

Fast non-reversible Markov chains in statistical physics

Werner Krauth

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02 March 2022 Seminar

King's College London, London (Great Britain)

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)

B. Li, Y. Nishikawa, P. Höllmer, L. Carillo, A. C. Maggs, W. Krauth, arXiv 202203XXX
Hard-disk computer simulations—a historic perspective

P. Höllmer, L. Qin, M. F. Faulkner, A. C. Maggs, W. Krauth (2020)
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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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

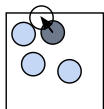
AND

EDWARD TELLER,* *Department of Physics, University of Chicago, Chicago, Illinois*
(Received March 6, 1953)

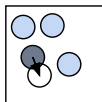
A general method, suitable for fast computing machines, for investigating such properties as equations of state for substances consisting of interacting individual molecules is described. The method consists of a modified Monte Carlo integration over configuration space. Results for the two-dimensional 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.



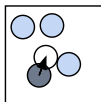
Metropolis et al (1953) (2/3)



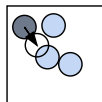
$i = 1$ (rej.)



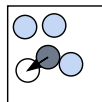
$i = 2$



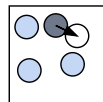
$i = 3$



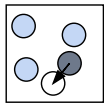
$i = 4$ (rej.)



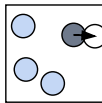
$i = 5$



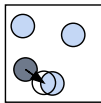
$i = 6$



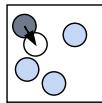
$i = 7$



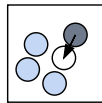
$i = 8$ (rej.)



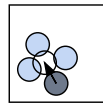
$i = 9$ (rej.)



$i = 10$

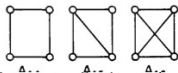


$i = 11$



$i = 12$ (rej.)

1092 METROPOLIS, ROSENBLUTH, ROSENBLUTH, TELLER, AND TELLER



distinguished by primes. For example, A_{33} is given schematically by the diagram



and mathematically as follows: if we define $f(r_{ij})$ by

$$f(r_{ij}) = 1 \quad \text{if } r_{ij} < d,$$

$$f(r_{ij}) = 0 \quad \text{if } r_{ij} > d,$$

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 $f_{12}=f_{23}=f_{34}=f_{13}=1$. The number of trials for which $f_{45}=1$, divided by the total number of trials, is just $A_{5,5}$.

The data on $A_{4,5}$ 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.

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.

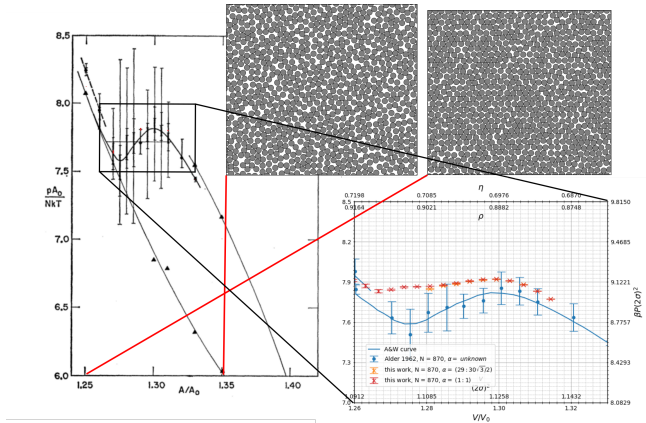
A STUDY has been made of a two-dimensional system consisting of 870 hard-disk particles. Simultaneous motions of the particles have been calculated by means of an electronic computer as described previously.¹ The disks were again placed in a periodically repeated rectangular array. The computer program

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

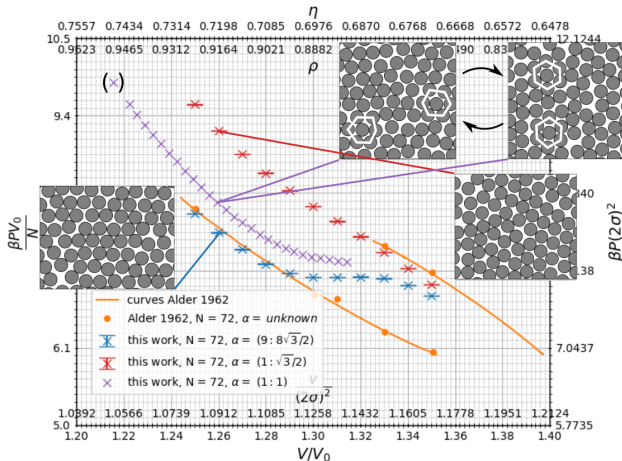


Alder–Wainwright (1962) (2/5)



