Reconsidering long-range forces in Monte Carlo
Do we still need Ewald sums?

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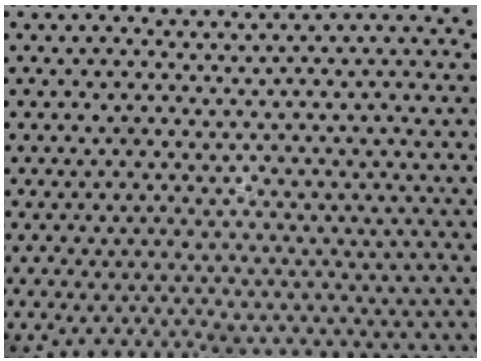
CompPhys16, Leipzig, 22 November 2016

Département de Physique
École Normale Supérieure

Ivanhoe Reservoir (Los Angeles, Photo: National Geographic)

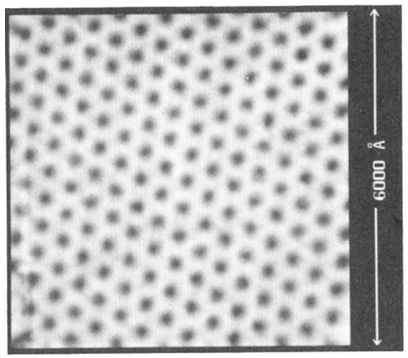
A very brief history of 2D Melting

- 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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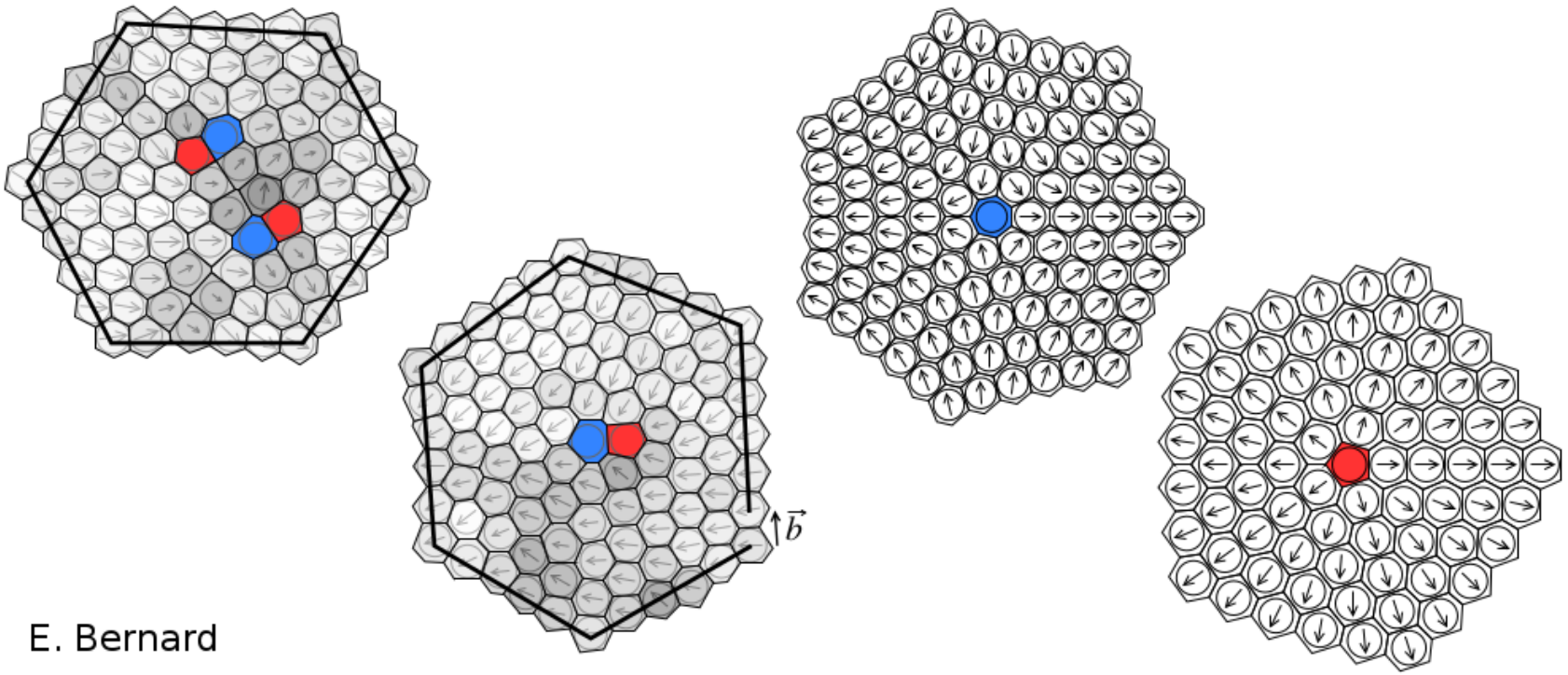

