Monte Carlo algorithms for hard spheres, 2D melting transition

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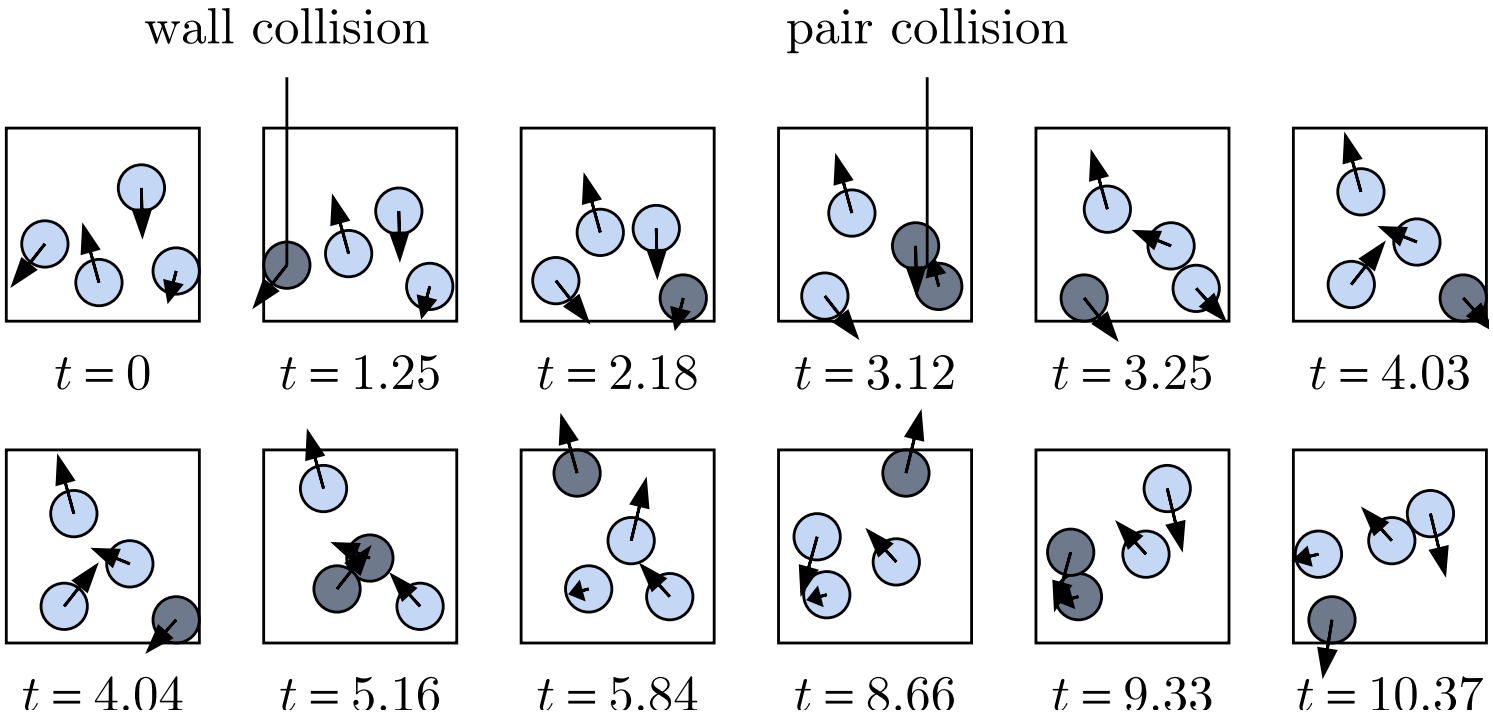
Melbourne, 28 July 2010

Table of contents

Molecular dynamics ('Newton')

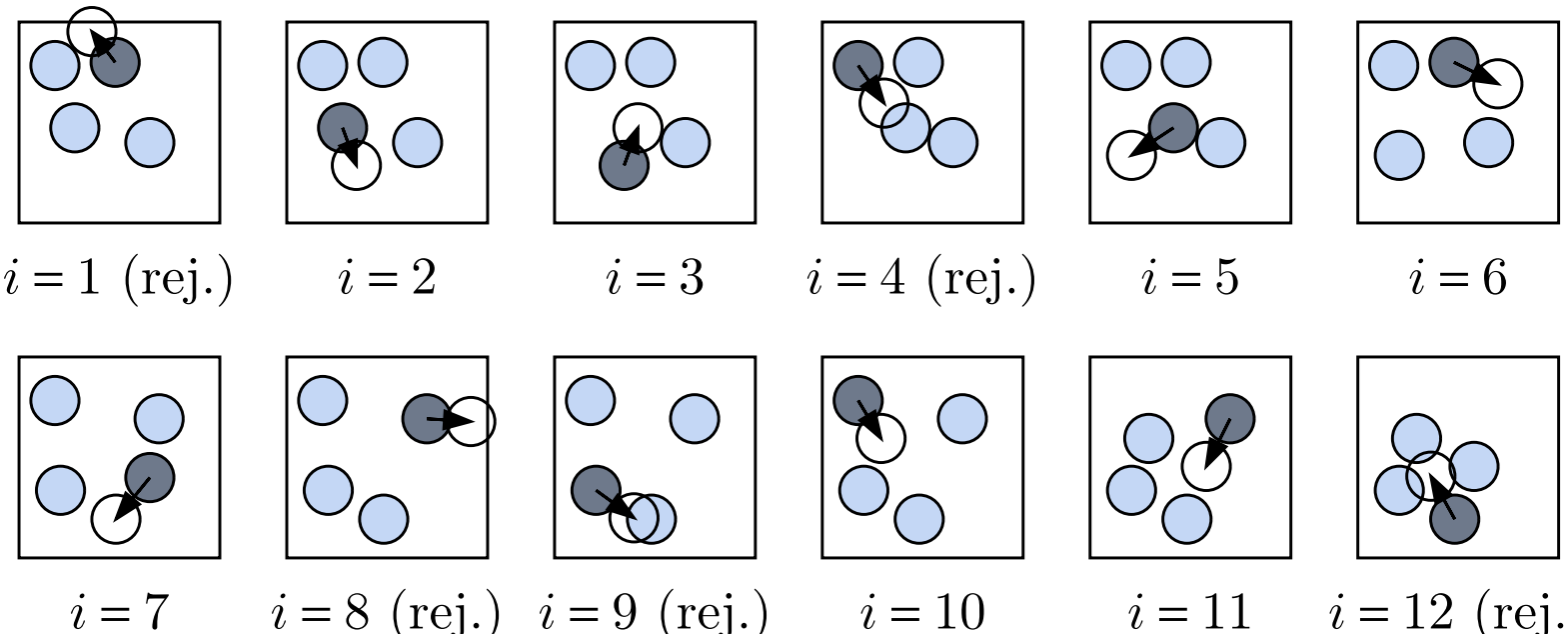
- A molecular dynamics algorithm for hard spheres (billiard):



- . . . starting point of Molecular dynamics, in 1957 . . .
- . . . treats positions and velocities . . .
- . . . useful for $N \gg 4$, but times extremely short . . .
- . . . converges towards thermal equilibrium.

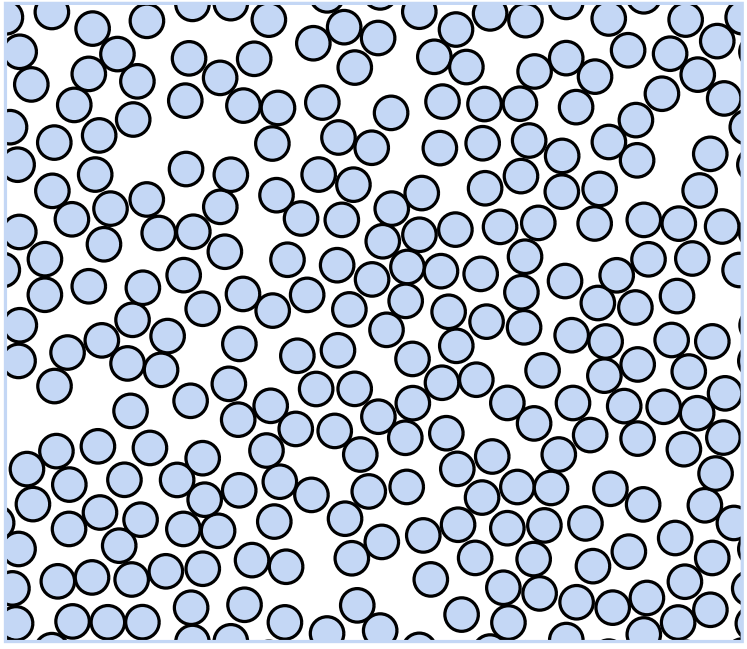
Markov-chain Monte Carlo ('Boltzmann')

- A local Markov-chain Monte Carlo algorithm for hard spheres (billiard):

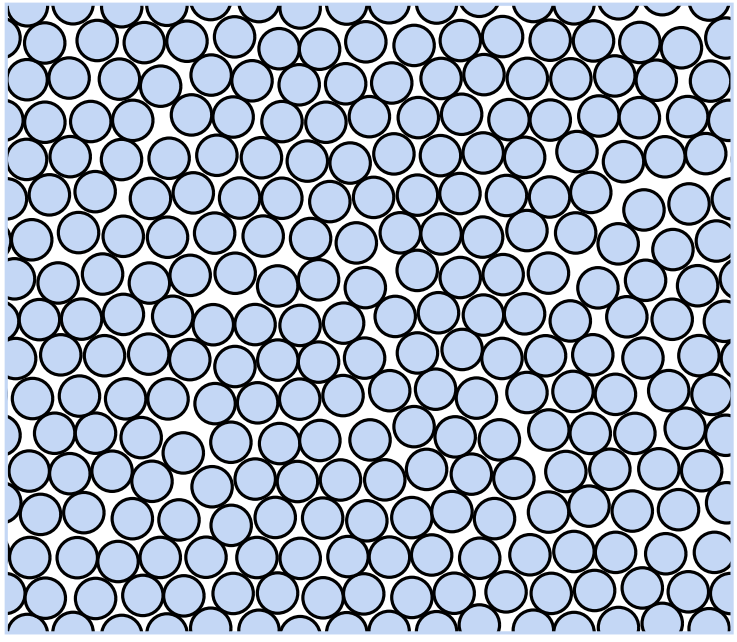


- . . . starting point of Markov chain Monte Carlo, in 1953 . . .
- . . . treats only positions . . .
- . . . useful for $N \gg 4$ . . .
- . . . converges towards thermal equilibrium.

