Université
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Accelerating sampling
by irreversible methods

Frédéric van Wijland, Matière et Systèmes Complexes

YITP, Kyoto, July 25th , 2024
Long-term Workshop on
Frontiers in Non-equilibrium Physics

YUKAWA INSTITUTE FOR
THEORETICAL PHYSICS

Active particles
to the rescue of passive ones

Frédéric van Wijland, Matière et Systèmes Complexes

YITP, Kyoto, July 24th , 2024
Long-term Workshop on
Frontiers in Non-equilibrium Physics

Acknowledgements

Federico Ghimenti

Université Paris Cité

Ludovic Berthier

Grzegorz Szamel

Acknowledgements

Jorge Kurchan

ENS
ÉCOLE NORMALE SUPÉRIEURE

Yoshihiko Nishikawa

なりたい、を超えていく
北里大学 理学部
Kitasato University School of Science

& Werner Krauth,
Manon Michel,
Camille Scalliet

Based on

Ghimenti, Berthier, Szamel, FvW, PRL (2023) (acceleration)
Ghimenti, Berthier, Szamel, FvW, PRE (2024 (infinite dimension)
Ghimenti, Berthier, FvW, PRL (2024) (algorithm)
Ghimenti, Berthier, Szamel, FvW, PRE (2024) (mode-coupling)
Ghimenti, Berthier, FvW, JCP (2024) (3d)

Ghimenti, Berthier, Kurchan, FvW, in preparation, time-permitting

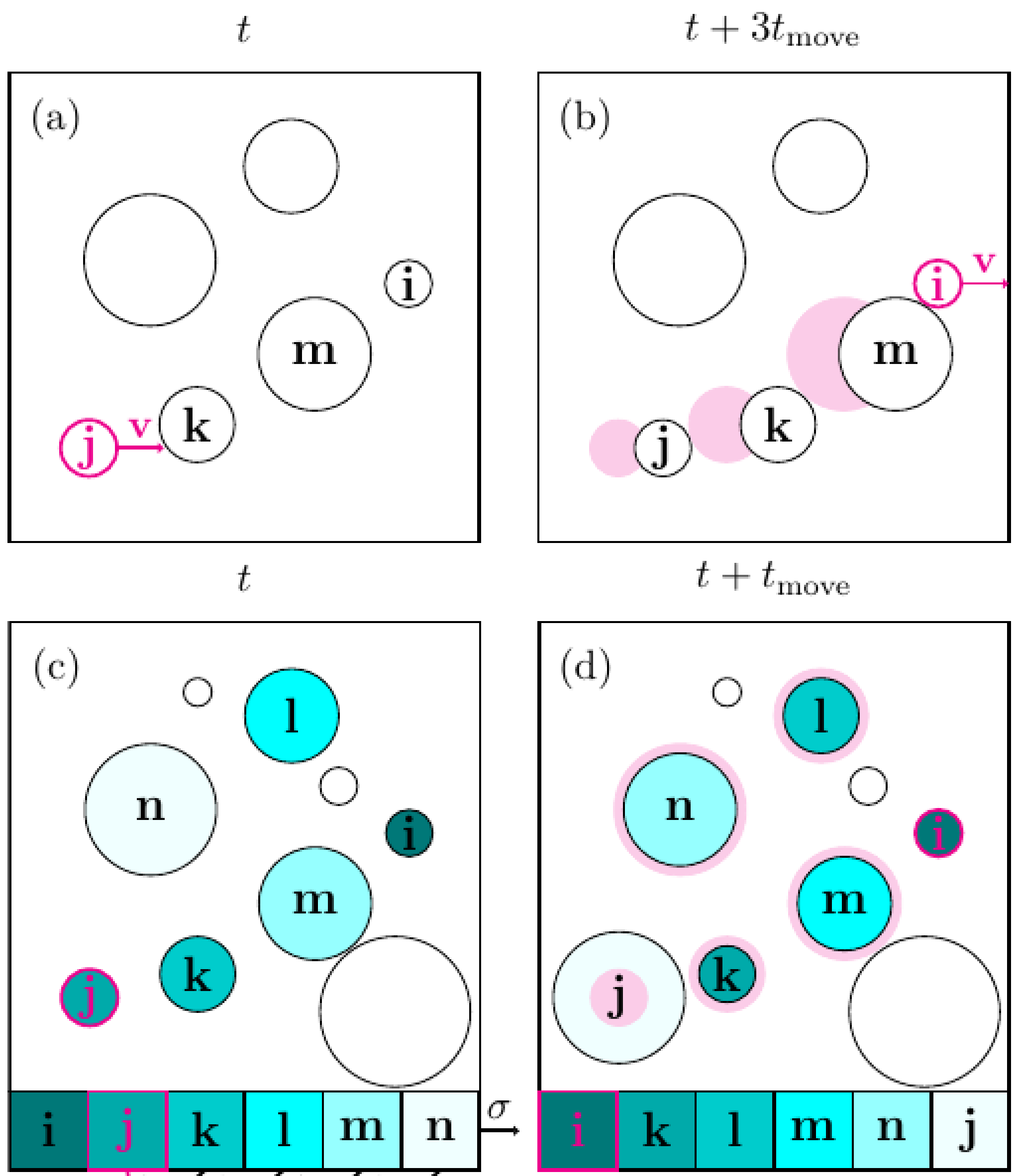
YITP Colloquium：Time-reparametrization invariance: from glasses to toy black holes

Jorge Kurchan (Laboratoire de Physique, Ecole Normale Superieure)

2024/07/30 15:30 --

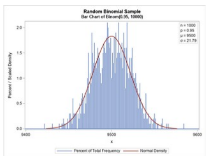
Panasonic Auditorium, Yukawa Hall, Yukawa Institute, Kyoto U. &【Zoom】

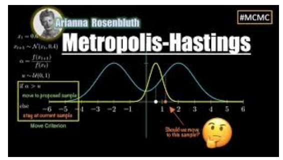
Speed-up of 40



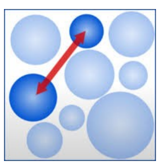
Menu

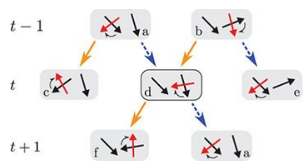
Sampling



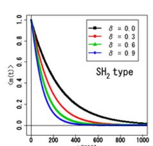


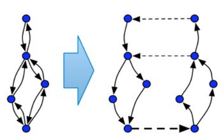
Faster, in, or out of equilibrium





A case where irreversibility works at its best

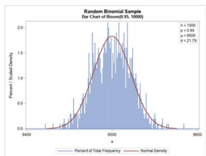


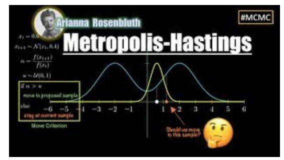


Glasses

Menu

Sampling





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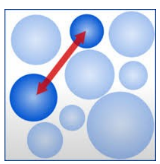
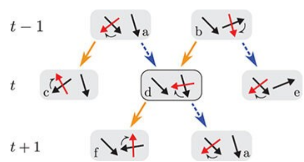
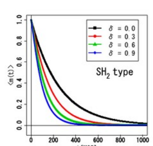
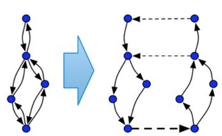




A case where irreversibility works at its best





Glasses

Sampling

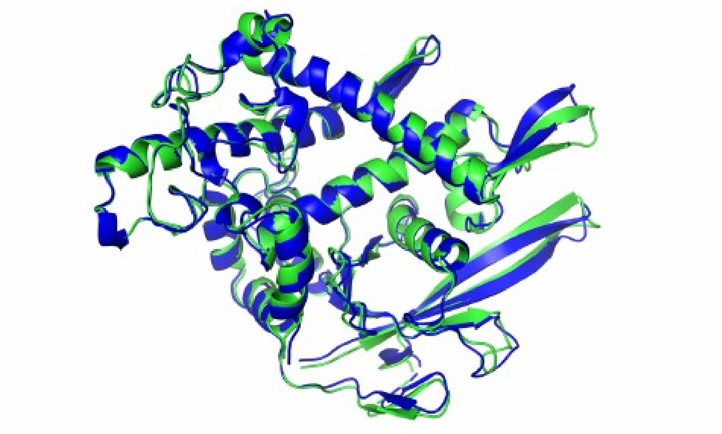
Consider a system with many degrees of freedom $\mathbf{r}$

and with energy $V(\mathbf{r})$

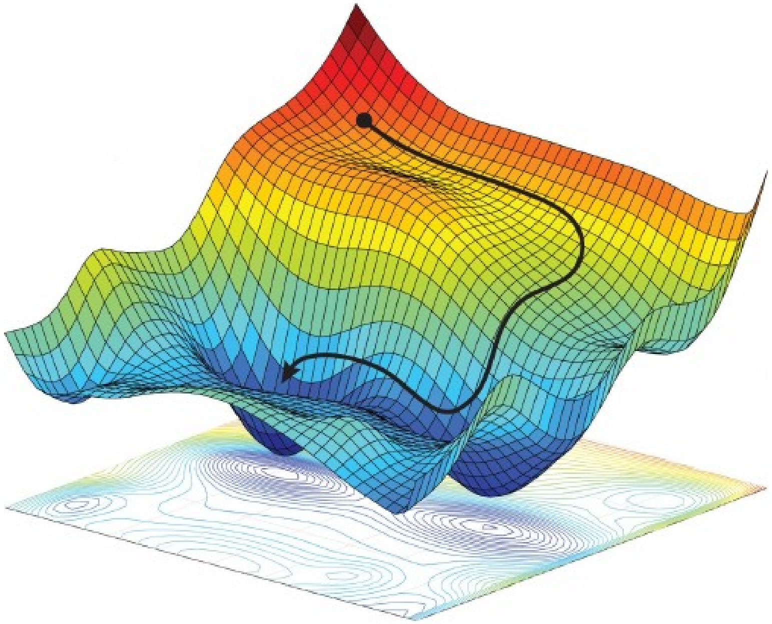
Goal: sample $p_{\mathrm{B}}(\mathbf{r}) = \mathrm{e}^{-\frac{V(\mathbf{r})}{T}}$

Sampling

This can sometimes be very hard.



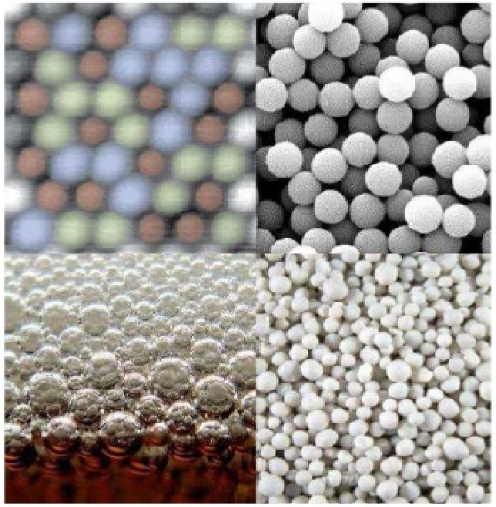
Protein folding
DeepMind



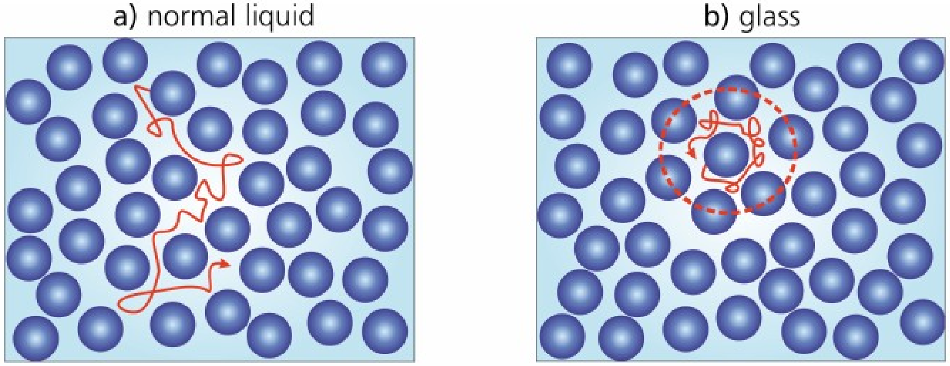
Machine Learning & Optimization
Amini *et al.*, NIPS 2017

Sampling

This can sometimes be very hard.



