Fast irreversible Markov chains beyond the Metropolis paradigm

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COmputational Statistics and MOlecular Simulation

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M. Isobe, N. Yoshihiko, K. Hukushima,
E. P. Bernard, D. B. Wilson

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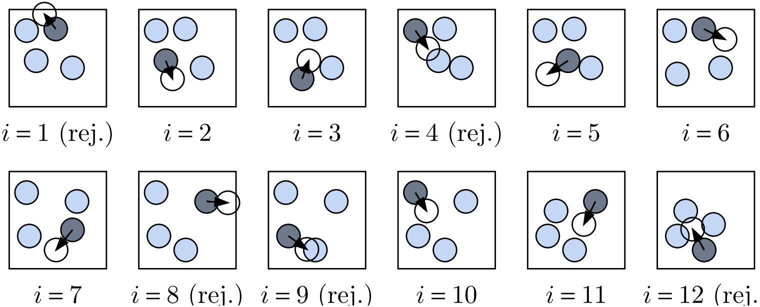
Metropolis et al (1953)

- Local hard-sphere Monte Carlo:



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- . . . is reversible (satisfies detailed balance) . . .
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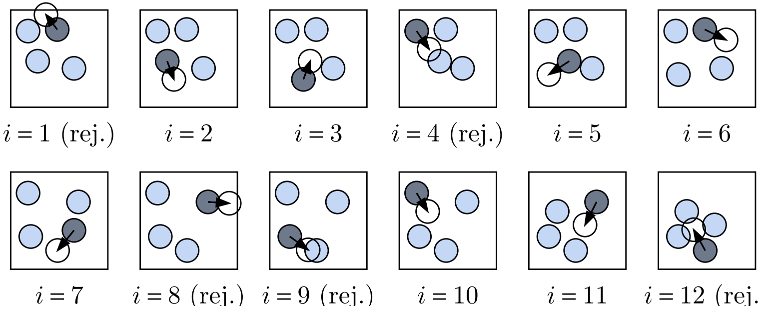

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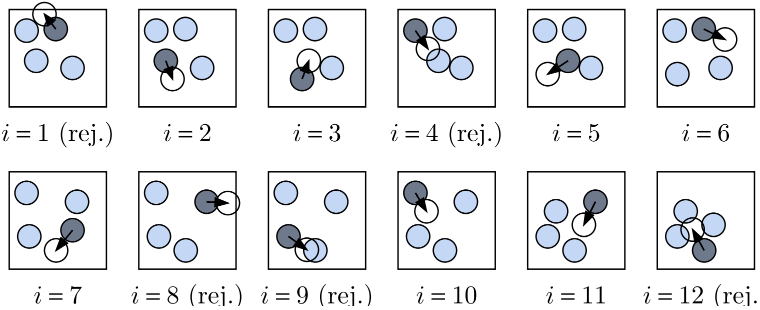

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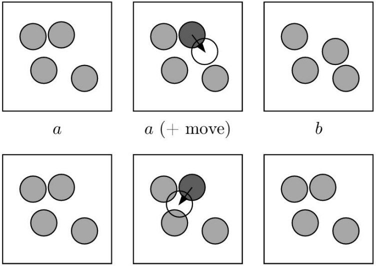
Hard spheres



- Displacements (δ_x, δ_y) sampled uniformly in $([-\delta, \delta], [-\delta, \delta])$
- Algorithm satisfies detailed balance:

$$\pi(a)p(a \to b) = \pi(b)p(b \to a)$$

with $\pi(a) = \pi(b) = \pi(c)$, for all legal configurations of hard spheres

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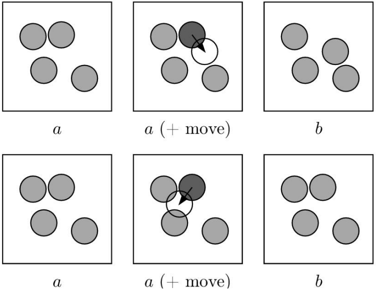

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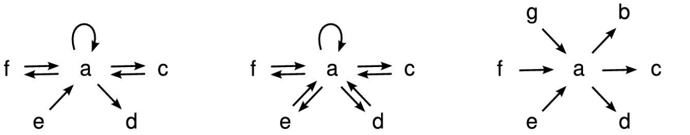
Detailed balance - global balance



global balance — detailed balance — maximal global balance

- flow in $\equiv$ flow out (global balance condition):

