Complex dynamics made simple: colloidal dynamics

Paolo Sibani

Chemnitz, June 2010
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Terminology

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- Aging: After a quench, complex glassy materials (glasses, polymers spin glasses) undergo a slow change of physical properties called aging\(^1\).
- Age: time elapsed from the initial quench
- Time homogeneous dynamics: e.g. diffusion, no changes of mesoscopic rates with time.
- Time inhomogeneous dynamics: e.g. aging: rate of significant events goes down with age.
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The resulting dynamics may be simple: e.g. diffusion in sinusoidal potential

Or complex: e.g. spin glass dynamics, where averages have power-law or logarithmic dependences.
Hard sphere colloidal systems-only short range interactions
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• Entropy driven dynamics.
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- Clusters of highly correlated groups of particles (spatial coarse graining)
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- Entropy driven dynamics.
- Clusters of highly correlated groups of particles (spatial coarse graining)
- Dynamics described in terms of the probability per unit of time that a cluster survives the random forces from the rest of the system.
What does ‘trivial’ or ‘simple’ mean?

- Trivial dynamics $\overset{\text{def}}{=} \text{time homogeneous (but perhaps not stationary)}$
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- For stationary processes:
- Correlation and response functions only depend on time differences
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For stationary processes:

- Correlation and response functions only depend on time differences
- Can be expanded in eigenvalue expansions
Add random and independent ‘position’ increments
The simplest stochastic process

- Add random and independent ‘position’ increments
- Use linearity of the variance
The simplest stochastic process

- Add random and independent ‘position’ increments
- Use linearity of the variance
- $MSD \propto t$: diffusion
Trivializing aging dynamics

Record dynamics

- record sized fluctuations
Record dynamics

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- in the stationary white noise impinging on the system (e.g. thermal noise)
Trivializing aging dynamics

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- record sized fluctuations
- in the stationary white noise impinging on the system (e.g. thermal noise)
- drive the aging dynamics in marginally stable (glassy) systems
- no. of records is a Poisson process in logarithmic time
- the dynamics appears simple in logarithmic time
Brief overview of results for *thermally activated* dynamics
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Experimental\(^1\) colloidal data re-analyzed.
Brief overview of results for *thermally activated* dynamics

Experimental\(^1\) colloidal data re-analyzed.

A cluster model for colloidal behavior numerically analyzed.
The rest of this talk

- Brief overview of results for *thermally activated* dynamics
- Experimental\(^1\) colloidal data re-analyzed.
- A cluster model for colloidal behavior numerically analyzed.
- Trees, record dynamics and complexity
Aging set-up

The age $t$ starts at the 'initial quench', and a field is (possibly) switched on at $t = t_w = 100$. In a colloid, the system is centrifuged to a high density (quench). No fields are applied.
The Edwards Anderson spin-glass is an Ising spin model where interacting spins $\sigma_i = \pm 1$ are placed on a lattice. The Hamiltonian is

$$\mathcal{H} = \sum_{n.n.} \sigma_i \sigma_j J_{ij}.$$
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- For nearest neighbors $J_{ij}$ are Gaussian standard random variables, independent for $i < j$. 
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- The thermal equilibrium properties of the model are complex
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- The thermal equilibrium properties of the model are complex.
- The time evolution, as given by a MC algorithm (Metropolis acceptance rule or equivalent) is complex and very similar to experimental data.
The p-spin model is an Ising spin model, The Hamiltonian is 
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\[ \mathcal{H} = - \sum_{\text{Plaq.}} \sigma_i \sigma_j \sigma_k \sigma_l \]

- The thermal equilibrium properties of the model are **trivial**.
- The time evolution is nevertheless complex, featuring metastability and aging.
The Restricted Occupancy Model is a lattice model describing vortex creep in type II superconductors in terms of the number $n_i$ of vortices on site $i$.

- the energy includes repulsive interactions between vortex lines on neighbor sites

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- the energy includes repulsive interactions between vortex lines on neighbor sites
- pinning to random sites
- the configuration is updated with Metropolis dynamics

The time variation of the total number of vortices $N(t)$ on the system for a single realization of the pinning potential and the thermal noise in a $8 \times 8 \times 8$ lattice for $T = 0.1$.

