Memory Effects in Model Glasses Under Cyclic Deformation

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Outline

- ✧ Memory formation generalities
- ✧A model glass subjected to oscillatory shear
- ✧ A non-equilibrium phase transition
- ✧ Memory Effects
- ✧ NK Model
- ✧ Transition Matrix Model
- ✧ Sheared soft sphere assemblies
- ✧Summary

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Fiocco, Foffi, Sastry, Phys Rev E 88, 020301(R) (2013)
Phys Rev Lett 112 025702 (2014)
JPCM (2015)
Adhikari and Sastry, in preparation

Memory Formation in Matter

- Memory connotes the ability to encode, access and erase signatures of past history in the state of a system.
- Systems capable of memory display multiple (symmetry or ergodicity broken) states they can reside in. The choice depends on history.
- Simple examples involve instances of symmetry breaking or being trapped in locally stable states that are easy to characterize.
- Driven, out of equilibrium systems may reach steady states in which they persist even after the driving is removed, which carry memory of the driving.
- Interesting to understand different types of memory formation, and comparison of different instances helpful.
- Cyclically shear deformed particle assemblies is a recently well studied case.
- Sheared glasses, soft sphere assemblies, and related model systems will be discussed.

Model Glass subjected to Oscillatory Shear

Mechanical response of amorphous solids subjected to shear deformation of interest in diverser contexts.

Model glass subjected to athermal quasi-static, oscillatory shear deformation.

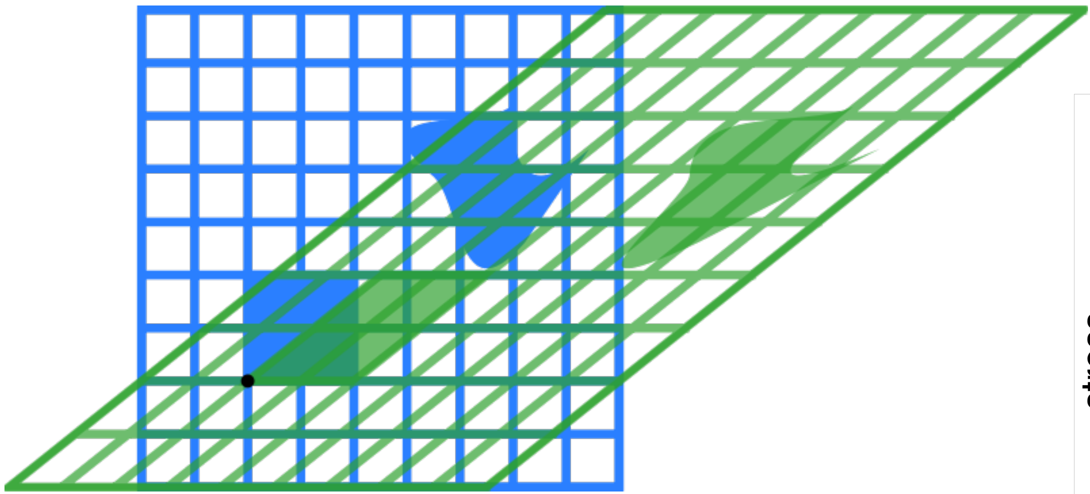
Amplitude of oscillatory strain is the control parameter.

Transition from a localized to diffusive state.

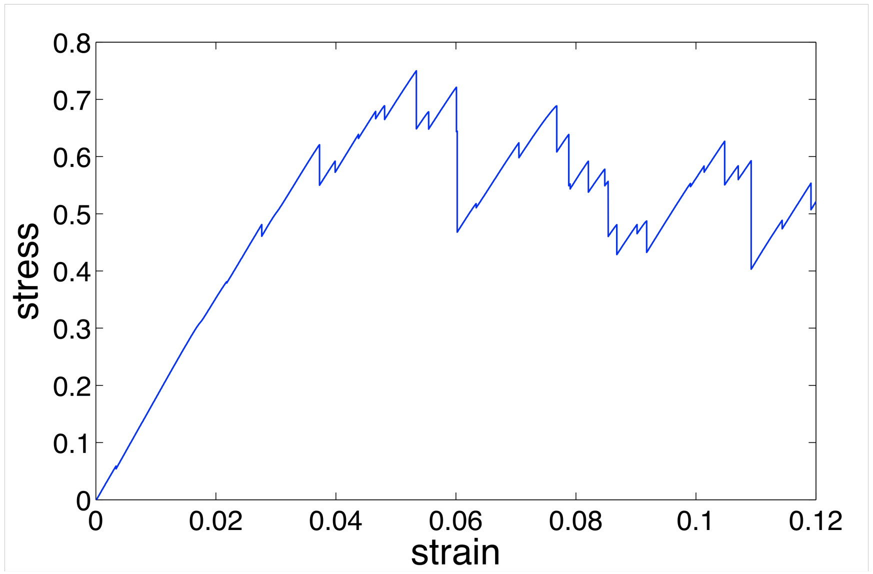
Memory effects in the localized state.

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 energy/stress interrupted by discontinuous change.
6. Discontinuous changes correspond to rearrangements.



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



Energy landscape picture: Schematic

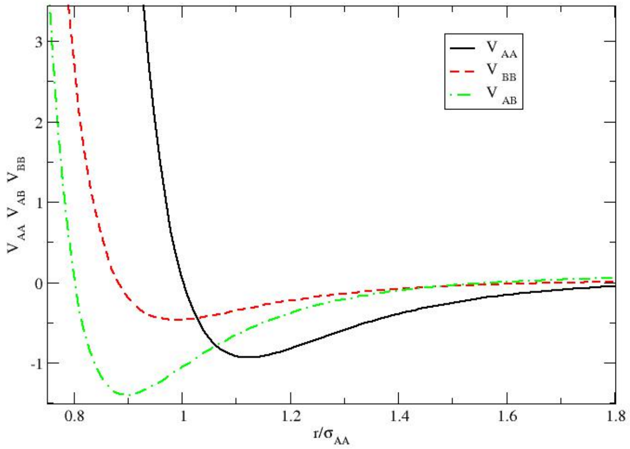
Shear deformation modifies the potential energy landscape and destabilizes the system, eventually leading to irreversible rearrangements.

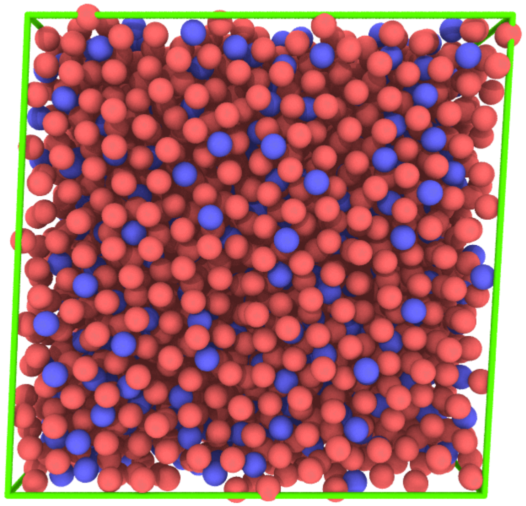
How does such deformation modify the properties of the glasses?

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

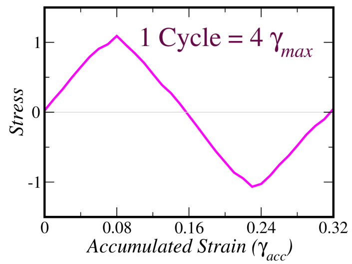
Kob-Andersen binary glass forming model.
(Constant Volume AQS)

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





$0 \rightarrow \gamma_{max} \rightarrow 0 \rightarrow -\gamma_{max} \rightarrow 0$



Different system sizes: Wide range from 2000 to 256000, but memory effects studied for 4000 particles.

Local minima from liquids states runs at: **T = 1, density = 1.2**

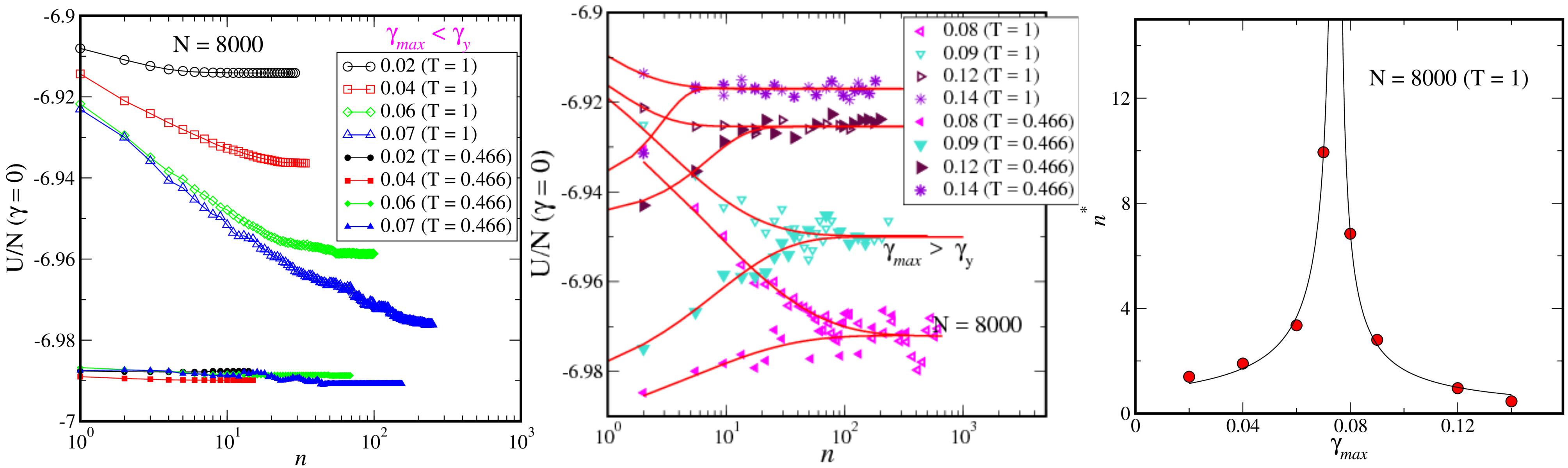
Cyclic shear for range of γ_{max} values with strain step dγ= 2x10^{-4}.

Stroboscopic configurations were used to compute various quantities, i.e. energy, MSD etc …

Later: Binary 50:50 soft sphere mixture with diameter ratio 1:1.4, with N = 2000, density 0.61, interaction potential $V_{ij} = \epsilon_{ij}(1 - \frac{r_{ij}}{\sigma_{ij}})^2$

Potential Energy vs. Cycle Number

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.
- Relaxation to the steady state **becomes more sluggish as γ_y is approached.**

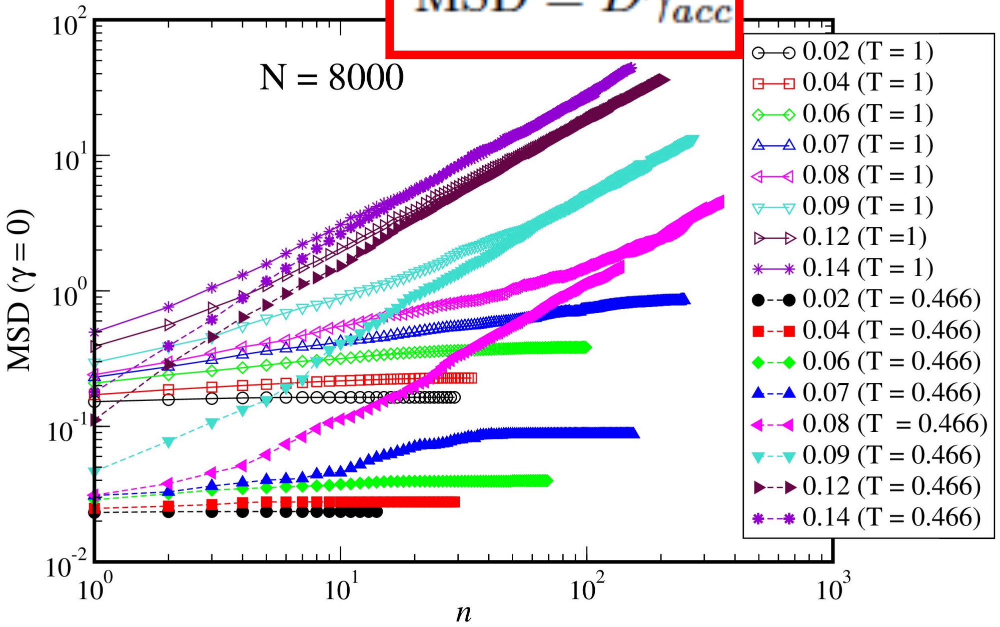
Change in behavior across a critical strain amplitude γ_c

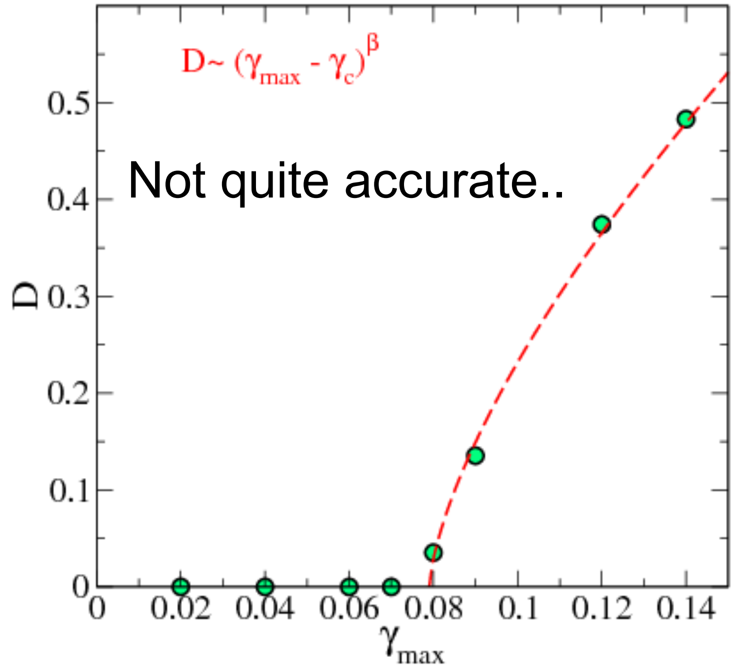
Mean Squared Displacement vs. Cycle #: Diffusion Coefficient

Depending on γ_{max} systems are either diffusive or non-diffusive.

In the diffusive regime, asymptotic slopes depend only on γ_{max}.

$$\boxed{\mathrm{MSD} = D\gamma_{acc}^{*}}$$



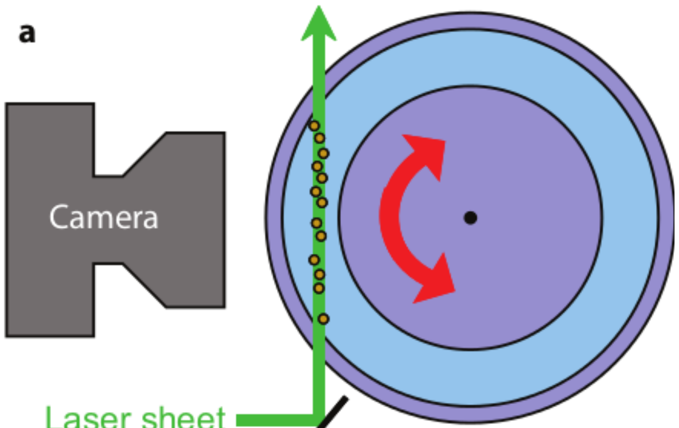


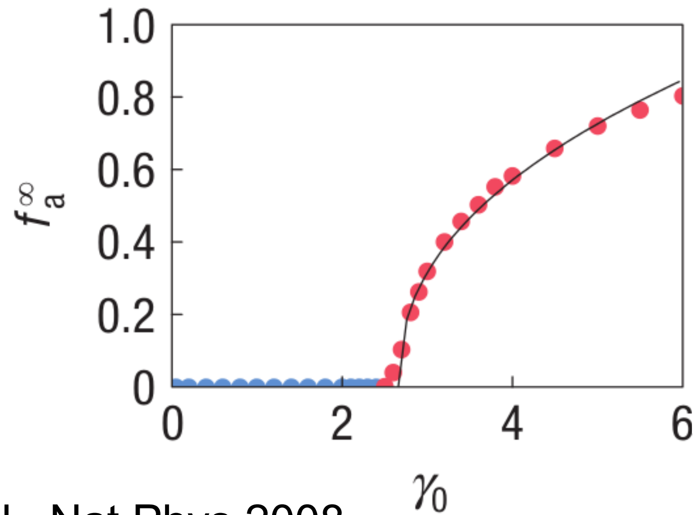
- The diffusion coefficient vanishes below a finite value of γ_{max}
- Critical γ_{max} a function of system size… but approach finite value asymptotically.

