Markov-chain Monte Carlo: A modern primer 1/2

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B. Li, Y. Nishikawa, P. Höllmer, L. Carillo, A. C. Maggs, W. Krauth; arXiv 202205XXXX
Hard-disk computer simulations—a historic perspective

W. Krauth; Front. Phys. (2021)
Event-Chain Monte Carlo: Foundations, Applications, and Prospects

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Metropolis et al. (1953) (1/5)

URNAL OF CHEMICAL PHYSICS VOLUME 21, NUMBER 6 JUN

Equation of State Calculations by Fast Computing Machines

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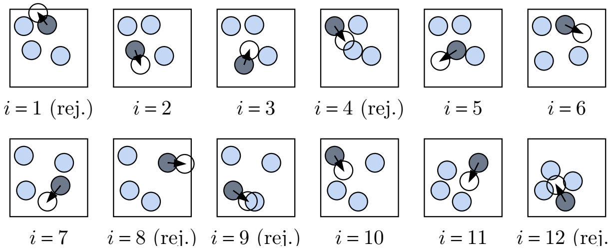
(Received March 6, 1953)

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) (2/5)



Metropolis et al. (1953) (3/5)

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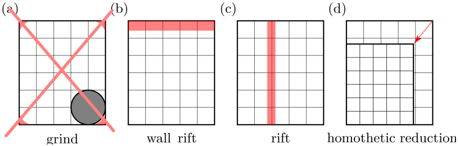
- EoS $\supset$ isotherm $\equiv P(V)$



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Translation of terms

- Disks in box $\rightarrow$ sample space Ω.
- Moves $\rightarrow$ Markov chain: Sequence of random variables $(X_0, X_1, \dots)$ where X_0 represents the initial distribution and X_{t+1} depends on X_t through a transition matrix P.
- A priori probability$\rightarrow$ split matrix: $P_{ij} = \mathcal{A}_{ij}\mathcal{P}_{ij}$ for $i \neq j$
  $\mathcal{A} \Leftrightarrow$ a priori probability; $\mathcal{P} \Leftrightarrow$ filter
  Examples: Metropolis filter, heatbath filter.
- Monte Carlo rejections $\rightarrow$ $P_{ii} \Leftrightarrow$ (filter) rejection probability.
  NB: Modern MCMC algorithms often have no rejections.

NB: Double role of P:

1. For probability distributions: $\pi^{\{t+1\}} = \pi^{\{t\}} P$ (with $\pi^{\{t\}}, \pi^{\{t+1\}}$ non-explicit objects, often even for $t \rightarrow \infty$).
2. For samples i, j: P_{ij}: explicit probability to move from i to j.

Irreducibility

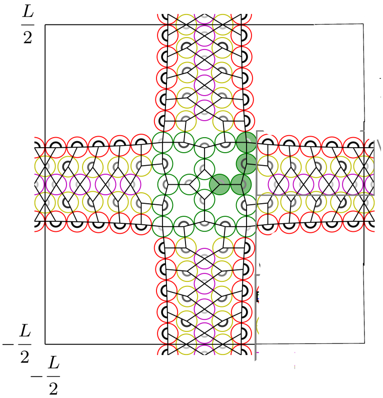
- P irreducible $\Leftrightarrow$ any i can be reached from any j.
- $\pi^{\{0\}}$: Initial probability (explicit, user-supplied). Often concentrated on a single sample $x \in \Omega$.
- P irreducible $\Rightarrow$ unique stationary distribution π with

$$\pi_i = \sum_{j \in \Omega} \pi_j P_{ji} \quad \forall i \in \Omega.$$

NB: Transition matrix P is stochastic, that is, $\sum_j P_{ij} = 1$.

Irreducibility of hard-disk problem

Is the Metropolis algorithm for hard disks irreducible?
Rather not ...



