Out of equilibrium simulation

Pascal Viot

December 10, 2020
Introduction: systems out of equilibrium

- Relaxation time exceeds simulation time or observation time
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  - Supercooled liquids
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  2. Glasses
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- Systems in contact with several reservoirs: Non equilibrium stationary states
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Glassy systems

Angell plot for supercooled liquids
From Arrhenius to super-Arrhenius behavior

\[ \tau = \tau_0 \exp\left(\frac{E}{T}\right) \]
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- if \( E \) is constant, Arrhenius behavior. The relaxation is associated with a barrier crossing.
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- if \( E \) is constant, Arrhenius behavior. The relaxation is associated with a barrier crossing.
- If \( E = E(T) \) with \( E \uparrow \) when \( T \downarrow \), Super Arrhenius behavior. The height of the barrier increases when the temperature is decreased.
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Simulation models

- Bidisperse or polydisperse systems avoiding the crystallization. Molecular dynamics (LAMMPS) and swap Monte Carlo method.
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Simulation models

- Bidisperse or polydisperse systems avoiding the crystallization. Molecular dynamics (LAMMPS) and swap Monte Carlo method.
- Lattice models (Kinetically constrained spin models)
For fragile glasses, several proposed fits are associated with the absence of a specific temperature relevant to the phenomenon; A possible scenario is the existence of a temperature (below the glass transition) and a putative transition not accessible to experiments. The Vogel-Fulscher-Thalmann (VFT) law provides accurate fits of the relaxation time versus temperature and is given by the relation

$$\tau = \tau_0 \exp\left(\frac{A}{T - T_0}\right)$$

The temperature $T_0$ is often interpreted as a transition temperature, where the transition can be reached experimentally. An alternative interpretation consists of considering the ratio $A/(T - T_0)$ as an activation energy which increases rapidly when the system is cooled.
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Consider a lattice (in one-dimension, for the sake of simplicity). On each site, one has a boolean variable, denoted by \( n_i \). The Hamiltonian reads

\[
H = \sum_{i=1}^{N} n_i
\]

At a given temperature \( T \) (the inverse temperature is \( \beta = 1/k_B T \)), one has the density of (“mobile”) \( n \) in the state 1, which is given by

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n = \frac{1}{1 + \exp(\beta)}
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Particles which are mobile are in the state 1 whereas particles in the state 0 are sluggish. This model mimics a heterogeneous dynamics. At low temperature, the density of mobile particles is small $n \sim \exp(-\beta)$. 

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Consider a lattice (in one-dimension), Using Metropolis rules, four elementary configuration changes have to be considered. The rule corresponding to a state change does not depend on the neighborhood, but one has

...000... ⇔ ...010...
...100... ⇔ ...110...
...001... ⇔ ...011...
...101... ⇔ ...111...

The Friedrickson-Andersen model removes the configuration change of the first of the four situations, which corresponds to preventing the creation or destruction of a mobile particle surrounded by immobile particles. By restricting the dynamics, one can explore all configurations of the phase space except one configuration where all particles are immobile and cannot be reached.

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\tau = \exp(3\beta)
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This model is inspired by the preceding model: the Hamiltonian is the same, but the dynamics is more restrictive with a left-right symmetry breaking. Indeed, the dynamic rules are the same as the preceding model, except when no mobile exists on the right.

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Relaxation time grows as

\[
\tau = \exp\left(1/(T^2 \ln(2))\right)
\]

Fragile behavior
Random Sequential Adsorption: motivation

When a solution of macromolecules (proteins, colloids) is placed in contact with a solid surface, one observes a surface adsorption as a monolayer of macromolecules. This process is slow; the adsorption can take from several minutes to several weeks. Once adsorption performed, if one replaces the solution with a buffer solution, little or no desorption is observed and there are few changes in the structure of the adsorbed monolayer. When the experiment is repeated with different concentrations of macromolecules, the saturation coverage is always the same.
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Close to solid interface, the particle-surface interaction is strongly attractive on a short distance and strongly repulsive when the particle goes into the surface. The interaction potential can be approximated as a strongly attractive contact potential. Once adsorbed, particles cannot desorb or move on the surface. Because particles in solution follow Brownian trajectories, one can assume that particles reach the surface randomly. If the particle first reaches an adsorbed particle, it is pushed away from the surface and returns to the bulk. If the particle reaches the solid surface, it is “glued” to the surface, definitively.
Model

Particles are dropped randomly on the surface. If the particle overlaps previously adsorbed particles, it is rejected. If not the particle is adsorbed definitively (no move).
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Algorithm

A kinetic time step is the following:

1. One selects randomly and uniformly positions of a trial particle within the simulation cell.

\[
\begin{align*}
    x_0 &= \text{rand} \\
    y_0 &= \text{rand}
\end{align*}
\]  

(1)

Time is increased by 1: \( t = t + 1 \).