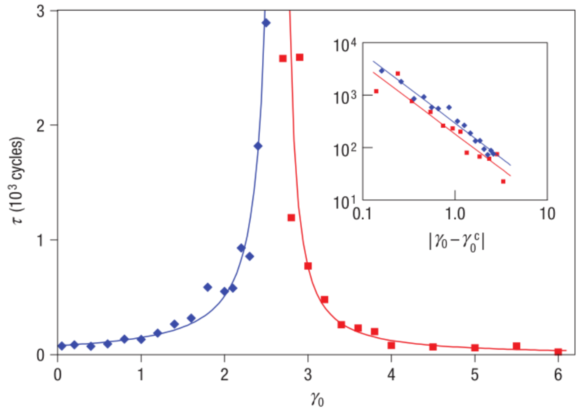
Non-equilibrium transition from localized to diffusive regimes!

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”.

Behavior reproduced in a model where particles that would overlap during a shear cycle are given random kicks.

The fraction of active particles, and the time to reach steady states indicate a absorbing to ‘ergodic’ state transition.

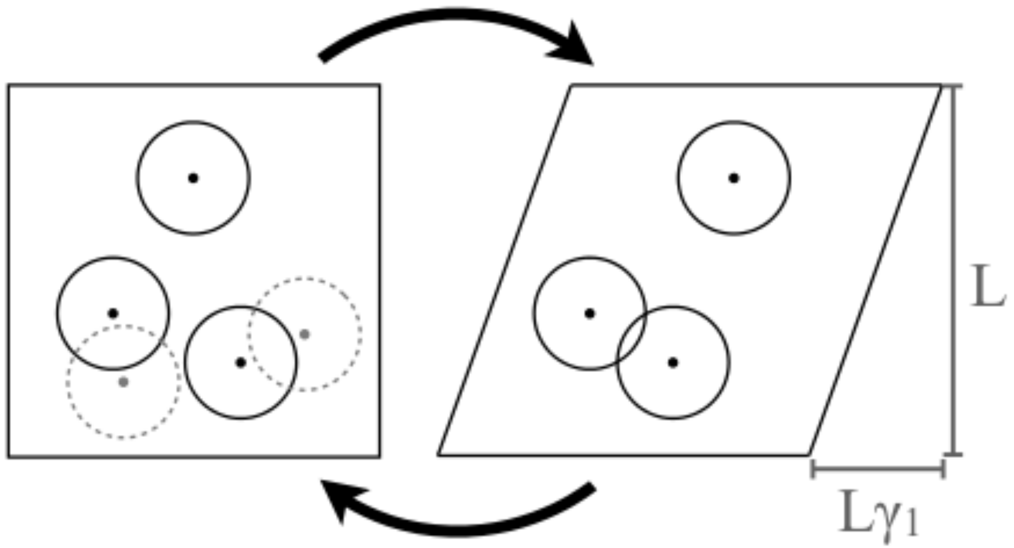
In the absorbing state, particles reach positions where they do not collide with each other during the shear cycle.

Memory

Do the absorbing state configurations exhibit memory of the shear amplitude at which they were obtained?

Question addressed for a computational model for the colloidal suspensions experiment by Keim and Nagel (2011), using simulations of the model system of Corte et al.

Subsequently studied experimentally (Paulsen, Keim, Nagel 2013).



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

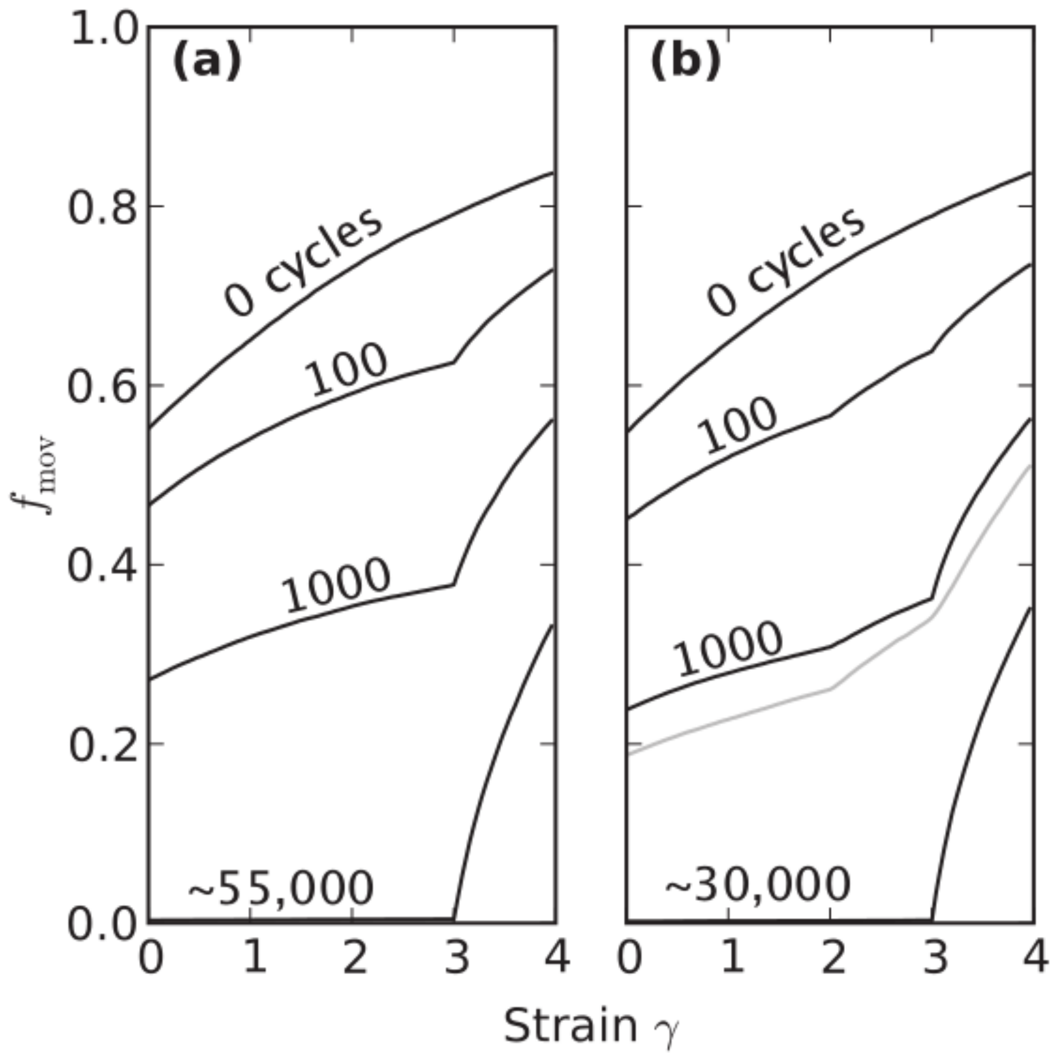
The "read off" at any stage is the number of "active" particles in **one** cycle.

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 the Glass

Given the similarity in behavior between the colloidal suspension and glass models, what do we expect as memory effects in the latter?

We follow the procedures of training and read off:

Training: Repeated oscillatory strain at a given (single) amplitude or cycling through multiple amplitudes.

Reading: Measure mean squared displacement (MSD) for one cycle, for range of amplitudes.
Parallel – read cycle starting with trained configuration for each read amplitude.

Sequential – read cycle starting with configuration after previous read operation at a lower amplitude.

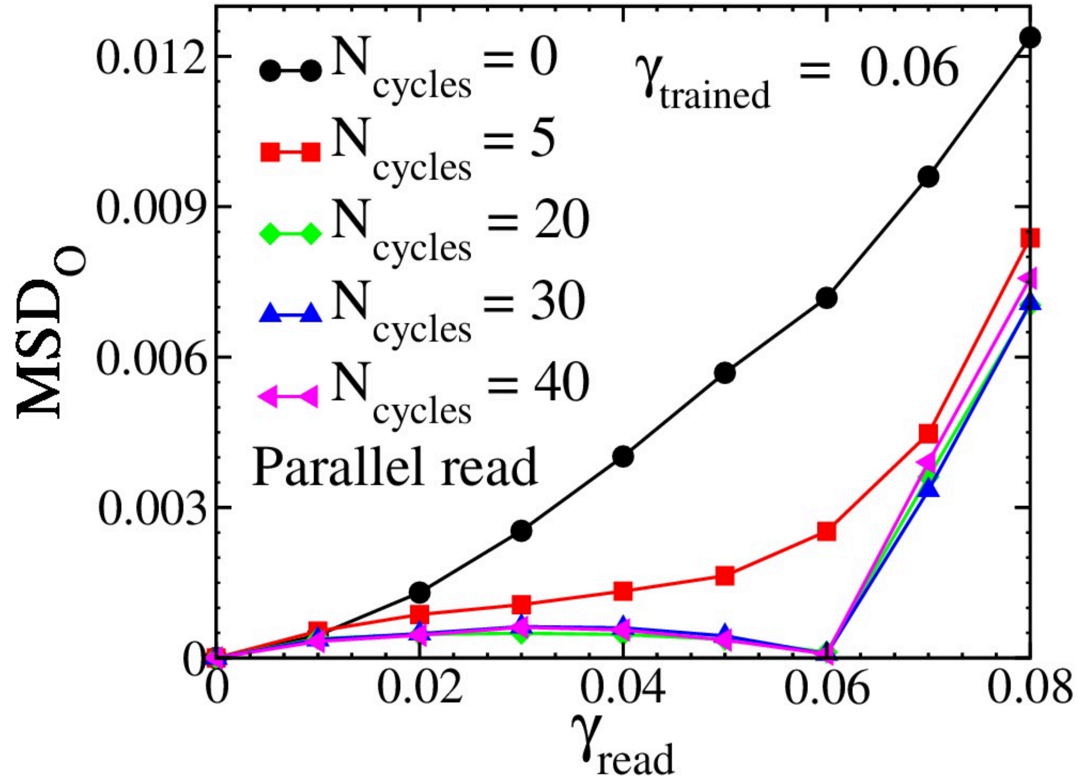
MSD_0 = with respect to the trained configuration.
MSD(I,i-1) = with respect to the previous read amplitude.
f_{active} = particles that move beyond a cutoff distance.

Single memory: parallel read

Equilibrated Sample (undeformed)

Shear for N cycles(N_{cycles} at γ_{max} (training)

Reading



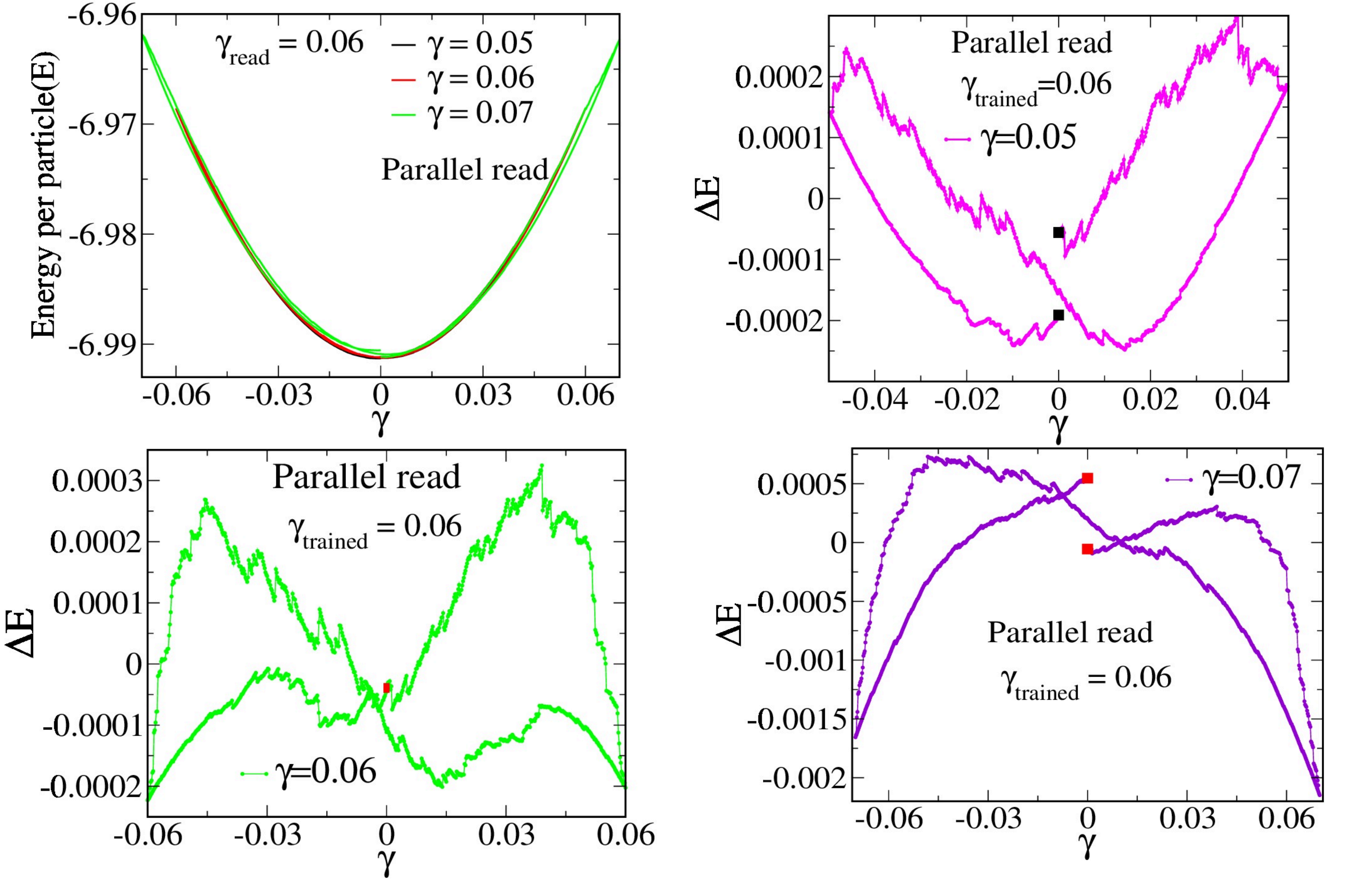
Memory of training amplitude: $MSD_0 = 0$ ONLY at training amplitude. Why?

Parallel reading:

Make n copies of trained sample

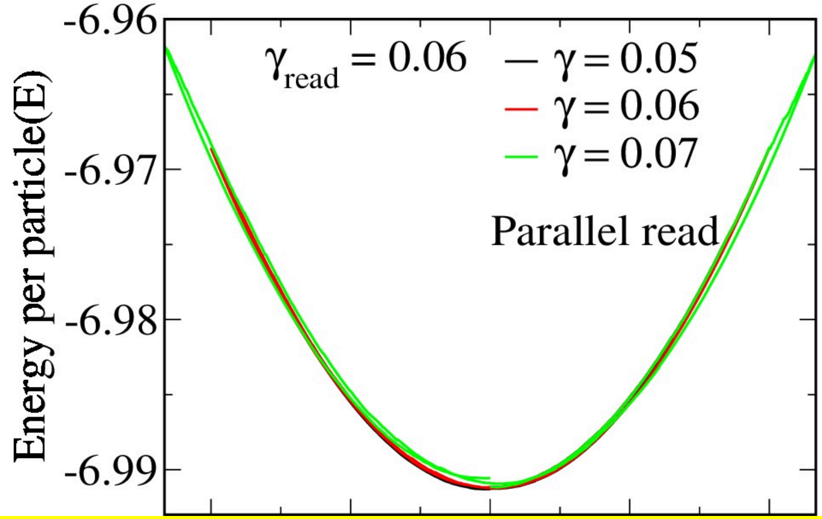
Apply shear for one cycle with different γ_{read} for different copies.

