Der Schmelzübergang der harten Scheiben

First-order liquid-hexatic transition in hard disks

Werner Krauth

Département de physique
Ecole normale supérieure
Paris, France

Institutskolloquium Institut für Physik, Universität Oldenburg
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References

- E. P. Bernard, W. Krauth, and D. B. Wilson 'Event-chain Monte Carlo algorithm for hard-sphere systems' PRE **80** 056704 (2009)
- E. P. Bernard and W. Krauth 'First-order liquid-hexatic transition in hard disks' arXiv:1102.4094

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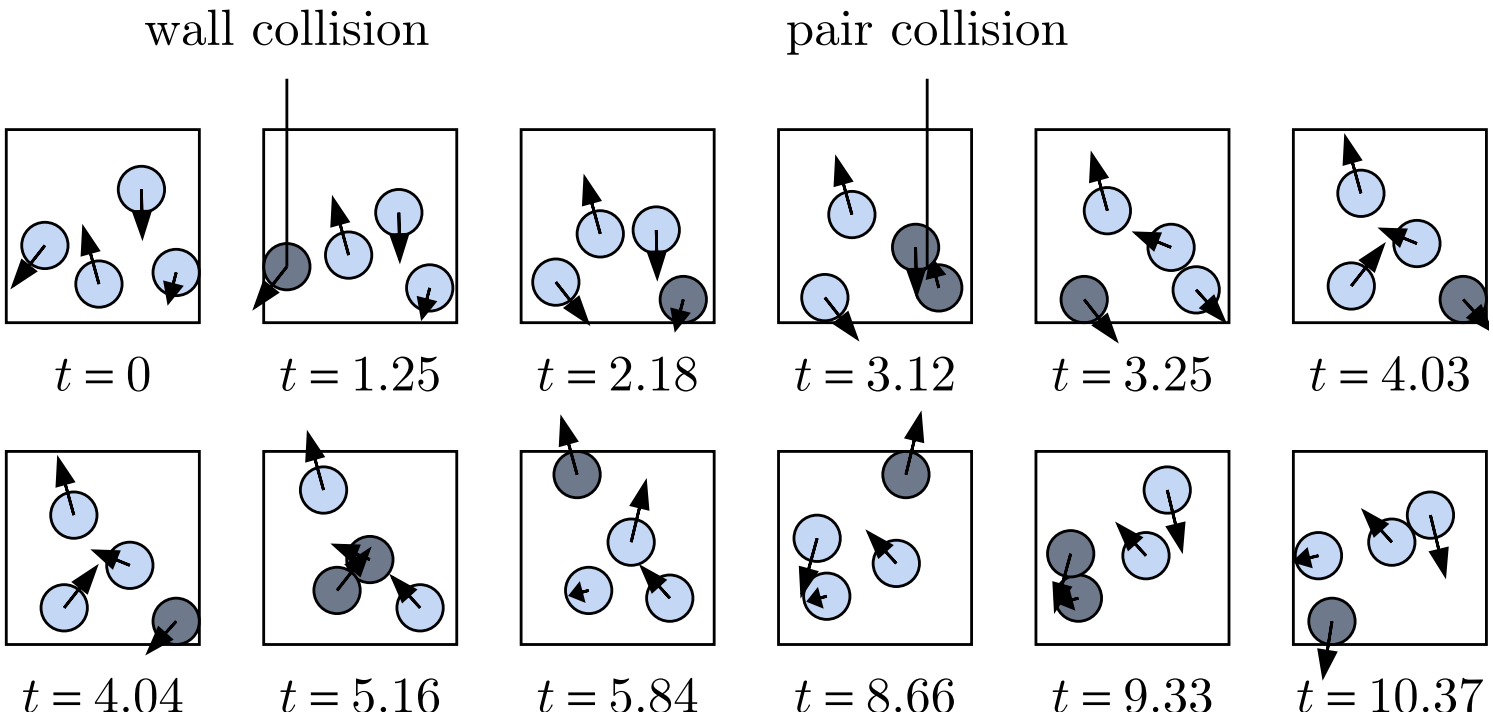
Molecular dynamics ('Newton')

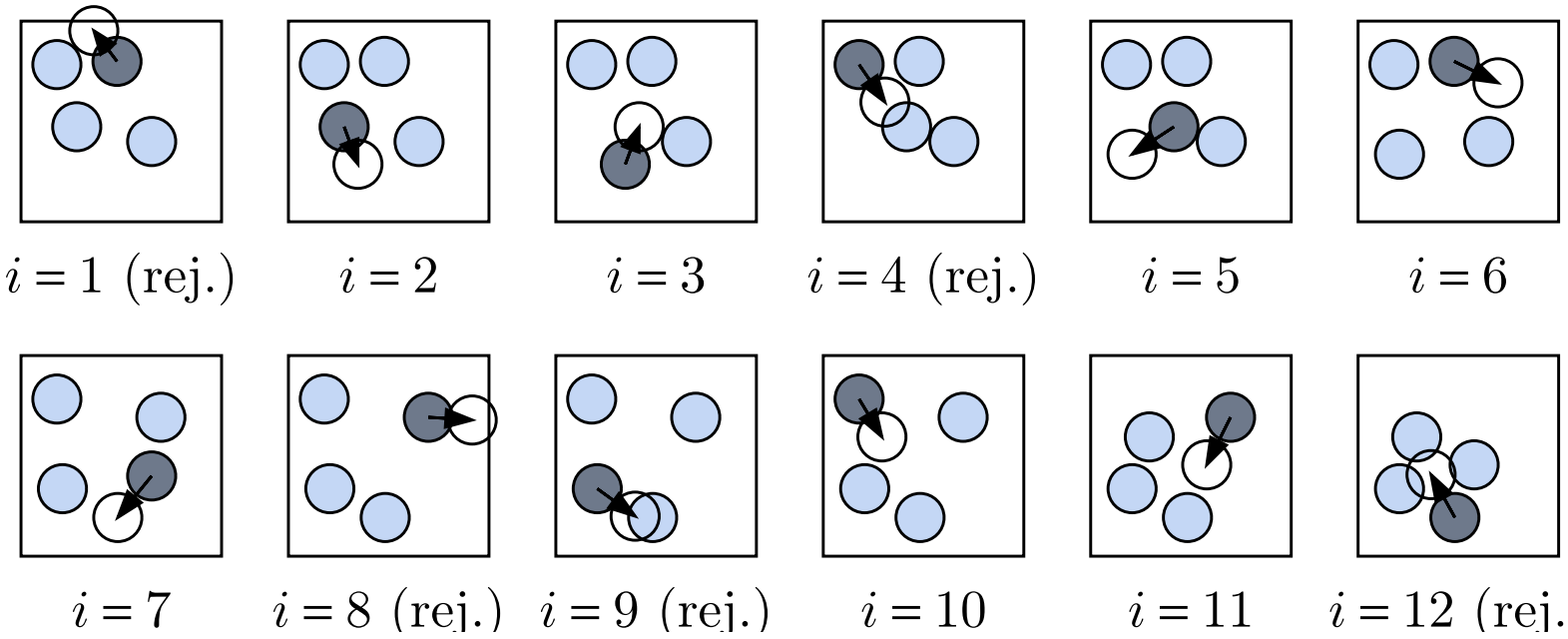
- A molecular dynamics algorithm for hard spheres (disks):



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

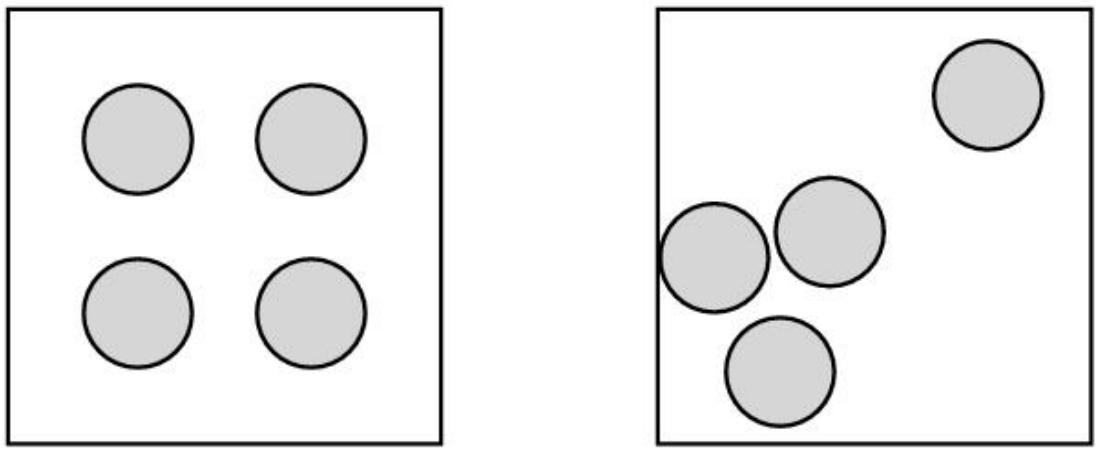
Markov-chain Monte Carlo ('Boltzmann')