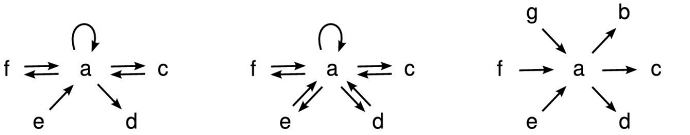
$$\underbrace{\sum_k \pi(k)p(k \to a)}_{\text{flow into } a \ \sum_k \varphi(k \to a)} = \underbrace{\sum_k \pi(a)p(a \to k)}_{\sum_k \varphi(a \to k) \text{ flow out of } a}$$

- flow $\varphi(a \to b) \equiv$ flow $\varphi(b \to a)$ (detailed balance condition):
  - Metropolis algorithm (for flows and cond. probabilities)

$$\varphi(a \to b) = \min(\pi(a), \pi(b))$$

$$p(a \to b) = \min\left(1, \frac{\pi(b)}{\pi(a)}\right)$$

Detailed balance - global balance



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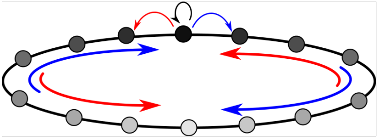
Lifting - one (hard) sphere 1/2



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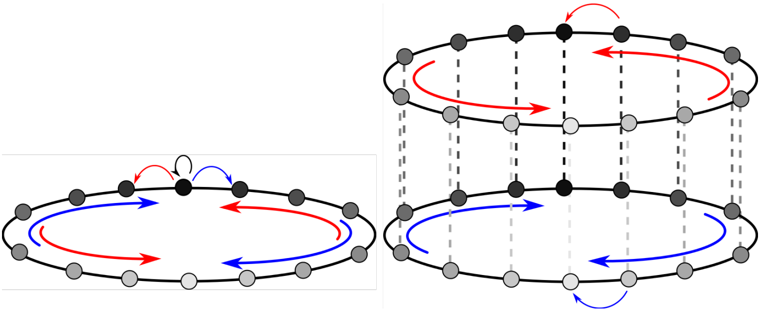

- Diaconis et al (2000)
- lifting ≡ additional variable
- Dynamical critical exponent $z = 1$ rather than $z = 2$
- Irreversible Markov chain

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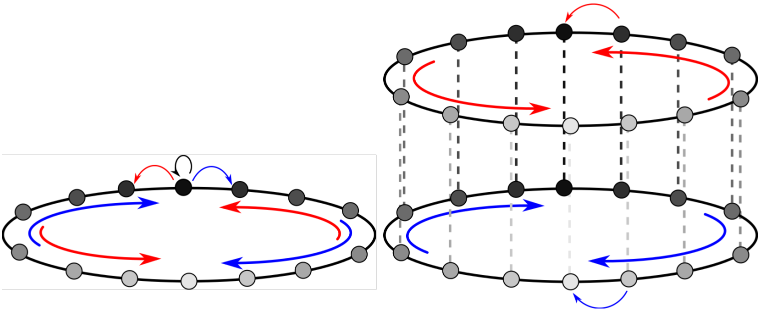

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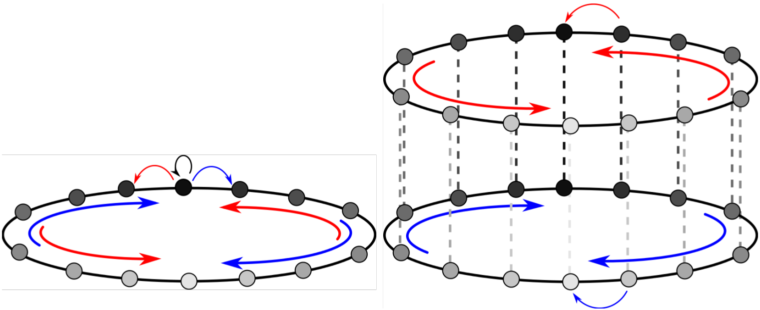

