Rejection-free, irreversible, and infinitesimal (!) Monte Carlo algorithms

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Preprint: arXiv201308xx (coming soon)

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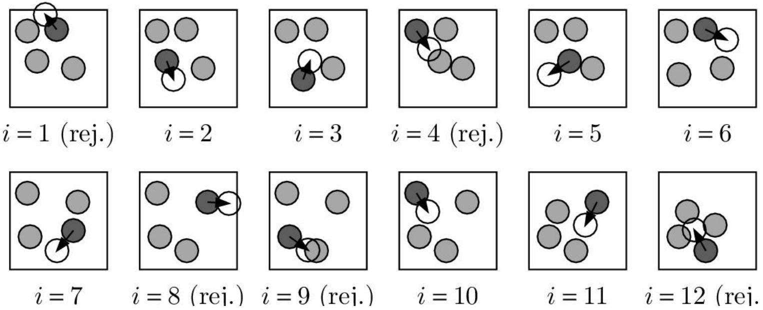
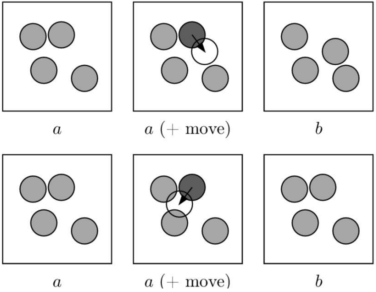
Metropolis et al (1953)

- Local hard-sphere Monte Carlo:



- . . . has rejections . . .
- . . . is reversible (satisfies detailed balance) . . .
- . . . makes finite moves . . .
- . . . has been generalized to arbitrary potentials.

Motivation - hard spheres



- displacements (δ_x, δ_y) sampled uniformly in $([-\delta, \delta], [-\delta, \delta])$
- Algorithm satisfies detailed balance:

$$\pi(a)p(a \to b) = \pi(b)p(b \to a)$$

with $\pi(a) = \pi(b) = \pi(c)$, for all legal configurations of hard spheres

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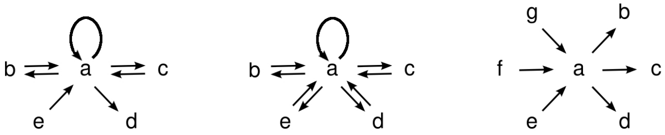
Detailed balance - global balance



global balance — detailed balance — maximal global balance

- flow in $\equiv$ flow out (global balance condition):

$$\sum_k \underbrace{\pi(k)p(k \to a)}_{\varphi(k \to a)} = \sum_k \underbrace{\pi(a)p(a \to k)}_{\varphi(a \to k)}$$

- flow $\varphi(a \to b) \equiv$ flow $\varphi(b \to a)$ (detailed balance condition):
  - Metropolis algorithm (for flows and cond. probabilities)

$$\varphi(a \to b) = \min(\pi(a), \pi(b))$$

$$p(a \to b) = \min\left(1, \frac{\pi(b)}{\pi(a)}\right)$$

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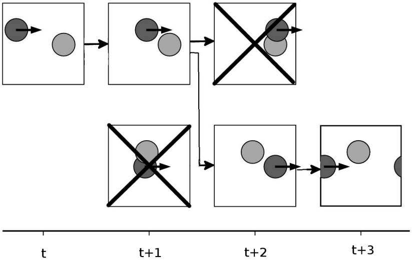
Lifting - two hard spheres



- Lifting: add variables to the system (here: one fixed displacement vector Δ)
- This algorithm satisfies maximal global balance (two hard disks, fixed Δ, periodic boundary conditions).
- This works just as well for arbitrary potentials

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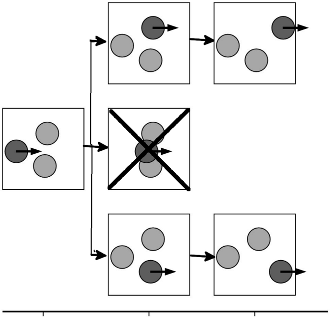
Lifting - N hard spheres



