

Hard-sphere MCMC algorithms,  
and  
Physics of two-dimensional melting  
and  
Perfect sampling  
Physics of algorithms, Santa Fe 2009

Werner Krauth

CNRS-Laboratoire de Physique Statistique  
Ecole Normale Supérieure, Paris

3 September 2009

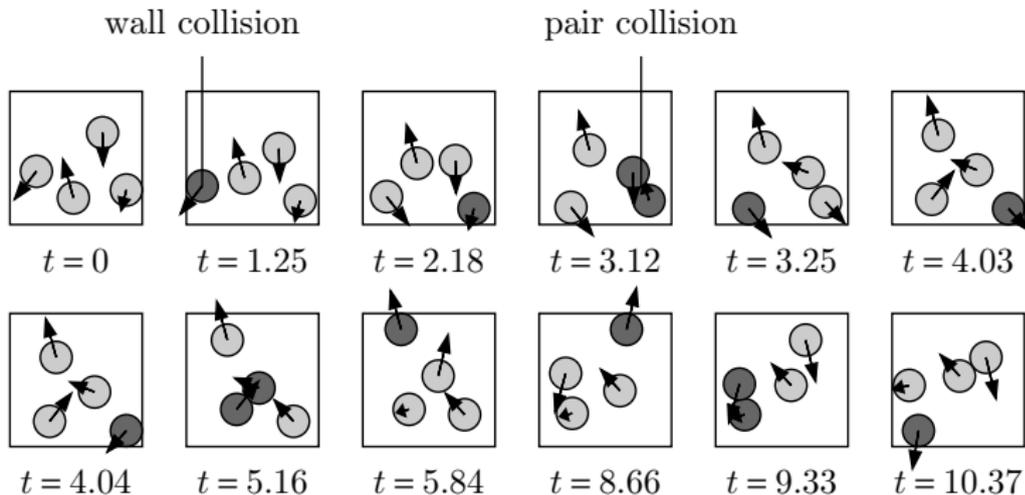


- **Monte Carlo methods and hard spheres**
  - MD and MC
  - Transfer matrices
  - The physics of melting
  - General remarks on MC algorithms
- **Cluster Monte Carlo algorithms, Event chains**
  - Estimating mixing times
  - Event chains
  - Breaking detailed balance
  - Applications
- **Perfect sampling**
  - Infinitely long Monte Carlo simulations (Propp & Wilson)
  - Monte Carlo simulations with an equilibration guarantee
  - More transfer matrices
  - Application to spin glasses & hard spheres
- **Conclusion**
  - Statistical Mechanics  $\equiv$  Algorithms & Computations



# Molecular dynamics ('Newton')

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

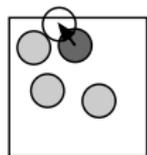


- ... starting point of Molecular dynamics, in 1957 ...
- ... treats positions and velocities ...
- ... useful for  $N \gg 4$ , but times extremely short ...
- ... converges towards thermal equilibrium.

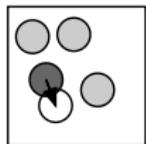


# Markov-chain Monte Carlo ('Boltzmann')

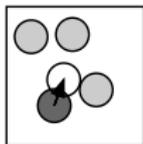
- A local Markov-chain Monte Carlo algorithm for hard spheres (billiard):



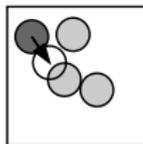
$i = 1$  (rej.)



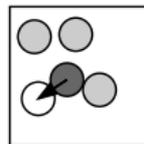
$i = 2$



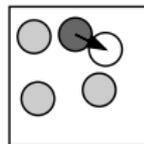
$i = 3$



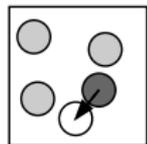
$i = 4$  (rej.)



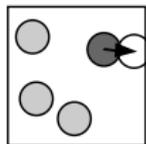
$i = 5$



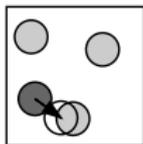
$i = 6$



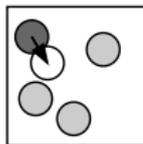
$i = 7$



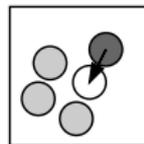
$i = 8$  (rej.)



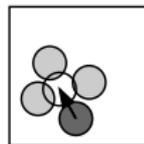
$i = 9$  (rej.)