Heat transfer PDF for a spin glass model (PS & H J Jensen, Europhysics Lett. 2005)

Heat transfer $H$ over small time $\delta t$ in the E-A spin glass model has a Gaussian part and an intermittent tail. Six different ages are considered with $\delta t/t_w = .01$. 
The average rate of energy flow is plotted versus the age for the temperatures shown. The full line has the form $y = C(T)t_w^{-1}$.
**Complex dynamics made simple: colloidal dynamics**

p-spin model, quakes in real space

\[ t_w = 10^5; \quad t_{\text{obs}} = 10^6; \quad T=1.5 \]

S. Christiansen
& PS, *New J. of Physics*
The PDF of the heat exchanged between system and thermal bath over a time $\delta t = 100$. $T = 1.5$. 

$t_w = 1000; t_{obs} = 10000; \delta t = 100$.
p-spin model, magnetic fluctuations $H = 0$

The PDF of the spontaneous magnetic fluctuations over a time $\delta t = 100$ and $T = 1.5$.
p-spin model, magnetic fluctuations $H = 0.3$

The magnetic response is SUBORDINATED to the quakes.

PDF of the spontaneous magnetic fluctuations over a time $\delta t = 100$. $T = 1.5$. 

PDF

$t_w = 1000; t_{\text{obs}} = 10000; \delta t = 100$

$\delta E > -5$
The evolution of aggregate variables (i.e. the energy and magnetization) is controlled by extremely rare and irreversible events quakes.
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Reversible fluctuation of zero average with Gaussian PDF’s describe the dynamics in quasi-equilibrium.
Experimental data

- Tracking data obtained by confocal microscopy

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- Trajectories \([x(t), y(t), z(t)]\) available for thousands of tagged particles

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- dense colloids $\rho > 0.62$ sub-diffusive behavior, aging

Experimental data

- Tracking data obtained by confocal microscopy
- Particle radius $1.18 \mu$
- Trajectories $[x(t), y(t), z(t)]$ available for thousands of tagged particles
- Dense colloids $\rho > 0.62$ sub-diffusive behavior, aging
- ‘Glass formers’ $\rho < 0.62$ diffusive behavior, time homogeneous

Experimental procedure

- Centrifuge the sample to desired density
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- Centrifuge the sample to desired density
- Stir the sample
Experimental procedure

- Centrifuge the sample to desired density
- Stir the sample
- Wait (age $t_w$ calculated from the end of the stirring phase)
Centrifuge the sample to desired density

Stir the sample

Wait (age $t_w$ calculated from the end of the stirring phase)

Start tracking. Scanning through sample $\approx 20$ s
MSD vs time. Glass-former

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MSD vs time. Dense

MSD (μ^2) vs t/t_w

Complex dynamics made simple: colloidal dynamics

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Partition the system volume in a set of subvolumes
Persistence analysis

- Partition the system volume in a set of subvolumes
- Pick for each sub-volume a pair of colloidal particle which are initially ‘in touch’
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- Identify the time at which each pair splits
Persistence analysis

- Partition the system volume in a set of subvolumes
- Pick for each sub-volume a pair of colloidal particle which are initially ‘in touch’
- Identify the time at which each pair splits
- Calculate the fraction of pairs which survive at time $t$. 

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Persistence curves

Pair Survival probability

$t (s)$

$10^{-1}$

$10^{0}$

$10^{1}$

$10^{2}$

$10^{3}$

$10^{4}$

$t/t_w$

Thr.=0.4

Thr.=0.6

Thr.=0.8

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Intermittency curves

‘Glass former’

\[ \Delta t = 18 \]
\[ \Delta t = 180 \]
\[ \Delta t = 360 \]

PDF

\[ |\Delta r| \quad (\mu) \]

\[ \text{MSD} \quad (\mu^2) \]

0 0.5 1 1.5

0 10^{-4} 10^{-2} 10^0 10^2

0 0.05 0.1

0 500 1000

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Complex dynamics made simple: colloidal dynamics
Intermittency curves

Dense colloid

PDF

MSD (µ²)

