Melting in 2D and a Fresh Perspective on Monte Carlo

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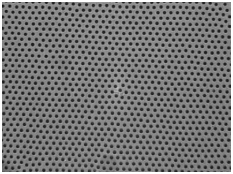
Ivanhoe Reservoir (Los Angeles, Photo: National Geographic)

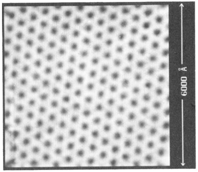
A very brief history of 2D Melting

- Experiments: Wigner lattices, Plasma crystals...



Magnetic Colloids

(P. Keim & G. Maret)



Abrikosov lattice (H. Hess et al)

- No long-ranged positional order in 2D (Wagner Mermin 1966)
  No crystals in 2D

- Theory of two-step melting with intermediate **hexatic** phase ("KTHNY", Halperin Nelson Young 1978/79)
  Dissociation of topological defects; two continuous transitions

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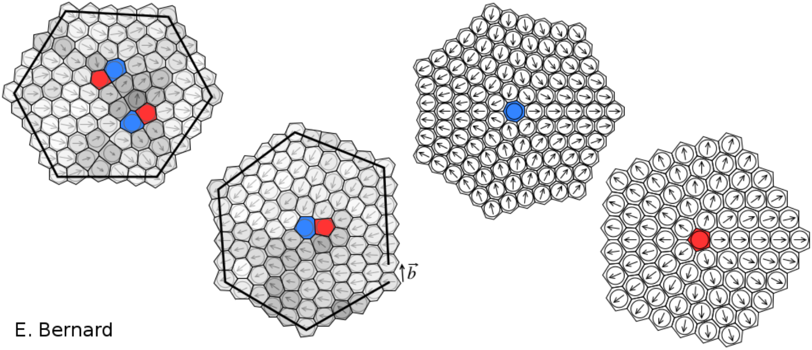

E. Bernard

A very brief history of 2D Melting

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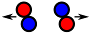
- Theories of first-order liquid/solid transitions (Chui 1983, Janke Kleinert 1988)
  Collective behavior of defects drives transition first-order

- Liquid/hexatic coexistence in experiment (Marcus Rice 1996)
  ... and more recent experiments, 2017

- But also KTHNY in paramagnetic colloids (Maret, Keim 1999–2000s)

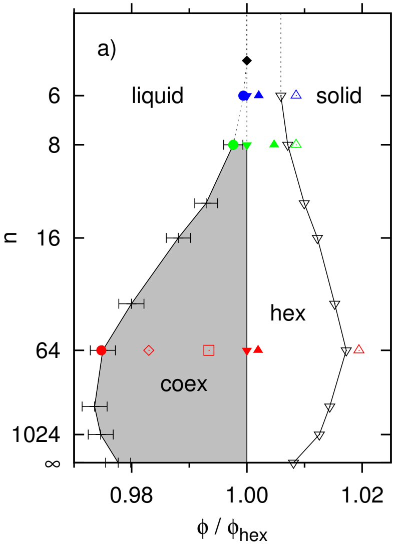
	phase	orientational order g_6	positional order g
	solid	long-ranged $\to$ const	quasi-long-ranged $\propto 1/r^{\eta}$
	hexatic	quasi-long-ranged $\propto 1/r^{\eta_6}$	short-ranged $\propto \exp(-r/\xi_{\mathrm{pos}})$
	liquid	short-ranged $\propto \exp(-r/\xi_6)$	short-ranged $\propto \exp(-r/\xi_{\mathrm{pos}})$

Translates to structure factor $S(\boldsymbol{k}) = 1 + \int \mathrm{d}^2 r \exp(-\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{r}) g(\boldsymbol{r})$

Two questions:

- Does the hexatic exist?
- Continuous transition or coexistence?