2. Nonoverlap checking: \((\vec{r}_0 - \vec{r}_i)^2 > \sigma^2\) with \(i\) running from 1 to the index of the last adsorbed particle (at time \(t\)) denoted \(n_a\). If this test is false, the particle is rejected and one selects a new trial particle. If this test is true, the particle is added to the container.
Adsorption kinetics is slow at long time. Few small areas are available for a new adsorption.

Real-time simulation (Python code)
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Real-time simulation (Python code)
In 1D, the model is solvable

\[ \rho(t) = \int_0^t du \exp \left( -2 \int_0^u dv \frac{1 - e^{-v}}{v} \right). \]
Results

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Asymptotic behaviors:

- When \( t \to \infty \), the density goes to \( \rho(\infty) = 0.7476 \ldots \).
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\[ g(r, \rho_{\infty}) \sim \ln \left( \frac{r - 1}{\sigma} \right). \]
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- \( \rho(\infty) - \rho(t) \sim \left( \frac{e^{-2\gamma}}{t} \right) \), where \( \gamma \) is the Euler’s constant.
- \( g(r, \rho_\infty) \sim \ln \left( \frac{(r - 1)}{\sigma} \right) \).

Non trivial solution in 1D helps to find predictions in higher dimensions.
Motivation

Granular matter (powders, sands, ...) properties: particle size is much larger than the atomic scales (at least several hundreds micrometers); the range of interaction between particles is less than the typical particle size; when particles collide, a fraction of the kinetic energy is lost and transformed in plastic deformations; the particle mass being much larger than atoms, the thermal energy is negligible compared to gravitational energy and power supply (generally, provided by vibrations).

In the absence of a continuous power supply, a granular system looses rapidly this initial kinetic energy.
Inelastic hard sphere model

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Model

Taking account of the time scale separation, one can considers that the collision time is negligible compared to the characteristic time of free steaming. Because the interactions are short ranged and particle shape is not modified with collisions (we consider “gentle” collisions), one can assume that the interaction potential is a hard core potential.
The total momentum of the two particles involved in a collision is conserved:

\[ v_1 + v_2 = v_1' + v_2'. \]  \hspace{1cm} (2)
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During the collision, the relative velocity of the point of impact is changed as follows: Assuming that the tangential component of the velocity is conserved (which corresponds to a tangential coefficient of restitution equal to 1) one has the following relation

\[ (v'_1 - v'_2).n = -e(v_1 - v_2).n \]  

(3)

where \( e \) is the normal coefficient of restitution and \( n \) is a normal unit vector, whose direction is given by the straight line joining the two centers of colliding particles.

\[ 0 \leq e < 1 \ (e = 1 \text{ corresponds to an elastic collision}) \]
Inelastic hard sphere model

Algorithm

Combining the conservation of the total impulse and the collision rules gives

\[ v'_{i,j} = v_{i,j} \pm \frac{1 + e}{2} [(v_j - v_i).\hat{n}]\hat{n} \] (4)

with \( \hat{n} = \frac{r_1 - r_2}{|r_1 - r_2|} \).
Combining the conservation of the total impulse and the collision rules gives

\[ v'_{i,j} = v_{i,j} \pm \frac{1 + e}{2} [(v_j - v_i) \cdot \hat{n}] \hat{n} \]  

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- Start from an initial configuration, consider all pairs and determine the collision time occurring in the future. Store the collision times for all particle pairs.
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- Start from an initial configuration, consider all pairs and determine the collision time occurring in the future. Store the collision times for all particle pairs.
- Select the shortest collision time and the pair associated with it.
Inelastic hard sphere model

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- Move all particles up to this time.
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- Start from an initial configuration, consider all pairs and determine the collision time occurring in the future. Store the collision times for all particle pairs.
- Select the shortest collision time and the pair associated with it.
- Move all particles up to this time.
- Update the velocities for the colliding pair.
Inelastic hard sphere model

**Algorithm**

Combining the conservation of the total impulse and the collision rules gives

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- Start from an initial configuration, consider all pairs and determine the collision time occurring in the future. Store the collision times for all particle pairs.
- Select the shortest collision time and the pair associated with it.
- Move all particles up to this time.
- Update the velocities for the colliding pair.
- Update the collision time between those two particles and the others.
Inelastic hard sphere model

Algorithm

Combining the conservation of the total impulse and the collision rules gives

\[ v_{i,j}' = v_{i,j} \pm \frac{1 + e}{2} [(v_j - v_i) \cdot \hat{n}] \hat{n} \]  

(4)

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- Start from an initial configuration, consider all pairs and determine the collision time occurring in the future. Store the collision times for all particle pairs.
- Select the shortest collision time and the pair associated with it.
- Move all particles up to this time.
- Update the velocities for the colliding pair.
- Update the collision time between these two particles and the others.
- Select the shortest collision time again...
Inelastic hard sphere model

Inelastic collapse

The kinetic energy decreases with time in the absence of power supply and the simulation seems to be stopped.