2D melting transition



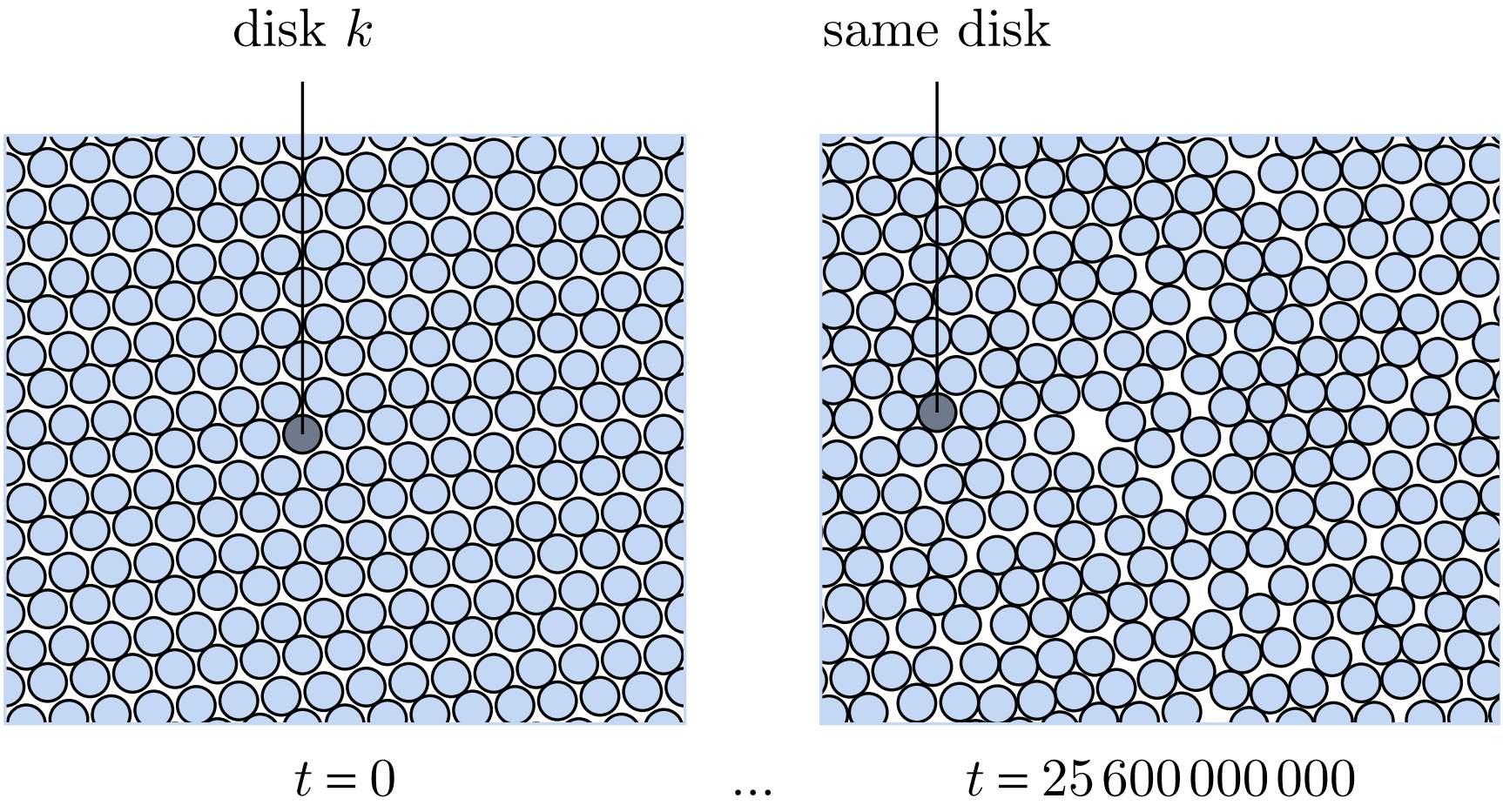
density $\eta = 0.48$



density $\eta = 0.72$

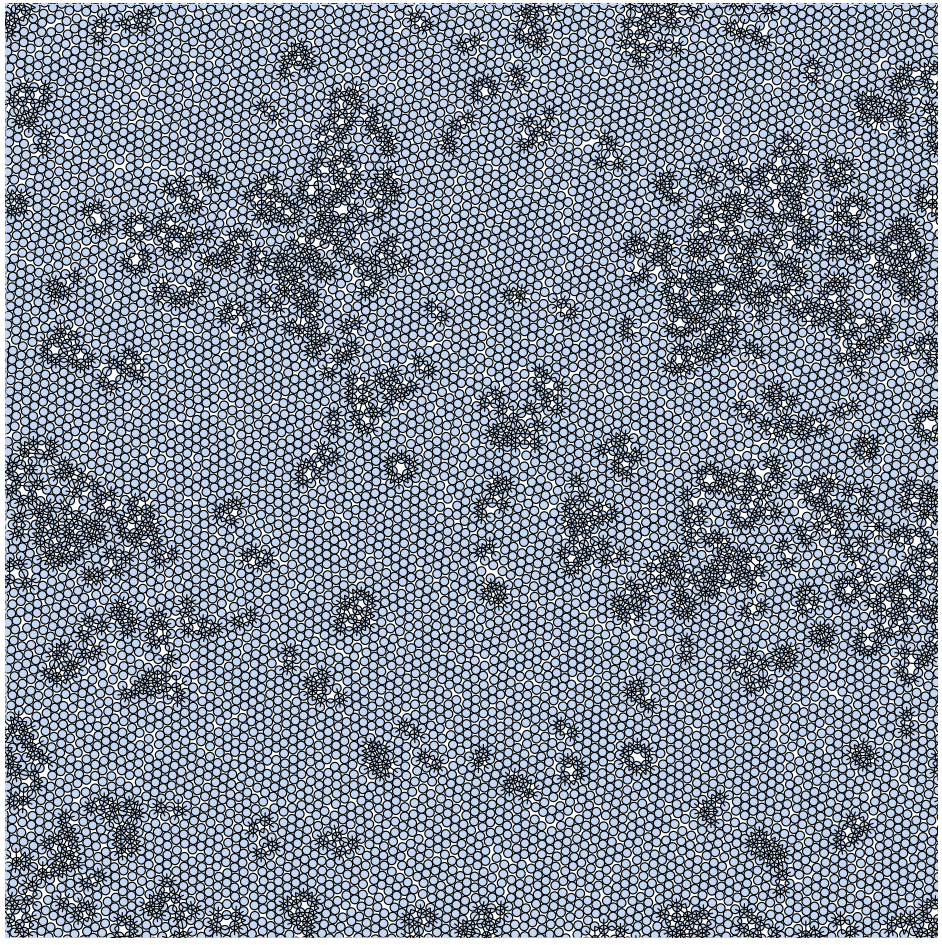
- At low density, disks move easily (liquid)
- . . . at high density, MC algorithms slow down and disks crystallize . . .
- . . . but nature of transition long disputed (first order vs. KTHNY)
- cf. Blöte et al. (2002); van Enter, Schlosman (2002)

Correlation time in larger simulations



- τ exists, but it is large ($\tau \gg 25\,600\,000\,000$).

