Totally asymmetric Markov chains with rapid convergence towards equilibrium

Werner Krauth

Laboratoire de Physique statistique
Département de Physique
Ecole normale supérieure
Paris, France

Work with Sebastian C. Kapfer (FAU Erlangen, Germany),
arXiv201705XXXX (next week)
arXiv201705XXXX (Invited EPJB Colloquium)

April 27, 2017

Département de Physique
École normale supérieure

Metropolis et al (1953) 1/4

URNAL OF CHEMICAL PHYSICS VOLUME 21, NUMBER 6 JUN

Equation of State Calculations by Fast Computing Machines

NICHOLAS METROPOLIS, ARIANNA W. ROSENBLUTH, MARSHALL N. ROSENBLUTH, AND AUGUSTA H. TELLER,
Los Alamos Scientific Laboratory, Los Alamos, New Mexico

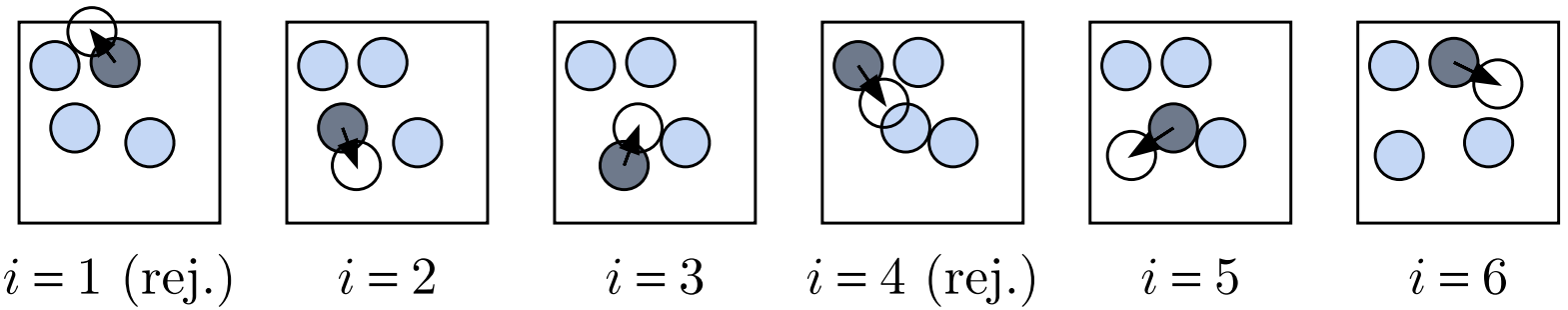
AND

EDWARD TELLER,* *Department of Physics, University of Chicago, Chicago, Illinois*

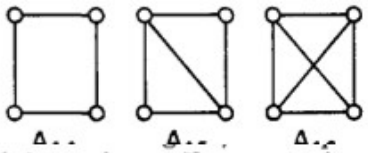
(Received March 6, 1953)

A general method, suitable for fast computing machines, for investigating such properties as equations of state for substances consisting of interacting individual molecules is described. The method consists of a modified Monte Carlo integration over configuration space. Results for the two-dimensional rigid-sphere system have been obtained on the Los Alamos MANIAC and are presented here. These results are compared to the free volume equation of state and to a four-term virial coefficient expansion.

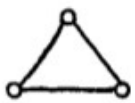
Metropolis et al (1953) 2/4



Metropolis et al (1953) 3/4



distinguished by primes. For example, A_{33} is given schematically by the diagram

$A_{3,3}$: 

and mathematically as follows: if we define $f(r_{ij})$ by

$$f(r_{ij})=1 \quad \text{if} \quad r_{ij}<d,$$
$$f(r_{ij})=0 \quad \text{if} \quad r_{ij}>d,$$

then

$$A_{3,3}=\frac{1}{\pi^2 d^4}\int\cdots\int dx_1 dx_2 dx_3 dy_1 dy_2 dy_3 (f_{12}f_{23}f_{31}).$$

The schematics for the remaining integrals are indicated in Fig. 6.