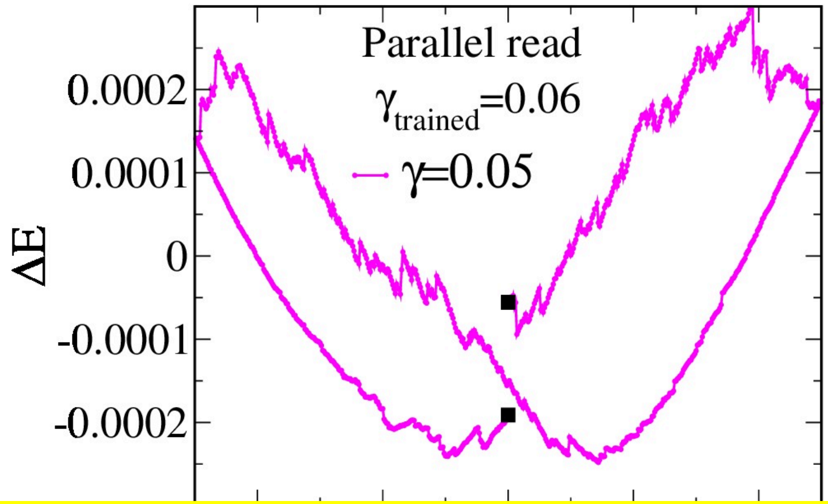
Energy curves



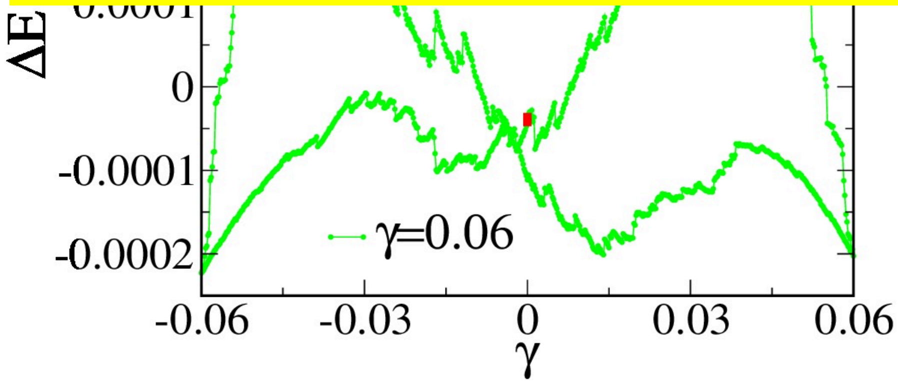
γ **trained=γread**

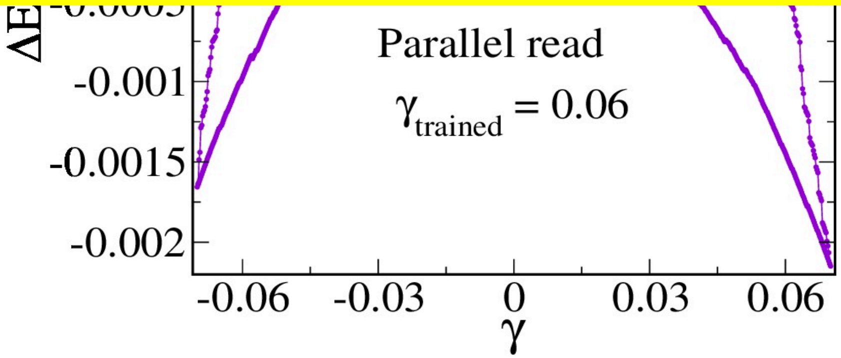
Energy curves





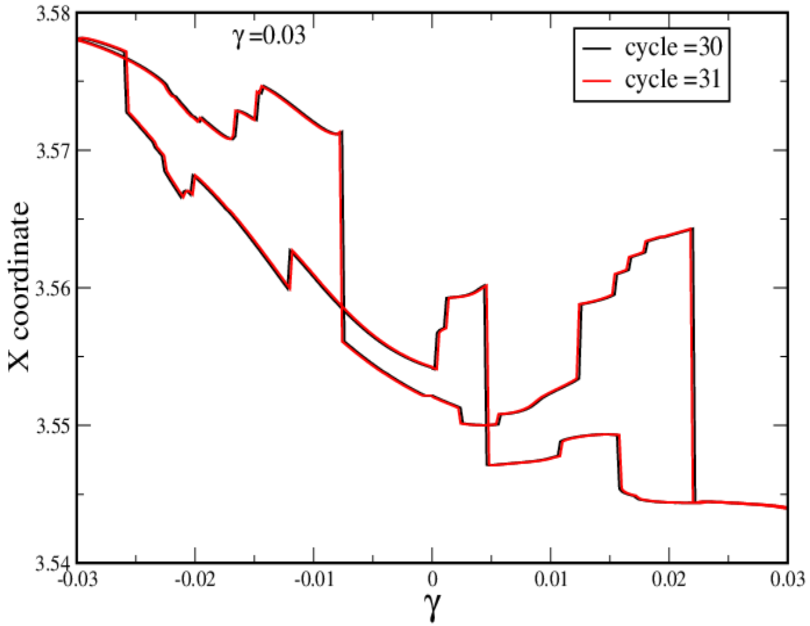
After a sequence of inherent structure transition system returns to original position. If the sequence breaks, then the system won't come back to original position. Energy loops are closed at $\gamma_{trained}$. Otherwise, they are open.

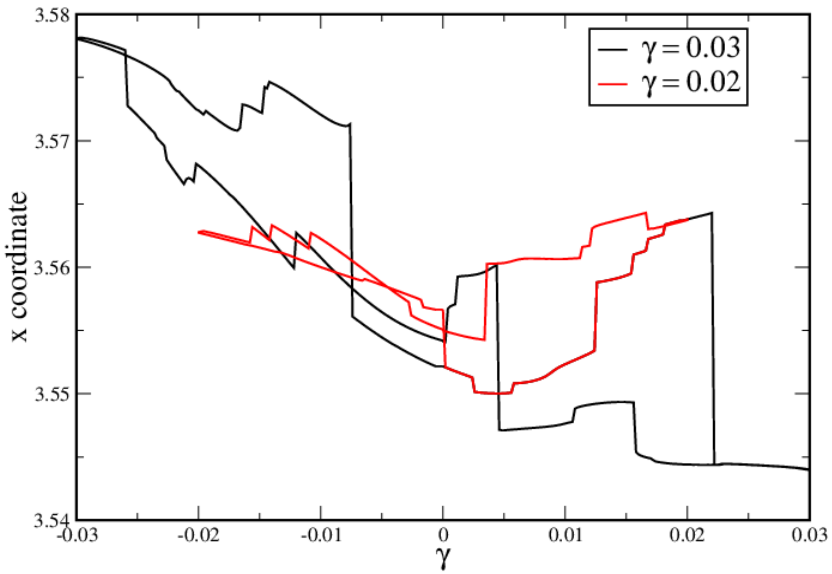


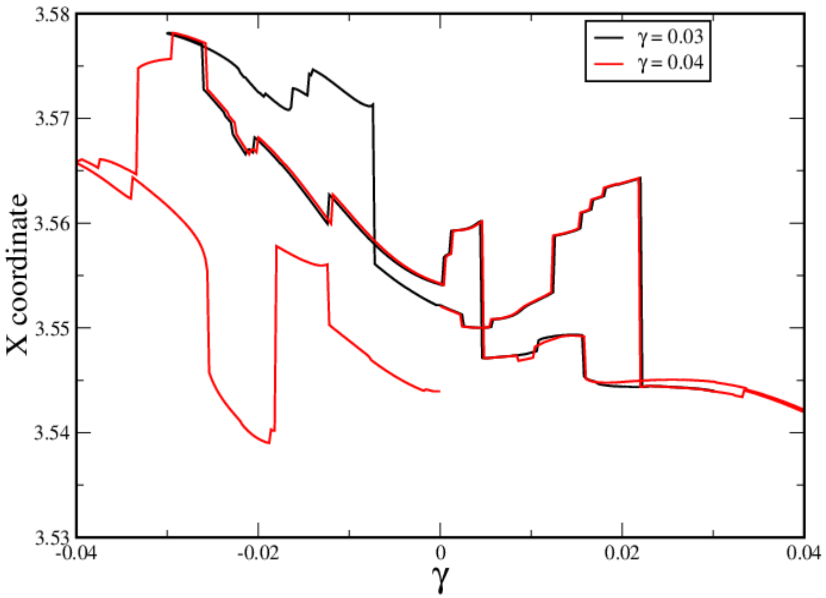


$\gamma_{trained=\gamma read}$

Loop reversibility

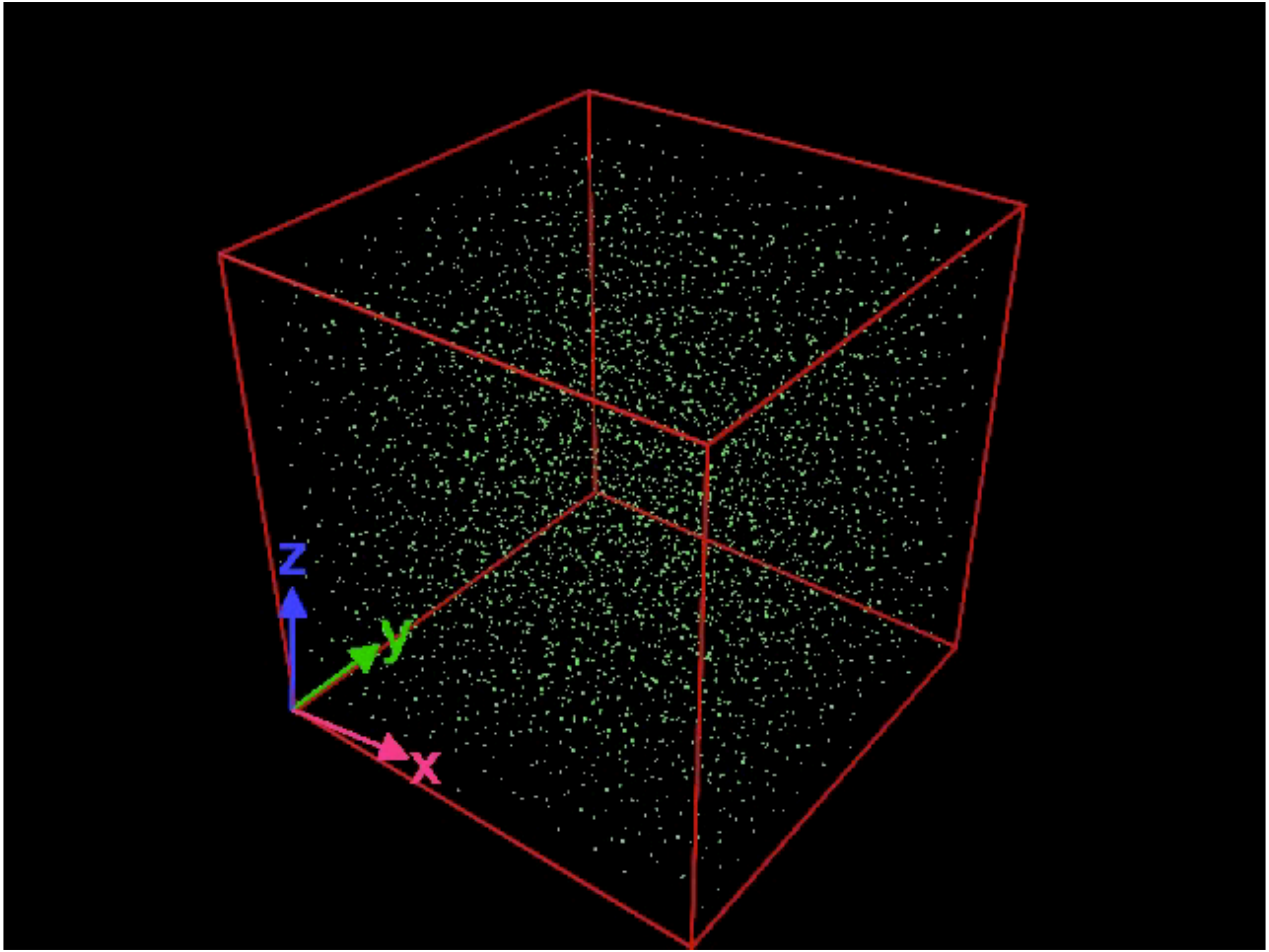






Evolution of a single particle coordinate during reading for diffrent γ_{read}. Particles return to original position when $\gamma_{read} = \gamma_{trained}$. Otherwise loop is open.

Particle Displacements



More questions

How do memory effects depend upon *amplitude* of deformation?

***Parallel read* is not possible for experimental samples. Are the memory effect seen robust and present for sequential read?**

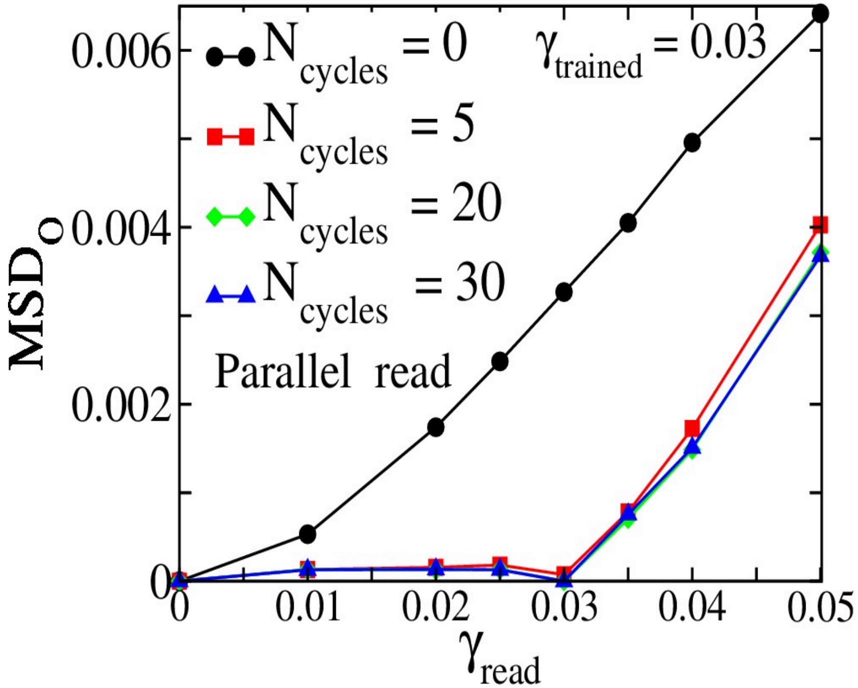
Can one encode *multiple memories* in the system ?

Once a memory is encoded how can one *erase* that memory?

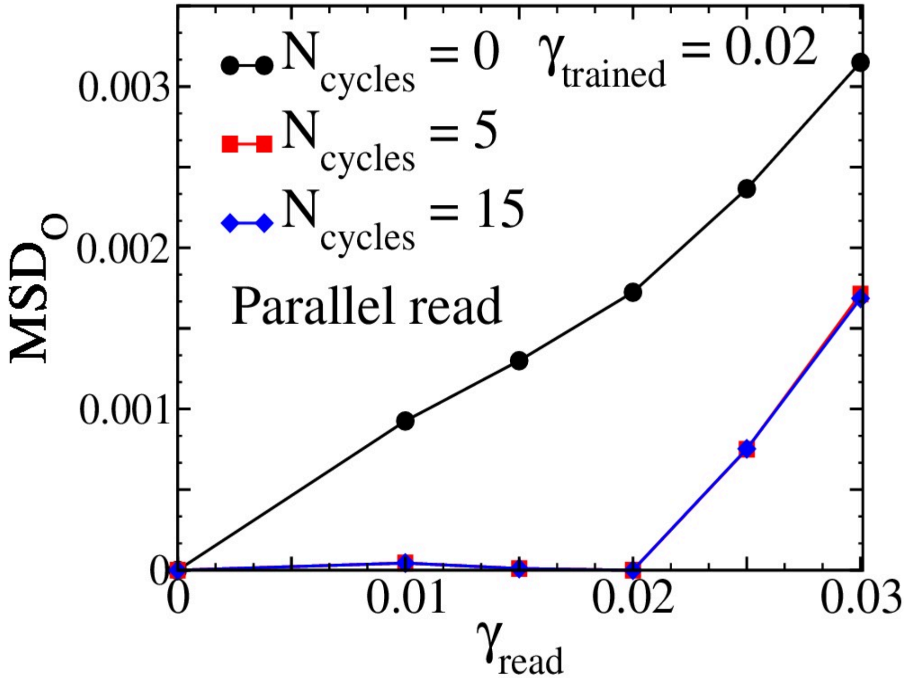
Parallel read: different amplitudes

We studied memory effects at different amplitudes below γ_c

Training amplitude γ_1 = 0.03



Training amplitude γ_1 = 0.02



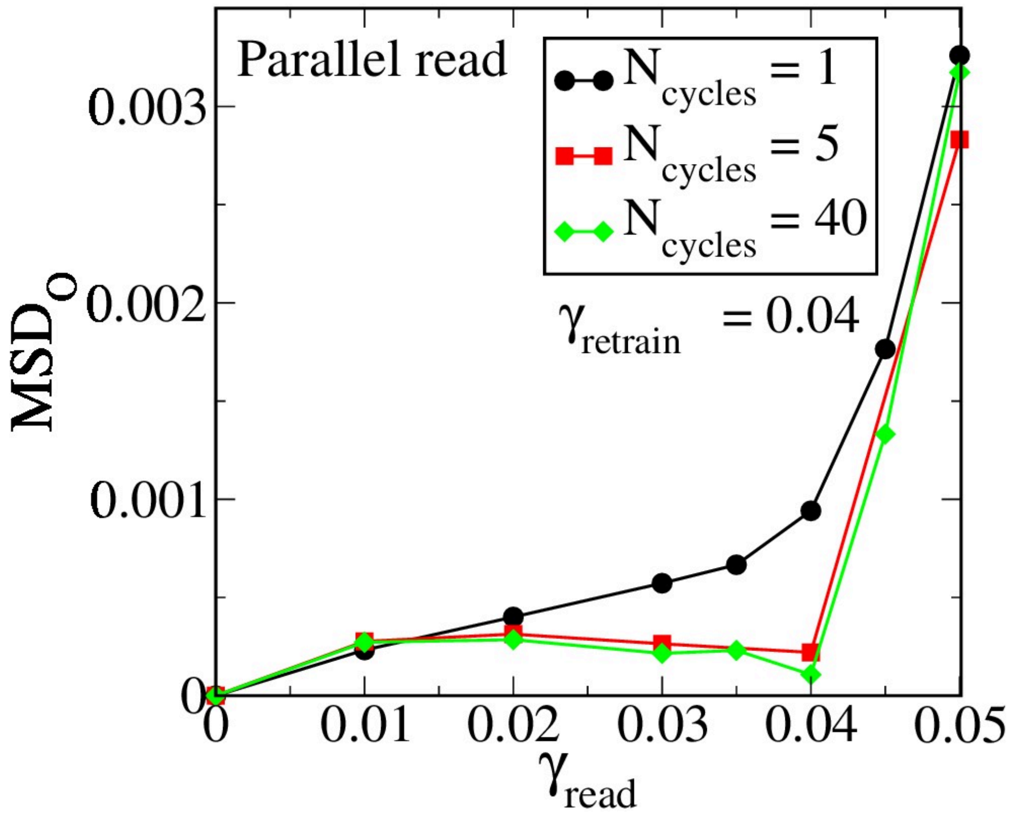
Memory is observed at all γ below γ_c

Stronger as training amplitude increases. [Ref Ajay Sood talk]