Hoellmer et al. (2022), following Böröczky (1964)

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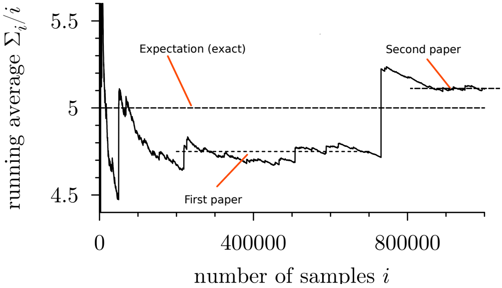
Ergodic theorem

- P irreducible $\Rightarrow \pi$ unique, but maybe $\pi^{\{t\}} \not\to \pi$ for $t \to \infty$.
- P irreducible $\Rightarrow$ Ergodic theorem $(\mathbb{E}(\mathcal{O}) := \sum_{i\in\Omega} \mathcal{O}_i \pi_i)$:

$$\mathbb{P}_{\pi^{\{0\}}}\left[\lim_{t\to\infty} \frac{1}{t} \sum_{i_t} \mathcal{O}(i_t) = \mathbb{E}(\mathcal{O})\right] = 1$$

(Strong law of large numbers for running average)



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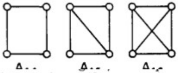
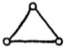
Metropolis et al. (1953) (4/5)



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

$$A_{3,3}=\frac{1}{\pi^2 d^4}\int\cdots\int dx_1dx_2dx_3dy_1dy_2dy_3(f_{12}f_{23}f_{31}).$$

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 $A_{5,5}$.

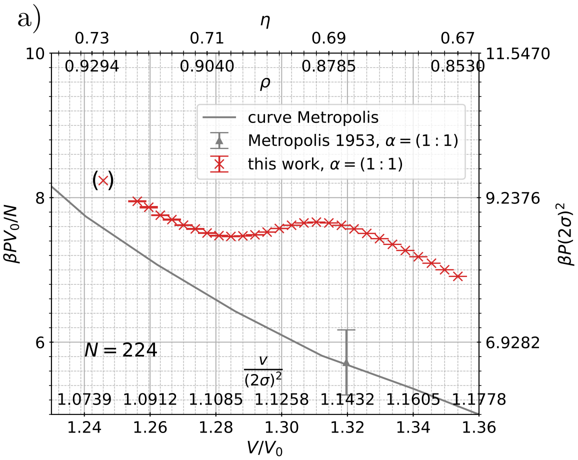
The data on $A_{4,6}$ is quite reliable. We obtained

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.

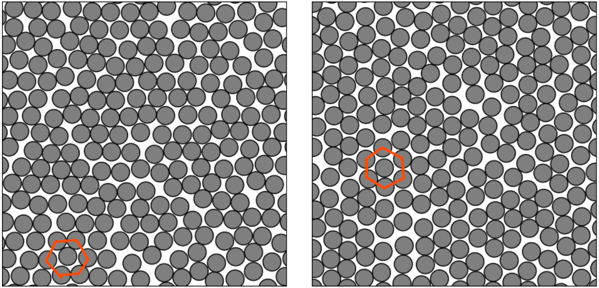
Metropolis et al. (1953) (5/5)



- Li et al. (2022)

‘Base’ and ‘tip’ configurations

$N = 224$ in square box (NB: $224 = 16 \times 14$) with $16\sqrt{3}/2 \simeq 14$.



$$\Psi_6 = \frac{1}{N} \sum_l \frac{1}{\mathrm{nbr}(l)} \sum_{j=1}^{\mathrm{nbr}(l)} \exp\left(6 i \phi_{lj}\right),$$

NB: $\mathbb{E}\left(\Psi_6\right) = (0, 0)$ (Ergodic theorem as a diagnostic tool).

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Alder–Wainwright (1962) (1/4)

PHYSICAL REVIEW VOLUME 127, NUMBER 2 JULY 15, 1962

Phase Transition in Elastic Disks*

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University of California, Lawrence Radiation Laboratory, Livermore, California

(Received October 30, 1961)

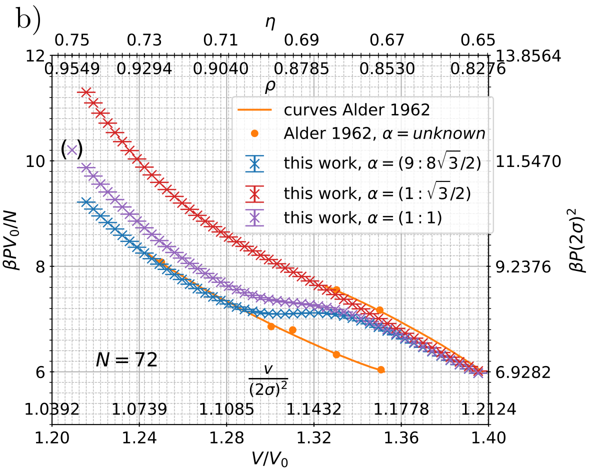
The study of a two-dimensional system consisting of 870 hard-disk particles in the phase-transition region has shown that the isotherm has a van der Waals-like loop. The density change across the transition is about 4% and the corresponding entropy change is small.