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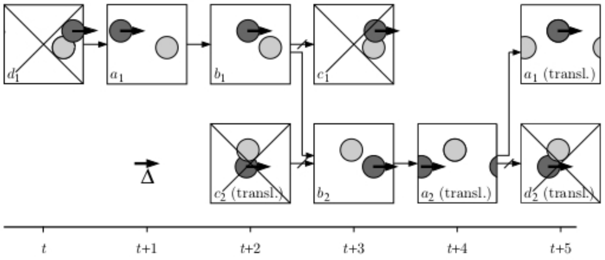
Lifting - two hard spheres 1/1



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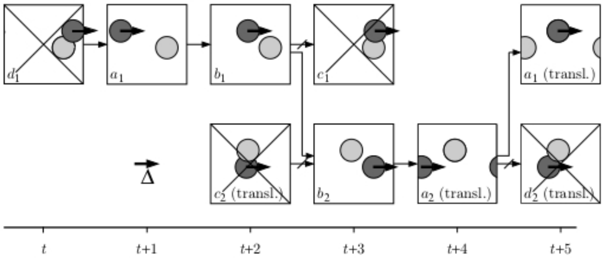

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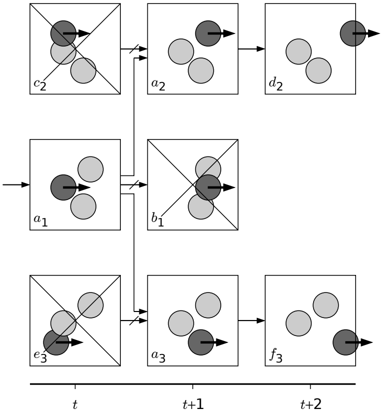
Lifting - N hard spheres



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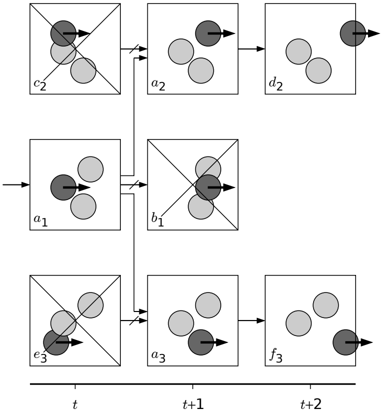

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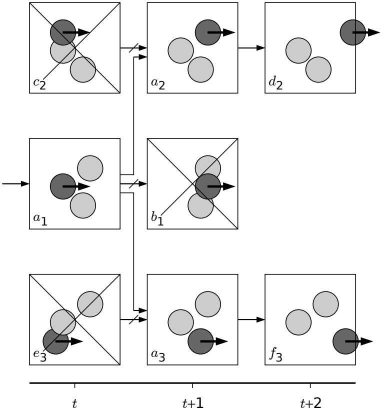

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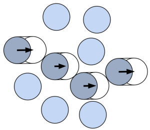
Lifting algorithm for general potentials



- Infinitesimal physical moves
- Liftings rather than rejections.
- Global balance rather than detailed balance.
- Bernard, Krauth, Wilson, (2009).

For general pair potentials, replace Metropolis by factorized filter

- $p^{\text{Met}}(a \to b) = \min\left[1, \exp(-\beta \sum_{i<j}(E_{ij}^b - E_{ij}^a))\right]$
- $p^{\text{Met}}(a \to b) = \min\left[1, \prod_{i<j} \exp(-\beta(E_{ij}^b - E_{ij}^a))\right]$
- $p^{\text{fact}}(a \to b) = \prod_{i<j} \min\left[1, \exp(-\beta(E_{ij}^b - E_{ij}^a))\right]$
- Michel, Kapfer & Krauth JCP (2014)

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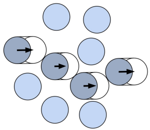

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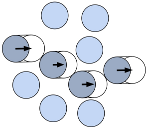

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Metropolis filter

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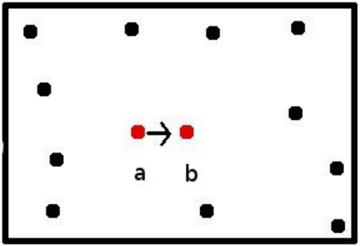

- Energy-based: MCMC knows its own weight.

