Fast irreversible Markov chains in statistical physics

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10 September 2019
CECAM50
CECAM EPFL, Lausanne (Switzerland)

E. P. Bernard, W. Krauth, D. B. Wilson, PRE (2009)
Event-chain algorithms for hard-sphere systems

E. P. Bernard, W. Krauth, PRL (2011)
M. Michel, S. C. Kapfer, W. Krauth, JCP (2014)
S. C. Kapfer, W. Krauth, PRL (2015, 2017)
Z. Lei, W. Krauth EPL (2018, 2019)
M. F. Faulkner, L. Qin, A. C. Maggs, W. Krauth, JCP (2018)

P. Höllmer, L. Qin, M. F. Faulkner, A. C. Maggs, W. Krauth, arXiv:1907.12502 (2019)
JeLLyFysh (Version 1.0) - a Python application for all-atom event-chain Monte Carlo

Work supported by A. v. Humboldt Foundation

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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

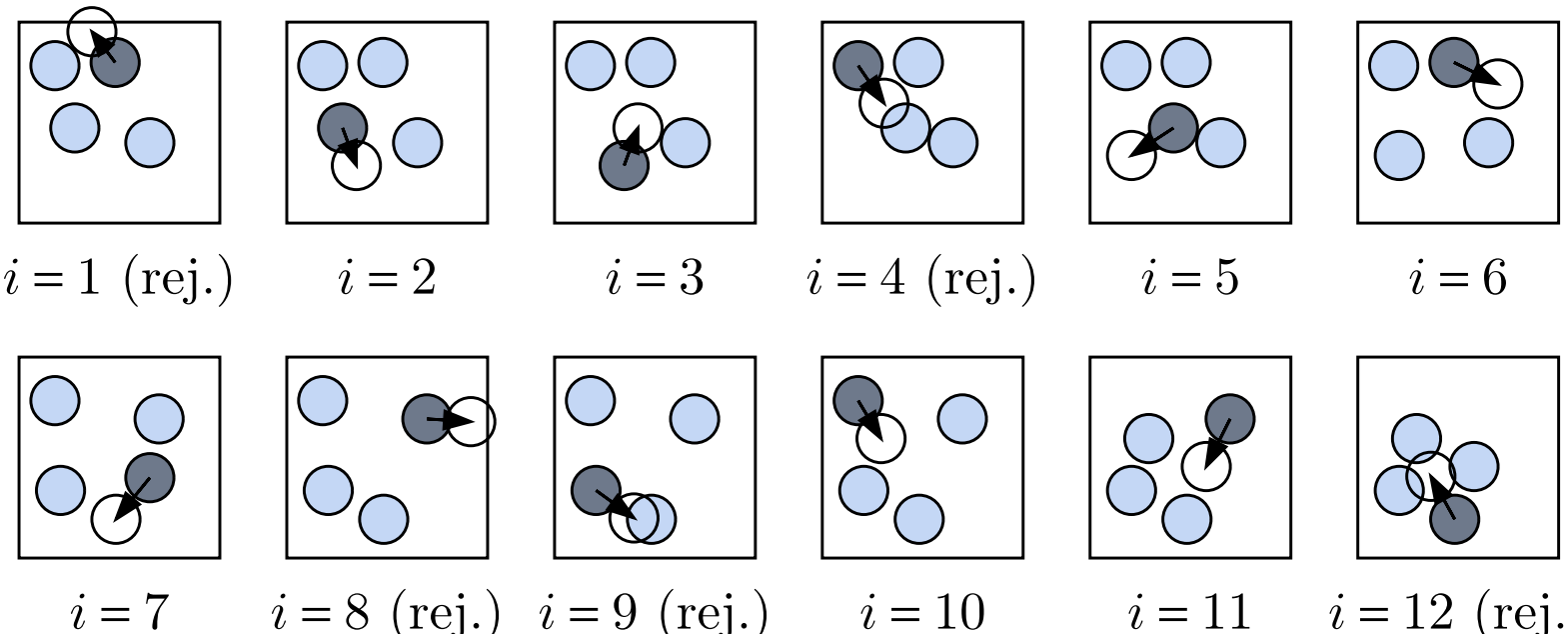
AND

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

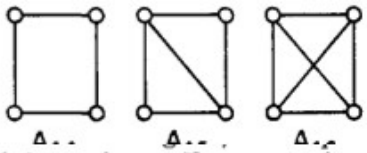
(Received March 6, 1953)

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.

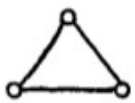
Metropolis et al (1953) (2/4)



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.

Alder–Wainwright (1962)

PHYSICAL REVIEW VOLUME 127, NUMBER 2 JULY 15, 1962

Phase Transition in Elastic Disks*

B. J. ALDER AND T. E. WAINWRIGHT
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

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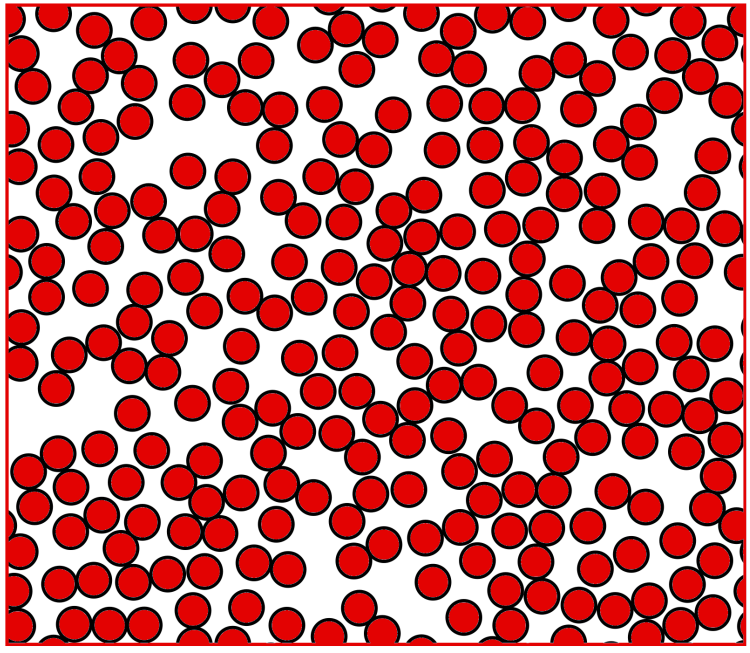
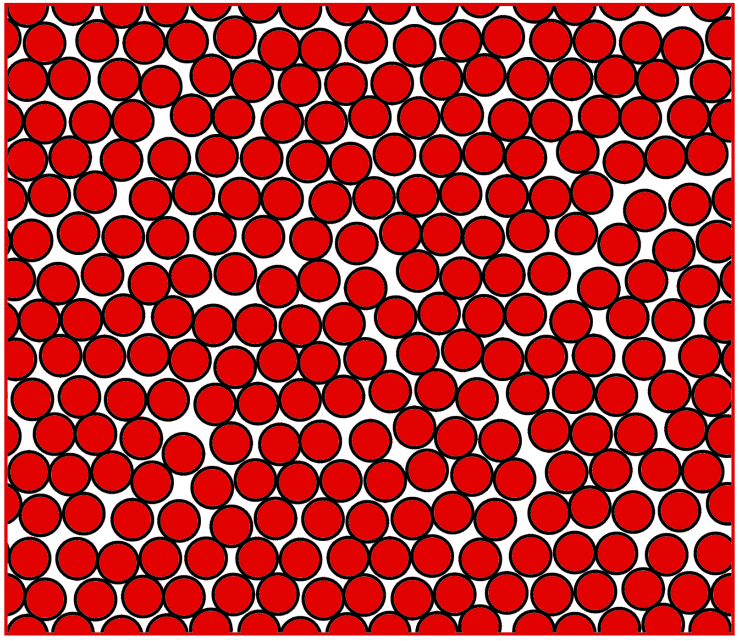
$2D$ melting transition



$\eta = 0.48$



$\eta = 0.72$

- Generic 2D systems cannot crystallize (Peierls, Landau 1930s) but they can turn solid (Alder & Wainwright, 1962).
- Nature of transition disputed for decades.

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Kosterlitz–Thouless (1973)

Ordering, metastability and phase transitions in two-dimensional systems

J M Kosterlitz and D J Thouless
Department of Mathematical Physics, University of Birmingham, Birmingham B15 2TT, UK

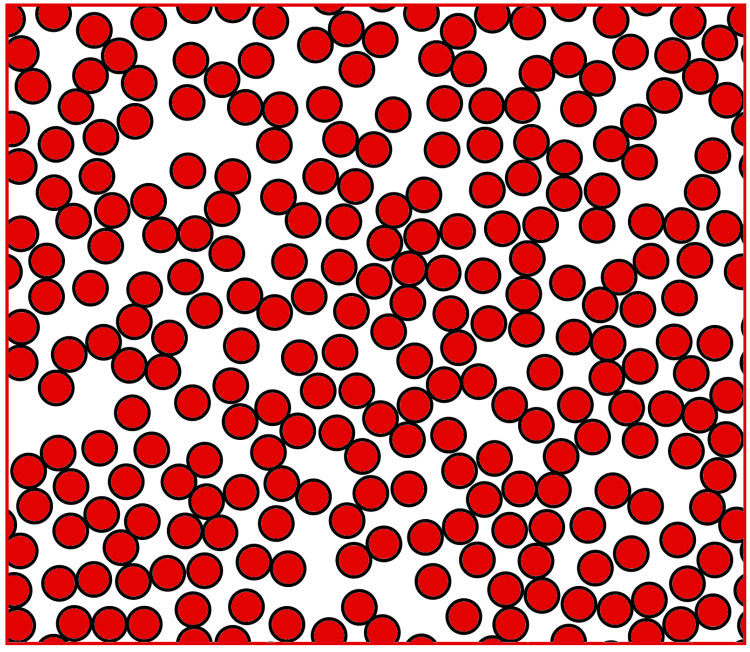
Received 13 November 1972

1. Introduction

Peierls (1935) has argued that thermal motion of long-wavelength phonons will destroy the long-range order of a two-dimensional solid in the sense that the mean square deviation of an atom from its equilibrium position increases logarithmically with the size of the system, and the Bragg peaks of the diffraction pattern formed by the system are broad instead of sharp. The absence of long-range order of this simple form has been shown by Mermin (1968) using rigorous inequalities. Similar arguments can be used to show that there is no spontaneous magnetization in a two-dimensional magnet with spins with more than one degree of freedom (Mermin and Wagner 1966) and that the expectation value of the superfluid order parameter in a two-dimensional Bose fluid is zero (Hohenberg 1967).