Phase diagram for Soft-disk interactions, $U = 1/r^n$

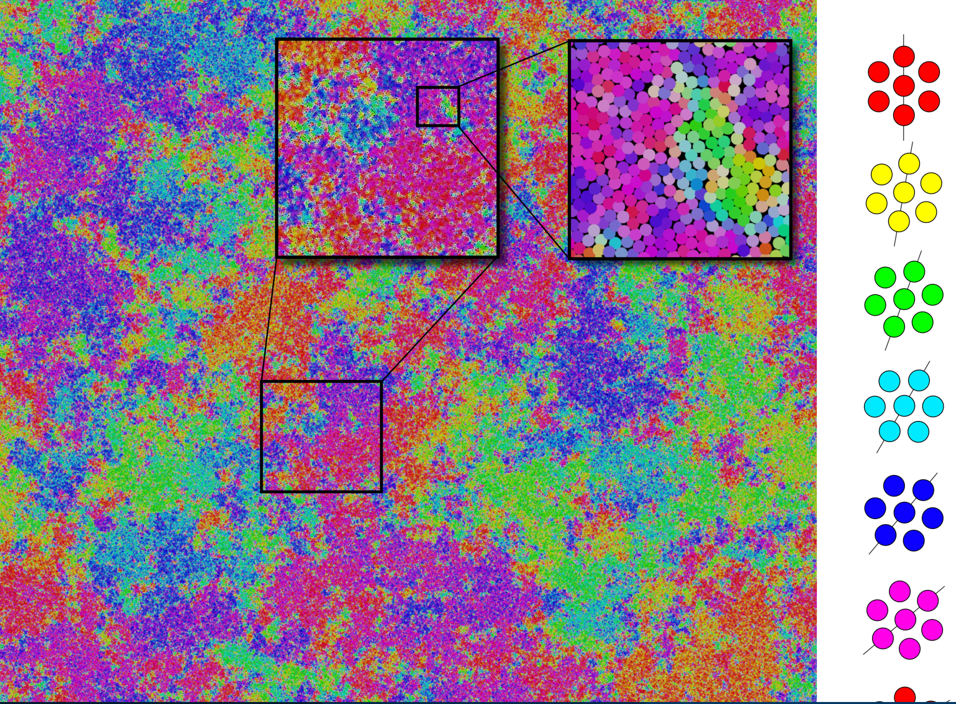


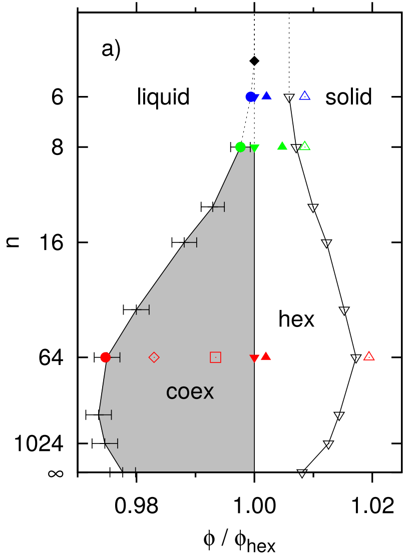
Long-range EC
Kapfer & Krauth 2016, 2017