A STUDY has been made of a two-dimensional system consisting of 870 hard-disk particles. Simultaneous motions of the particles have been calculated by means of an electronic computer as described previously.[1] The disks were again placed in a periodically repeated rectangular array. The computer program

interchanges it was not possible to average the two branches.

Two-dimensional systems were then studied, since the number of particles required to form clusters of particles of one phase of any given diameter is less than in three dimensions. Thus, an 870 hard-disk system is

Alder–Wainwright (1962) (2/4)



- Li et al. (2022)

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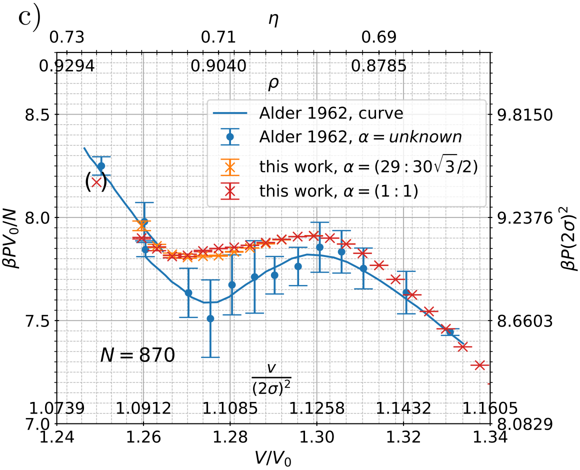
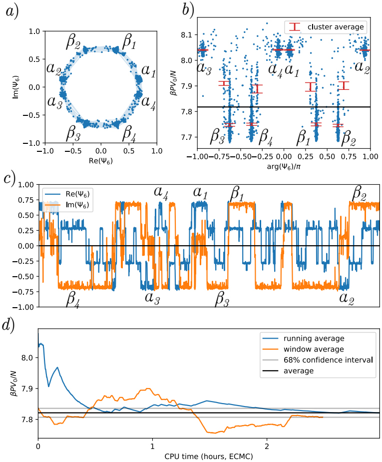
Alder–Wainwright (1962) (3/4)



- Li et al. (2022)

Alder–Wainwright (1962) (4/4)



NB: Hours of 2022 CPU time (ECMC algorithm) to equilibrate 870 disks in a box.

- Li et al. (2022)

Probability flows

- Uniqueness of $\pi \Rightarrow$ balance condition on P:

$$\pi_i = \sum_{j\in\Omega} \pi_j P_{ji} \quad \forall i \in \Omega.$$

- 'flow' from j to $i \Leftrightarrow$ weight of j $\times$ probability to move from j to i:

$$\mathcal{F}_{ji} \equiv \pi_j P_{ji} \quad \Leftrightarrow \pi_i = \overbrace{\sum_{j\in\Omega} \mathcal{F}_{ji}}^{\text{flows entering } i} \quad \forall i \in \Omega,$$

$$\mathcal{F}_{ji} \equiv \pi_j P_{ji} \quad \Leftrightarrow \overbrace{\sum_{k\in\Omega} \mathcal{F}_{ik}}^{\text{flows exiting } i} = \overbrace{\sum_{j\in\Omega} \mathcal{F}_{ji}}^{\text{flows entering } i} \quad \forall i \in \Omega,$$

(NB: stochasticity condition used $\sum_{k\in\Omega} P_{ik} = 1$).

