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

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26 April 2024
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This work was supported by a grant from the Simons Foundation

This work was supported by the Alexander von Humboldt Foundation

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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)

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,
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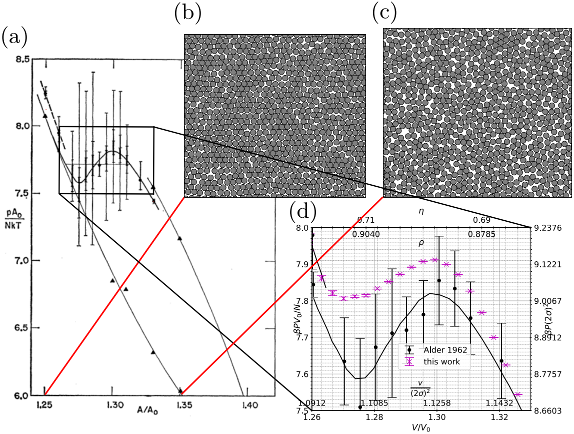
(Received March 6, 1953)

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.

Example I: Equilibrated (?) samples



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

Markov chains (2/2)

- Sample space Ω (e.g. hard disks, water molecules, quarks, ...)
- Markov chain $\leftarrow$ Sequence of random variables
  $(X_0 \sim \pi^{\{0\}}, X_1 \sim \pi^{\{1\}}, X_2 \sim \pi^{\{2\}} \dots)$
  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:

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

- Distance:

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

- Mixing time:

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

- Usually $\epsilon = 1/4$ is taken, $\epsilon = 1/e$ would be better.

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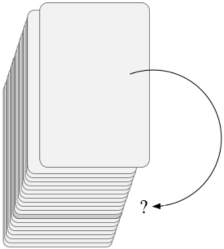
Shuffling of cards 1/5



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

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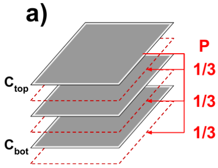
Shuffling of cards 2/5



moves

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.

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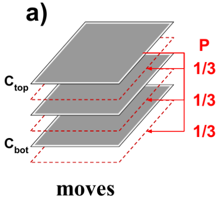
Shuffling of cards 3/5

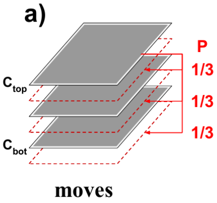


- $\Omega_3^{\text{shuffle}} = \{1 \equiv \{1,2,3\}, 2 \equiv \{1,3,2\}, 3 \equiv \{2,1,3\}, 4 \equiv \{2,3,1\}, 5 \equiv \{3,1,2\}, 6 \equiv \{3,2,1\}\}$.
- $$P = \frac{1}{3}\begin{pmatrix} 1 & 0 & 1 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 1 \\ 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 \\ 1 & 1 & 0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

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

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

Shuffling of cards 5/5




```
procedure top2random-stop
input {c_1, ..., c_n}
c_first-n ← c_n
for t = 1, 2, ... do
  { c̃_1 ← c_1
  { {c_1, ..., c_n} ← top2random({c_1, ..., c_n})
  { if (c̃_1 = c_first-n) break
output {c_1, ..., c_n, t}
```

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

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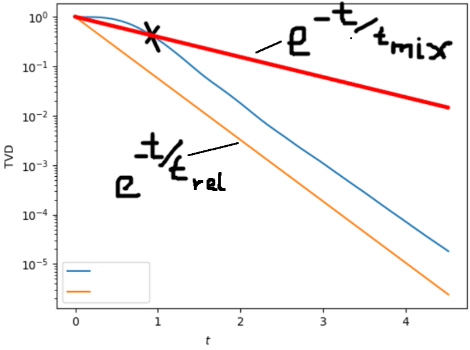
Mixing and Relaxation



- $t_{\text{mix}} = ||\pi^{\{t_{\text{mix}}\}} - \pi||_{\text{TV}} = 1/e$, (non-asymptotic time scale).
- $t_{\text{rel}} =$ 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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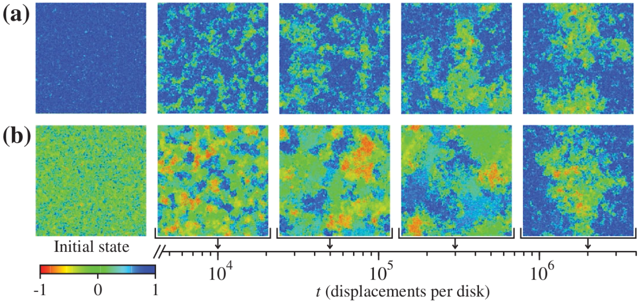
Example II: A non-asymptotic time scale