On the other hand there is inconclusive evidence from the numerical work on a two-dimensional system of hard discs by Alder and Wainwright (1962) of a phase transition between a gaseous and solid state. Stanley and Kaplan (1966) found that high-temperature series expansions for two-dimensional spin models indicated a phase

Possible phases in two dimensions



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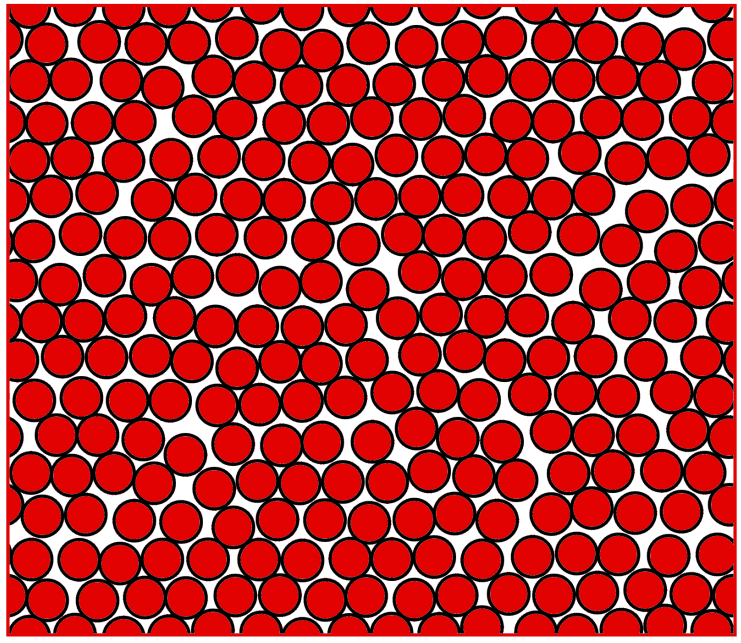

$\eta = 0.72$

Phase	positional order	orientational order
solid	algebraic	long-range
hexatic	short-range	algebraic
liquid	short-range	short-range

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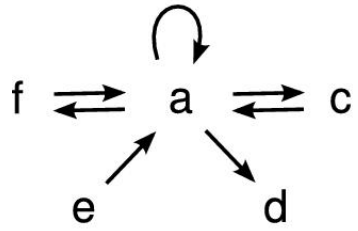
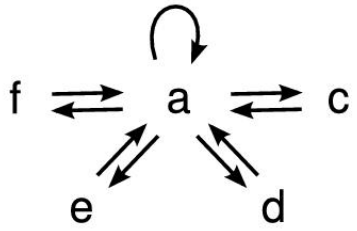
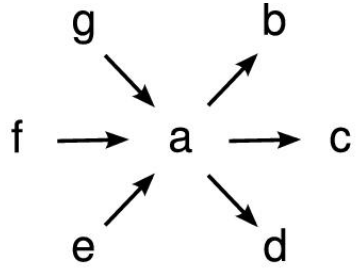
Detailed balance - global balance



global balance



detailed balance



maximal global balance

- flow into a = Boltzmann weight $\pi(a)$ (global balance condition):

$$\underbrace{\sum_k \pi^{(t-1)}(k) p(k \to a)}_{\text{flow into } a \ \sum_k \mathcal{F}(k \to a)} = \pi^{(t)}(a)$$

- flow $\mathcal{F}(a \to b) \equiv$ flow $\mathcal{F}(b \to a)$ (detailed balance condition):

$$\underbrace{\pi(b) p(b \to a)}_{\text{flow from } b \text{ to } a \ \mathcal{F}(b \to a)} = \underbrace{\pi(a) p(a \to b)}_{\mathcal{F}(a \to b) \text{ flow from } a \text{ to } b}$$

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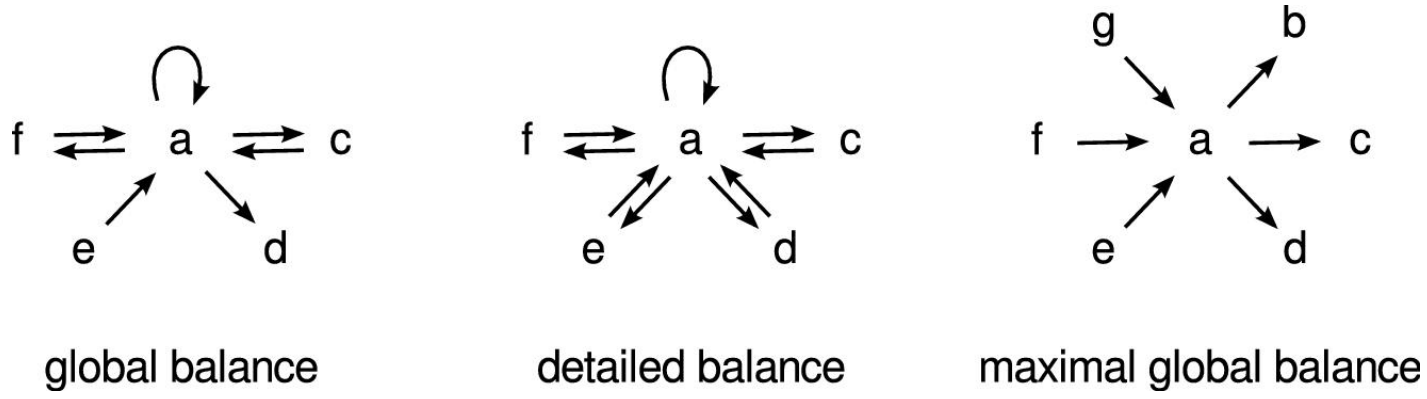
Detailed balance - global balance



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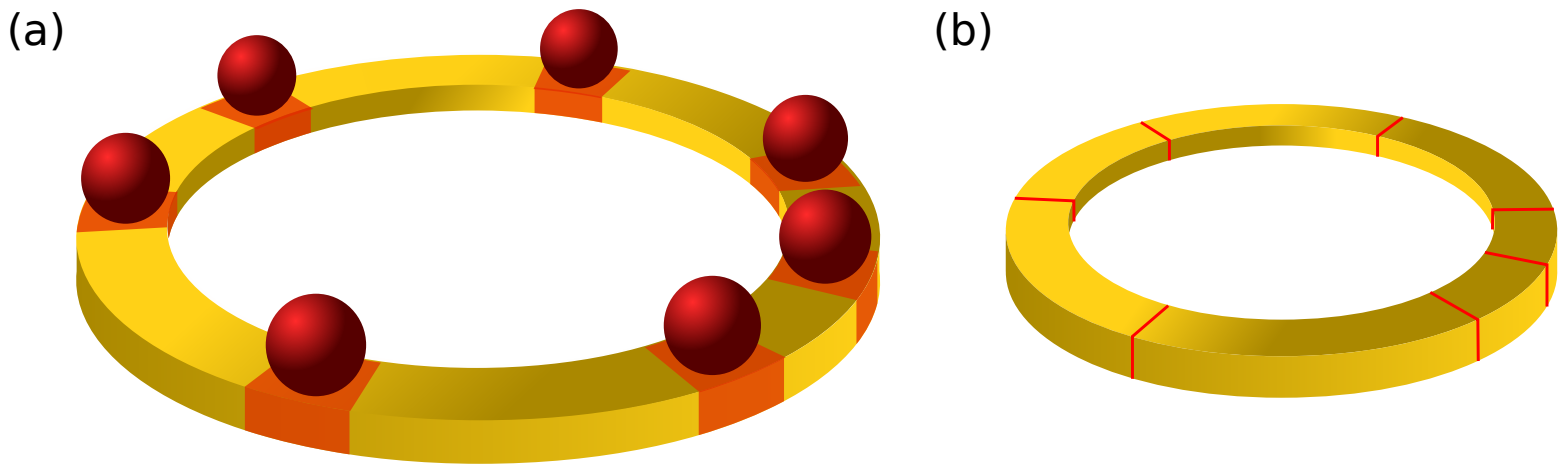
1d hard spheres with periodic boundary conditions



- N spheres, diameter σ, interval L, $\pi(a) = 1 \quad \forall a$
- N spheres, diameter 0, interval $L - N\sigma$.
- Equivalent if local moves (no change of order).

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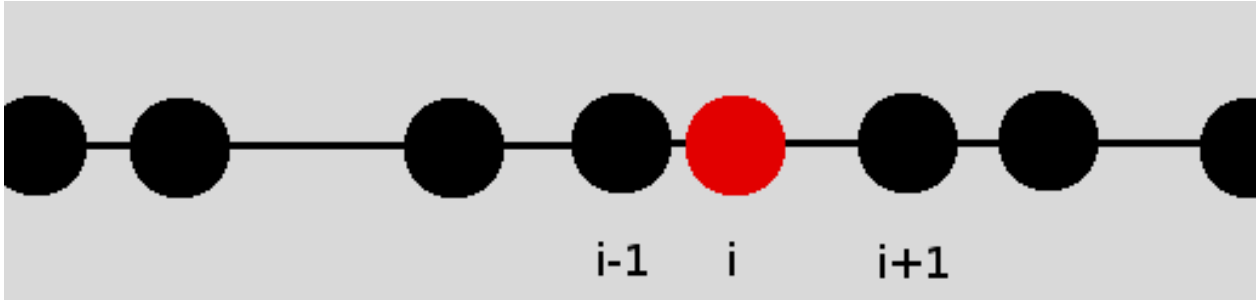
Reversible Metropolis algorithm, 1d (detailed balance)



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

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

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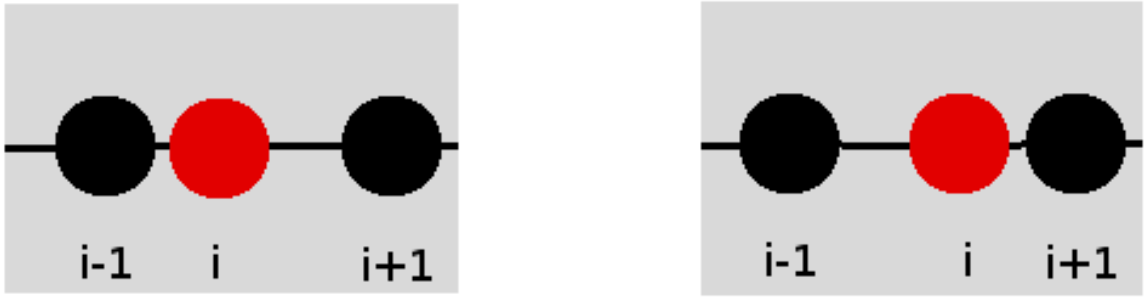
Reversible Metropolis algorithm, 1d (detailed balance)