Correlation time in systems of current interest

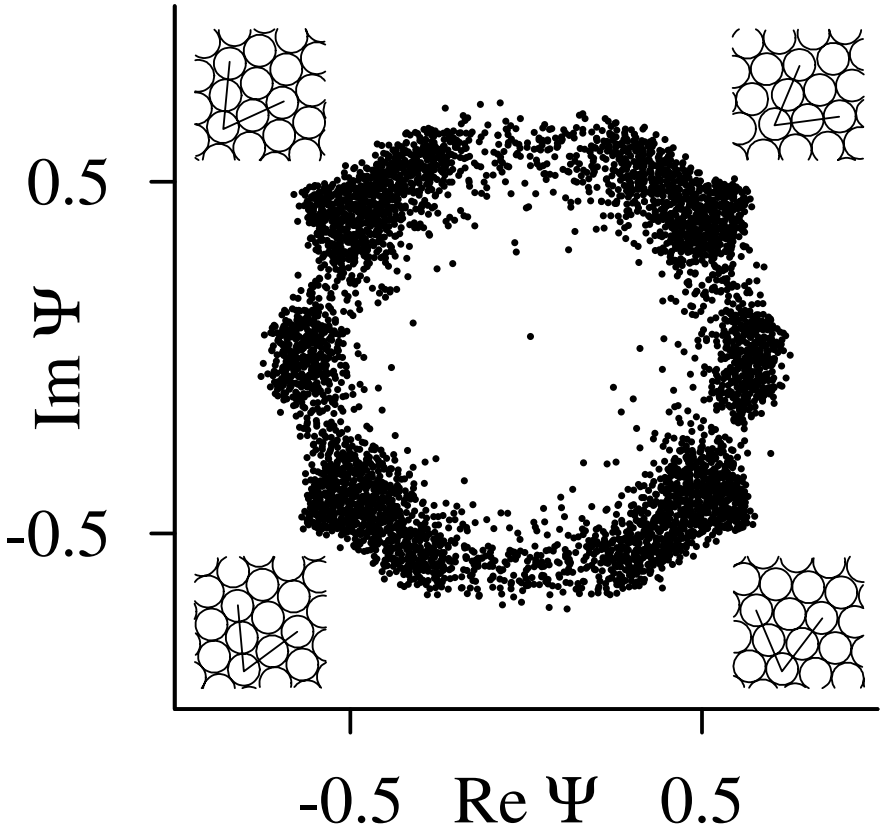


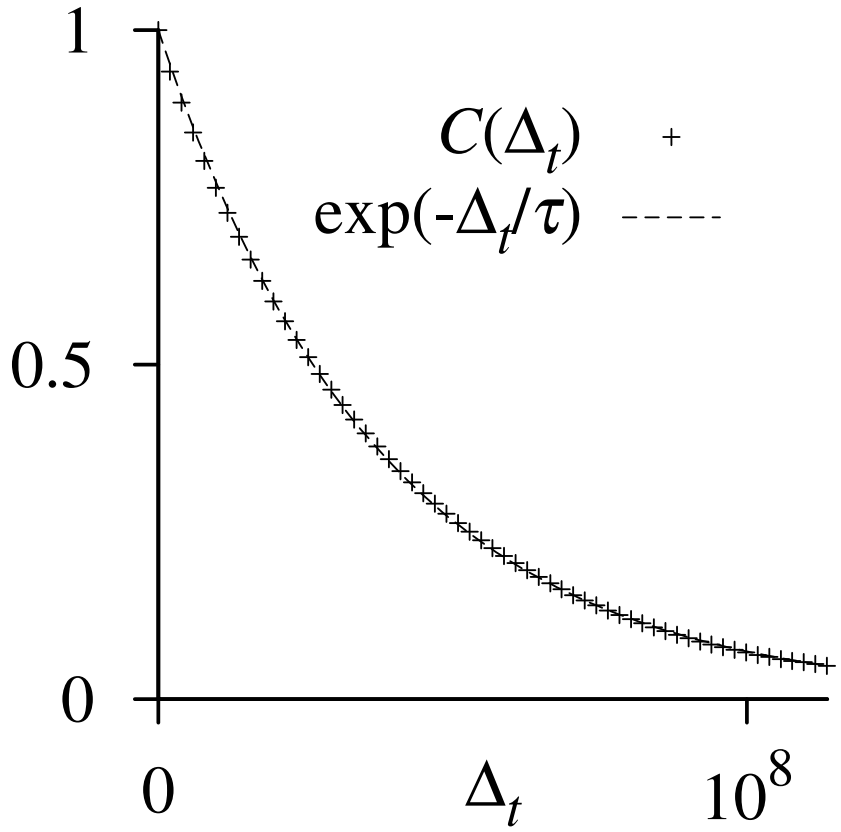
- τ still exists . . .

Things we want to do

- Knowing correlation time τ would be nice (Part I).
- Faster algorithms would be nice (Part II).
- Understanding why they are faster would be nice.
- Doing interesting physics with them would be nice (Part III).
- An infinitely long simulation is best (Part IV).

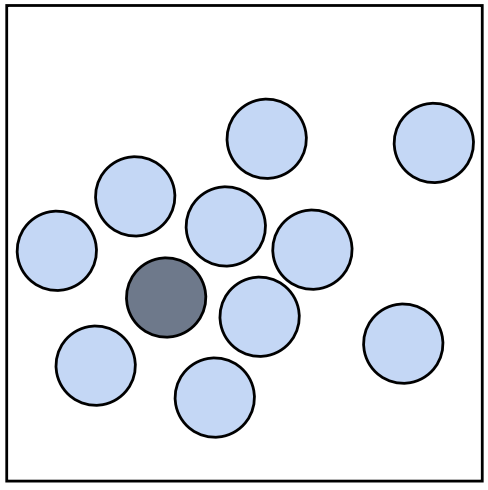
Correlation time (square box)



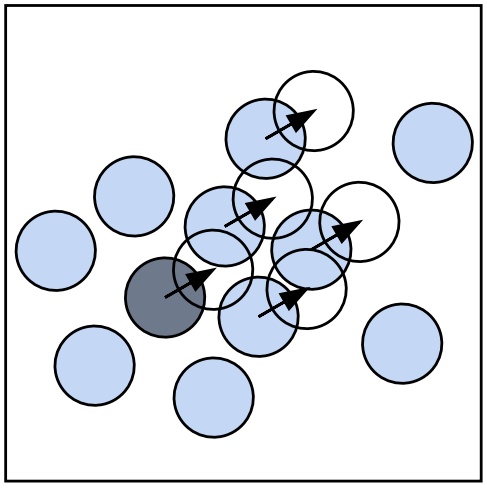


- Hypothesis: Correlation time $\equiv$ correlation time of order parameter
- . . . much more cautious than others . . .

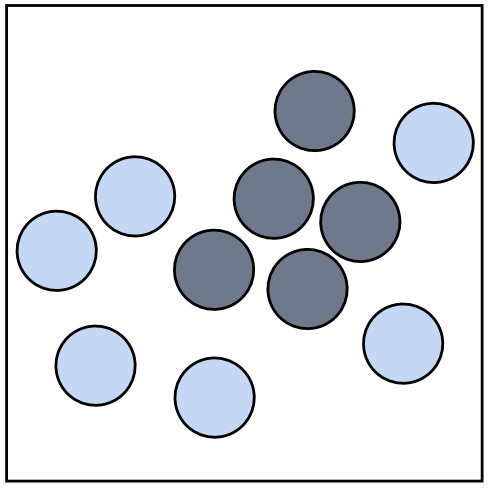
‘Avalanche’ Monte Carlo I



a

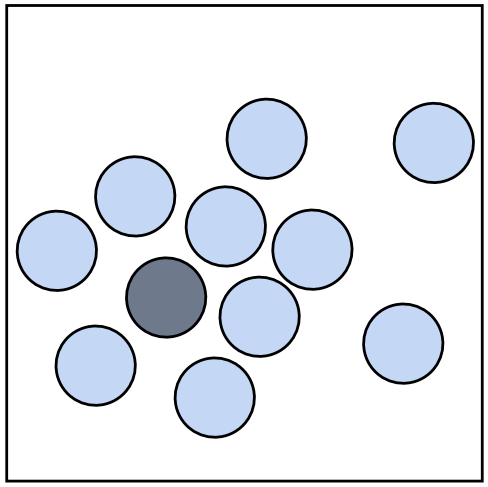


a (+ move)



b

‘Avalanche’ Monte Carlo II



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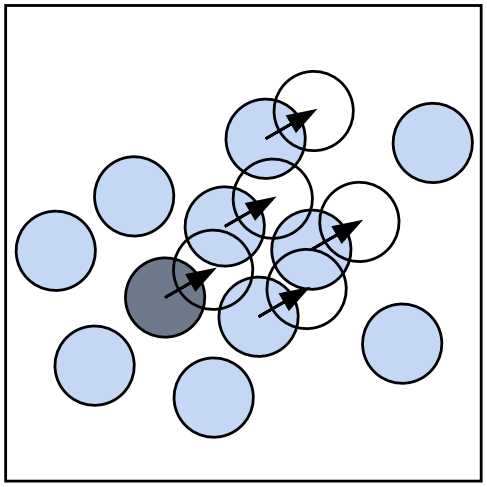
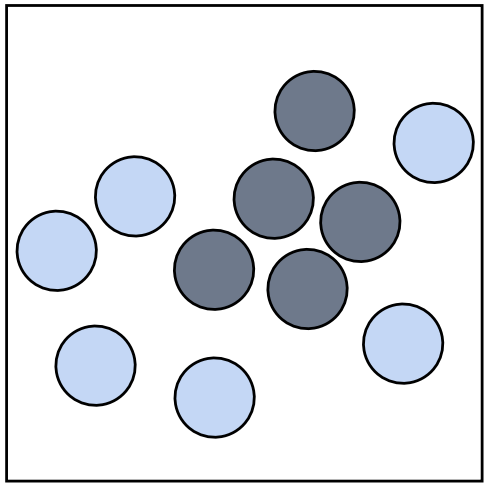
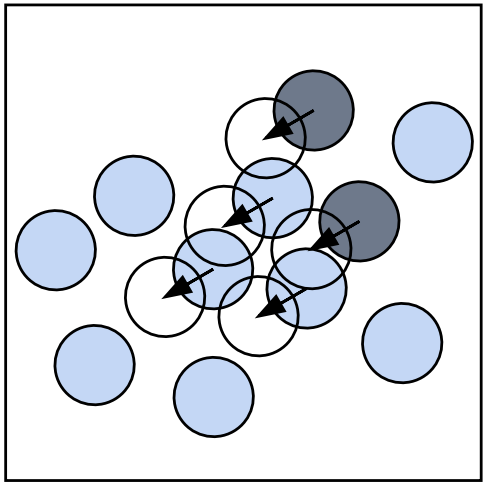


a (+ move)



b

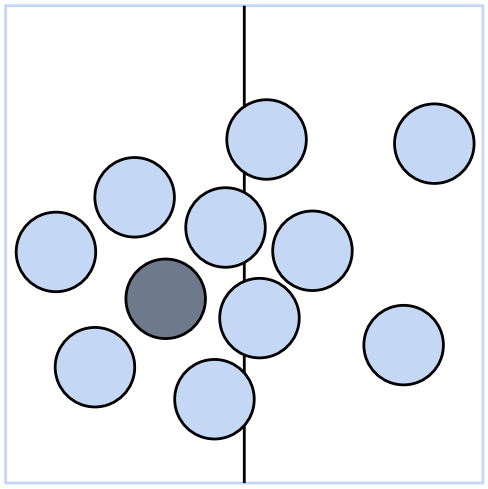


b (+ return move)

‘Avalanche’ Monte Carlo (conclusion)

- Avalanche Monte Carlo has problems with detailed balance
- . . . and is related to the ‘independent set’ problem. . .
- cf. Jaster (1999, 2004)