$i = 10$



$i = 11$

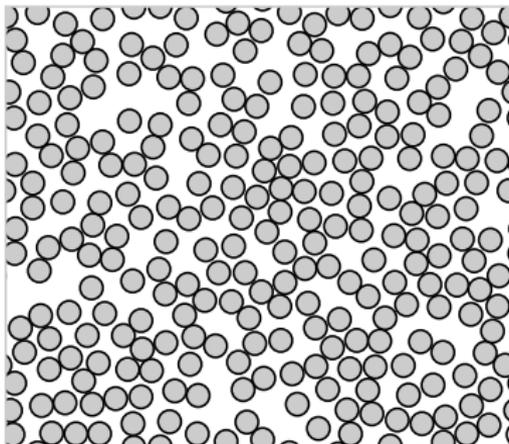


$i = 12$  (rej.)

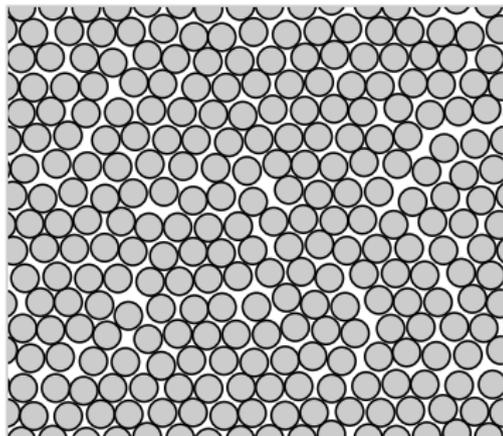
- ... starting point of Markov chain Monte Carlo, in 1953 ...
- ... treats only positions ...
- ... useful for  $N \gg 4$  ...
- ... converges towards thermal equilibrium.



# Physics of crystallization in 2D



density  $\eta = 0.48$



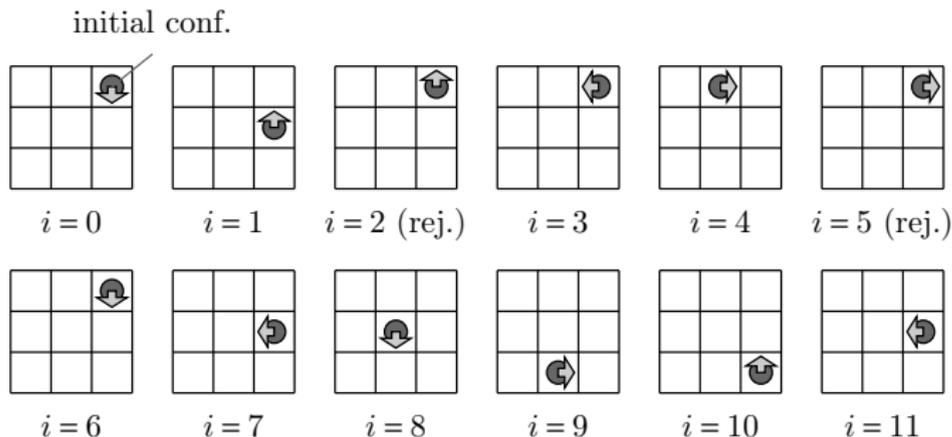
density  $\eta = 0.72$

- At low density, disks move easily (liquid)
- ... at high density, MC algorithms slow down and **disks crystallize** ...
- ... but the crystal cannot have long-range (positional) order



# Single discrete hard sphere ('3 × 3 pebble game')

- Monte Carlo algorithm for one hard sphere on a lattice:



- Move 'up', 'down', 'left', 'right', each with probability 1/4.
- Reject moves if necessary ( $i = 2$ ,  $i = 5$ ).



# Transfer matrix of $3 \times 3$ pebble game

- Transfer matrix of algorithmic probabilities  $p(a \rightarrow b)$ :