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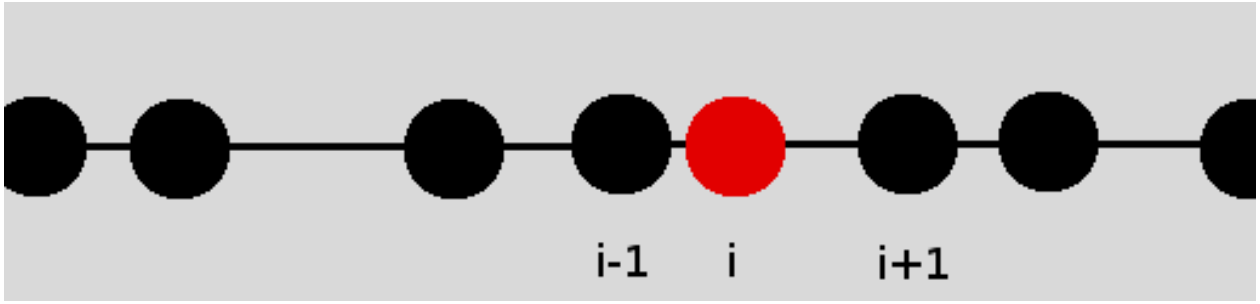
Reversible Metropolis algorithm, 1d (global balance)



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

$$\mathcal{F}_a^{\text{rev}} = \frac{1}{2N} \sum_i \underbrace{\left(\mathcal{A}_i^+ + \mathcal{R}_i^- + \mathcal{A}_i^- + \mathcal{R}_i^+\right)}_{=2 \text{ for any } \epsilon} = 1.$$

- NB: $\mathcal{A}_i^+(\epsilon) + \mathcal{R}_i^-(\epsilon) = 1$ also $\mathcal{A}_i^-(\epsilon) + \mathcal{R}_i^+(\epsilon) = 1$.

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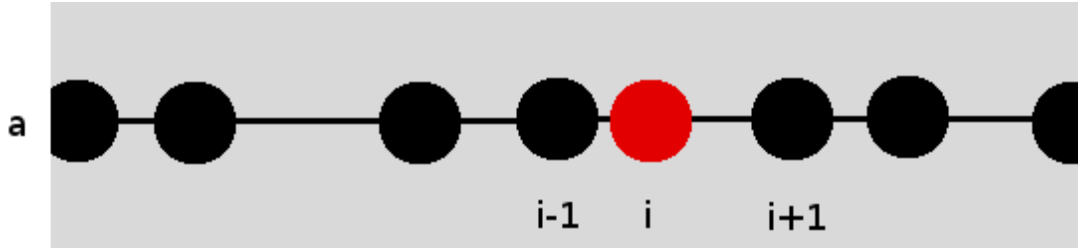
Sequential Metropolis algorithm, 1d (global balance)



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

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

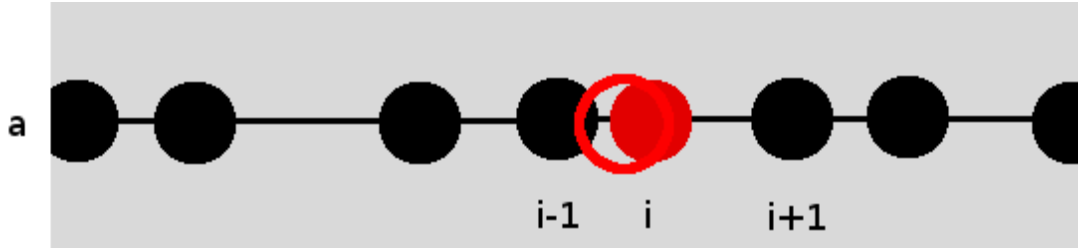
1088 METROPOLIS, ROSENBLUTH, ROSENBLUTH, TELLER, AND TELLER

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:

Sequential Metropolis algorithm, 1d (global balance)



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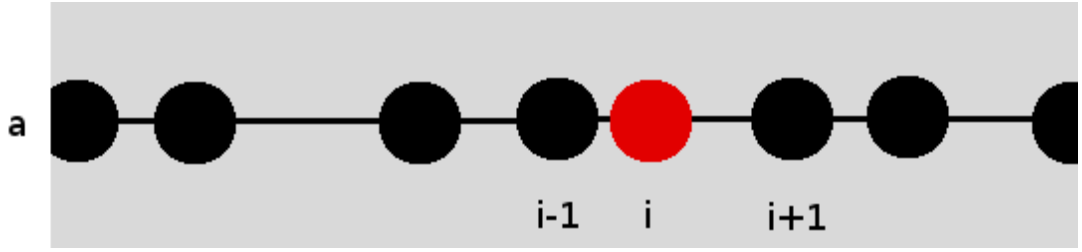

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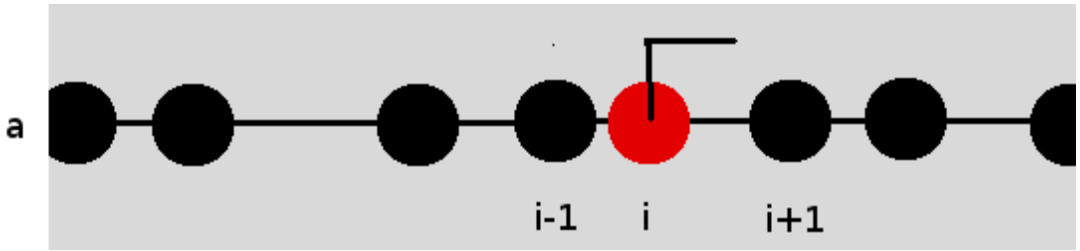
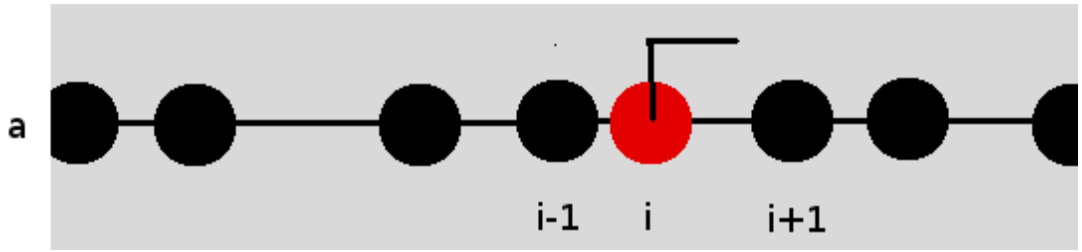
Forward Metropolis algorithm, 1d (global balance)



- 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 (Irreversible 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

- For Symmetric SEP mixing cf Lacoin (2014)
- For TASEP mixing cf Baik & Liu (2016)
- All others cf Kapfer & Krauth (2017)
- Mixing time for event-chain: Lei & Krauth (2018)

NB: All algorithms converge towards equilibrium

NNB: rigorous results, numerical results

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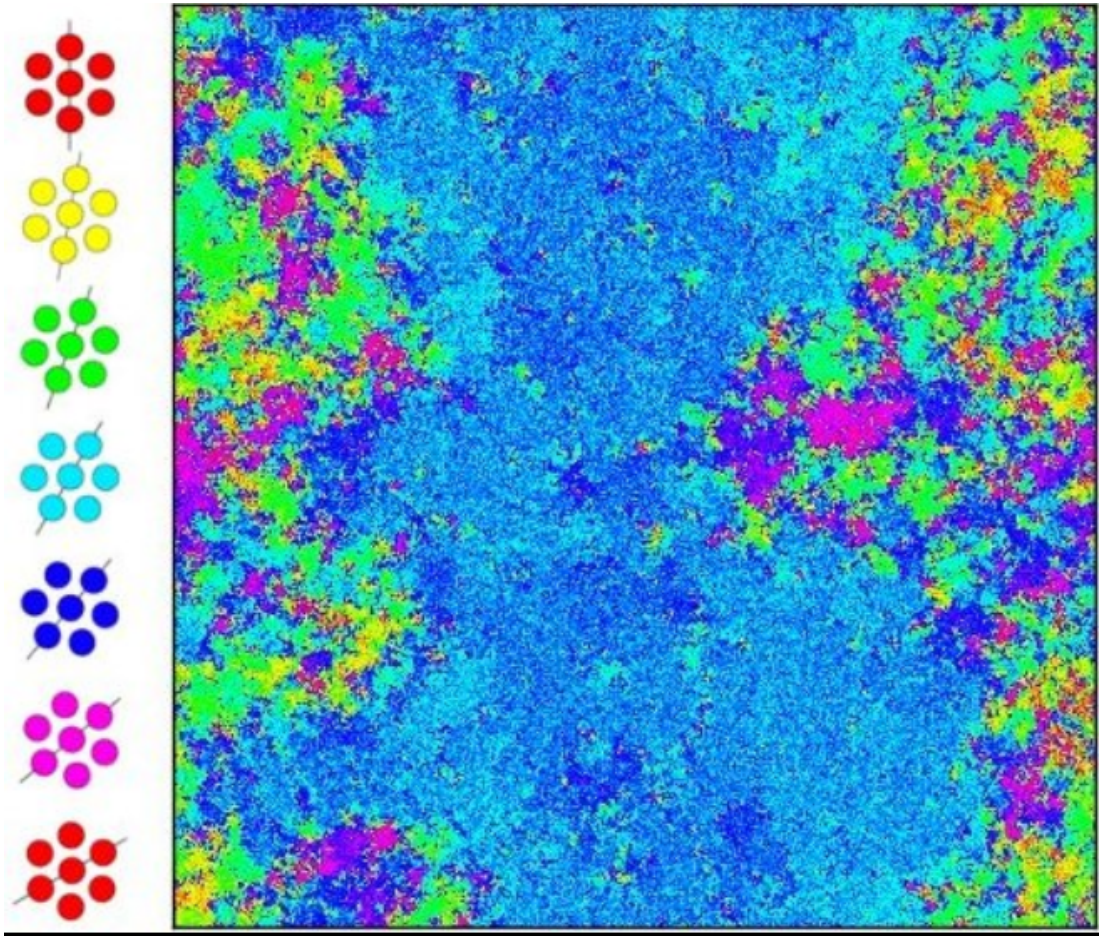
Hard-disk configuration