Disordered materials
Berthier & Biroli 2011



Janssen 2018

Hot questions (about cold liquids)

• Equilibrium liquid to glass phase transition: complete mean-field theory with Kauzmann transition, and very strong but incomplete numerical hints.

• Nature of equilibrium relaxation dynamics close to the experimental T_g where $\tau_\alpha \sim 10^2$ s: cooperativity, facilitation, spatially heterogeneous dynamics.

• Basic properties of the glassy state: transport, thermal excitations, linear and non-linear defects, rheology, plasticy and failure.

• New physics revealed by the discovery of ultrastable glassy films: melting, annealing, aging, excitations.

Attacking these problems numerically requires efficient methods to equilibrate, sample, or prepare glasses with various degrees of annealing.

The Langevin paradigm

$$\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t} = -\mu \boldsymbol{\nabla} V(\mathbf{r}) + \sqrt{2\mu T}\boldsymbol{\eta}$$

$$\langle \eta_i(t) \eta_j(t') \rangle = \delta_{ij} \delta(t - t')$$

The Langevin paradigm

$$\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t} = -\mu \boldsymbol{\nabla} V(\mathbf{r}) + \sqrt{2\mu T}\boldsymbol{\eta}$$

$$\langle \eta_i(t)\eta_j(t')\rangle = \delta_{ij}\delta(t-t')$$

$$\partial_t p(\mathbf{r},t) = -\boldsymbol{\nabla}\cdot\mathbf{j},\ \mathbf{j} = -T\boldsymbol{\nabla} p - \boldsymbol{\nabla} V p$$

The Langevin paradigm

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$$\partial_t p(\mathbf{r},t) = -\boldsymbol{\nabla}\cdot\mathbf{j},\ \mathbf{j} = -T\boldsymbol{\nabla}p - \boldsymbol{\nabla}Vp$$

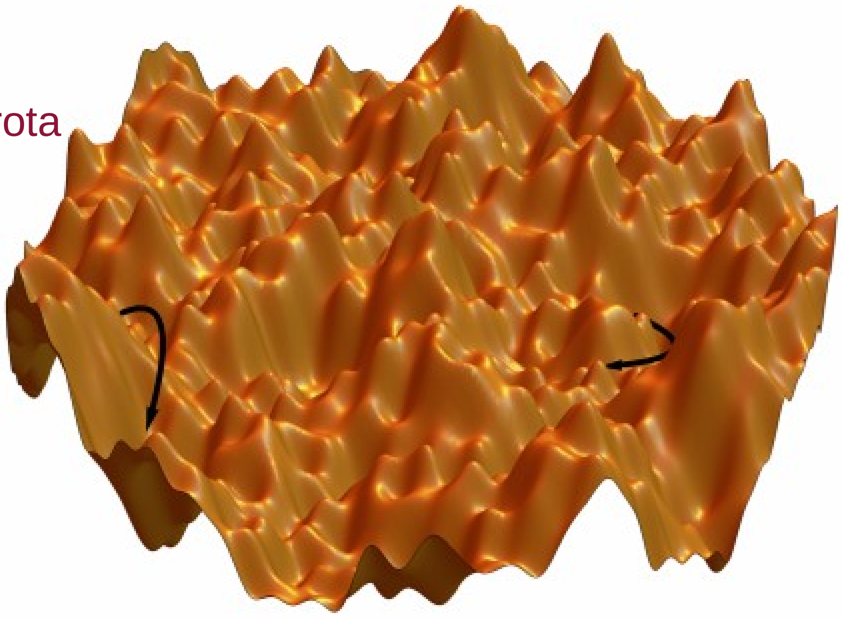
$$p(\mathbf{r},t) = p_{\mathrm{B}}(\mathbf{r}) + \mathrm{e}^{-\frac{t}{\tau_{\mathrm{relax}}}}\phi(\mathbf{r}) + \ldots$$

The Langevin paradigm

$$p(\mathbf{r},t) = p_{\mathrm{B}}(\mathbf{r}) + \mathrm{e}^{-\frac{t}{\tau_{\mathrm{relax}}}}\phi(\mathbf{r}) + \ldots$$

but what if τ_{relax} becomes very large

C. Cammarota



The Langevin paradigm

$$p(\mathbf{r},t) = p_{\mathrm{B}}(\mathbf{r}) + \mathrm{e}^{-\frac{t}{\tau_{\mathrm{relax}}}}\phi(\mathbf{r}) + \ldots$$

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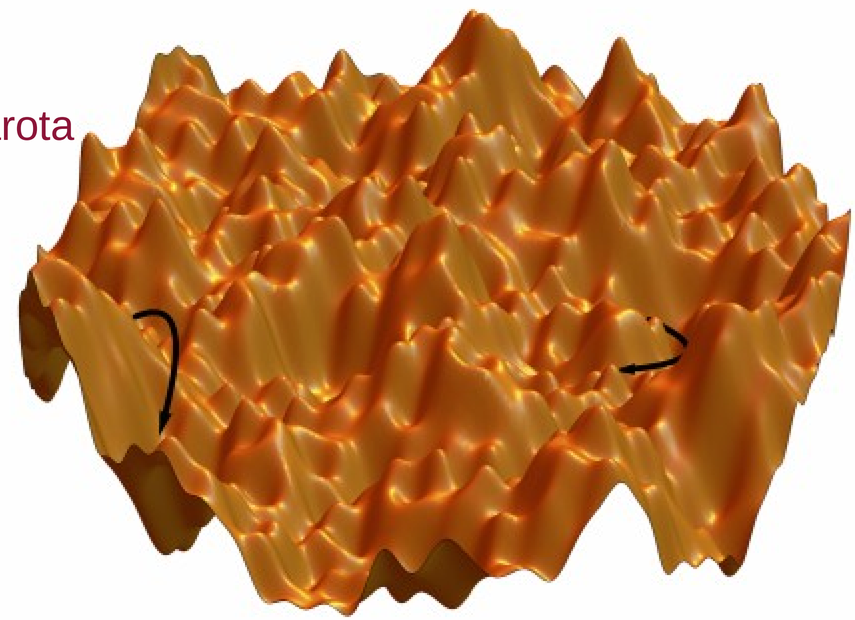
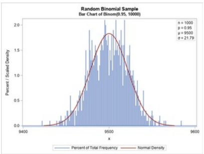
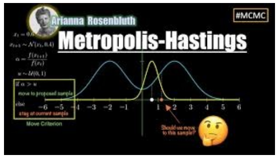


τ_{relax} or τ_{mixing} or τ_{first}

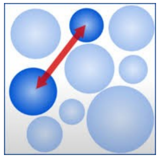
Menu

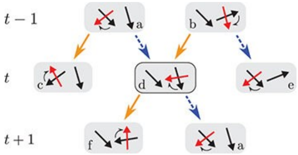
Sampling



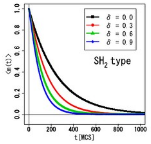


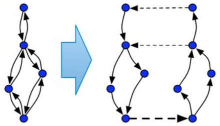
Faster, in, or out of equilibrium





A case where irreversibility works at its best





Glasses

Equilibrium

is a dynamical concept

Statistical time reversibility of trajectories

aka Detailed Balance, Zero entropy production, etc.

What we don't want

$$\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t} = -\mu \boldsymbol{\nabla} V(\mathbf{r}) + \sqrt{2\mu T}\boldsymbol{\eta}$$

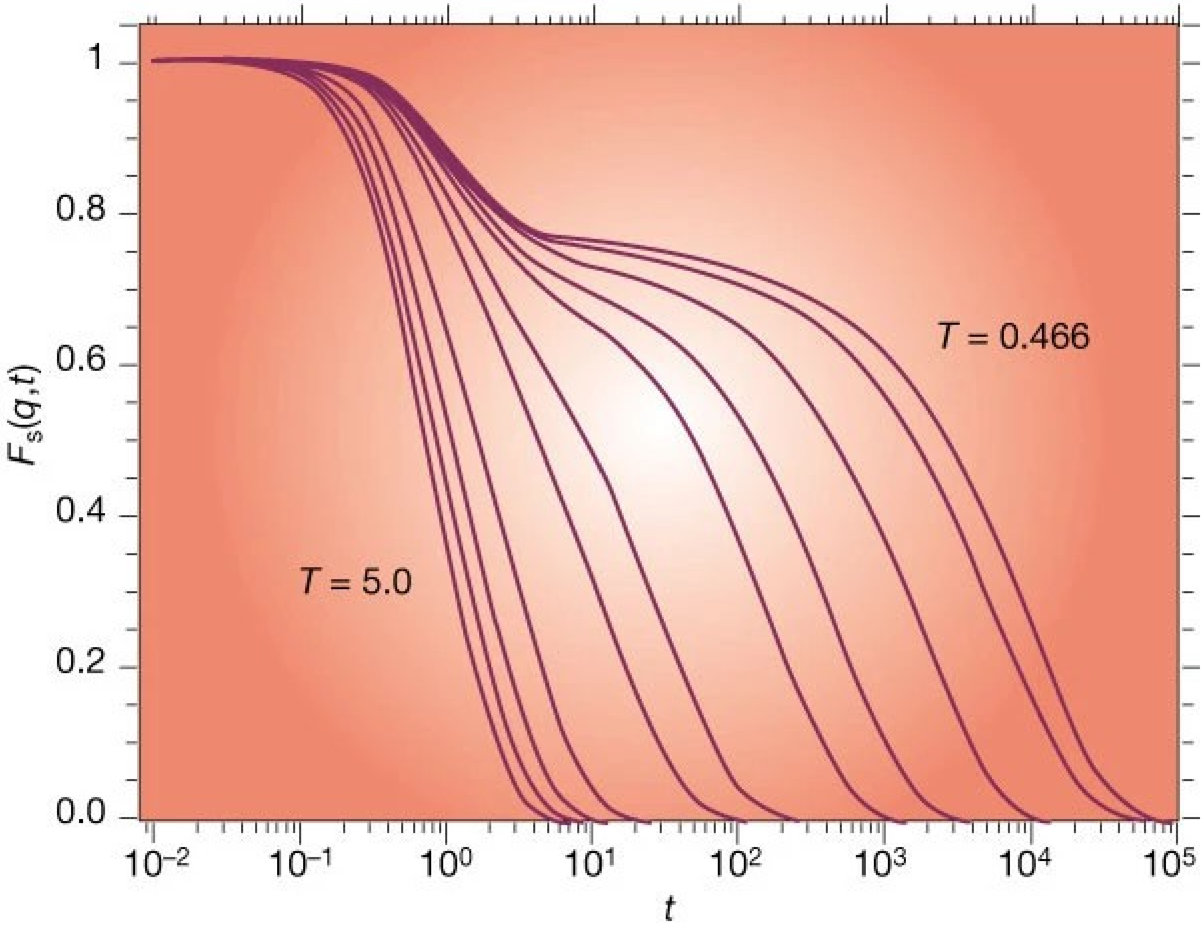
$$\langle \eta_i(t)\eta_j(t')\rangle = \delta_{ij}\delta(t - t')$$

