Efficient algorithms for hard spheres and related systems, Applications

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DPG Summer School Bad Honnef
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see also lecture's webpage

http://cours-physique.lps.ens.fr/index.php/Bad_Honnef_Lecture_2012

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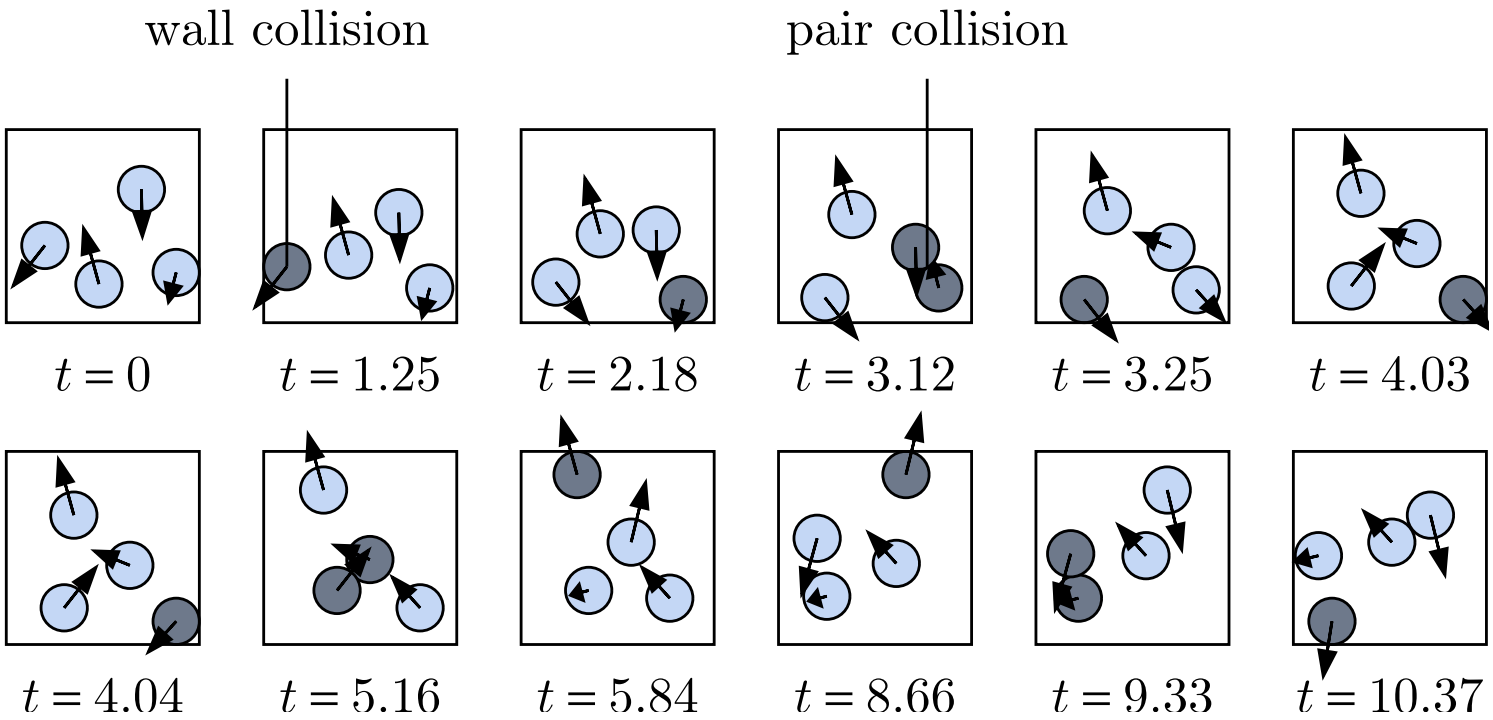
Molecular dynamics ('Newton')

- A molecular dynamics algorithm for hard disks:



- . . . starting point of Molecular dynamics, in 1957 . . .
- . . . converges towards thermal equilibrium.

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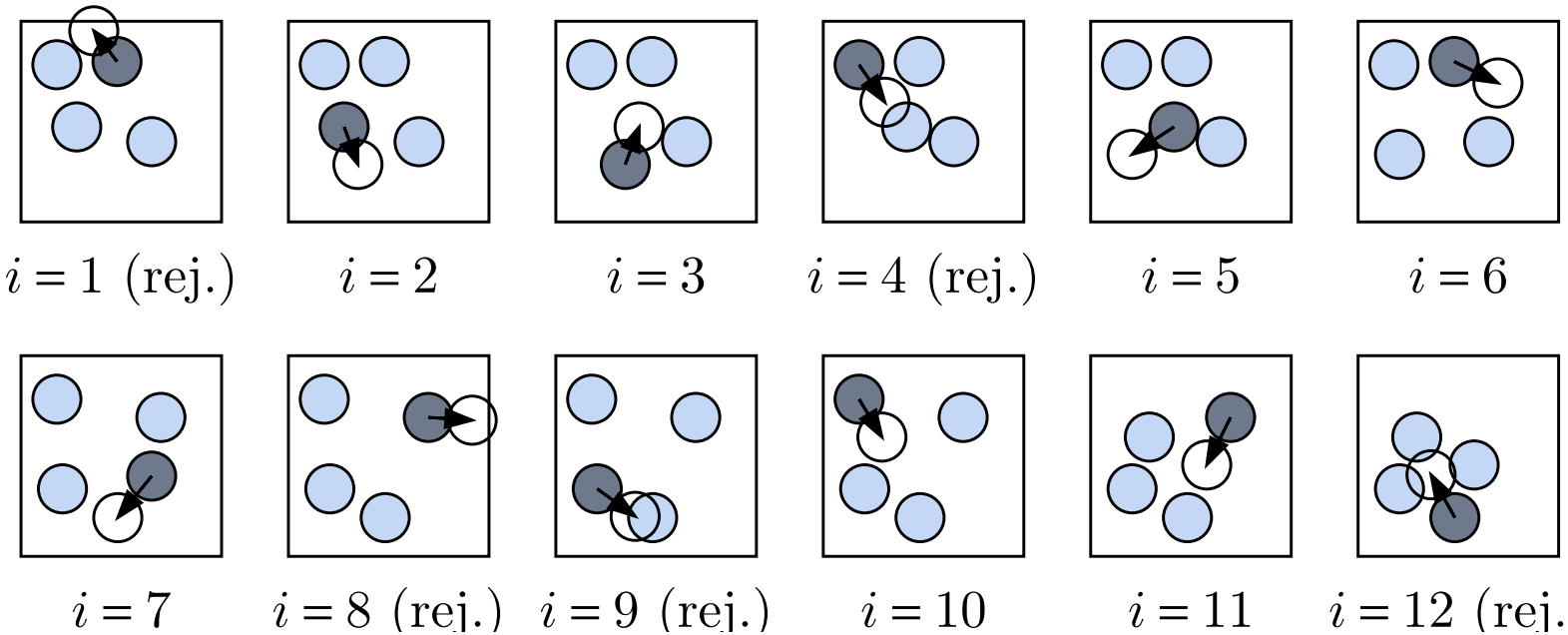
Markov-chain Monte Carlo ('Boltzmann')

- A local Markov-chain Monte Carlo algorithm for hard disks:



- . . . starting point of Markov chain Monte Carlo, in 1953
- . . . converges towards thermal equilibrium.