The coefficients $A_{3,3}$, $A_{4,4}$, and $A_{4,5}$ were calculated were put down at random, subject to $f_{12}=f_{23}=f_{34}=f_{15}=1$. The number of trials for which $f_{45}=1$, divided by the total number of trials, is just $A_{5,5}$.

The data on $A_{4,6}$ is quite reliable. We obtained

VI. CONCLUSION

The method of Monte Carlo integrations over configuration space seems to be a feasible approach to statistical mechanical problems which are as yet not analytically soluble. At least for a single-phase system a sample of several hundred particles seems sufficient. In the case of two-dimensional rigid spheres, runs made with 56 particles and with 224 particles agreed within statistical error. For a computing time of a few hours with presently available electronic computers, it seems possible to obtain the pressure for a given volume and temperature to an accuracy of a few percent.

In the case of two-dimensional rigid spheres our results are in agreement with the free volume approximation for $A/A_0<1.8$ and with a five-term virial expansion for $A/A_0>2.5$. There is no indication of a phase transition.

Metropolis et al (1953) 4/4

, 155704 (2011) PHYSICAL REVIEW LETTERS week 7 OCT

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

Etienne P. Bernard* and Werner Krauth†

oire de Physique Statistique Ecole Normale Supérieure, UPMC, CNRS 24 rue Lhomond, 75231 Paris Cedex 05

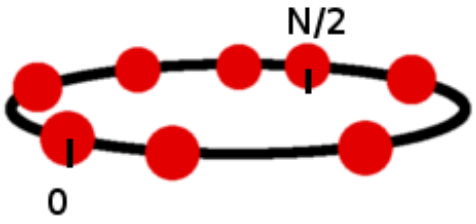
(Received 6 July 2011; published 7 October 2011)

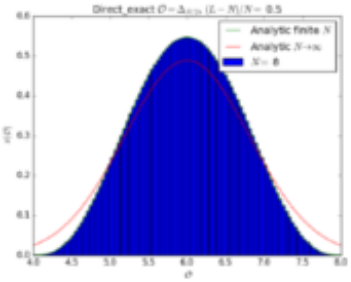
Melting in two spatial dimensions, as realized in thin films or at interfaces, represents one of the most fascinating phase transitions in nature, but it remains poorly understood. Even for the fundamental hard-disk model, the melting mechanism has not been agreed upon after 50 years of studies. A recent Monte Carlo algorithm allows us to thermalize systems large enough to access the thermodynamic regime. We show that melting in hard disks proceeds in two steps with a liquid phase, a hexatic phase, and a solid. The hexatic-solid transition is continuous while, surprisingly, the liquid-hexatic transition is of first order. This melting scenario solves one of the fundamental statistical-physics models, which is at the

- Event-chain algorithm (Bernard, Krauth, Wilson (2009))
- Beyond-Metropolis (Michel, Kapfer, Krauth (2014))
- Two-dimensional melting (Kapfer, Krauth (2014))
- Reduced dynamical scaling in Heisenberg spin systems (Nishikawa, Michel, Hukushima, Krauth (2015))

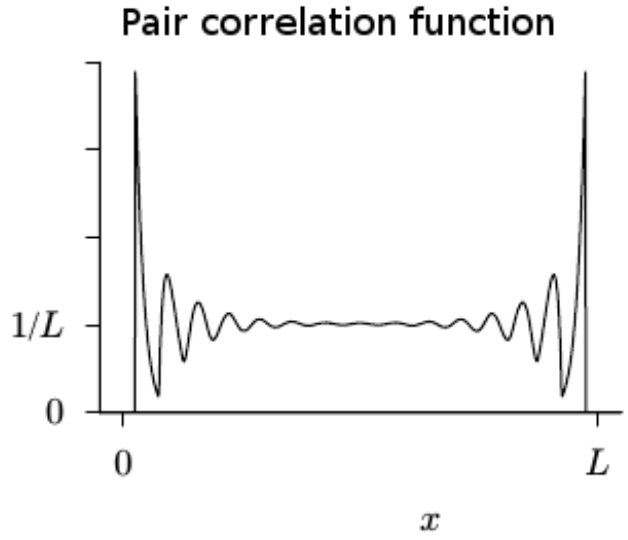
Département de Physique
École normale supérieure

One-dimensional hard spheres





Half-system distance



- N one-dimensional hard spheres of diameter $\sigma = 1$ (on interval of length L with periodic boundary conditions)
  - $L_{\text{free}} = L - N\sigma$, partition function $Z = (L_{\text{free}})^N$
  - $\ell_{\text{free}} = (L - N\sigma)/N$
- Non-trivial pair correlation function
- Half-system-distance distribution known exactly.