Larger μ means faster dynamics = trivial

Glassy dynamics

$$\tau_\alpha = \text{density relaxation time}$$

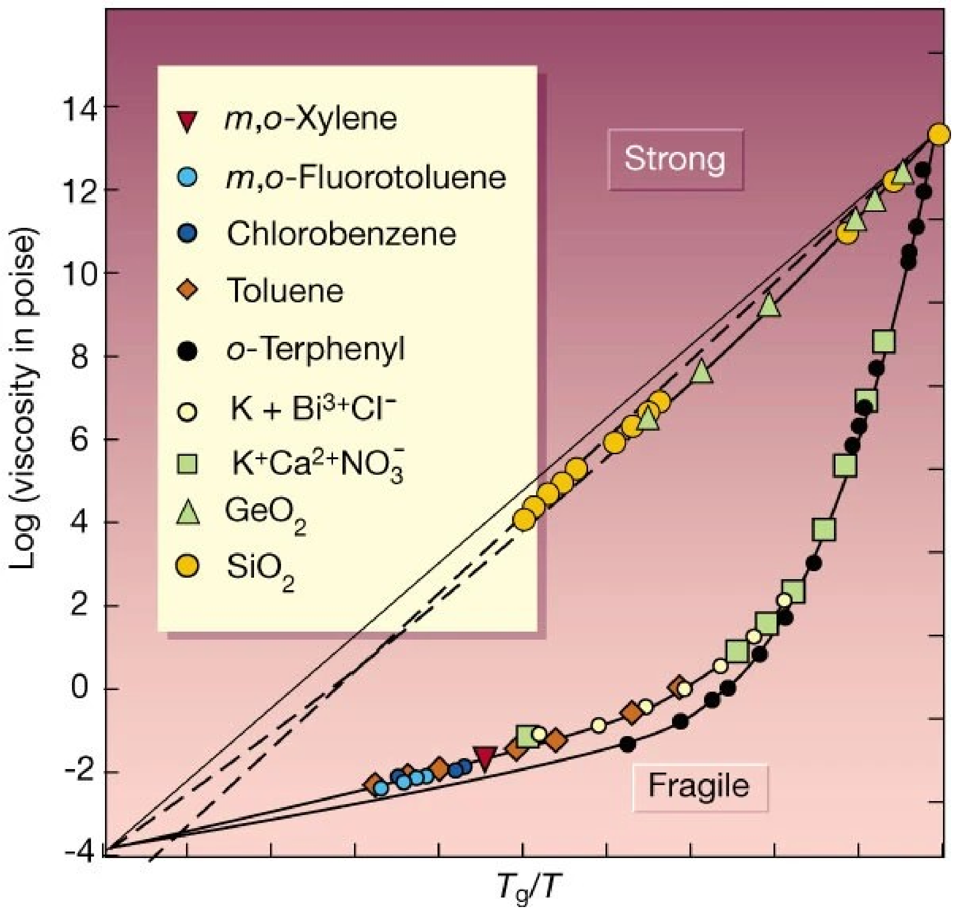
LJ mixture



Debenedetti & Stillinger, Nature (2001)

Glassy dynamics

$$\tau_\alpha = \text{density relaxation time}$$



Debenedetti & Stillinger, Nature (2001)

What ‘s on the market

• Molecular Dynamics (MD) and local Monte Carlo (MC) capture physical dynamics, but are then the slowest methods $\tau_{\text{sampling}} \sim \tau_\alpha$.

• Non-local, cluster and collective Monte Carlo moves: apriori require a great deal of physical understanding. Swap MC leads to $\tau_{\text{sampling}} \lll \tau_\alpha$.

• Parallel tempering and population annealing techniques: equilibrium variations of simulated annealing to climb barriers in complex landscapes.

• Random pinning/bonding.

• Machine learning assisted Monte Carlo techniques: learning MC moves, learning Boltzmann distribution.

Optimal transport formulation

Start from $p(\mathbf{x}, t = 0)$ uniform

Find an evolution such that $p(\mathbf{x}, t \to +\infty) = p_B(\mathbf{x})$

Optimal transport formulation

Start from $p(\mathbf{x}, t = 0)$ uniform

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while minimizing the relaxation time

Optimal transport formulation

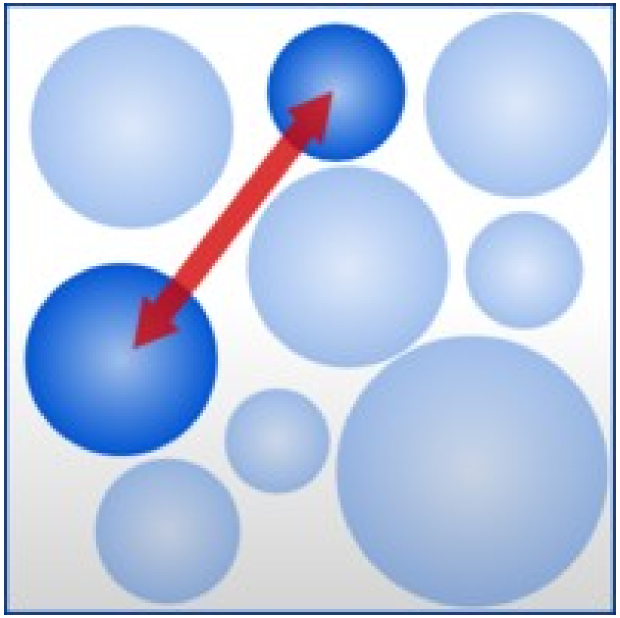
Start from $p(\mathbf{x}, t = 0)$ uniform

Find an evolution such that $p(\mathbf{x}, t \to +\infty) = p_B(\mathbf{x})$

while minimizing the relaxation time

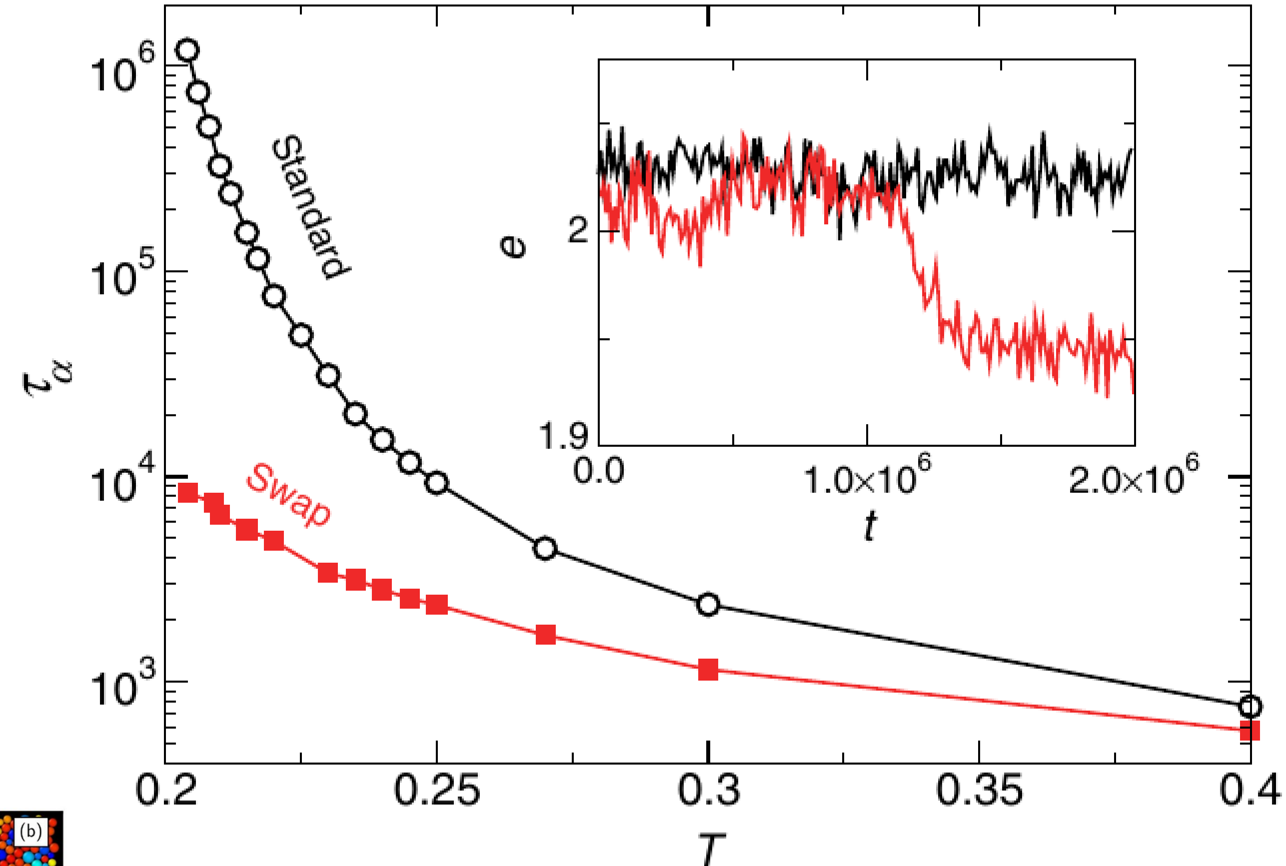
Find an evolution, what does it mean?
Minimizing the relaxation time, what does it mean?

SWAP

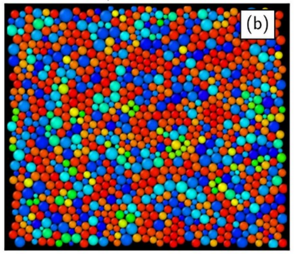


SWAP

$$\tau_\alpha = \text{density relaxation time}$$

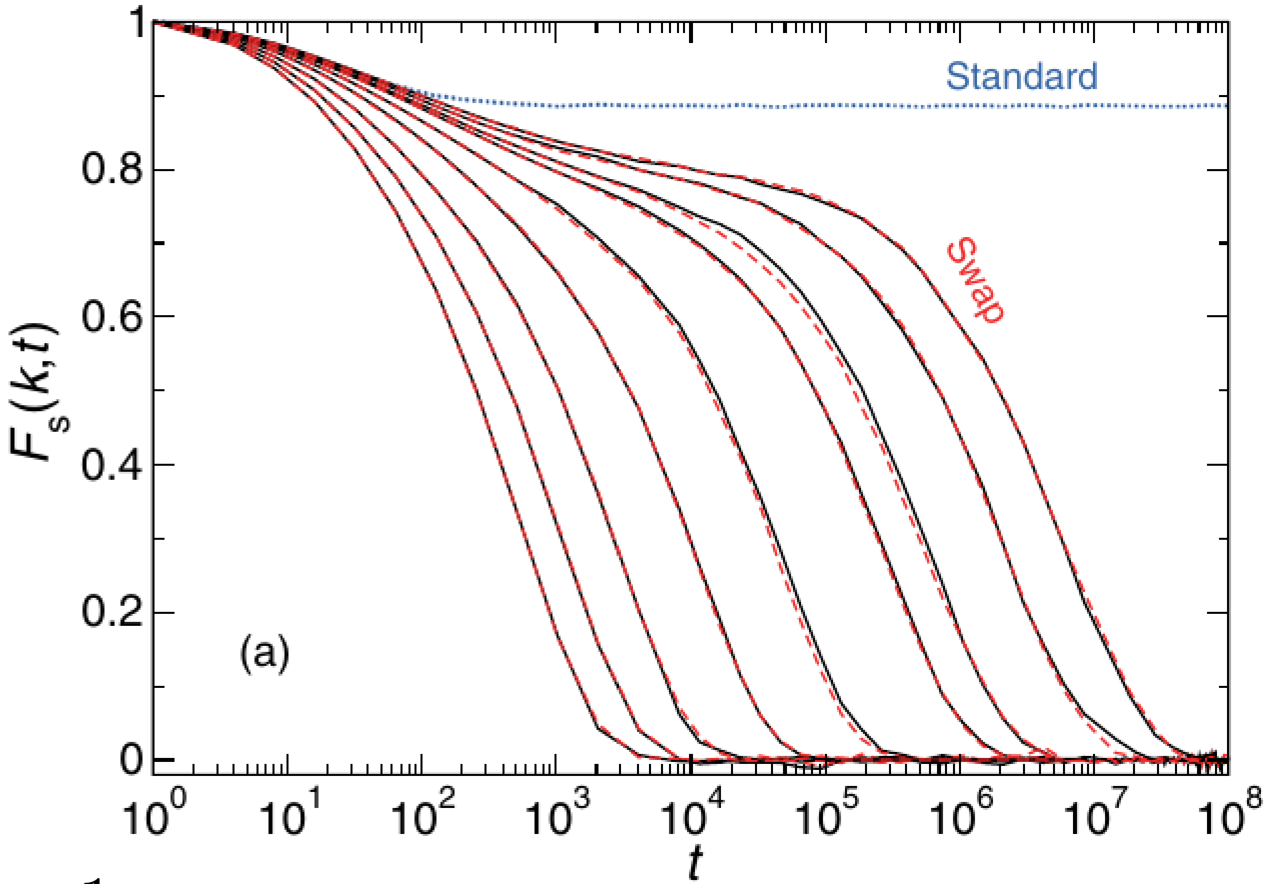


$\phi = 0.9029$



Ninarello, Berthier & Coslovich, PRX (2017)