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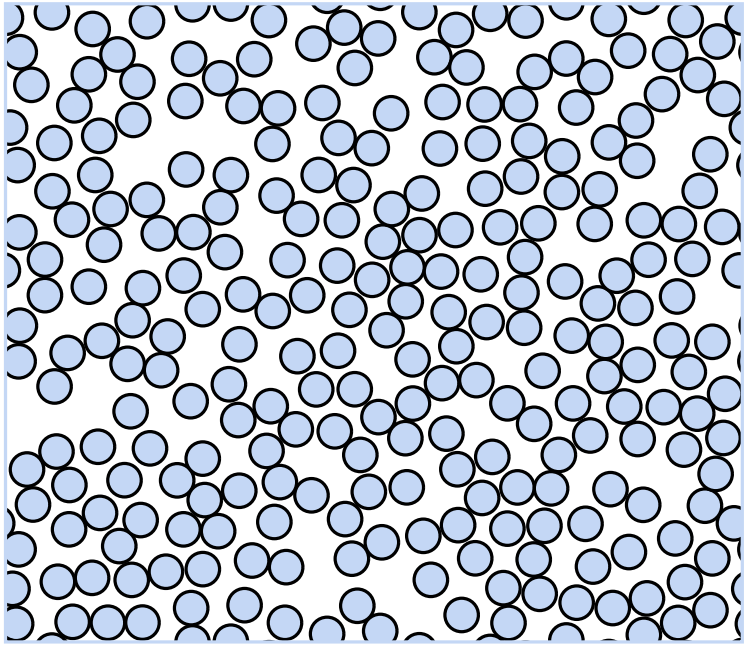
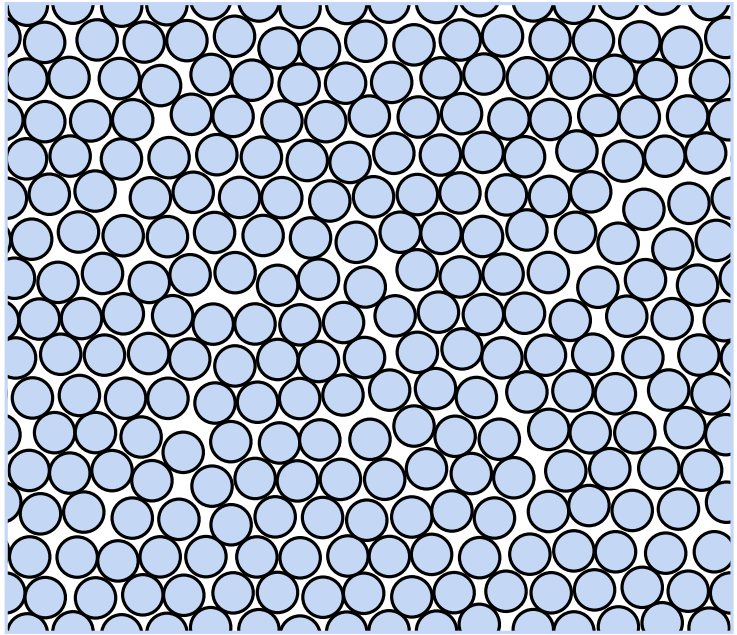
2D melting transition



density $\eta = 0.48$



density $\eta = 0.72$

- generic 2D systems cannot crystallize yet they can turn solid (Alder & Wainwright, 1962) ...
- ... nature of transition long disputed (first order vs. KTHNY (1973-1979))

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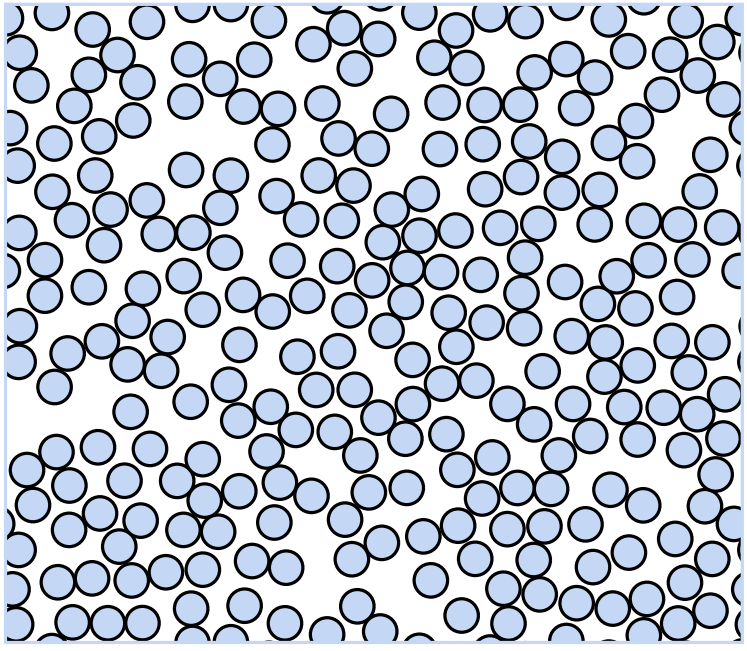
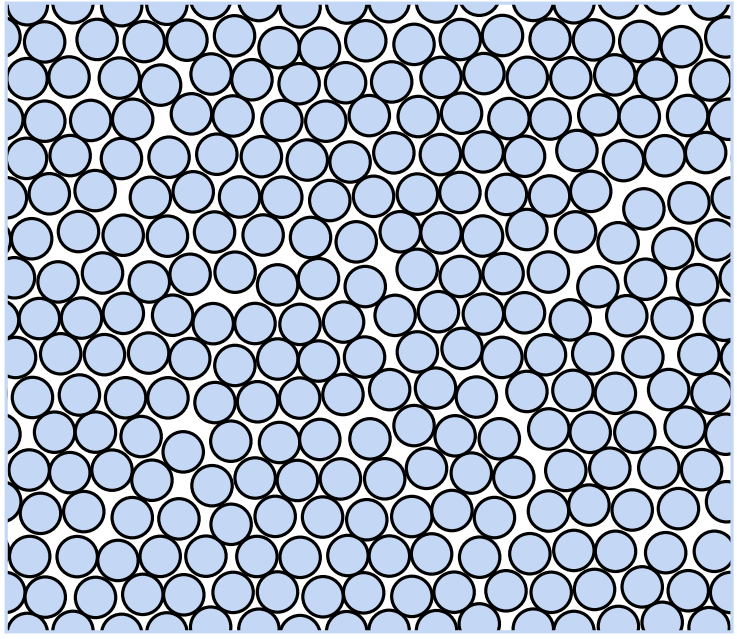
Possible phases in two dimensions



density $\eta = 0.48$



density $\eta = 0.72$

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

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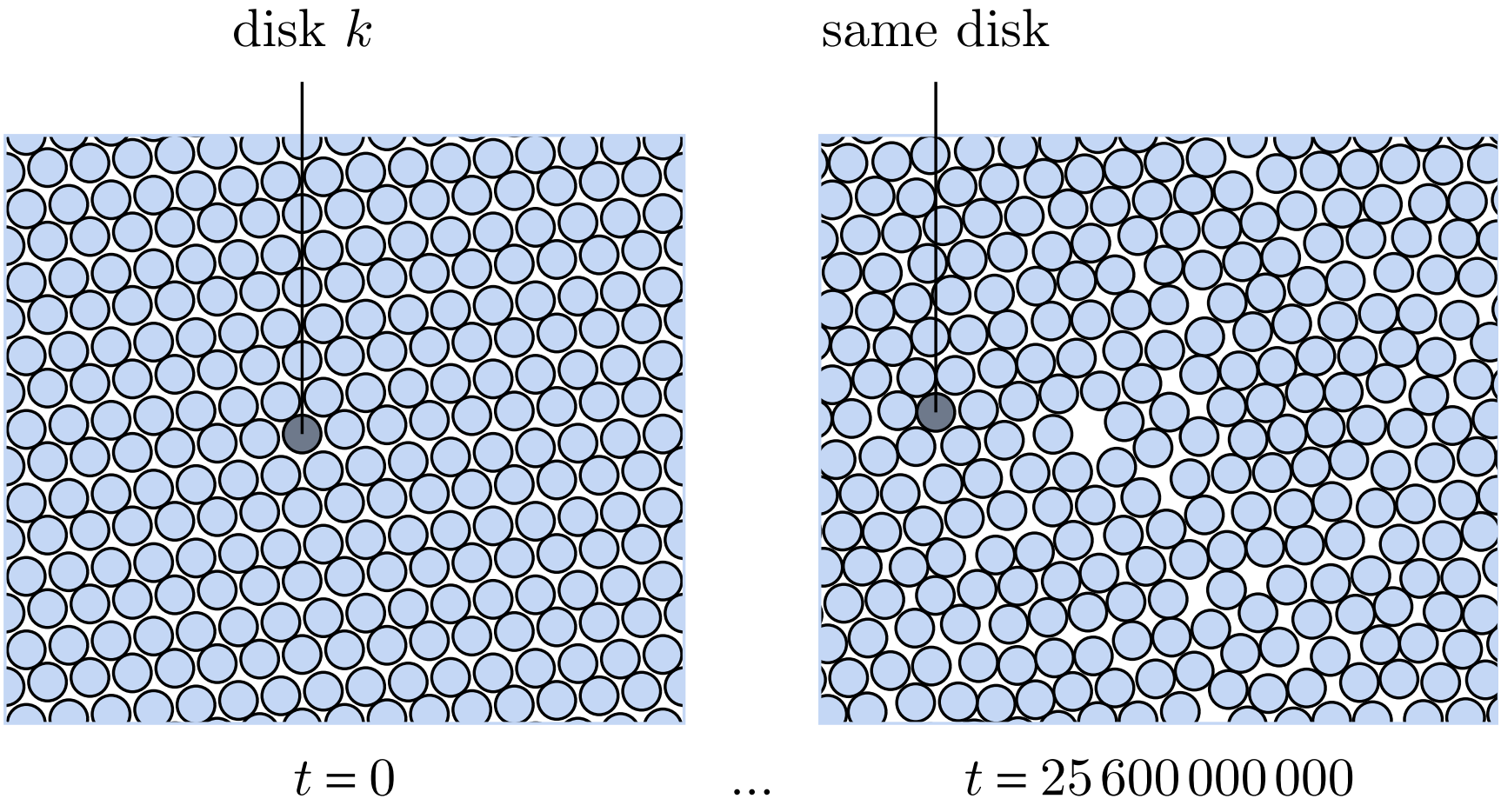
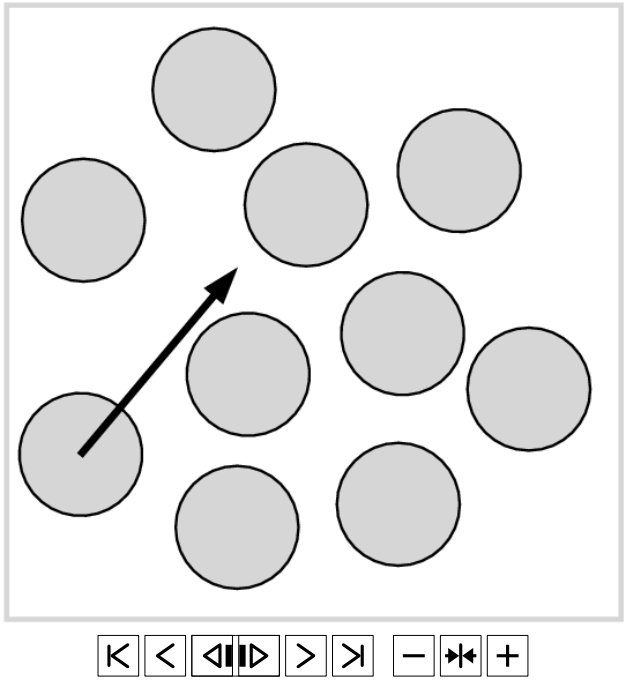
Correlation time in larger simulations