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



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

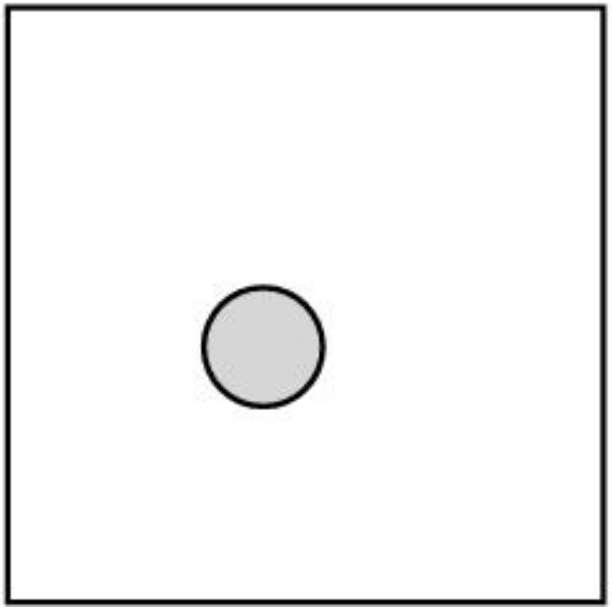
Equal-probability principle



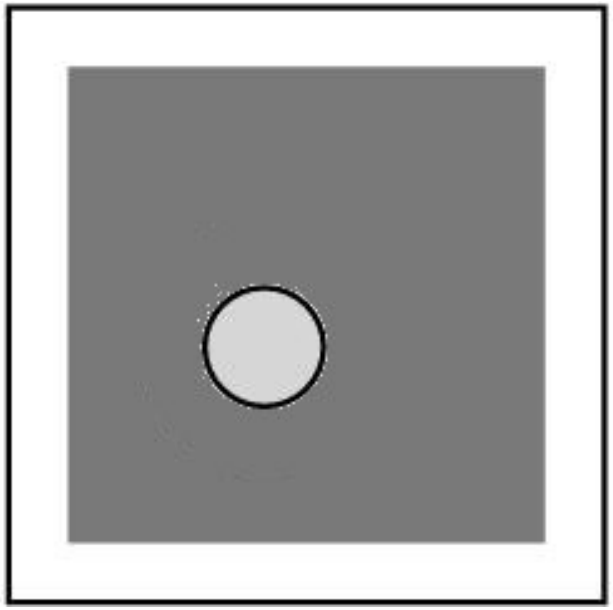
a b

- $\pi(a) = \pi(b)$,
- Equal-probability principle (Boltzmann distribution)

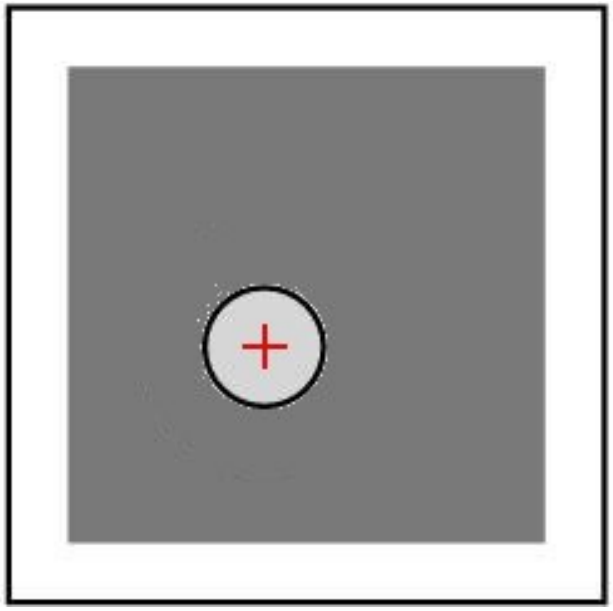
Hard-disk interaction (1/3)



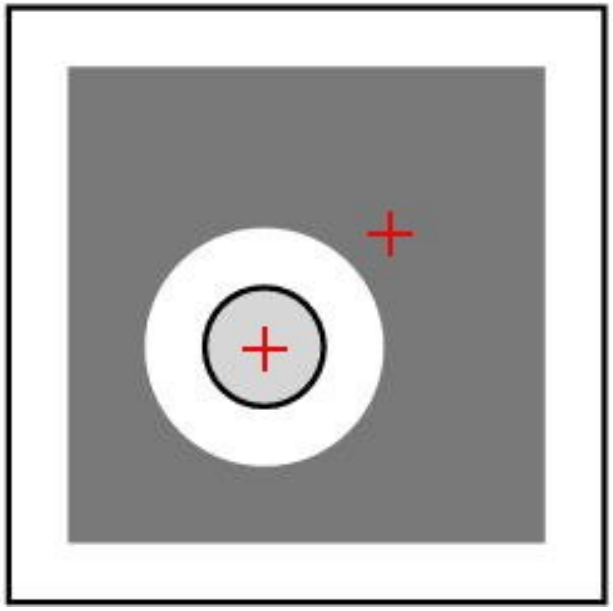
Hard-disk interaction (2/3)



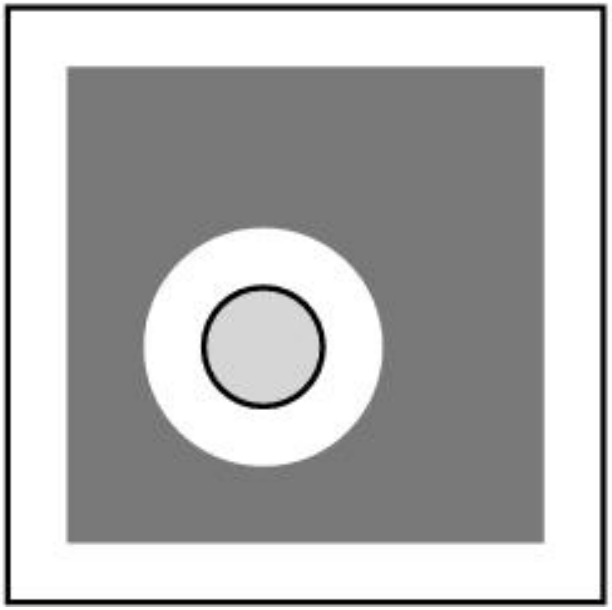
Hard-disk interaction (2/3)



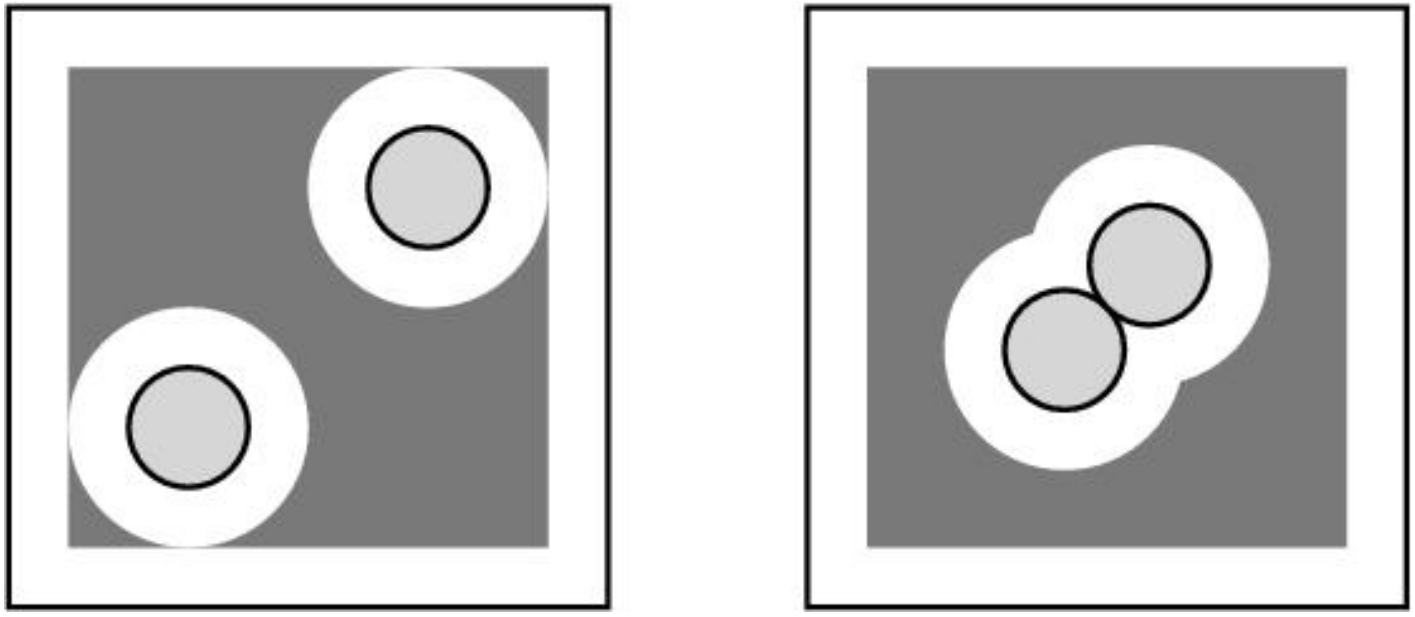
Hard-disk interaction (2/3)