Pivot cluster algorithm I



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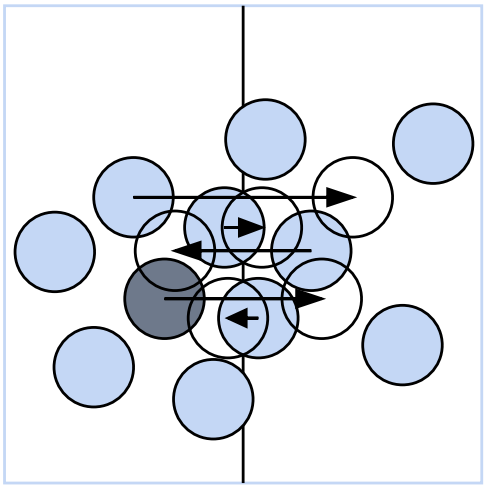
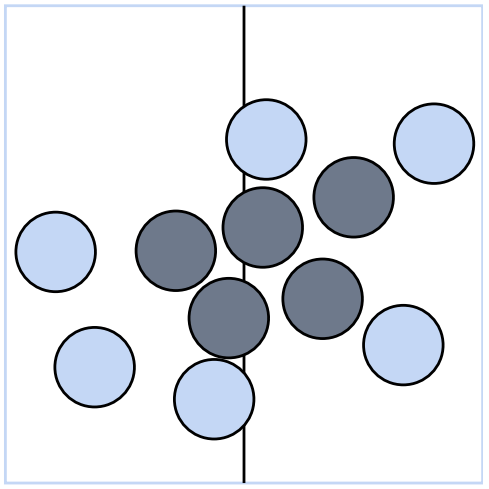
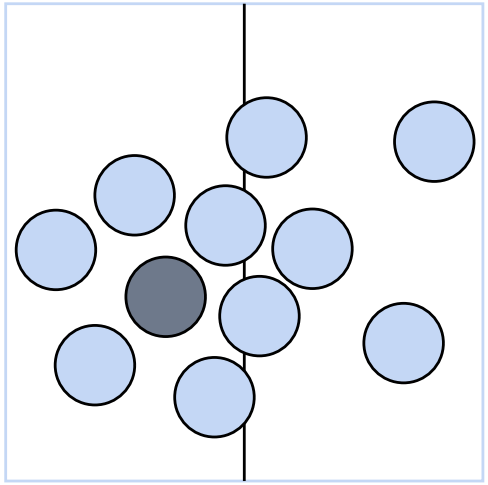


a (+ move)

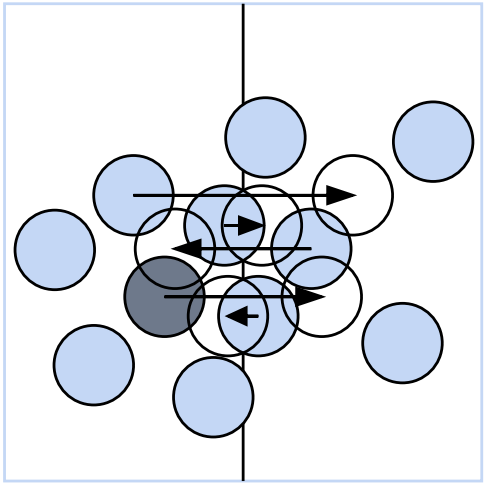


b

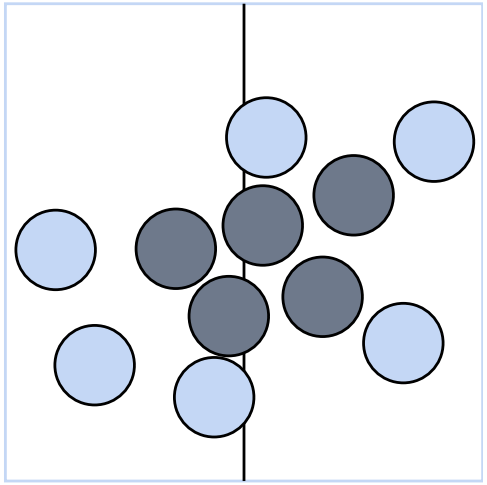
Pivot cluster algorithm II



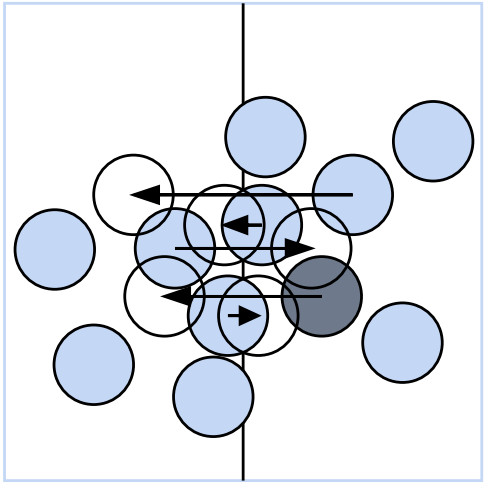
a



a (+ move)

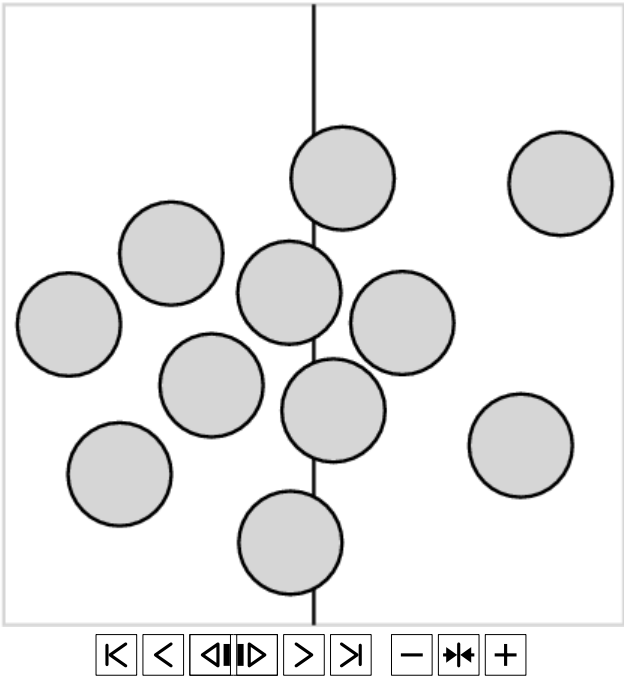


b



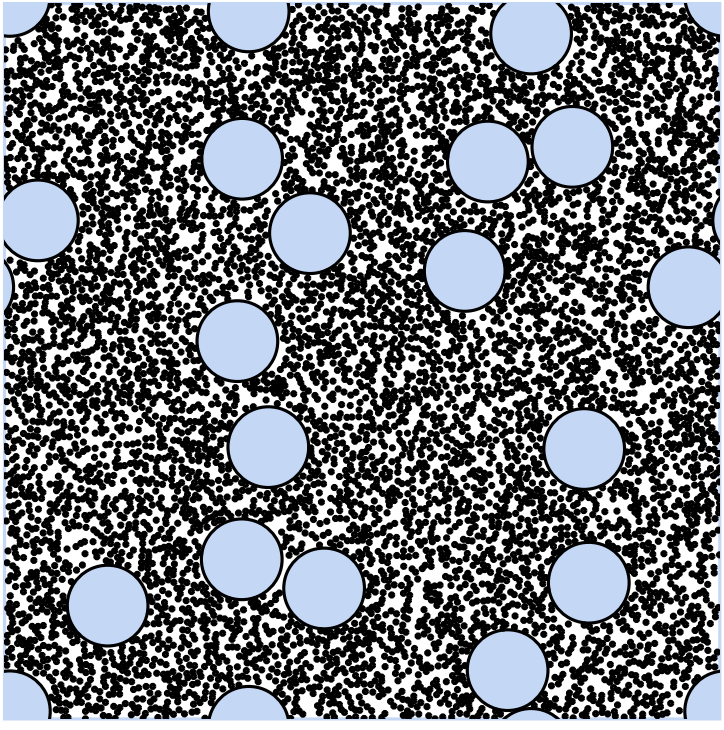
b (+ return move)

Pivot cluster algorithm for hard spheres

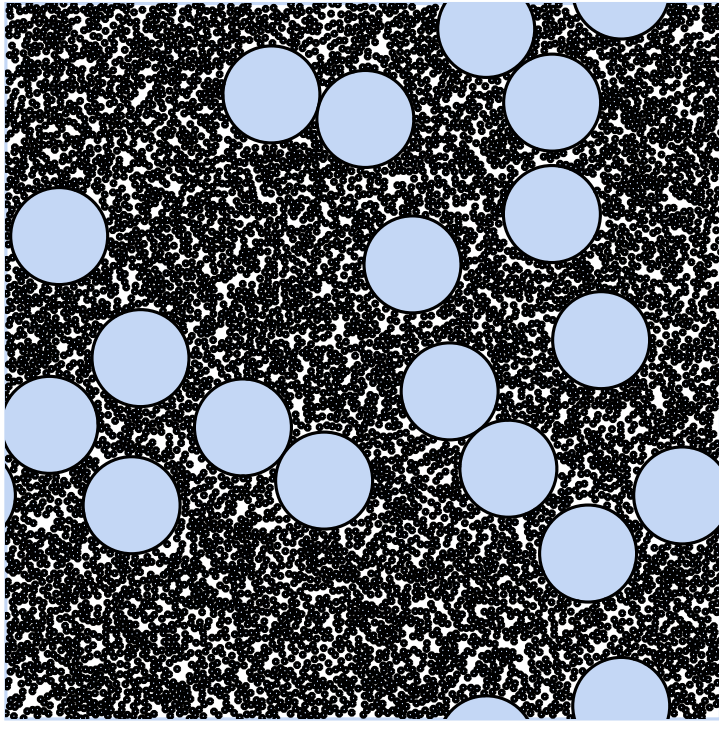


- Dress, Krauth (1995)
- Many applications, but fails for 2d melting.

