Large scale dynamics of non-reversible Monte Carlo algorithms

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Molecular simulation in condensed matter

A subject of tremendous practical importance:

- Chemistry
  - Battery technology
- Biology
  - DNA, Protein structure
- Physics
  - Phase transitions

Linking new non-reversible Monte Carlo methods to true self-avoiding walk.

Simulation methods

Historic Simulation Methods

- Either use molecular dynamics integrate Newtons equations:

$$\dot{x} = v$$
$$m\dot{v} = F$$

- Or perform a reversible Monte Carlo simulation with acceptance probability $\exp(-\beta \Delta U)$ (Metropolis),
- Main workhorses of almost all molecular simulation.

No one ever tells you that there are no better methods.

In specialised fields there are adapted sampling methods: cluster algorithms for the Ising model.

Large scale dynamics

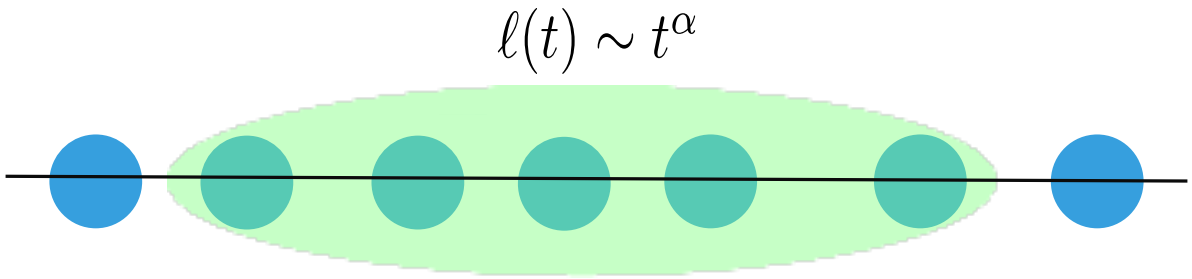
Main philosphy

- Molecular dynamics implements Navier-Stokes at large scale.
- Partial differential equations for mass, momentum, energy.
- Allow one to understand propagation and relaxation – sound waves, thermal diffusion.

PDE describing algorithms can tell you a lot about their dynamics.

Can we have such a picture of non-reversible Monte Carlo.

A dream simulation process in one dimension

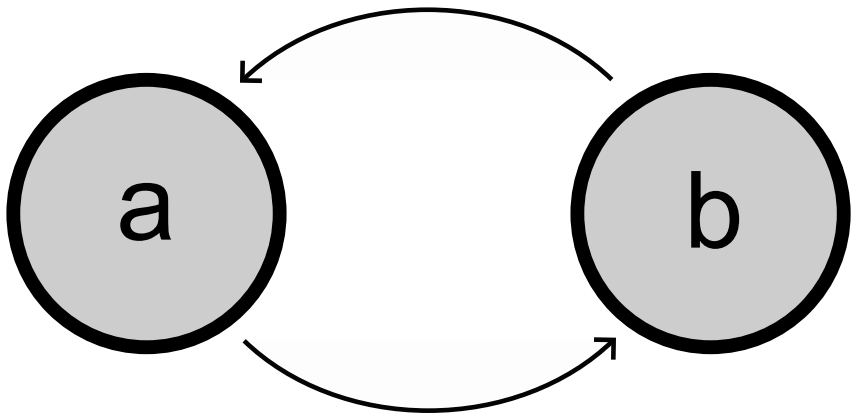


Local updates in some region of size ℓ should perfectly equilibrate that region in t steps:

- Spreading with an exponent α, $\quad \ell \sim t^{\alpha}$.
- We want perfect equilibration so that (from Peierls/random walk) the origin is visited $L_0 = \ell^{1/2}$ times:
- in scaling $L_0 = t/\ell = \ell^{1/2}$,
- giving $\ell \sim t^{2/3}$,
- $t \sim \ell^{(1+z)}$ with $z = 1/2$ (dynamic exponent).