Factorized filter 1/2

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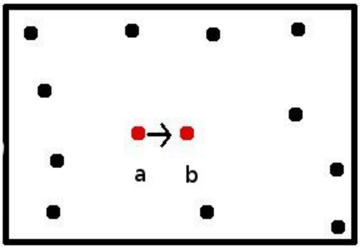

- pair-energy based
- bad idea, because $p^{\text{fact}}(a \to b) \leq p^{\text{Met}}(a \to b)$

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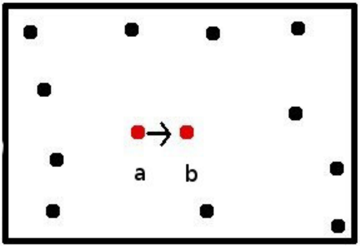

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Factorized filter 2/2

Acceptance probability

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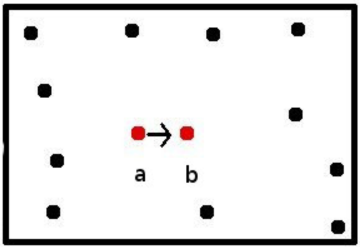

- pair-energy based.
- consensus rule (European-union like)
- Infinitesimal move: at most a single rejection
- lifting framework applicable

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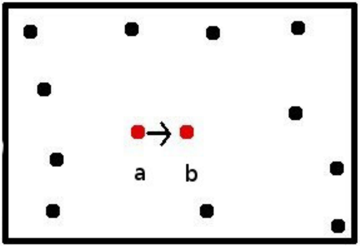

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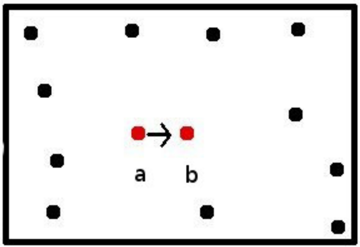

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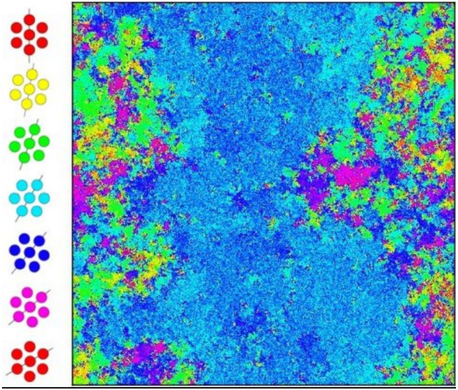
Applications - Hard disks



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- First-order liquid-hexatic transition in hard disks.

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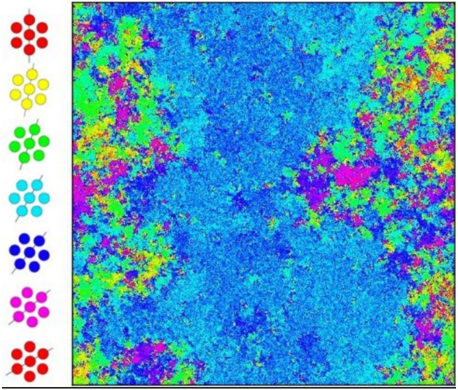

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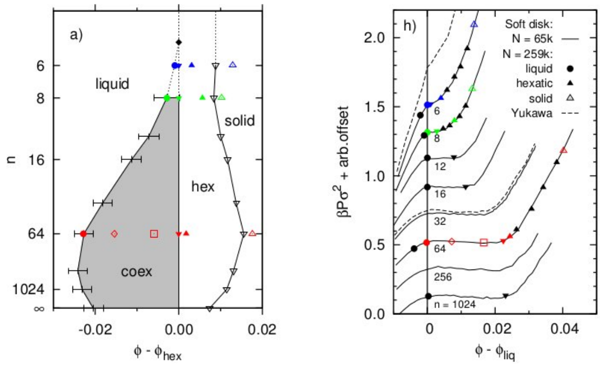
Applications - Soft disks

- Soft disks: $V \propto (\sigma/r)^n$.
- Mapping to Yukawa potentials.



- Kapfer & Krauth (PRL 2015).
- Two melting scenarios depending on softness n of potential.

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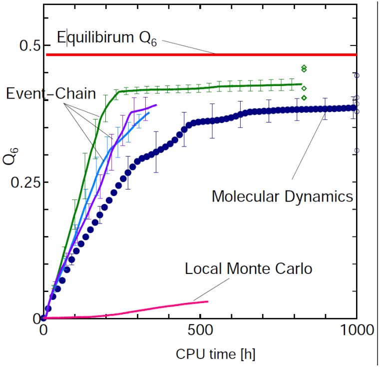
Applications - Hard spheres

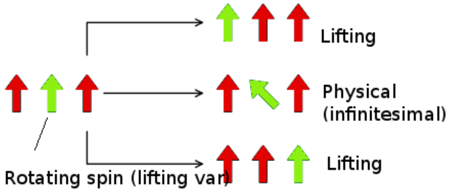
- Crystallization from liquid initial configurations ($\nu = 0.548$, $N = 1$Mio).



