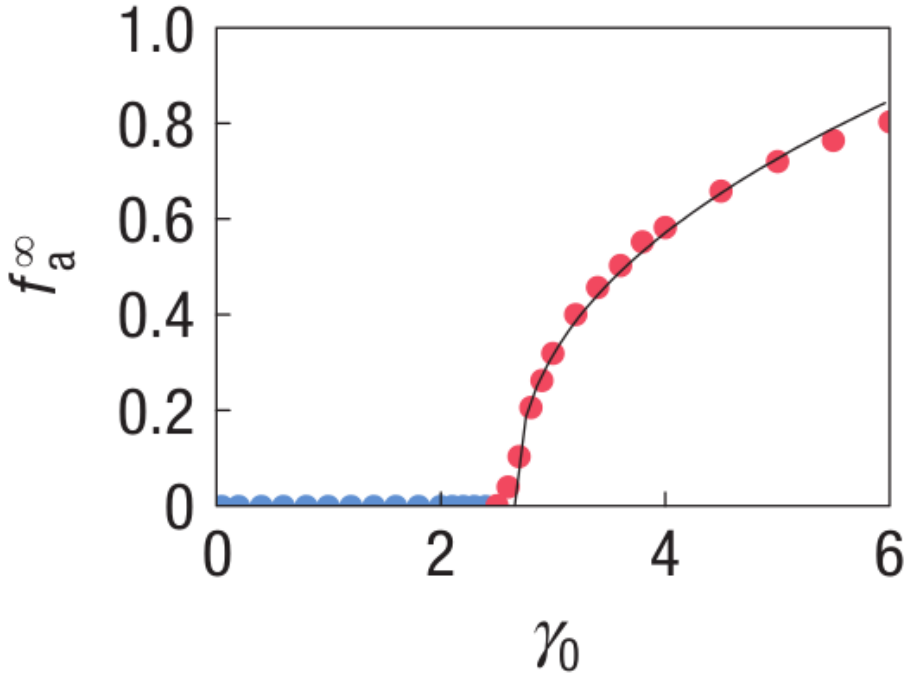


Pine et al Nature 2005
Corté et al., Nat Phys 2008

After a full oscillation, colloids in the cylinder return to the starting point or move a little. Those that move are named “active”.

Non-equilibrium phase transitions

After a long number of cycles the fraction f_a of the colloids that are still “active” depends on the maximum amplitude g0 of the cylinder oscillations



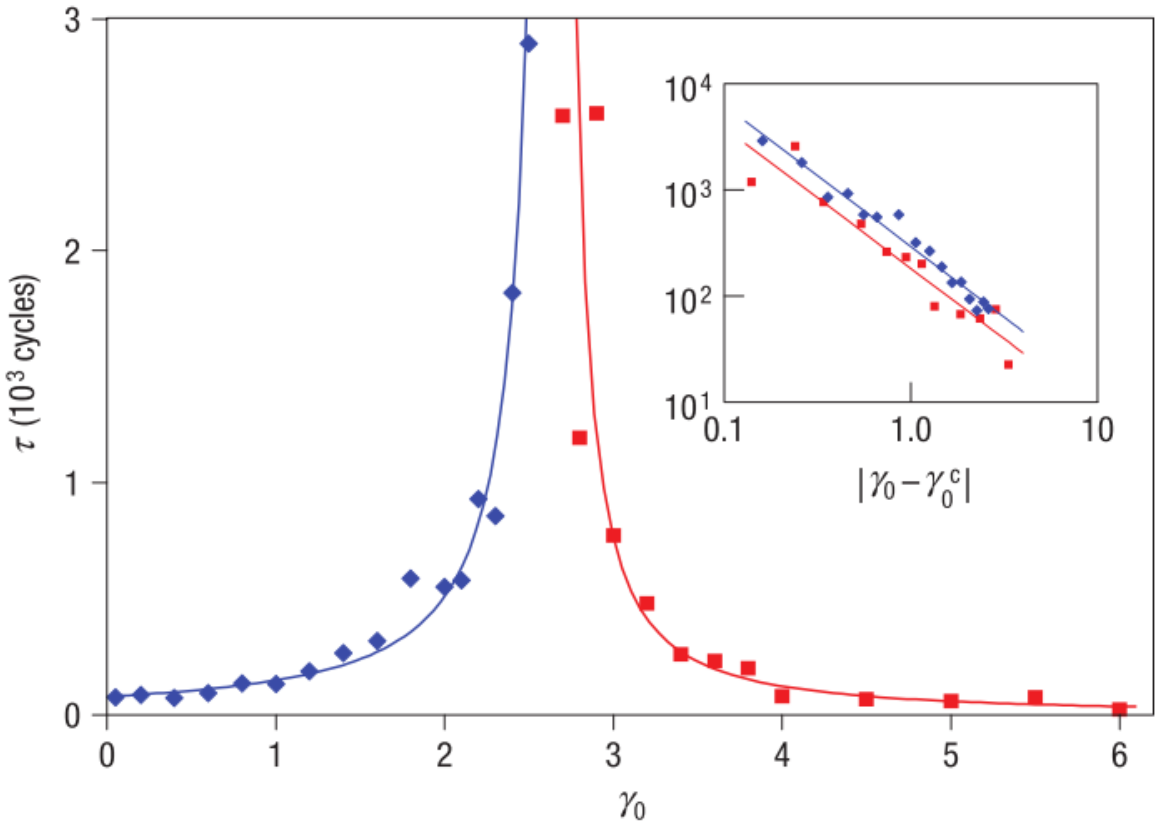
Corté et al., 2008

In this case the data have been interpreted as a non-equilibrium phase transition, possibly in the same universality class of directed percolation with a conserved order parameter (C-DP).