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Reversibility

- Reversible P satisfies the 'detailed-balance' condition:

$$\underbrace{\pi_i P_{ij}}_{\mathcal{F}_{ij}} = \underbrace{\pi_j P_{ji}}_{\mathcal{F}_{ji}} \quad \forall i, j \in \Omega.$$

- General P satisfies 'global-balance' condition

$$\pi_i = \sum_{j \in \Omega} \pi_j P_{ji} \quad \forall i \in \Omega.$$

- Detailed balance implies global balance.
- Global balance:

$$\overbrace{\sum_{k \in \Omega} \mathcal{F}_{ik}}^{\text{flows exiting } i} = \overbrace{\sum_{j \in \Omega} \mathcal{F}_{ji}}^{\text{flows entering } i} \qquad \forall i \in \Omega,$$

- DBC more restrictive, but far easier to check than GBC.

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Spectrum of reversible transition matrix

- Reversible P:

$$\pi_i P_{ij} = \pi_j P_{ji} \quad \forall i, j \in \Omega.$$

- Reversible P: $A_{ij} = \pi_i^{1/2} P_{ij} \pi_j^{-1/2}$ is symmetric.
- Reversible P:

$$\sum_{j \in \Omega} \underbrace{\pi_i^{1/2} P_{ij} \pi_j^{-1/2}}_{A_{ij}} x_j = \lambda x_i \Leftrightarrow \sum_{j \in \Omega} P_{ij} \left[\pi_j^{-1/2} x_j \right] = \lambda \left[\pi_i^{-1/2} x_i \right].$$

- P and A have same eigenvalues.
- A symmetric: (Spectral theorem): All eigenvalues real, can expand on eigenvectors.
- Irreducible, aperiodic: Single eigenvalue with $\lambda = 1$, all others smaller in absolute value.

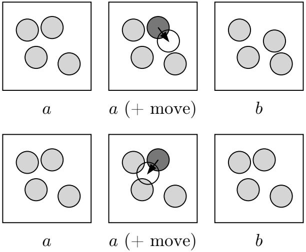
Classes for non-reversible transition matrix

Non-reversible P can be 'unhappy' in different ways:

- P can be non-reversible, real eigenvalues, eigenvectors non-orthogonal.
- P can be non-reversible, real eigenvalues: Non-diagonalizable. (algebraic multiplicity $\neq$ geometric multiplicity).
- P can be non-reversible, pairs of complex eigenvalues.
- Most common case: Complex eigenvalues.
- For simple examples, see Weber (2017)

Metropolis algorithm / reversibility

1. The Metropolis et al. algorithm is reversible.



2. The algorithm used by Metropolis et al. is non-reversible.

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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:

Total variation distance, mixing time

- Total variation distance:

$$||\pi^{\{t\}} - \pi||_{\text{TV}} = \max_{A \subset \Omega} |\pi^{\{t\}}(A) - \pi(A)| = \frac{1}{2} \sum_{i \in \Omega} |\pi_i^{\{t\}} - \pi_i|.$$

- (Above) first eq.: definition; second eq.: (tiny) theorem
- Distance:

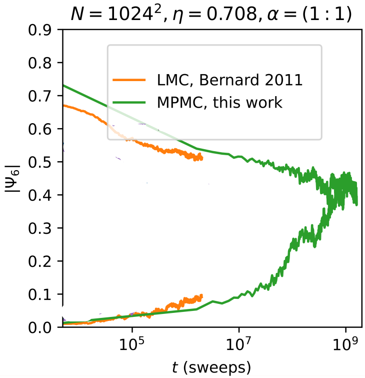
$$d(t) = \max_{\pi^{\{0\}}} ||\pi^{\{t\}}(\pi^{\{0\}}) - \pi||_{\text{TV}}$$

- Mixing time:

$$t_{\text{mix}}(\epsilon) = \min\{t : d(t) \leq \epsilon\}$$

- Usually $\epsilon = 1/4$ is taken (arbitrary, must be smaller than $\frac{1}{2}$): $t_{\text{mix}} = t_{\text{mix}}(1/4)$

Mixing time (poor man's)



- Metropolis algorithm on a sequential CPU $\simeq 10^{10}$ moves/hour
- 1 sweep $\simeq 10^6$ moves
- $10^{9+6-10}/24/365 \simeq 11.4$ years.
- Li et al. (2022, mod)

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Conductance (bottleneck ratio)

$$\Phi \equiv \min_{S\subset\Omega,\pi_S\leq\frac{1}{2}} \frac{\mathcal{F}_{S\to\overline{S}}}{\pi_S} = \min_{S\subset\Omega,\pi_S\leq\frac{1}{2}} \frac{\sum_{i\in S,j\notin S}\pi_i P_{ij}}{\pi_S}.$$