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

Faster algorithm: Event-chain



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

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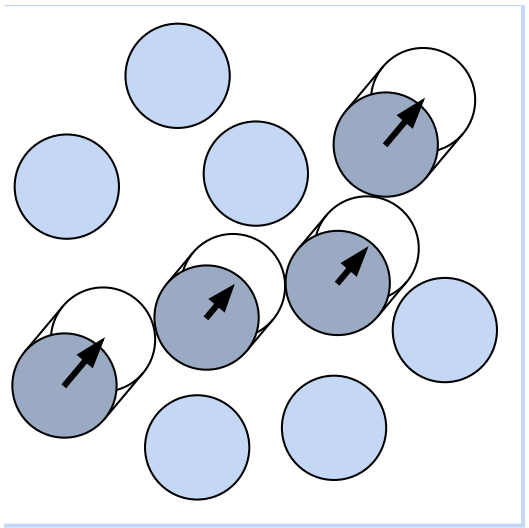
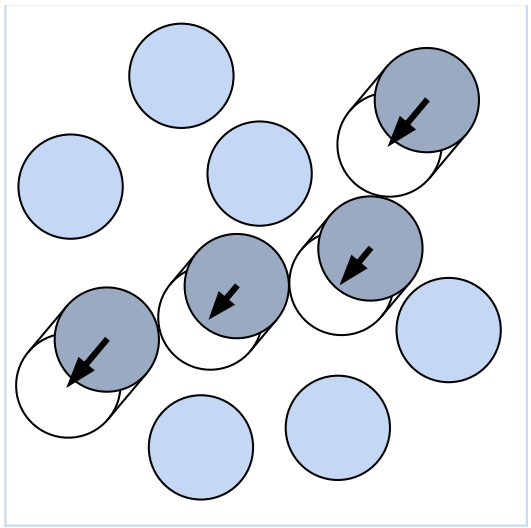
Faster algorithm: Event-chain



i



f

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

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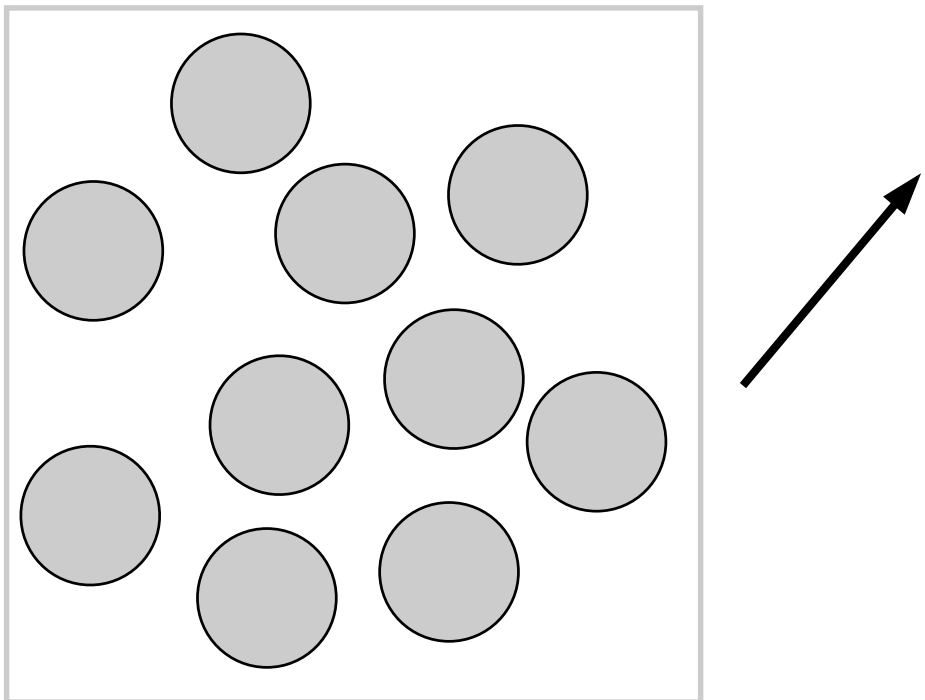
Breaking detailed balance



- . . . speeds up event-chain algorithm . . .