Menon and Ramaswamy, 2009

Non-equilibrium phase transitions

Close to the transition the time needed to reach a steady state (so that the fraction of active colloids doesn't change with time) diverges as a power-law.



Corté et al., 2008

In our case, the increased number of cycles to converge to the final energies is an indication that a similar behavior exists.

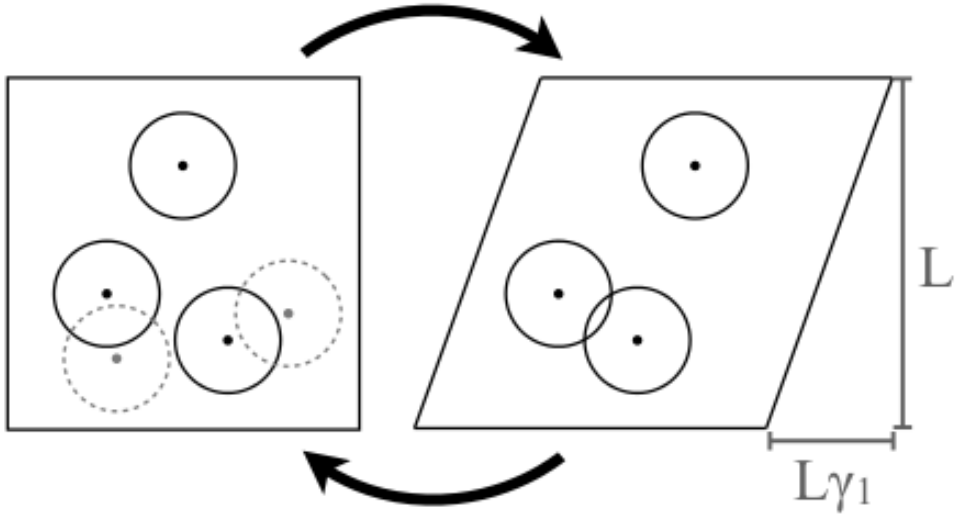
Memory

Systems not in equilibrium have the possibility to retain memory.

Amorphous solids under strain belong in this category.

Can they be used to store and retrieve information?

Addressed for a computational model for the colloidal suspensions experiment by Keim and Nagel (2011). [KN]



The system is “trained” by the application of oscillatory strain for some number of cycles.

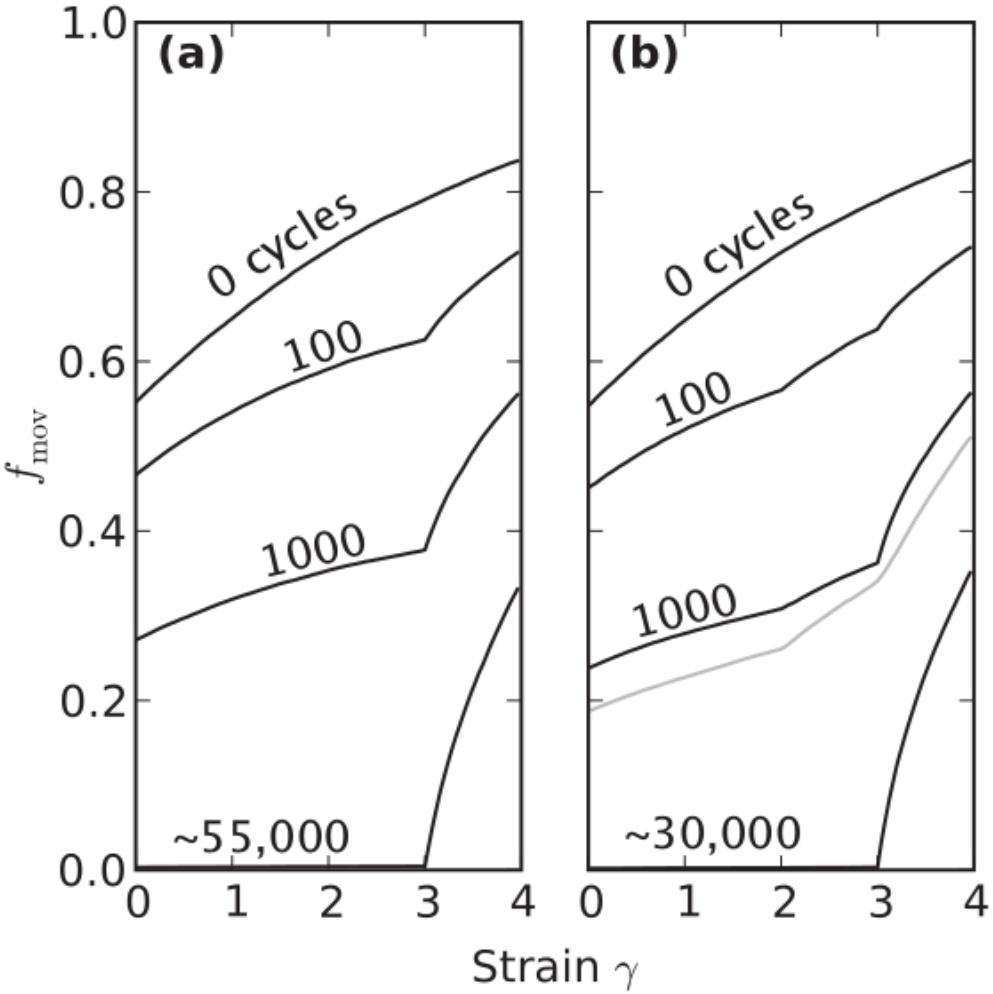
The “read off” at any stage is the number of “active” particles in one cycle.