Such a process corresponds to non-reversible MC.

Time reversibility in reversible Monte Carlo



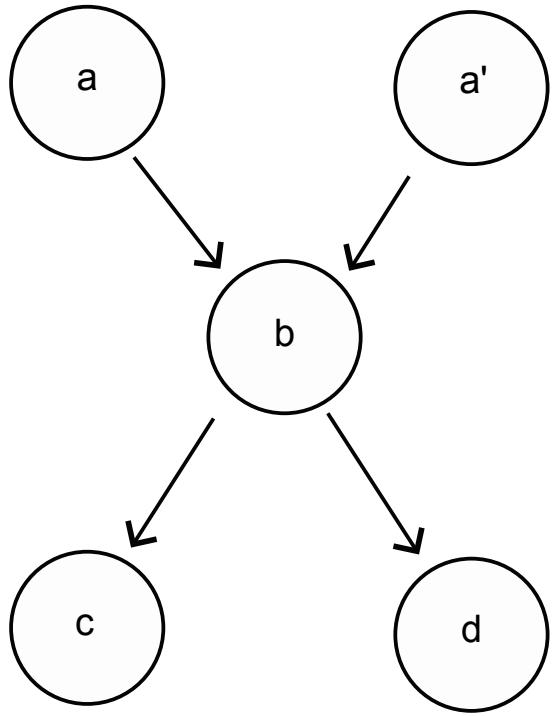
In Monte Carlo

- Detailed balance: $J(a \to b) = J(b \to a)$, currents for states a, b.
- If you can go forwards, then you can go back — diffusion.

Non-reversible Monte Carlo

- Monte Carlo with global balance, rather than detailed balance.
- Weaker condition, giving more freedom:

$$\sum_a \pi(a) T(a \to b) = \pi(b)$$



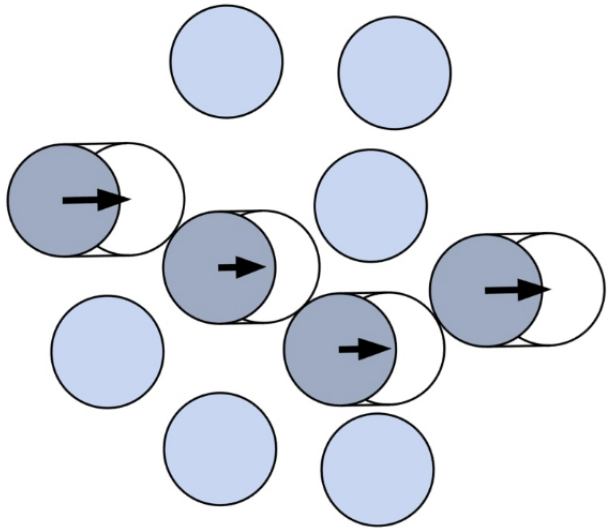
- Only move forwards, never back.
- Looks a little like a driven/active system.

Motivation: new algorithms coming from W. Krauth et al.

Event Chain Monte Carlo

Use for physical systems

Bernard, Krauth, Wilson (2009): Algorithm for hard spheres:



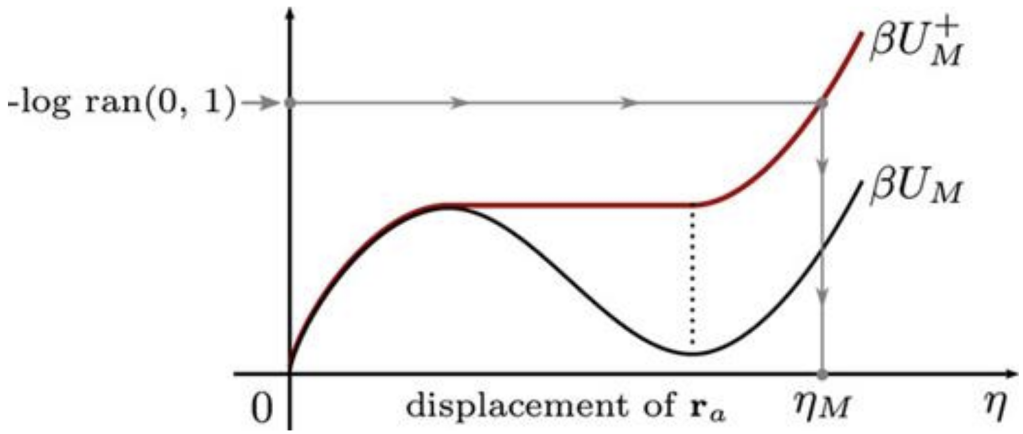
- Only one particle moving at any moment: it carries a "pointer".
- Only move forwards/up. Global balance, not detailed balance.
- Success for studying (hexatic) phase transitions in 2D.
- Study algorithm in one-dimension.

INSERT VIDEO

General potentials, beyond hard spheres

Michel, Kapfer, Krauth (2013):

- Split potential into components: $U = \sum_M U_M$.
- Convexify the components:



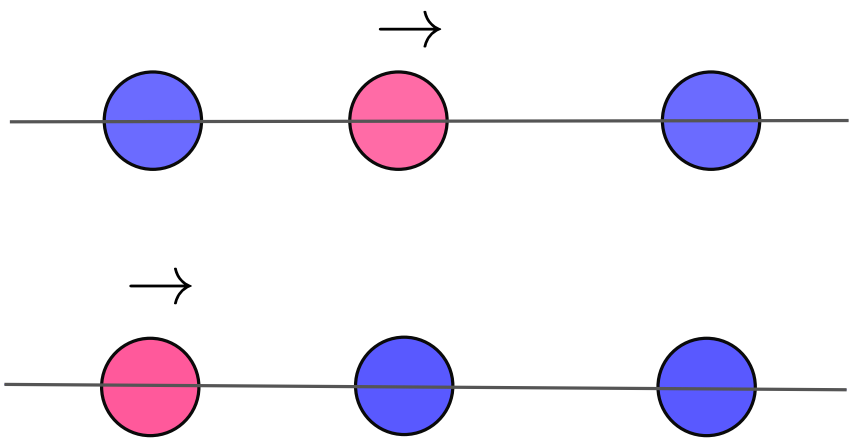
- For each component find first rejection point as particle moves: $\exp(-\beta U_M^+) = \mathit{rand}$.
- Select the smallest root as the collision partner, M.
- Transfer motion to new component.

This process generates equilibrated systems.