Hard-disk interaction (2/3)

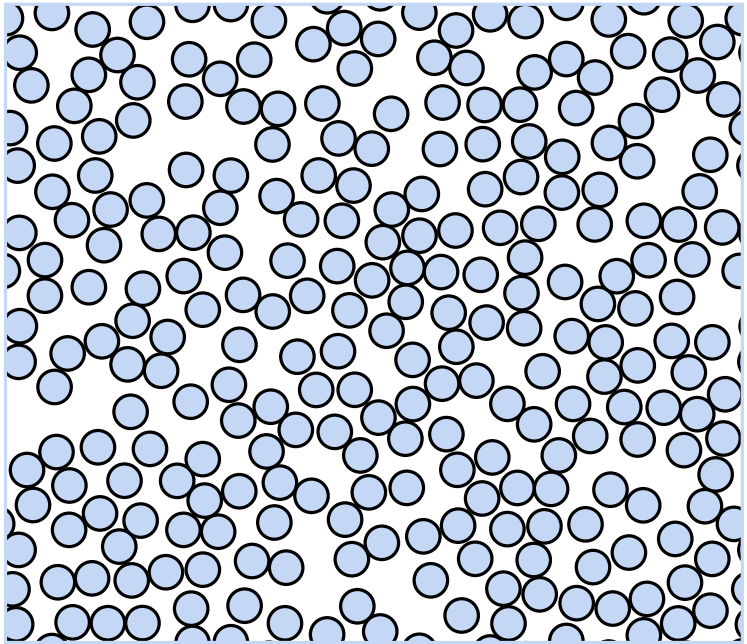


Hard-disk interaction (3/3)

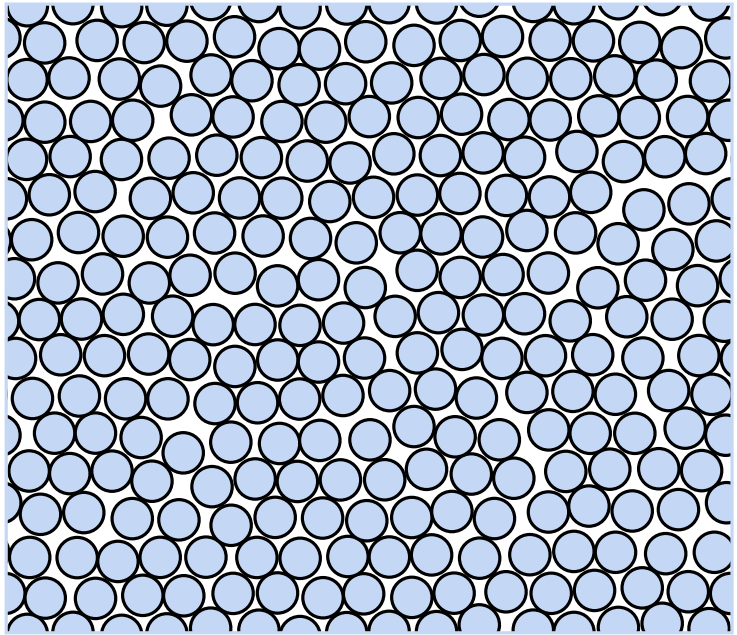


- Asakura-Oosawa (1954) depletion interaction

$2D$ melting transition

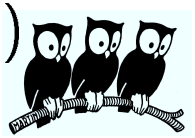


density $\eta = 0.48$

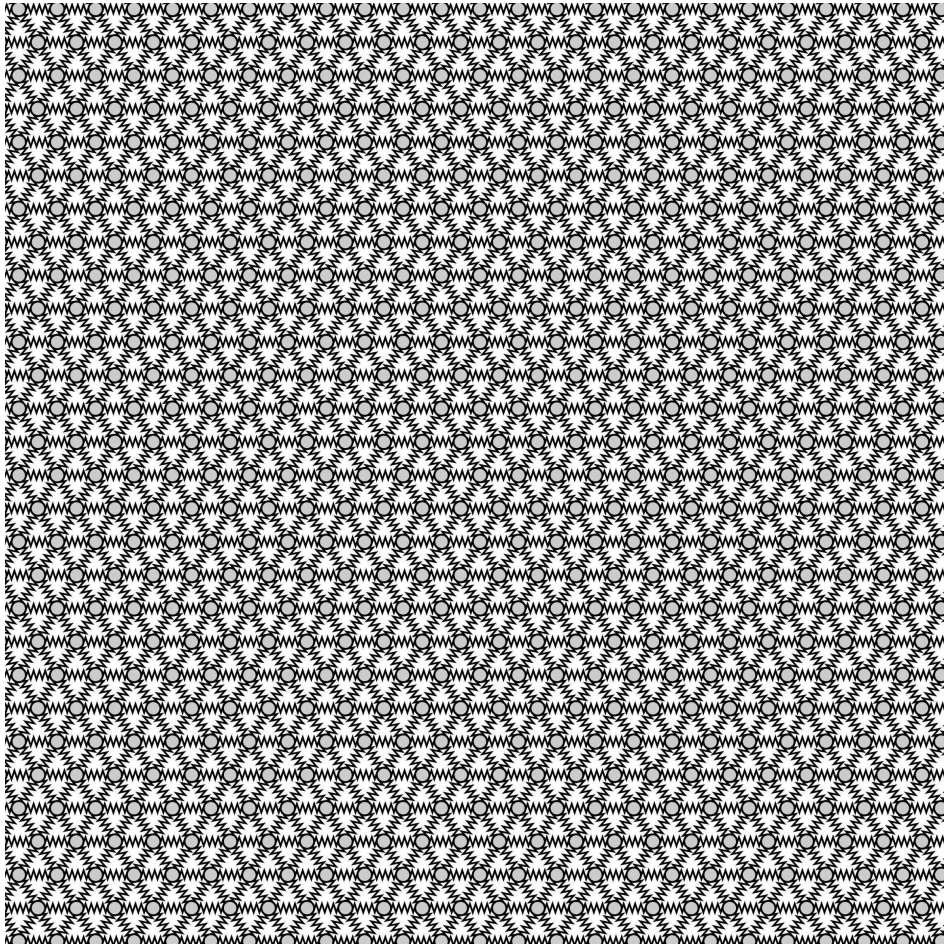


density $\eta = 0.72$

- At low density, disks move easily (liquid)
- . . . at high density, MC algorithms slow down and disks turn solid (but cannot crystallize) . . .
- . . . nature of transition long disputed (first order vs. KTHNY)
- cf. Blöte et al. (2002); van Enter, Schlosman (2002)



Harmonic solid - Peierls' argument (1938)