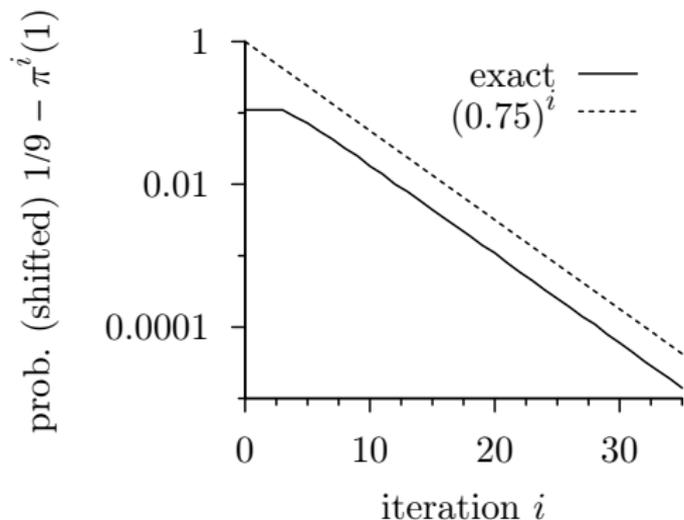
$$\{p(a \rightarrow b)\} = \begin{bmatrix} \boxed{\frac{1}{2}} & \frac{1}{4} & \cdot & \frac{1}{4} & \cdot & \cdot & \cdot & \cdot & \cdot \\ \frac{1}{4} & \boxed{\frac{1}{4}} & \frac{1}{4} & \cdot & \frac{1}{4} & \cdot & \cdot & \cdot & \cdot \\ \cdot & \frac{1}{4} & \boxed{\frac{1}{2}} & \cdot & \cdot & \frac{1}{4} & \cdot & \cdot & \cdot \\ \frac{1}{4} & \cdot & \cdot & \boxed{\frac{1}{4}} & \frac{1}{4} & \cdot & \frac{1}{4} & \cdot & \cdot \\ \cdot & \frac{1}{4} & \cdot & \frac{1}{4} & \boxed{0} & \frac{1}{4} & \cdot & \frac{1}{4} & \cdot \\ \cdot & \cdot & \frac{1}{4} & \cdot & \frac{1}{4} & \boxed{\frac{1}{4}} & \cdot & \cdot & \frac{1}{4} \\ \cdot & \cdot & \cdot & \frac{1}{4} & \cdot & \cdot & \boxed{\frac{1}{2}} & \frac{1}{4} & \cdot \\ \cdot & \cdot & \cdot & \cdot & \frac{1}{4} & \cdot & \frac{1}{4} & \boxed{\frac{1}{4}} & \frac{1}{4} \\ \cdot & \cdot & \cdot & \cdot & \cdot & \frac{1}{4} & \cdot & \frac{1}{4} & \boxed{\frac{1}{2}} \end{bmatrix}.$$

- $\{\pi(1), \dots, \pi(9)\} = \{\frac{1}{9}, \dots, \frac{1}{9}\}$  is eigenvector.



# Exponential convergence in the $3 \times 3$ pebble game

- $\pi^i$ (site 1) for simulation started in the right upper corner (site 9):

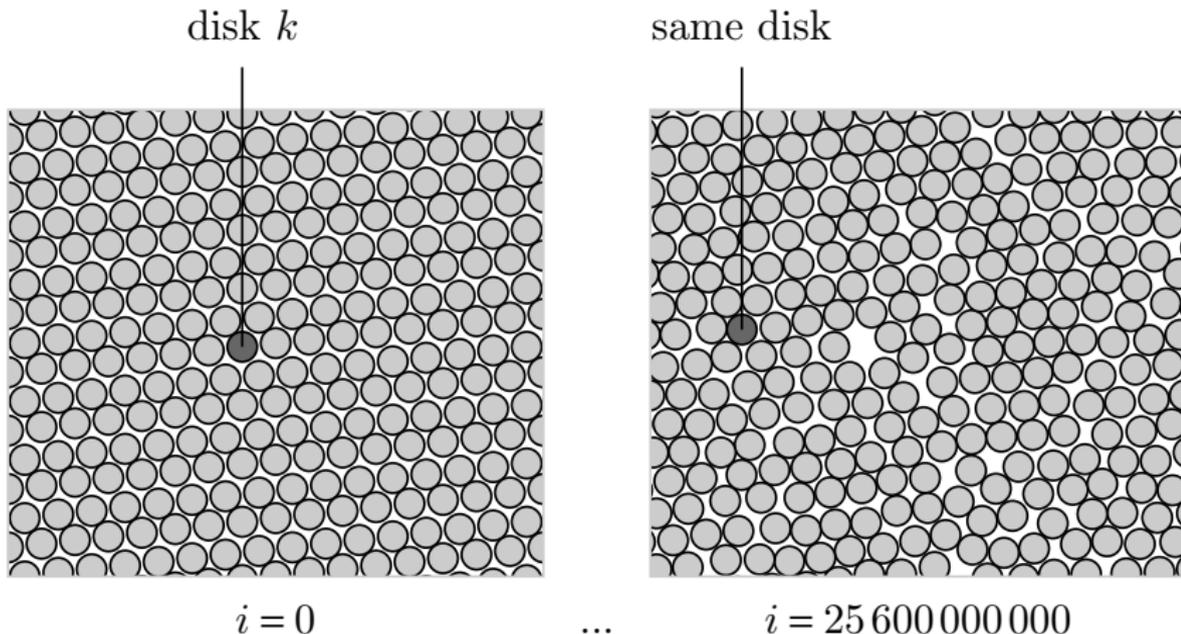


- Exponential convergence  $\equiv$  scale:

$$(0.75)^i = \exp [i \cdot \log 0.75] = \exp \left[ -\frac{i}{3.476} \right].$$



# Correlation time in larger simulations



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

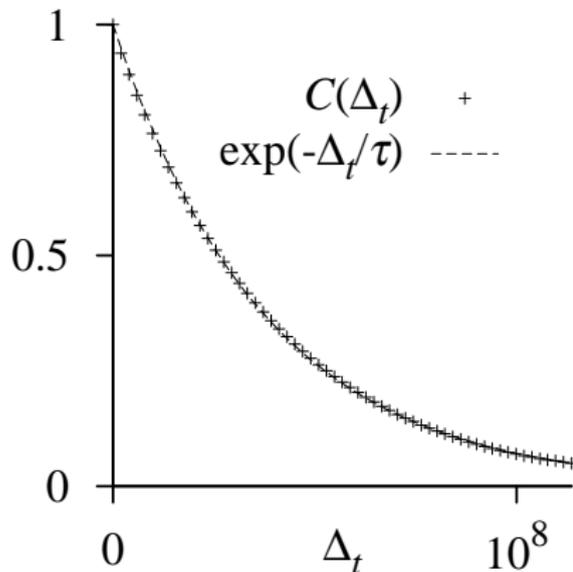
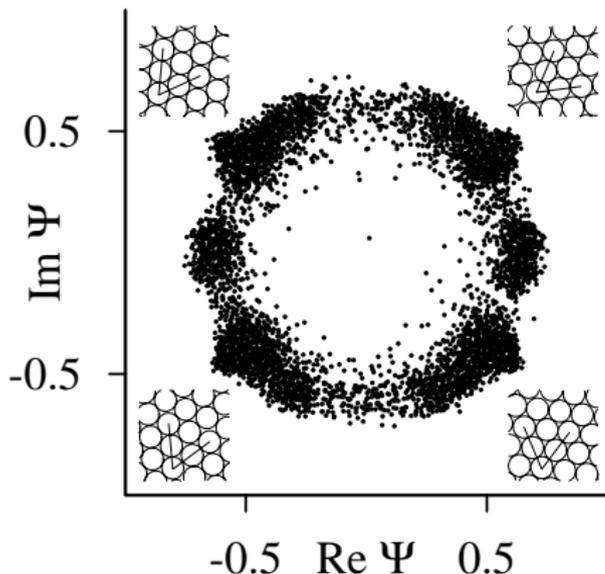


# Minimum running time of a Monte Carlo algorithm

- Knowing correlation time  $\tau$  would be nice (Part I).
- A faster algorithm would be nice (Part II).
- An infinitely long simulation would be nice (Part III).



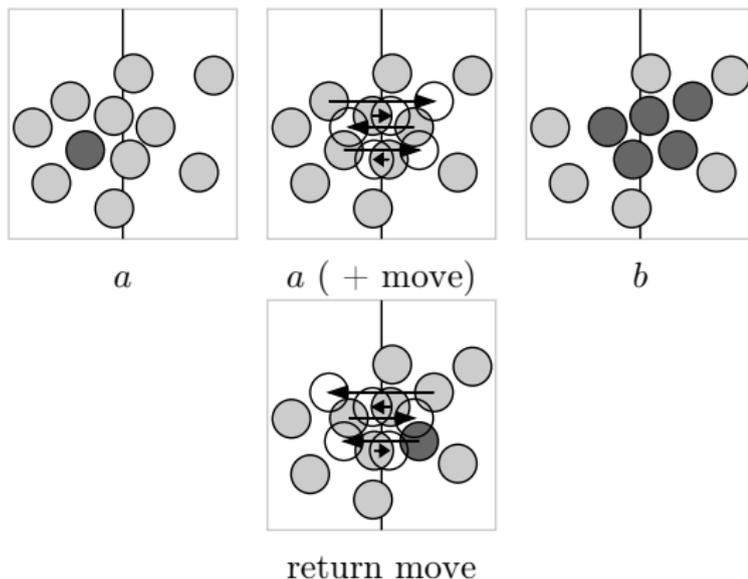
# Mixing time (square box)



- Correlation time  $\equiv$  correlation time of order parameter
- much better than diffusion-constants criterion ...
- ... hypothesis, but more cautious than what others do...