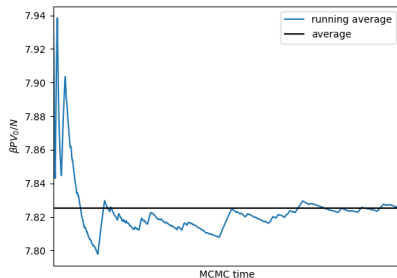
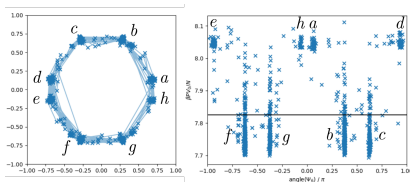
- Equation of state (Alder–Wainwright 1962)
- Revisited by Li et al. (2022)

Alder–Wainwright (1962) (3/5)



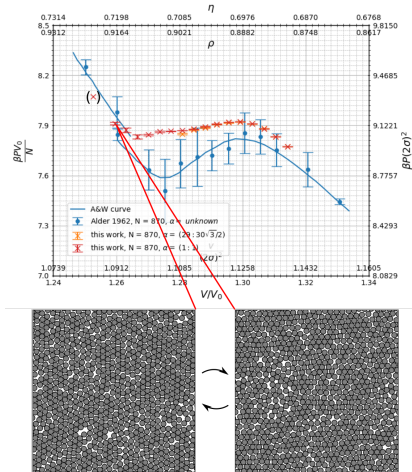
- Equation of state $N = 72$ (Alder–Wainwright 1962)
- Revisited by Li et al. (2022)

Alder–Wainwright (1962) (4/5)



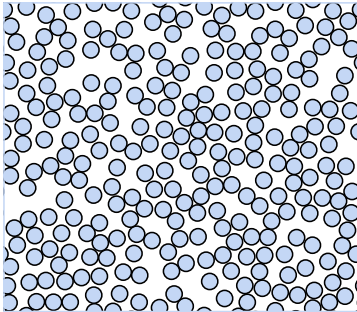
- Pressure (running average).
- 5-hour computation, state-of-the-art non-reversible code (2022)
- Density $\eta = 0.716$, 870 disks, square box.
- Li et al. (2022)

Alder–Wainwright (1962) (5/5)

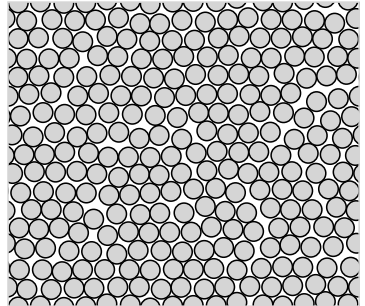


- Equation of state $N = 870$ (Alder–Wainwright 1962)
- Revisited by Li et al. (2022)

2D melting transition



density $\eta = 0.48$



$\eta = 0.72$

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

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

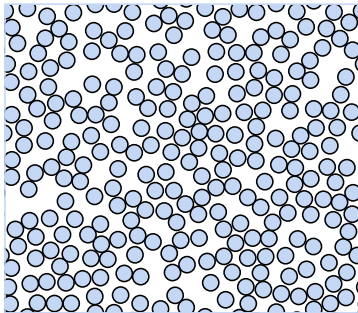
Received 13 November 1972

1. Introduction

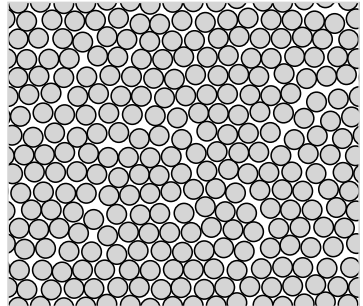
Peierls (1935) has argued that thermal motion of long-wavelength phonons will destroy the long-range order of a two-dimensional solid in the sense that the mean square deviation of an atom from its equilibrium position increases logarithmically with the size of the system, and the Bragg peaks of the 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



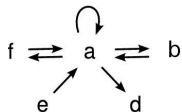
density $\eta = 0.48$



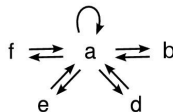
$\eta = 0.72$

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

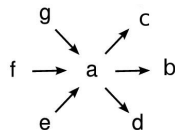
Detailed balance - global balance



global balance



detailed balance



maximal global balance

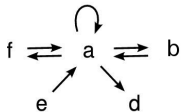
- flow into a = Boltzmann weight $\pi(a)$ (global balance condition):