Soft-disk EC

Michel, Kapfer, Krauth 2014, Kapfer & Krauth 2015

Hard-disk EC
Bernard & Krauth 2009/11




a)
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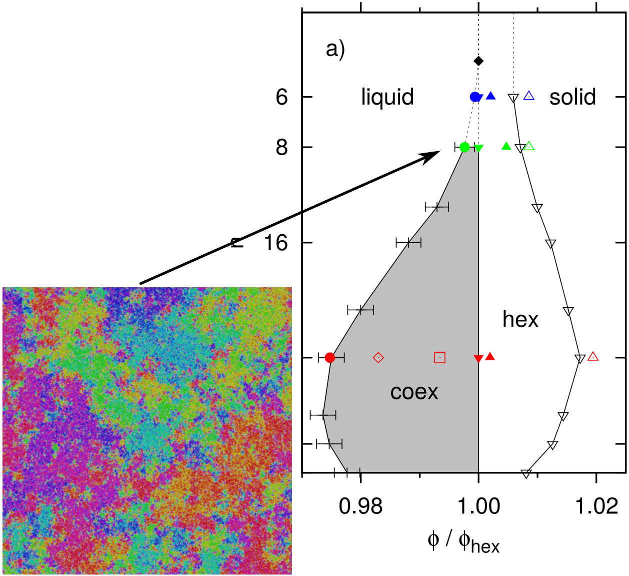
ϕ / ϕ_{hex}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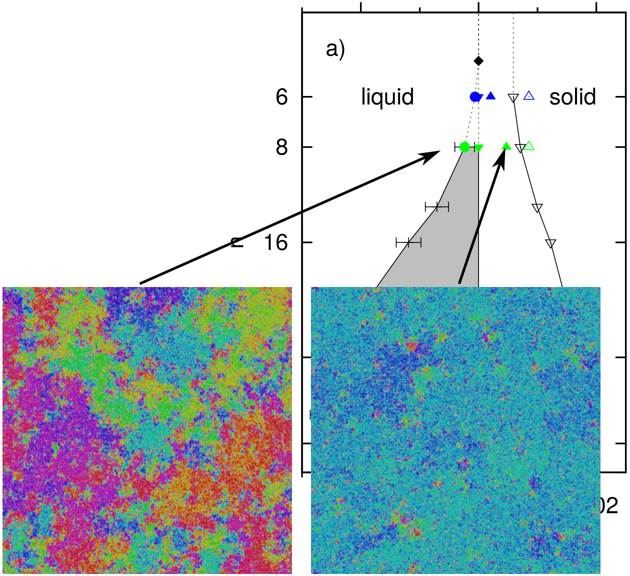
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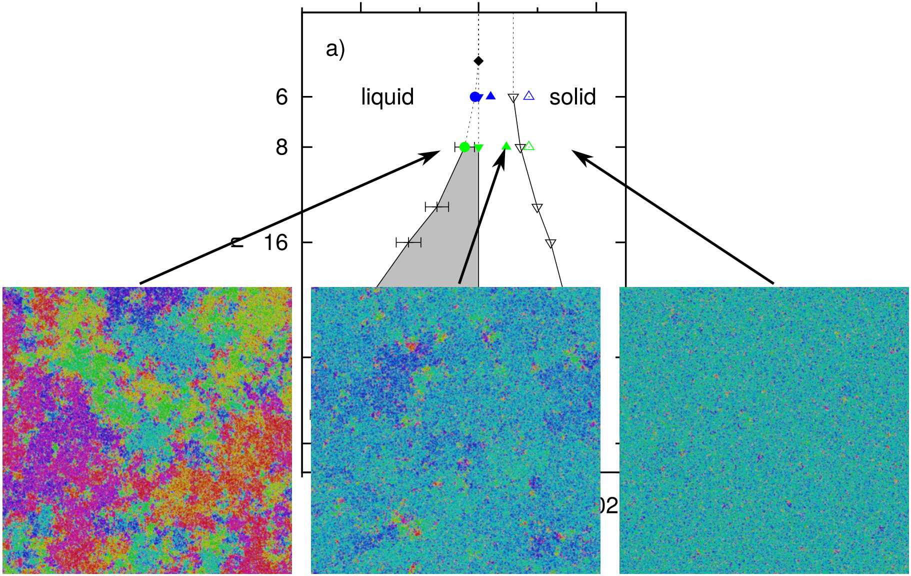
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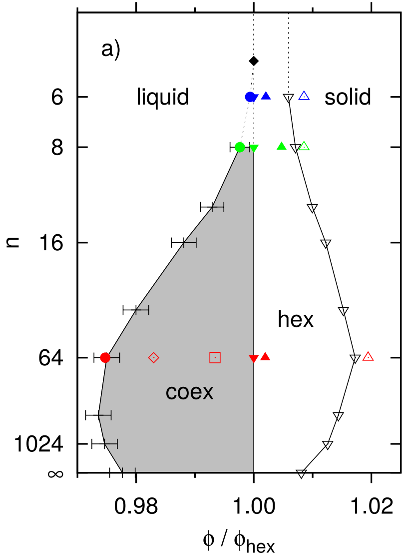
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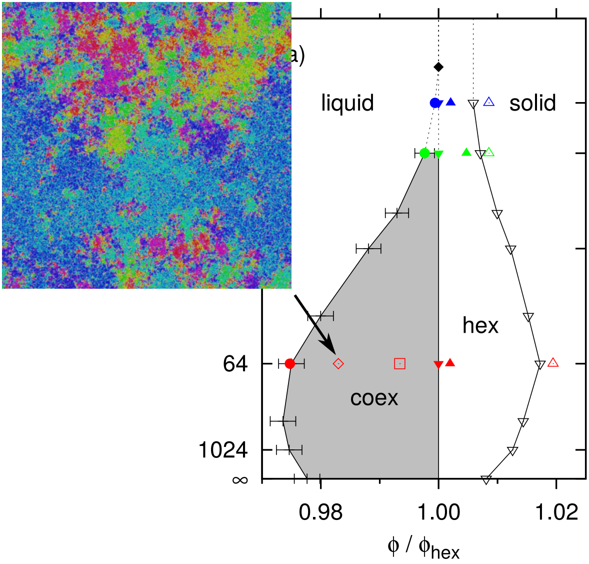
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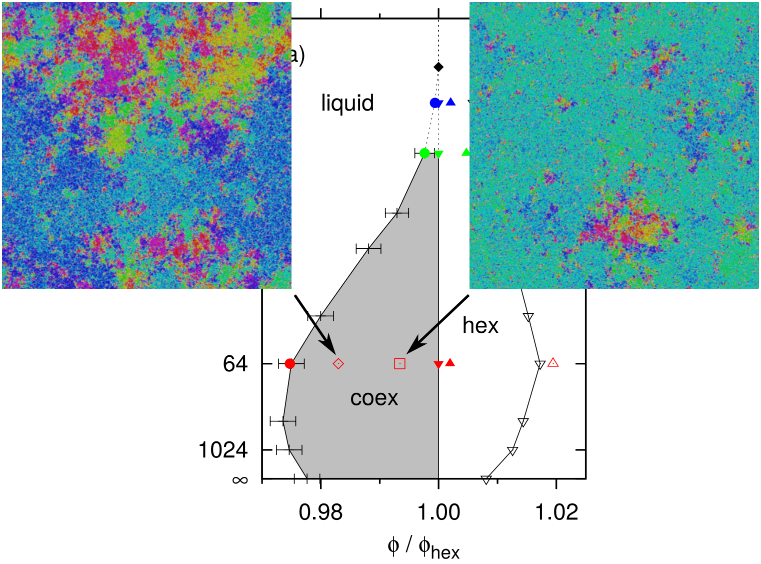
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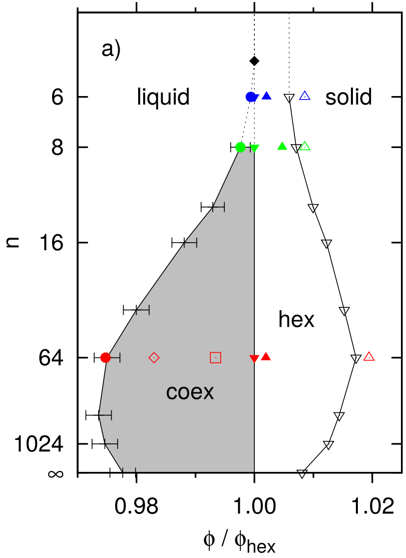