Département de Physique
École normale supérieure

Direct sampling

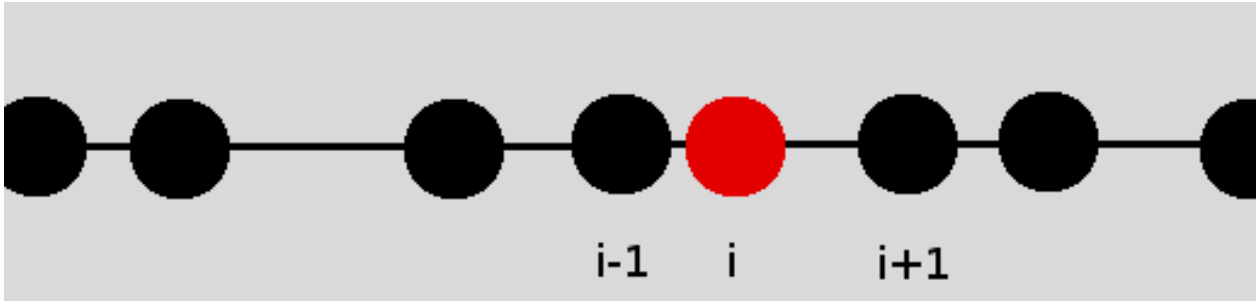
with L_{free} = free space, σ = sphere diameter:

procedure `direct-pin-circle`
for $k = 1, \ldots, N-1$ **do**
$\{\ \tilde{y}_k \leftarrow \texttt{ran}\,(0, L_{\text{free}})$
$\{y_1, \ldots, y_{N-1}\} \leftarrow \texttt{sort}[\{\tilde{y}_1, \ldots, \tilde{y}_{N-1}\}]$
$x_0 \leftarrow \texttt{ran}\,(0, L)$
for $k = 1, \ldots, N-1$ **do**
$\{\ x_k \leftarrow \texttt{mod}(x_0 + y_k + k\sigma, L)$
output $\{x_0, \ldots, x_{N-1}\}$

- Configurations at different densities through scaling with L_{free}

Département de Physique
École normale supérieure

Local heat bath algorithm, Metropolis



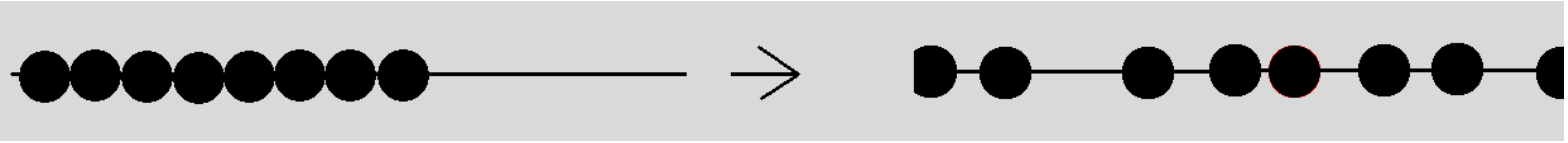
- Local heat bath algorithm: $x_i \to \text{ran}[x_{i-1} + \frac{\sigma}{2}, x_{i+1} - \frac{\sigma}{2}]$
- Local Metropolis: $x_i \to x_i + \text{ran}[-1, 1]$ (reject if overlap)
- Detailed balance:

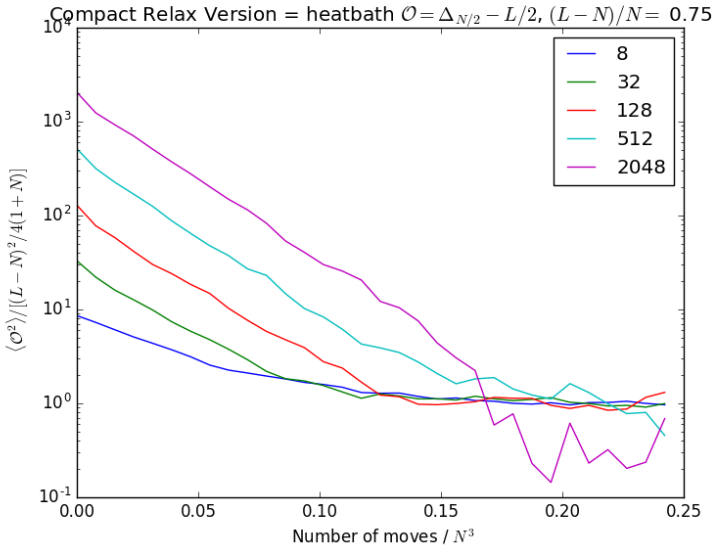
$$\pi_a p(a \to b) = \pi_b p(b \to a)$$

(satisfied if i sampled randomly)

Département de Physique
École normale supérieure

Compact relaxation, mixing (local heat bath)

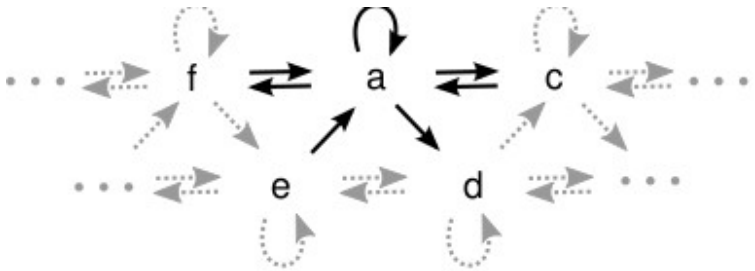




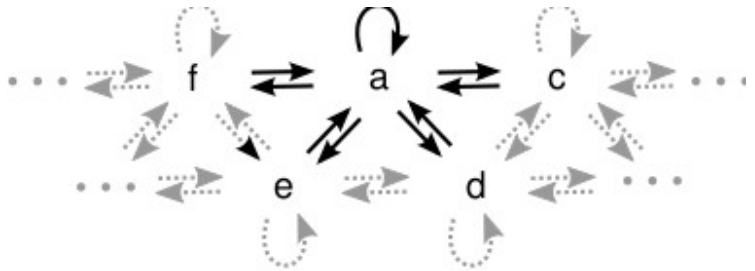
- Mixing time $N^3 \log N$ from compact relaxation.
- Randall & Winkler (2005): Mixing time $N^3 \log N$ or N^3.
- NB: Mixing time independent of density.

Département de Physique
École normale supérieure

Detailed balance and global balance



global balance



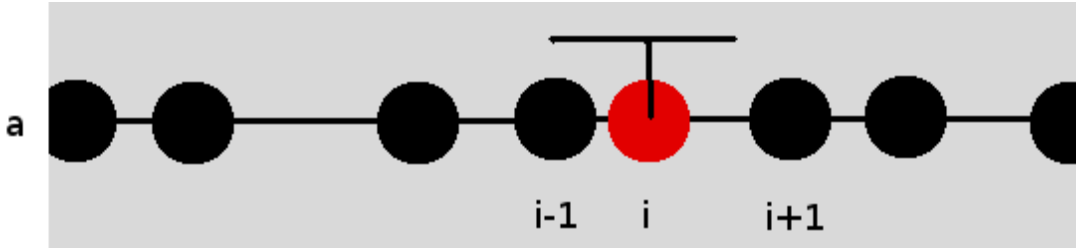
detailed balance

$$\pi_a p(a \to b) = \pi_b p(b \to a) \quad \text{detailed balance}$$

$$\sum_b \pi_b p(b \to a) = \pi_a \quad \text{global balance}$$

Département de Physique
École normale supérieure

Sequential Metropolis ('soft' breaking of detailed balance)