Application of shear with different amplitude to a trained sample

Amplitude is higher than trained amplitude : Erasure of Memory

Systems are trained at γ = 0.03



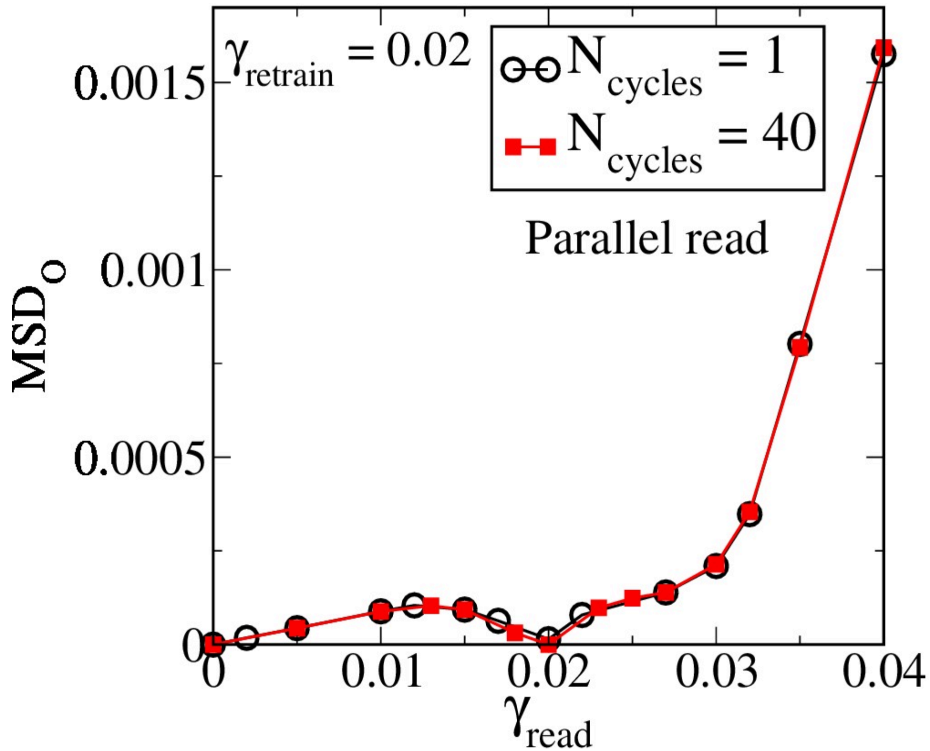
Apply shear with γ = 0.04 (1 cycle) : memory erased

Apply shear γ = 0.04 (40 cycles): memory encoded at γ = 0.04

Application of shear with different amplitude to a trained sample

Amplitude lower than trained amplitude : Multiple Memories

System trained at γ = 0.03

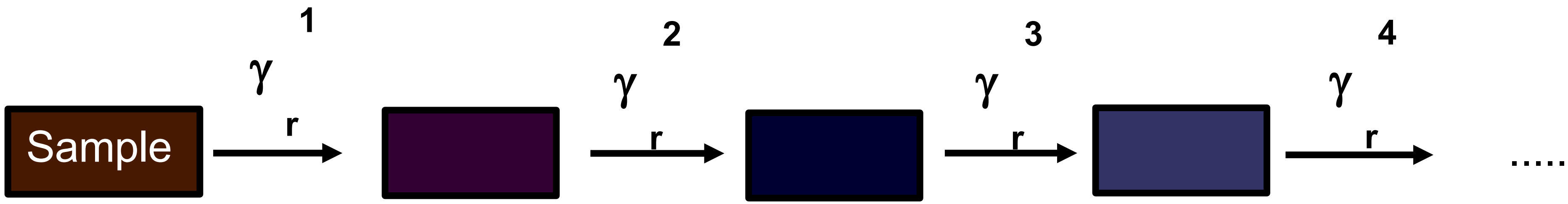


Apply shear with γ = 0.02 (1 cycle) : multiple memories (not clear)

Apply shear with γ = 0.02 (40 cycles): both memories present

Sequential read

After training, apply one cycle of shear with lower γ and use the resultant configuration for next cycle of shear with higher γ and so on. This is termed sequential read.



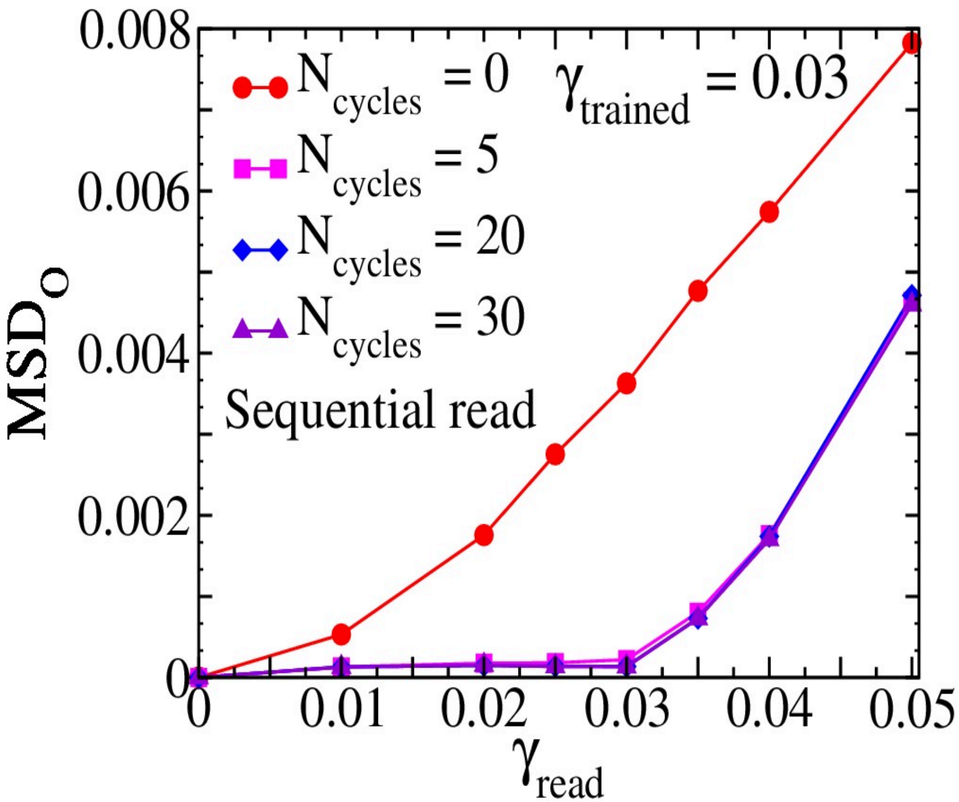
$\gamma_r^1 < \gamma_r^2 < \gamma_r^3 < \gamma_r^4$ ..

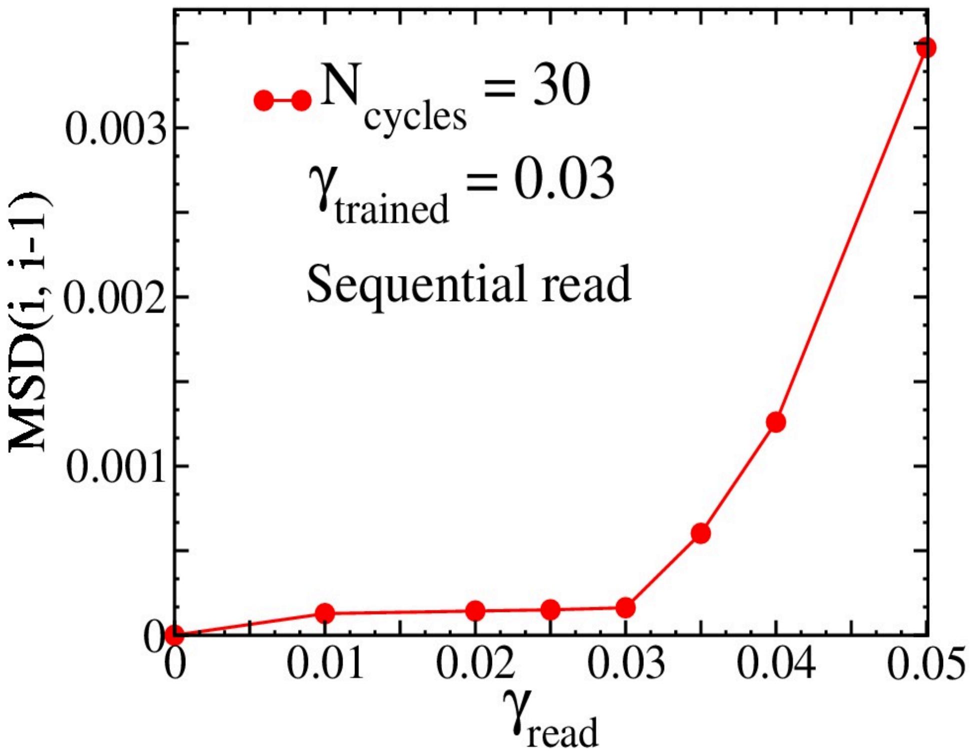
MSD was measured earlier with respect to 1. original configuration.
2. Also measured with respect to previous read configuration.

Sequential read

MSD was measured with respect to original configuration

MSD was measured with respect to previous configuration





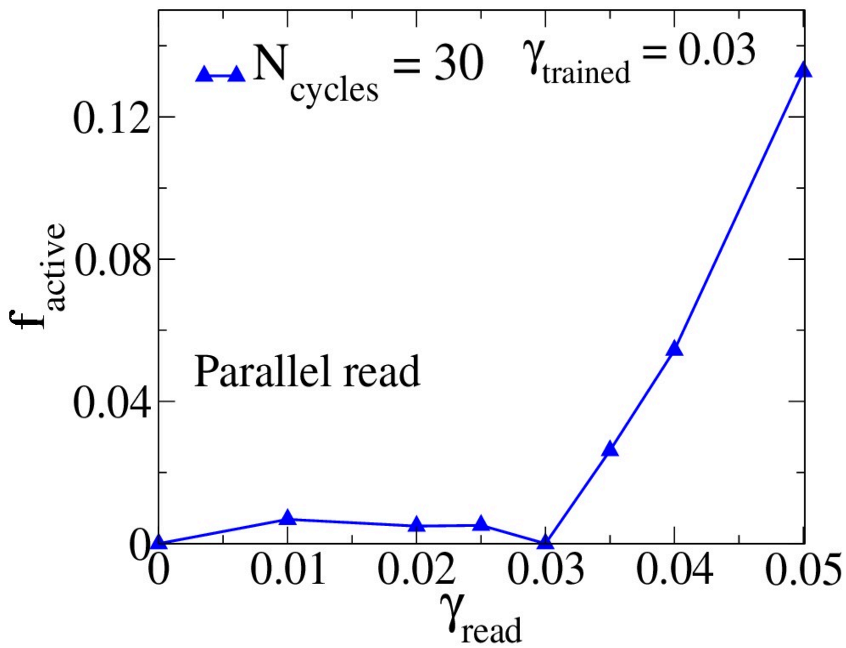
Memory can also be read sequentially.

Fraction of Active Particles

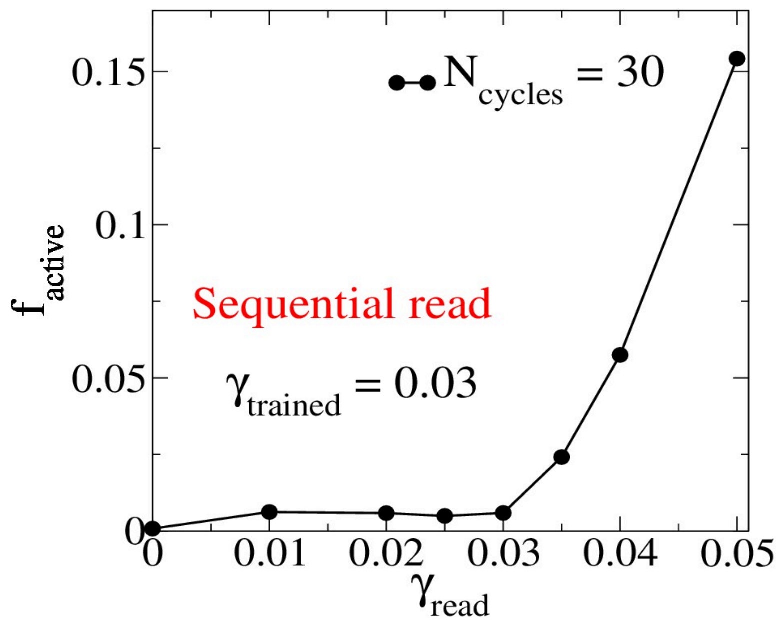
Different metric for reading: fraction of active particle (f_{active}), particle which has moved larger than some cutoff (0.1)

Works equally well.