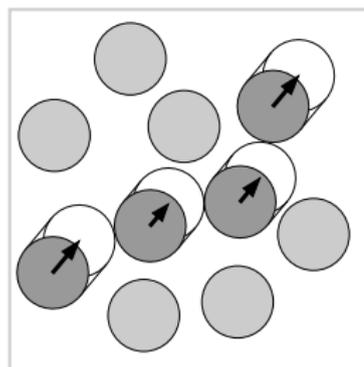
# Cluster algorithm for hard spheres



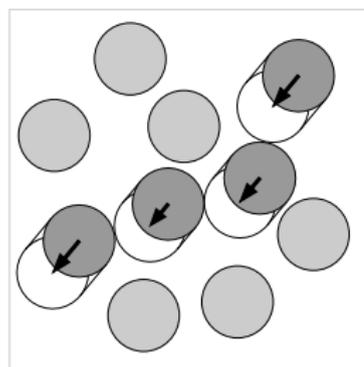
- Satisfies  $p(a \rightarrow b) = p(b \rightarrow a)$ , is ergodic.
- Cluster move, rejection-free (Dress & Krauth '95).
- Many applications, but algorithm no good for 2d melting.



# Event-chain . . . maximizing local moves



*i*

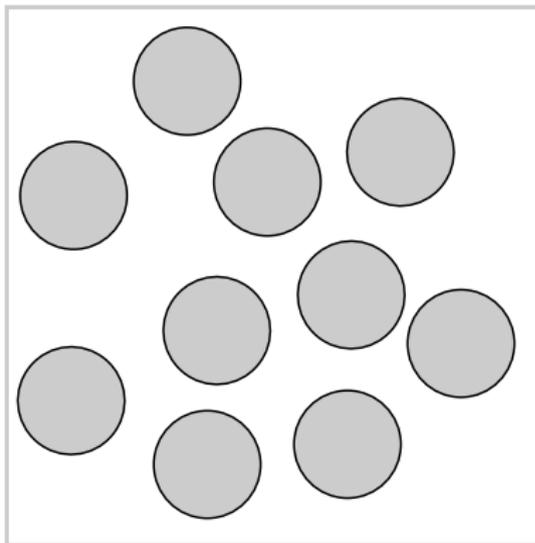


*f*

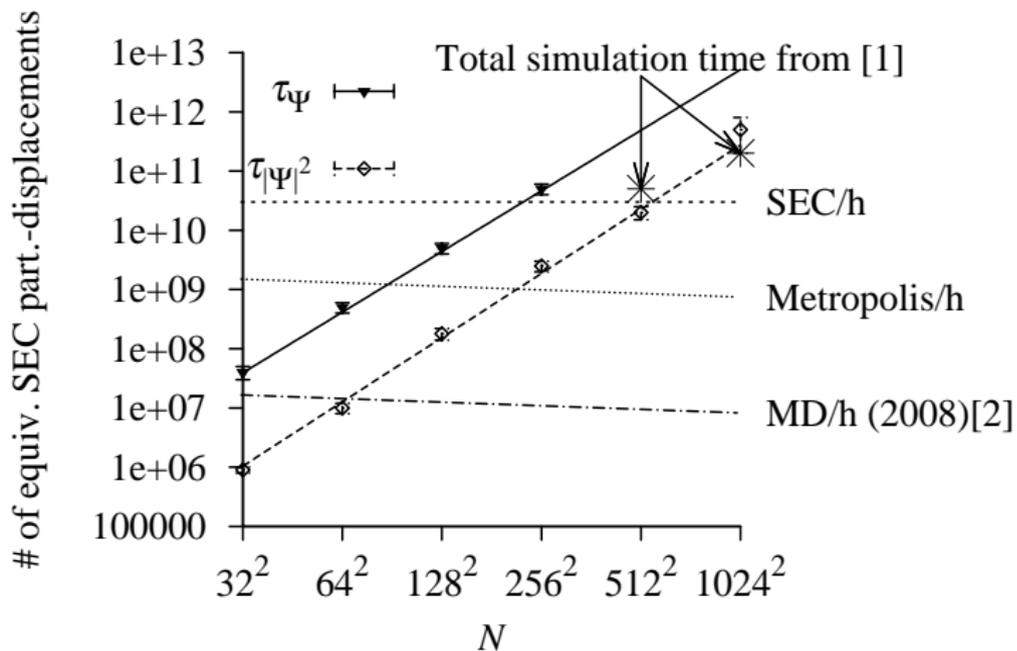
- rejection-free
- detailed balance OK ( $\theta \in [0, 2\pi]$ )
- moves each disk as far as possible
- E. Bernard, W. Krauth, D. B. Wilson (arXiv:0903.2954)