- 1024^2 hard disks
- Bernard, Krauth (PRL 2011)

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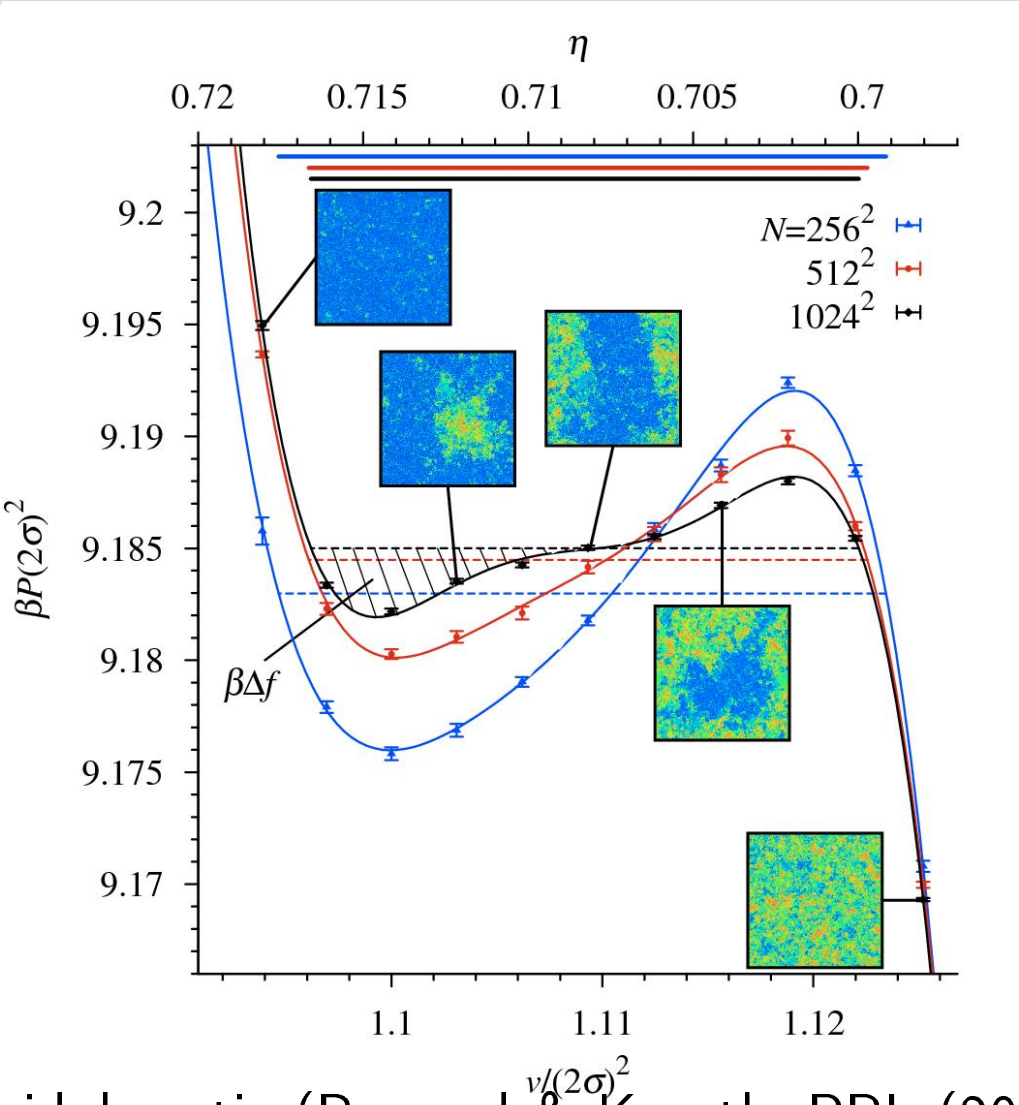
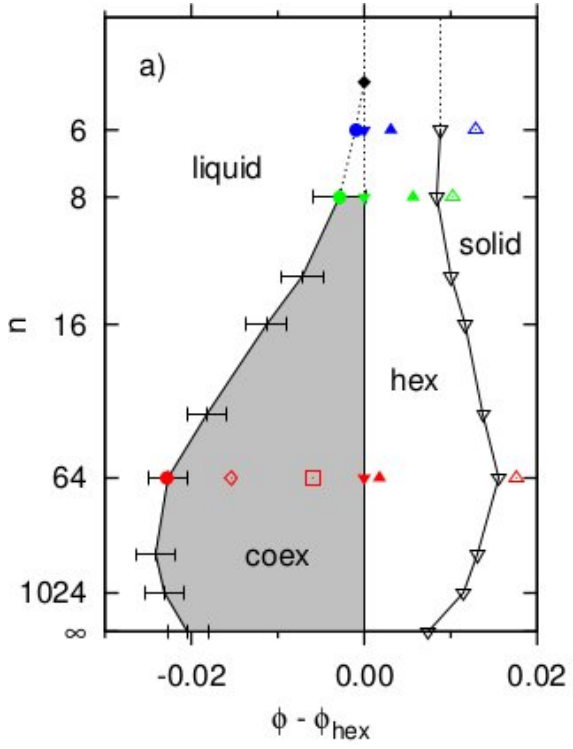
Equilibrium equation of state

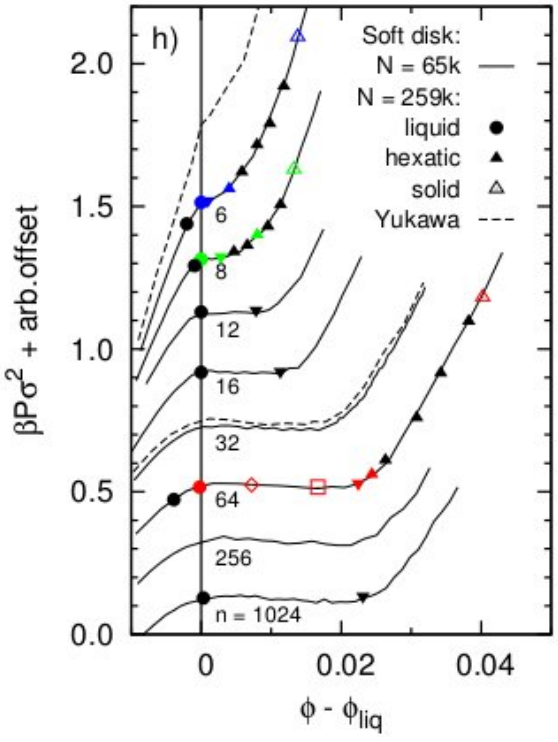


- 1st-order liquid–hexatic (Bernard & Krauth, PRL (2011)).
- Many confirmations (Engel, Anderson, Glotzer, Isobe, Bernard, Krauth, PRE Milestone (2013)).

Soft disks

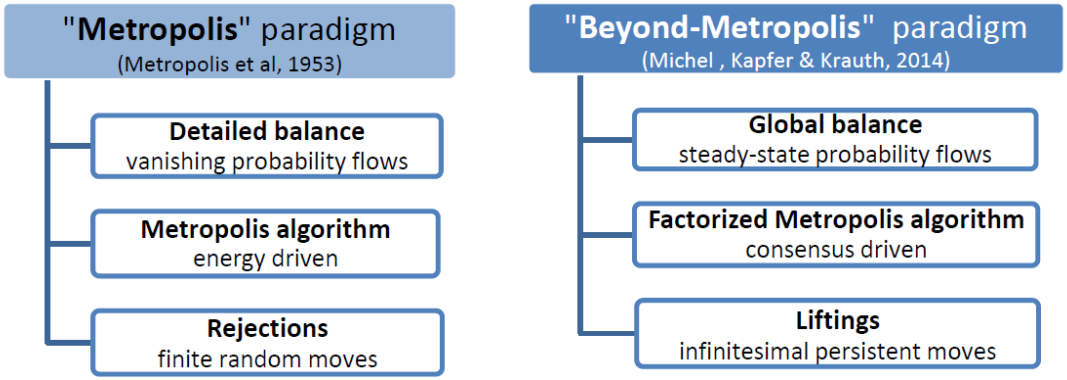
- Soft disks: $V \propto (\sigma/r)^n$.





- Kapfer & Krauth (PRL 2015).
- Two melting scenarios depending on softness n of potential.

Factorized Metropolis algorithm (1/2)



- Metropolis algorithm

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

- Factorized Metropolis algorithm (Michel, Kapfer, Krauth 2014)

$$p^{\text{Fact.}}(a \to b) = \prod_{i<j} \min\left[1, \exp\left(-\beta \Delta U_{i,j}\right)\right].$$

$$X^{\text{Fact.}}(a \to b) = X_{1,2} \wedge X_{1,3} \wedge \cdots \wedge X_{N-1,N}$$

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Factorized Metropolis algorithm (2/2)

- Total system potential

$$U(\{\mathbf{s}_1, \ldots, \mathbf{s}_N\}) = \sum_{M \in \Omega} U_M(\{\mathbf{s}_i : i \in I_M\}).$$

- $M = (I_M, T_M)$ factor, I_M: index set, T_M: factor type.
- Factorized Metropolis algorithm:

$$p^{\text{Fact}}(c \to c') = \prod_M \min\left[1, \exp\left(-\beta \Delta U_M\right)\right],$$

