Mixing, stopping, coupling, lifting, and other keys to the second Markov-chain revolution

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Plan of talk

1. Introduction (+ Example I)
2. Mixing and Relaxing (+ Example II)
3. Stopping and Coupling (+ Example III)
4. Equilibrium out of Equilibrium (+ Example IV)
5. Conclusion

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Markov chains (1/2)

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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

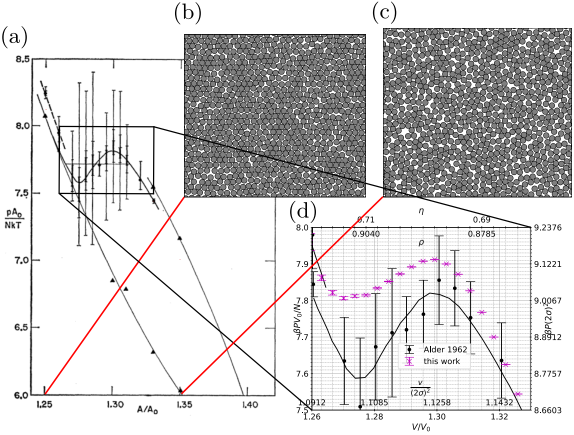
AND

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.

Example I: Equilibrated (?) samples



- Original figure from Alder & Wainwright 1962, see Li et al. (2022)

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Markov chains (2/2)

- Sample space Ω (e.g. hard disks, water molecules, quarks, ...)
- Markov chain ← Sequence of random variables
  $(X_0 \sim \pi^{\{0\}}, X_1 \sim \pi^{\{1\}}, X_2 \sim \pi^{\{2\}} \ldots)$
  X_{t+1} depends only on X_t, t is a 'time'
- Transition matrix P:
  - P_{ij}: conditional probability to move from sample i to sample j.
  - $\pi^{\{t+1\}} = \pi^{\{t\}} P$: Evolve probability distribution at time t to probability distribution at time $t+1$ (with $\pi^{\{t\}}, t > 0$ often non-explicit,even for $t \to \infty$).
- Move set $\mathcal{L}$: ... from which moves are sampled.
- Equilibrium distribution π: Satisfies global balance:

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

  NB: P irreducible $\implies$ π unique.
- Aperiodicity: Absence of cycles. P irreducible and aperiodic:

$$\pi^{\{t\}} \to \pi \quad \text{for } t \to \infty$$

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Total variation distance, mixing time

- Total variation distance:

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

- 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, $\epsilon = 1/e$ would be better.

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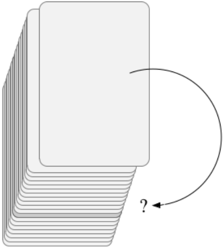
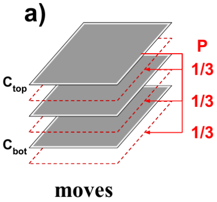
Shuffling of cards 1/5



- $\Omega_N^{\text{shuffle}} = \{\text{Permutations of } \{1, \ldots, N\}\}$
- For $N = 3$:
  $\Omega_3^{\text{shuffle}} = \{1 \equiv \{1,2,3\}, 2 \equiv \{1,3,2\}, 3 \equiv \{2,1,3\}, 4 \equiv \{2,3,1\}, 5 \equiv \{3,1,2\}, 6 \equiv \{3,2,1\}\}$.
- $\pi^{t=0} = \delta((1, , \ldots, N))$

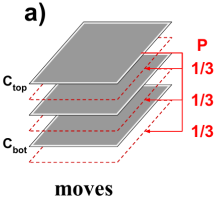
Shuffling of cards 2/5



procedure top-to-random
input $\{c_1, \ldots, c_n\}$
$i \leftarrow \texttt{choice}(\{1, \ldots, n\})$
$\{\hat{c}_1, \ldots, \hat{c}_n\} \leftarrow \{c_2, \ldots, c_i, c_1, c_{i+1}, \ldots, c_n\}$
output $\{\hat{c}_1, \ldots, \hat{c}_n\}$

- Insert upper card (c_1) after card i and before card $i + 1$
- NB: if $i = 1$, put it back on top.