- Sequential Metropolis: Update $0, 1, 2, \ldots$
- This configuration, a (with i moving) can be reached:
  - from a, if the proposed move of i creates overlaps with $i-1$ or $i+1$.
  - from other configurations of i, by moving to a,
- the two contributions add up to 1 $\Longrightarrow$ global balance (because of underlying detailed balance)

1088 METROPOLIS, ROSENBLUTH, ROSENBLUTH, TELLER, AND TELLER

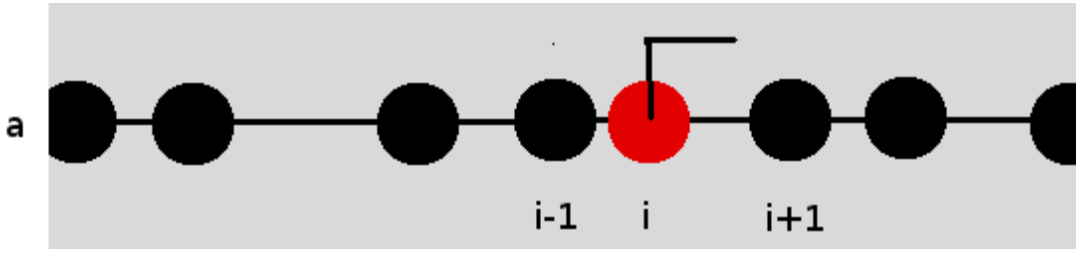
Our method in this respect is similar to the cell method except that our cells contain several hundred particles instead of one. One would think that such a sample would be quite adequate for describing any one-phase system. We do find, however, that in two-phase systems the surface between the phases makes quite a perturbation. Also, statistical fluctuations may be

configurations with a probability $\exp(-E/kT)$ and weight them evenly.

This we do as follows: We place the N particles in any configuration, for example, in a regular lattice. Then we move each of the particles in succession according to the following prescription:

Forward Metropolis

- Sequential Metropolis breaks the sequence of moves.
- Forward Metropolis instead breaks the symmetry of directions.

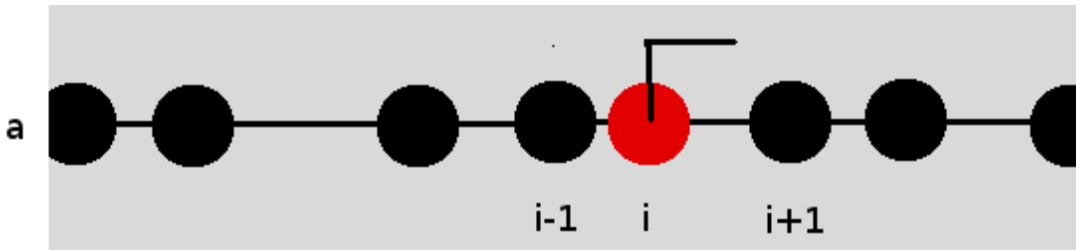


- Forward Metropolis: $x_i \to x_i + \text{ran}[0,1]$ (reject if overlap)
- This configuration, a, can be reached:
  - from a, if the move of $i-1$ is rejected by i.
  - from another position of i, if the proposed forward move is small.
- the two contributions (for all i) add up to 1 $\Longrightarrow$ global balance.

Département de Physique
École normale supérieure

Lifted Forward Metropolis (infinite chain)

- 'Lifted' Metropolis $\equiv$ sequential forward moves.
- cf. Diaconis et al (2000), Chen et al (1999)
- Move i forward until it is rejected by $i+1$.
- Then increment lifting variable $i \to i+1$.
- Move $i+1$ forward until it is rejected, etc.