SWAP



$$F_s(\mathbf{k},t) = \frac{1}{N}\langle \sum_i \mathrm{e}^{i\mathbf{k}\cdot(\mathbf{r}_i(t)-\mathbf{r}_i(0))} \rangle$$

SWAP

PHYSICAL REVIEW X **12**, 041028 (2022)

Thirty Milliseconds in the Life of a Supercooled Liquid

Camille Scalliet,[1] Benjamin Guiselin,[2] and Ludovic Berthier[3,4,*]

Think out of equilibrium

The Annals of Applied Probability
1993, Vol. 3, No. 3, 897–913

ACCELERATING GAUSSIAN DIFFUSIONS[1]

BY CHII-RUEY HWANG,[2] SHU-YIN HWANG-MA AND SHUENN-JYI SHEU

Academia Sinica, Soochow University and Academia Sinica

Let $\pi(x)$ be a given probability density proportional to $\exp(-U(x))$ in a high-dimensional Euclidean space $\mathbb{R}^m$. The diffusion $dX(t) = -\nabla U(X(t))\,dt + \sqrt{2}\,dW(t)$ is often used to sample from π. Instead of $-\nabla U(x)$, we consider diffusions with smooth drift $b(x)$ and having equi-

The Annals of Applied Probability
2000, Vol. 10, No. 3, 726–752

ANALYSIS OF A NONREVERSIBLE MARKOV CHAIN SAMPLER

BY PERSI DIACONIS,[1] SUSAN HOLMES AND RADFORD M. NEAL[2]

Stanford University, Stanford University and INRA and University of Toronto

We analyze the convergence to stationarity of a simple nonreversible Markov chain that serves as a model for several nonreversible Markov chain sampling methods that are used in practice. Our theoretical and numerical results show that nonreversibility can indeed lead to improvements over the diffusive behavior of simple Markov chain sampling schemes. The analysis uses both probabilistic techniques and an explicit diagonalization.

Lifting Markov Chains to Speed up Mixing

Fang Chen
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Igor Pak †
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Simulation of quantum walks and fast mixing with classical processes

Simon Apers, Alain Sarlette, and Francesco Ticozzi
Phys. Rev. A **98**, 032115 – Published 20 September 2018

Think out of equilibriuum

PHYSICAL REVIEW E **80**, 056704 (2009)

Event-chain Monte Carlo algorithms for hard-sphere systems

Etienne P. Bernard,[1,*] Werner Krauth,[1,†] and David B. Wilson[2,‡]
[1]*CNRS–Laboratoire de Physique Statistique, Ecole Normale Supérieure, 24 rue Lhomond, 75231 Paris Cedex 05, France*
[2]*Microsoft Research, One Microsoft Way, Redmond, Washington 98052, USA*
(Received 19 March 2009; revised manuscript received 15 October 2009; published 18 November 2009)

In this paper we present the event-chain algorithms, which are fast Markov-chain Monte Carlo methods for hard spheres and related systems. In a single move of these rejection-free methods, an arbitrarily long chain of particles is displaced, and long-range coherent motion can be induced. Numerical simulations show that event-chain algorithms clearly outperform the conventional Metropolis method. Irreversible versions of the algorithms, which violate detailed balance, improve the speed of the method even further. We also compare our method with a recent implementations of the molecular-dynamics algorithm.

Irreversible Monte Carlo algorithms for efficient sampling

Konstantin S. Turitsyn [a,b,*], Michael Chertkov [a,c], Marija Vucelja [a,c]
[a] *Center for Nonlinear Studies & Theoretical Division, LANL, Los Alamos, NM 87545, USA*
[b] *Landau Institute for Theoretical Physics, Moscow 142432, Russia*
[c] *Department of Physics of Complex Systems, Weizmann Institute of Sciences, Rehovot 76100, Israel*

Lifting—A nonreversible Markov chain Monte Carlo algorithm

Marija Vucelja[a)]
Center for Studies in Physics and Biology, The Rockefeller University, 1230 York Avenue, New York, New York 10065 and Department of Physics, University of Virginia, Charlottesville, Virginia 22904
(Received 2 February 2015; accepted 11 August 2016)

Think out of equilibriuum

A theorem

$$\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t} = -\mu\boldsymbol{\nabla}V + \mathbf{f} + \sqrt{2\mu T}\boldsymbol{\eta}$$

$$\boldsymbol{\nabla}\cdot\mathbf{f} - \beta\boldsymbol{\nabla}V\cdot\mathbf{f} = 0$$

Think out of equilibriuum

A theorem

$$\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t} = -\mu \boldsymbol{\nabla} V + \mathbf{f} + \sqrt{2\mu T}\boldsymbol{\eta}$$

$$\boldsymbol{\nabla} \cdot \mathbf{f} - \beta \boldsymbol{\nabla} V \cdot \mathbf{f} = 0$$

$$\text{then } \tau_{\mathrm{relax}}(\mathbf{f}) \leq \tau_{\mathrm{relax}}(\mathbf{0})$$

Think out of equilibriuum

$$\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t} = -\mu\boldsymbol{\nabla}V + \mathbf{f} + \sqrt{2\mu T}\boldsymbol{\eta}$$

$$\boldsymbol{\nabla}\cdot\mathbf{f} - \beta\boldsymbol{\nabla}V\cdot\mathbf{f} = 0$$

$$\text{Choose }\ \mathbf{f} = -A\boldsymbol{\nabla}V,\ \ A^T = -A$$

Think out of equilibriuum

$$\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t} = -\mu\boldsymbol{\nabla}V + \mathbf{f} + \sqrt{2\mu T}\boldsymbol{\eta}$$

$$\underbrace{\boldsymbol{\nabla}\cdot\mathbf{f}}_{=0} - \beta\underbrace{\boldsymbol{\nabla}V\cdot\mathbf{f}}_{=0} = 0$$

$$\text{Choose }\ \mathbf{f} = -A\boldsymbol{\nabla}V,\ \ A^T = -A$$

Trial and error

$$\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t} = -\mu \boldsymbol{\nabla} V + \mathbf{f} + \sqrt{2\mu T}\boldsymbol{\eta}$$

a small of self-propelled particles

Trial and error

$$\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t} = -\mu \boldsymbol{\nabla} V + \mathbf{f} + \sqrt{2\mu T}\boldsymbol{\eta}$$

RTP, ABP, AOUP

Loss of (mathematical) control

Trust RTPs

$$\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t} = -\mu \boldsymbol{\nabla} V + \mathbf{f} + \sqrt{2\mu T}\boldsymbol{\eta}$$

Choose $\mathbf{f} = v_0 \mathbf{u}$, $||\mathbf{u}|| = 1$

$\mathbf{u} =$ Runs and Tumbles with a fine-tuned rate

$$\Gamma(\mathbf{u} \to \mathbf{u}') = \frac{1}{\Omega_d} \beta v_0 \boldsymbol{\nabla} V \cdot (\mathbf{u} - \mathbf{u}') \text{ or 0 if negative}$$

And even set $\mu = 0$

Trust RTPs

$$\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t} = v_0 \mathbf{u}$$

$$\Gamma(\mathbf{u} \to \mathbf{u}') = \frac{1}{\Omega_d} \beta v_0 \boldsymbol{\nabla} V \cdot (\mathbf{u} - \mathbf{u}') \text{ or } 0 \text{ if negative}$$

(the theorem is lost)

Boltzmann is safe

$$\Gamma(\mathbf{u} \to \mathbf{u}') = \frac{1}{\Omega_d} \beta v_0 \boldsymbol{\nabla} V \cdot (\mathbf{u} - \mathbf{u}') \text{ or 0 if negative}$$

$$\partial_t p(\mathbf{r}, \mathbf{u}, t) = -v_0 \mathbf{u} \cdot \nabla p$$

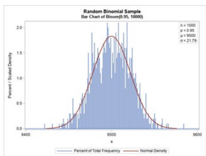
$$+ \int \mathrm{d}^{d-1} u' \left[\Gamma(\mathbf{u}' \to \mathbf{u}) p(\mathbf{r}, \mathbf{u}', t) - \Gamma(\mathbf{u} \to \mathbf{u}') p(\mathbf{r}, \mathbf{u}, t) \right]$$

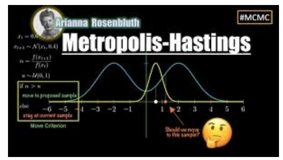
$$\text{Check:} p_{\mathrm{ss}}(\mathbf{r}, \mathbf{u}) = p_{\mathrm{B}}(\mathbf{r}) \frac{1}{\Omega_d} \text{ is a stationary solution}$$

$$\text{with } p_{\mathrm{B}}(\mathbf{r}) = \frac{\mathrm{e}^{-\beta V(\mathbf{r})}}{Z}$$

Menu

Sampling





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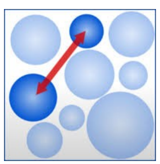
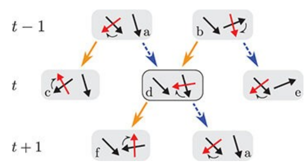
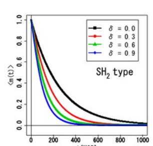
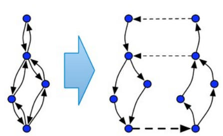