Shuffling of cards 3/5



- $\Omega_3^{\text{shuffle}} = \{1 \equiv \{1,2,3\}, 2 \equiv \{1,3,2\}, 3 \equiv \{2,1,3\}, 4 \equiv \{2,3,1\}, 5 \equiv \{3,1,2\}, 6 \equiv \{3,2,1\}\}$.
- $$P = \frac{1}{3}\begin{pmatrix} 1 & 0 & 1 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 1 \\ 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 1 & 0 & 1 \end{pmatrix}$$

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Shuffling of cards 4/5

- $$P_3^{\text{shuffle}} = \frac{1}{3}\begin{pmatrix} 1 & 0 & 1 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 1 \\ 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 1 & 0 & 1 \end{pmatrix}$$
- Eigenvalues of P_N^{shuffle}: $0, \frac{1}{N}, \frac{2}{N}, \ldots, 1 - \frac{2}{N}, 1$
- Degeneracies:

$$N = 2 : [1, 0, 1]$$
$$N = 3 : [2, 3, 0, 1]$$
$$N = 4 : [9, 8, 6, 0, 1]$$
$$N = 5 : [44, 45, 20, 10, 0, 1]$$
$$N = 6 : [265, 264, 135, 40, 15, 0, 1]$$
$$N = 7 : [1854, 1855, 924, 315, 70, 21, 0, 1]$$

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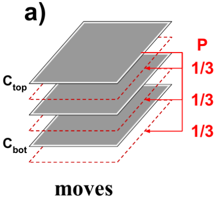
Shuffling of cards 5/5



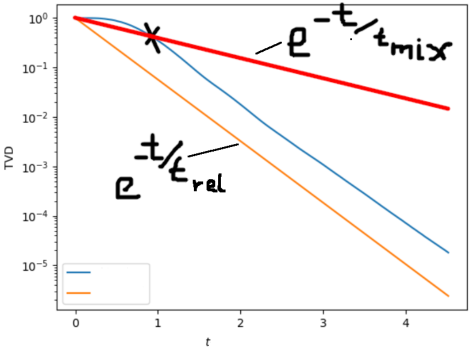
procedure `top2random-stop`
input $\{c_1, \ldots, c_n\}$
$c_{\text{first-n}} \leftarrow c_{\text{n}}$
for $t = 1, 2, \ldots$ **do**

$$\begin{cases} \tilde{c}_1 \leftarrow c_1 \\ \{c_1, \ldots, c_n\} \leftarrow \texttt{top2random}(\{c_1, \ldots, c_n\}) \\ \textbf{if } (\tilde{c}_1 = c_{\text{first-n}}) \ \textbf{break} \end{cases}$$

output $\{c_1, \ldots, c_n, t\}$

- Expected running time: $n \log n$.
- Time scale $n \log n$ larger than inverse gap $n/2$.

Mixing and Relaxation



- $t_{\text{mix}} = ||\pi^{\{t_{\text{mix}}\}} - \pi||_{\text{TV}} = 1/e$, (non-asymptotic time scale).
- t_{rel} = inverse gap, (asymptotic time scale).
- $t_{\text{mix}} \gg t_{\text{rel}}$ leads to cutoff phenomenon.
- Aldous–Diaconis (1986)
- Diaconis–Fill-Pitman (1992)

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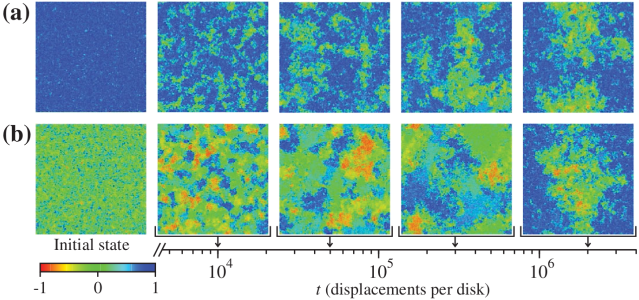
Example II: A non-asymptotic time scale



- Coarsening in hard disks (from Bernard & Krauth 2011)...
- ... an example of a non-asymptotic mixing-time scale