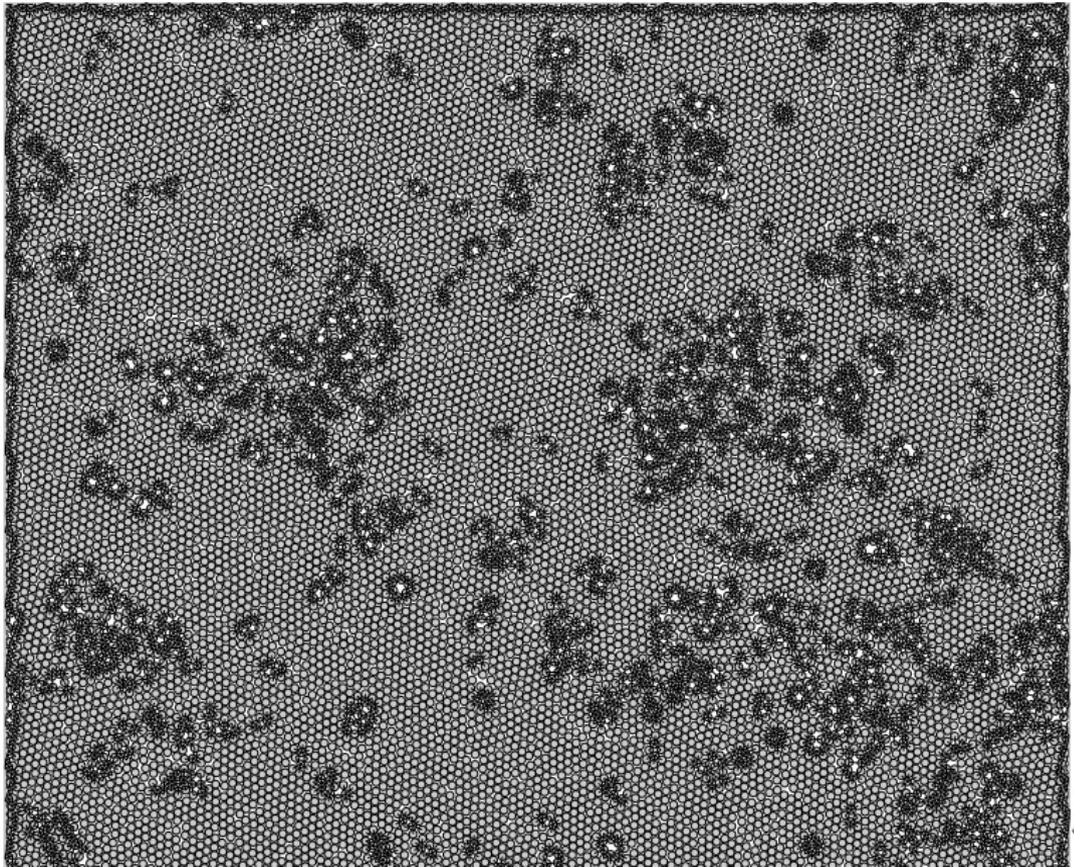
# Giving up detailed balance



# Timing issues



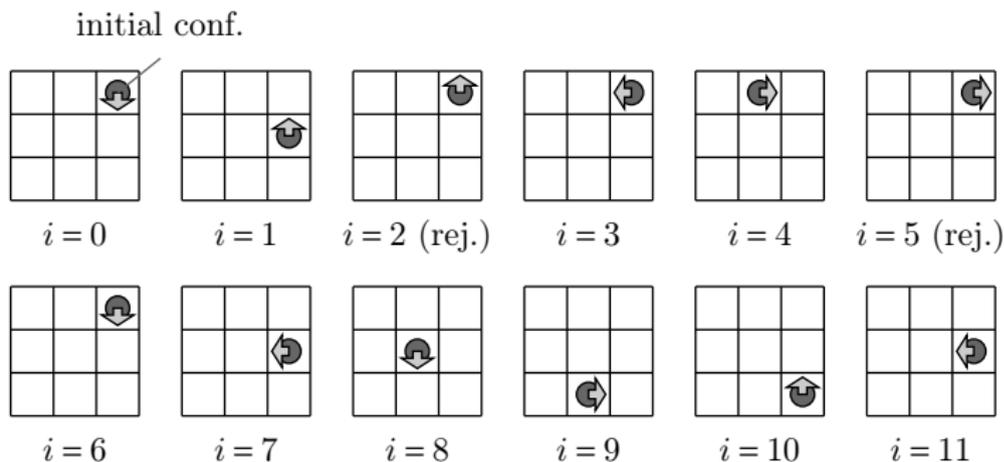
# Equilibrated configuration



# Dislocations



# Return of the '3 × 3 pebble game'



To prove that Monte Carlo simulation is in equilibrium, we must

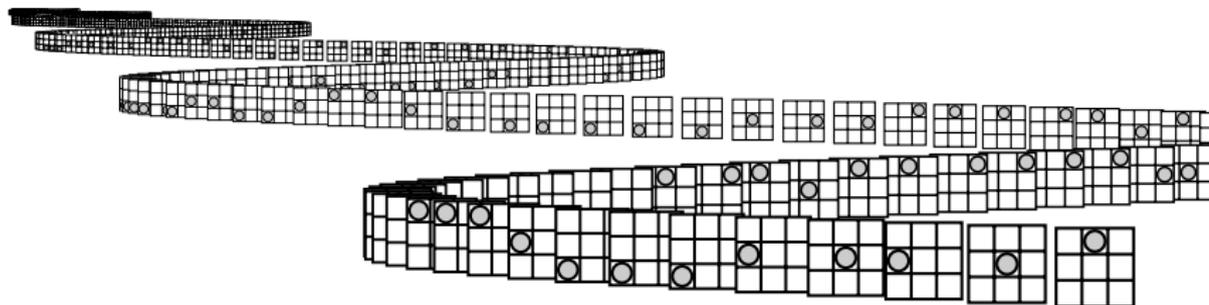
- either compute correlation time  $\tau = 3.476 \dots$
- or do an infinitely long simulation (reach  $i = \infty$ ) ...
- or both



# Infinite simulations (in $3 \times 3$ pebble game)

- Do not start at  $t = 0$ , **start in the past, at  $i = -\infty$** :

$i = -\infty$

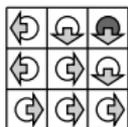


$i = 0$  (now)

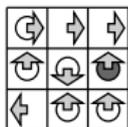
- The configuration at  $i = 0$  is an 'exact sample'.



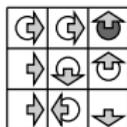
# Coupling random maps in the $3 \times 3$ pebble game



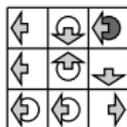
$i = -17$



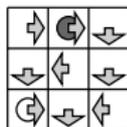
$i = -16$



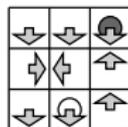
$i = -15$



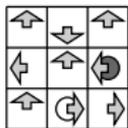