Observations:

For a single training strain, memory is generated after a small number of training cycles.

For multiple training strains, memory is present at intermediate number of training cycles, but in the long term, only the largest strain is remembered.

But if a small amount of noise is added, multiple memories become stabilized.



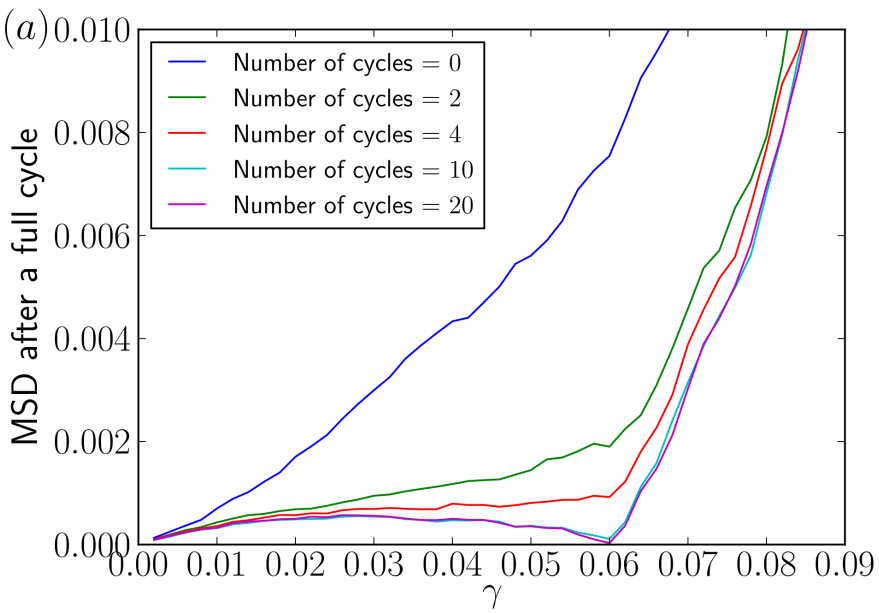
Memory in our Amorphous Solid

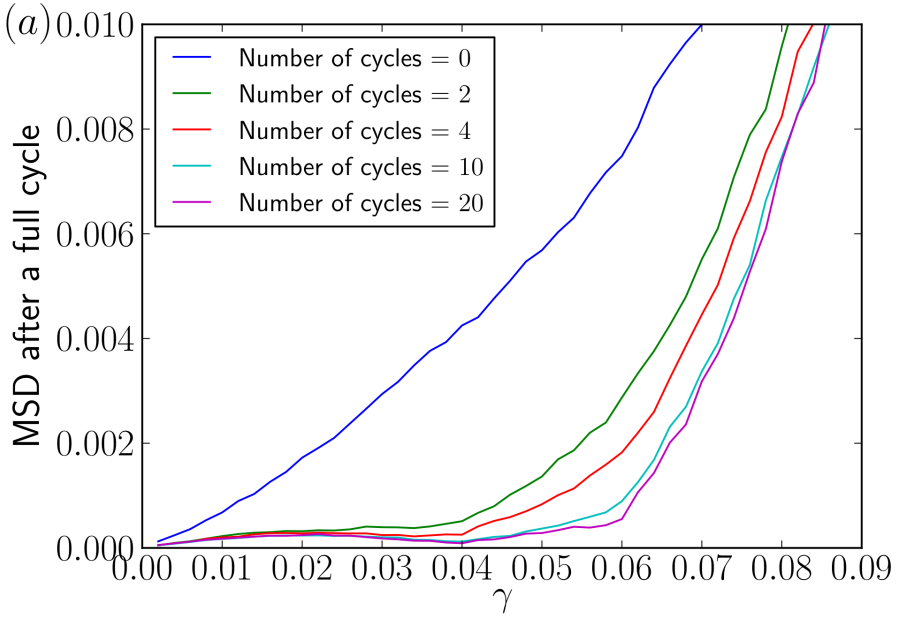
We use the same protocol for training as Keim and Nagel. However, we use the MSD in one cycle as the read off.

Similar behavior as KN for single memory, but MSD non-monotonic with reading strain.

But – stable multiple memories without noise!!