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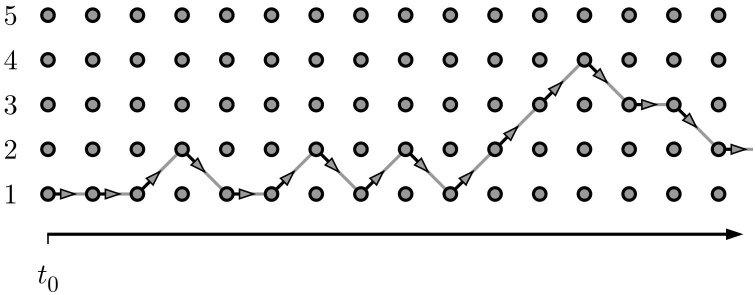
Markov chain



- Configuration c_t, move δ_t.
- Set $t_0 = 0$.

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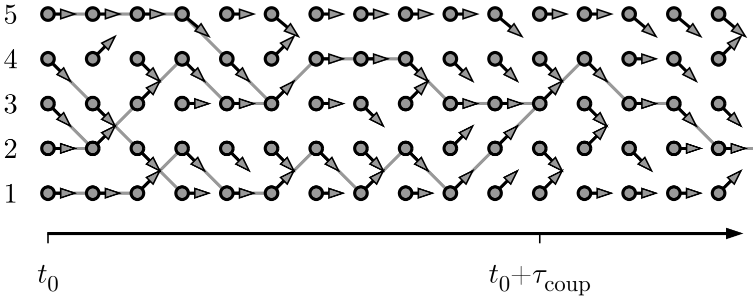
Markov chain (random maps), coupling 1/3



- Each configuration has its move at each time step.
- Coupling (Doeblin, 1930s).

Markov chain (random maps), coupling 2/3

procedure `forward-coupling`

$\mathcal{P} \leftarrow \{1, \ldots, N\}$

$t \leftarrow 0$

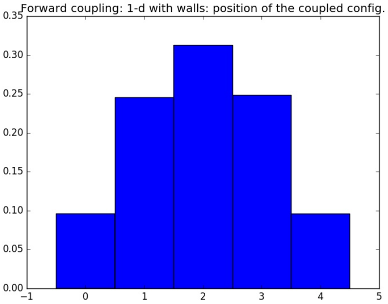
while True:

$$\begin{cases} t \leftarrow t + 1 \\ \mathcal{P} \leftarrow \{\min\left[\max(b + \mathbf{choice}\{-1, +1\}, 1), N\right] \text{ for } b \in \mathcal{P}\} \\ \mathbf{if}\ |\mathcal{P}| = 1\mathbf{:}\ \mathbf{break} \end{cases}$$

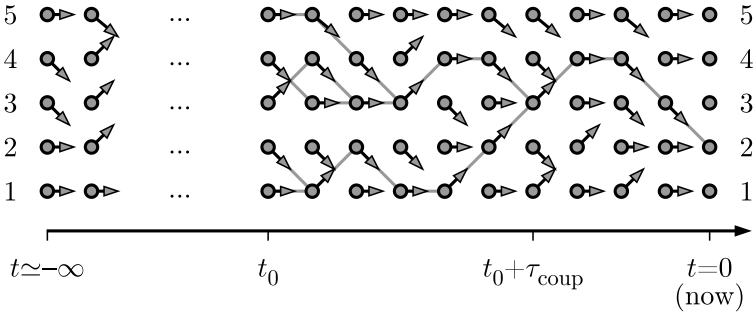
output $\mathcal{P}, t$ (position, time of coupling)

- Position of coupling not uniform.
- Coupling time larger than mixing time.

Markov chain (random maps), coupling 3/3



- Histogram of coupling position.