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

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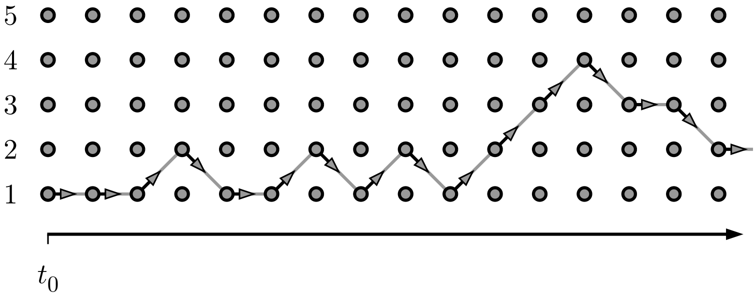
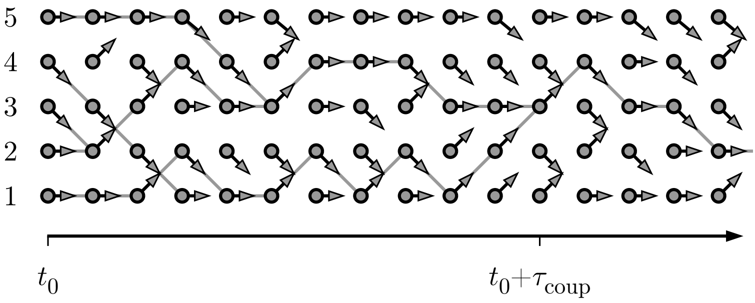
Markov chain



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

Markov chain (random maps), coupling 1/3



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

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Markov chain (random maps), coupling 2/3

procedure `forward-coupling`
$\mathcal{P} \leftarrow \{1, \ldots, N\}$
$t \leftarrow 0$
while True:
$$\begin{cases} t \leftarrow t + 1 \\ \mathcal{P} \leftarrow \{\min\left[\max(b + \textbf{choice}\{-1, +1\}, 1), N\right] \text{ for } b \in \mathcal{P}\} \\ \textbf{if } |\mathcal{P}| = 1\textbf{: break} \end{cases}$$
output $\mathcal{P}, t$ (position, time of coupling)

———

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

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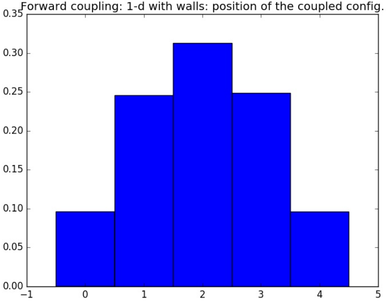
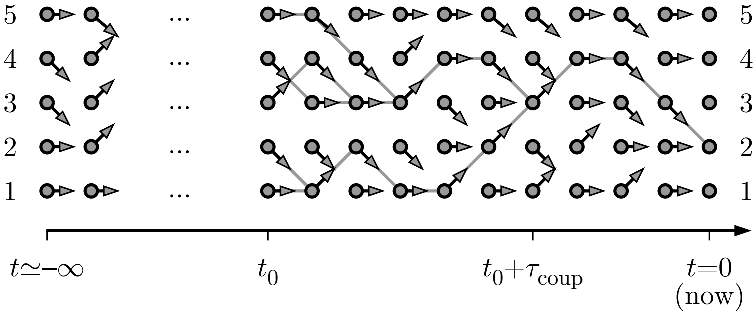
Markov chain (random maps), coupling 3/3



- Histogram of coupling position.