A case where irreversibility works at its best





Glasses

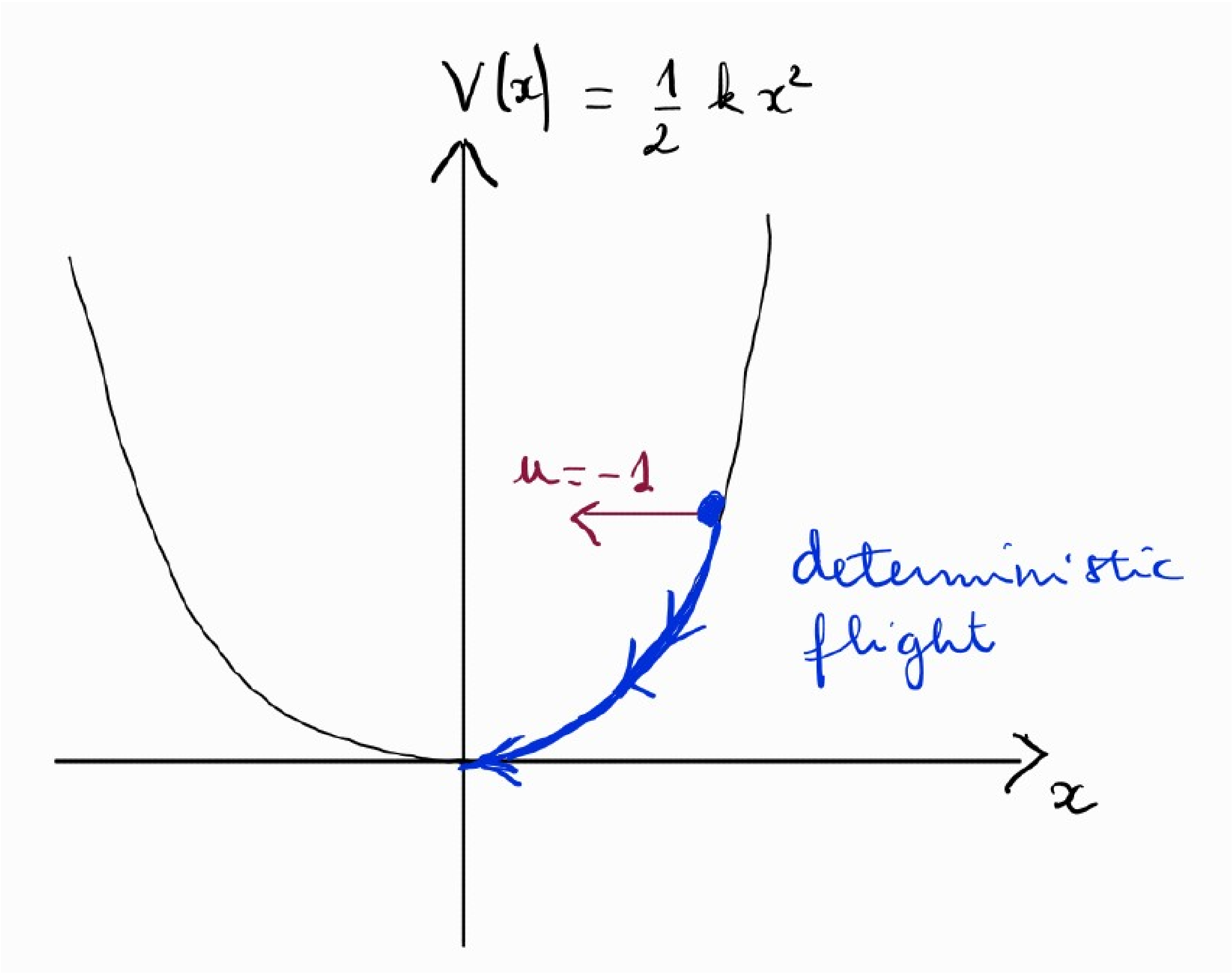
Harmonic potential

$$\frac{\mathrm{d}x}{\mathrm{d}t} = v_0 u, \;\; u = \pm 1$$

$$\Gamma(u \to -u) = \beta v_0 V' u \theta(uV')$$

$$V(x) = \frac{1}{2} k x^2$$

Harmonic potential



Harmonic potential/Langevin

$$V(x) = \frac{1}{2}kx^2$$

$$\dot{x} = -\mu k x + \sqrt{2\mu T}\eta$$

$$\tau_{\mathrm{relax}}^{-1} = \mu k \propto k^1$$

Harmonic potential/Lifted

$$V(x) = \frac{1}{2} k x^2$$

$$\dot{x} = v_0,\ u = \pm 1$$

$$\tau_{\mathrm{relax}}^{-1} = \sqrt{\beta {v_0}^2}\sqrt{k}\,(1.0034 + i3.209) \propto k^{1/2}$$

Monthus, JSTAT (2021) $\tau_{\mathrm{first}}^{-1} \propto \sqrt{k}$

Phase transitions

$$V(x) = \frac{1}{2}kx^2 \to V(M) = \frac{T - T_c}{2}M^2 + \ldots$$

$$\tau_{\text{relax}} = \xi^z, \quad z = 1 \text{ in mean-field}$$

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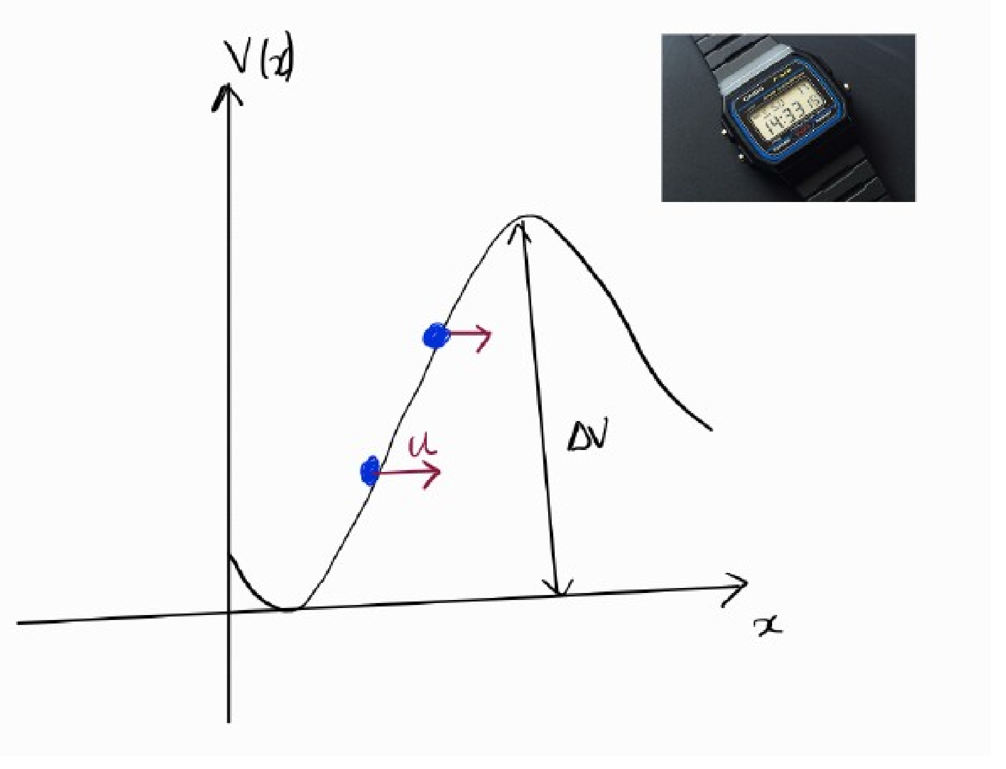
Two-Step Melting in Two Dimensions: First-Order Liquid-Hexatic Transition

Etienne P. Bernard* and Werner Krauth†

Many papers over the years by Krauth, Kapfer, Michel, Hukushima, Nishikawa, and even Sasa

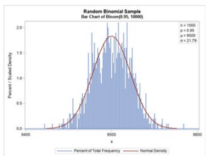
How about a potential barrier ?

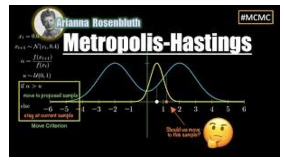


$$\tau_{\text{Kramers}} \sim \mathrm{e}^{\beta \Delta V}$$

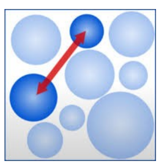
Menu

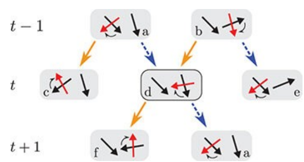
Sampling



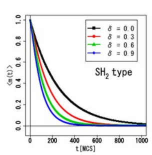


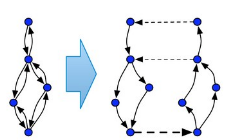
Faster, in, or out of equilibrium





A case where irreversibility works at its best





Glasses

Glasses

Many particles, repulsive potential

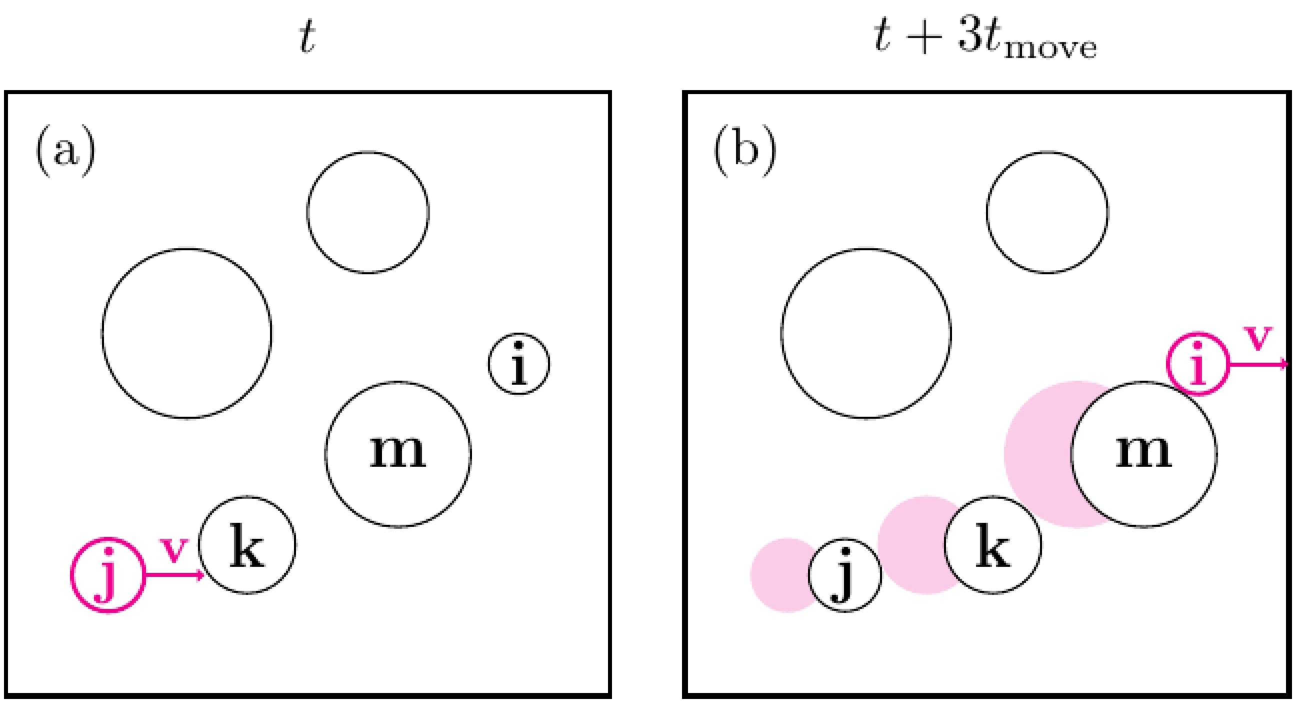
$$\mathbf{r}_i(t), \quad H = \sum_{i<j} V(\mathbf{r}_i - \mathbf{r}_j)$$

Control temperature or density.

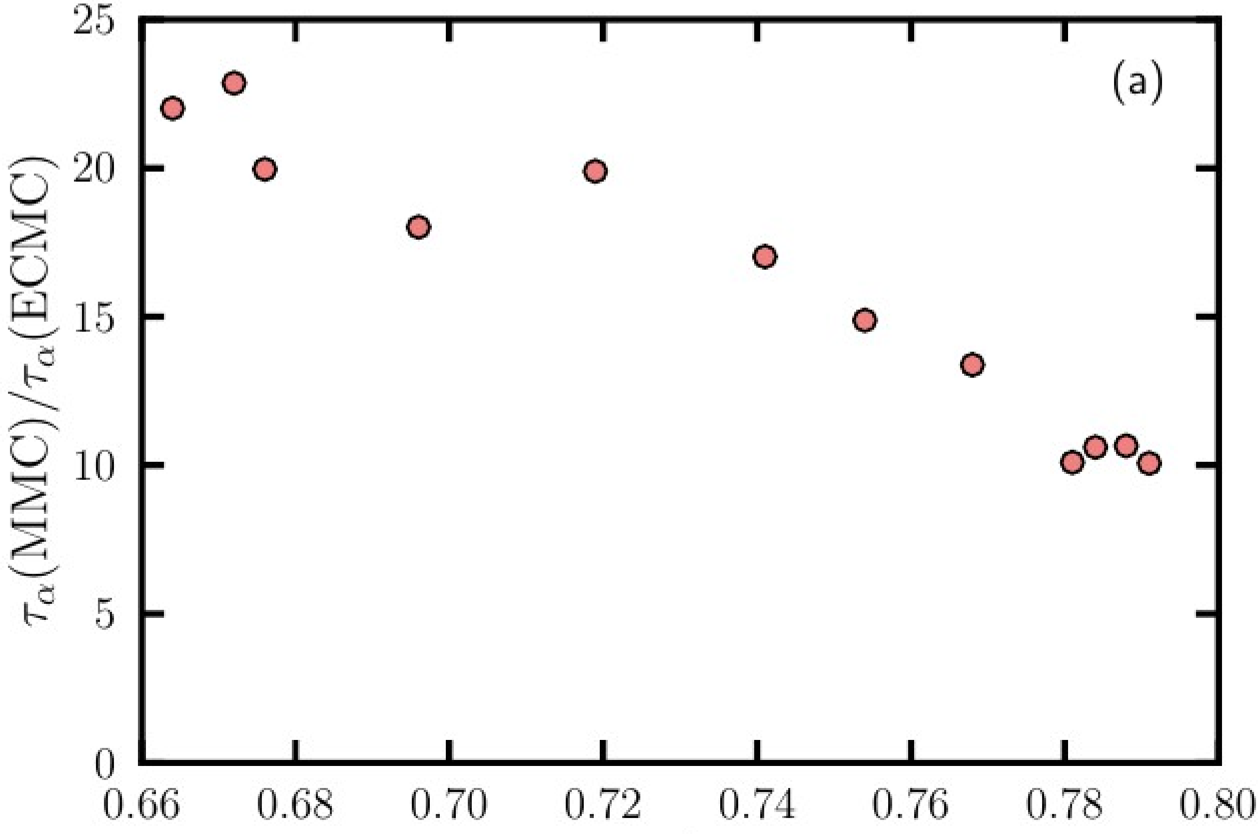
$$\frac{\mathrm{d}\mathbf{r}_i}{\mathrm{d}t} = v_0 \mathbf{u}_i$$