Binary mixtures of disks



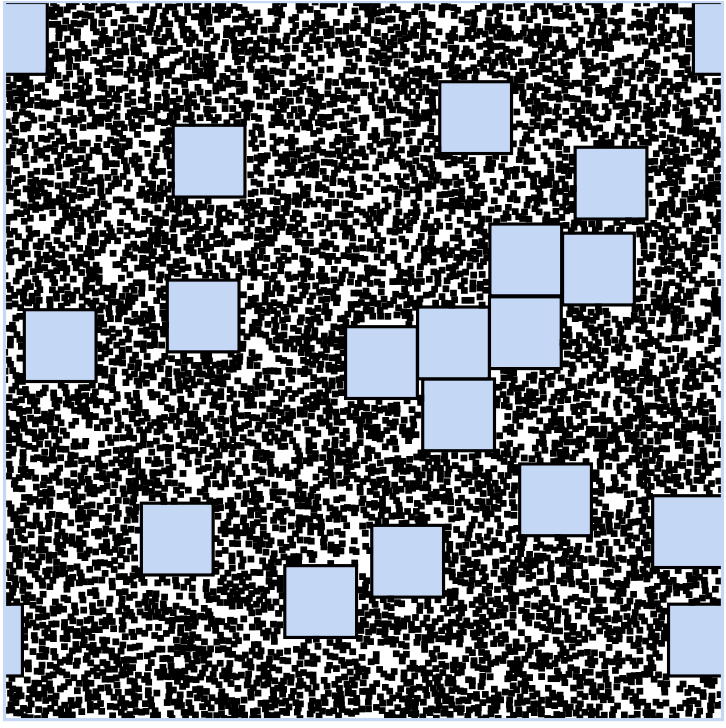
$\eta_B = \eta_S = 0.18$



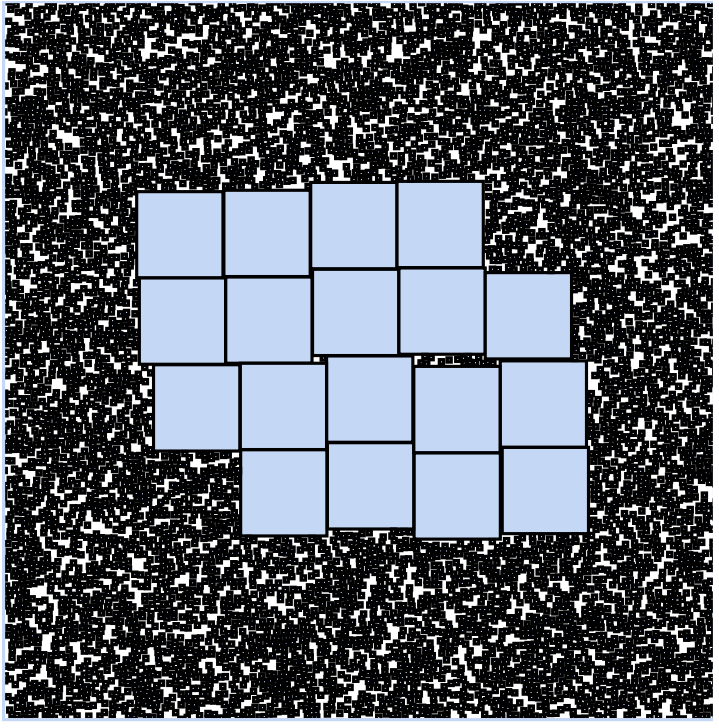
$\eta_B = \eta_S = 0.26$

- homogeneous mixtures up to high densities...

Binary mixtures of squares



$\eta_{\mathrm{B}} = \eta_{\mathrm{S}} = 0.18$



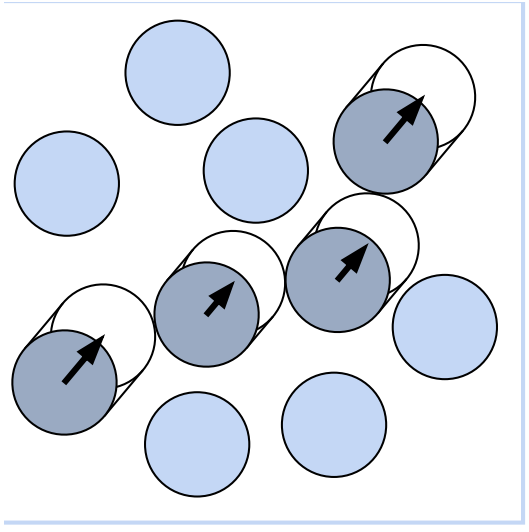
$\eta_{\mathrm{B}} = \eta_{\mathrm{S}} = 0.26$

- solid–liquid phase separation

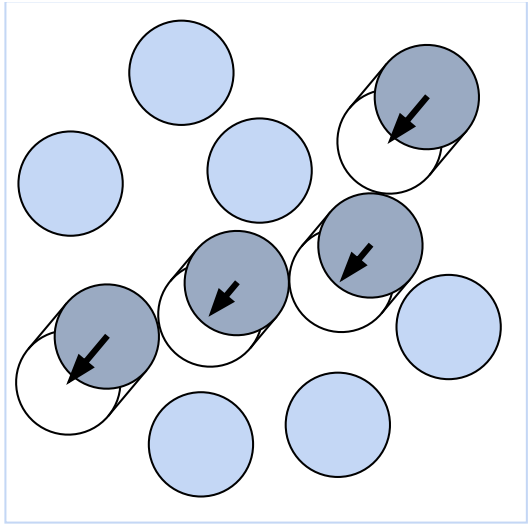
Binary mixtures (conclusion)

- Liquid–solid phase separation in $2d$ (squares) and $3d$ (spheres, cubes) (Buhot, Krauth '98, '99).
- . . . verified experimentally (Dinsmore et al. '95).

Event-chain algorithm for hard spheres



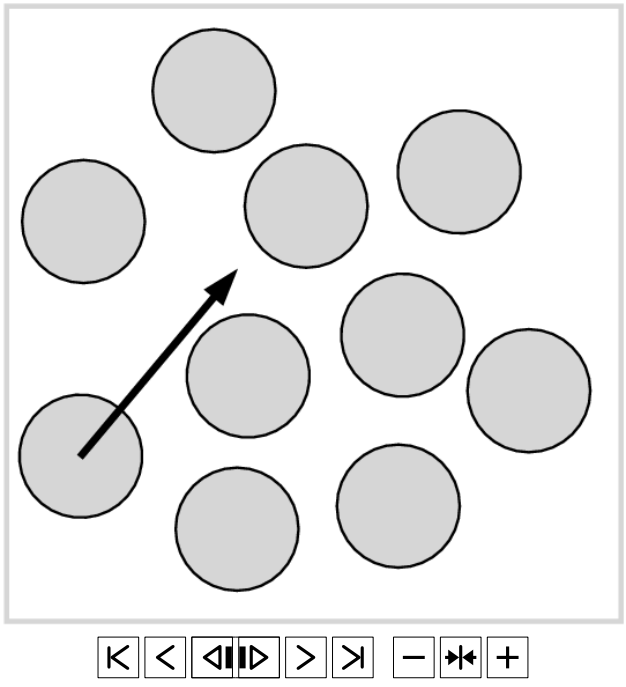
i



f

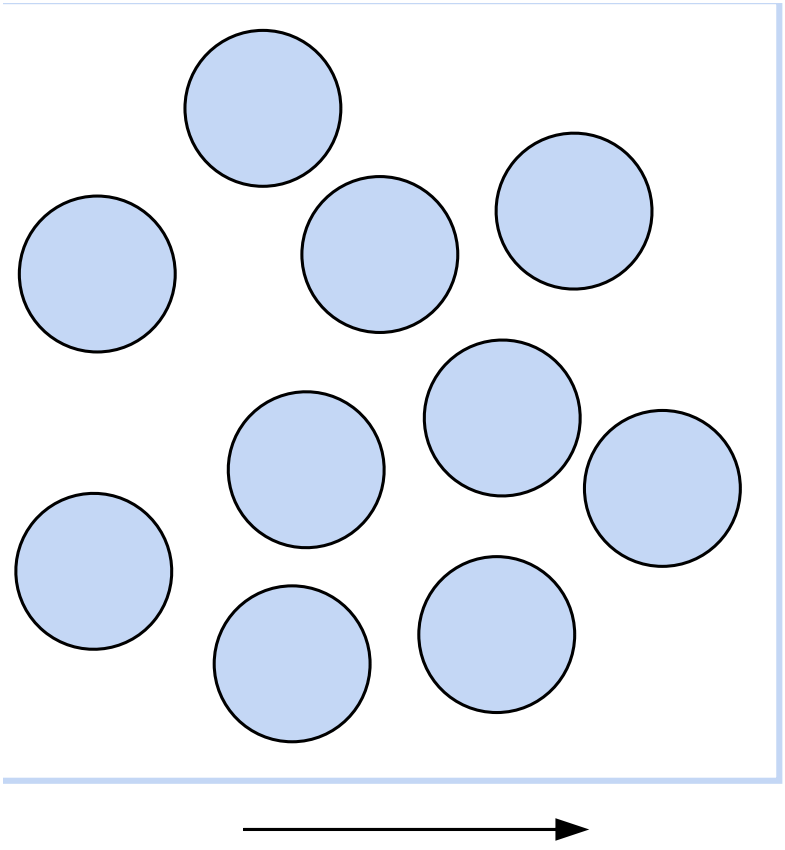
- fast even at high density . . .

Event-chain algorithm for hard spheres



- rejection-free
- detailed balance OK ($\theta \in [0, 2\pi]$)
- Bernard, Krauth, Wilson (2009)

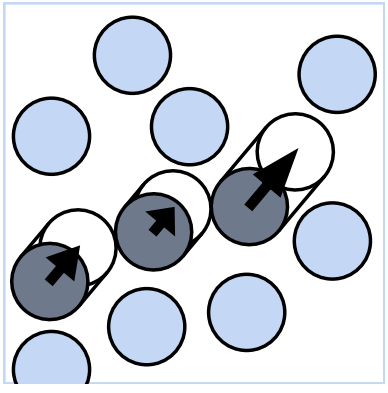
Giving up detailed balance



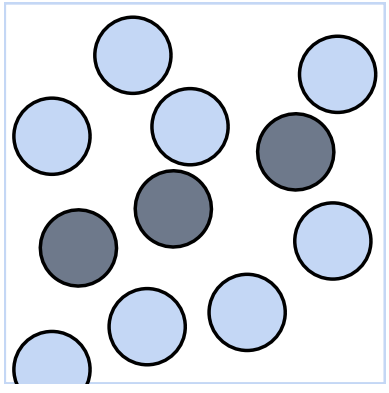
MC without detailed balance

- breaking detailed balance speeds up algorithms . . .
- . . . not so common (cf. Diaconis et al (2000))
- cf. Turitsyn et al (2008); Suwa, Todo (2010)