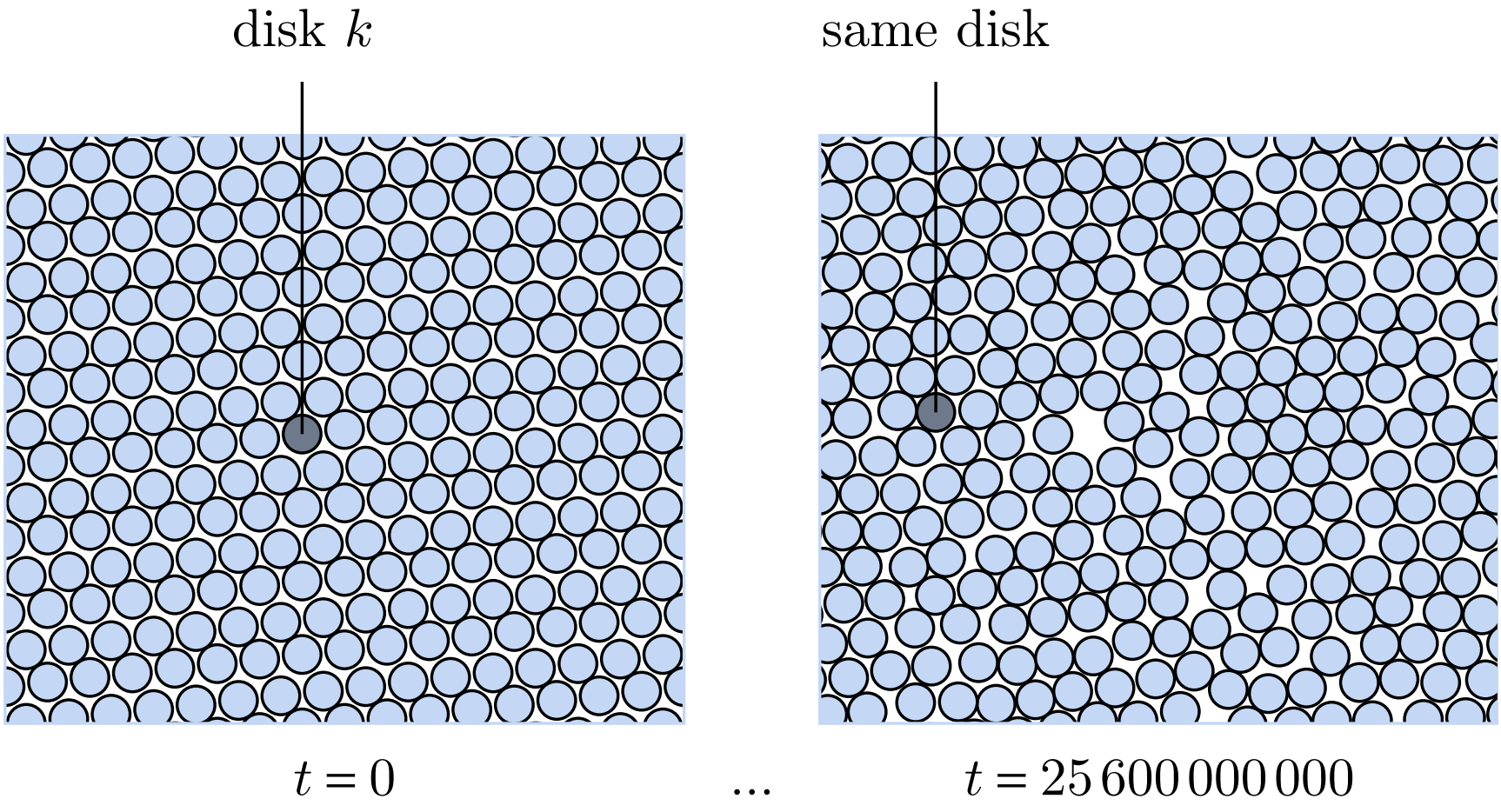
Harmonic solid - Mermin's observation (1968)

In the harmonic solid

- positional order decays algebraically...
- ... but *orientational* order is truly long-ranged...

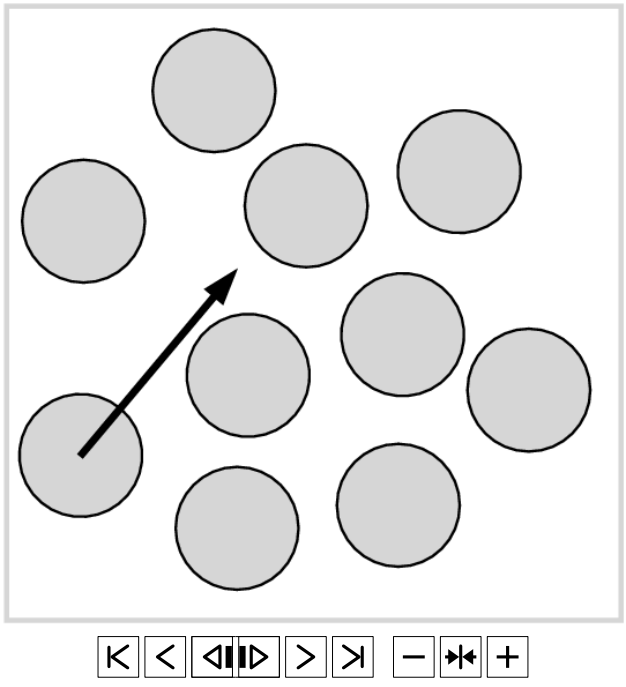
... 'no long-range order in two dimensions...'

Correlation time in larger simulations



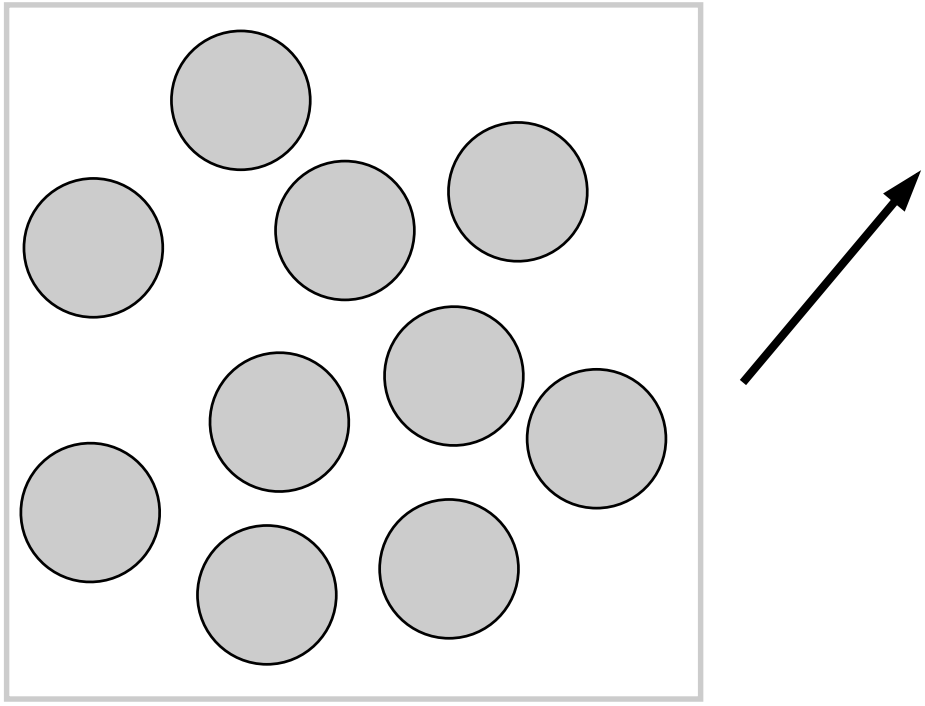
- τ exists, but it is large ($\tau \gg 25\,600\,000\,000$).

Event-chain algorithm



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

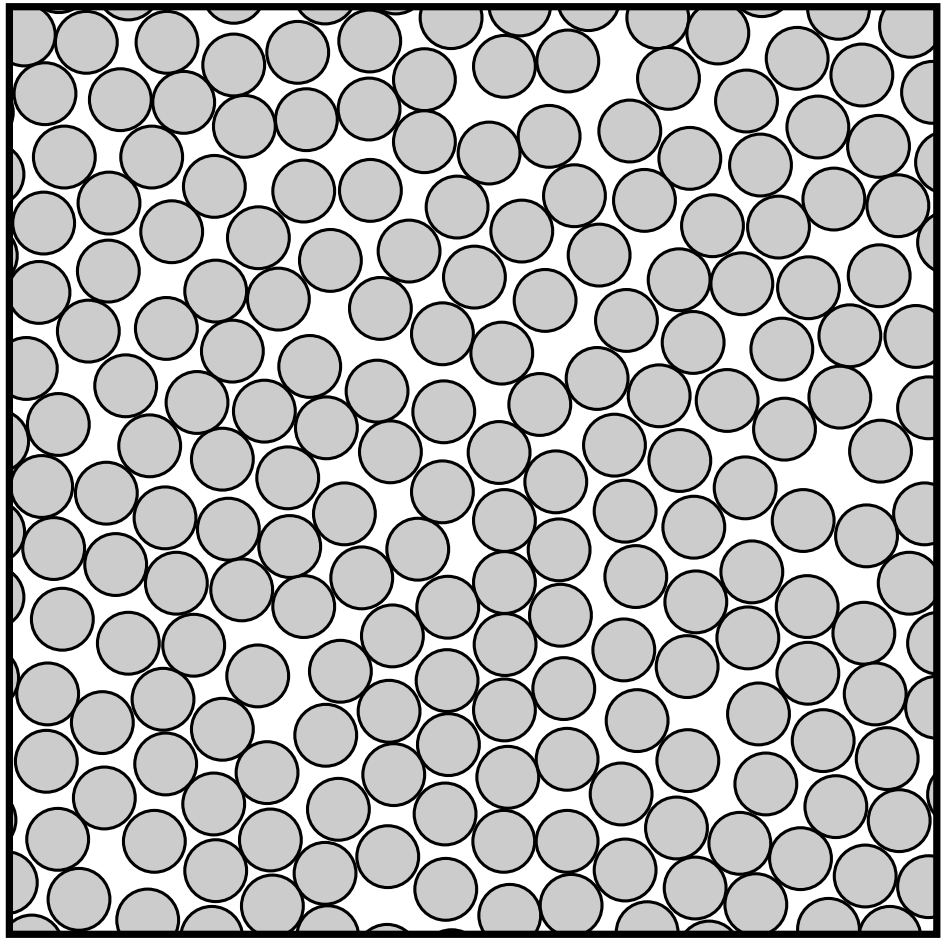
Giving up detailed balance (1/2)