Non-reversible MC simulation of harmonic chain, 2024

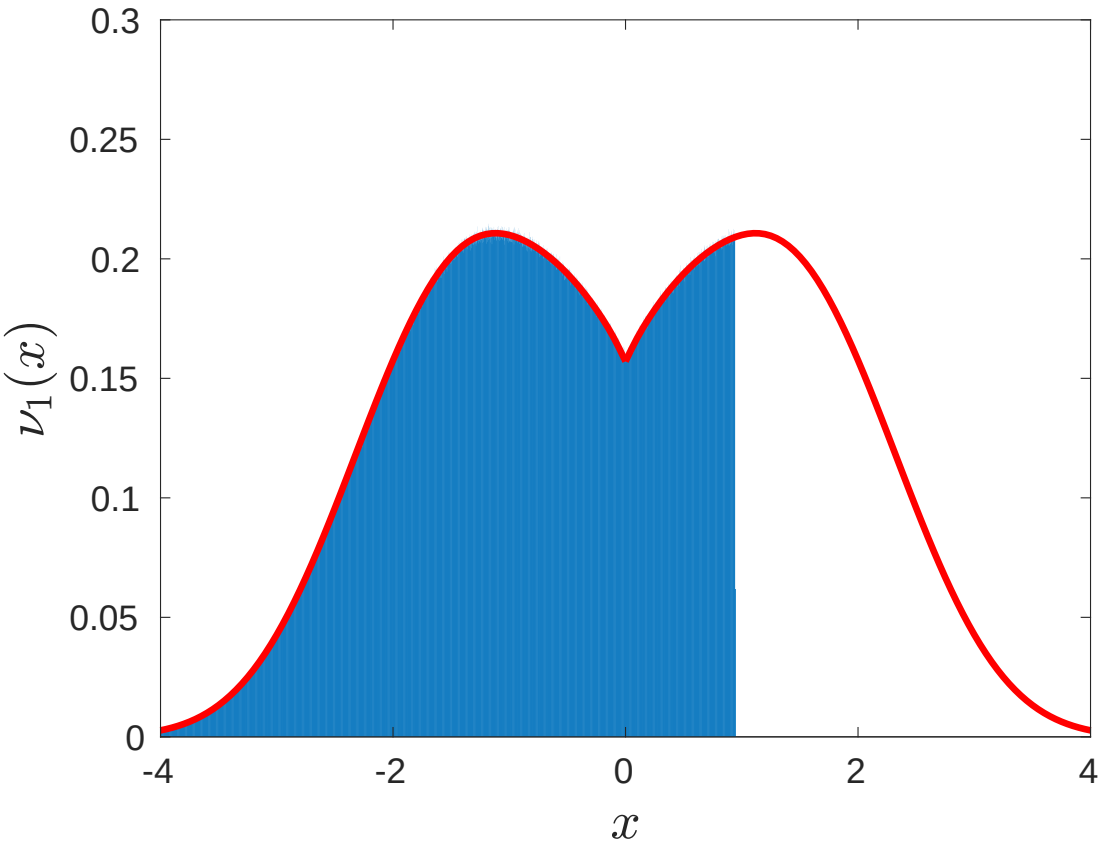
$$U = \frac{1}{2}\sum_p (y_p - y_{p+1})^2$$

Two components are important: left/right.



- path: -1, -1 , -1, +1, -1, sum, $s = -3$
- Bin distribution of final s from non-reversible simulation.

Simulation results + True self-avoiding walk



blue: binned simulation
red: true self-avoiding walk

Link to true self-avoiding walk

True self-avoiding walk: Amit, Parisi, Peliti (82)

I heard Peliti in '83

- Amit et al. (82) Random walk on sites of lattice, l

$$p_l(t+1) \sim e^{-\lambda L_l(t)}$$

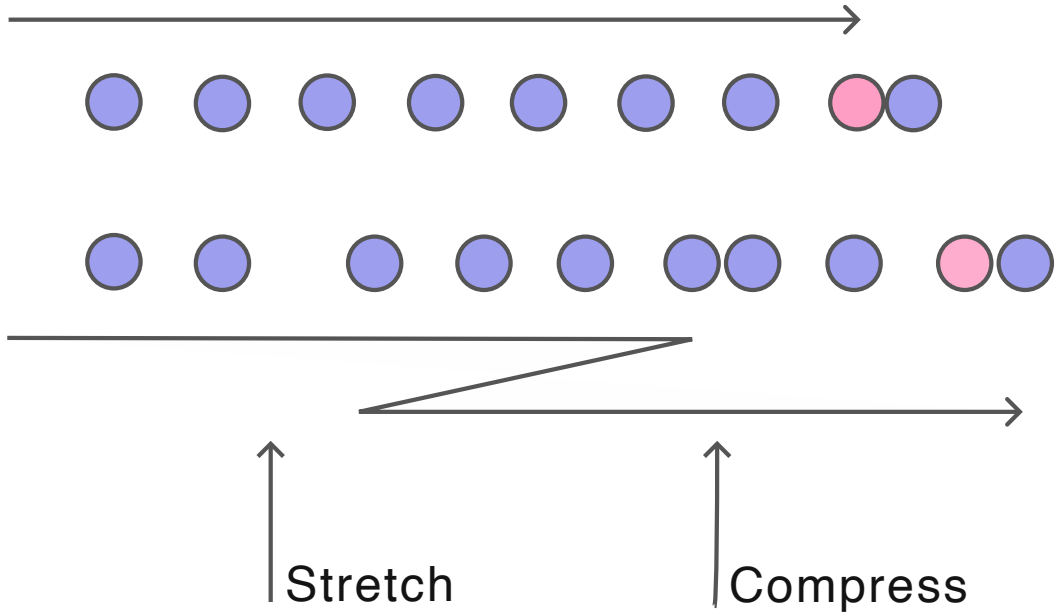
- $L_l(t)$ number of previous visits to site l.
- Continuous version: walk is repelled from previous visits giving:

$$\frac{d\mathbf{X}(t)}{dt} = -\nabla L(t, \mathbf{X}(t))$$
$$\frac{\partial L(t,\mathbf{x})}{\partial t} = \delta(\mathbf{x} - \mathbf{X}(t)).$$

- L looks a little like a repulsive potential for the motion of $\mathbf{X}$.
- $\mathbf{X}(t)$ position of the end of the walk.

Why should ECMC be TSAW?

- Stressless chain: zero drift velocity (Michel et al. 2013).
- Drift speed of pointer == Pressure/stress.
- Each visit of the activity to a site displaces $O(1)$.
- If all sites are visited same number of times, all displacements are the same == no stress, no mean speed.



- Pointer speed couples to gradient in number of visits, == Amit et al.

Solution: our dream dynamical system

Balint Tóth, Wendelin Werner, Laure Dumaz

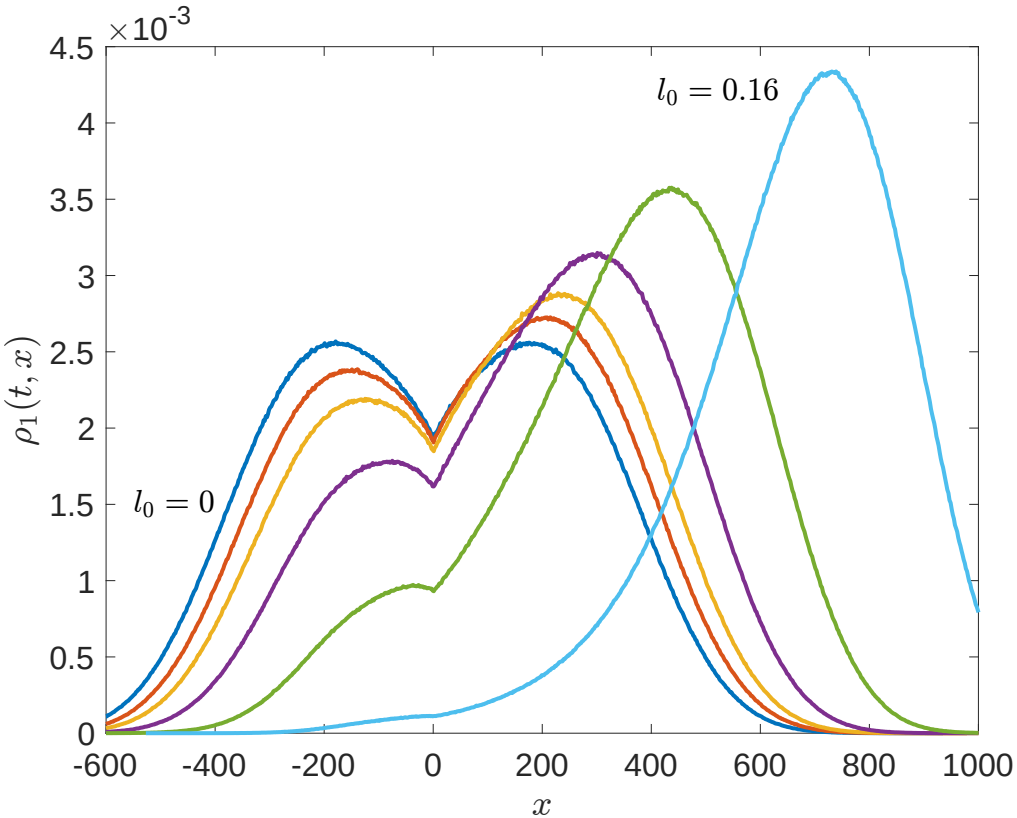
- Density in x after t steps:

$$\rho(t,x) = t^{-2/3}\nu(x/t^{2/3}).$$

- Superdiffusive motion: $x \sim t^{2/3}$.
- Equilibrates in $\tau \sim N^{3/2}$ in effort: Superfast relaxation.
- With a choice of U_M works for all potentials: LJ, hard-spheres.

Stressed chains

Tension in the chain is !=0, $\Longrightarrow$ mean propagation speed in the position of the pointer.



Perhaps

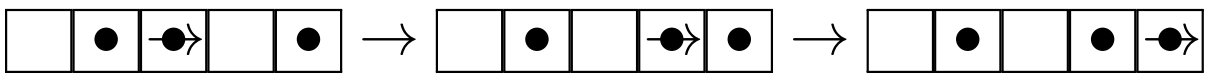
$$\frac{d\mathbf{X}(t)}{dt} = -\nabla L(t, \mathbf{X}(t)) + \mathbf{u}_0$$

Modification to the local rules kill drift (Lei, Krauth, ACM 2018)

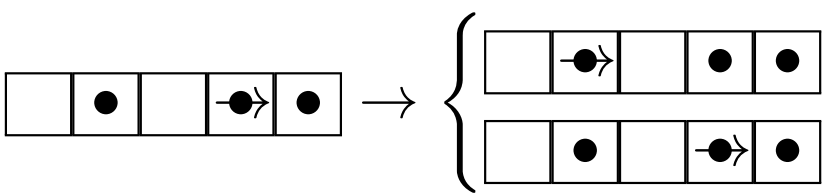
Lifted TASEP

Essler, Krauth, Brune Massoulié, Cristina Toninelli
Bethe Ansatz

Move forwards particle: Like original MC.