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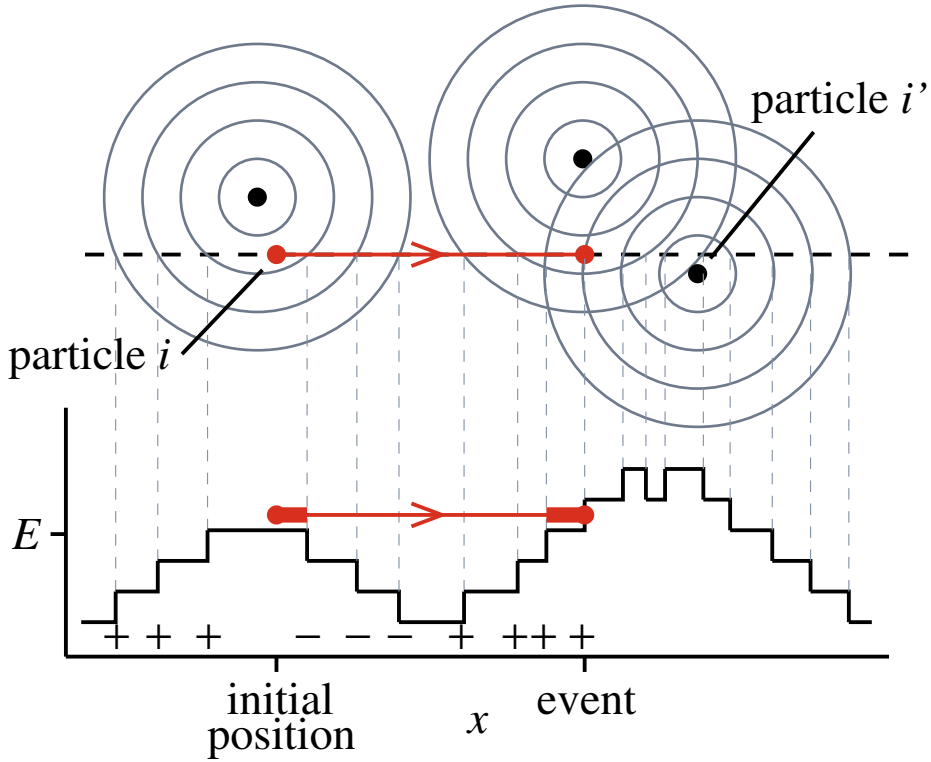
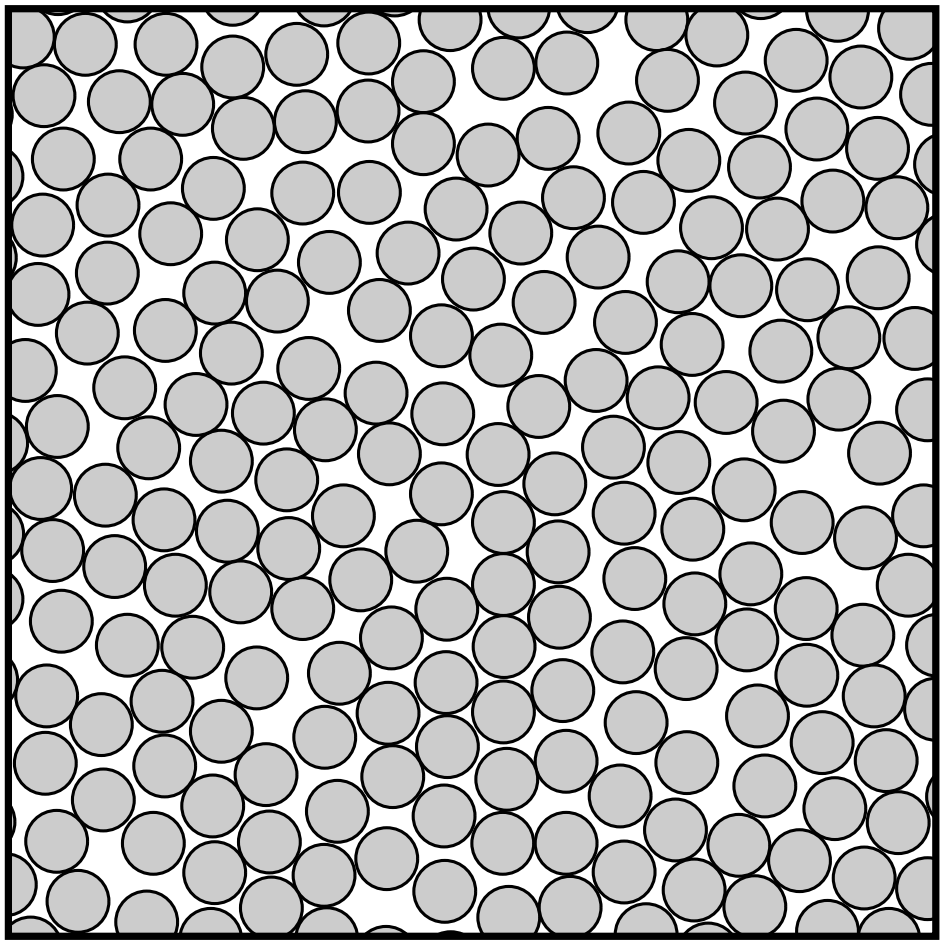
Generalization for stepped/smooth potentials

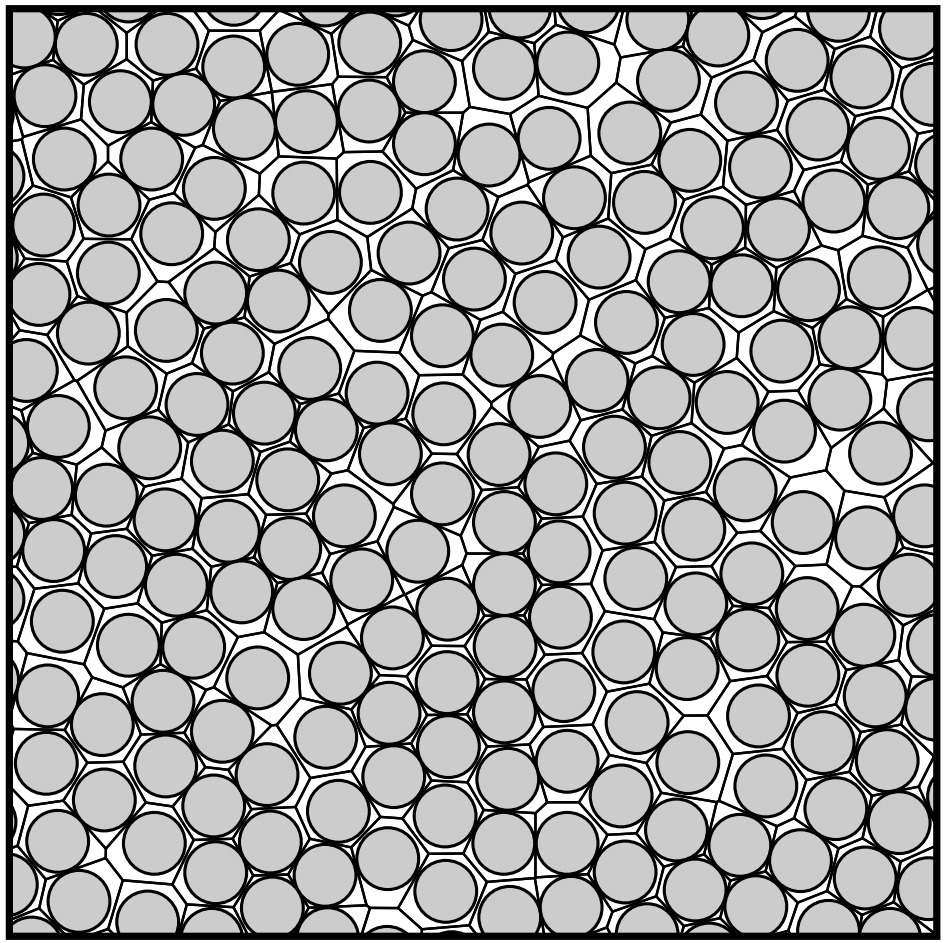


- Microcanonical version, breaking detailed balance
- faster than local Monte Carlo
- Python example code (on WK home page)
- infinite # of steps possible (see home page)
- see lecture webpage

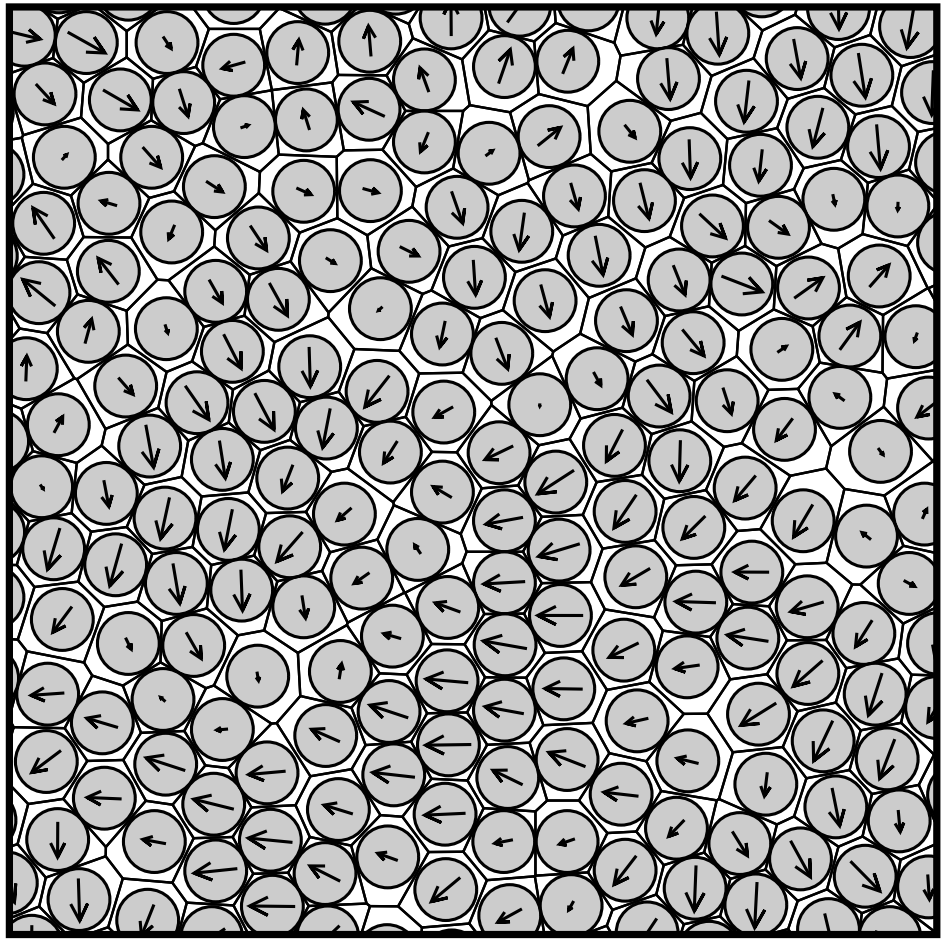
Configurations (1/5)