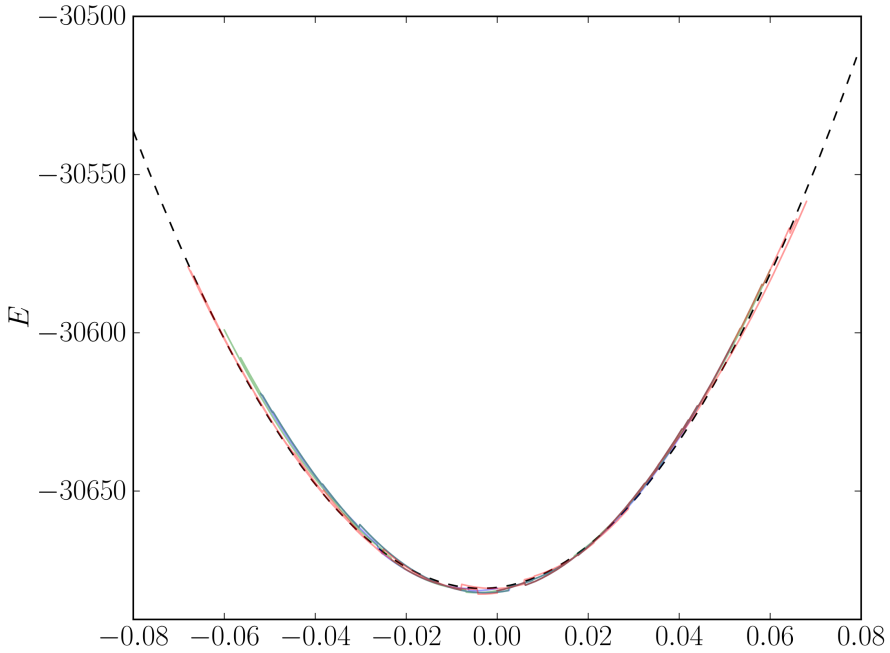
Why the difference?

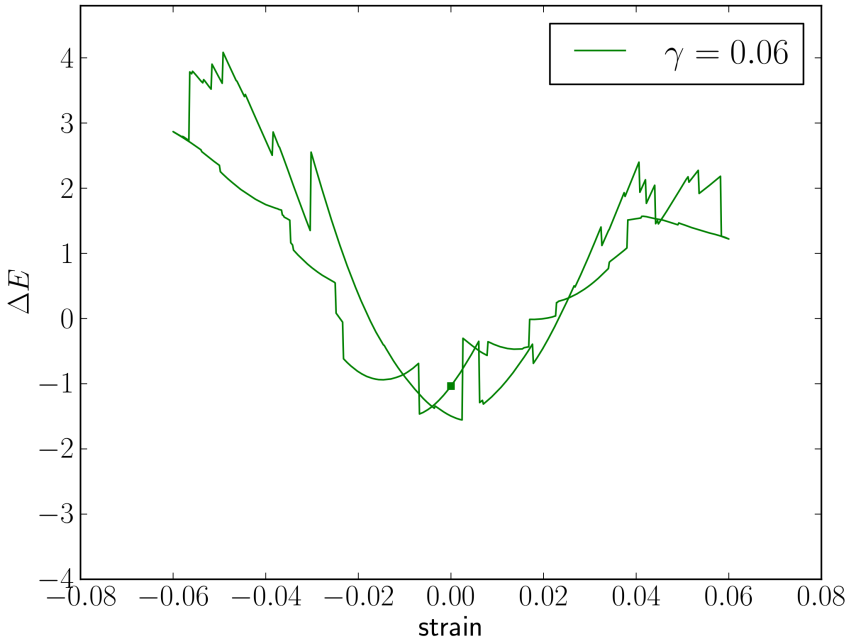




Once the system reaches steady state, the model used by KN has entirely uninteresting dynamics/landscape below the threshold strain.