- Consensus:

$$X^{\text{Fact}}(c \to c') = \bigwedge_{M \in \Omega} X_M(c_M \to c'_M).$$

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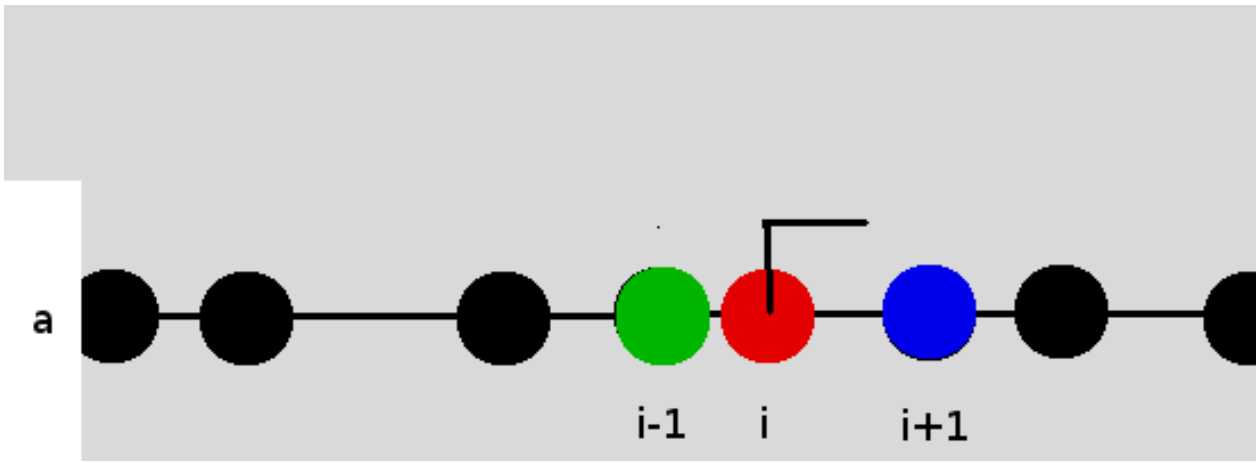
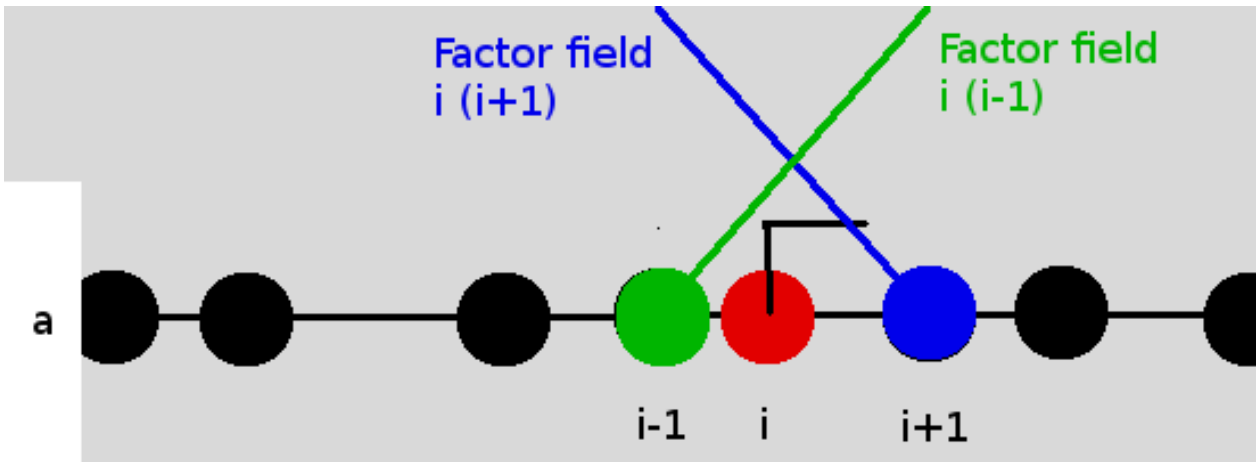
Event-chain algorithm with factor fields (1/4)

- Hard-sphere event-chain algorithm (standard version):



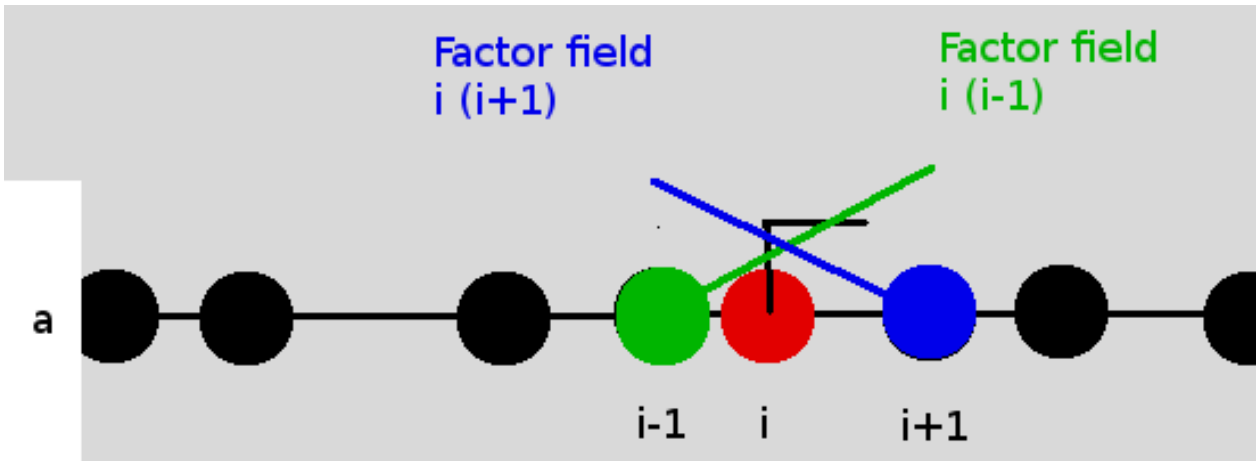
Event-chain algorithm with factor fields (2/4)

- Hard-sphere event-chain algorithm (factor field version):



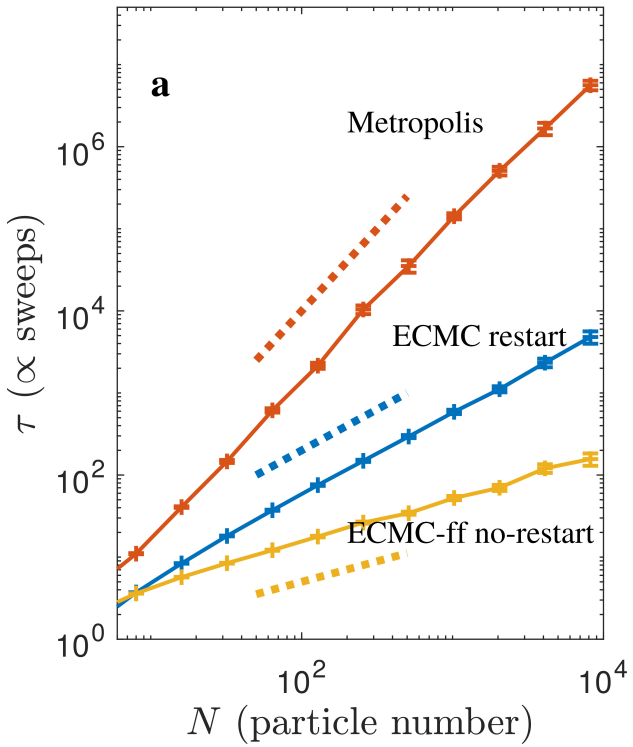
Event-chain algorithm with factor fields (3/4)

- Hard-sphere event-chain algorithm (variable factor field):



Event-chain algorithm with factor fields (4/4)

- Scaling of auto-correlation times (optimal factor field):



- Algebraic correlations of event steps $u \in \{-1, 1\}$ with event time s: $\langle u(0)u(s)\rangle \sim s^{-2/3}$.
- Lei, Krauth, Maggs (PRE, 2019).

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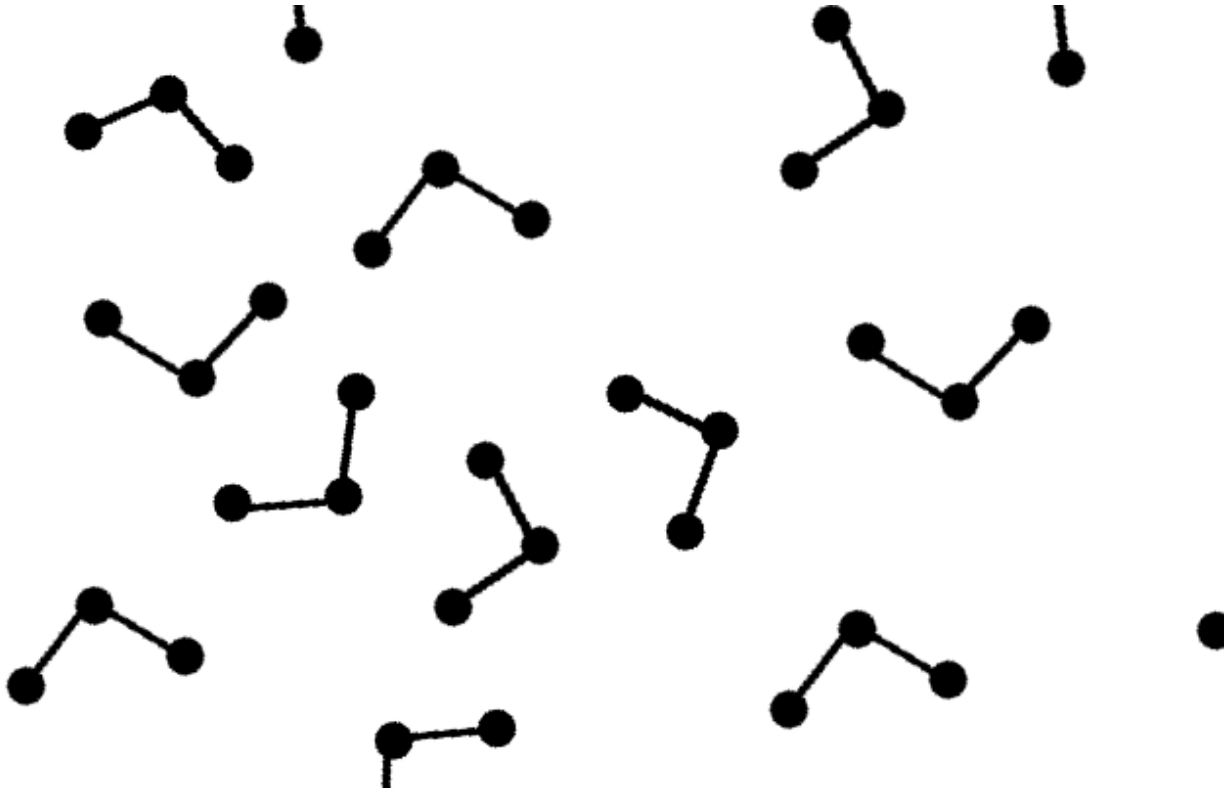
All-Atom Coulomb problem (1/5)



- 3D water model: bond, bending, Lennard-Jones, Coulomb (SPC/Fw).