Coupling from the past 1/3



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

Coupling from the past 2/3

procedure `coupling-from-past`

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

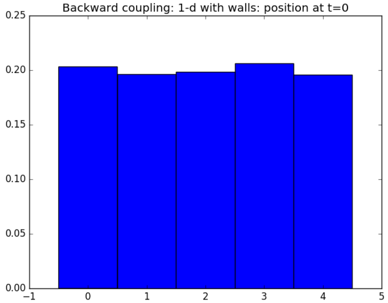
while True:

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

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

- Propp & Wilson (1997)

Coupling from the past 3/3



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

Example III: Perfect Monte Carlo samples of hard disks

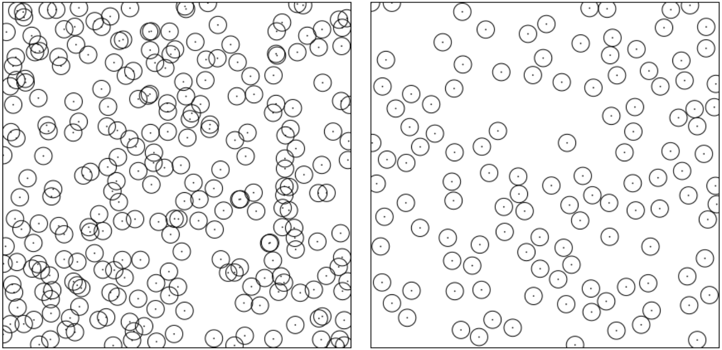
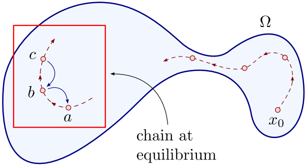


Figure 10: Perfectly random samples of the Strauss point process. In both panels the point

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

Plan of talk

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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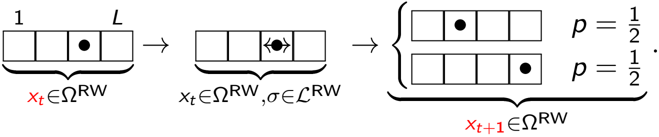
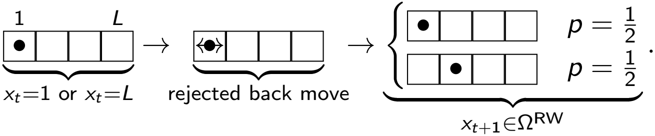
Random walk (RW) on the one-dimensional lattice

- In the bulk:



(1)

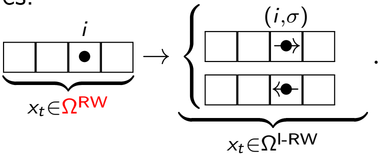
- At the boundary:



(2)

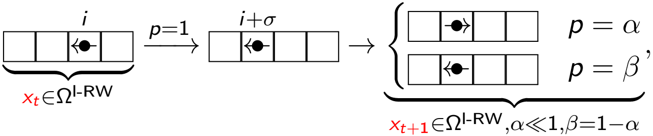
Lifted random walk (l-RW)

- Lifting of samples:



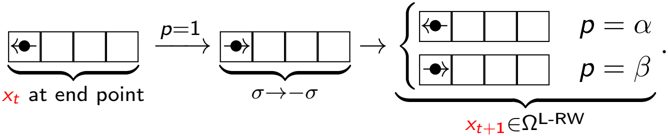
(3)

- In the bulk:



(4)

- At the boundary:



(5)

Diaconis, Holmes, Neal (2000)

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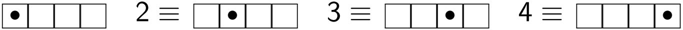
Random walk, lifted random walk (examples)

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

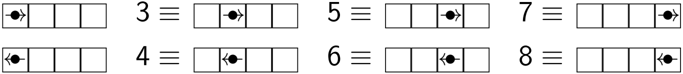


$$P^{RW}_{\text{walls}} = \frac{1}{2}\begin{bmatrix} 1 & 1 & \cdot & \cdot \\ 1 & \cdot & 1 & \cdot \\ \cdot & 1 & \cdot & 1 \\ \cdot & \cdot & 1 & 1 \end{bmatrix}$$

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

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

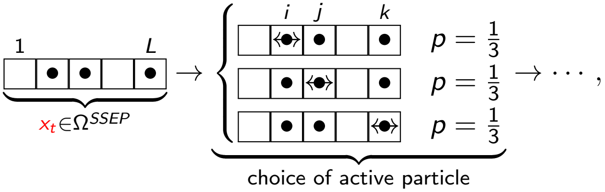
$2 \equiv$ $4 \equiv$ $6 \equiv$ $8 \equiv$



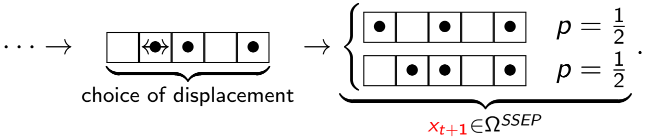
$$P^{\text{lRW}}_{\text{walls}} = \begin{bmatrix} \cdot & \cdot & \beta & \alpha & \cdot & \cdot & \cdot & \cdot \\ \beta & \alpha & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \beta & \alpha & \cdot & \cdot \\ \alpha & \beta & \cdot & \cdot & \cdot & \cdot & \cdot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

Symmetric simple exclusion process (SSEP)

- Move (first part ...)