∆t = 20
∆t = 60
∆t = 100

|∆r| (µ)

Δt (s)

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Complex dynamics made simple: colloidal dynamics
the MSD is linear in $t$ (glass formers) and in $\ln(t) - \ln(t_w)$ (dense)
Conclusion from colloid data analysis

- the MSD is linear in $t$ (glass formers) and in $\ln(t) - \ln(t_w)$ (dense)
- The persistence probability is exponential in $t$ (glass formers) and $\ln(t) - \ln(t_w)$ (dense)
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- Transformation $t \rightarrow \ln(t/t_w)$ trivializes the dynamics of dense colloids
Conclusion from colloid data analysis

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- The persistence probability is exponential in $t$ (glass formers) and $\ln(t) - \ln(t_w)$ (dense)
- Transformation $t \rightarrow \ln(t/t_w)$ trivializes the dynamics of dense colloids
- Highly intermittent and correlated motion
Not much changes in a colloid

- Particle density is constant
Not much changes in a colloid

- Particle density is constant
- Energy density is constant
Not much changes in a colloid

- Particle density is constant
- Energy density is constant
- Particle displacement over observation time of the order of particle radius
Not much changes in a colloid

- Particle density is constant
- Energy density is constant
- Particle displacement over observation time of the order of particle radius
- Particle motion is jerky and spatially correlated
A cluster model

particles in a cluster moves in fully correlated fashion on average zero CM displacement as long as the cluster persists
when a cluster is destroyed
 Particle motion

- when a cluster is destroyed
- the particles join neighboring clusters
• when a cluster is destroyed
• the particles join neighboring clusters
• and move in real space
when a cluster is destroyed
the particles join neighboring clusters
and move in real space
Probability (per MC query) that a cluster of size \( h \) is destroyed
when a cluster is destroyed
the particles join neighboring clusters
and move in real space
Probability (per MC query) that a cluster of size $h$ is destroyed
$P_k(h) = \frac{1}{\sum_{j=0}^{k} h^j / j!}$; $P_\infty(h) = e^{-h}$; $P_1(h) = 1/(1+h)$
Particle motion

- when a cluster is destroyed
- the particles join neighboring clusters
- and move in real space
- Probability (per MC query) that a cluster of size \( h \) is destroyed
  \[ P_k(h) = \frac{1}{\sum_{j=0}^{k} h^j / j!}; \quad P_\infty(h) = e^{-h}; \quad P_1(h) = 1/(1 + h) \]
- for all \( k \): \( P_k(h \to 0) \) for \( h \to \infty \)
The algorithm

- Markov chain, $L$ clusters
The algorithm

- Markov chain, $L$ clusters
- pick a cluster at random
The algorithm

- Markov chain, $L$ clusters
- pick a cluster at random
- destroy it with probability $P_k(h)$
The algorithm

- Markov chain, $L$ clusters
- pick a cluster at random
- destroy it with probability $P_k(h)$
- or choose to another cluster
The algorithm

- Markov chain, $L$ clusters
- pick a cluster at random
- destroy it with probability $P_k(h)$
- or choose to another cluster
- iff cluster is destroyed:
  - partition its particles randomly in two groups
  - each sub-group joins neighboring cluster
  - particles move one random unit step on the lattice
$P_1(h) = \frac{1}{1 + h}$, ‘glass former’, diffusive

\[
\langle \chi^2 \rangle \sim \frac{1}{h}
\]

\[
L = 512, 256, 128, 64, 32, 16
\]

\[
\sim t
\]

Sweeps
Diffusive behavior II

\[ P_\infty(h) = e^{-h} \]

dense colloid, log diffusive

\[ \langle x^2 \rangle \]

Sweeps

\[ \text{L=512} \]
\[ \text{L=256} \]
\[ \text{L=128} \]
\[ \text{L=64} \]
\[ \text{L=32} \]
\[ \text{L=16} \]

\[ P(h) \sim e^{-h} \]

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Complex dynamics made simple: colloidal dynamics
$P_1(h) = \frac{1}{1+h}$  
‘glass former’, exponential decay