- Isobe & Krauth J. Chem. Phys. (2015)
- Considerable speedup of crystallization dynamics

Applications - Spin systems (XY, Heisenberg)

- Continuous spin systems:



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- Michel, Mayer & Krauth (EPL 2015)
  fast, but $z \sim 2$ dynamical scaling in 2D XY model.
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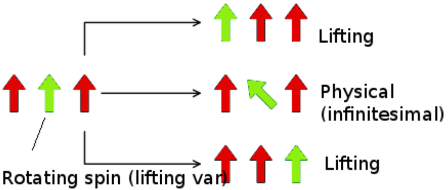

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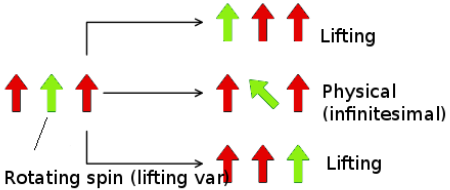

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Applications - Long-range systems 1/2

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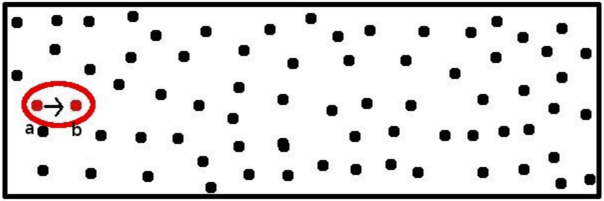
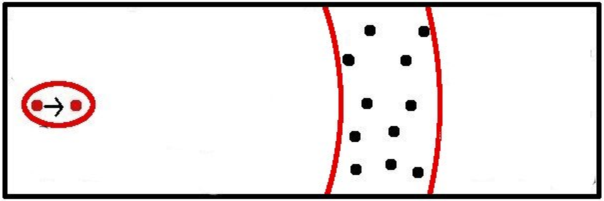
- Long-range particle system:



- Energy criterium problematic

Applications - Long-range systems 2/2

- $p^{\text{fact}}(a \to b) = \prod_{i<j} \underbrace{\min\left[1, \exp(-\beta(E_{ij}^b - E_{ij}^a))\right]}_{p_{ij}^{\text{accept}}}$



- if $p_{ij}^{\text{reject}} \ll 1$: consider subset of pairs.
- no more Ewald summation, no more Fourier methods.
- treat Coulomb forces directly.
- Kapfer & Krauth (manuscript in preparation).

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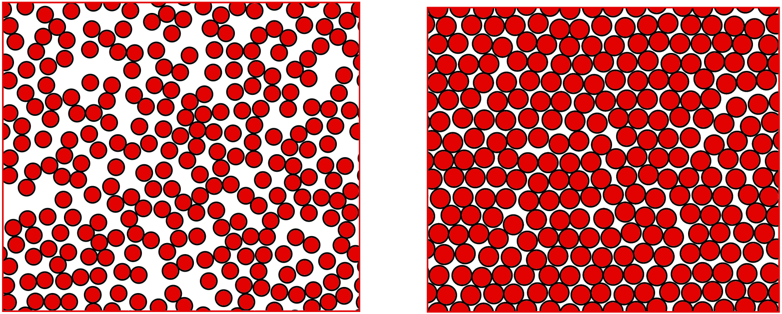
$2D$ melting transition



$\eta = 0.48$ $\eta = 0.72$

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- Nature of transition disputed for decades (quid KTHNY?, quid hexatic?)