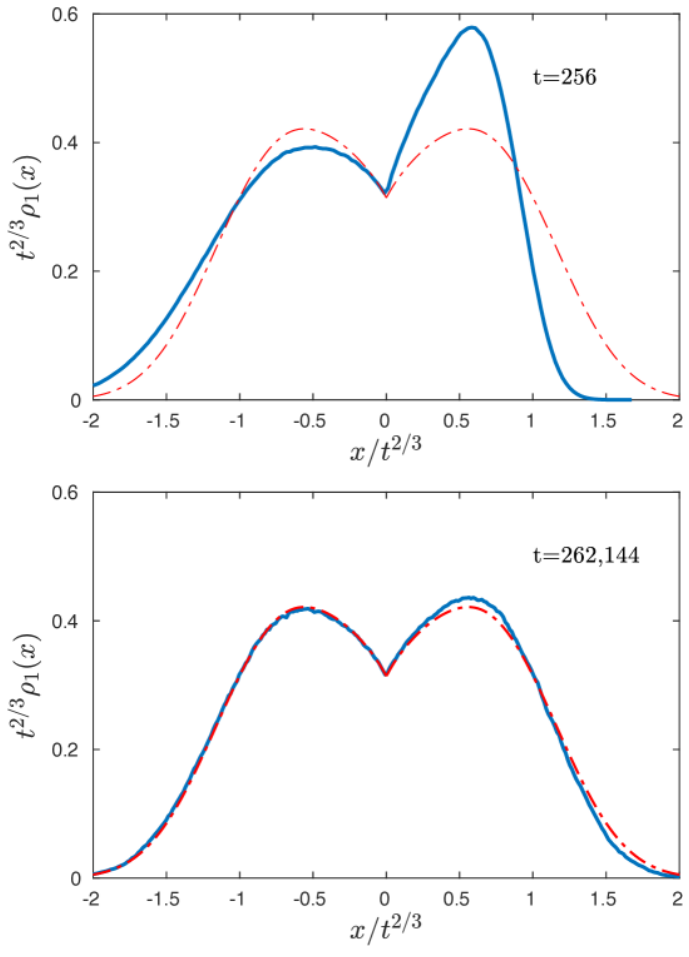


Back jumps of pointer cancel average drift:



Lifted TASEP

Pointer distribution



Back-forwards symmetry only seen on long times.

Multi-agent simulations

Parallel updates: every computer has many processors

- Parallel implementation of the non-reversible algorithm: Li, Todo, ACM, Krauth (2020) 2D implementation.
- Inspire us to study the multi-agent generalisation of TSAW: Tóth, Werner (2002).

$$\frac{dX}{dt} = -\frac{\partial L}{\partial x} \qquad \frac{\partial \rho}{\partial t} + \frac{\partial (u\rho)}{\partial x} = 0$$

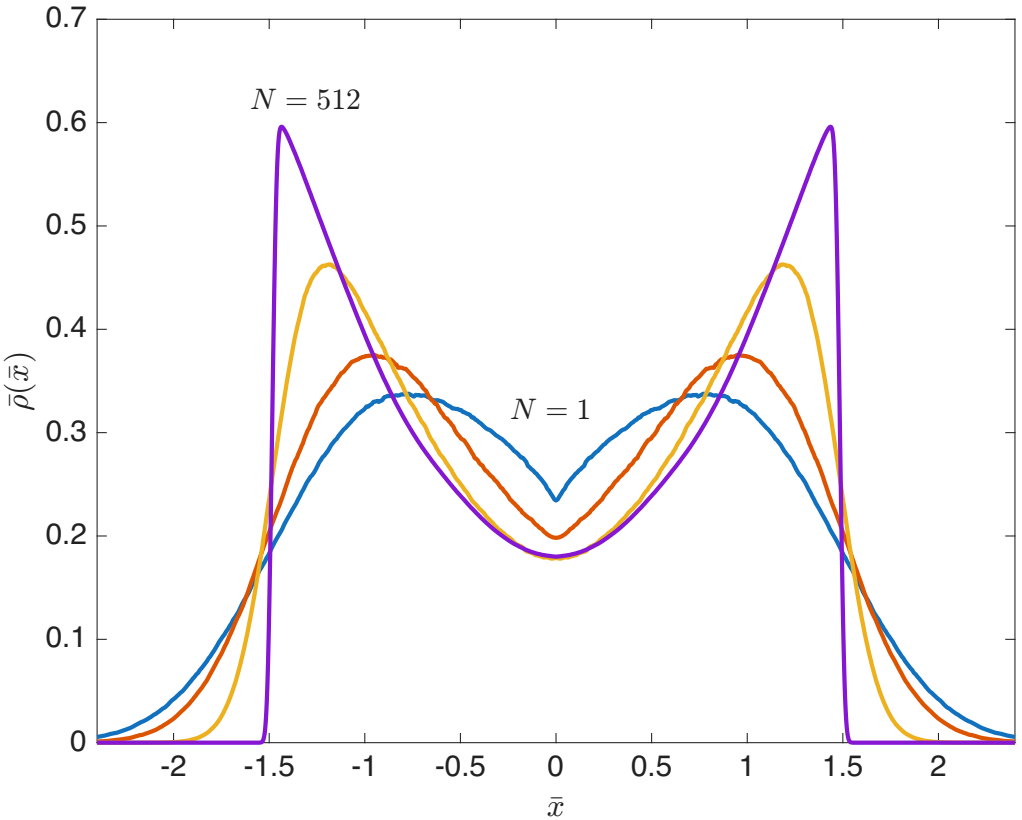
$$\frac{\partial L(x)}{\partial t} = \delta(x - X(t)) \qquad \frac{\partial u}{\partial t} + \frac{\partial \rho}{\partial x} = 0$$