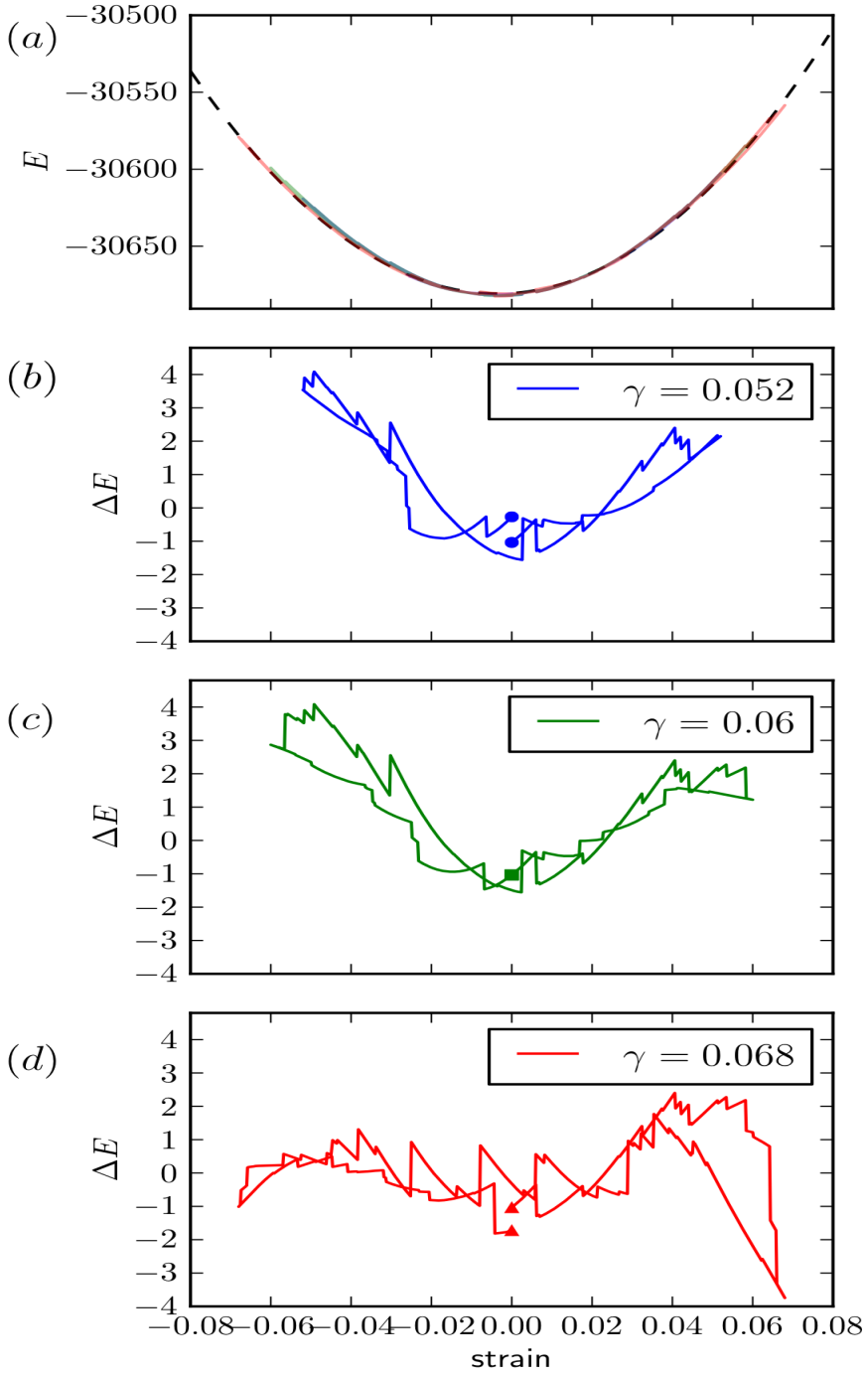
In contrast, our system can have steady state, cyclic, behavior for a given maximum strain that involves multiple transitions between energy minima.





A different maximum strain, even smaller than the one that produces the steady state, will disrupt the cycle, and hence will be registered.

Thus, multiple memories possible without the addition of noise.