Configurations (2/5)



Configurations (3/5)



$$\Psi_k = \frac{1}{\#\text{ of neighbors } l} \sum_l e^{6i\phi_{kl}}$$

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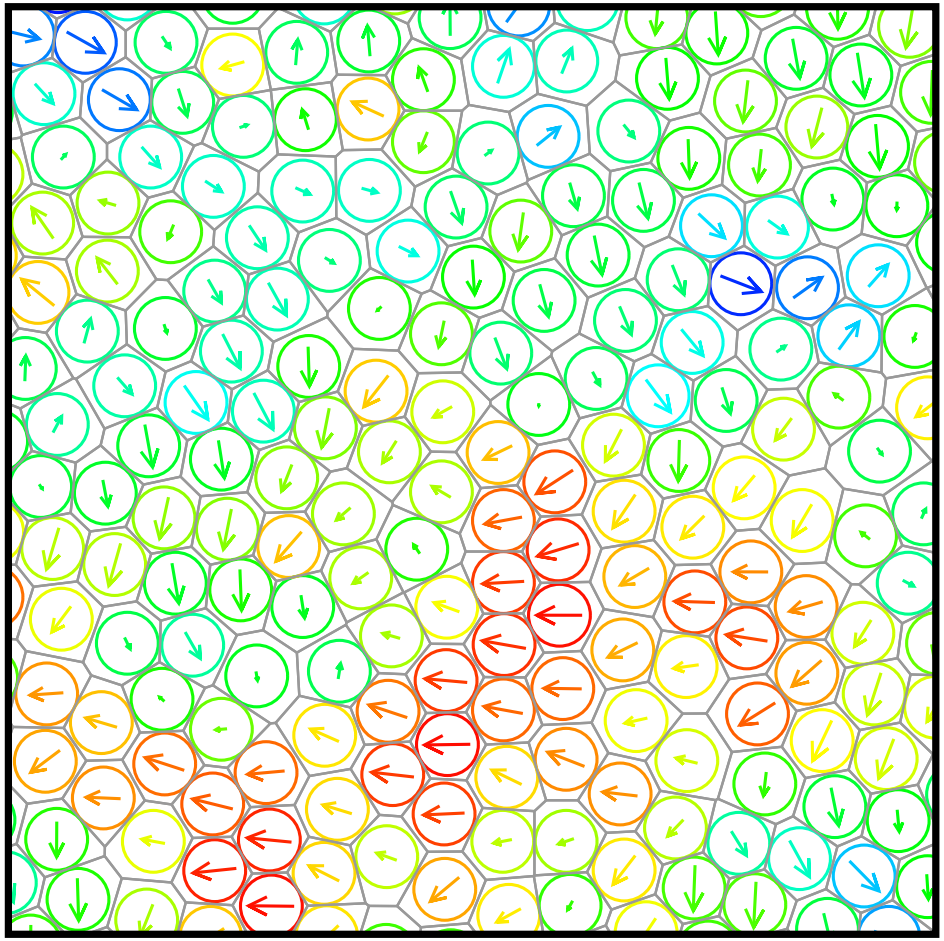
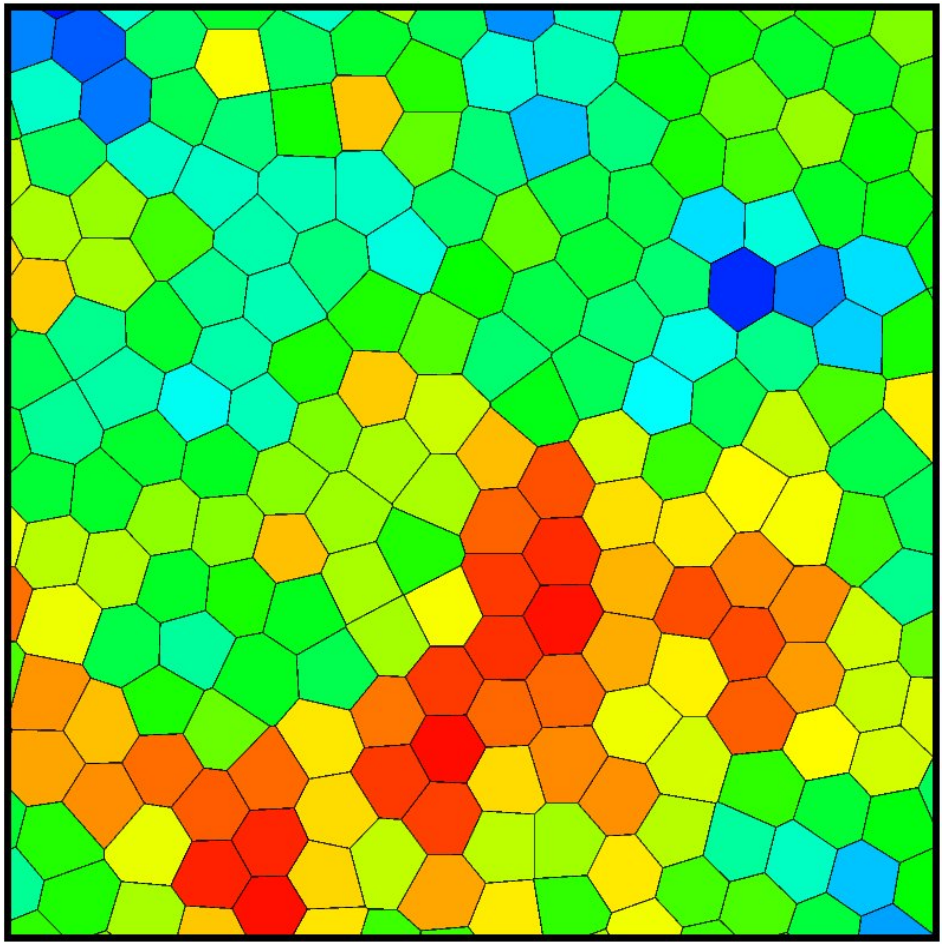
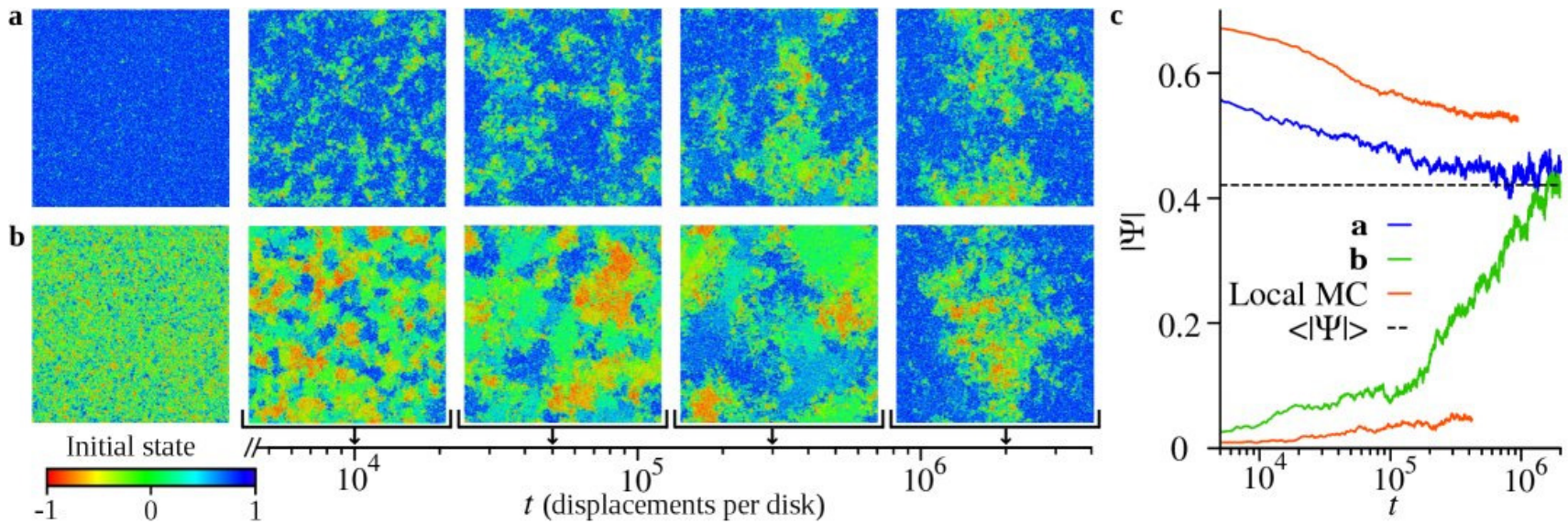
Configurations (4/5)