- Starting an MCMC simulation at $t = -\infty$
- Propp & Wilson (1997)

Coupling from the past 2/3

procedure `coupling-from-past`

$t_{\text{tot}} \leftarrow 0$

while True:

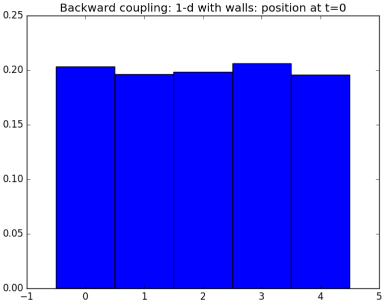
$$\begin{cases} t_{\text{tot}} \leftarrow t_{\text{tot}} - 1 \\ \mathcal{A}_{t_{\text{tot}}} \leftarrow \texttt{draw-arrows} \text{ (draw arrows at time } t_{\text{tot}}) \\ \mathcal{P} \leftarrow \{1, \ldots, N\} \\ \textbf{for } t = t_{\text{tot}}, t_{\text{tot}} + 1, \ldots, -1\textbf{:} \\ \quad \{ \mathcal{P} \leftarrow \{b + \mathcal{A}_t(b) \text{ for } b \in \mathcal{P}\} \\ \textbf{if } |\mathcal{P}| = 1\textbf{: break} \end{cases}$$

output $\mathcal{P}$ ((perfect) sample)

———

- Propp & Wilson (1997)

Coupling from the past 3/3



- Propp & Wilson (1997)
- see `CouplingFromThePast.py` on my website

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Example III: Perfect Monte Carlo samples of hard disks

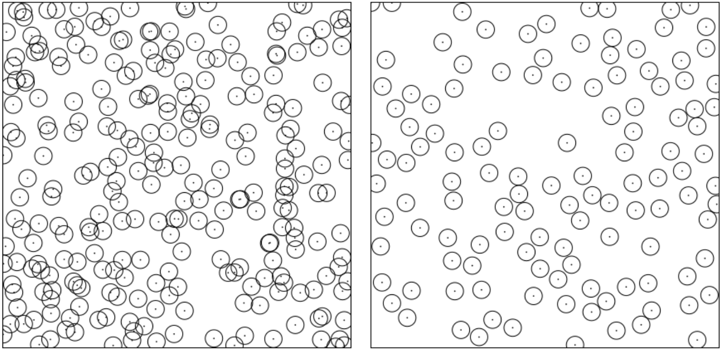

Figure 10: Perfectly random samples of the Strauss point process. In both panels the point

- Perfect sample of hard disks (right) from Wilson (2000)

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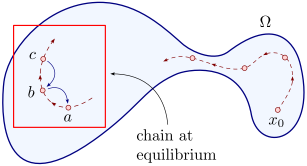
Detailed balance, global balance, lifting



- Reversible transition matrices P satisfy the 'detailed-balance' condition:

$$\pi_a P_{ab} = \pi_b P_{ba}$$

- Non-reversible transition matrices P only satisfy 'global balance':

$$\pi_a = \sum_{b \in \Omega} \pi_b P_{ba}$$

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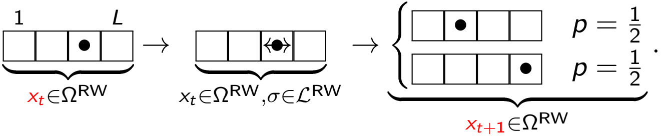
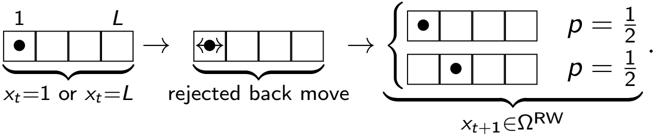
Random walk (RW) on the one-dimensional lattice

- In the bulk:



(1)

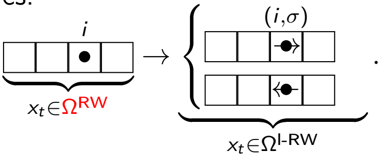
- At the boundary:



(2)

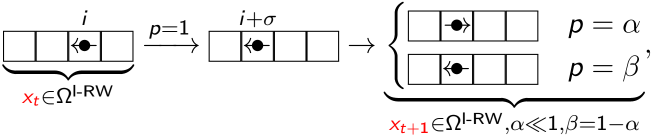
Lifted random walk (l-RW)

- Lifting of samples:



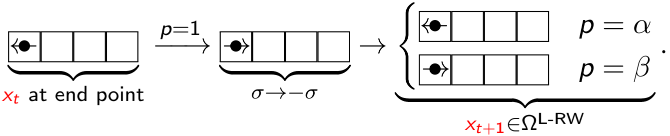
(3)

- In the bulk:



(4)

- At the boundary:



(5)

Diaconis, Holmes, Neal (2000)

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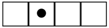
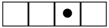
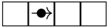
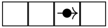
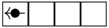
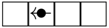
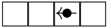
Random walk, lifted random walk (examples)

- $1 \equiv$  $2 \equiv$  $3 \equiv$  $4 \equiv$ 

$$P^{RW}_{\text{walls}} = \frac{1}{2} \begin{bmatrix} 1 & 1 & \cdot & \cdot \\ 1 & \cdot & 1 & \cdot \\ \cdot & 1 & \cdot & 1 \\ \cdot & \cdot & 1 & 1 \end{bmatrix}$$

- Lifted random walk (NB: $\alpha + \beta = 1, \quad \alpha \sim 1/L$)

$1 \equiv$  $3 \equiv$  $5 \equiv$  $7 \equiv$ 

$2 \equiv$  $4 \equiv$  $6 \equiv$  $8 \equiv$ 

$$P^{\text{lRW}}_{\text{walls}} = \begin{bmatrix} \cdot & \cdot & \beta & \alpha & \cdot & \cdot & \cdot & \cdot \\ \beta & \alpha & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \beta & \alpha & \cdot & \cdot \\ \alpha & \beta & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \beta & \alpha \\ \cdot & \cdot & \alpha & \beta & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \alpha & \beta \\ \cdot & \cdot & \cdot & \cdot & \alpha & \beta & \cdot & \cdot \end{bmatrix},$$

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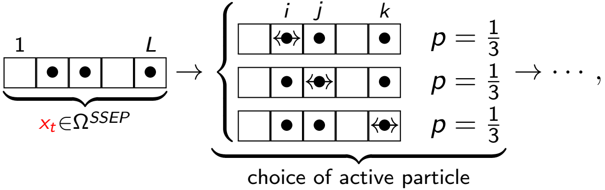
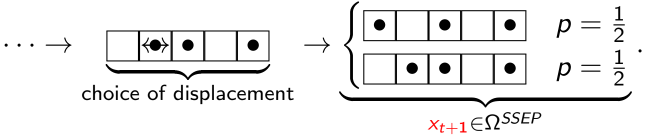
Symmetric simple exclusion process (SSEP)

- Move (first part ...)

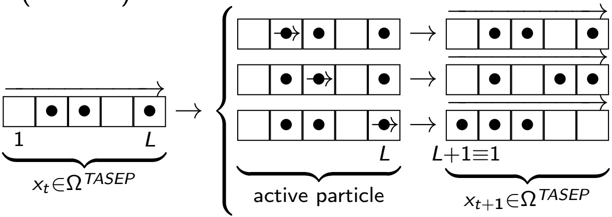


- Move (... second part)

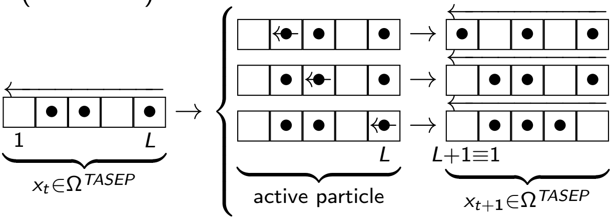


Totally asymmetric simple exclusion process (TASEP)

- Move (forward)



- Move (backward)

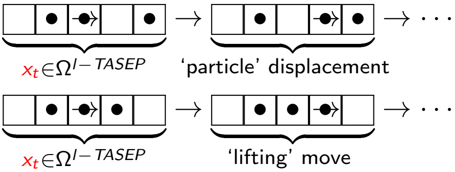


- forward–backward coupling (ad-hoc, or boundary conditions).

NB: Non-reversible, i.e. non-equilibrium, but samples equilibrium Boltzmann distribution.

Lifted TASEP (definition)

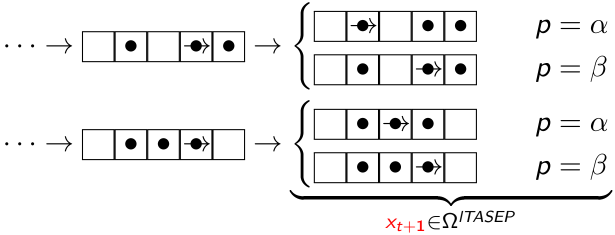
- $\Omega^{l-TASEP} = \Omega^{SSEP} \times \{-1, +1\} \times \{1, \ldots, N\}$, $\mathcal{L} = \emptyset$
- Move (first part ...)