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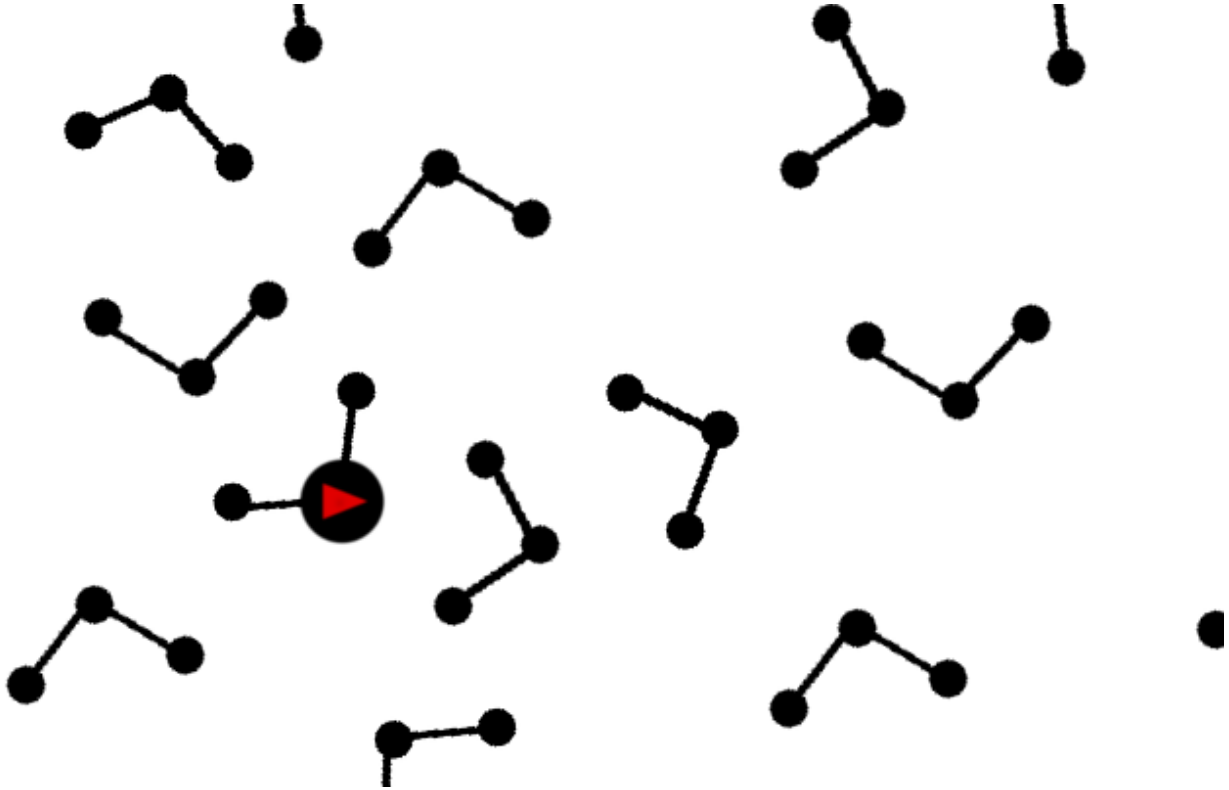
All-Atom Coulomb problem (2/5)



- 3D water model: bond, bending, Lennard-Jones, Coulomb (SPC/Fw).
- Factors and types.

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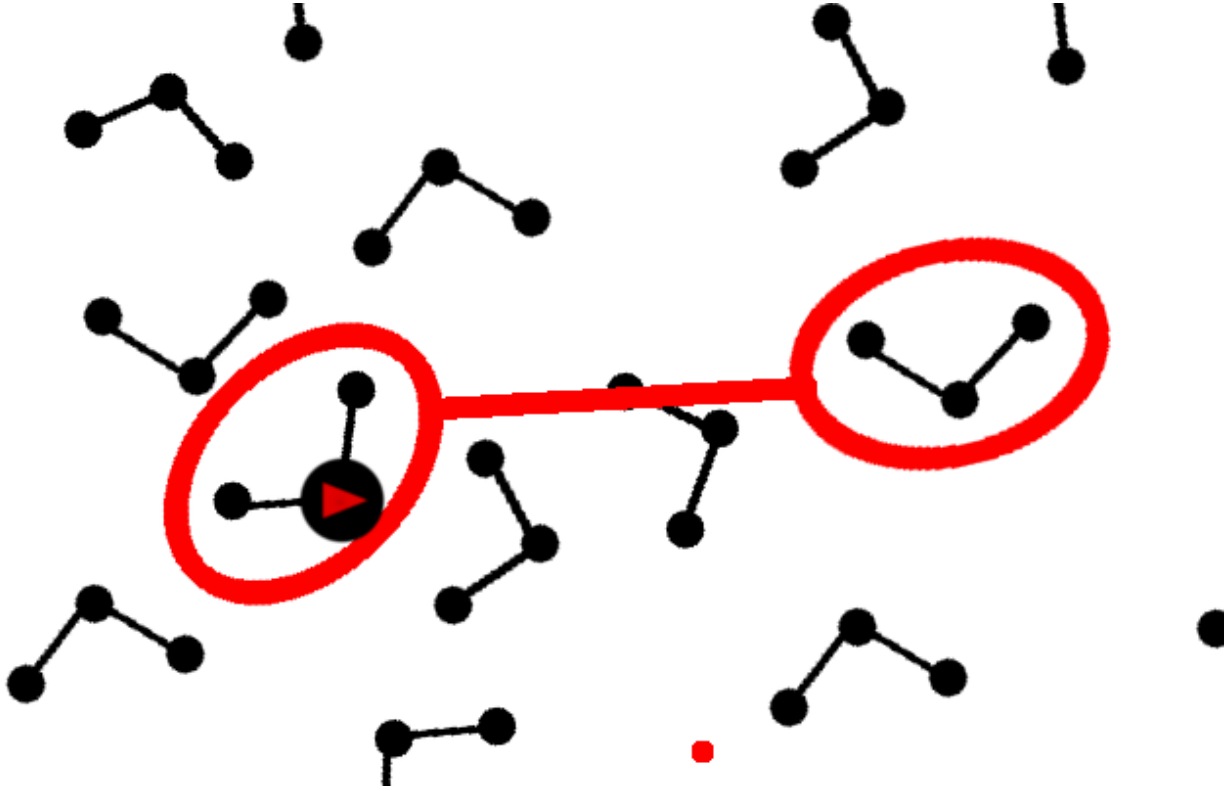
All-Atom Coulomb problem (3/5)



- Factor $M = (I_M, T_M)$: $|I_M| = 6$, two molecules. $T_M =$ 'Coulomb'.

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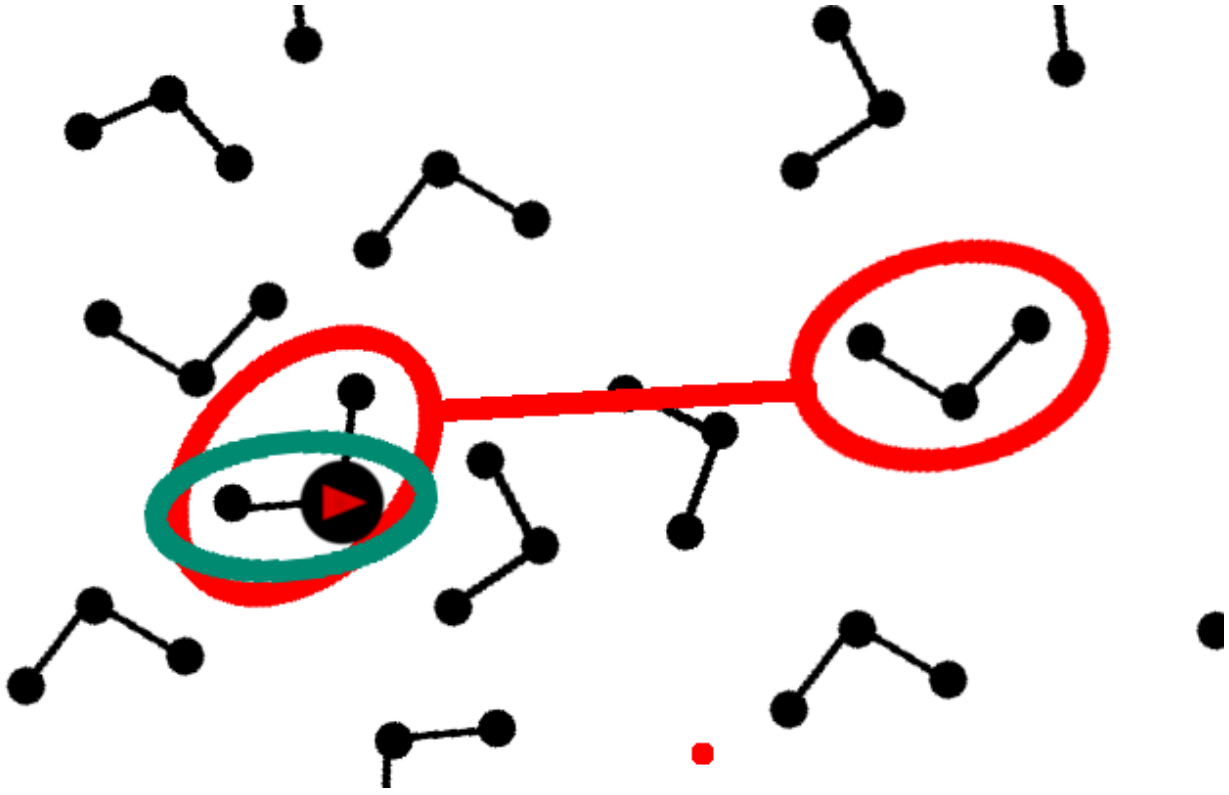
All-Atom Coulomb problem (4/5)



- Water model: bond, bending, Lennard-Jones, Coulomb (SPC/Fw).