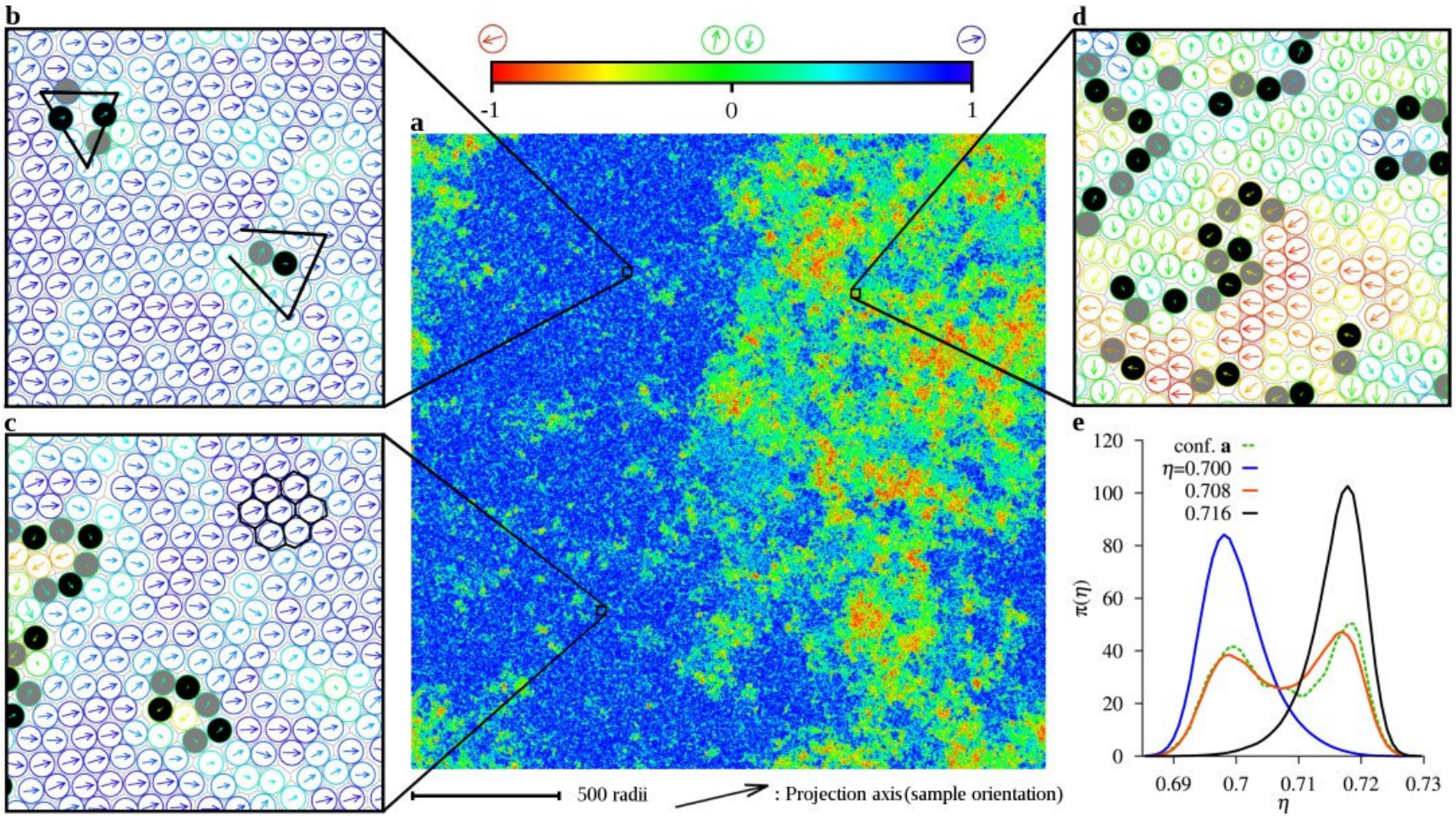
Configurations (5/5)



Correlation times



Phase separation



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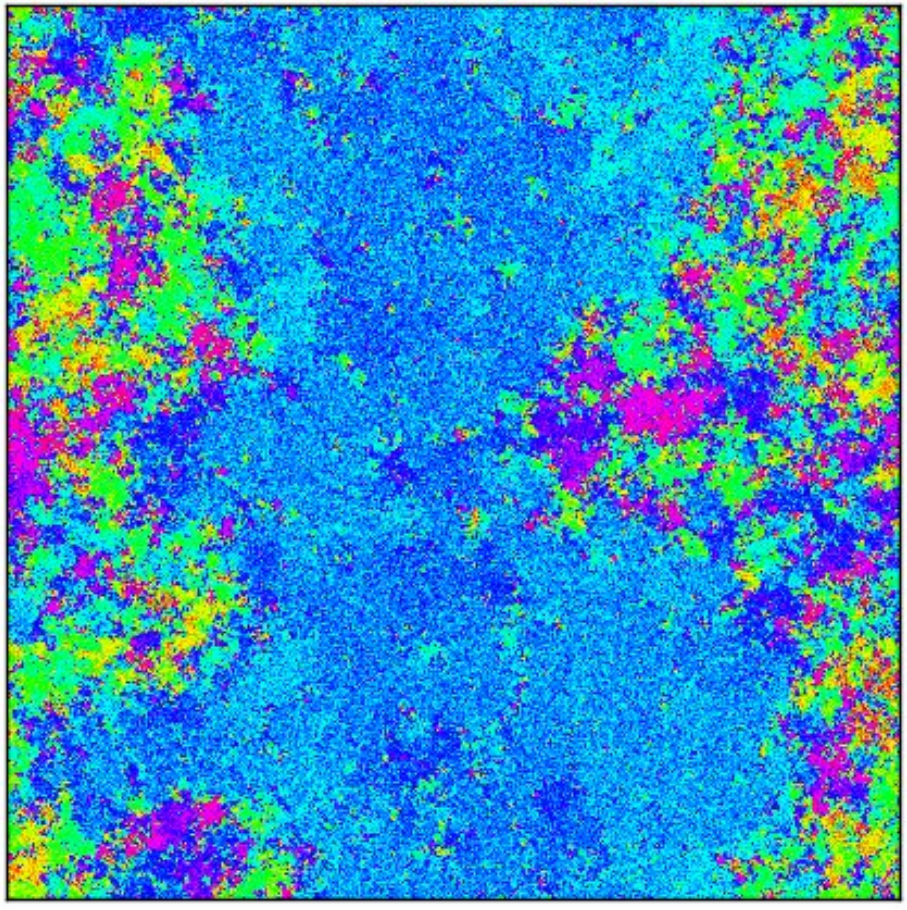
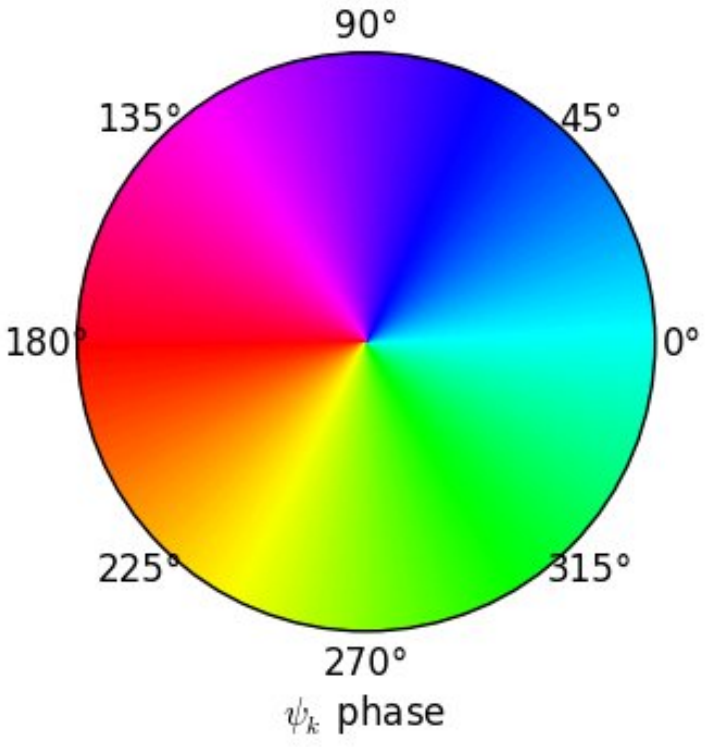
Phase separation (other color code)