- Reversible Markov chains:

$$\frac{1}{\Phi} \leq \tau_{\text{corr}} \leq \frac{8}{\Phi^2}$$

('$\leq$': Sinclair & Jerrum (1986), Lemma (3.3))

- Arbitrary Markov chain (see Chen et al. (1999)):

$$\frac{1}{4\Phi} \leq \mathcal{A} \leq \frac{20}{\Phi^2},$$

(set time: Expectation of $\max_S (t_S \times \pi_S)$ from equilibrium)

NB: One bottleneck, not many. Lower and upper bound.

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Lifting (Chen et al. (1999)) (1/2)

- Markov chain $\Pi \Leftrightarrow$ Lifted Markov chain $\hat{\Pi}$
- $\Omega \ni v$ (sample space) $\Leftrightarrow \hat{\Omega} \ni i$ (lifted sample space)
- P (transition matrix) $\Leftrightarrow \hat{P}$ (lifted transition matrix)
- π_v (stationary probability) $\Leftrightarrow \hat{\pi}_i$
- **Condition 1**: sample space is copied ('lifted'), π preserved

$$\pi_v = \hat{\pi}\left[f^{-1}(v)\right] = \sum_{i \in f^{-1}(v)} \hat{\pi}_i,$$

- **Condition 2**: flows are preserved

$$\underbrace{\pi_v P_{vu}}_{\text{collapsed flow}} = \sum_{i \in f^{-1}(v), j \in f^{-1}(u)} \overbrace{\hat{\pi}_i \hat{P}_{ij}}^{\text{lifted flow}} .$$

- Usually: $\hat{\Omega} = \Omega \times \mathcal{L}$, with $\mathcal{L}$ a set of lifting variables σ

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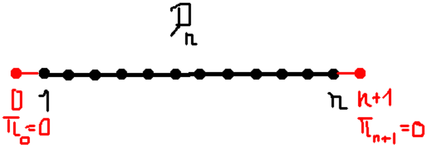
Lifting (Chen et al. (1999)) (2/2)

- Required: Mapping from $\hat{\Omega}$ (lifted sample space) to Ω that preserves stationary probability distribution.
- Required: Lifted transition matrix $\hat{P}$ that preserves flow.
- Optional: $\hat{\Omega} = \Omega \times \mathcal{L}$ (with $\mathcal{L}$: set of lifting variables).
- Optional:

$$\frac{\hat{\pi}(u,\sigma)}{\pi(u)} = \frac{\hat{\pi}(v,\sigma)}{\pi(v)} \quad \forall\ u, v \in \Omega; \forall\ \sigma \in \mathcal{L}. \tag{1}$$

- There are many liftings $\hat{P}$ for a given lifted sample space $\hat{\Omega}$.
- Liftings are popular for transfering parts of the moves into the sample space.
- Lifting do not increase conductance.

Metropolis algorithm on path graph (1/4)



- Path graph $\mathcal{P}_n$ so that $\Omega_n = \{1, \ldots, n\}$.
- Phantom vertices and edges.

Metropolis algorithm (NB: $P_{ij} = \mathcal{A}_{ij}\mathcal{P}_{ij}$ for $i \neq j$):

1. Move set $\mathcal{L} = \{+, -\}$.
2. $\mathcal{A}$ flat $\rightarrow \sigma = \text{choice}(\mathcal{L})$.
3. Metropolis filter: Accept with probability $\min(1, \pi_j/\pi_i)$.

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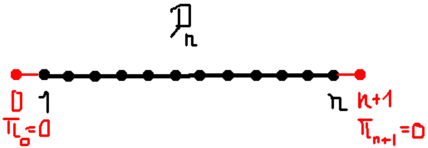
Metropolis algorithm on path graph (2/4)



- Detailed balance:

$$\underbrace{\pi_i P_{ij}}_{\mathcal{F}_{ij}} = \underbrace{\pi_j P_{ji}}_{\mathcal{F}_{ji}}$$