Parallel reading



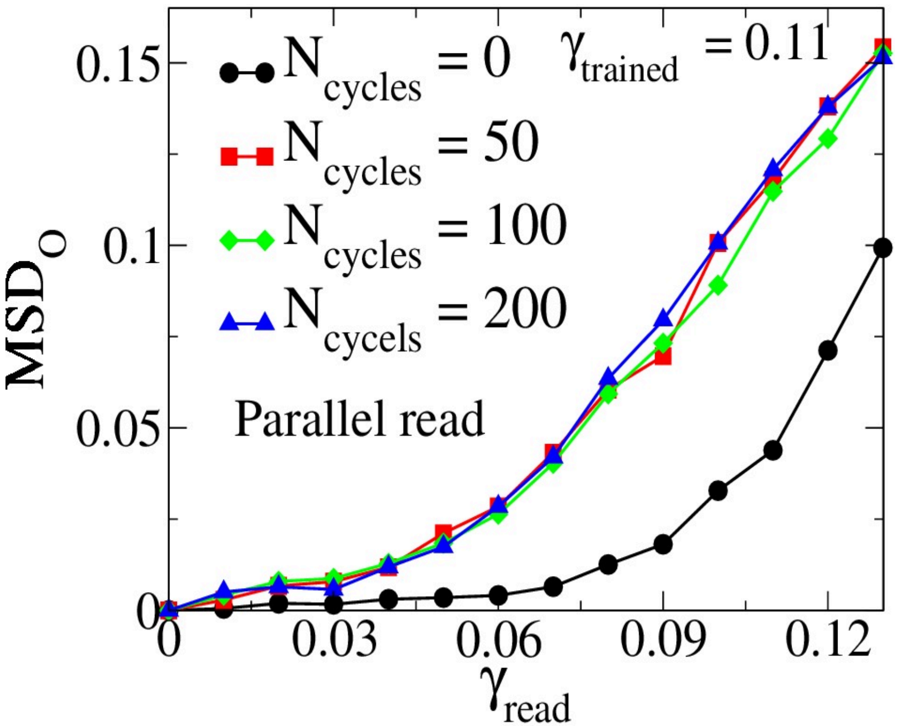
Sequential reading



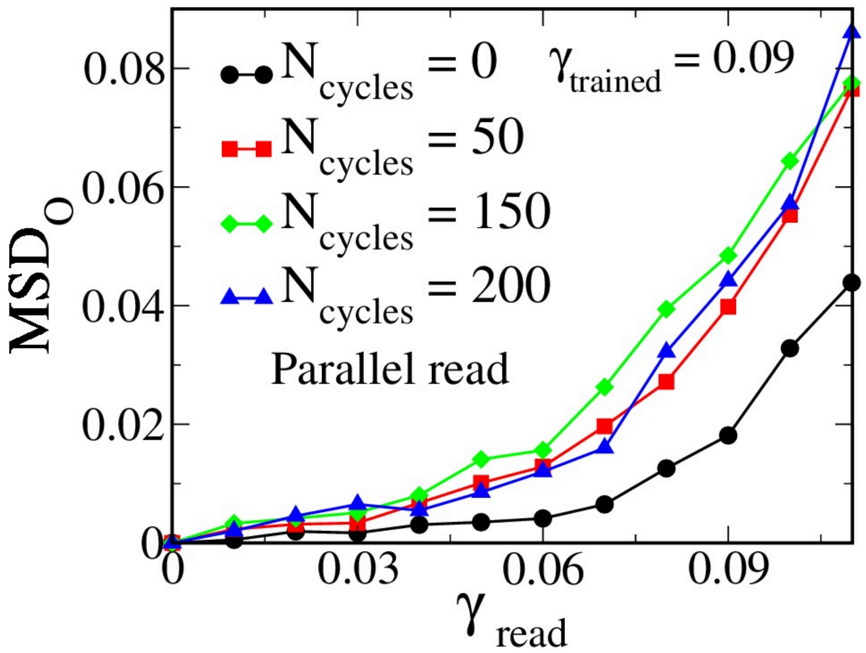
Memory effects in diffusive state

We studied memory effects at two amplitudes which belong to diffusing state

Training amplitude γ_1 = 0.11



Training amplitude γ_1 = 0.09



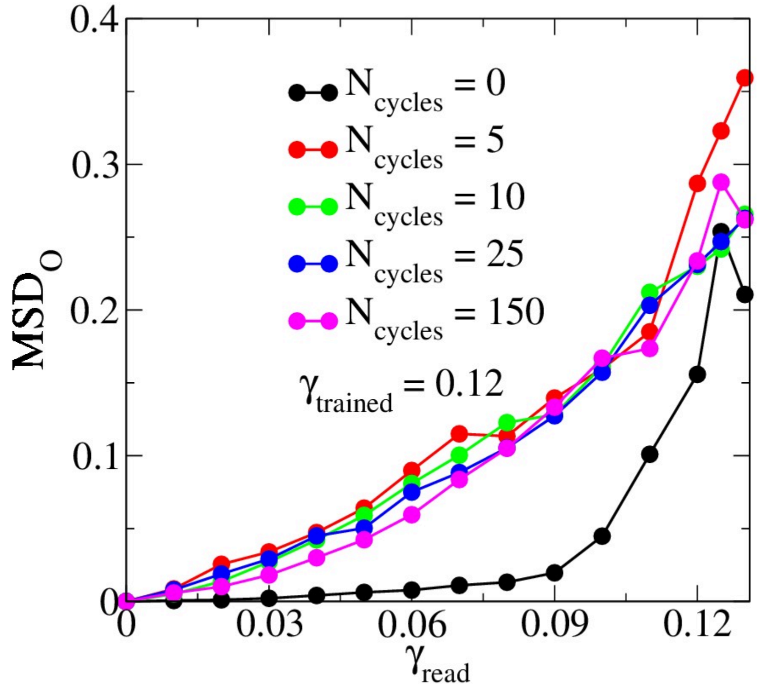
Memory is not observed above γ_c

At variance with bubble raft results [Ref. Ajay Sood talk]

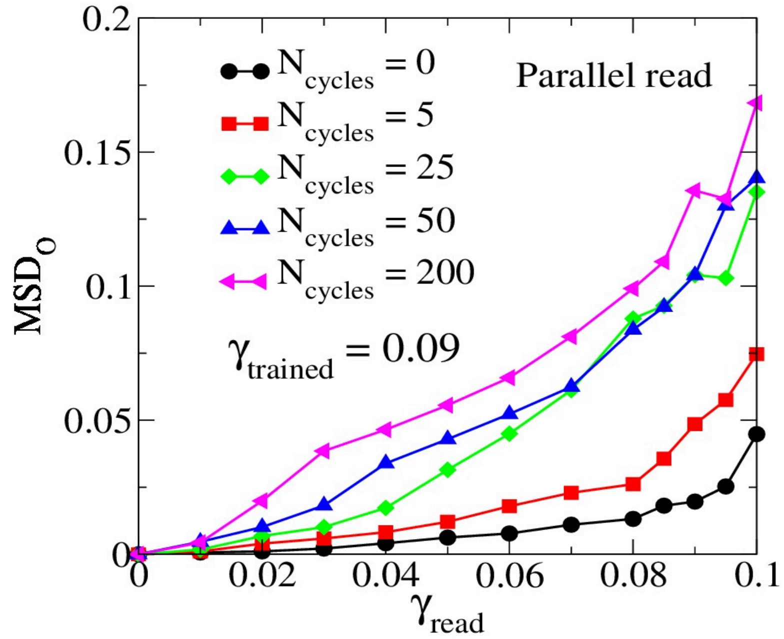
Memory effects in diffusing state

Larger system size : 64000 particles [which shows shear banding]

Training amplitude $\gamma_{trained}$ = 0.12



Training amplitude $\gamma_{trained}$ = 0.09

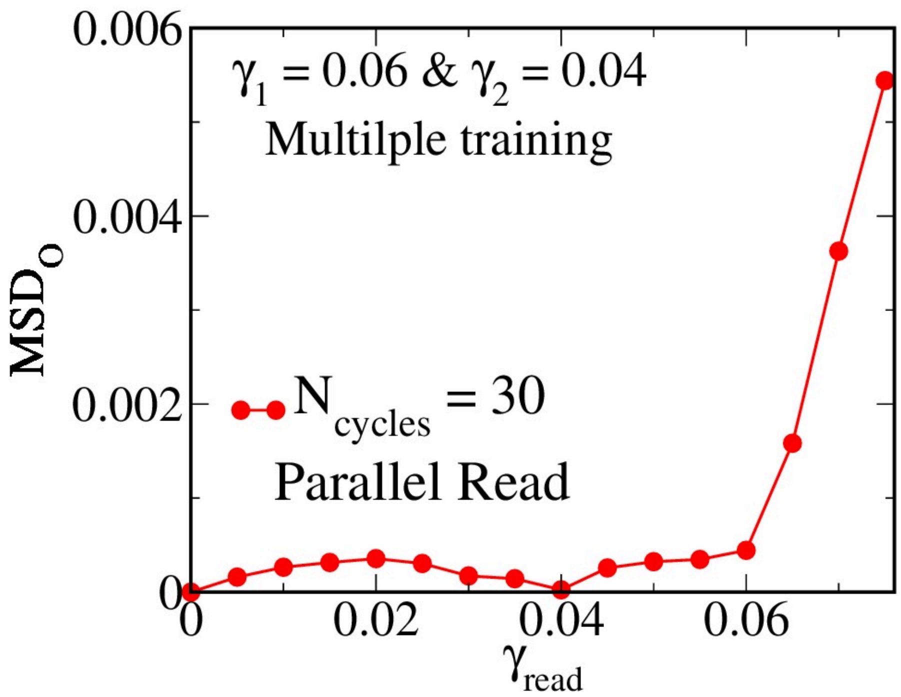


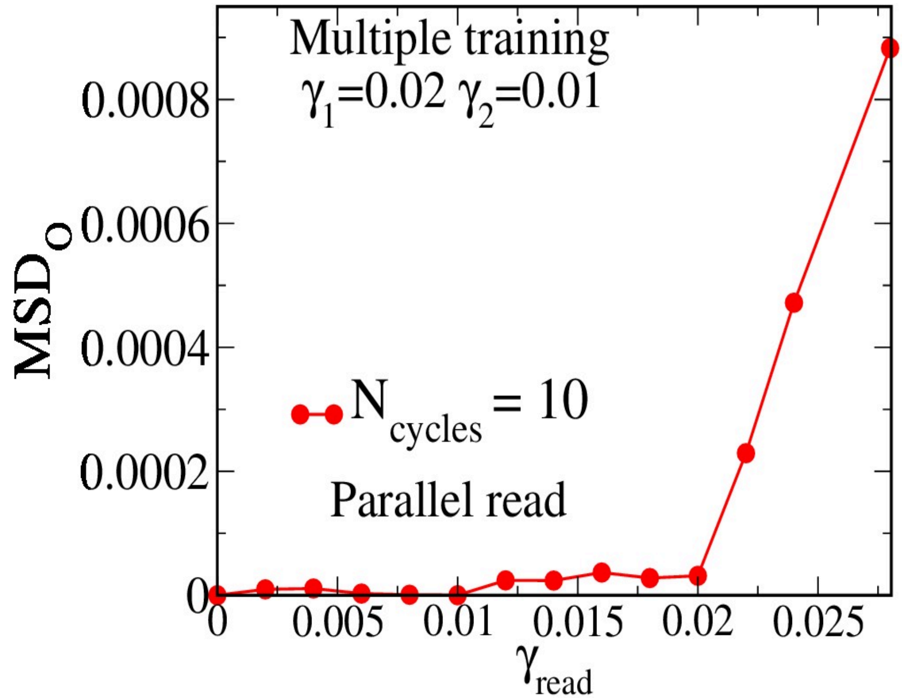
Memory is not observed above γ_c

Multiple Memories

Training cycle : Repeation of alternating cycles with two different amplitudes ($0 \longrightarrow \gamma_1 \longrightarrow -\gamma_1 \longrightarrow 0 \longrightarrow \gamma_2 \longrightarrow -\gamma_2 \longrightarrow 0$)

γ_1 and γ_2 are the amplitudes of deformation in training

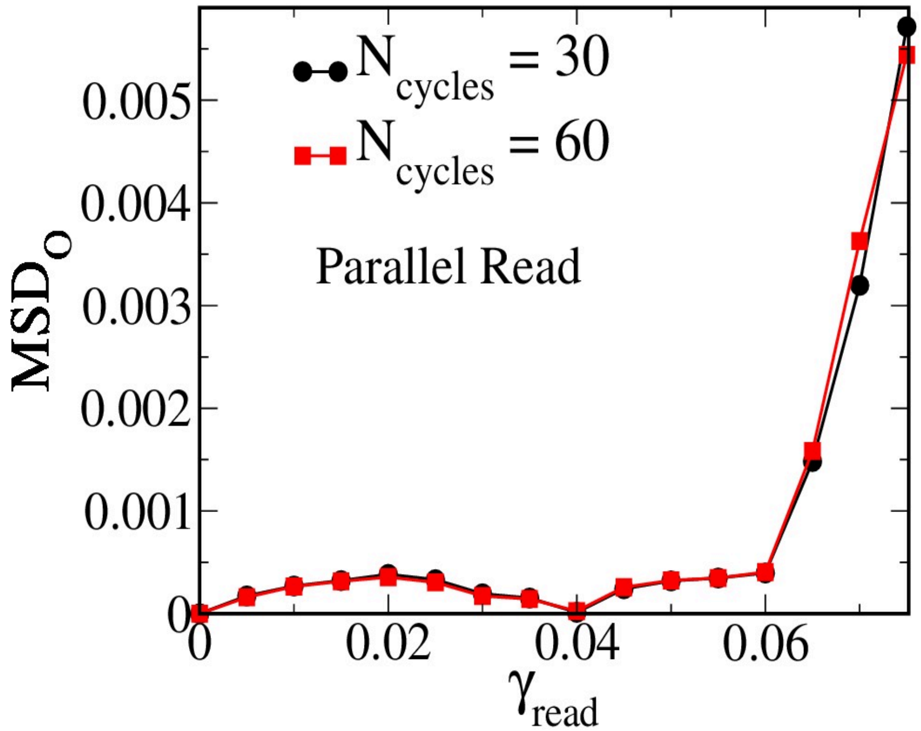


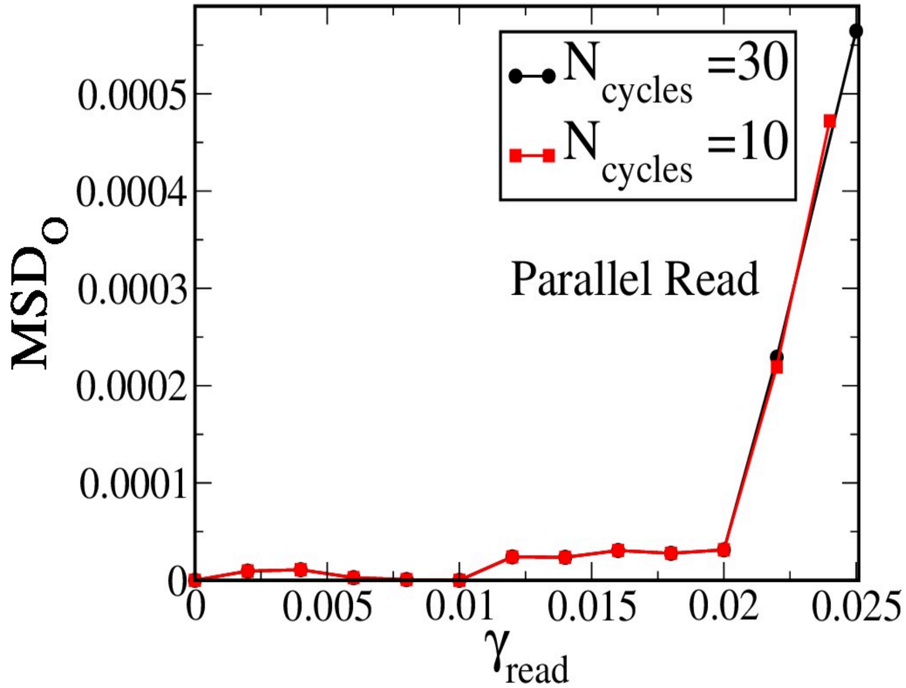


Two clear kinks were observed in MSD vs γ_{read} plot.
System can remember multiple memories

Multiple Memories: persistence

Both the memories are present after large number of training cycles





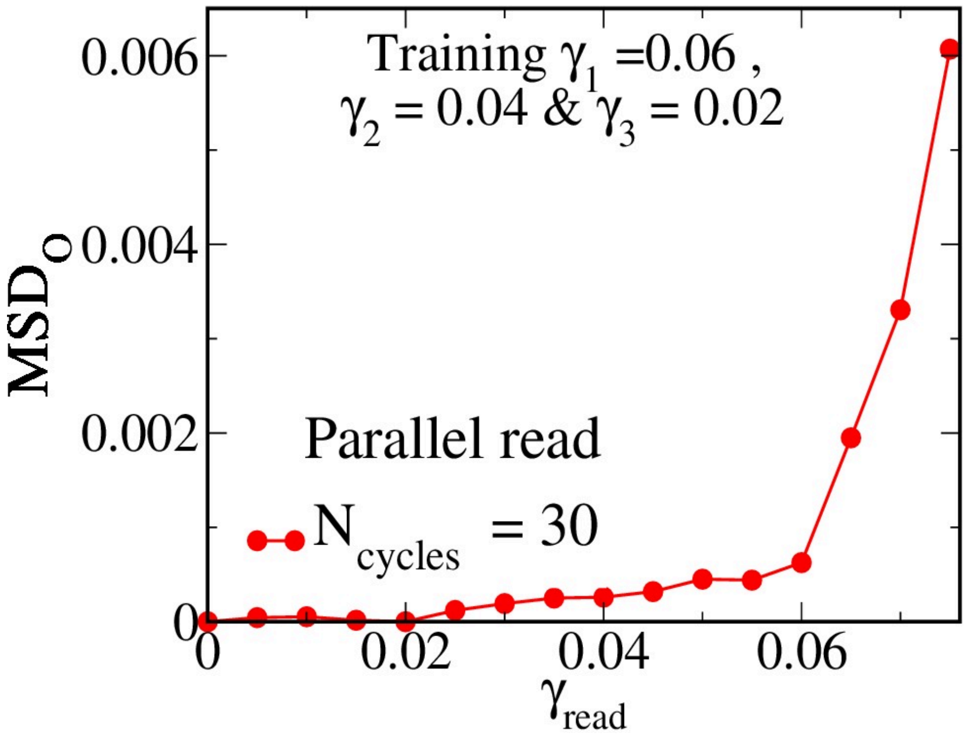
Multiple memories are persistent : Important difference form the previously discussed model

Multiple memories

Is this generally true for more than two amplitudes in training cycles ?