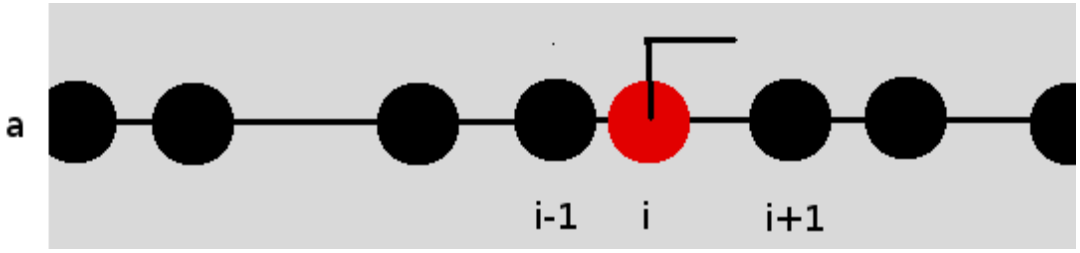
- This configuration, a, can be reached:
  - by a forward proposal of $i-1$ that goes too far and is rejected.
  - by a small forward move of i.
- the two contributions add up to 1 $\implies$ global balance.

This algorithm is asymmetric in displacements and asymmetric in particle labels

Département de Physique
École normale supérieure

Lifted Forward Metropolis (stochastic termination) 1/2

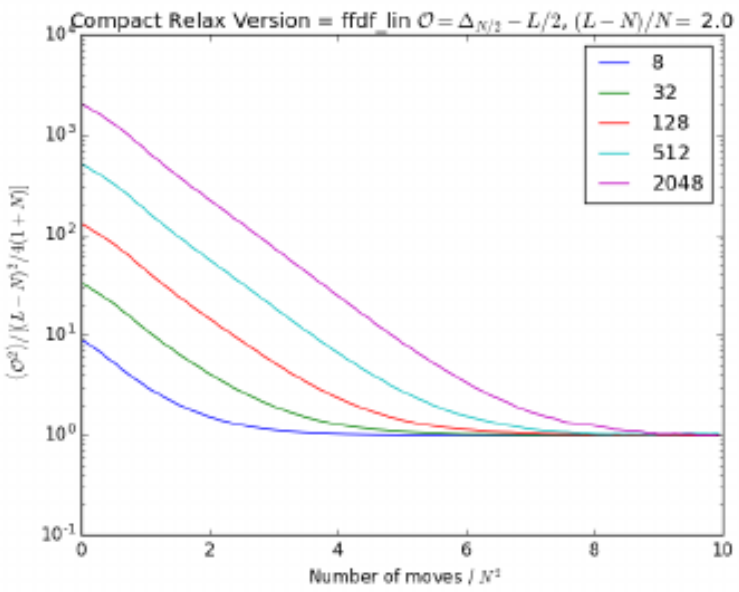
- sample starting disk
- sample chain length $\propto N$
- Then perform the lifted forward Metropolis algorithm

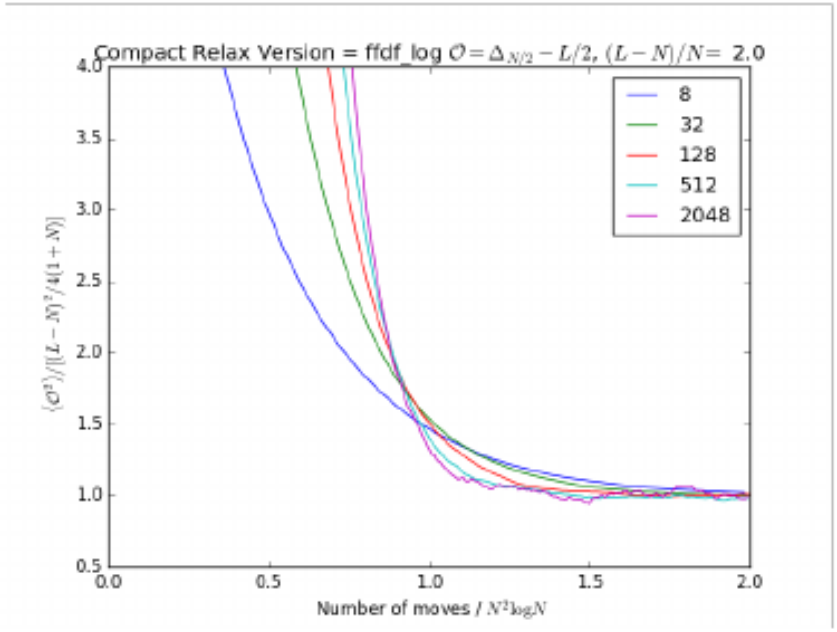


- Two variants:
  - Use a displacement vector $\in [0, 1]$ for the entire chain.
  - Sample a displacement vector for each move.
- Mixing in $N^2 \log N$ moves.