(6)

(7)

- Move (second part ...)



(6b)

(7b)

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TASEP (example)

NB: Consider only the forward-moving sector (pbc):

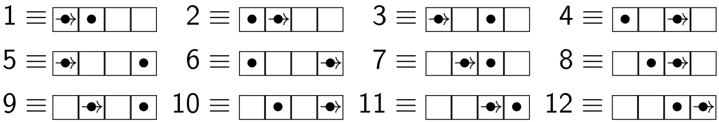
$$1 \equiv \overrightarrow{\boxed{\bullet}\boxed{\bullet}\boxed{}\boxed{}} \quad 2 \equiv \overrightarrow{\boxed{\bullet}\boxed{}\boxed{\bullet}\boxed{}} \quad 3 \equiv \overrightarrow{\boxed{\bullet}\boxed{}\boxed{}\boxed{\bullet}}$$

$$4 \equiv \overrightarrow{\boxed{}\boxed{\bullet}\boxed{\bullet}\boxed{}} \quad 5 \equiv \overrightarrow{\boxed{}\boxed{\bullet}\boxed{}\boxed{\bullet}} \quad 6 \equiv \overrightarrow{\boxed{}\boxed{}\boxed{\bullet}\boxed{\bullet}}$$

$$P^{\mathrm{TASEP}} = \frac{1}{2}\begin{bmatrix} 1 & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & 1 & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & 1 & 1 & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & 1 & \cdot & \cdot & \cdot & 1 \end{bmatrix} .$$

Lifted TASEP (example)

NB: Consider only the forward-moving sector (pbc):



$$P = \begin{bmatrix}
\alpha & \beta & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \alpha & \beta & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \beta & \alpha & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \alpha & \beta & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \beta & \alpha & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \beta & \alpha & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \alpha & \beta & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \alpha & \beta & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \beta & \alpha \\
\beta & \alpha & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \alpha & \beta \\
\cdot & \cdot & \beta & \alpha & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot
\end{bmatrix}$$

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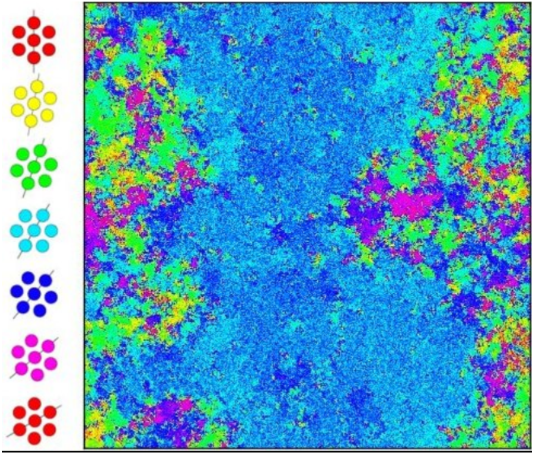
Synopsis of mixing and relaxation times

Algorithm	mixing	relaxation (inverse gap)
SSEP	$N^3 \log N$	N^3
TASEP	$N^{5/2}$	$N^{5/2}$
Lifted TASEP	N^2	N^2

- continuous-space versions available (Kapfer & Krauth (2017))
- see Essler & Krauth (2023)

Example IV: Equilibrium non-equilibrium



- Equilibrated sample of 10^6 disks (from Bernard & Krauth 2011, see also Li et al. 2022)

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Conclusion & Outlook

Conclusion:

- A second revolution in Markov-chain Monte Carlo underway.
- Time scales of MCMC much better understood.
- Coupling: a way to perfect simulations.
- Non-reversible MCMC is what comes after the revolution.
- Lifting: a practical method to create non-reversible algorithms.

Outlook:

- Sampling $\exp(-\beta U)$ without evaluating U.
- 'Natively cutoff-free' MCMC (Coulomb, LJ) in $\mathcal{O}(1)$.
- Applications in chemical physics.

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