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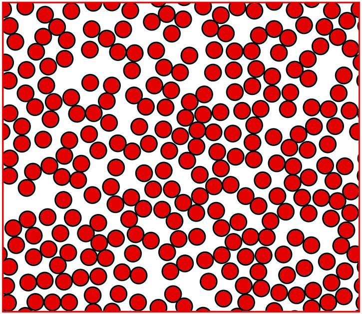

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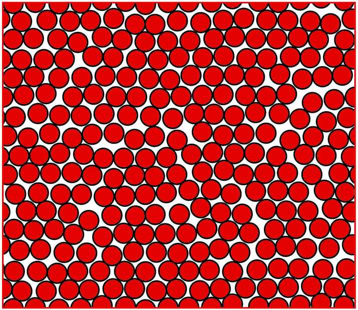

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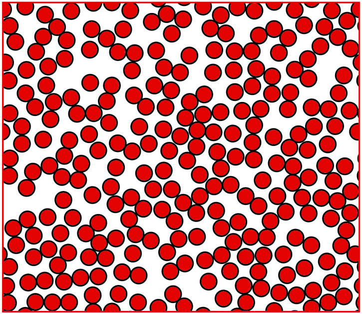
Possible phases in two dimensions



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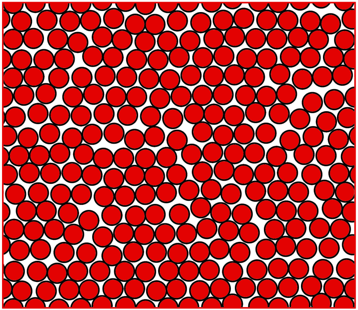

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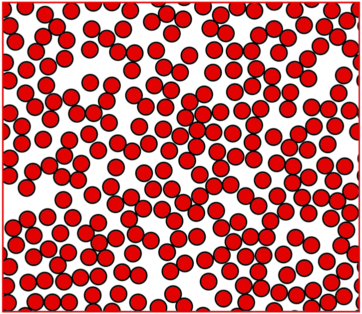
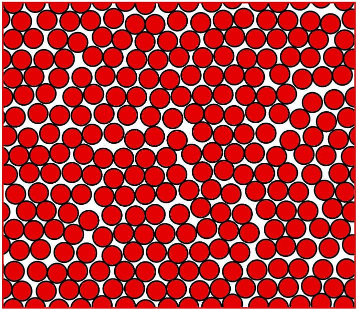
Phase	positional order	orientational order
solid	algebraic	long-range
hexatic	short-range	algebraic
liquid	short-range	short-range

Possible phases in two dimensions



$\eta = 0.48$



$\eta = 0.72$

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

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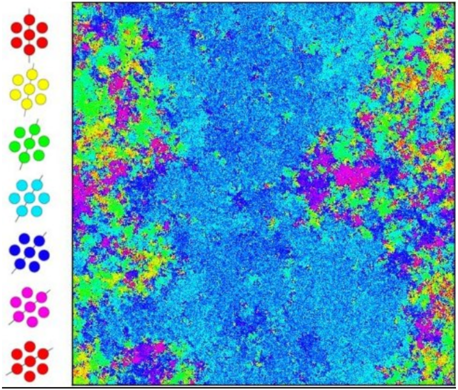
Hard-disk configuration



- 1024^2 hard disks
- circular color code for orientational order
- Bernard, Krauth (PRL 2011)

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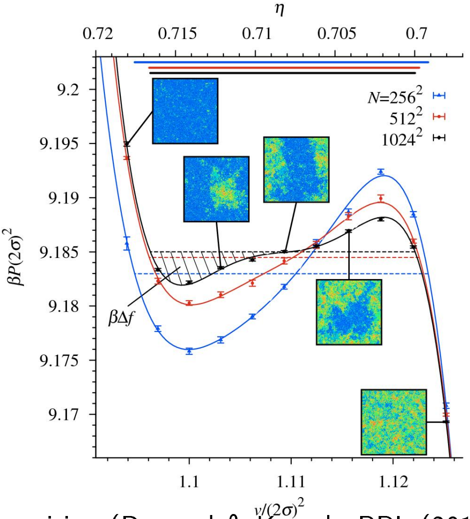
Equilibrium equation of state



- First-order transition (Bernard & Krauth, PRL (2011)).
- Many confirmations.