Glasses, in practice

For hard-spheres, Event Chain Monte Carlo :



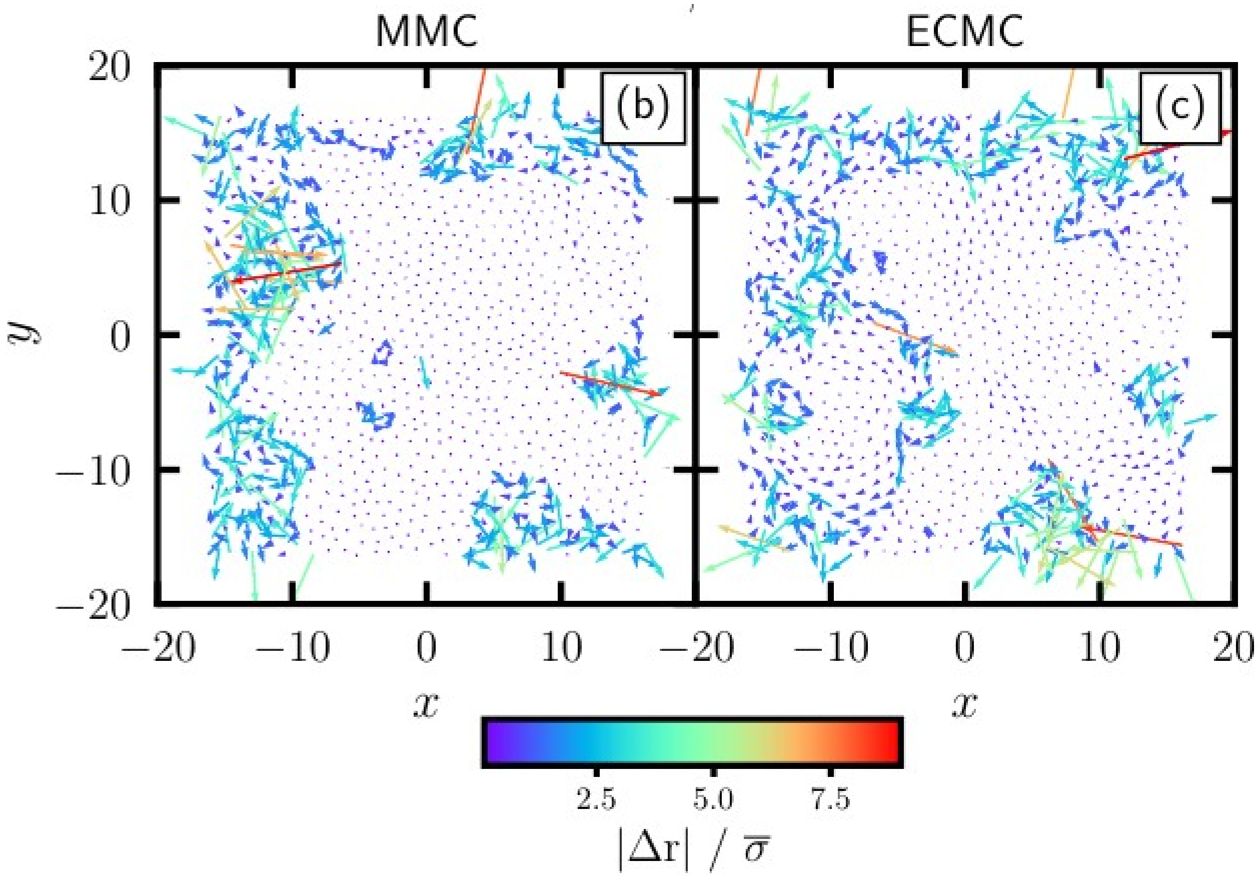
What's the gain ?



$\rightarrow$ Speedup about 20 wrt Metropolis MC in dense fluids

$\rightarrow$ Speedup decreases as density increases

Similar dynamical pathways

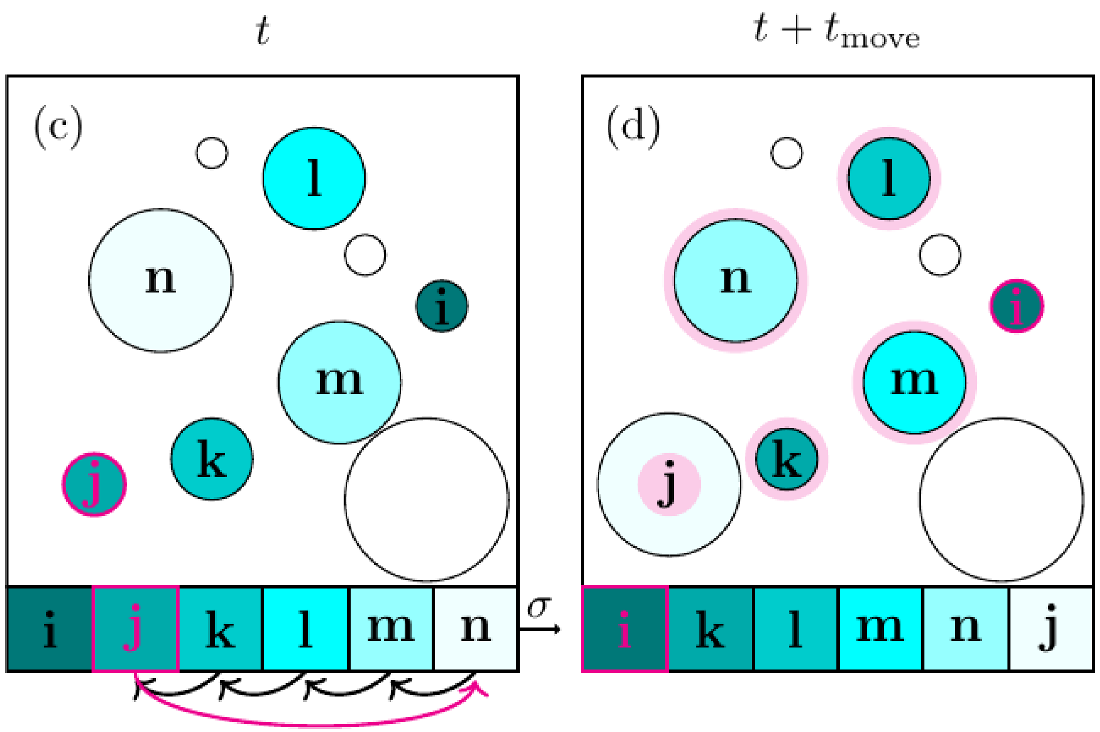


$\rightarrow$ Speedup about 20 wrt Metropolis MC in dense fluids

$\rightarrow$ Speedup decreases as density increases

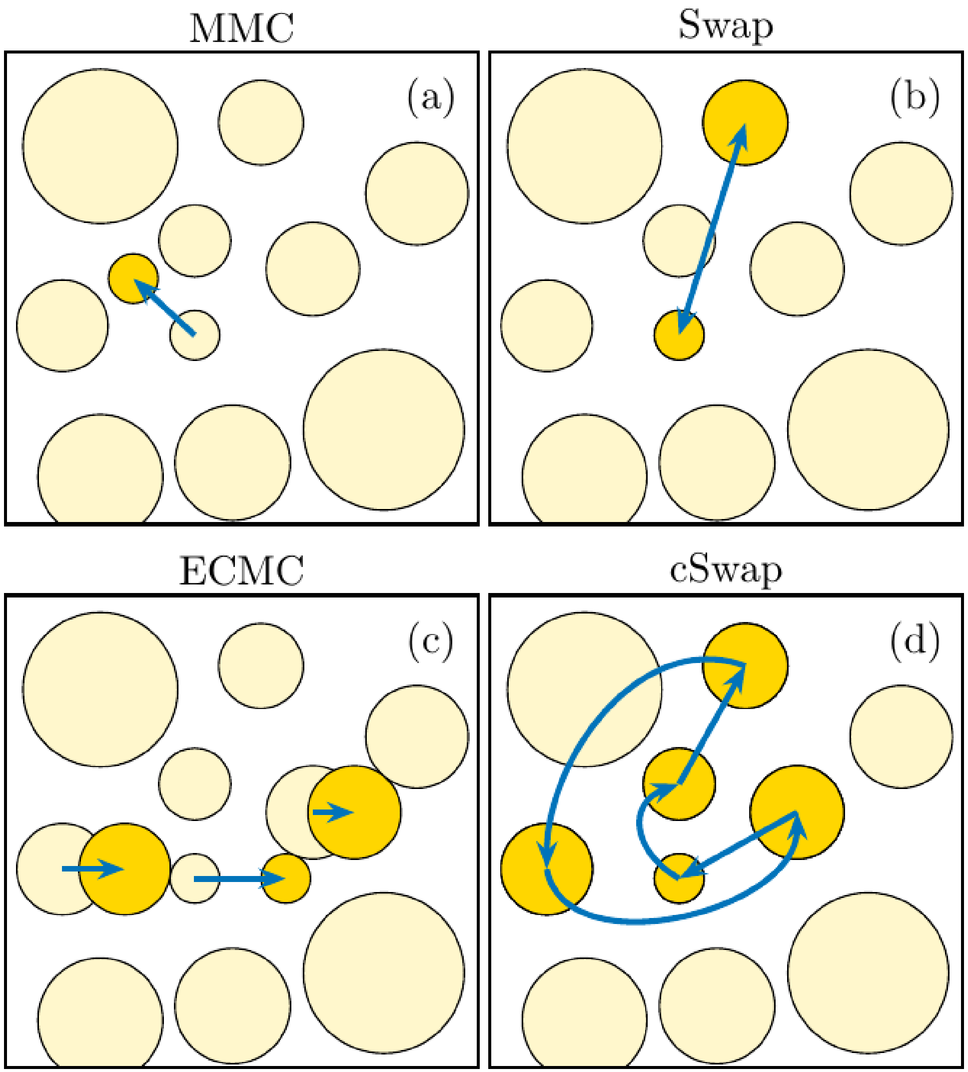
New algorithm

Idea: perform rejection-free, irreversible, collective moves in diameter space, i.e. a collective swap.