P(h)~1/h
Persistence II

\[ P_\infty(h) = e^{-h} \]

dense colloid, exponential decay in \( \log t \)

Int. Persistence

\[ P_\infty(h) \sim e^{-h} \]

Sweep time \( t \)
\[ P_1(h) = \frac{1}{1+h} \]

‘glass former’, approaches stationary state

Deviation $\sigma$ vs. sweeps for different system sizes $L$. The plot shows the deviation $\sigma$ as a function of the number of sweeps for various system sizes, with each line representing a different $L$ value. The sizes considered are $L = 512, 256, 128, 64, 32, 16$. The data suggests a trend where larger system sizes approach a stationary state more quickly than smaller ones.
$P_\infty(h) = e^{-h}$

dense colloid, equilibrium is out of reach

![Graph showing the deviation $\sigma$ as a function of sweeps for different system sizes $L$. The graph illustrates the trend of $\sigma$ increasing with increasing number of sweeps, with distinct markers for $L=512$, $L=256$, $L=128$, $L=64$, $L=32$, and $L=16$.](image-url)
Collapses of clusters of different sizes are widely separated in time.

All clusters of size $\sigma(t)$ only provide background of mobile particles.

A quake on a time scale $t$ corresponds to the collapse of the smallest cluster $>\sigma$. 
Quakes in thermally activated aging

- Energy fluctuations which are negative
Energy fluctuations which are negative
And not reversible on the time scale \( t \) at which they occur
Energy fluctuations which are negative
And not reversible on the time scale $t$ at which they occur
Size $-\delta e/T \gg \log t$
In the aging regime, each cluster collapse is called a ‘quake’

$$P(h) \sim e^{-h}$$

**Graph:**
- **Y-axis:** Rate of Quakes/L
- **X-axis:** Sweeps
- **Legend:**
  - L=512
  - L=256
  - L=128
  - L=64
  - L=32
  - L=16
  - ~1/t
Temporal statistics of ‘quakes’ II

\[ \tau_k = \log(t_k) - \log(t_{k-1}) : \text{waiting log-times} \]

\[ P(h) \sim e^{-h} \]

\[
\begin{array}{c|c|c|c}
L & P(\tau) & h \\
32 & \bullet & -1.1 \\
128 & \bullet & -1.2 \\
512 & + & -1.3 \\
\end{array}
\]
The distribution of the logarithmic differences \( \log(t_k) - \log(t_{k-1}) \) is approximately exponential.
The ‘log’ Poisson distribution

- \( P(n, t_1, t_2) \) probability that \( n \) quakes occur in \([t_1, t_2]\).
The ‘log’ Poisson distribution

- $P(n, t_1, t_2)$ probability that $n$ quakes occur in $[t_1, t_2)$.

$$P(n, t_1, t_2) = \frac{\mu^n}{n!} \exp(-\mu) \quad \mu(t_1, t_2) = \alpha \log(\frac{t_2}{t_1}) \quad (1)$$
The ‘log’ Poisson distribution

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- The statistics applies to e.g. spin-glasses, colloids, evolutionary dynamics etc.
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\]

- The statistics applies to e.g. spin-glasses, colloids, evolutionary dynamics etc.
- Where can it possibly come from?
• In colloids: The dynamics decelerates once a smallest cluster marginally larger than its predecessor is formed
• This cluster is toppled by a record sized fluctuation on a time scale $t_2 > t_1$...
• Sequence of magnitude records in the probability of toppling the smallest cluster marks the evolution of the dynamics.
Relation to hierarchies and trees?

- Two different ways to describe the same generic situation

( Fischer Hoffmann & Sibani, PRE 2008 )
Two different ways to describe the same generic situation
Record dynamics needs an underlining hierarchical structure

(Fischer Hoffmann & Sibani, PRE 2008)
Two different ways to describe the same generic situation
Record dynamics needs an underlining hierarchical structure
work with Andreas Fischer and KH elaborates on this point

( Fischer Hoffmann & Sibani, PRE 2008 )
Colloid analysis in collaboration with Stefan Boettcher, Emory University, GA, USA. Thanks to Eric Weeks Emory University, for kindly providing the colloidal data.
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