- Move (... second part)



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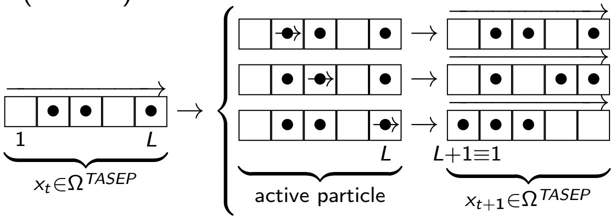
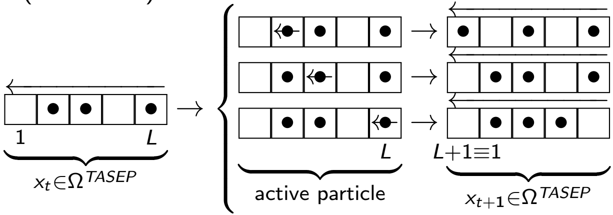
Totally asymmetric simple exclusion process (TASEP)

- Move (forward)



- Move (backward)



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

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

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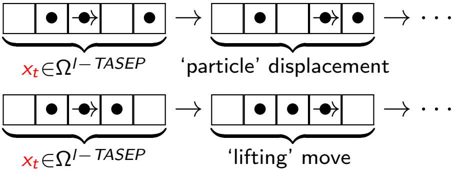
Lifted TASEP (definition)

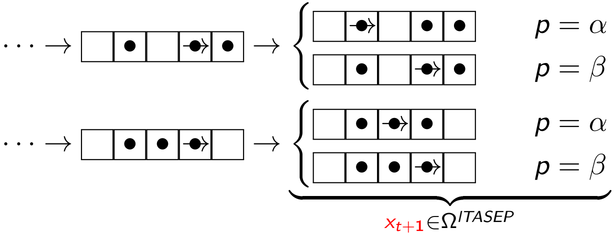
- $\Omega^{l-TASEP} = \Omega^{SSEP} \times \{-1, +1\} \times \{1, \dots, N\}$, $\mathcal{L} = \emptyset$
- Move (first part ...)



(6)

(7)

- Move (second part ...)



(6b)

(7b)

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

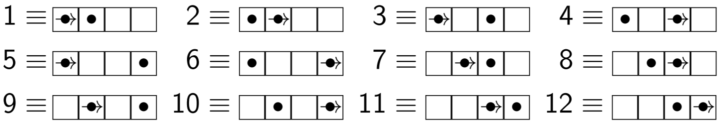
$$1 \equiv \overrightarrow{\boxed{\bullet}\boxed{\bullet}\boxed{}\boxed{}} \quad 2 \equiv \overrightarrow{\boxed{\bullet}\boxed{}\boxed{\bullet}\boxed{}} \quad 3 \equiv \overrightarrow{\boxed{\bullet}\boxed{}\boxed{}\boxed{\bullet}}$$

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

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

Lifted TASEP (example)

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



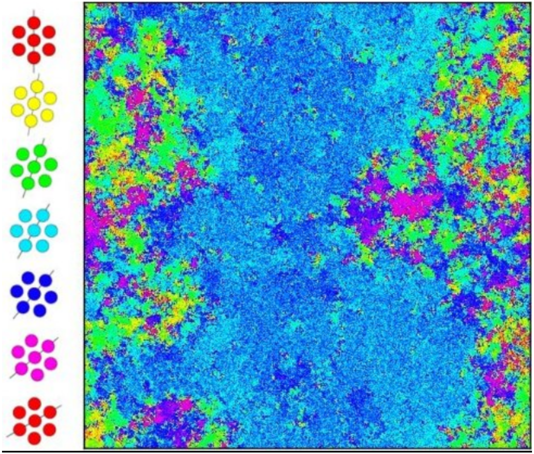
$$P = \begin{bmatrix} \alpha & \beta & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \alpha & \beta & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \beta & \alpha & \cdot & \cdot & \cdot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

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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