Lifted Forward Metropolis (stochastic termination) 2/2

- Mixing in $N^2 \log N$ moves
  - from compact relaxation
  - Observable: Variance of mid-system distance

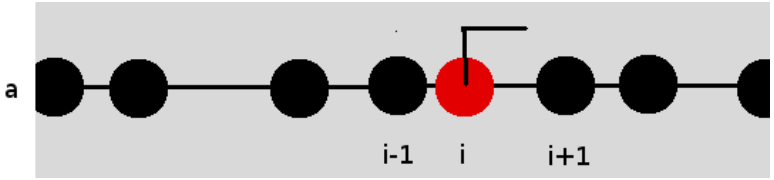




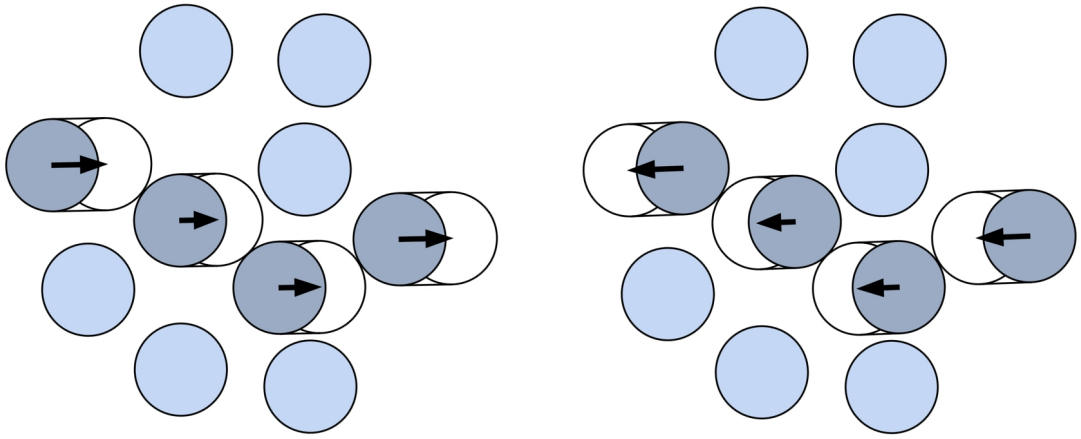
Département de Physique
École normale supérieure

Infinitesimal Lifted Forward Metropolis ≡ event-chain algorithm

- Lifted forward Metropolis algorithm, infinitesimal moves, stochastic termination.



- Mixing in $N^2 \log N$ liftings.
- This is the event-chain algorithm.



Département de Physique
École normale supérieure

Synopsis

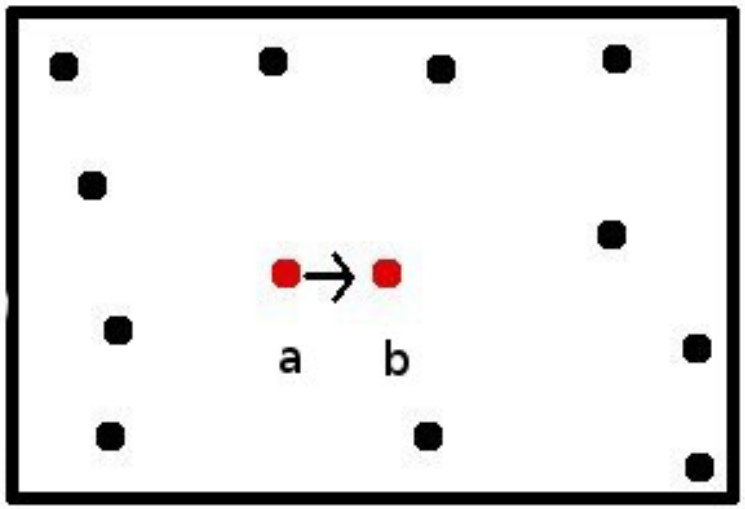
Algorithm	convergence	discrete analogue
Heatbath, Metropolis	$N^3 \log N$	Kawasaki
Forward Metropolis, Lifted (∞)	$N^{5/2}$	TASEP
Event-chain, Lifted (term)	$N^2 \log N$	lifted TASEP