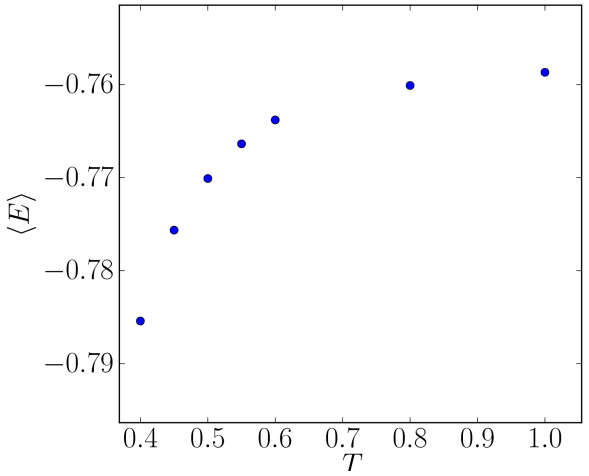


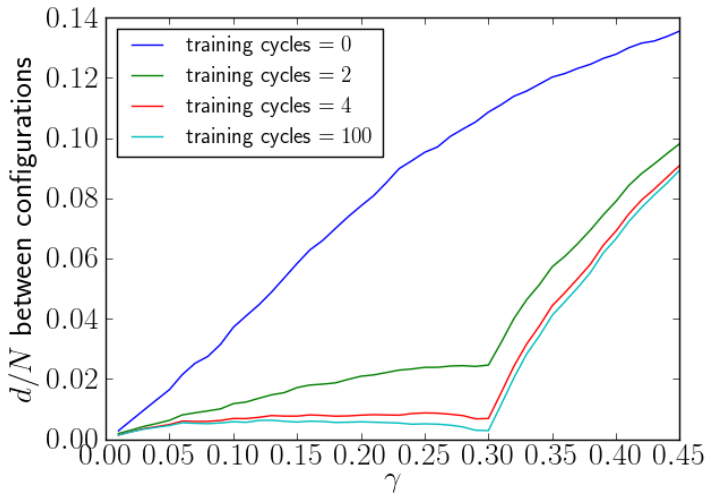
Memory in the NK model

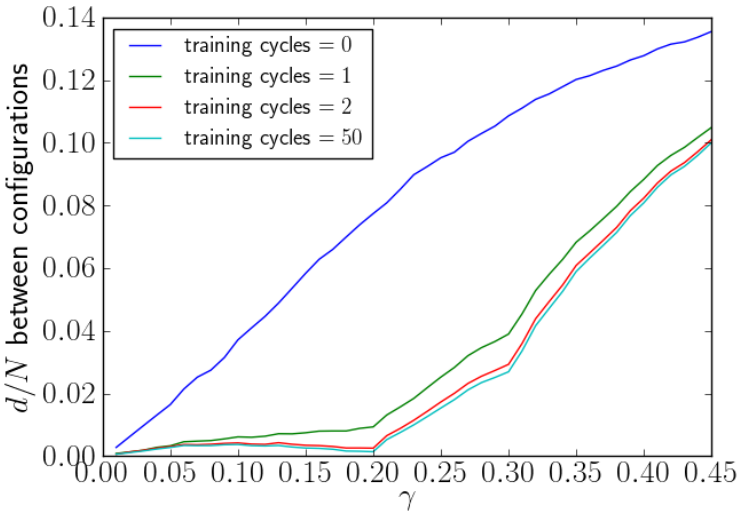
NK Model: A spin model with disordered and *deformable* interactions, and a rugged, deformable landscape.

$$E = -\frac{1}{N}\sum_{i=1}^{N}(1+\sin(2\pi(a_i+\gamma b_i)))$$

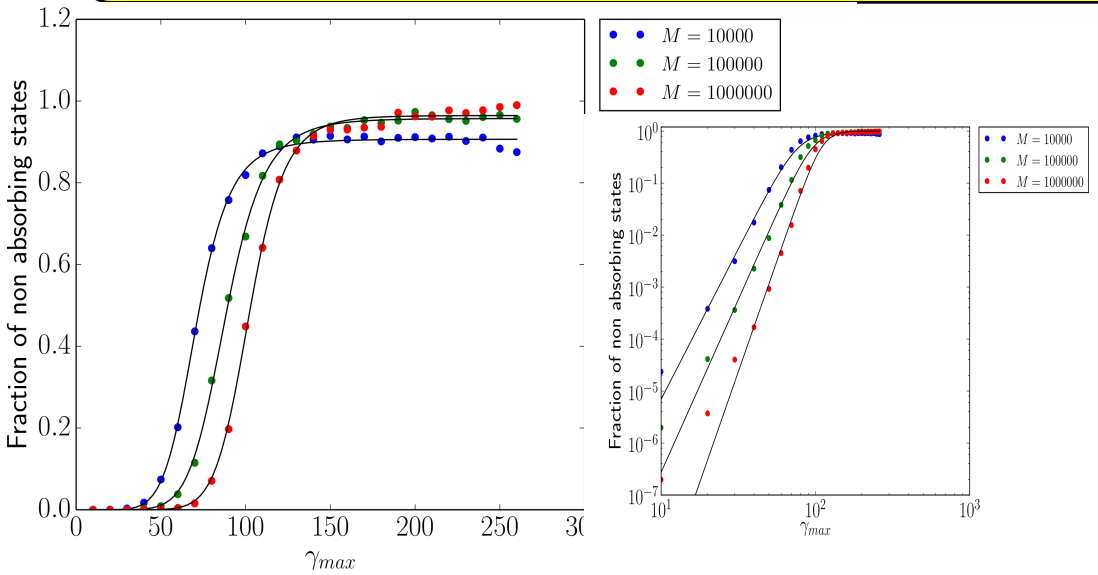
Behavior similar to structural glass formers.







Memory in the transition matrix model

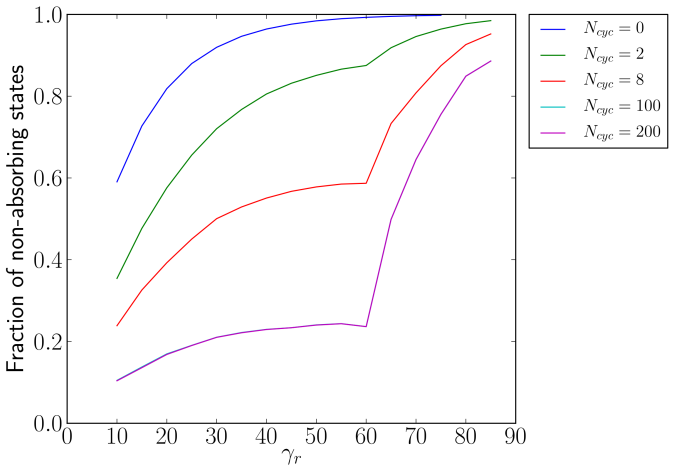


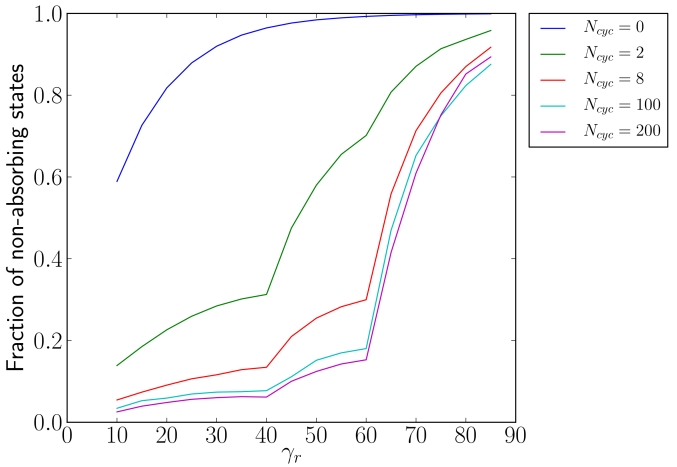
Transition Matrix Model: Define a transition matrix for transitions of inherent structures onto another for one cycle of oscillatory deformation.