We try encoding memory with three different amplitudes $\gamma_1 \rightarrow 0 \rightarrow -\gamma_1 \rightarrow \gamma_2 \rightarrow 0 \rightarrow -\gamma_2 \rightarrow \gamma_3 \rightarrow 0 \rightarrow -\gamma_3$

$\gamma_1 = 0.06$, $\gamma_2 = 0.04$ $\gamma_3 = 0.02$



Only two memories are observed by the protocol we used for training and reading

Multiple memories

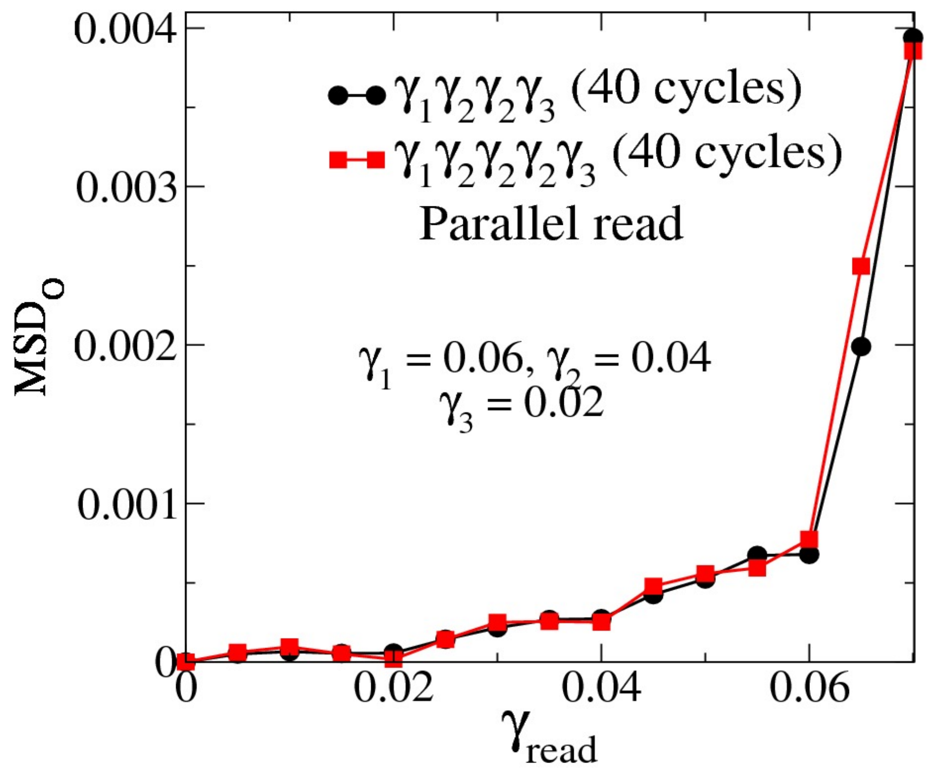
Memory for more than two amplitudes

Systems trained with three different amplitudes.

We follow here these sequences

1. $\gamma_1\gamma_2\gamma_2\gamma_3$
2. $\gamma_1\gamma_2\,\gamma_2\gamma_2\gamma_3$

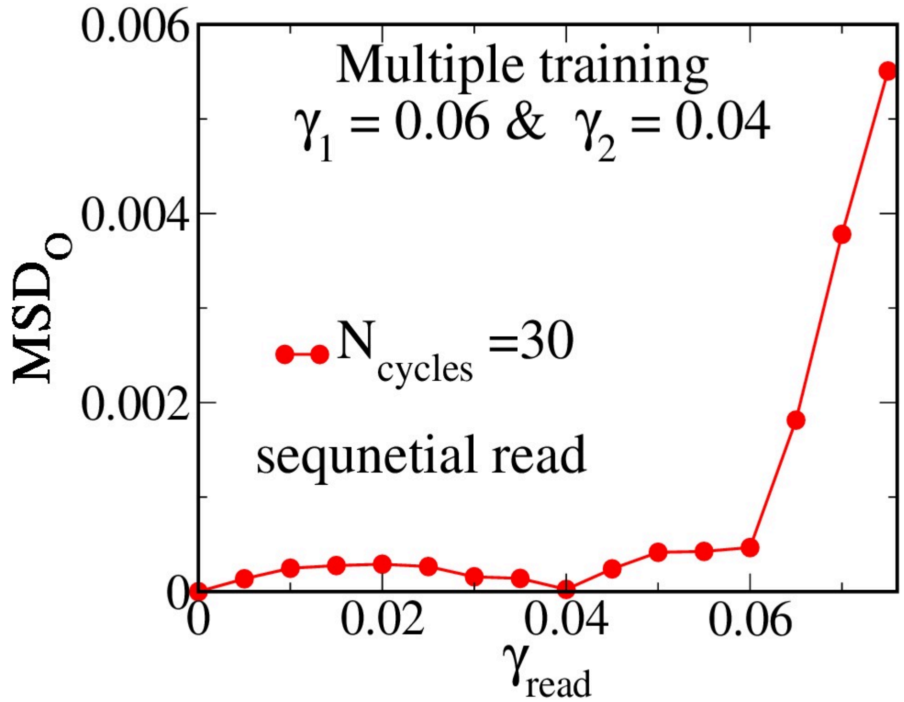
All the kinks were observed at trained amplitudes($\gamma_1 = 0.06\,, \gamma_2 = 0.04, \gamma_2 = 0.02$ **)**



All three memories are clearly observed

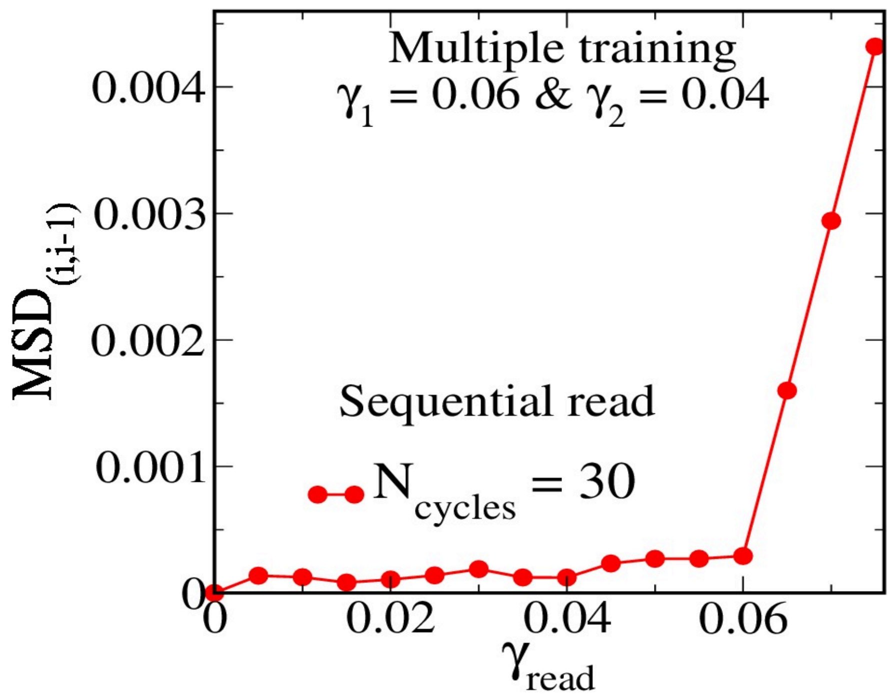
Sequential read

MSD with respect to **original** configuration



Two kinks are also observed

MSD with respect to **previous** configuration



Memory at lower γ is not clear

Summary so far

Model glass under cyclic deformation exhibits memory effects.

Both single and multiple memories are seen persistently.

Different protocols for reading lead to consistent results.

Application of an amplitude of shear larger than the training amplitude leads to erasure of memory.

Training at amplitudes larger than yield strain lead to no memory effects.

Interesting features attributed to presence of periodic orbits to which sheared glasses map, in the landscape of the system.

Do other models with such landscape features show similar behavior?

Simple Model I: The NK Model

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

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

Parameters a_i and b_i are random and depend on the state of i and K neighbors.

Each spin associated with K neighbors: $m_i \xrightarrow{J} \{m_i^1, \ldots, m_i^K\}$

a and **b** have randomly chosen values for each (K+1)-tuple:

$$\{0,1\}^{K+1} \xrightarrow{a} [-1,1] \qquad \{0,1\}^{K+1} \xrightarrow{b} [0,1]$$

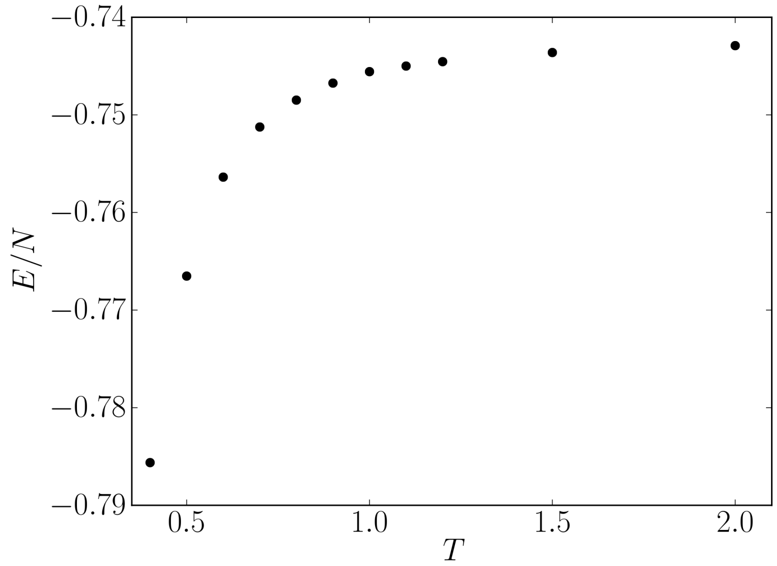
Varying γ mimicks the application of strain.

Varying **K** varies the ruggedness of the landscape.

We study M = 0 states.

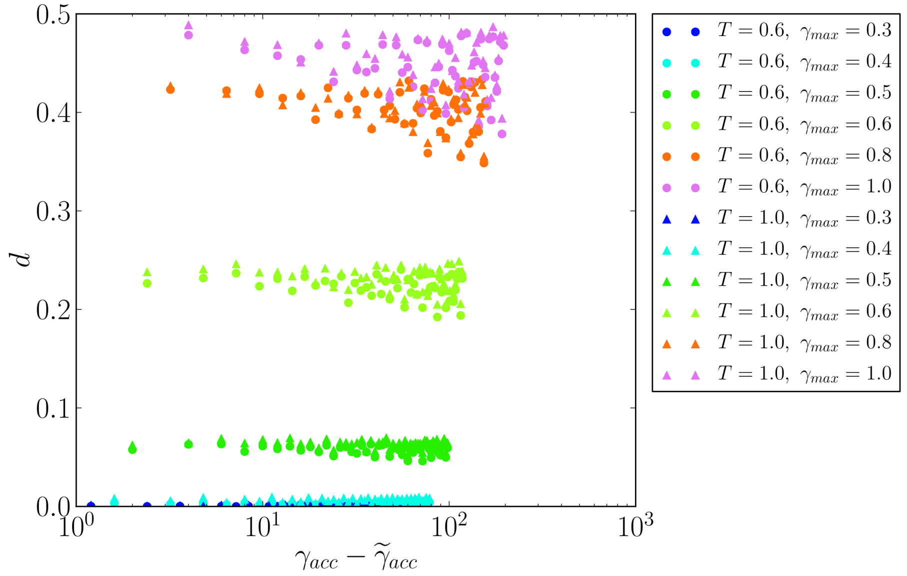
Dynamical Transition in the NK model

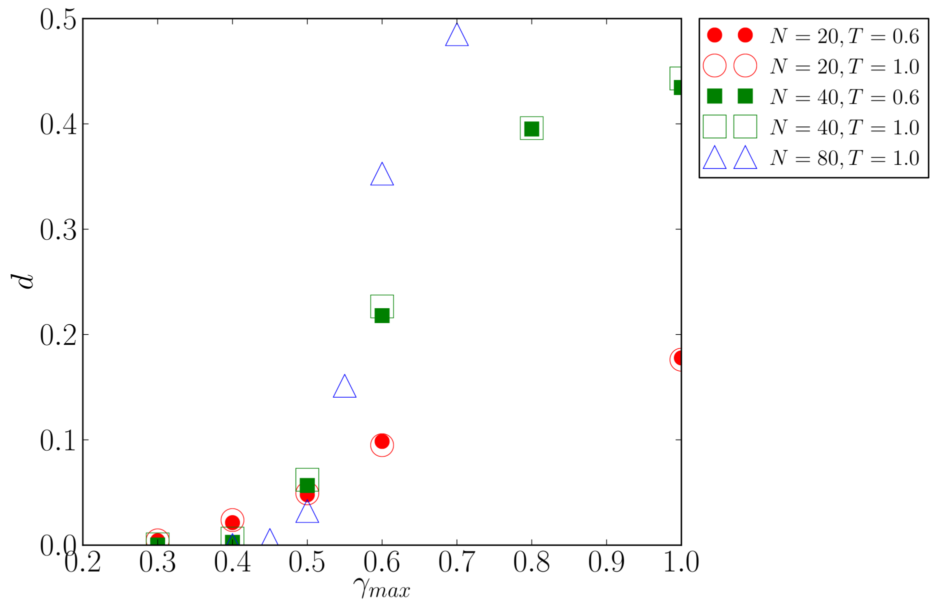
Energy of minima vs T similar to structural glass formers.



Using Hamming distance from initial configuration as measure, one observes dynamical transition similar to model glass.

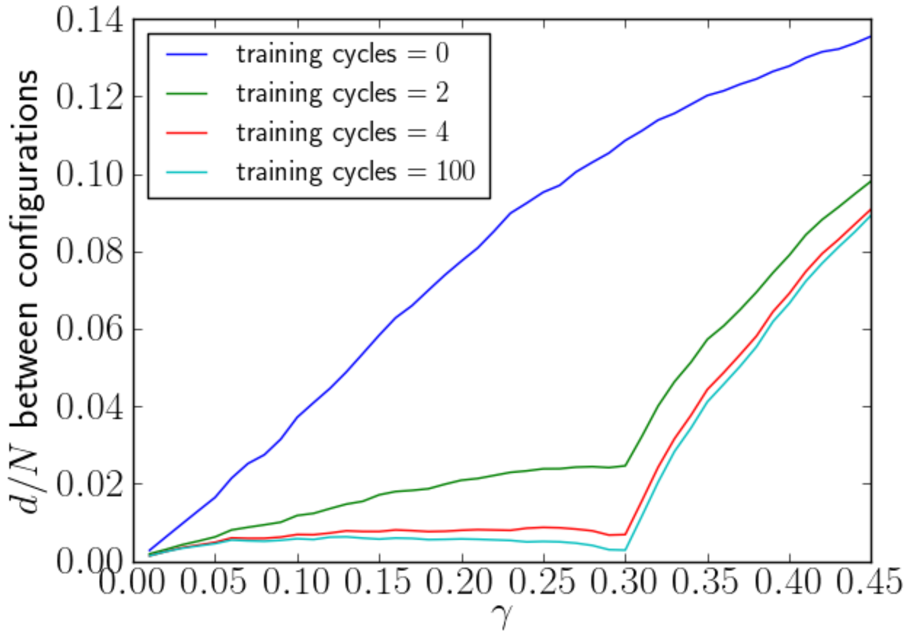
Sharpness of transition in large N limit needs to be ascertained.

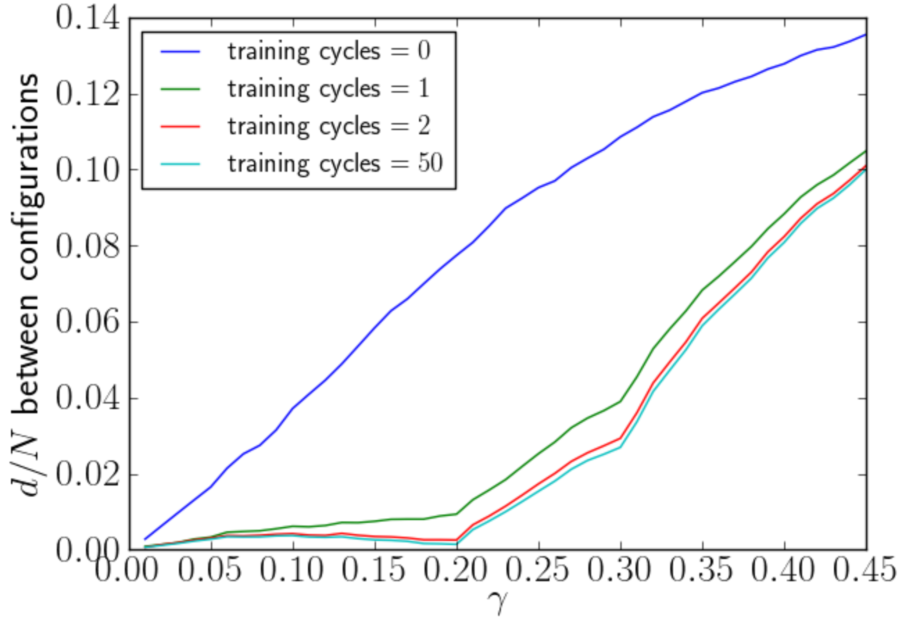




Memory in the NK model

Ability to store single and multiple memories similar to model glass.