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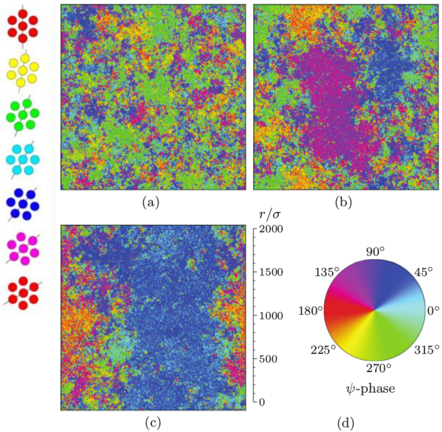
Phase coexistence in hard disks

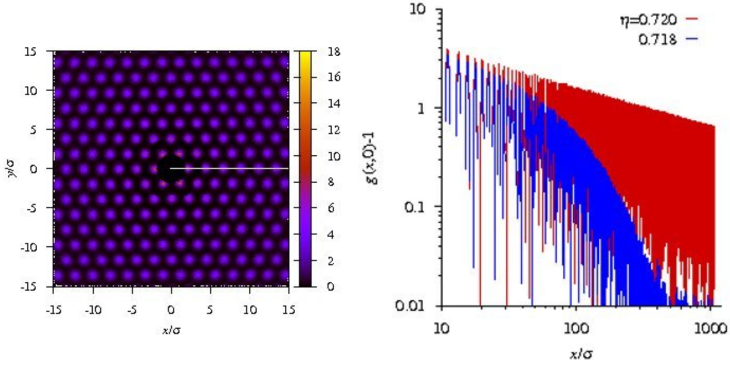


- 1024^2 systems.
- Densities $\eta = 0.700$ (a), $\eta = 0.704$ (b), $\eta = 0.708$ (c).
- Phase coexistence $\Longrightarrow$ Coarsening $\Longrightarrow$ Slow dynamics.
- cf. Engel et al (2013).

Possible phases (again)

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.
- At $\eta \sim 0.720$: solid.
- Bernard & Krauth (PRL 2011).
- Many confirmations.

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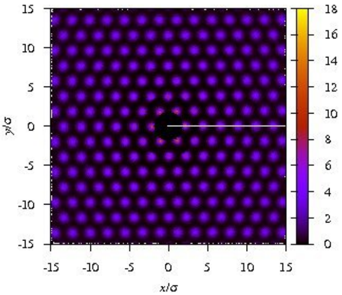
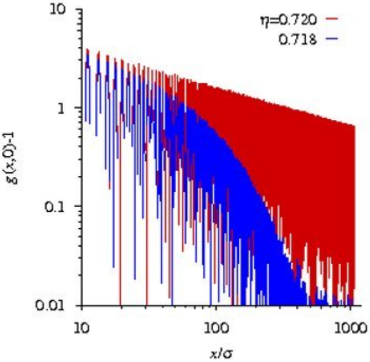
Spatial correlations at $\eta = 0.718$ and 0.720

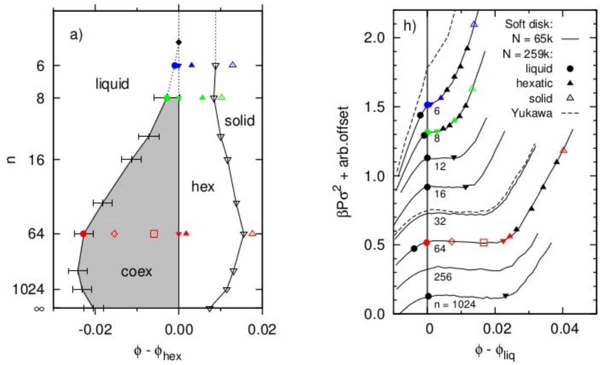




- Two-dimensional pair correlations, sample-averaged.
- At $\eta = 0.718$; hexatic.
- At $\eta \sim 0.720$: solid.
- Bernard & Krauth (PRL 2011).
- Many confirmations.

Applications - Soft disks

- Soft disks: $V \propto (\sigma/r)^n$.
- Mapping to Yukawa potentials.



- Kapfer & Krauth (PRL 2015).
- Two melting scenarios depending on softness n of potential.

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Conclusions

- Event-chain, factorized Metropolis, lifting:
  - 'Beyond Metropolis' paradigm for Monte Carlo computations, mathematically challenging, completely general, many applications.
  - Makes infinitesimal moves.
  - Uses lifting.
  - Breaks detailed balance.
  - Ignores its own energy.
- Hard disks:
  - The mother of MCMC models & of 2D physics.
  - Hexatic phase exists, first-order liquid-hexatic transition.
  - Hexatic-solid transition is KT.
  - Communities A and B were wrong.
- Many extensions, both for physics and for algorithms.