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

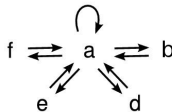
- flow $\mathcal{F}(a \rightarrow b) \equiv \text{flow } \mathcal{F}(b \rightarrow a)$ (detailed balance condition):

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

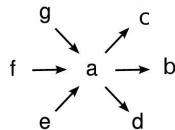
Detailed balance - global balance



global balance



detailed balance



maximal global balance

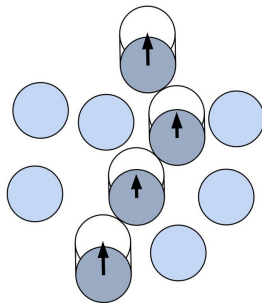
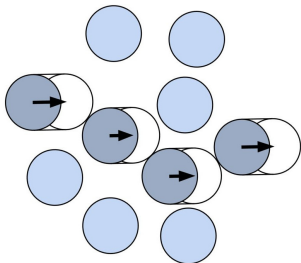
- flow into a = Boltzmann weight $\pi(a)$ (global balance condition):

$$\underbrace{\sum_k \pi(k) p(k \rightarrow a)}_{\text{flow into } a \sum_k \mathcal{F}(k \rightarrow a)} = \pi(a)$$

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

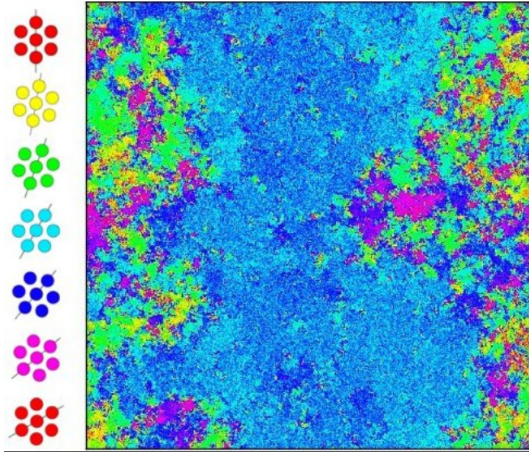
$$\underbrace{\pi(b) p(b \rightarrow a)}_{\text{flow from } b \text{ to } a \mathcal{F}(b \rightarrow a)} = \underbrace{\pi(a) p(a \rightarrow b)}_{\mathcal{F}(a \rightarrow b) \text{ flow from } a \text{ to } b}$$

Event-chain Monte Carlo



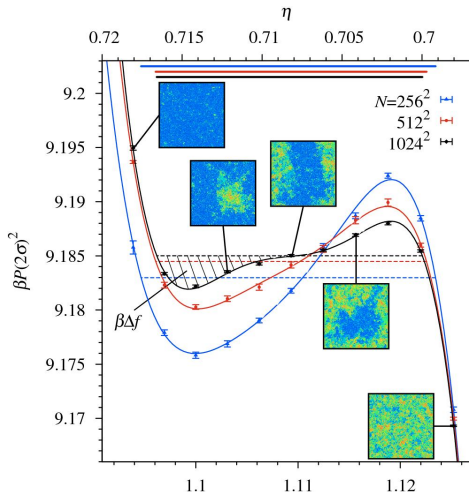
- Bernard et al. (2009)
- Simplest of many variants
- See Krauth (2021) Front. Phys.

Hard-disk configuration



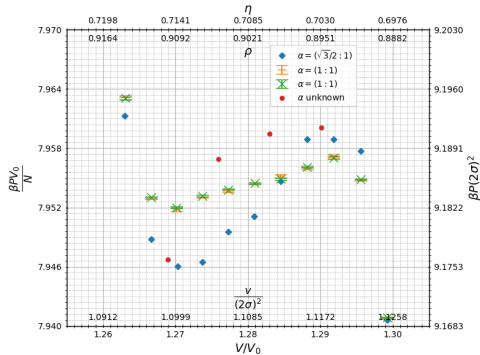
- 1024^2 hard disks
- Bernard, Krauth (PRL 2011)

Equilibrium equation of state



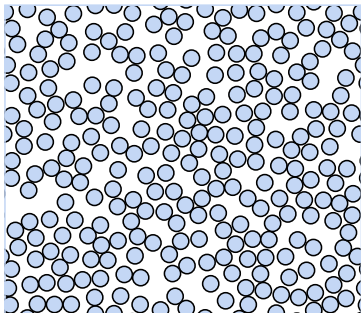
- 1st-order liquid-hexatic (Bernard & Krauth, PRL (2011)).
- Many confirmations (Engel, Anderson, Glotzer, Isobe, Bernard, Krauth, PRE Milestone (2013)).