- For Heatbath convergence cf Randall & Winkler (2005)
- For TASEP convergence cf Baik & Liu (2016)
- All others cf Kapfer & Krauth (2017, soon)

Département de Physique
École normale supérieure

Factorized filter 1/2

- $p^{\text{fact}}(a \to b) = \prod_{i<j} \min\left[1, \exp(-\beta(E_{ij}^b - E_{ij}^a))\right]$

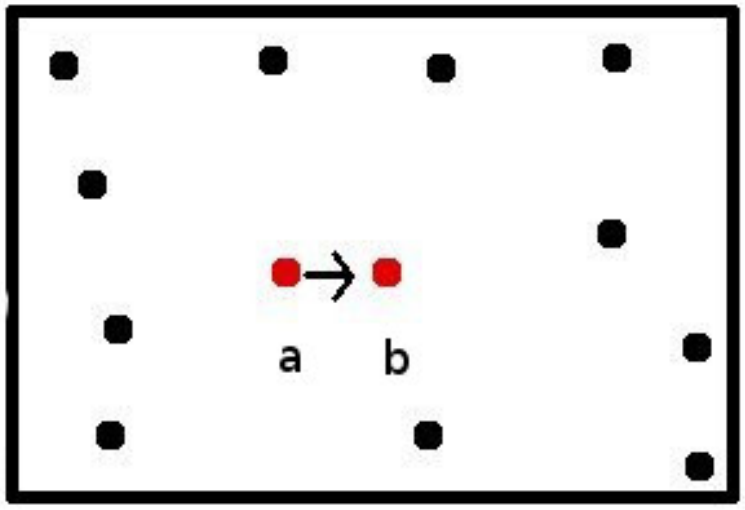


- pair-energy based.
- satisfies detailed balance.
- Michel, Kapfer, Krauth (2014).

Département de Physique
École normale supérieure

Factorized filter 2/2

- $p^{\text{fact}}(a \to b) = \prod_{i<j} \underbrace{\min\left[1, \exp(-\beta(E_{ij}^b - E_{ij}^a))\right]}_{p_{ij}^{\text{accept}}}$



- consensus based (European union).
- satisfies global balance.
- Michel, Kapfer, Krauth (2014).

Département de Physique
École normale supérieure

Beyond-Metropolis paradigm

"Metropolis" paradigm
(Metropolis et al, 1953)

- **Detailed balance**
  vanishing probability flows
- **Metropolis algorithm**
  energy driven
- **Rejections**
  finite random moves

"Beyond-Metropolis" paradigm
(Michel , Kapfer & Krauth, 2014)

- **Global balance**
  steady-state probability flows
- **Factorized Metropolis algorithm**
  consensus driven
- **Liftings**
  infinitesimal persistent moves

Département de Physique
École normale supérieure

Conclusions

- There has always been more to MCMC than reversible Markov chains.
- One-dimensional particle systems provide clear picture.

Algorithm	mixing	discrete analogue
Heatbath, Metropolis	$N^3 \log N$	Kawasaki
Forward Metropolis, Lifted (∞)	$N^{5/2}$	TASEP
Event-chain, Lifted (term)	$N^2 \log N$	lifted TASEP

- for further details:
  - on one-dimensional asymmetric Markov chains, including TASEP and lifted TASEP, shocks
  - on Beyond-Metropolis algorithms and applications,

cf Kapfer & Krauth
arXiv201705XXXX and arXiv201705XXXX ;)

Département de Physique
École normale supérieure