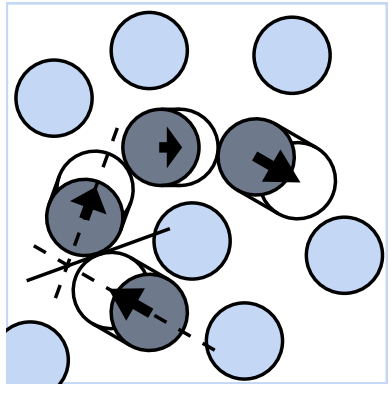
Other versions



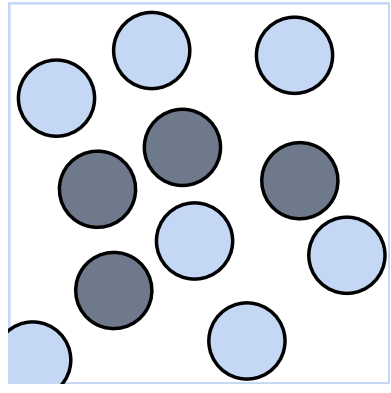
t_i



$t_f = t_i + 3$



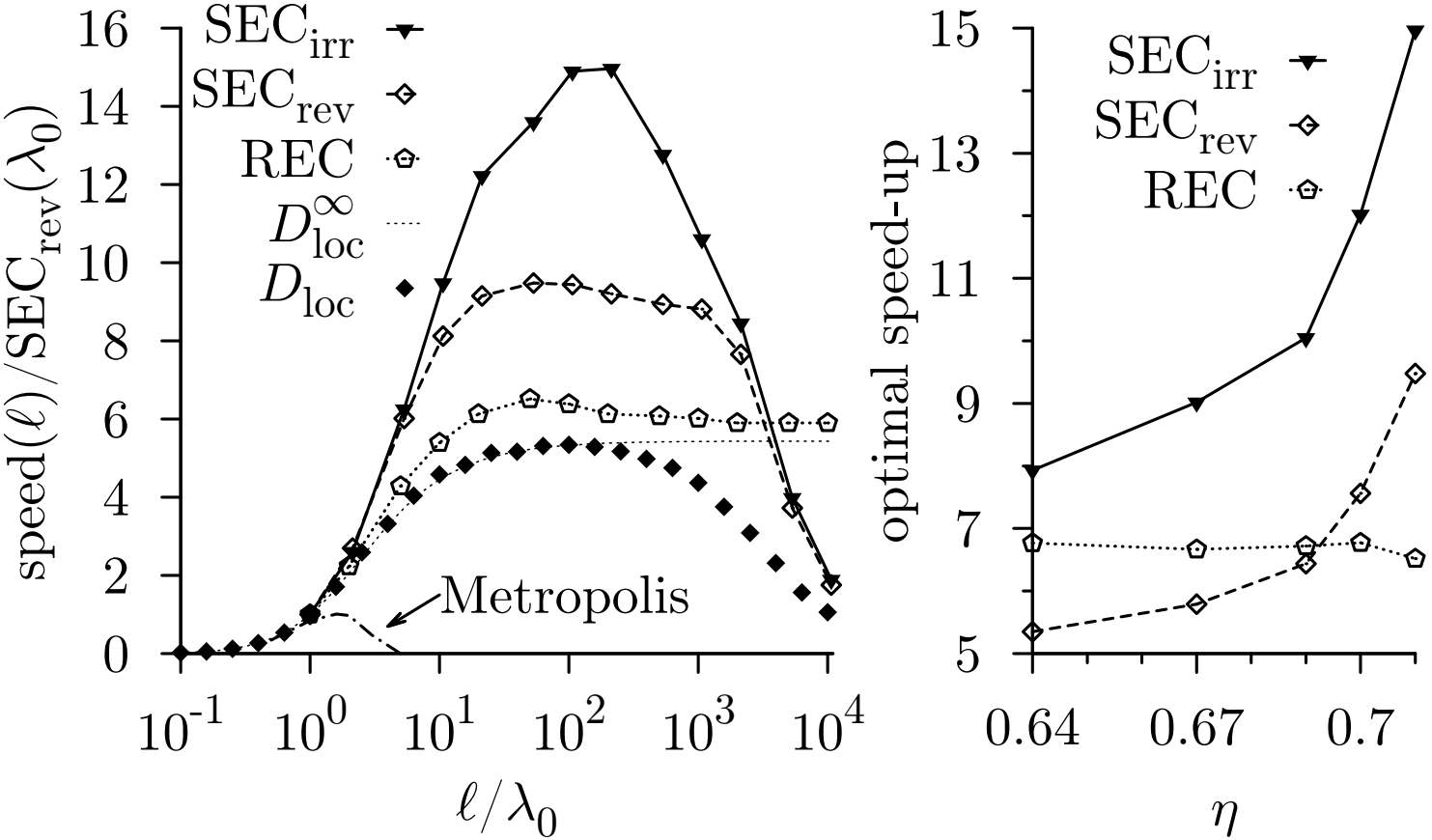
t_i



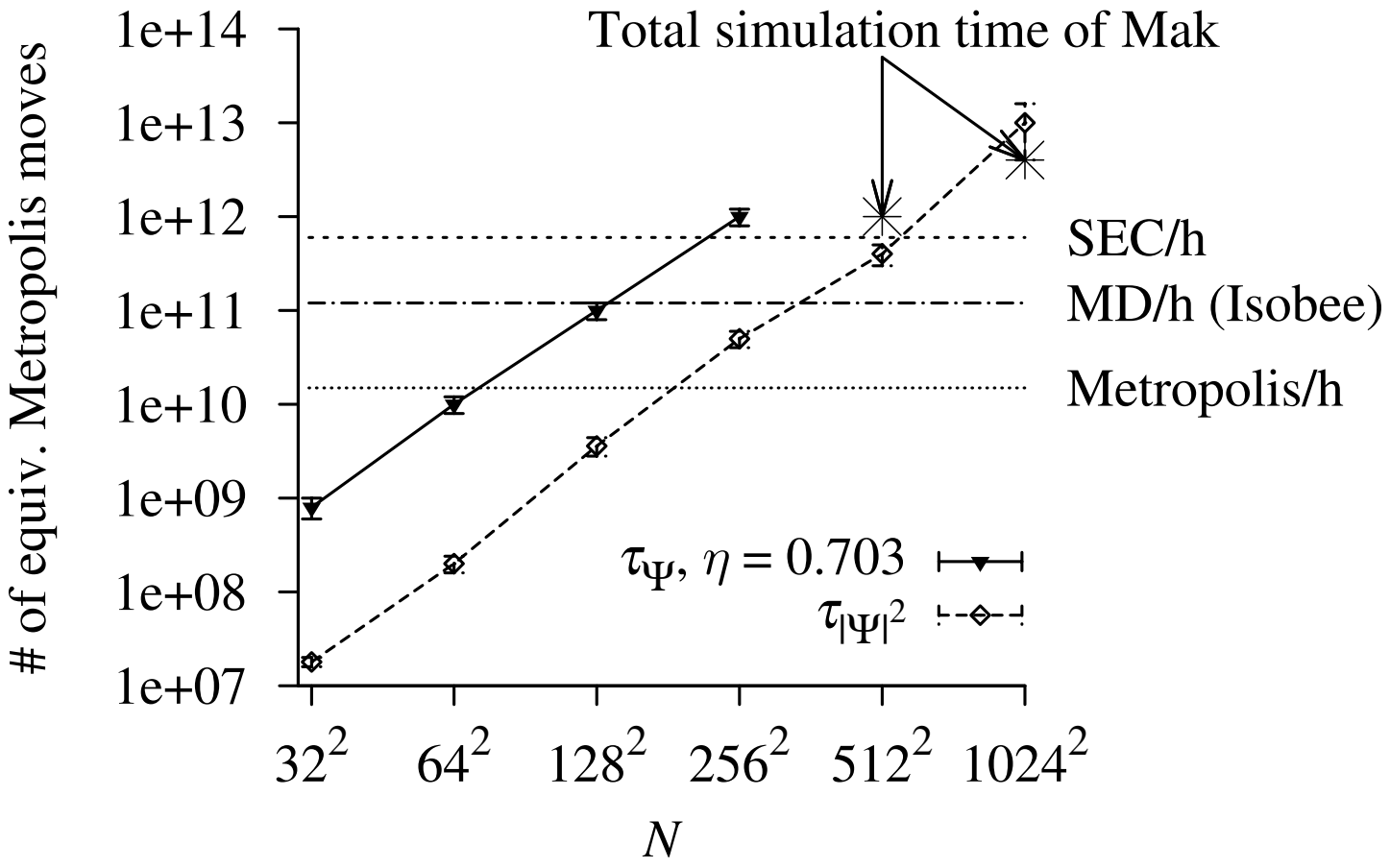
$t_f = t_i + 4$

- detailed balance = microreversibility & conservation of phase space volume

Relative timing issues



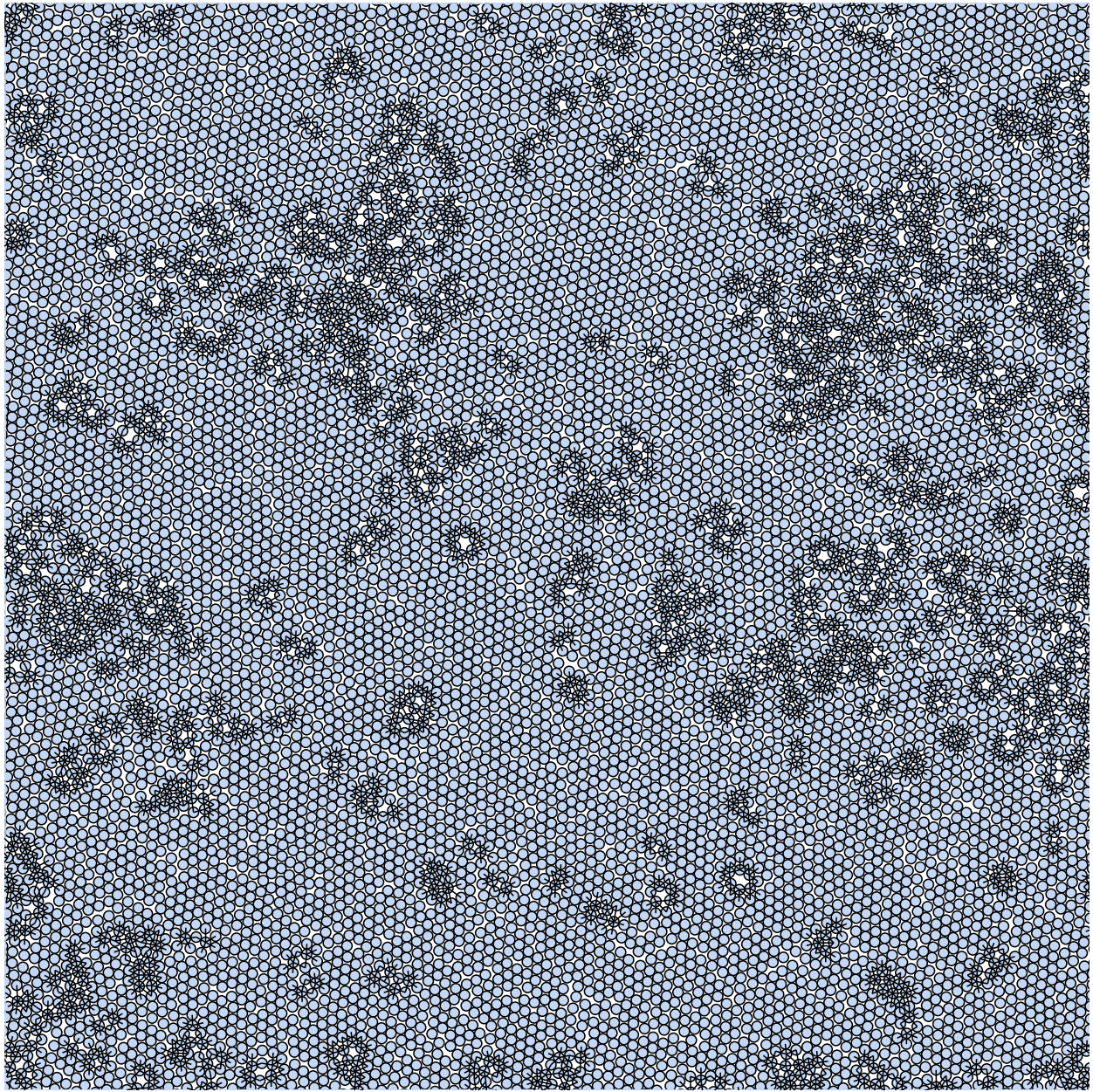
Absolute timing issues



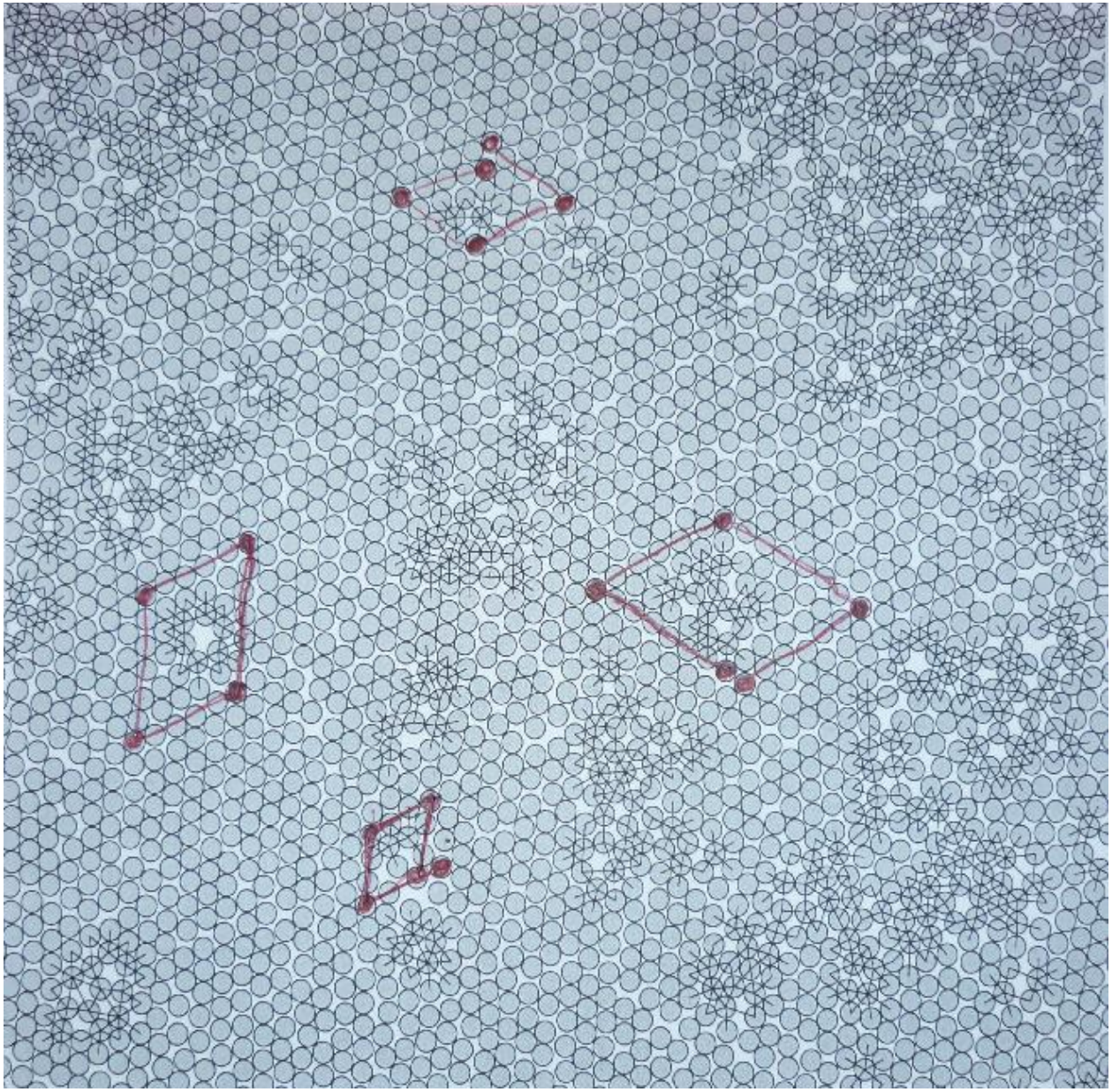
Comparison with Molecular dynamics

- Naively, MD seems orders of magnitude slower than MC