Let \( h \) denote the height at which the ball is dropped. At the first collision between the particle and the plane, the elapsed time is \( t_1 = \sqrt{\frac{2h}{g}} \) and the precollisional velocity is \( \sqrt{2gh} \). After the first collision, the velocity becomes \( e\sqrt{2gh} \). When the second collision occurs, the elapsed time is, \( t_2 = t_1 + 2et_1 \) and for the \( n \)th collision, one has \( t_n = t_1 \left( 1 + 2n - 1 \sum_{i=1}^{n-1} e^i \right) \rightarrow t_1 + e_{\infty} - e_1(5) \). A finite time of duration is elapsed until the bead comes to rest on the plane, whereas an infinite number of collisions were performed.
Inelastic hard sphere model

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Basic example for illustrating the inelastic collapse

Let $h$ denotes the height at which the ball is dropped. At the first collision between the particle and the plane, the elapsed time is $t_1 = \sqrt{\frac{2h}{g}}$ and the precollisional velocity is $\sqrt{2gh}$. After the first collision, the velocity becomes $e\sqrt{2gh}$. When the second collision occurs, the elapsed time is, $t_2 = t_1 + 2et_1$ and for the $n$ collision, one has

$$t_n = t_1 \left(1 + 2 \sum_{i=1}^{n-1} e^i\right) \to t_1 \frac{1 + e}{1 - e} \quad (5)$$

A finite time of duration is elapsed until the bead comes to rest on the plan, whereas an infinite number of collisions was performed.
With the assumption of a homogeneous system, the mean collision frequency is proportional to $\frac{l}{v}$, where $v$ is the mean velocity and $l$ the mean distance between particles. The mean energy loss is given by $\Delta E \approx -\epsilon (v)^2$ where $\epsilon = 1 - e^2$, which gives the evolution of the temperature (assuming that $E \approx T$)

$$\frac{dT}{dt} = -\epsilon T^3/2$$ (6)

and then the cooling law is

$$T(t) \approx 1/(1 + A\epsilon t)^2$$ (7)

This is known as the Haff's law (1983).
Inelastic hard sphere model

Free cooling state

Energy loss per collision

\[ \Delta E = -\frac{1 - e^2}{4} m((v_j - v_i) \cdot \hat{n})^2 \]

With the assumption of a homogeneous system, the mean collision frequency is proportional to \( l/v \), where \( v \) is the mean velocity and \( l \) the mean distance between particles. The mean energy loss is given by \( \Delta E \simeq -\epsilon(v)^2 \) where \( \epsilon = 1 - e^2 \), which gives the evolution of the temperature (assuming that \( E \simeq T \))

\[ \frac{dT}{dt} = -\epsilon T^{3/2} \quad (6) \]
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Inelastic hard sphere model

Free cooling state

- Scaling function of the velocity distributions
Inelastic hard sphere model

Free cooling state

- Scaling function of the velocity distributions
- Deviations from the Gaussian profiles
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Power supply

- Vibrating plate at the bottom allows one to reach a non equilibrium stationary state.
Inelastic hard sphere model

Free cooling state
- Scaling function of the velocity distributions
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Power supply
- Vibrating plate at the bottom allows one to reach a non equilibrium stationary state.
- Introduce the effect of the gravity
Exclusion models

Consider a one dimensional lattice of $N$ sites where $n$ particles are placed. Each particle has a hopping probability $p$ on the right if the nearest site is empty and a hopping probability $1 - p$ on the left if the nearest site is empty.
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Algorithms

- Parallel update: at the same time, all rules are applied to particles (synchronous update). The corresponding master equation is a finite difference equation in time.
Systems in contact with several reservoirs:

**Exclusion models**

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- Asynchronous update. This corresponds to the most used algorithm by choosing randomly and uniformly a particle at time $t$. The corresponding master equation is a differential equation.
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- Asynchronous update. This corresponds to the most used algorithm by choosing randomly and uniformly a particle at time $t$. The corresponding master equation is a differential equation.

- When the update is sequential and ordered, one considers successive sites of the lattice. Ordering can be chosen from the left to the right or conversely. The corresponding equation is also finite difference equation in time.
Systems in contact with several reservoirs:

### Exclusion models

- One-dimensional lattice of size $L$ with periodic boundary conditions (ring)

It is easy to find out that such a system has a stationary state where the probability of being on a site is independent of the site and is equal to $P_{st}(i) = 1/N$. Therefore, one has

$$\prod(i \rightarrow i + 1)P_{st}(i) = \frac{p}{N}$$

$$\prod(i + 1 \rightarrow i)P_{st}(i + 1) = \frac{1 - p}{N}$$

- Detailed balance broken except for $p = 1/2$.