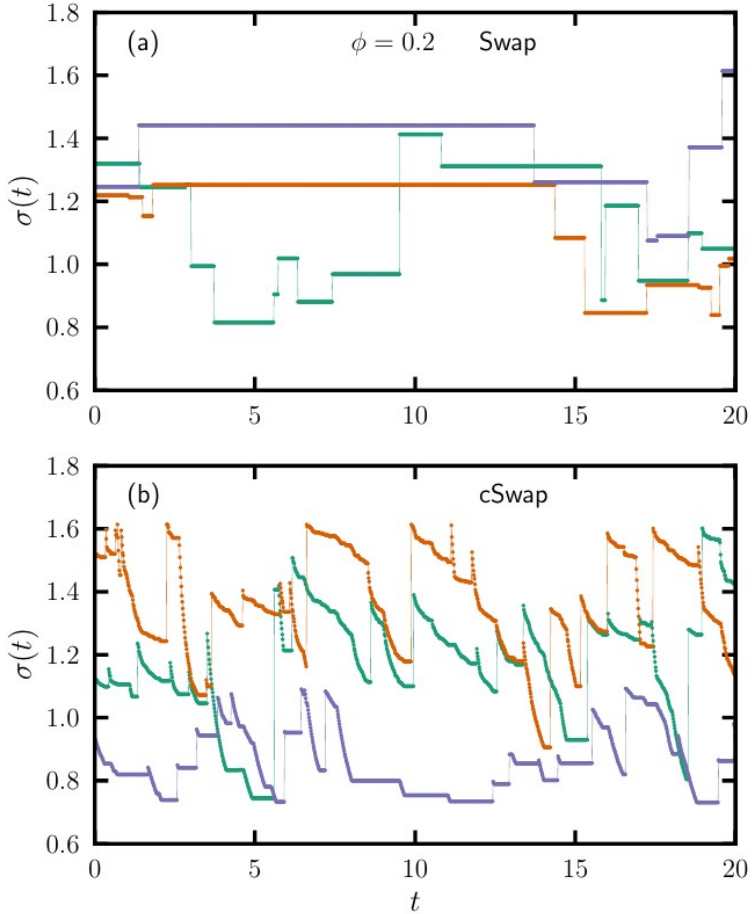
Like ECMC, it satisfies global balance and breaks detailed balance.

New algorithm

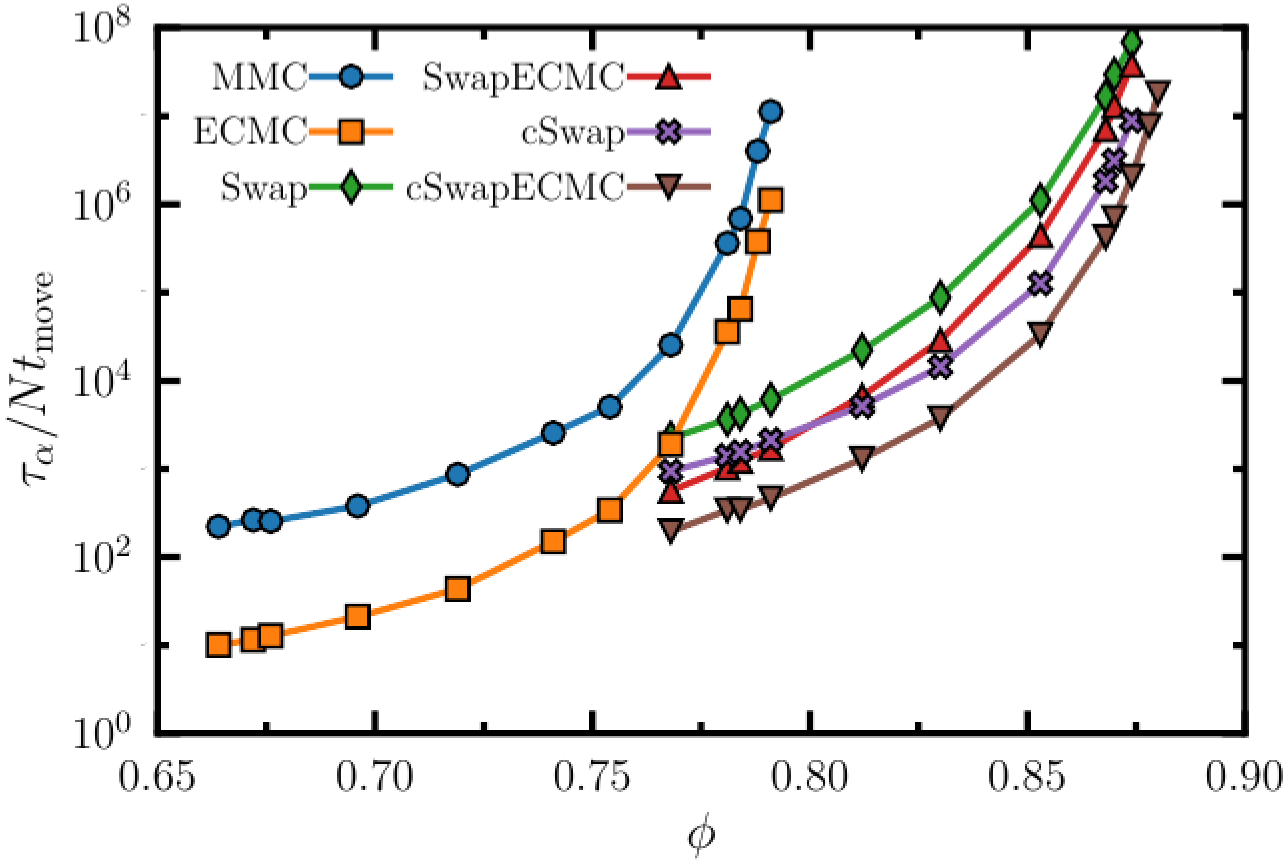


New algorithm

Biased random walk
Directed motion in diameter space

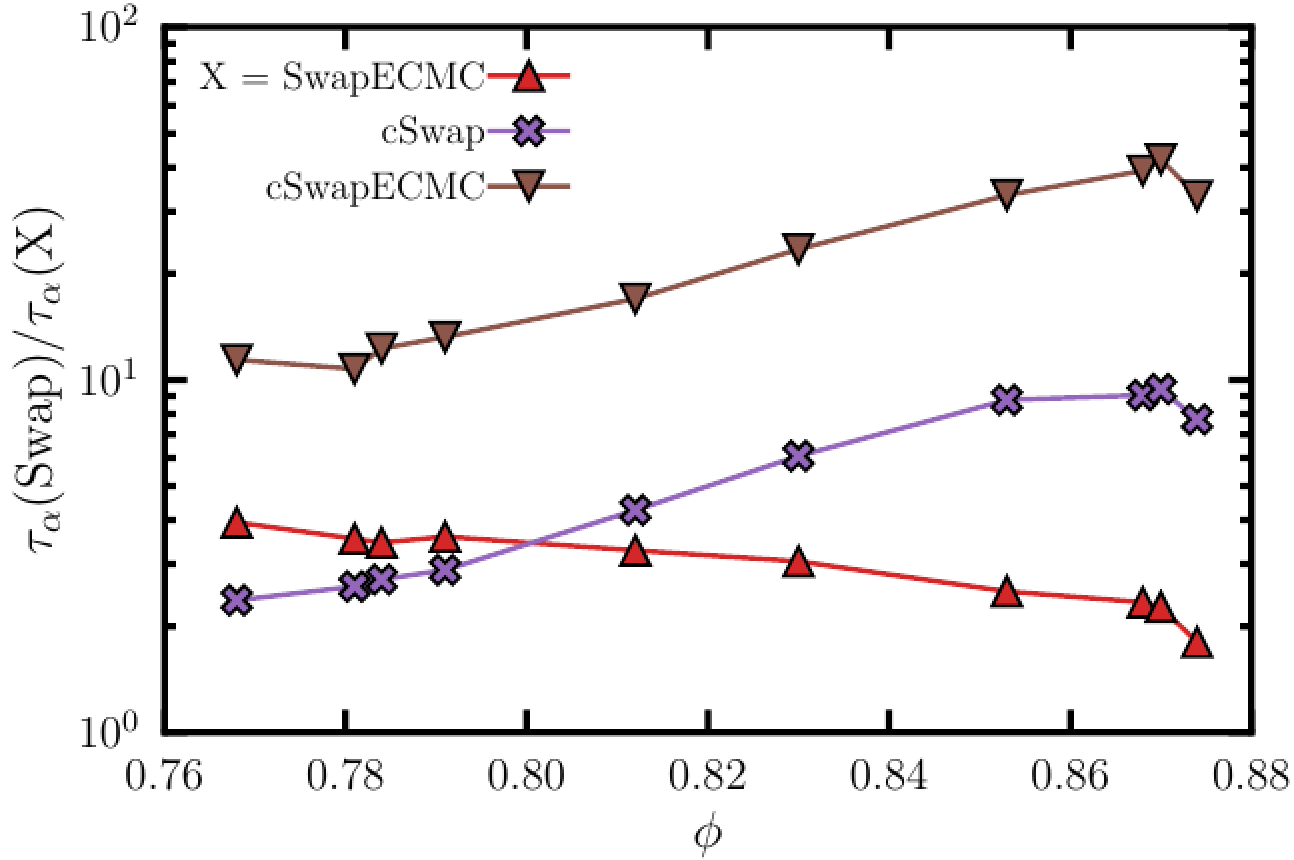


Acceleration ?



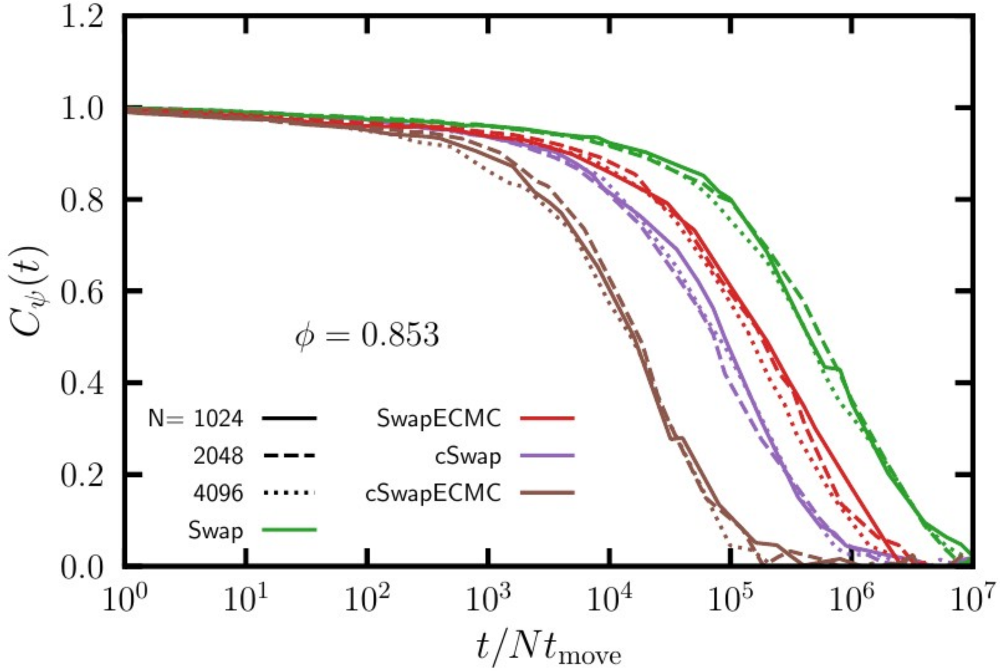
Swap moves (diameter space) badly needed, cSwapECMC the best.

Speedup



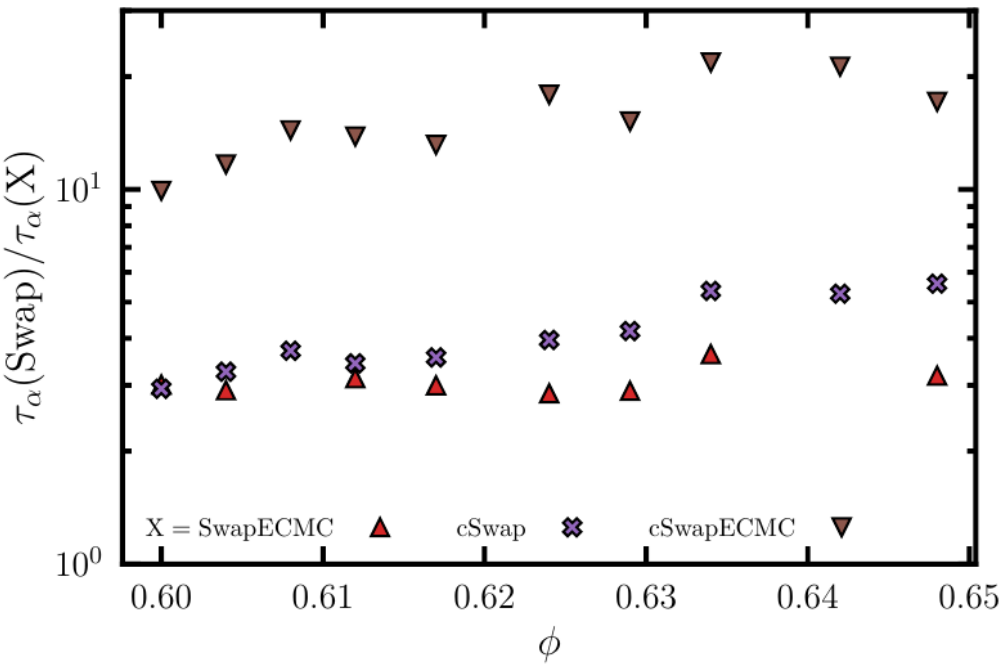
Combined cSwapECMC gets the best of both algorithms with speedup increasing to about 40 compared to swap at largest density.