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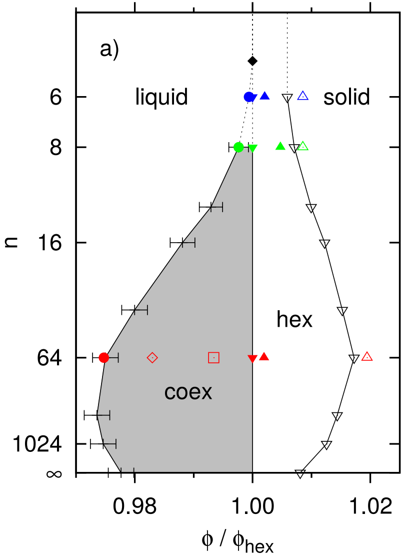
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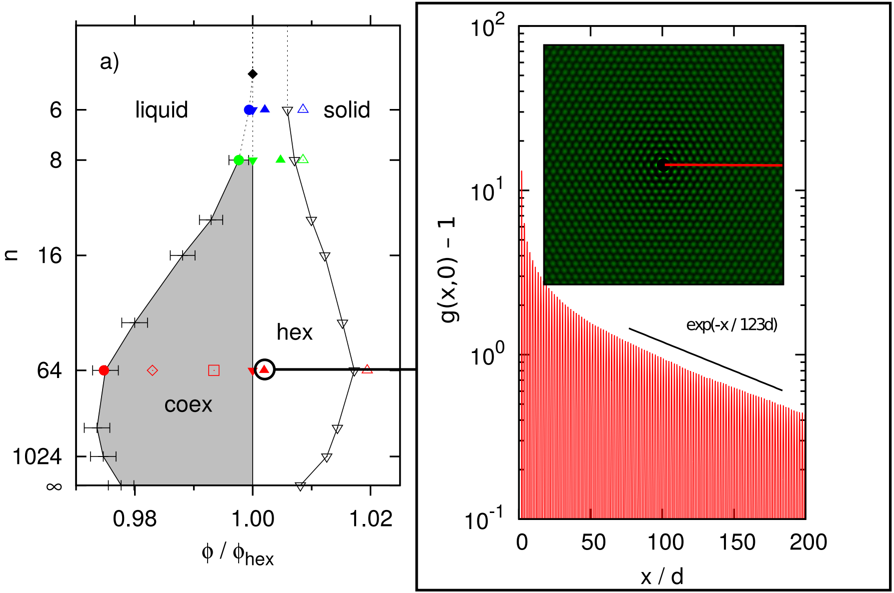
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64
1024
∞
hex
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0.98
1.00
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ϕ / ϕhex
g(x,0) − 1
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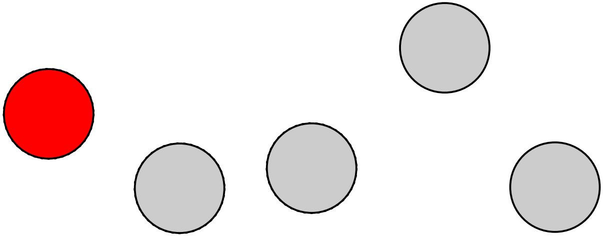
10^1
10^0
10^-1
exp(-x / 123d)
0
50
100
150
200
x / d

Evolution of a Hard-disk Event Chain



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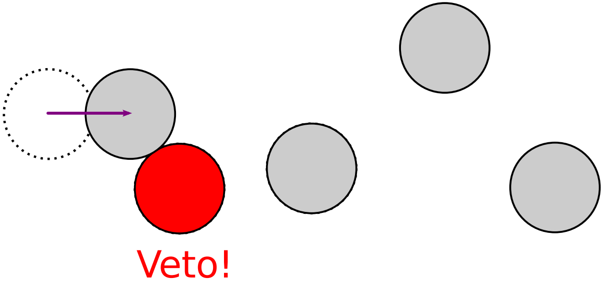

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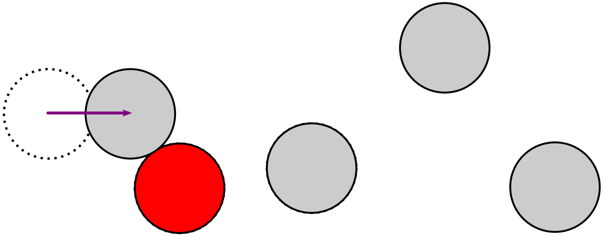

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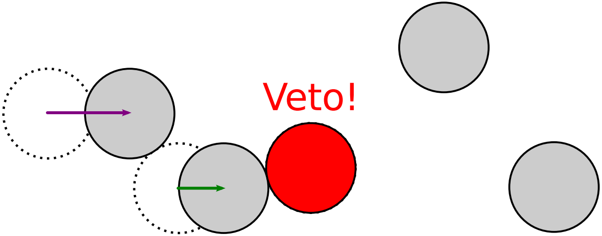

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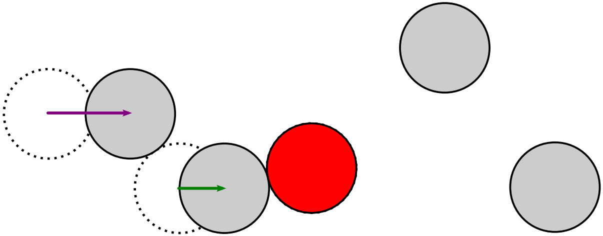