Simple Model II: The Transition Matrix Model

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

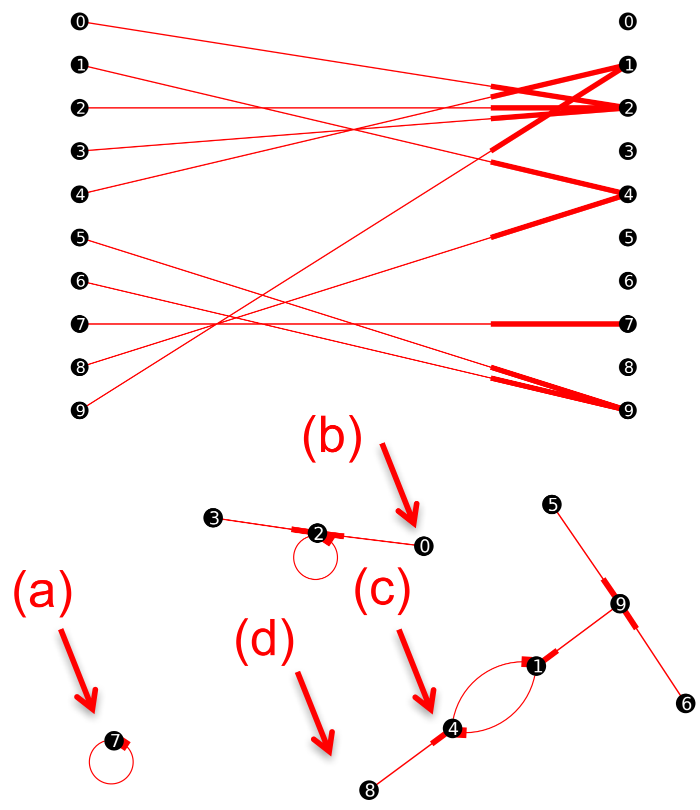
Probability of jumping to another inherent structure increases with strain amplitude.

For each maximum strain amplitude, a transition matrix **P** is constructed for a full cycle by considering mappings of of minima for successive strain increments.

Minima are classified into (a) absorbing states, (b) mapping to absorbing states, (c) recurring states, and (d) mapping to recurring states.

Repeated cycles correspond to the application of **P** repeatedly, and the number of nodes mapping to absorbing states and non-absorbing states is obtained.

We do not make a distinction based on size of recurring state loops at present.

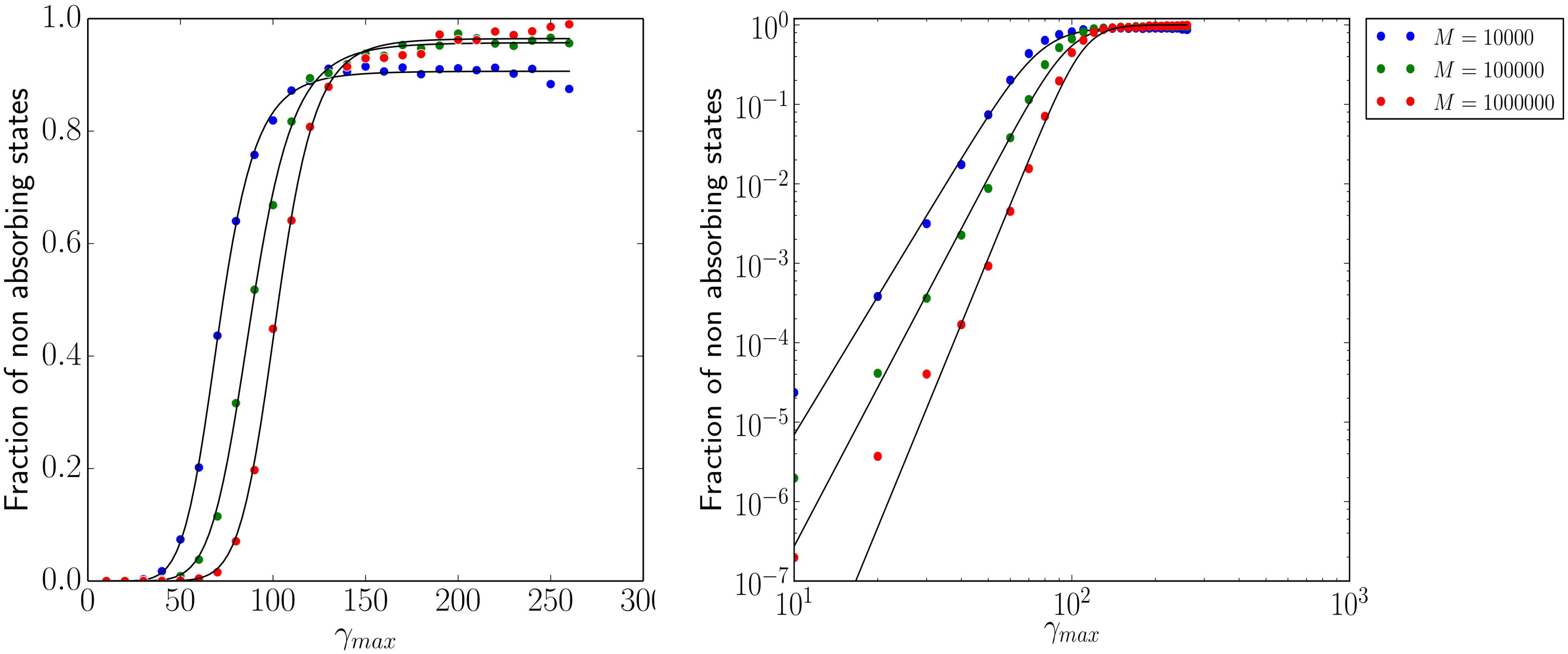


Directed graph representation

Dynamical Transition in the TM model

Transition matrices constructed for different sizes M, that indicate a sharp increase in the fraction of non-absorbing states beyond a critical amplitude.

Sharpness of transition in large N limit needs to be ascertained, in particular making the distinction between O(1) cycles and O(M) cycles among recurring states.



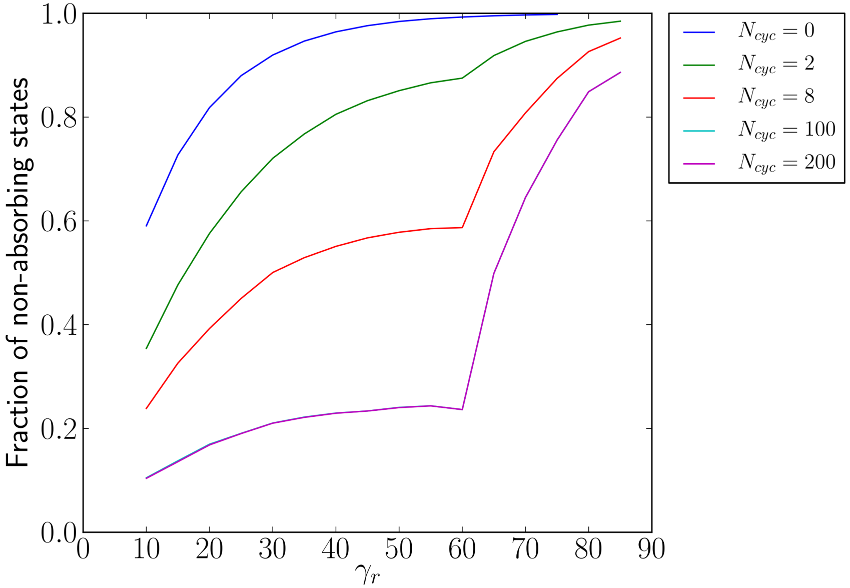
Memory in the TM model

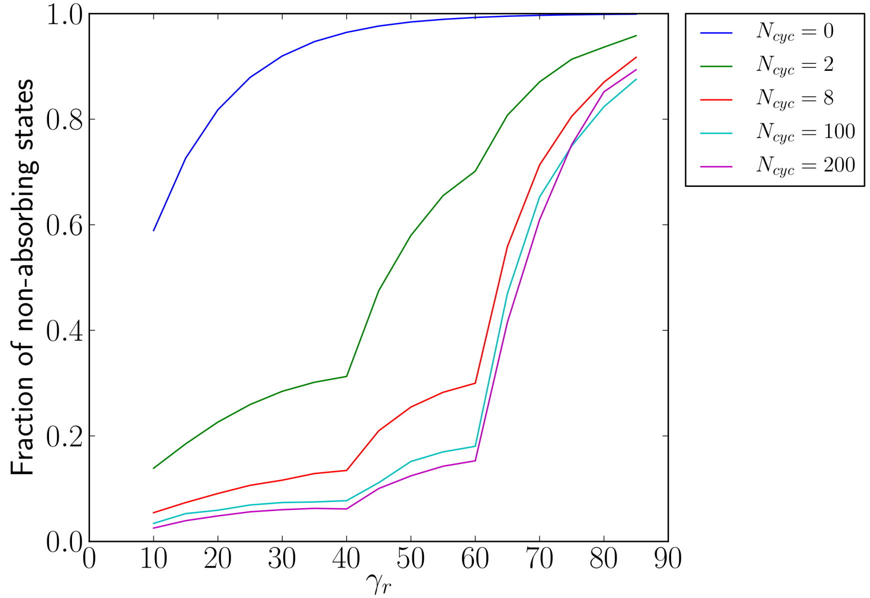
Generate subset of states after training for N cycles at (one or two) given amplitudes. These are states with finite weight after training.

These states are subjected to a reading cycle varying γ_r to test if they are absorbing states at γ_r.

Fraction of non-absorbing states displays behavior similar to model glass and the NK model.

Behavior appears generic. But very little has been assumed in constructing the TM model.. Consdiering a model without a nontrivial landcape sheds some light…next.





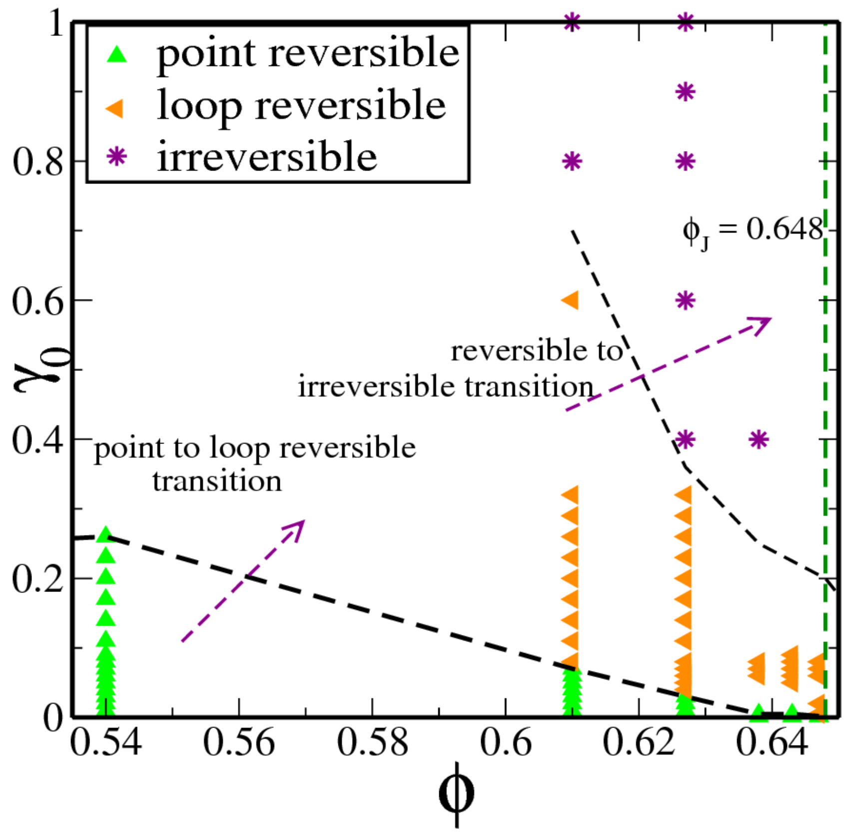
Soft Sphere Assemblies

At density 0.61:

Point reversible below 0.07

Loop reversible till 0.7 (est)

Irreversible beyond 0.7



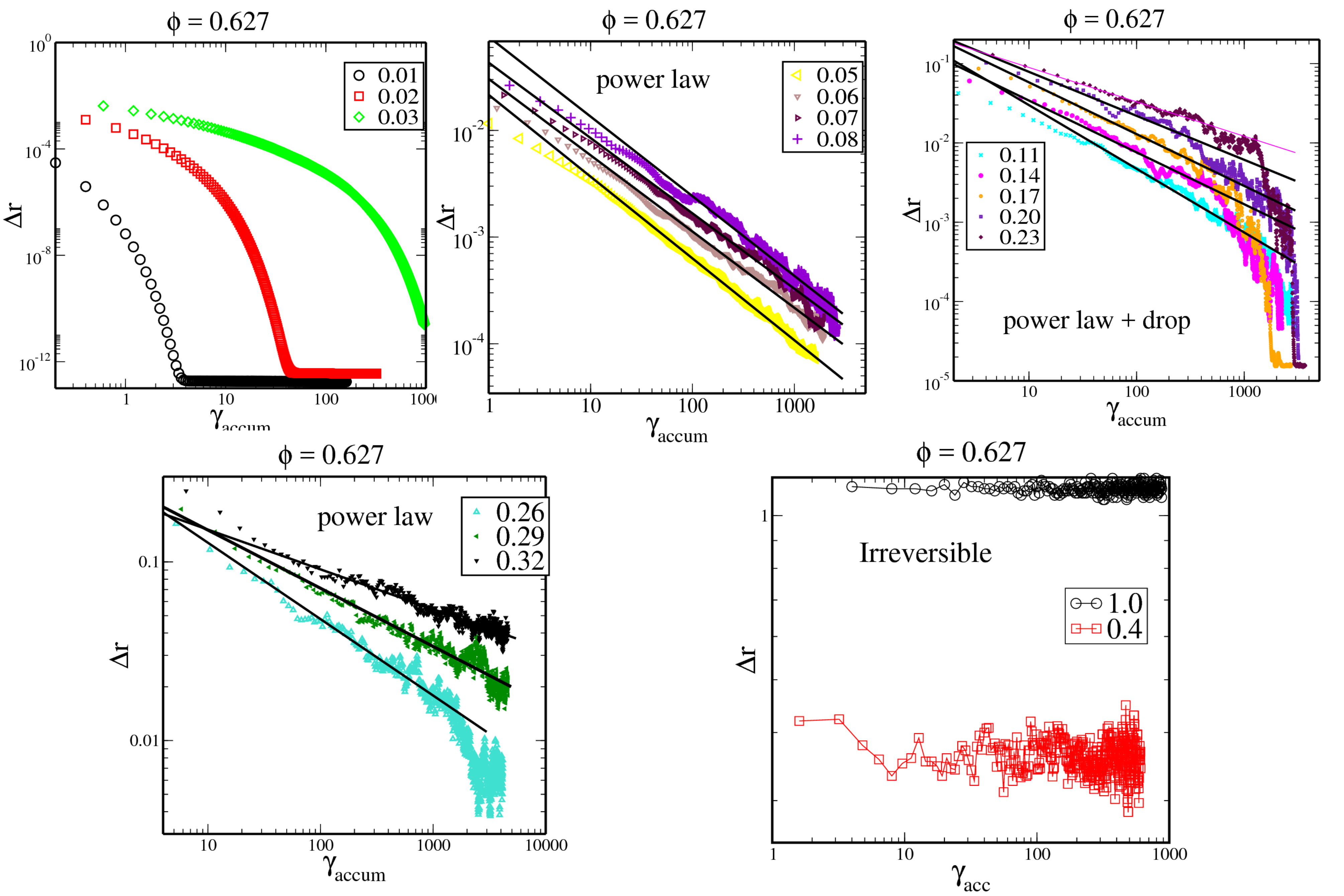
[Work in progress: Pallabi Das]

C. F. Schreck et al PRE 2013

Soft sphere assemblies subject to AQS cyclic shear, below the isotropic jamming density(Φ_J), display an intermediate regime, termed “Loop Reversible” – Stroboscopically invariant, but undergoing collisions during the cycle.

What to expect for memory effects in this regime?