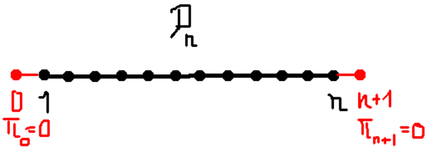
- Metropolis algorithm:

$$\mathcal{F}_{ij} = \frac{1}{2}\min(\pi_i, \pi_j) \Leftrightarrow P_{ij} = \frac{1}{2}\min(1, \pi_j/\pi_i)$$

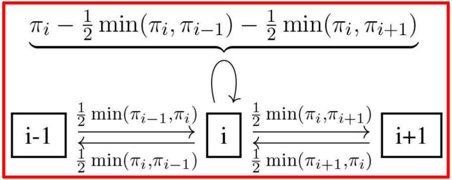
- Metropolis filter (NB: $P_{ij} = \mathcal{A}_{ij}\mathcal{P}_{ij}$):

$$\mathcal{P}_{ij} = \min(1, \pi_j/\pi_i)$$

Metropolis algorithm on path graph (3/4)

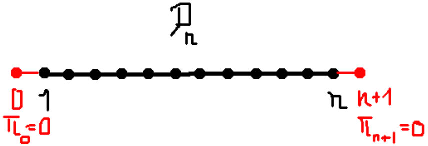


- Global balance ($\pi_i = \sum_j \pi_j P_{ji} = \sum_j \mathcal{F}_{ji}$):



- Irreducibility OK if no holes in π.
- Aperiodicity OK, thanks to boundaries

Metropolis algorithm on path graph (4/4)



procedure metro-path
input x
$\sigma \leftarrow \texttt{choice}(\mathcal{L})\ (\mathcal{L} = \{-1, +1\})$
if $(\texttt{ran}\,(0,1) < \pi_{x+\sigma}/\pi_x)$ **then**
$\quad \{\, x_i \leftarrow x_i + \sigma$
output x

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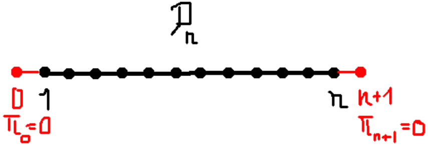
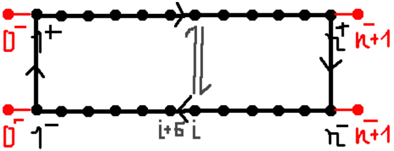
Lifting on the path graph (1/4)

General probability distribution $\pi = (\pi_1, \dots, \pi_n)$

- 'Collapsed' Markov chain:



- 'Lifted' Markov chain $\hat{\Omega} = \Omega \times \{-, +\}$:



- Replace all rejections by lifting moves.
- Diaconis et al. (2000)

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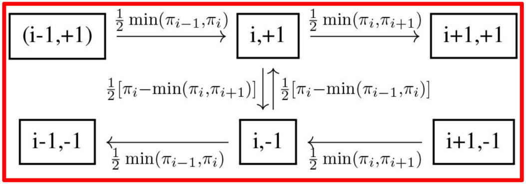
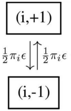
Lifting on the path graph (2/4)

- 'Lifted Markov chain: Transport'



NB: The $\frac{1}{2} \Leftrightarrow \hat{\pi}_{i,\sigma} = \frac{1}{2}\pi_i$

- 'Lifted Markov chain: Resampling'



- Resampling can often be dropped

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Lifting on the path graph (3/4)

- Transport

procedure transport-path
input $\{x, \sigma\}$ (configuration $\in \hat{\Omega} = \Omega \times \{+, -\}$)
if $(\text{ran}(0,1) < \pi_{x+\sigma}/\pi_x)$ **then**
  $\{ x_i \leftarrow x_i + \sigma$
else
  $\{ \sigma \leftarrow -\sigma$
output $\{x, \sigma\}$
———

- Resampling

procedure resample-path
input $\{x, \sigma\}$ (configuration $\in \hat{\Omega} = \Omega \times \{+, -\}$)
if $(\text{ran}(0,1) < p)$ **then** (p: resampling rate)
  $\{ \sigma \leftarrow -\sigma$
output $\{x, \sigma\}$
———

- Mix freely!