- . . . but recent improvements in algorithms

Equilibrated configuration



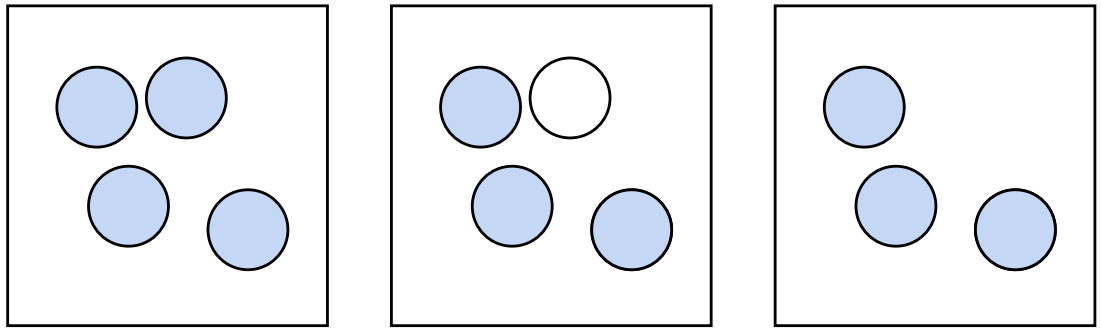
Dislocations



Exact sampling for hard spheres

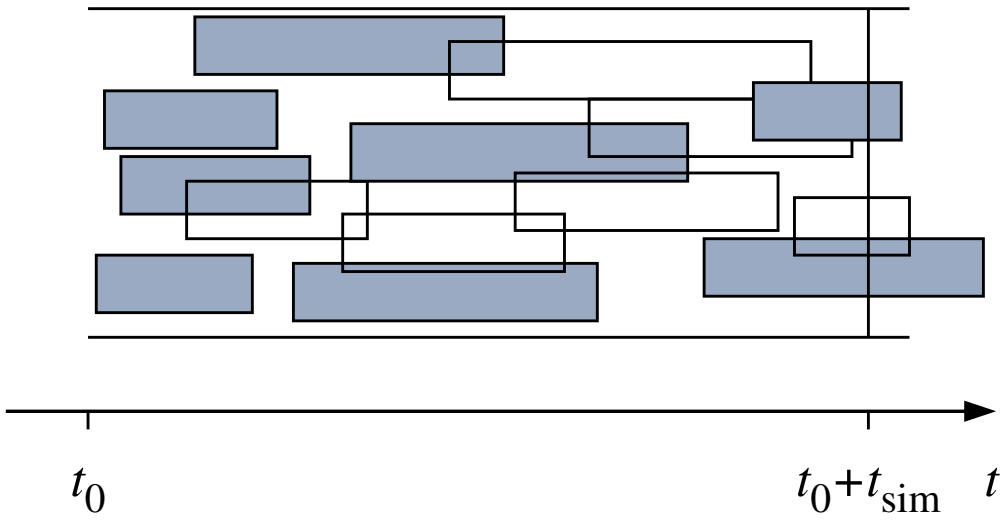
- Perfect sampling: Markov chains that are proven to converge....
- Continuous system...with hidden discrete structure...

Birth and death for hard spheres



- Space of configurations infinite...
- . . . yet underlying discrete structure
- Patch algorithm (Chanal and Krauth 2010)

Birth and death for hard spheres II



- Hidden discrete structure in a continuous model.