- circular color code
- by D. Fiocco

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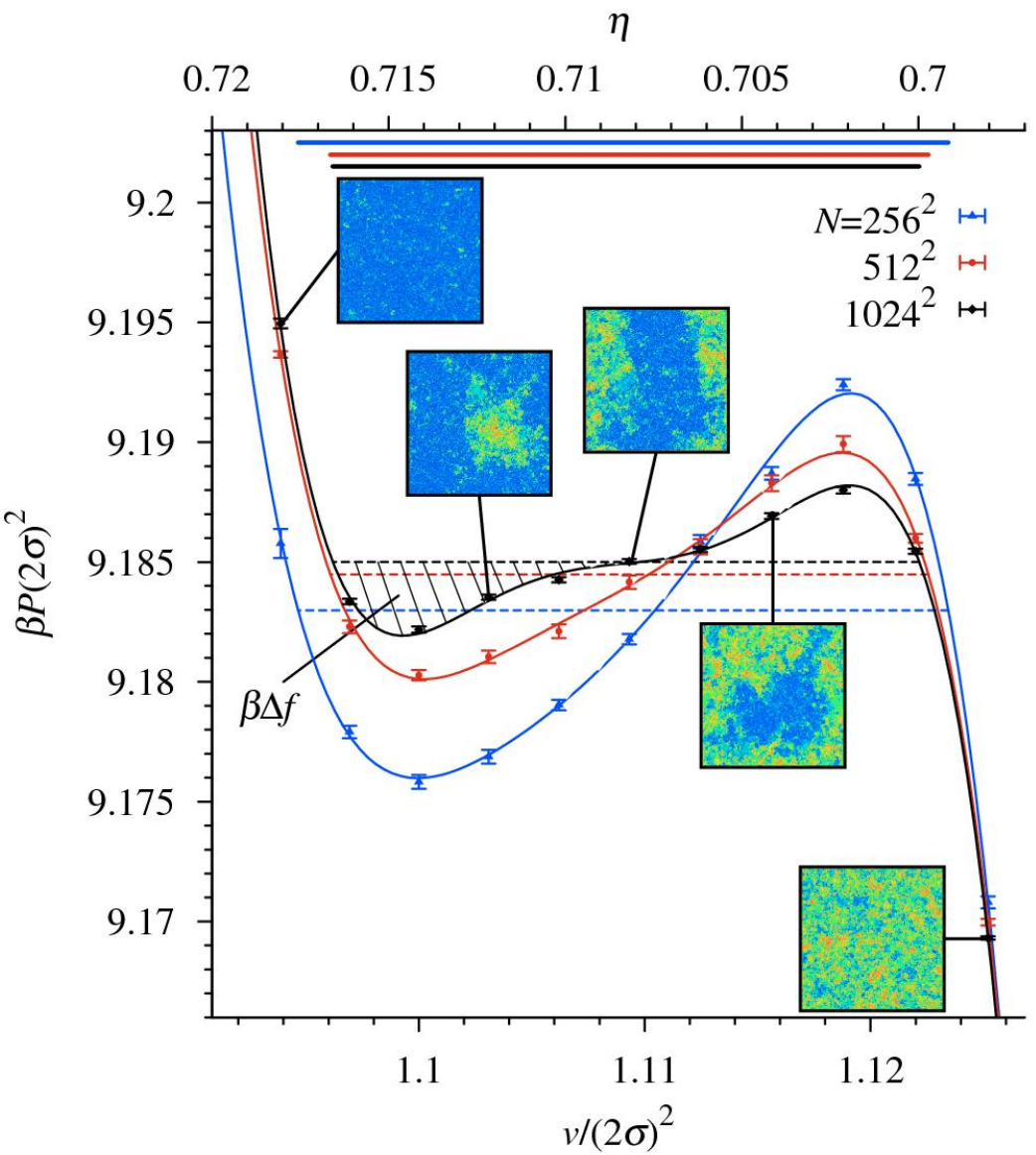
Equation of state



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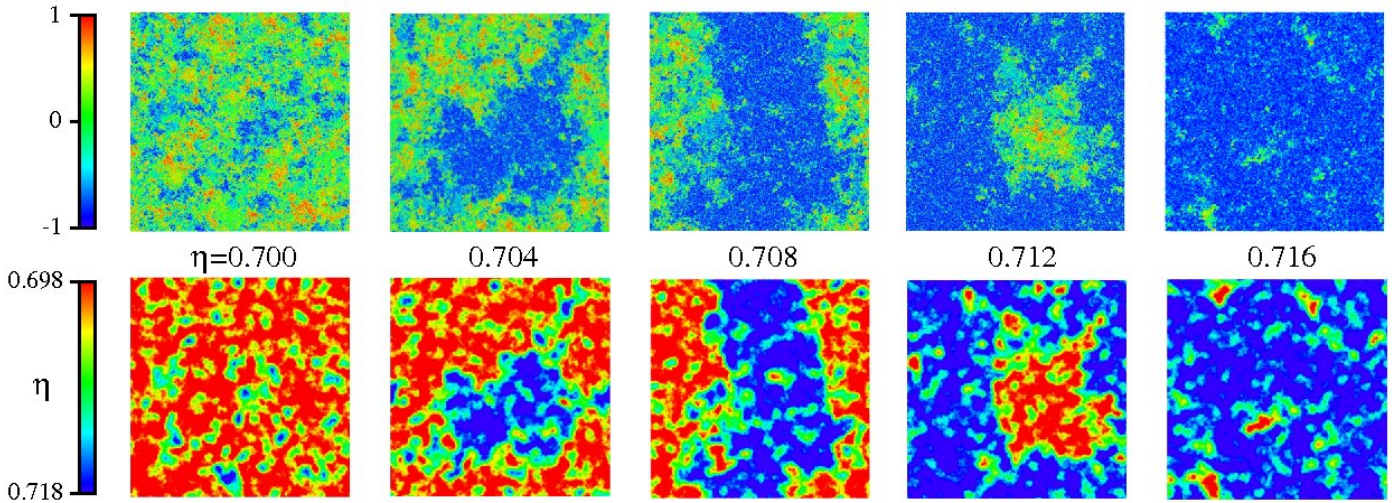
Synopsis of orientations and densities



- Upper: Orientations.
- Lower: Coarse-grained densities.
- Bernard, Krauth, PRL (2011)

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Possible phases (again)