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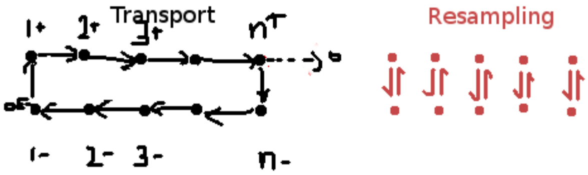
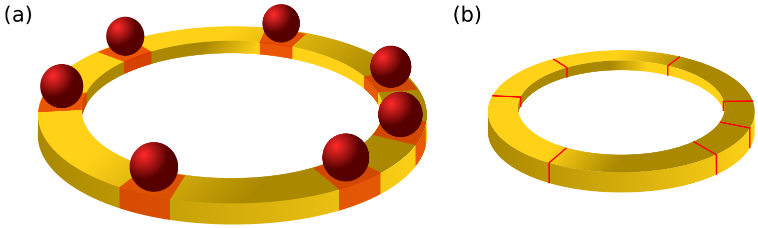
Lifting on the path graph (4/4)



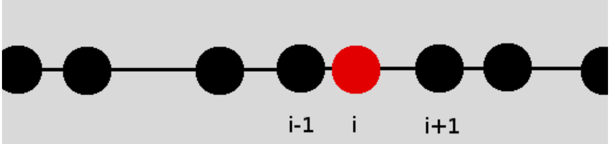
Model	Conductance	t_{mix} (collapsed)	t_{mix} (lifted)
Flat	$\mathcal{O}\left(1/n\right)$	$\mathcal{O}\left(n^2\right)$	$\mathcal{O}\left(n\right)$
Square	$\mathcal{O}\left(1/n\right)$	$\mathcal{O}\left(n^2\right)$	$\mathcal{O}\left(n^2\right)$
V-shape	$\mathcal{O}\left(1/n^2\right)$	$\mathcal{O}\left(n^2 \log n\right)$	$\mathcal{O}\left(n^2\right)$

1d hard spheres with periodic boundary conditions



- N spheres, diameter σ, interval L, $\pi(a) = 1 \quad \forall a$
- N spheres, diameter 0, interval $L - N\sigma$.

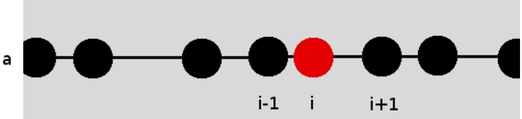
Reversible Metropolis algorithm, 1d (detailed balance)



- Local Metropolis: $x_i \to x_i \pm \epsilon$ (reject if overlap, $\epsilon > 0$)
- Detailed balance:

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

Sequential Metropolis algorithm, 1d (global balance)



- Sequential Metropolis: Update 0, then 1, then 2, . . .
- Global balance:

$$\mathcal{F}_a^{\text{seq}} = \frac{1}{2}\left(\mathcal{A}_i^+ + \mathcal{R}_i^+ + \mathcal{A}_i^- + \mathcal{R}_i^-\right) = 1.$$

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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:

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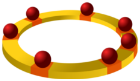
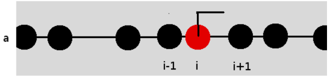
Forward Metropolis algorithm, 1d (global balance)

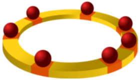


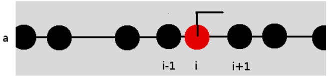


- Forward Metropolis: $x_i \to x_i + \epsilon$ (reject if overlap, $\epsilon > 0$)
- $$\mathcal{F}_a^{\text{forw}} = \frac{1}{N} \sum_i \underbrace{\left(\mathcal{A}_i^+ + \mathcal{R}_{i-1}^+\right)}_{=1 \text{ for any } \epsilon} = 1,$$

Lifted Forward Metropolis algorithm, 1d (global balance)

- Move i forward until it is rejected by $i+1$.
- Then move $i+1$ forward until it is rejected, etc.





- $\mathcal{F}^{\text{lift}}_{(a,i)} = \mathcal{A}^{+}_{i} + \mathcal{R}^{+}_{i-1} = 1.$
- NB: 1 time step: 1 particle move OR 1 lifting move.
- Infinitesimal $\epsilon \to 0$ version: Event-chain algorithm.