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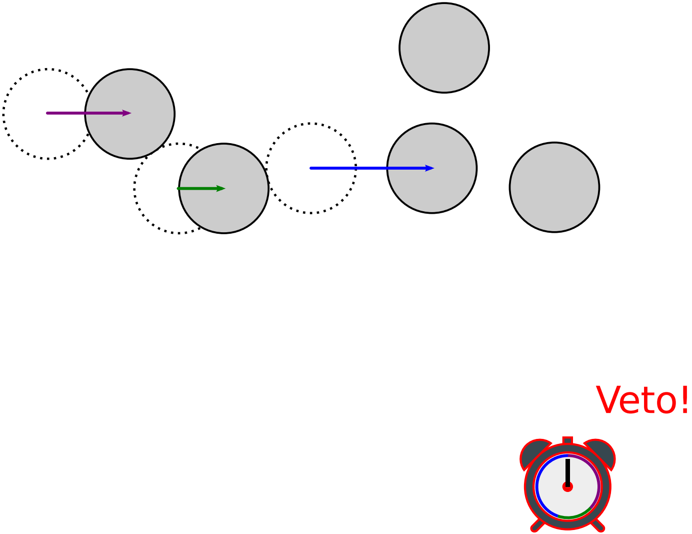

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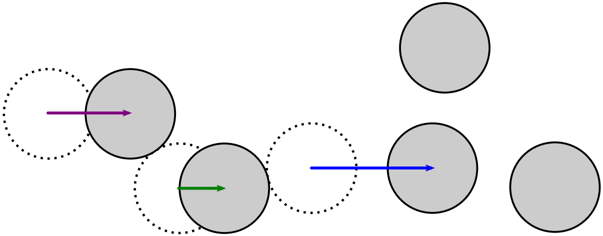
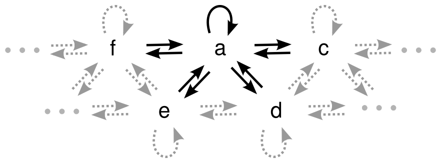
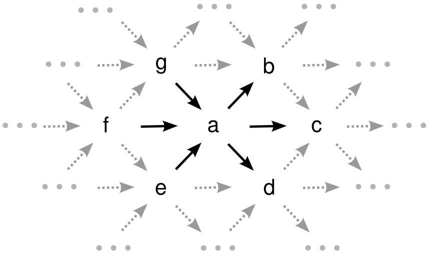


Detailed vs. Global Balance condition



detailed balance



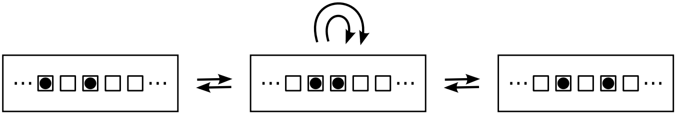
maximal global balance

GB: $\pi(a) = \pi(a) \underbrace{\sum_{a'} p(a \to a')}_{1} = \sum_{a'} \pi(a') p(a' \to a)$

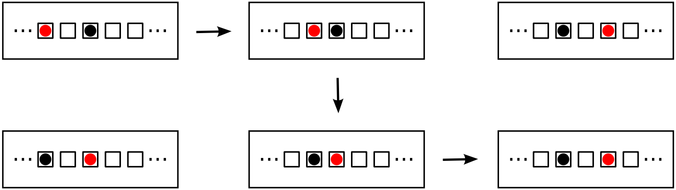
DB: $\pi(a) p(a \to a') = \pi(a') p(a' \to a)$

Discrete 1D Hard-Rod Event Chain

Detailed Balance



Global Balance (Lifted)



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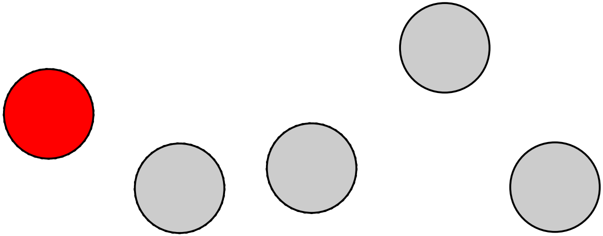

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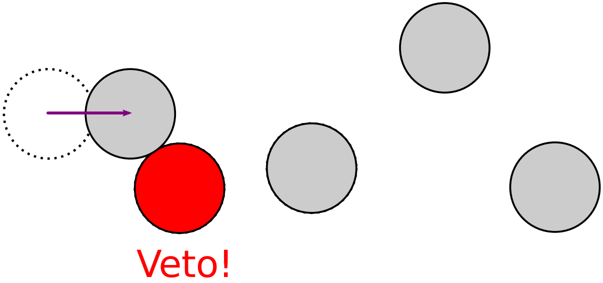

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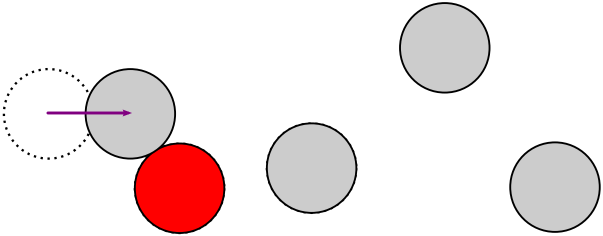

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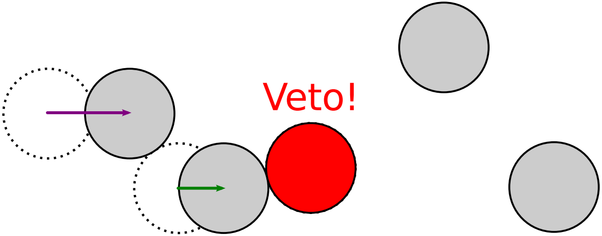