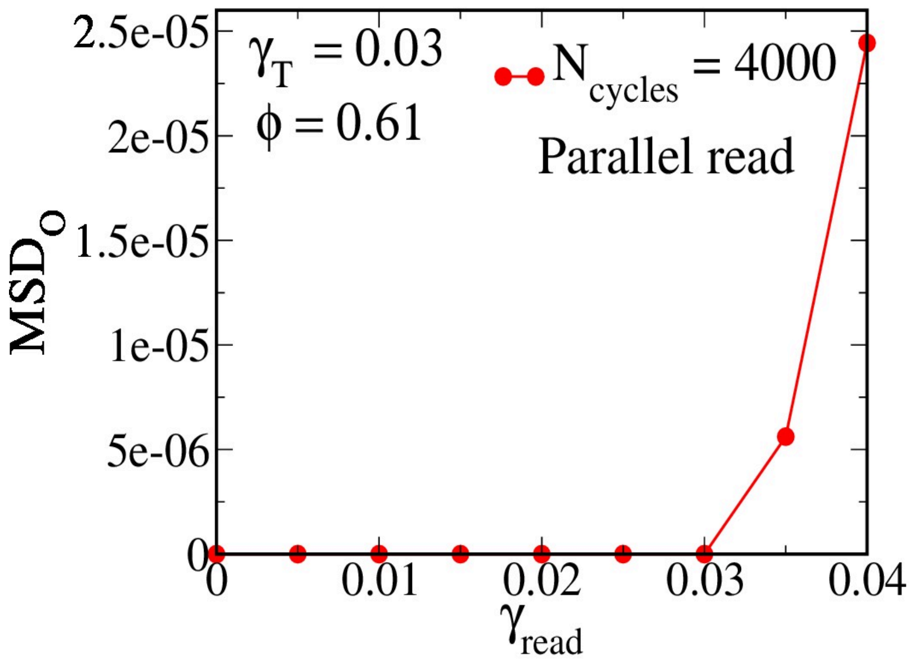
Different relaxation behaviour of Δr below Φ_J



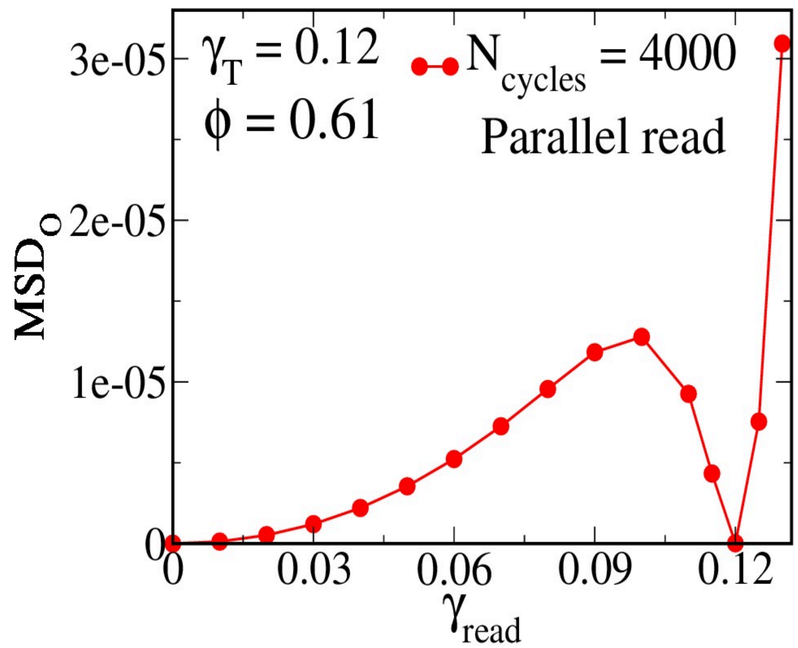
Single memory: Parallel read

We study memory effects at one amplitudes in the point reversible range and other in the loop reversible range.

Training amplitude γ_1 = 0.03



Training amplitude γ_1 = 0.12



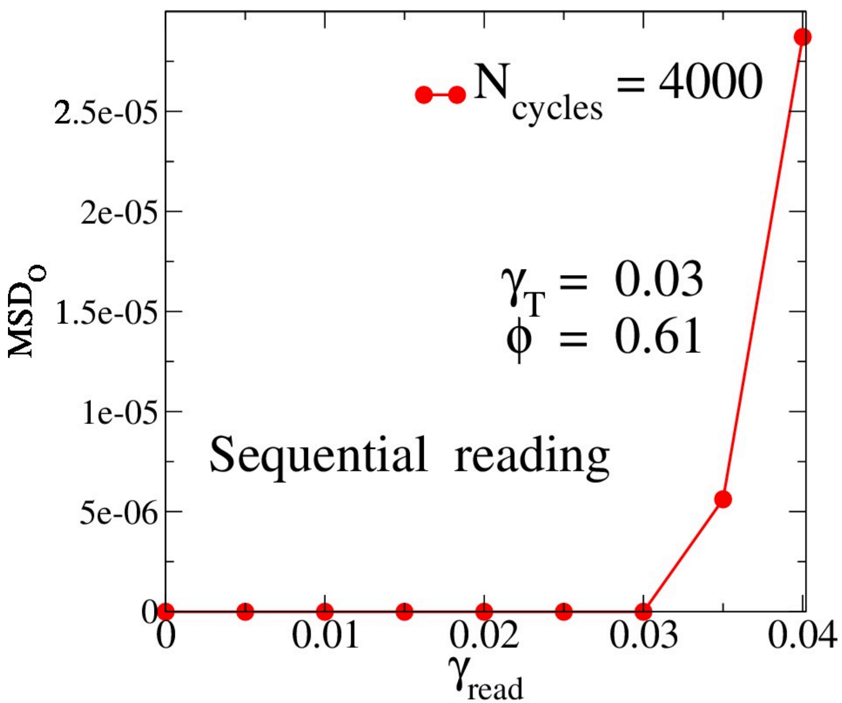
Memory is observed at all γ below γ_c

But the character is different.

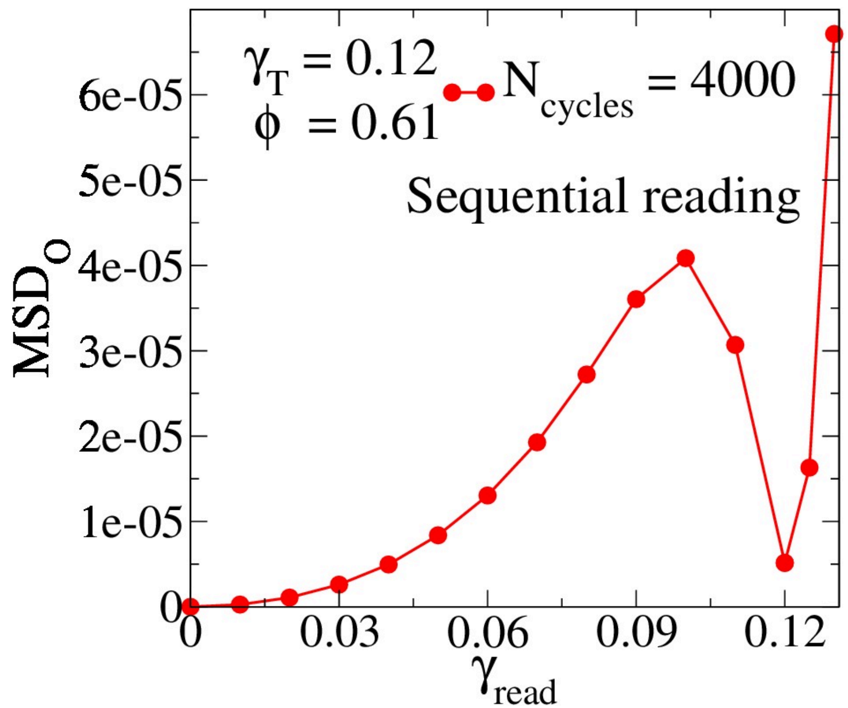
Single memory: Sequential read

We study memory effects at one amplitudes in the point reversible range and other in the loop reversible range.

Training amplitude γ_1 = 0.03



Training amplitude γ_1 = 0.12

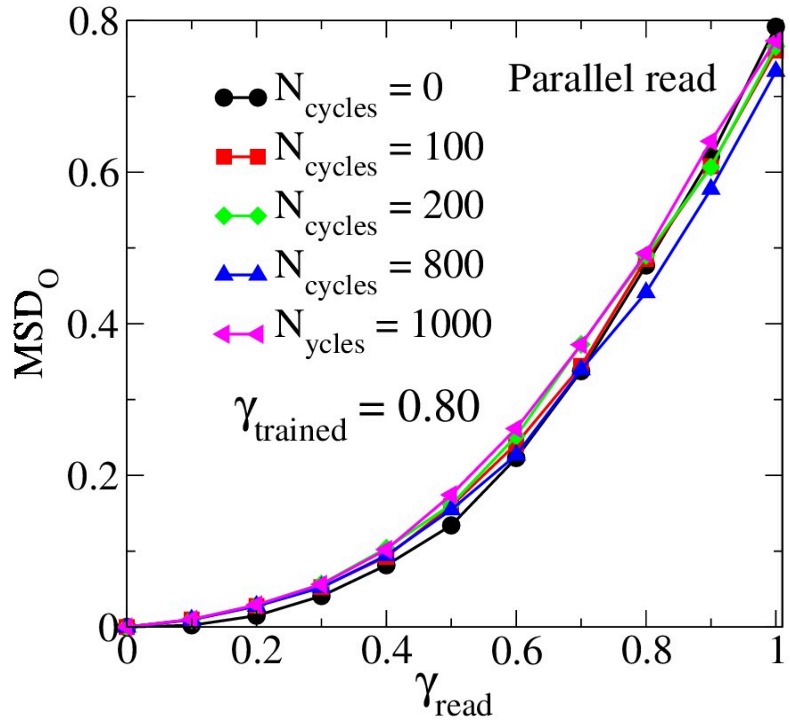


Memory is observed at all γ below γ_c
But the character is different.

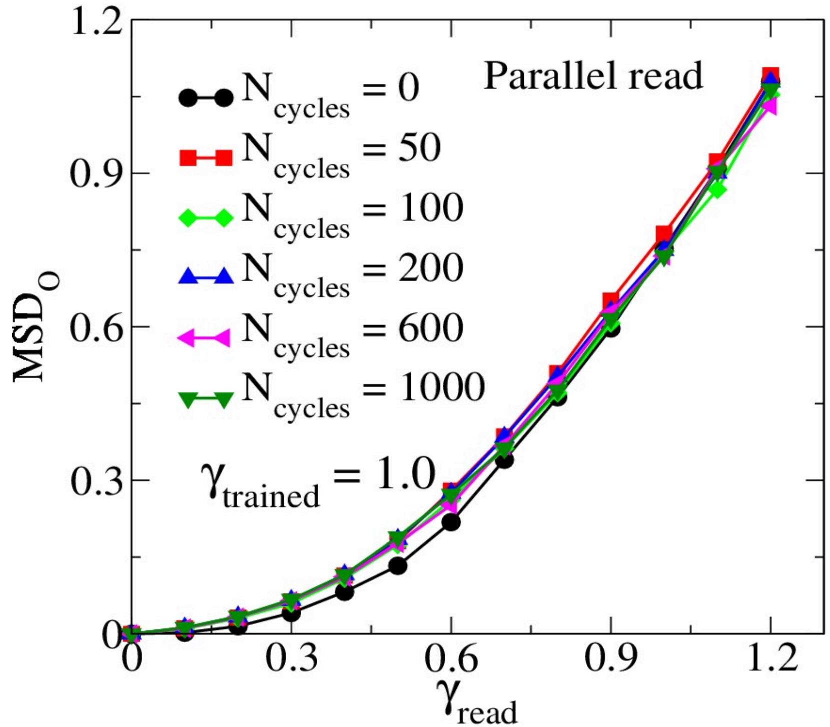
Memory effects in diffusing state

We studied memory effects at one amplitudes which belongs to diffusing state

Training amplitude $\gamma_{trained}$ = 0.8

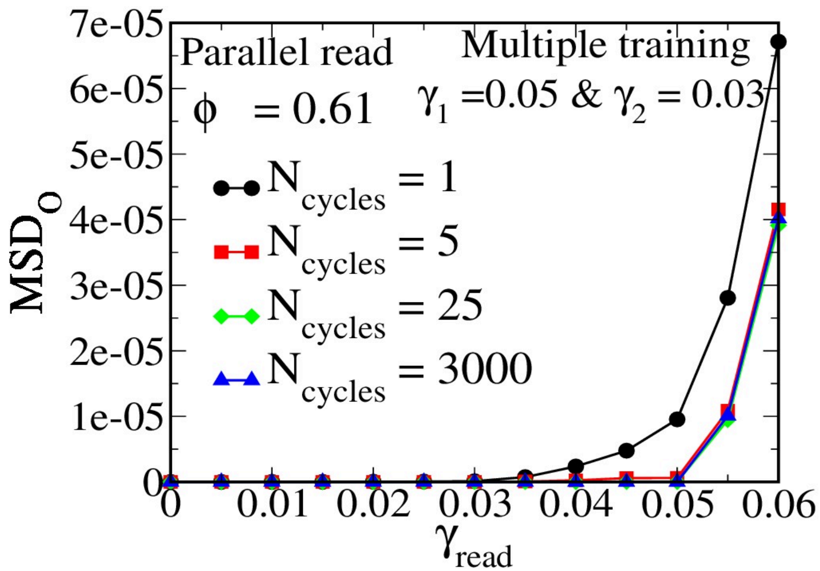


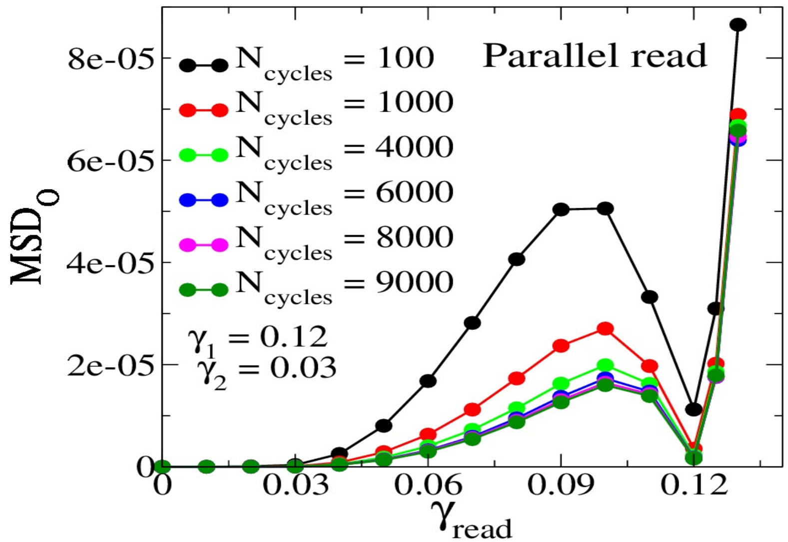
Training amplitude $\gamma_{trained}$ = 1.0

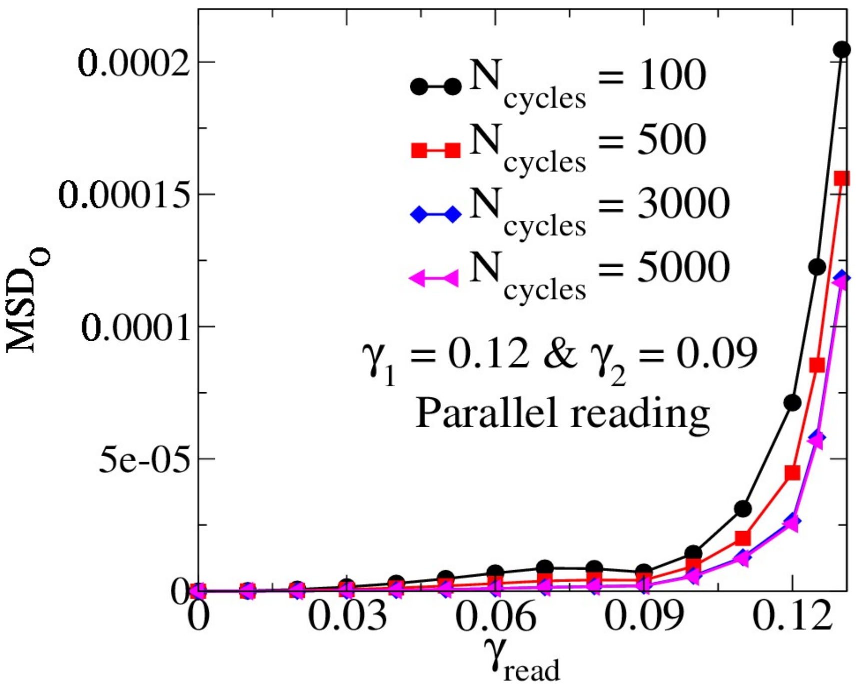


Memory is not observed above γ_c

Multiple Memories : Parallel read







amplitudes: both are in point reversible range, highest amplitude memory is persistent.

Amplitudes (loop and point) : both the memories are persistent.

Amplitudes (both are in loop reversible range) : memory at large amplitude not clear but both memories present.

Summary

Memory effects studies in model glasses, disordered spin model, a non-specific transition matrix model, and sheared sphere assemblies.

Sheared glasses exhibit signatures of single and multiple memories.

Persistent memory for multiple training amplitudes.

Simple models, the NK model and the Transition Matrix model, demonstrate similar behavior.

The behavior appears generic, but distinctions in memory effects in comparison with dilute colloidal suspensions should be better clarified.

The soft sphere model indicates how to understand these different effects – transient multiple memory in point reversible regime but persistent memory in the loop reversible regime with non-trivial orbits during shear cycle.

Do these specific set of memory effects (closely related but with variations) provide directions to classify memory effects more broadly?