Probability of jumping to another inherent structure increases with strain amplitude.

Transition similar to model glass former (but perhaps smooth), and memory effects, are seen, using fraction of (non) absorbing states as the observable.

The behavior we see appears very generic for 'landscape models'.





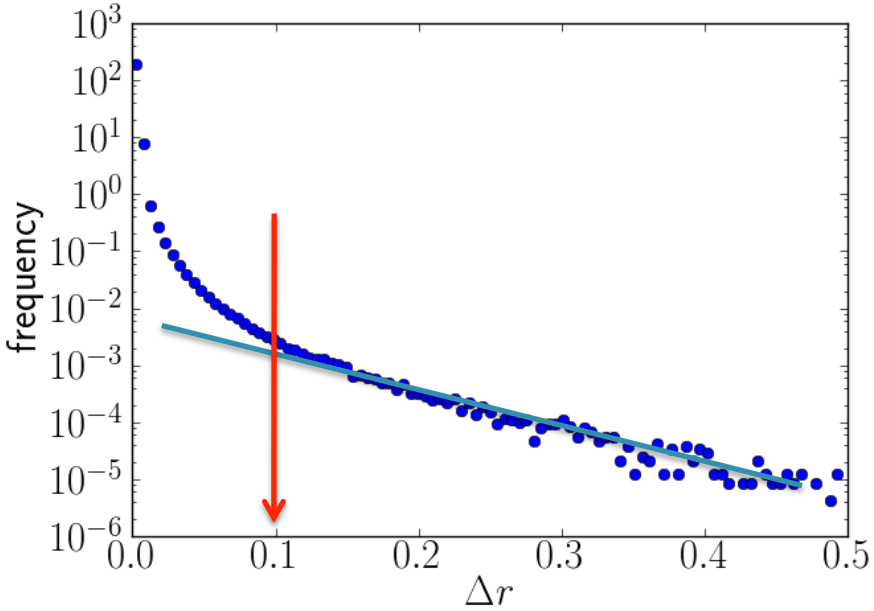
Events leading to Cycles

We consider single particle displacements during a jump in energy.

By defining a threshold for “plastic” displacement for single particles, and a cutoff for identifying neighbors, we can examine clusters of co-moving particles.

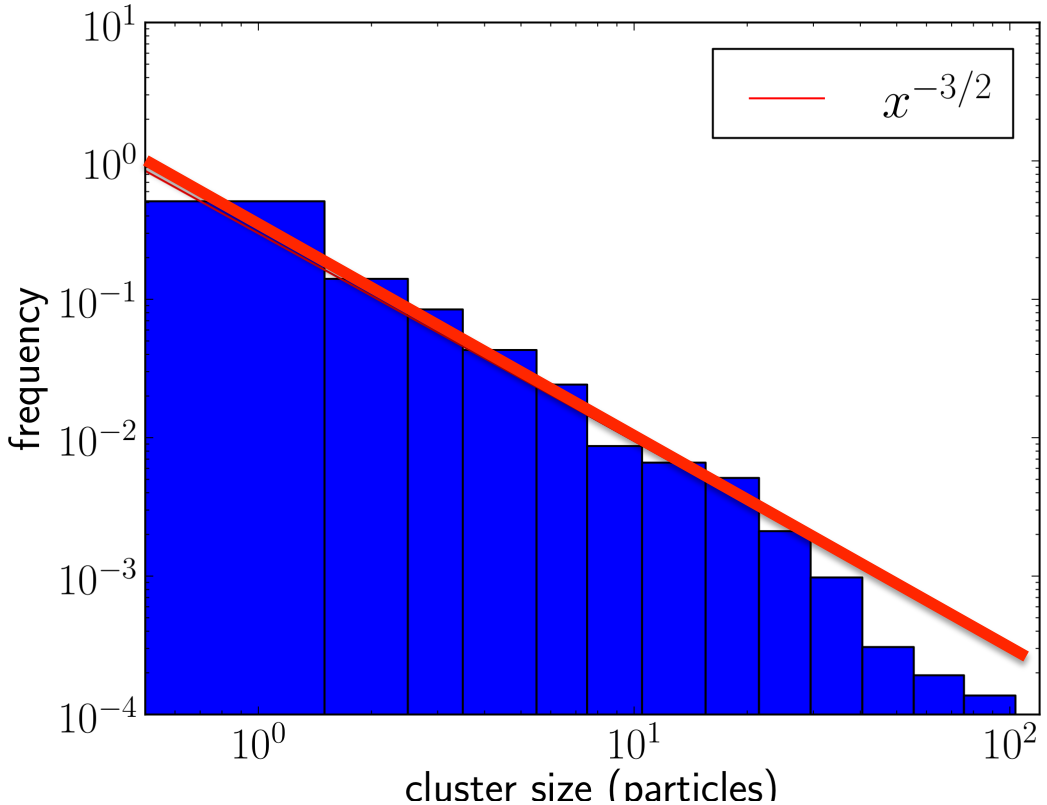
A choice of 0.01 σ or 0.3 σ would correspond to including all non-affine deformations or only the “players”. We choose 0.1σ.