$i = -14$



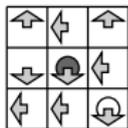
$i = -13$



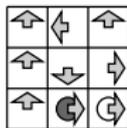
$i = -12$



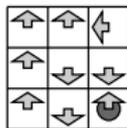
$i = -11$



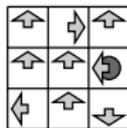
$i = -10$



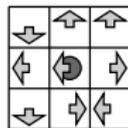
$i = -9$



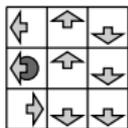
$i = -8$



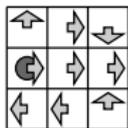
$i = -7$



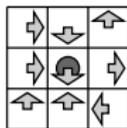
$i = -6$



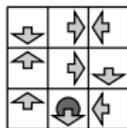
$i = -5$



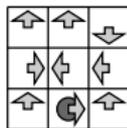
$i = -4$



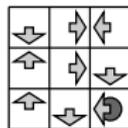
$i = -3$



$i = -2$



$i = -1$



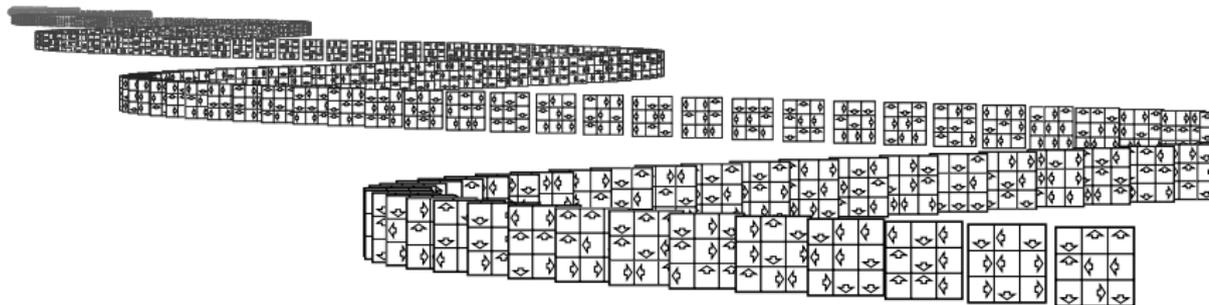
$i = 0$  (now)

NB: Proof of coupling by naive enumeration and exhaustion.



# Infinite simulation with random maps

$i = -\infty$



$i = 0$  (now)

- The configuration at  $i = 0$  is a perfect sample.
- It can be computed through finite back-track.
- Propp & Wilson (1995): landmark paper.
- Can work for spin glasses and hard spheres (Chanal & Krauth ('08, '09)).