with

$$u = -dL/dx \qquad \text{drift velocity}$$

Multi-agent generalisation of ECMC in higher dimensions?

Multiple walkers: bricklayer model, N builders



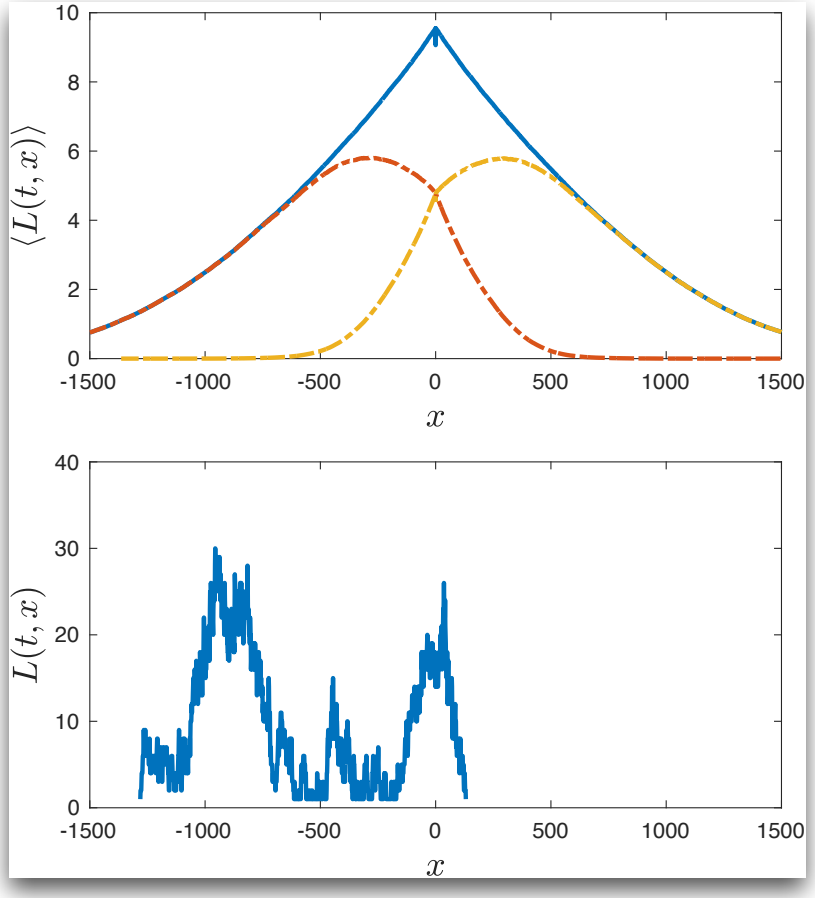
Large N: Parabolic density, width $w \sim N^{1/3} t^{2/3}$.
Analytic solution of PDE, (Ottinger, 1985).

Open Questions

Open questions

- Can we build better samplers in higher dimensions?
- How to couple to orientation, hexatic order etc?
- Same distributions for different local potentials eg LJ, hard sphere, 1st+2nd nearest neigbour. Universal distributions.
- Are there other, non-equilibrium dynamical systems that have the same universality class?
- Is active matter close in some sense? Or is it very different?
- Can one build parallel codes and describe their behaviour with hydrodynamics?

Shape of $L(x)$



Slope singularity in $L(x)$