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

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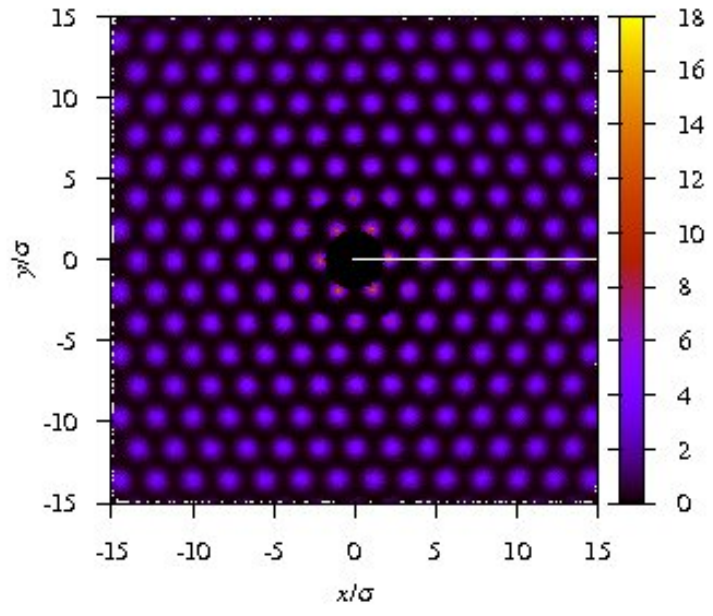
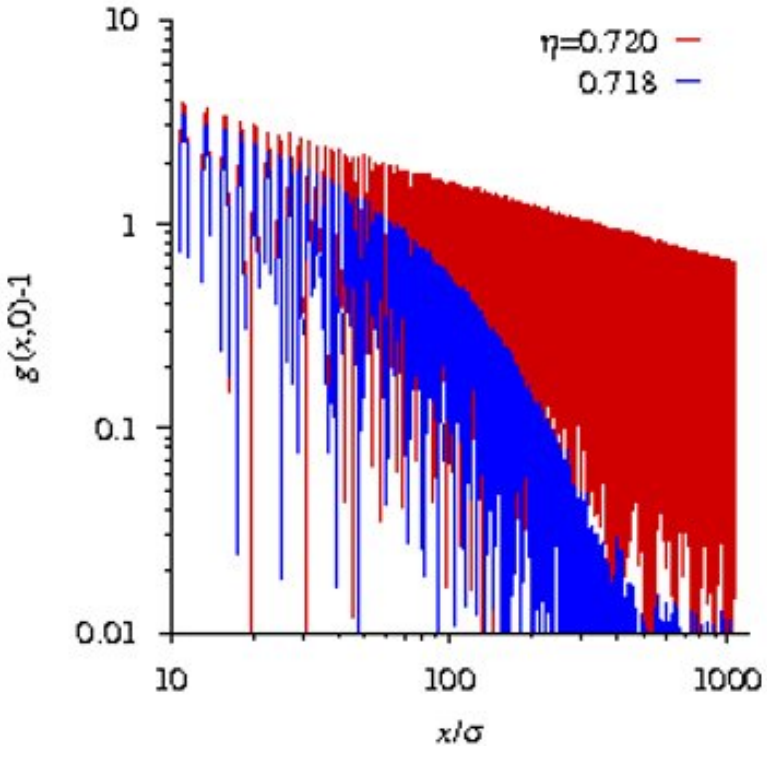
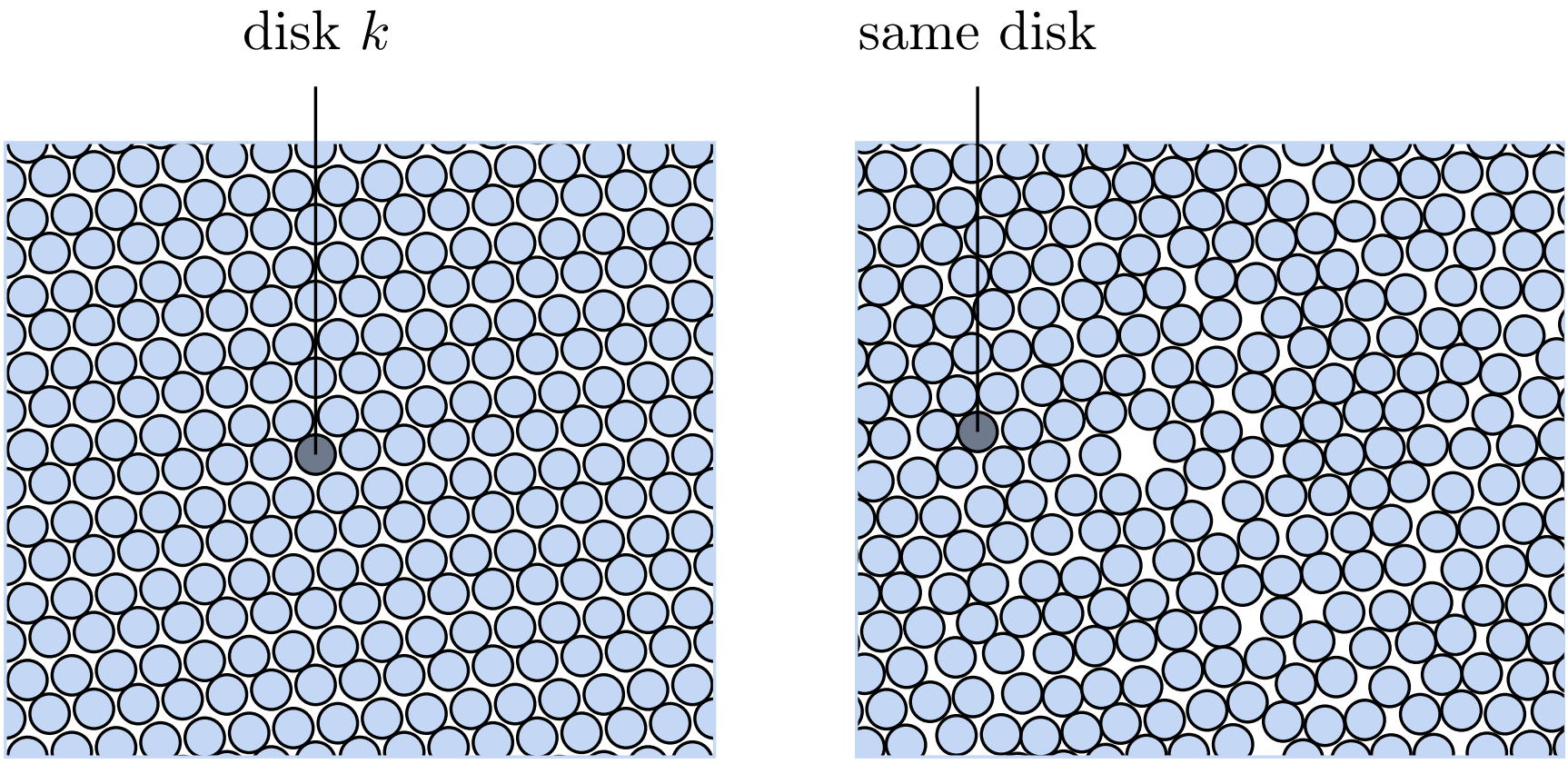
Spatial correlations at $\eta = 0.718$ (sample-averaged)





- Bernard, Krauth, PRL (2011)

Correlation times (2/2)



- Exact time of decorrelation can be computed
- This is the issue of "perfect sampling"

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

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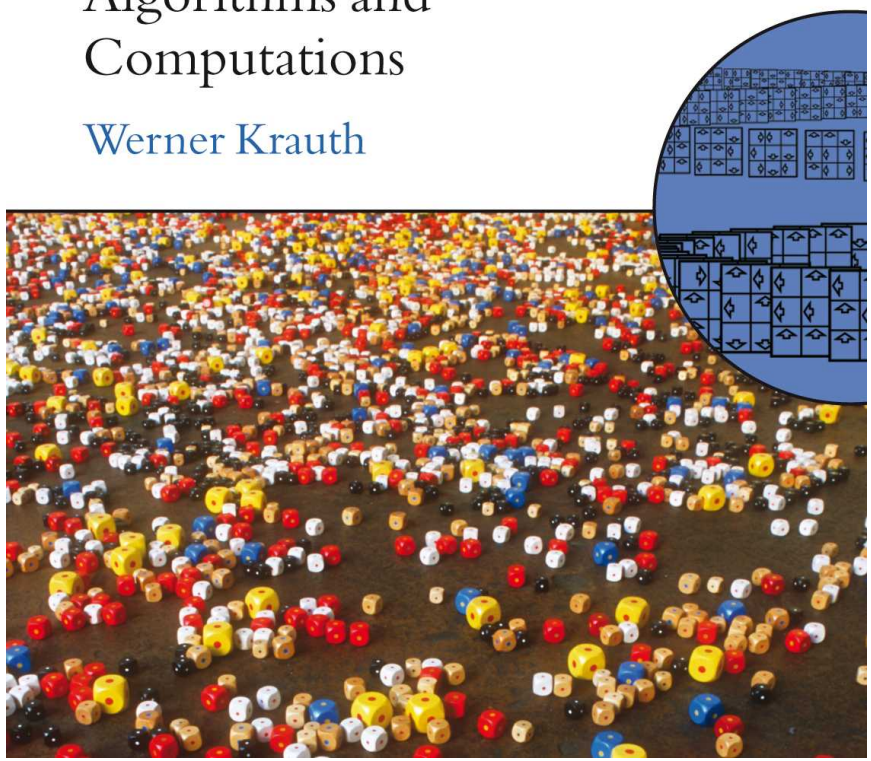

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