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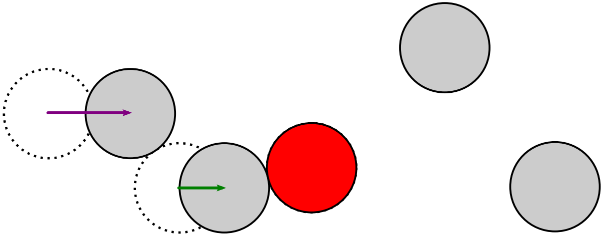

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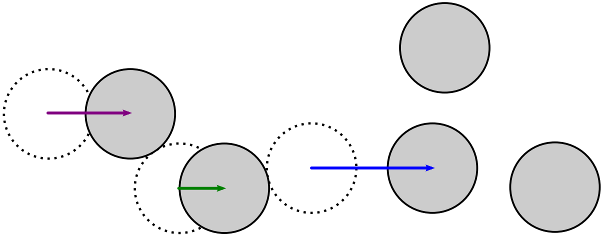
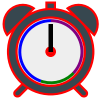


Veto!



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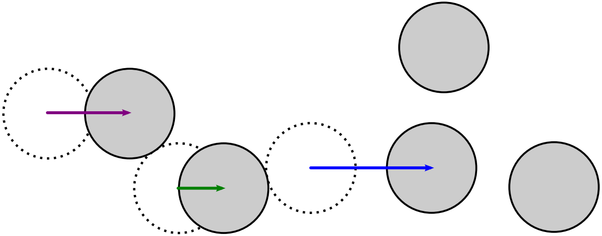


Factorized Metropolis Filter

Classical Metropolis filter (1950s)

$$p(a \to b) = \min\big(1, \exp(-\beta \sum_{(i,j)} \Delta U_{ij})\big)$$

New **Factorized Metropolis filter**

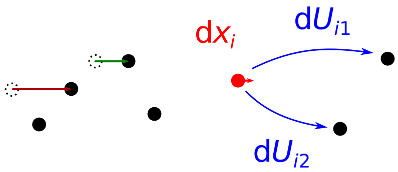
$$p^{\text{fact}}(a \to b) = \prod_{(i,j)} \min\big(1, \exp(-\beta \Delta U_{ij})\big)$$

Move is accepted **only by consensus** of all **pair terms**

$p^{\text{fact}}(a \to b)$ + infinitesimal moves + lifted Markov chain
= new Event-chain algorithm

Michel, Kapfer, Krauth, J. Chem. Phys. **140**, 054116 (2014)

Infinitesimal Moves and Lifting Events



Displacing particle i by $\mathrm{d}x_i$ costs energy $\mathrm{d}U_{ij}$ for each particle pair

$$p^{\mathrm{fact}}(a \to b) = \prod_{\langle i,j \rangle} \min\bigl(1, \exp(-\beta\, \mathrm{d}U_{ij})\bigr)$$
$$= 1 - \sum_{\langle i,j \rangle} \underbrace{\max(0, \beta\, \mathrm{d}U_{ij})}_{p_{\mathrm{veto}}}$$

With probability $\max(0, \beta\, \mathrm{d}U_{ij})$, particle j vetoes move of particle i
Then: **lifting event** $i \to j$, now j is the active particle

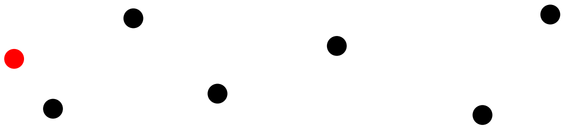
Recipe for an Event-chain algorithm

Three ingredients

- **Lifted Markov chain**
  extend physical configuration space (*particle coordinates*)
  by artificial variables *direction of motion* and *active particle*
  persistence ⇒ **cooperative moves**
- **Infinitesimal moves**
  continuous time evolution of system state
  interrupted by singular events
- **Pairwise-factorized acceptance criterion**
  replaces traditional Metropolis criterion
  operates on particle pair energies, **not total energies**

Result: Global-balance, rejection-free, cooperative moves, continuous time!
. . . but still Markov-chain Monte Carlo

Evolution of a Soft-disk Event Chain



Probabilistic veto radius set by *pairwise* energy increase $\propto \exp(-\beta \Delta U_{ij})$

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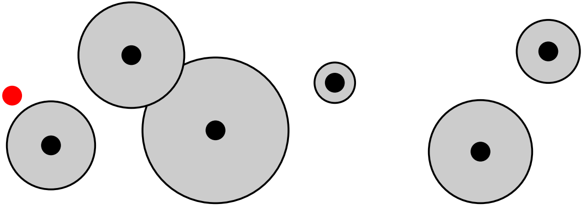

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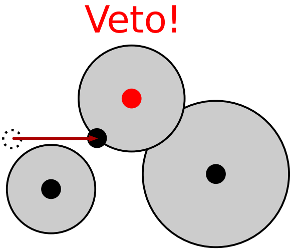

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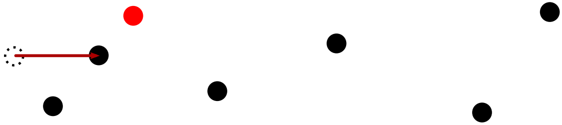