Yes, it survives *N*



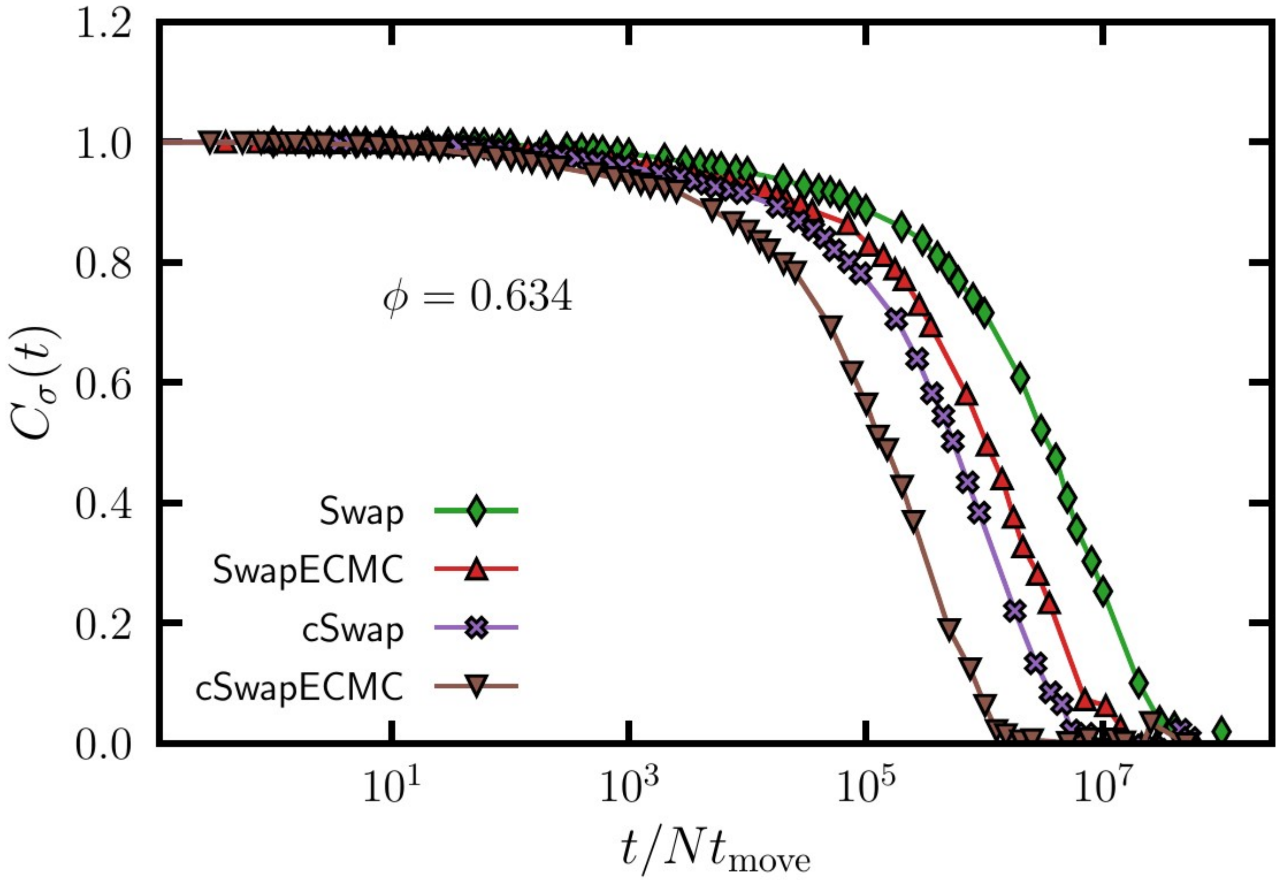
Time correlations of the hexatic order parameter

And *d*

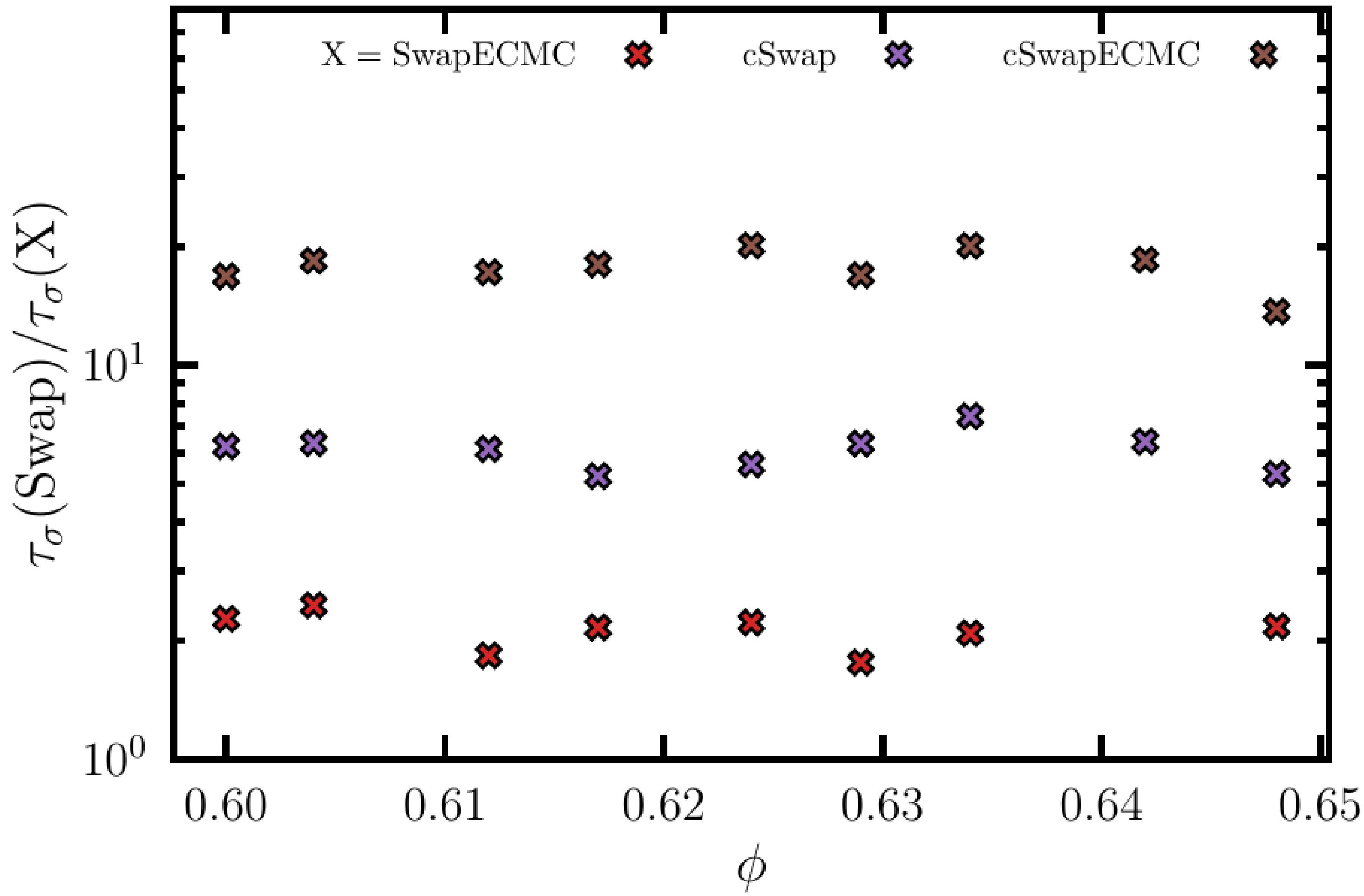


N=300 particles in a cubic box with periodic boundary conditions.

3d hard spheres



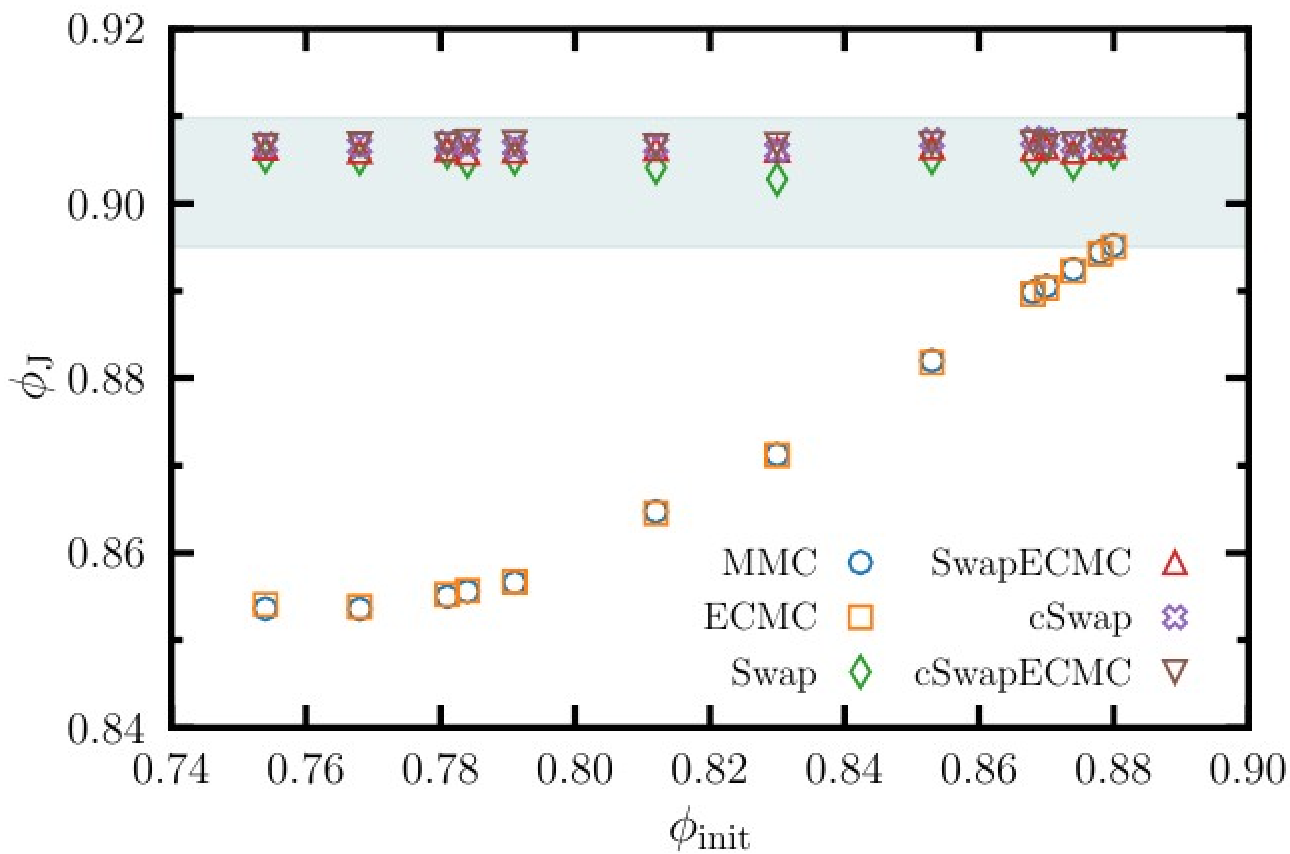
3d hard spheres



Where does this take us ?

- Faster than the fastest.
- This is just the beginning.
- Physics informed lifting.
- Physics informed learning.

Jamming competition



Jamming competition