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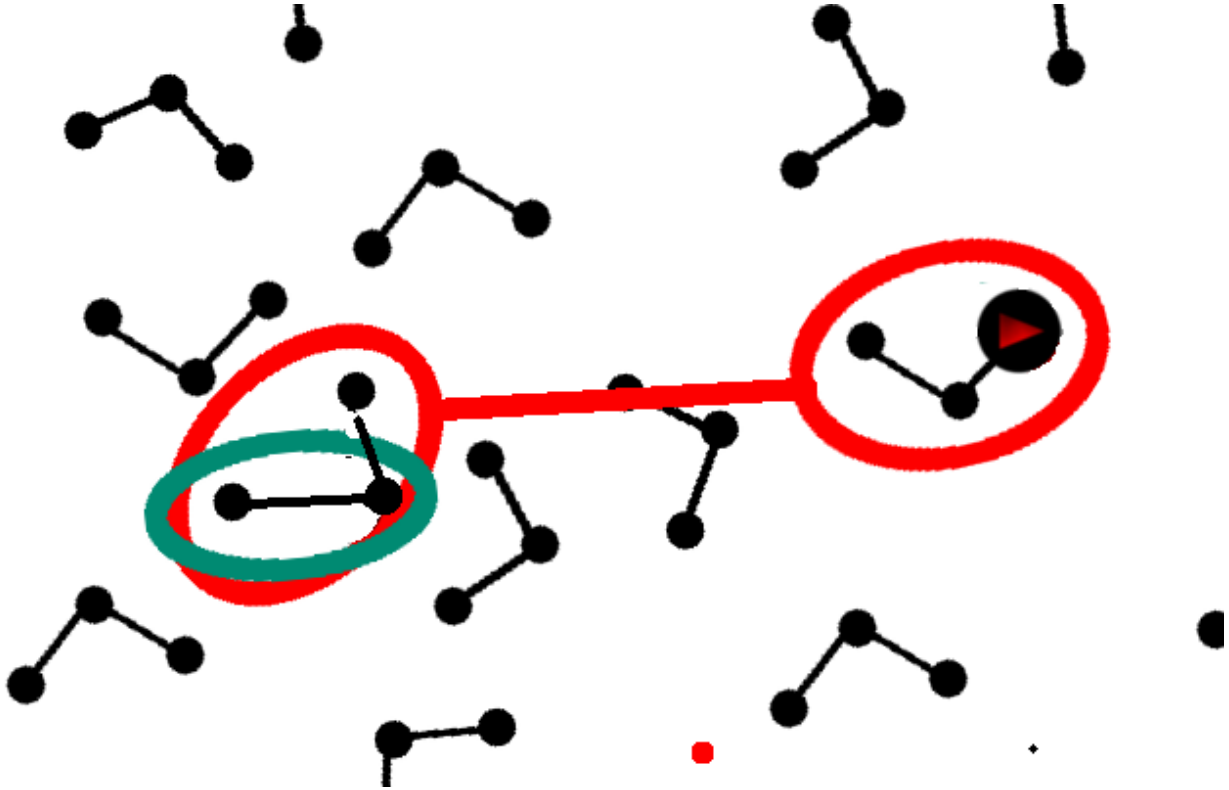
All-Atom Coulomb problem (5/5)



- Complexity $\mathcal{O}(1)$ per 'lifting' move.
- This is the cell-veto algorithm (Kapfer, Krauth (2016)).
- Thinning, Walker (1977).

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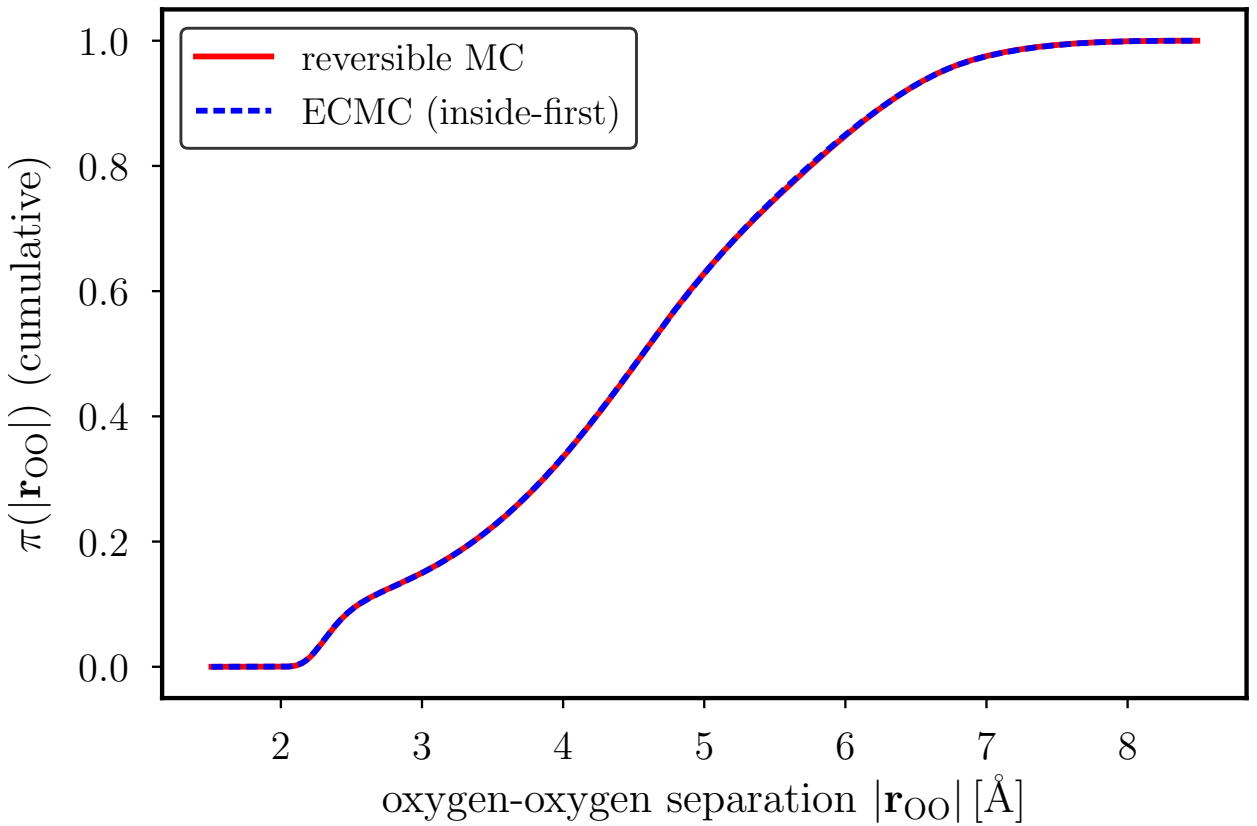
ECMC for all-atom water simulations

- ECMC: Event-driven, approximation-free, canonical.
- here oxygen–oxygen distance for 32 water molecules.



See: Faulkner, Qin, Maggs, Krauth (2018).

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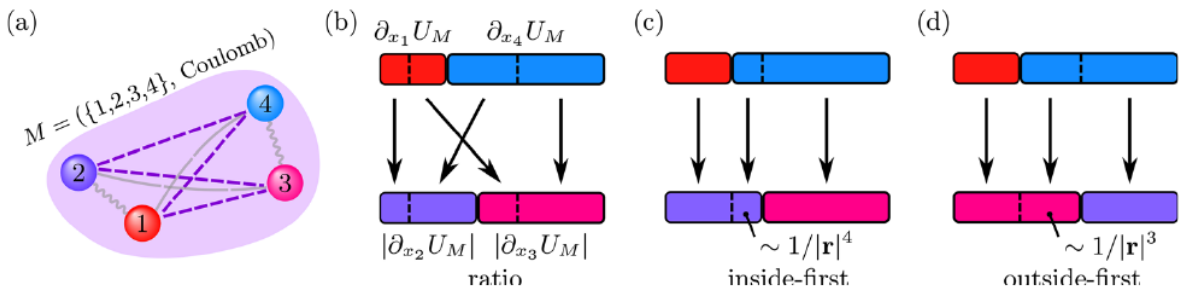
Lifting schemes and performance (1/3)

- Lifting schemes for factors M with $I_M > 2$ (here, $I_M = 4$)



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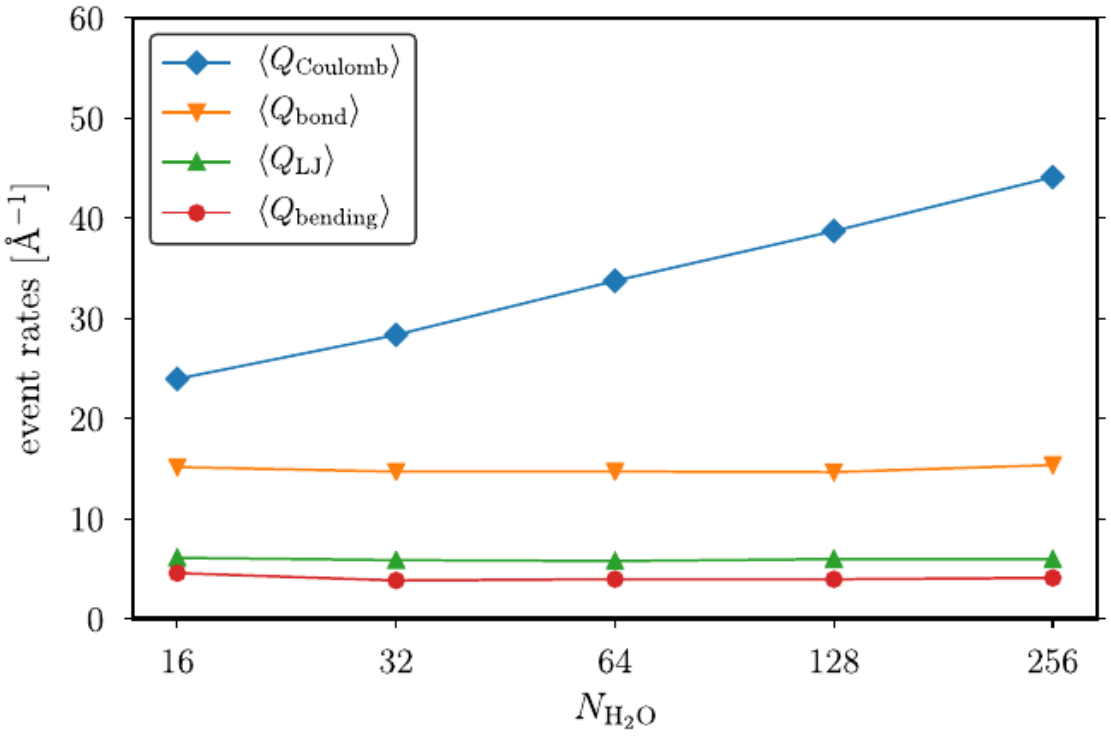
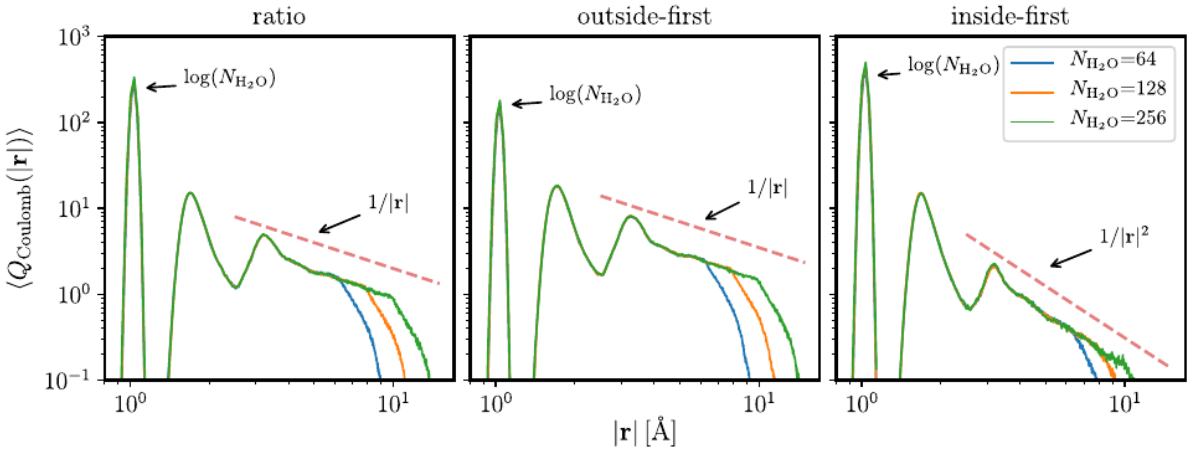
Lifting schemes and performance (2/3)