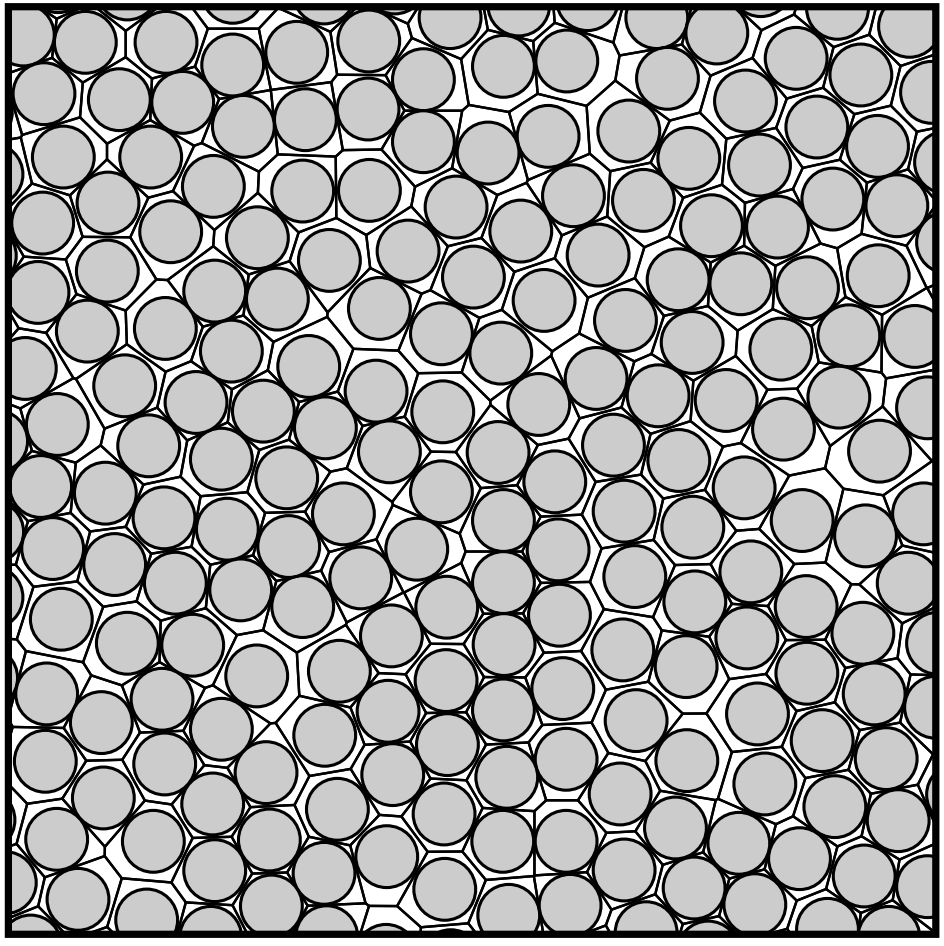
Giving up detailed balance (2/2)

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

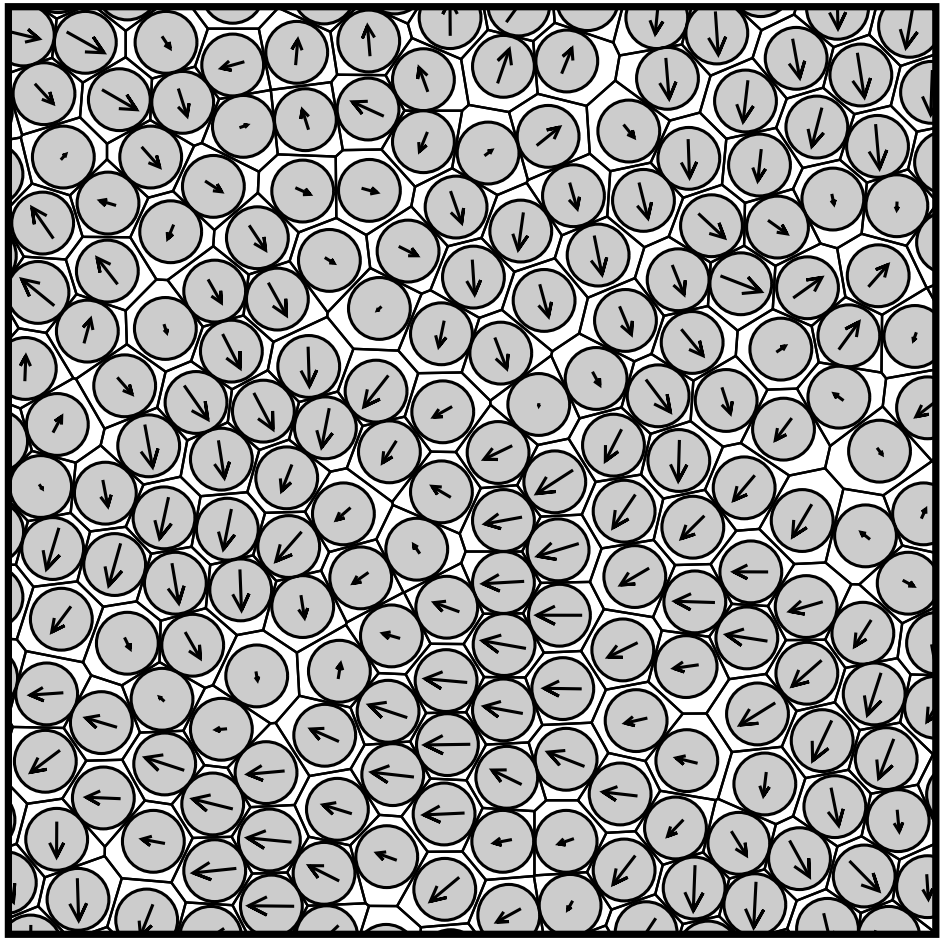
Configurations (1/5)



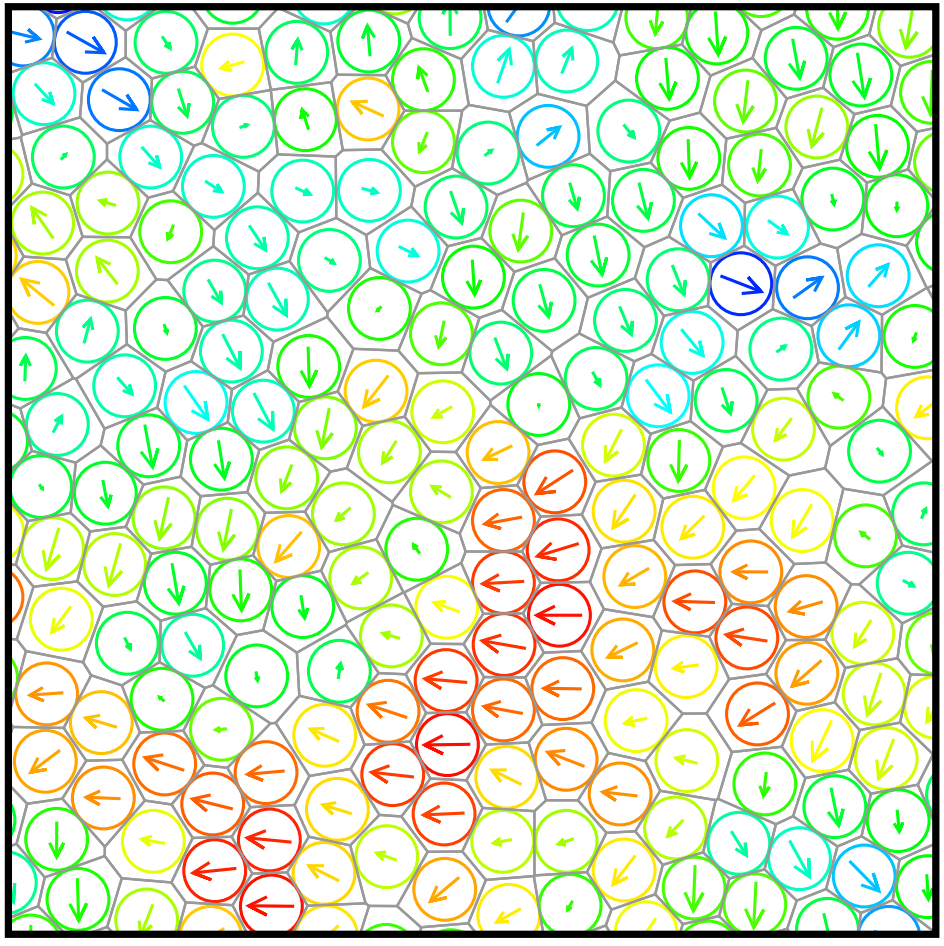
Configurations (2/5)