References

- J. G. Propp and D. B. Wilson 'Exact sampling with coupled Markov chains and applications to statistical mechanics' Random Structures & Algorithms 9, 223 (1995).
- W. Krauth 'Statistical Mechanics: Algorithms and Computations' (Oxford University Press, 2006)
  Wiki site **http://www.smac.lps.ens.fr**
- C. Chanal and W. Krauth 'Renormalization group approach to exact sampling' PRL (2008),
- C. Chanal and W. Krauth 'Convergence and coupling for spin glasses and hard spheres' PRE (2010)
- E. P. Bernard, W. Krauth, and D. B. Wilson 'Event-chain Monte Carlo algorithm for hard-sphere systems' PRE (2010)

http://www.smac.lps.ens.fr

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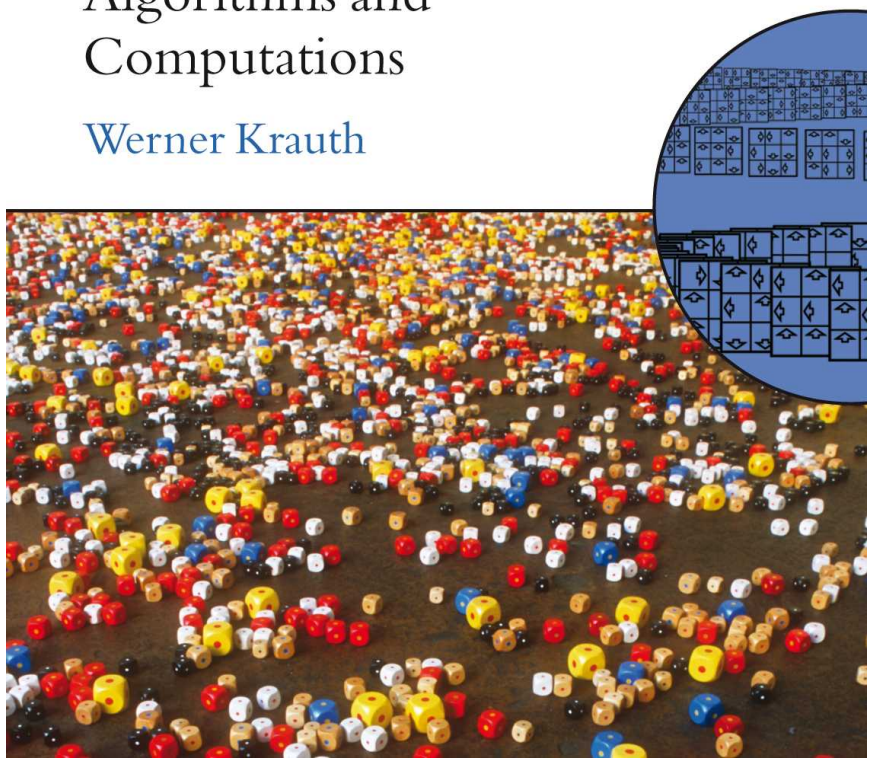
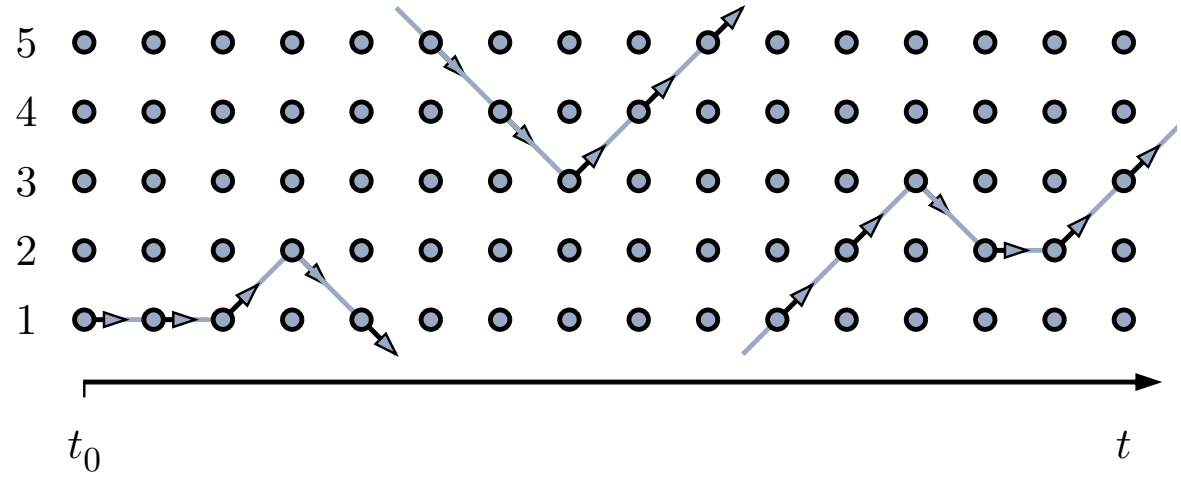
Werner Krauth

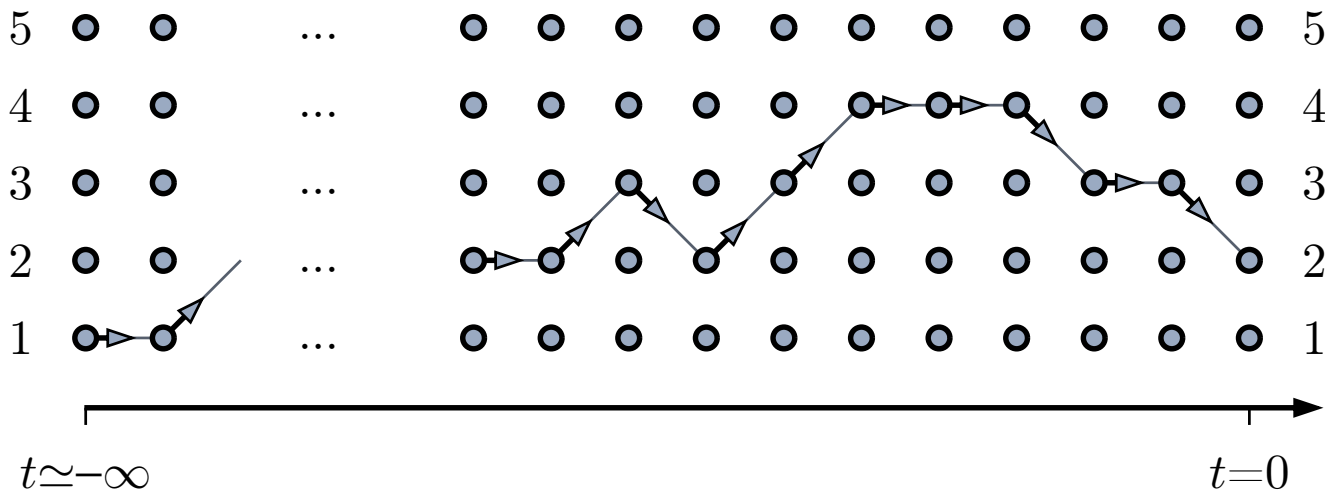


One-d convergence



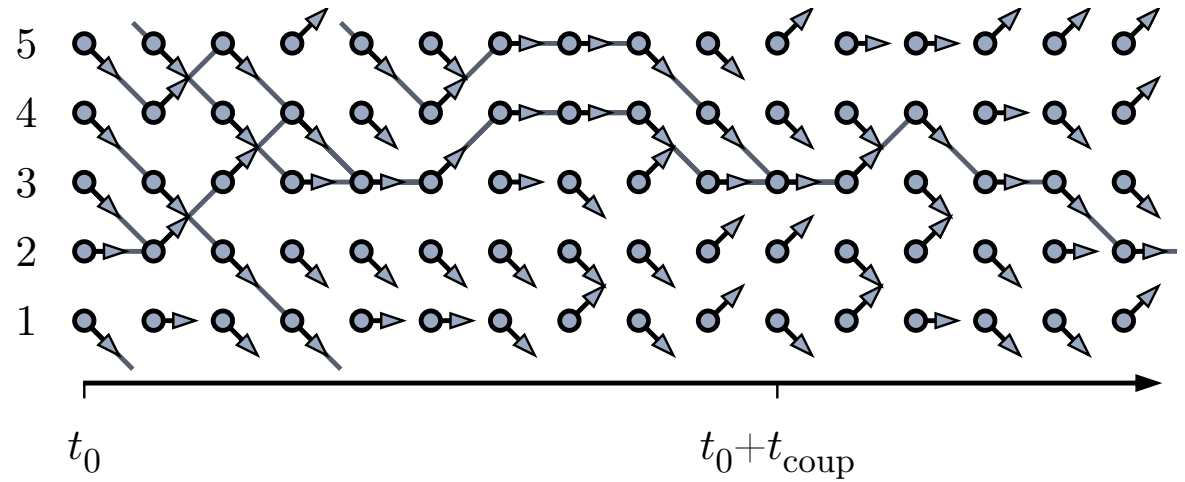
- Markov-chain Monte Carlo algorithm on 5 sites...
- ...converges as $\exp[-t/\tau]$ with finite correlation time τ ...

One-d calculation that finishes on time!



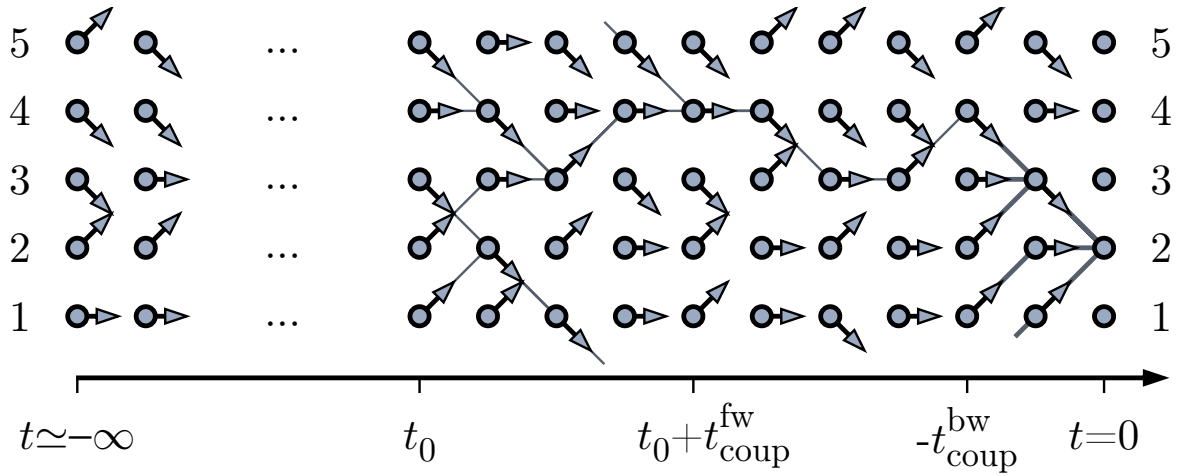
- . . . start earlier and earlier . . .
- . . . get done on time . . .
- . . . Propp, Wilson (1995).

Random maps, coupling



- Markov-chain Monte Carlo algorithm . . .
- . . . with random maps.
- This chain couples after 10 steps.

Correlations and coupling III (from the past)



- Simulation starts really early (at time $t \simeq -\infty$) ...
- ... At time $t = 0$, we are done ...
- ... infinite simulation.