- Events / Angstrom in SPC/Fw water



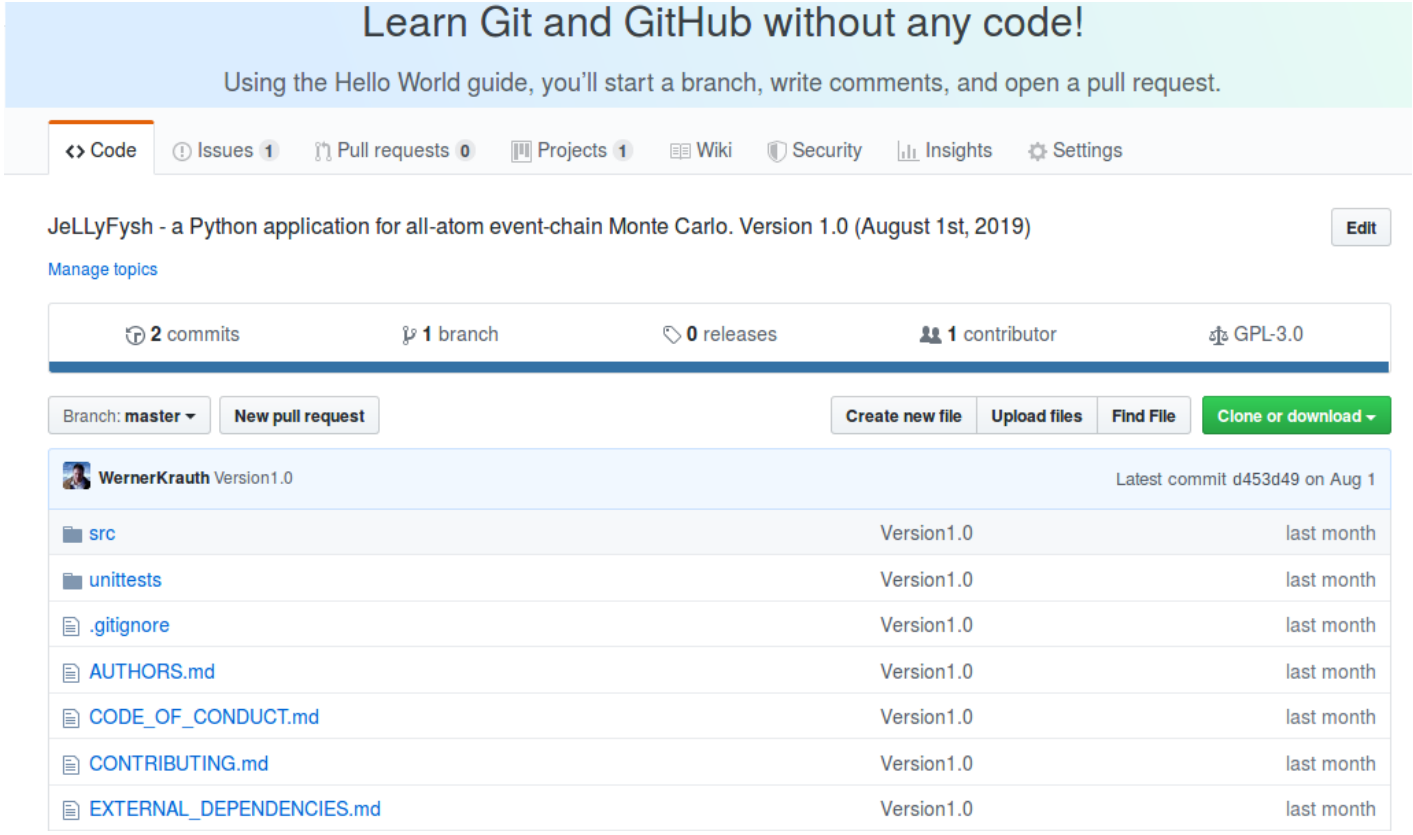
Lifting schemes and performance (3/3)

- Local moves with far-away mediators



See: Faulkner, Qin, Maggs, Krauth (2018).

ECMC - JeLLyFysh (1/2)



- cf Höllmer, Qin, Faulkner, Maggs & Krauth:
  - see arXiv:1907.12502 (2019)
  - 'JeLLyFysh' Open-source Python application for irreversible Markov chains

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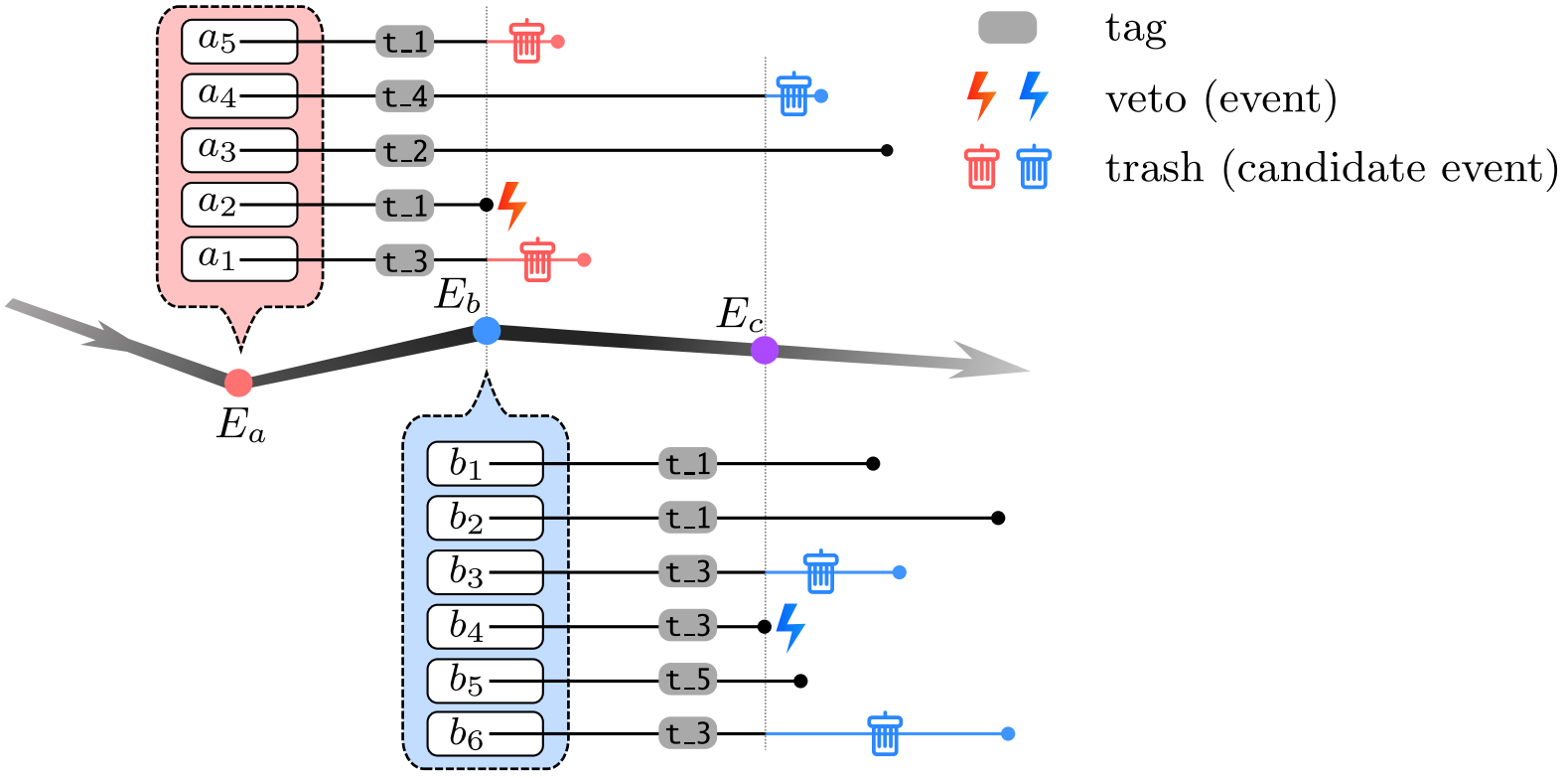
ECMC - JeLLyFysh (2/2)



- cf Höllmer, Qin, Faulkner, Maggs & Krauth:
  - see arXiv:1907.12502 (2019)
  - 'JeLLyFysh' Open-source Python application for irreversible Markov chains

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Conclusions

- From hard disks to SPC/Fw water all-atom
- Detailed balance - global balance
- Sampling $\exp(-\beta U)$ without knowing U

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Conclusions

- From hard disks to SPC/Fw water all-atom
- Equilibrium - steady state
- Consensus replacing force calculations

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Conclusions

- From hard disks to SPC/Fw water all-atom
- Equilibrium - steady state (indistinguishable from equilibrium)
- Factors & factorized Metropolis algorithm

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