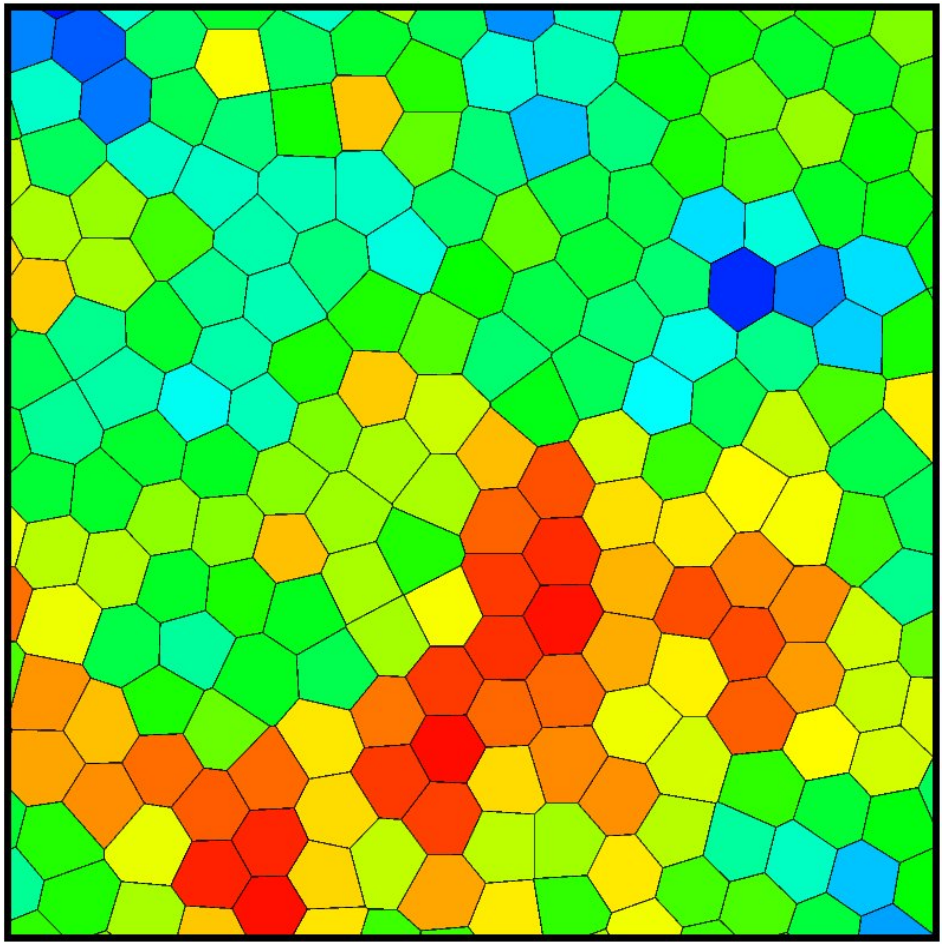
Configurations (3/5)



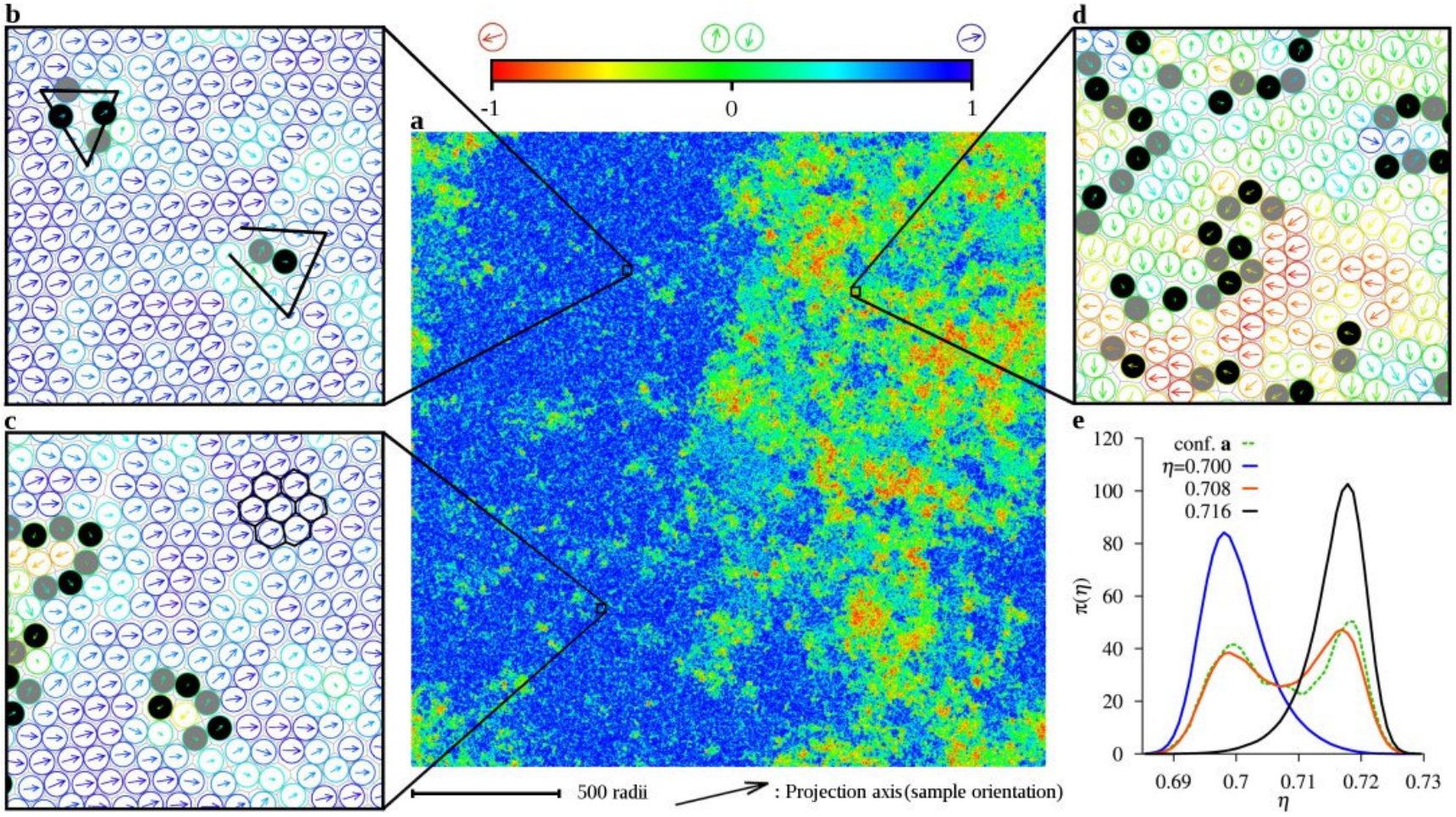
Configurations (4/5)



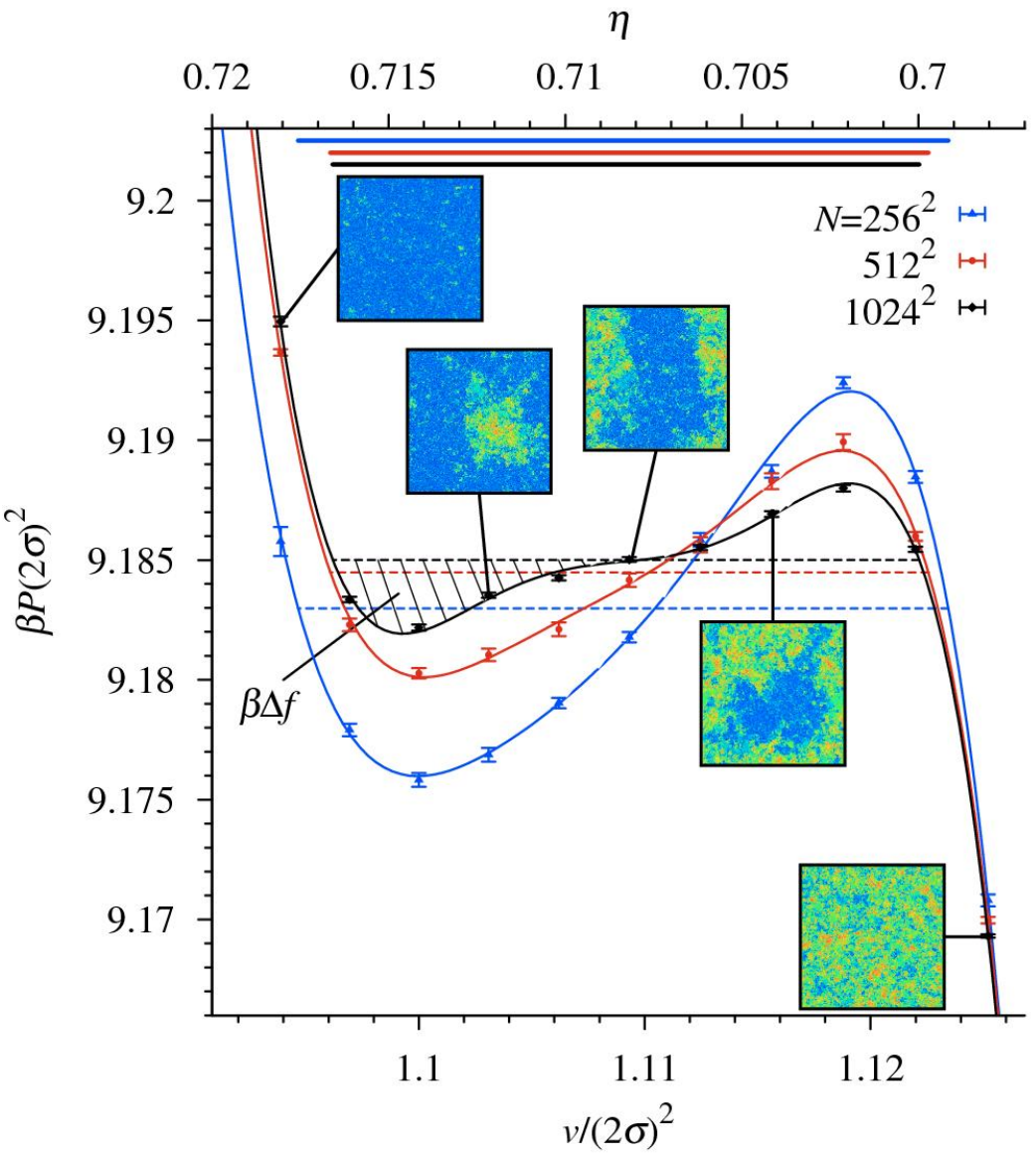
Configurations (5/5)