Equilibrium equation of state

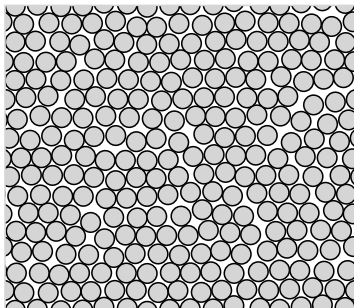


- Different views on the equation of state at $N = 1024^2$.

Possible phases (again)



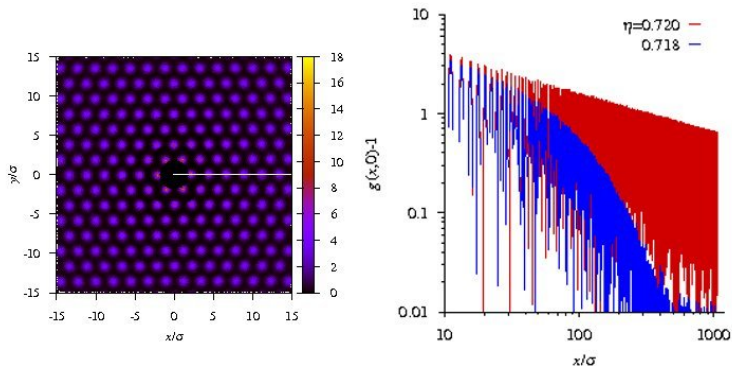
density $\eta = 0.48$



$\eta = 0.72$

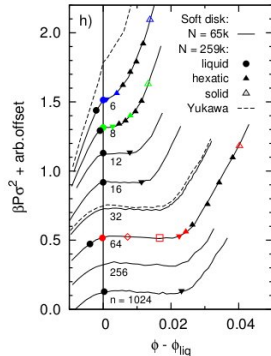
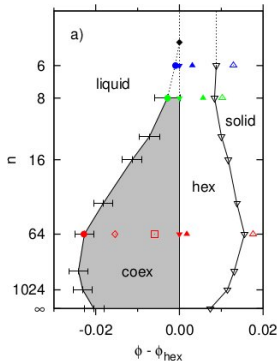
Phase	positional order	orientational order
solid	algebraic	long-range
hexatic	short-range	algebraic
liquid	short-range	short-range

Spatial correlations at $\eta = 0.718$ and 0.720



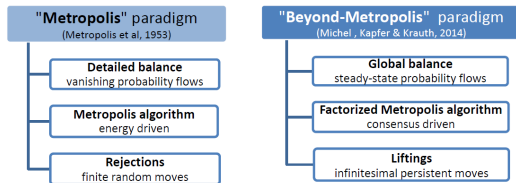
- Two-dimensional pair correlations, sample-averaged.
- At $\eta = 0.718$; hexatic: First-order liquid–hexatic transition.
- At $\eta \sim 0.720$: KT-type hexatic–solid transition.
- Bernard & Krauth (PRL 2011).
- Many confirmations.

- 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

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

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

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

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

Factorized Metropolis algorithm (2/2)

- Total system potential

$$U(\{s_1, \dots, s_N\}) = \sum_{M \in \Omega} U_M(\{s_i : i \in I_M\}).$$

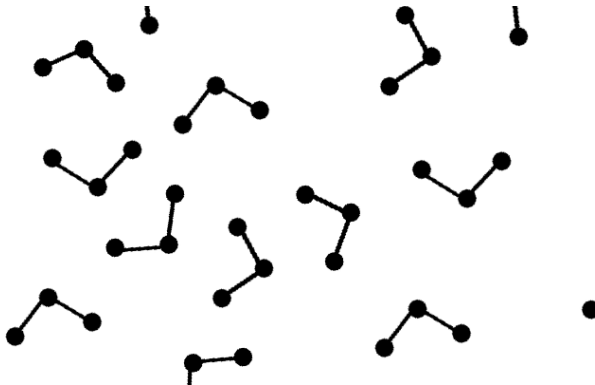
- $M = (I_M, T_M)$ factor, I_M : index set, T_M : factor type.
- Factorized Metropolis algorithm:

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

- Consensus:

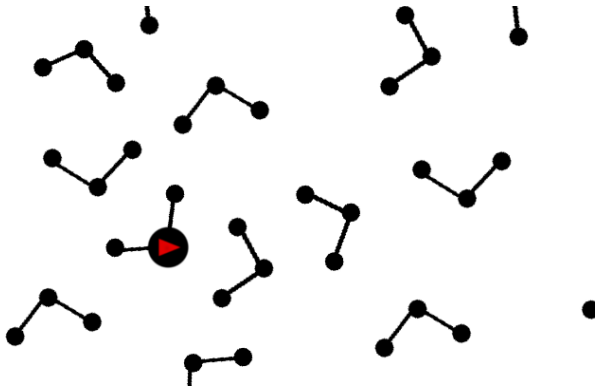
$$X^{\text{Fact}}(c \rightarrow c') = \bigwedge_{M \in \Omega} X_M(c_M \rightarrow c'_M).$$

All-Atom Coulomb problem (1/5)



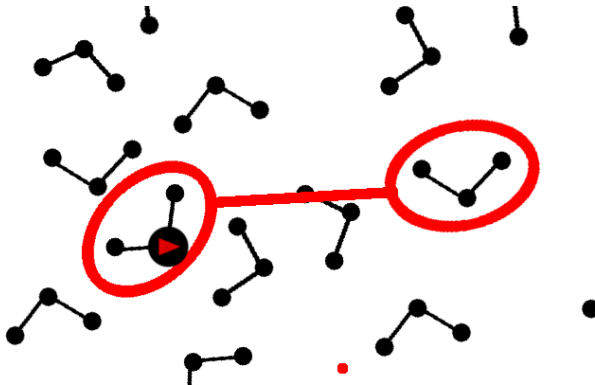
- 3D water model: bond, bending, Lennard-Jones, Coulomb (SPC/Fw).

All-Atom Coulomb problem (2/5)



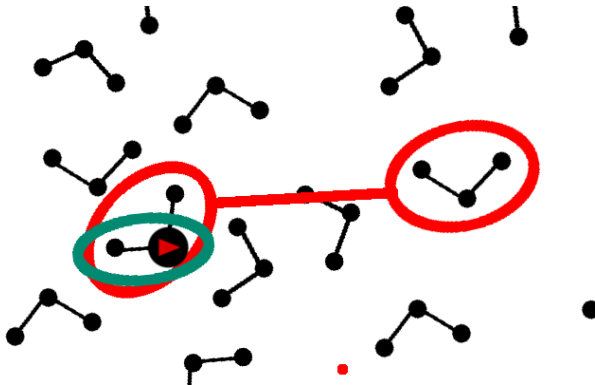
- 3D water model: bond, bending, Lennard-Jones, Coulomb (SPC/Fw).
- Factors and types.

All-Atom Coulomb problem (3/5)



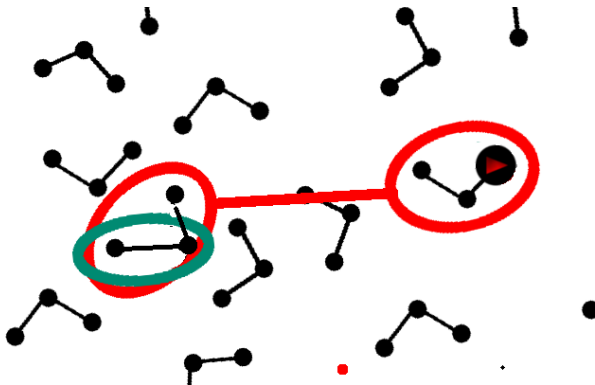
- Factor $M = (I_M, T_M)$: $|I_M| = 6$, two molecules. $T_M =$ 'Coulomb'.