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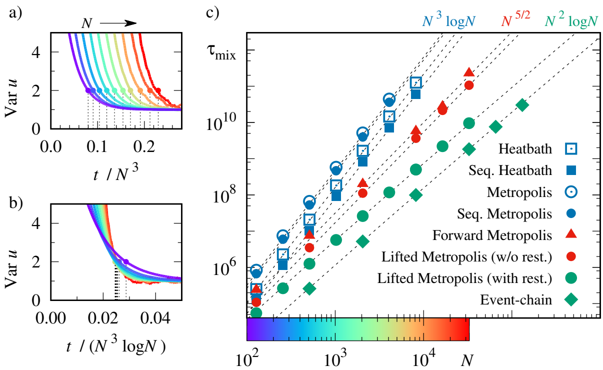
Synopsis (Non-reversible Markov chains in 1d)



Algorithm	mixing	discrete analogue
Rev. Metropolis	$N^3 \log N$	Symmetric SEP
Forward Metropolis, Lifted (∞)	$N^{5/2}$	TASEP
Event-chain, Lifted (restarts)	$N^2 \log N$	lifted TASEP

- Kapfer—Krauth (2017)

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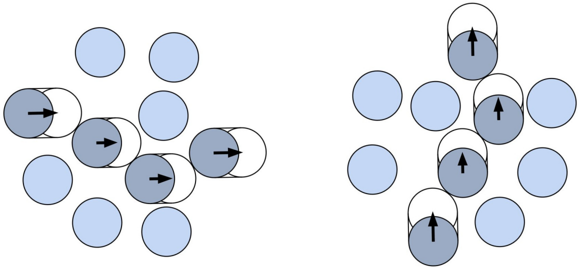
Higher-dimensional variant: event-chain algorithm



- Bernard, Krauth, Wilson (2009).
- Infinitesimal moves: No multiple overlaps, consensus.
- Michel, Kapfer, Krauth (2014) (smooth potentials).
- Many variants.

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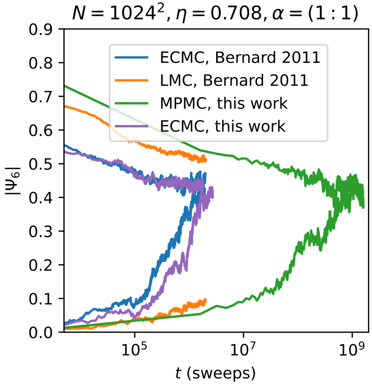
ECMC and the hard-disk model



- $10^{9+6-10}/24/365 = 11.4$ years
- $10^{6+6-10}/24 = 4.2$ days
- Li et al. (2022)

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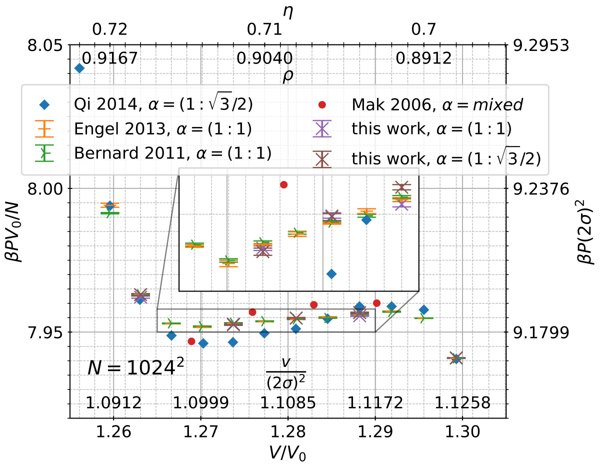
Synopsis large hard-disk system



- Li et al. (2022)

NB: Pressures are required precisely for further analysis.

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Conclusions (1/3)

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Equation of State Calculations by Fast Computing Machines

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(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.

- EoS $\supset$ isotherm $\equiv P(V)$
- Pressure unambiguous, even at finite N.

Conclusions (2/3)

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Equation of State Calculations by Fast Computing Machines

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- ‘vast subject...’

Conclusions (3/3)

We discussed:

- Markov chains, a priori probabilities, filters.
- Transition matrix P, and its double role.
- Irreducibility.
- Ergodic theorem, and its use as a diagostic tool.
- Flows and balance conditions.
- Reversibility, non-reversibility.
- Classes of non-reversible transition matrices.
- Total variation distances.
- Mixing times.
- Lifted Markov chains.