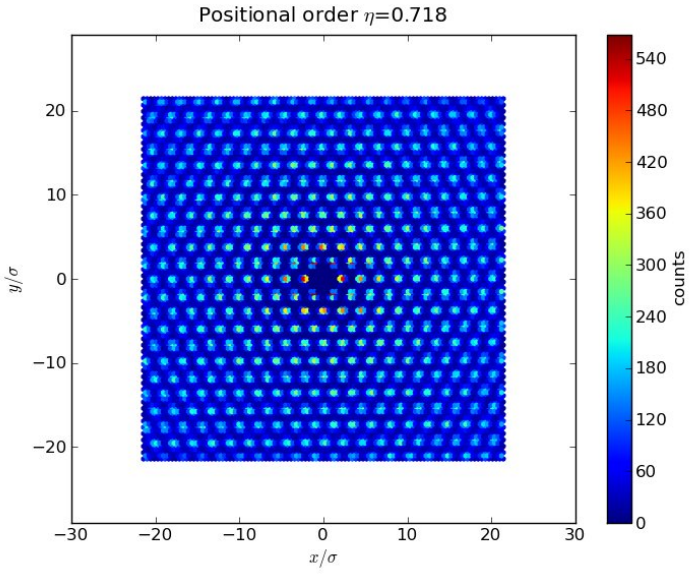
Phase separation

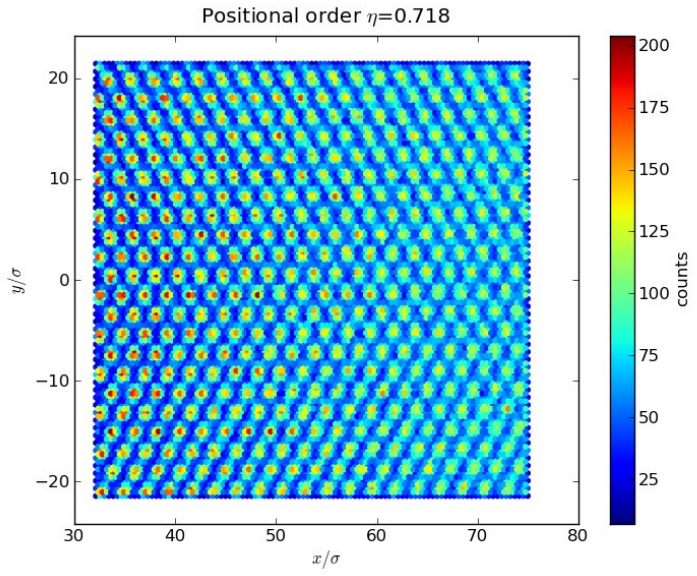


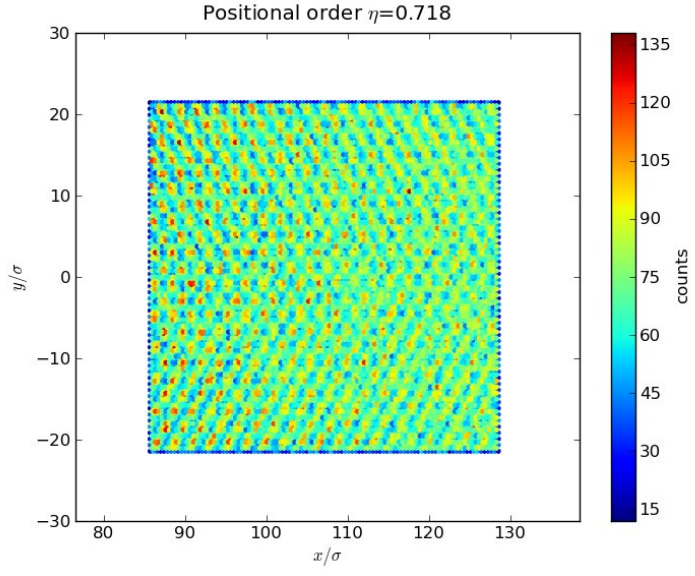
Equation of state

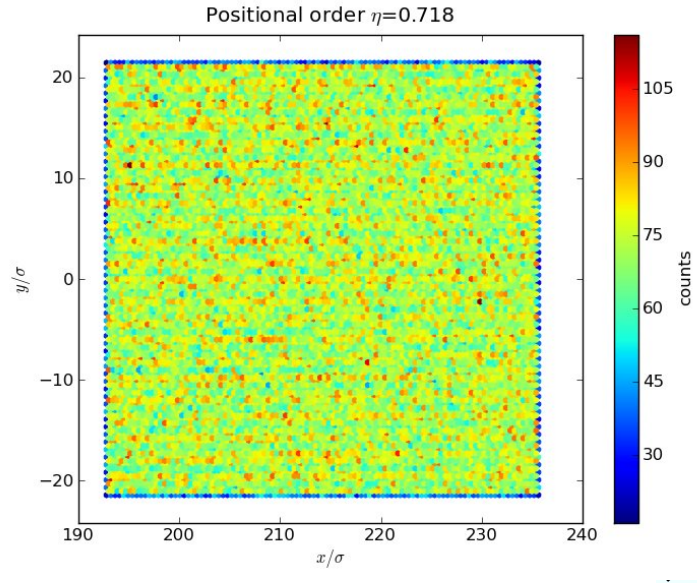


Spatial correlations at $\eta = 0.718$ (single sample)