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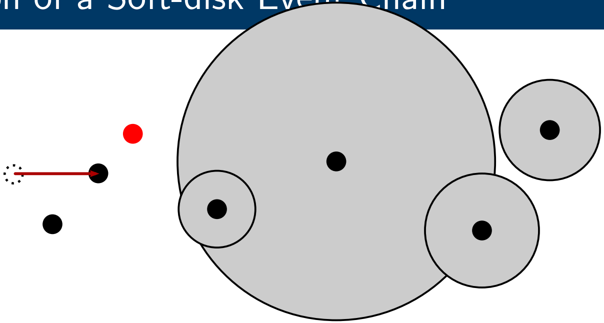

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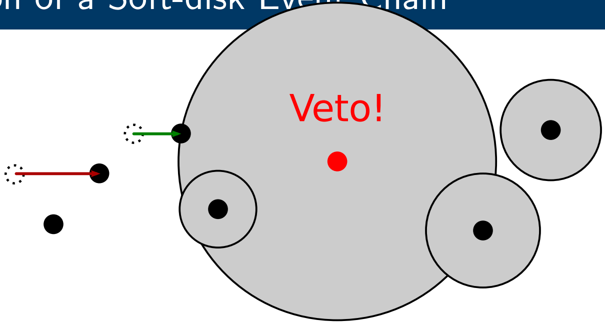

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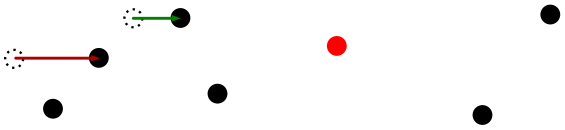

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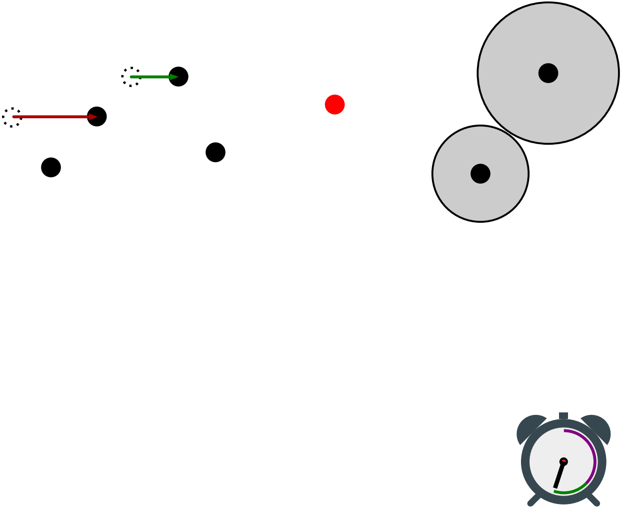

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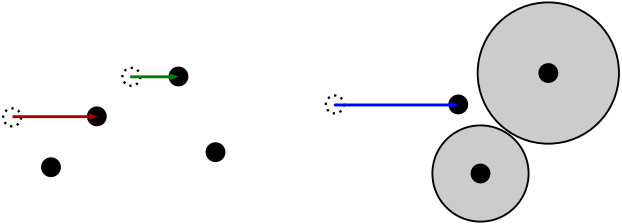

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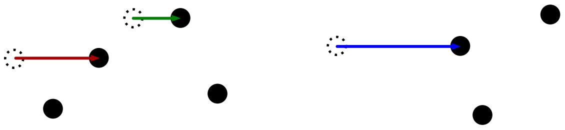

Probabilistic veto radius set by *pairwise* energy increase $\propto \exp(-\beta \Delta U_{ij})$

Handling ∞ pair interactions

For short-range forces: $\mathcal{O}(1)$ pairs to consider

For long-range forces: $\mathcal{O}(N)$ pairs, including periodic copies: ∞ pairs!

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...and in factorized Event-chain MC?

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. . . and in factorized Event-chain MC? **Probabilistic approach!**

Cell-veto Monte Carlo

Preparation stage

Put cell grid such that occupation < 1

For each non-nearby cell: precompute
cell veto rate $Q > q$ (particle event rate)

Finite total cell veto rate $Q_{\text{tot}} = \sum Q$

Event-driven simulation

Find time s of next cell veto in $\mathcal{O}(1)$:

$$s = -\frac{1}{Q_{\text{tot}}} \ln u$$

Find the cell which vetoed:

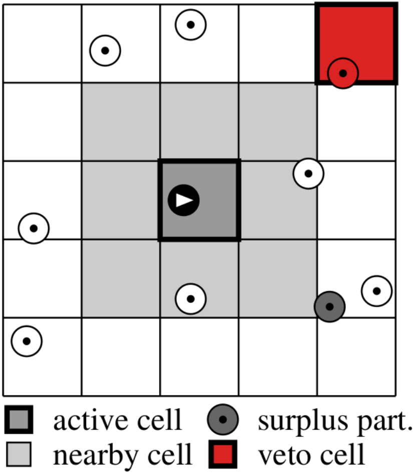
e.g. Walker's alias method, $\mathcal{O}(1)$

If vetoing cell contains a particle:

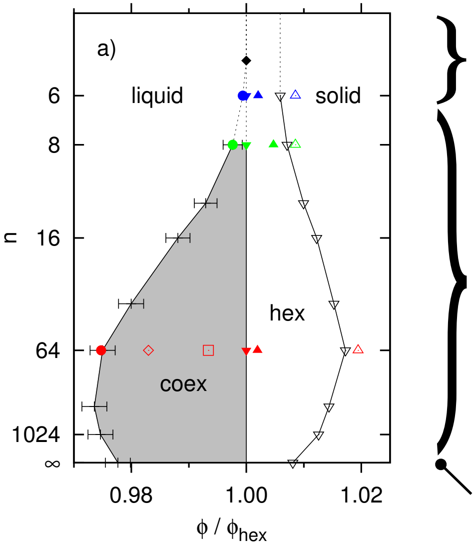
With probability q/Q:

Have a particle event, $\mathcal{O}(1)$

Next cell veto



Phase diagram for Soft-disk interactions, $U = 1/r^n$



Long-range EC
Kapfer & Krauth 2016, 2017

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Hard-disk EC
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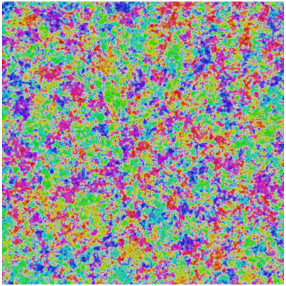
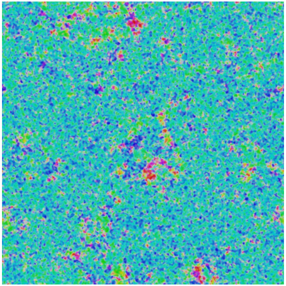
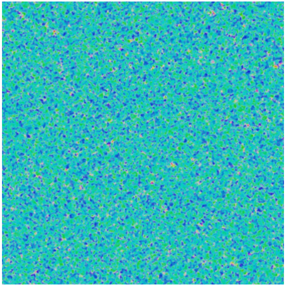
Soft disks with $U = 1/r^3$ interactions



liquid

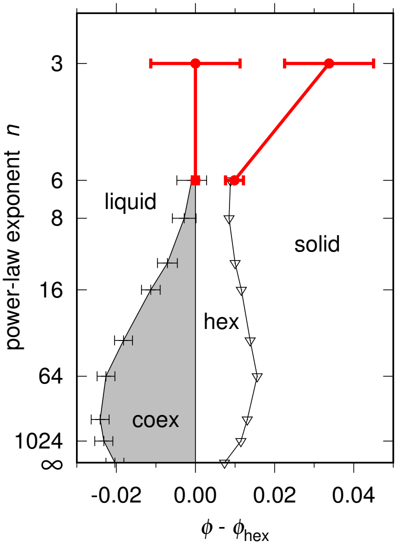


hexatic



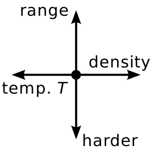
solid

Soft-disk phase diagram, including LR interactions

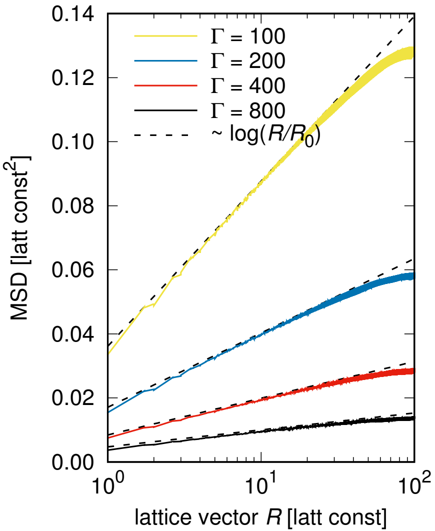


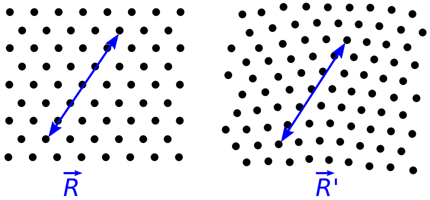
Long-ranged interactions $U \sim \dfrac{1}{r^n}$
Do not admit truncation
Two-step melting, twice continuous
= classical KTHNY

Short-ranged interactions $U \sim \dfrac{1}{r^n}$
(may be truncated)
Two-step melting,
liquid-hexatic 1st order
PRL **114**, 035702 (2015)



Solid phase: ‘Mermin-Wagner fluctuations’ in the LR limit





Mean-squared displacement:

$$\mathrm{MSD}(\boldsymbol{R}) := \left\langle \left(\boldsymbol{R} - \boldsymbol{R}'\right)^2 \right\rangle$$

Mermin-Wagner:

$$\mathrm{MSD}(\boldsymbol{R}) \sim \log \left| \frac{\boldsymbol{R}}{R_0} \right|$$

Summary

- **Hexatic/liquid coexistence** for short-range repulsive forces in 2D
  Continuous transition (**classical KTHNY**) for softer / long-ranged
  Paper: PRL **114**, 035702 (2015)
  Mermin-Wagner satisfied, even for long-ranged interactions
- Lifting, Factorized Metropolis, Infinitesimal moves
  allow to construct new MCMC algorithms of the Event-chain type
  Global balance, zero-rejection, cooperative, event-driven
  Paper: JCP **140**, 054116 (2014)
- Rigorous inclusion of **long-ranged interactions**
  $\mathcal{O}(1)$ for $1/r^3$ dipole forces, $\mathcal{O}(N^{1/3})$ for 3D Coulomb
  A replacement for $\mathcal{O}(N^{3/2})$ Ewald sums?
  Code: `https://github.com/cell-veto/`
  Paper: PRE **94**, 031302 (2016)

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FONDATION MEYER POUR LE DEVELOPPEMENT CULTUREL ET ARTISTIQUE

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