# More transfer matrices...

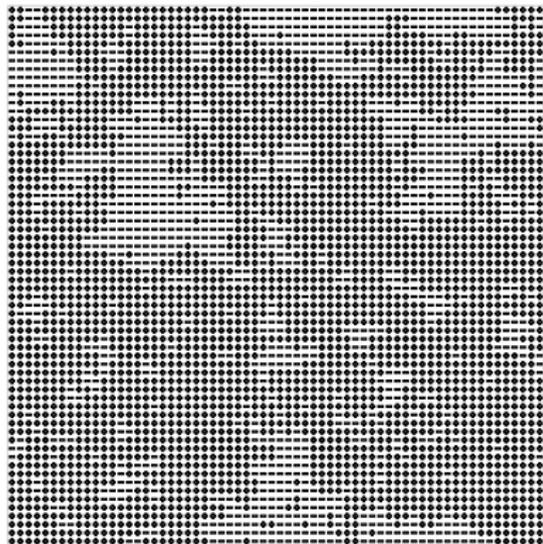
- The dynamics of the new pebble game is again described by a transfer matrix:

$$\mathcal{T}^{\text{forward}} = \begin{pmatrix} \mathcal{T}^{1,1} & \mathcal{T}^{2,1} & \dots & \dots \\ 0 & \mathcal{T}^{2,2} & \mathcal{T}^{3,2} & \dots \\ 0 & 0 & \mathcal{T}^{3,3} & \dots \\ \dots & & & \ddots \\ 0 & 0 & & \mathcal{T}^{N,N} \end{pmatrix}$$

- Triangular matrix: second-largest eigenvalue  $\geq$  second-largest eigenvalue of  $\mathcal{T}^{1,1}$ .
- therefore: coupling time  $\geq$  convergence time



# Updates on large lattices (spin systems)



- $64 \times 64$  Ising spin glass has  $2^{32 \times 64} \sim 3 \times 10^{616}$  states.
- We must rigorously show that they 'all' couple.
- Non-monotone model.

- Using patches  $k$  on the lattice, and sets of patches  $S_k$  on patch  $k$  ( $k = 1, \dots, N$ ), we define

$$\Omega = S_1 \otimes S_2 \otimes \dots \otimes S_N / (\text{pairwise compat.}).$$

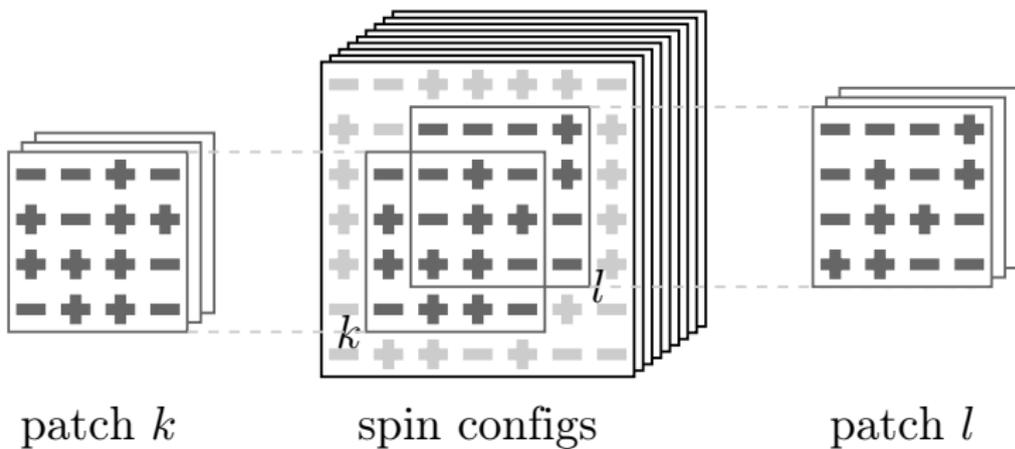
- $\Omega$  is overcomplete, but storage linear in lattice size

$$N \times 2^{m^2/2}$$

for  $N$  lattice sites and patches of size  $m \times m$ .



# Patches and compatibilities



# Exact sampling for hard spheres

- Continuous system...with hidden discrete structure...
- Patch algorithm reaches finite densities  $\eta \leq 0.3$  for  $N \rightarrow \infty$ ...
- ...improves on Wilson's algorithm.



We discussed Monte Carlo methods for hard spheres

- Convergence issues
- new algorithms
- new insight into melting transition..
- Exact sampling, coupling from the past (doing an infinitely long Monte Carlo simulation).
- ...