All-Atom Coulomb problem (4/5)



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

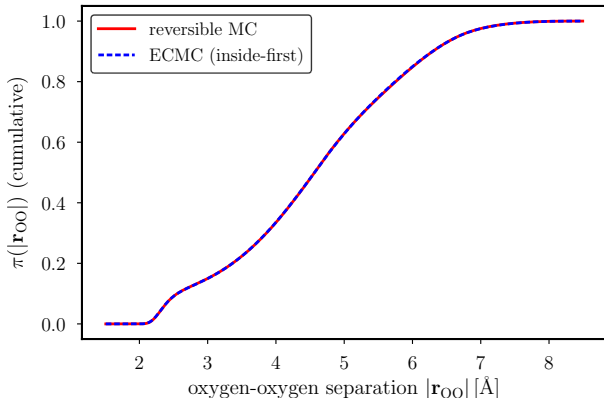
All-Atom Coulomb problem (5/5)



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

ECMC for all-atom water simulations

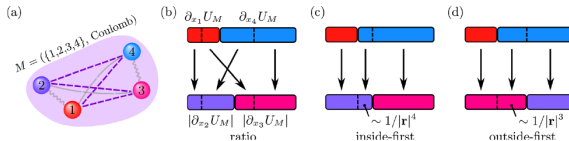
- ECMC: Event-driven, approximation-free, canonical.
- here oxygen–oxygen distance for 32 water molecules.



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

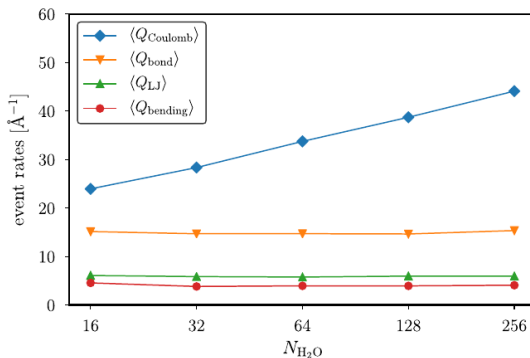
Lifting schemes and performance (1/3)

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



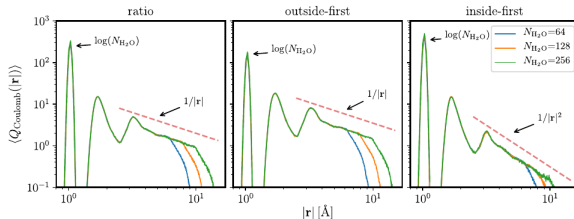
Lifting schemes and performance (2/3)

- 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)

Learn Git and GitHub without any code!

Using the Hello World guide, you'll start a branch, write comments, and open a pull request.


<> Code ⓘ Issues ⓘ 📁 Pull requests 0 📁 Projects 1 📖 Wiki 🛡 Security 📊 Insights ⚙ Settings

JeLLyFysh - a Python application for all-atom event-chain Monte Carlo. Version 1.0 (August 1st, 2019) [Edit](#)

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📁 2 commits 📁 1 branch 📁 0 releases 👤 1 contributor 📄 GPL-3.0

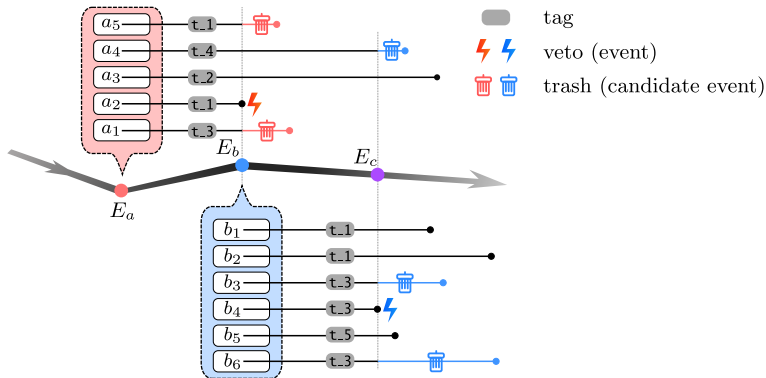
Branch: master ▾ [New pull request](#) [Create new file](#) [Upload files](#) [Find File](#) [Clone or download ▾](#)

 WernerKrauth Version 1.0 Latest commit d453d49 on Aug 1

src	Version 1.0	last month
unittests	Version 1.0	last month
.gitignore	Version 1.0	last month
AUTHORS.md	Version 1.0	last month
CODE_OF_CONDUCT.md	Version 1.0	last month
CONTRIBUTING.md	Version 1.0	last month
EXTERNAL_DEPENDENCIES.md	Version 1.0	last month

- cf Höllmer, Qin, Faulkner, Maggs & Krauth (2020):
 - ‘JeLLyFysh’ Open-source Python application for non-reversible Markov chains

ECMC - JeLLyFysh (2/2)



- cf Höllmer, Qin, Faulkner, Maggs & Krauth (2020):
 - ‘JeLLyFysh’ Open-source Python application for non-reversible Markov chains

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

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

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