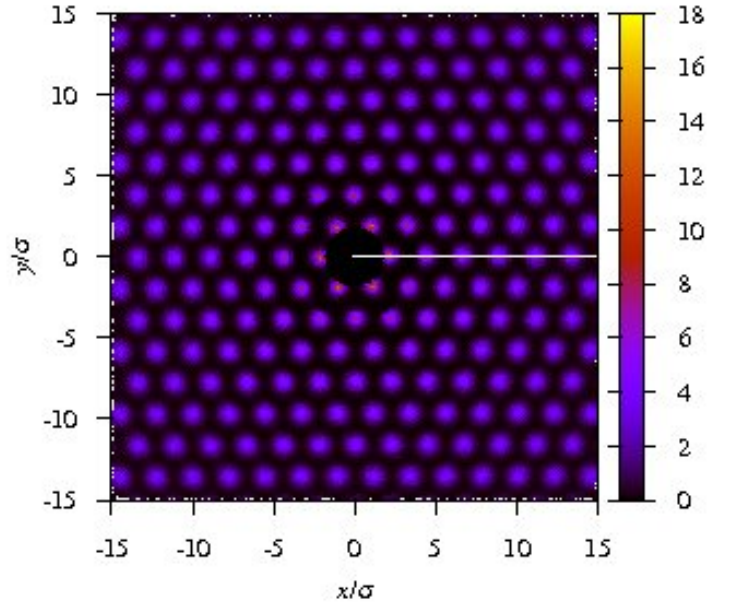


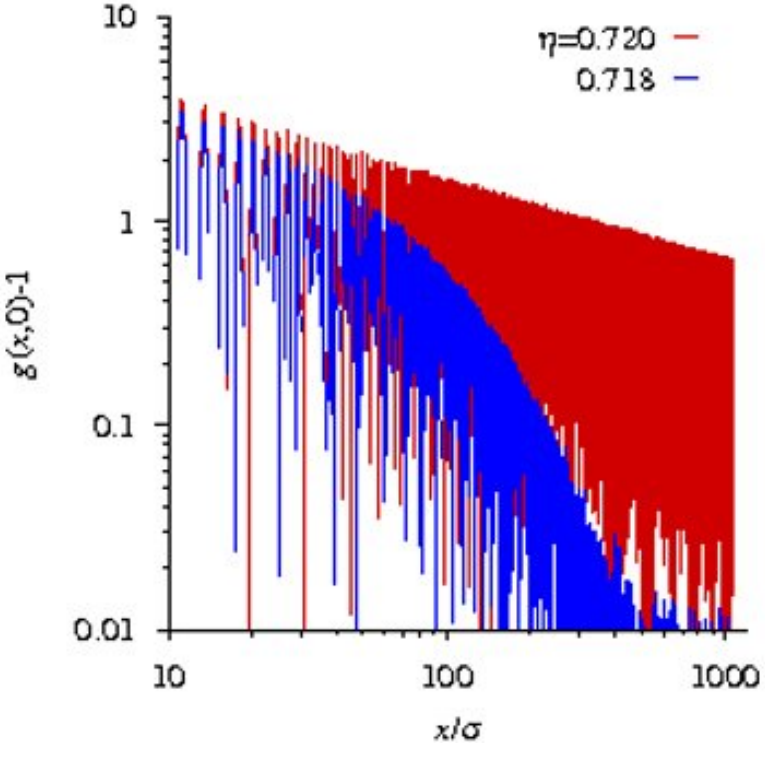




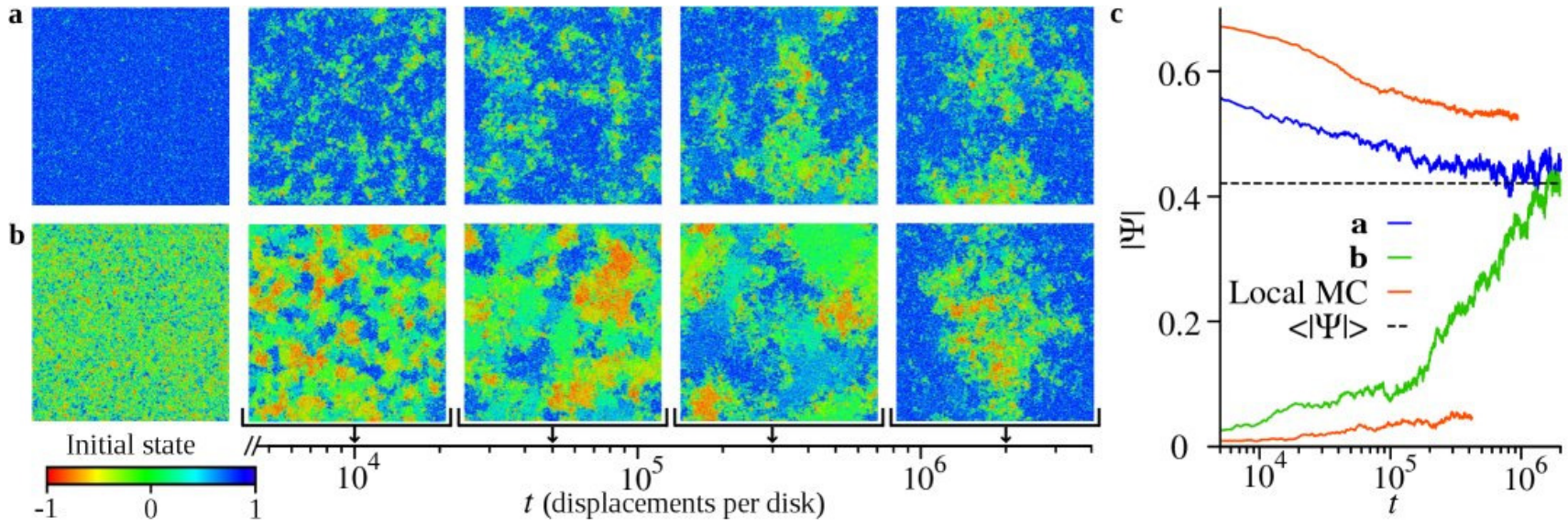


Spatial correlations at $\eta = 0.718$ (sample-averaged)





Correlation times



Conclusions

- **Interactions**
- **Phase transitions**
- **Algorithms - Event chains**
- **Graphics representations**
- **Two-dimensional melting**
  - Liquid-hexatic-solid
- **...solution of an old puzzle**

Extensions

- $2d$-$3d$ crossover (finite thickness in z)
- HS-LJ crossover (weaker potentials)
- Elastic constants - comparison with KTHNY theory

- Constant-pressure calculations
- Gibbs-ensemble calculations

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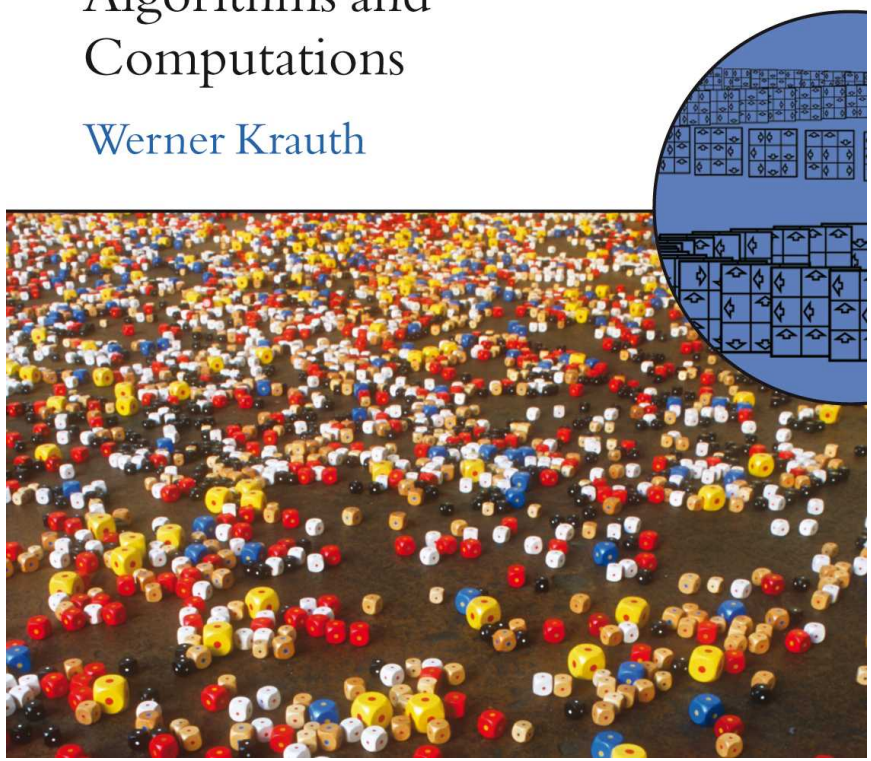
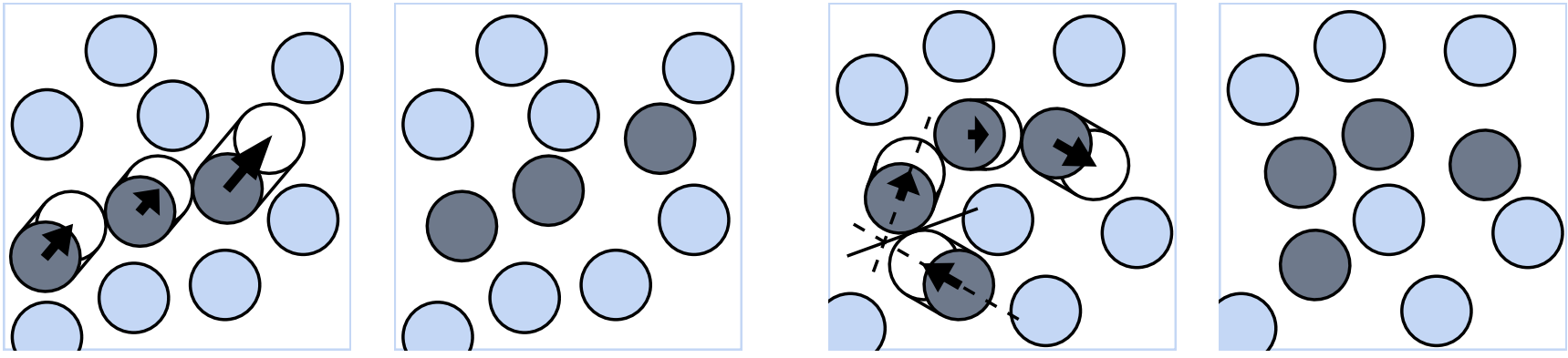


Other versions



- detailed balance = microreversibility & conservation of phase space volume

Error computations