A meaningful choice in between requires further understanding.



For threshold of 0.1, the distribution of sizes of events (or avalanches) is a power law with an exponent of -3/2

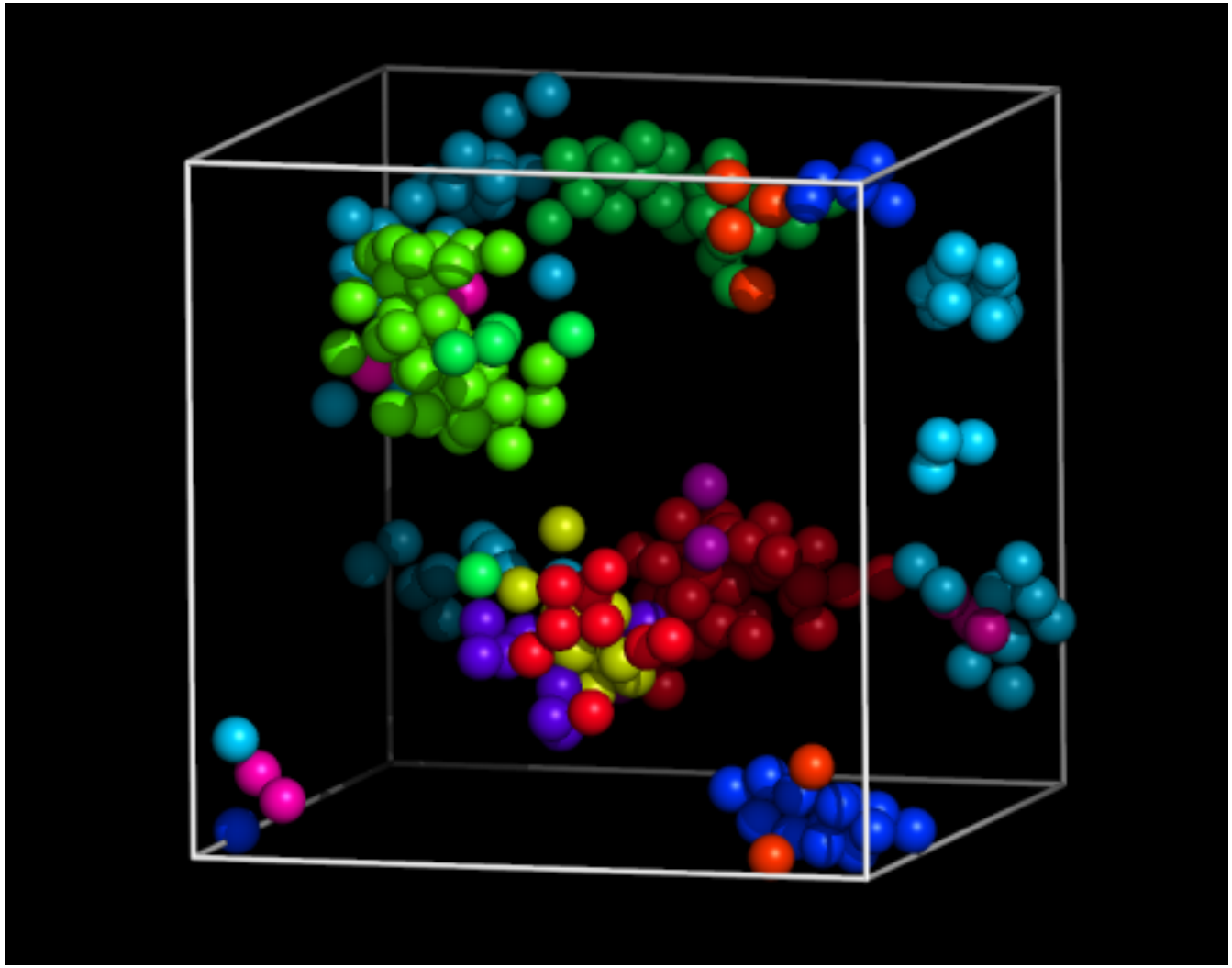
NB: Away from the nonequilibrium transition.



Related to avalanches in other contexts?

Needs further analysis.

How do the events look?



Summary

Evidence of a non-equilibrium transition from a localized to a diffusive state (in configuration space) that resembles the glass to liquid transition and other non-ergodic to ergodic transitions.

Steady state energies in the diffusive state do not depend on initial conditions.

Slow down of dynamics near the transition.

Finite dissipation in the diffusive state as measured by the stress-strain hysteresis curves.

Critical strain close to but not the same as yield strain.

Memory storage and read off similar to but different in interesting ways from model colloidal suspensions.

“Avalanches” with power law distribution of sizes involved in periodic cycles. Needs further analysis.