- Multiple collisions destroy global balance ($N > 2$).
- Infinitesimal moves $\Longrightarrow$ simple collisions only $\Longrightarrow$ lifting OK
- Event-chain algorithm (Bernard, Krauth, Wilson (2009))

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Metropolis vs. Pairwise Markov chains

Useful concept, useful identity:

- $[x]^- := \min(-x, 0) = -\max(x, 0) \quad (\leq 0)$
- $[x]^- - [-x]^- = -x$

Metropolis move $a \to b$

- $p(a \to b) = \min(1, \exp(-\Delta E)) = \exp[\Delta E]^-$
- $1 - p = 1 - \exp[\Delta E]^- \xrightarrow{\Delta E \sim 0} -[\Delta E]^- (\geq 0)$

Many-particle system, pair interactions $E = \sum_{i<j} E_{ij}$

- $p^{\text{Met}}(a \to b) = \exp\left(\left[\sum_{i<j} \Delta E_{ij}\right]^-\right)$
- $p^{\text{pair}}(a \to b) = \exp\left(\sum_{i<j} [\Delta E_{ij}]^-\right)$ new!
  (Michel, Kapfer, Krauth (2013)) use identity to prove

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Application - Lifting algorithm

Apply pair-wise rejections (Michel et al 2013)...

- $p^{\text{pair}}(a \to b) = \exp\left(\sum_{i<j} [\Delta E_{ij}]^-\right)$ (acceptance rate)
- $1 - p^{\text{pair}} \xrightarrow[\Delta E \to 0]{} -\sum_{i<j} [\Delta E_{ij}]^-$ (remarkable: sum over pairs!)

...for a lifting algorithm for general potentials:

- $(r_1, \ldots, r_N) \to (r_1, \ldots, r_i, \ldots, r_N)$ only particle i moving: $\Delta E \equiv \sum_{j(j \neq i)} \Delta E_{ij}$
- compensate for rejections through liftings: $p^{\text{lift}}(i \to j) = -[\Delta E_{ij}]^-$ depends only on i and j
- run in faster-than-the-clock mode (Bortz-Kalos-Lebowitz, 1975)
- cf. Peters and de With, 2012

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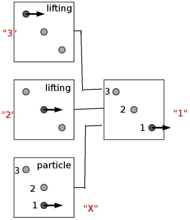

Let's compute flow into the configuration a (to first order):

$$\varphi_{2\to 1} = \pi(a)(-[\Delta E_{21}]^{-})$$

$$\varphi_{3\to 1} = \pi(a)(-[\Delta E_{31}]^{-})$$

$$\varphi_{X\to 1} = \varphi^{\text{pair}}_{X\to 1} = \varphi^{\text{pair}}_{1\to X} = \exp([\Delta E_{21}]^{-} + [\Delta E_{31}]^{-})$$

- Total flow into configuration 1 equals $\pi(a)$ in first order in Δ.
- Total flow out of configuration 1 equals $\pi(a)$.
- General MC algorithm with maximal global balance.

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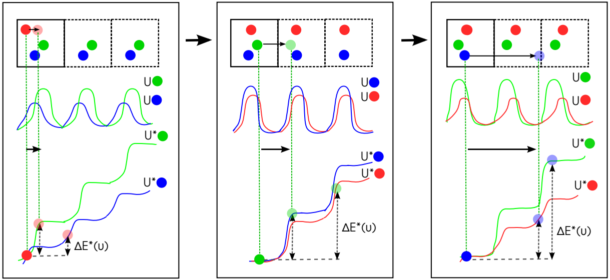
Lifting algorithm - Practical implementation



- Lifting probabilities are independent from each other
- Sampling of lifting event $i \to j$ through log of random number.
- General MC algorithm with maximal global balance.

Conclusion

- General Markov-chain Monte Carlo algorithm that is:
  - rejection-free,
  - irreversible,
  - infinitesimal,
  - faster than Metropolis.
- based on a pairwise Metropolis approach ....
- ...it generalizes the event-chain algorithm for hard spheres (Bernard et al., 2009), that has been very useful already (Bernard and Krauth, 2011; Engel et al., 2013).

In one word:

- No more rejections...
- ...No more detailed balance...

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