A stationary current appears!
State variable $\tau_i(t)$. If the site $i$ is occupied, it can be free if the particle located on site $i$ at time $t$ can hop on the site $i+1$, which must be empty. If the site $i$ is empty, it can be occupied if the site on the left is occupied.
**Totally asymmetric exclusion process (TASEP)**

**Kinetic description**

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\frac{d\langle \tau_i(t) \rangle}{dt} = -\langle \tau_i(t)(1 - \tau_{i+1}(t)) \rangle + \langle \tau_{i-1}(t)(1 - \tau_i(t)) \rangle
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\]

\[
\frac{d(\langle \tau_i(t)\tau_{i+1}(t) \rangle)}{dt} = -\langle \tau_i(t)\tau_{i+1}(t)(1 - \tau_{i+2}(t)) \rangle + \langle \tau_{i-1}(t)\tau_{i+1}(t)(1 - \tau_i(t)) \rangle
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- State variable $\tau_i(t)$. If the site $i$ is occupied, it can be free if the particle located on site $i$ at time $t$ can hop on the site $i+1$, which must be empty. If the site $i$ is empty, it can be occupied if the site on the left is occupied.

$$\frac{d\langle \tau_i(t) \rangle}{dt} = -\langle \tau_i(t)(1 - \tau_{i+1}(t)) \rangle + \langle \tau_{i-1}(t)(1 - \tau_i(t)) \rangle$$

$$\frac{d\langle \tau_i(t)\tau_{i+1}(t) \rangle}{dt} = -\langle \tau_i(t)\tau_{i+1}(t)(1 - \tau_{i+2}(t)) \rangle + \langle \tau_{i-1}(t)\tau_{i+1}(t)(1 - \tau_i(t)) \rangle$$

- Finally, one obtains an infinite hierarchy of equations involving clusters of increasing sizes. One has a simple solution of the stationary state, because one can show that all configurations have an equal weight given by the equation

$$P_{st} = \frac{P!(N-P)!}{N!} \quad (8)$$
Totally asymmetric exclusion process (TASEP)

Kinetic description

\[ \langle \tau_i \rangle = \frac{P}{N} \]  \hspace{1cm} (9)

\[ \langle \tau_i \tau_j \rangle = \frac{P(P - 1)}{N(N - 1)} \]  \hspace{1cm} (10)

\[ \langle \tau_i \tau_j \tau_k \rangle = \frac{P(P - 1)(P - 2)}{N(N - 1)(N - 2)} \]  \hspace{1cm} (11)

Open boundaries

One-dimensional lattice of \( N \) sites

Site 1: if free, a particle is coming from a reservoir with a probability \( \alpha \). If occupied, the particle is moved in the reservoir with the probability \( \gamma \).

Site \( N \): if occupied, the particle can be moved in the reservoir with the probability \( \beta \). If free, a particle is inserted from the reservoir with a probability \( \delta \).
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Open boundaries

- Boundary equations

\[
\frac{d\langle \tau_1(t) \rangle}{dt} = \alpha(1 - \langle \tau_1(t) \rangle) - \gamma\langle \tau_1(t) \rangle - \langle \tau_1(t)(1 - \tau_2(t)) \rangle
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Open boundaries

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- In a similar manner for the site \( N \), one has

\[
\frac{d\langle \tau_N(t) \rangle}{dt} = \langle \tau_{N-1}(t)(1 - \tau_N(t)) \rangle + \delta \langle (1 - \tau_N(t)) \rangle - \beta \langle \tau_N(t) \rangle
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Simpler rules
\[\gamma = \delta = 0\]
Totally asymmetric exclusion process (TASEP)

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Simpler rules

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Simple traffic car model.
The LDP (low density phase) region corresponds to a stationary density (in bulk) equal to $\rho_{LDP} = \alpha$ if $\alpha < 1/2$ and $\alpha < \beta$.

The HDP (high density phase) region corresponds to a stationary density $\rho_{HDP} = 1 - \beta$ and occurs for values of $\beta < 0$ and $\alpha > \beta$.

The dashed line denotes the boundary between the LDP and HDP phase and corresponds to a first-order transition line.
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Indeed, in the thermodynamic limit, crossing the transition line leads to a density discontinuity.
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\[ \Delta \rho = \rho_{HCP} - \rho_{LCP} \]
\[ = 1 - \beta - \alpha \]
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which is nonzero for \( \alpha < 0.5 \). For a simulation where one has a finite system, one obtains a rapidly variation with a increasing slope when the system size increases.
Indeed, in the thermodynamic limit, crossing the transition line leads to a density discontinuity

\[ \Delta \rho = \rho_{HCP} - \rho_{LCP} = 1 - \beta - \alpha = 1 - 2\alpha \]

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Real-time simulation