E. Bernard

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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
liquid	short-ranged	short-ranged
hexatic	**quasi-long-ranged**	short-ranged
solid	long-ranged	**quasi-long-ranged**

short-ranged: correlations $g, g_6 \propto \exp(-r/\xi)$

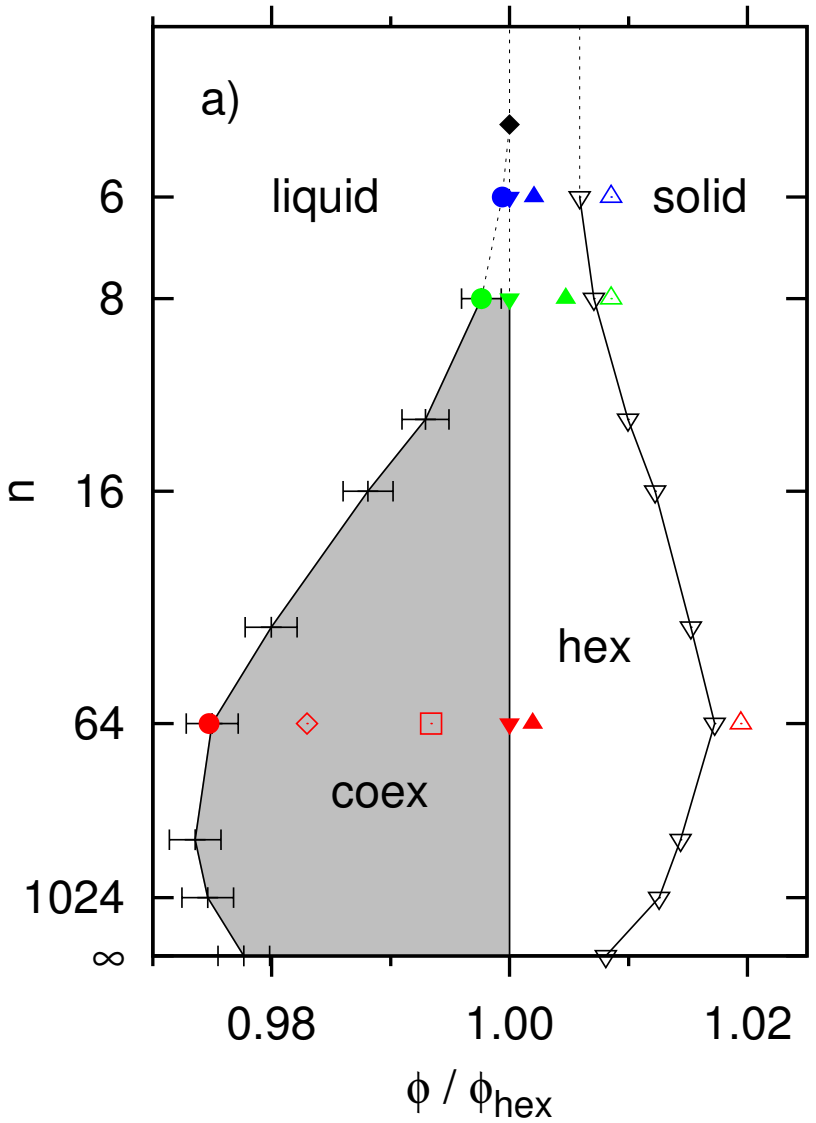
quasi-long-ranged: correlations $g, g_6 \propto r^{-\eta}$

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, $U = 1/r^n$

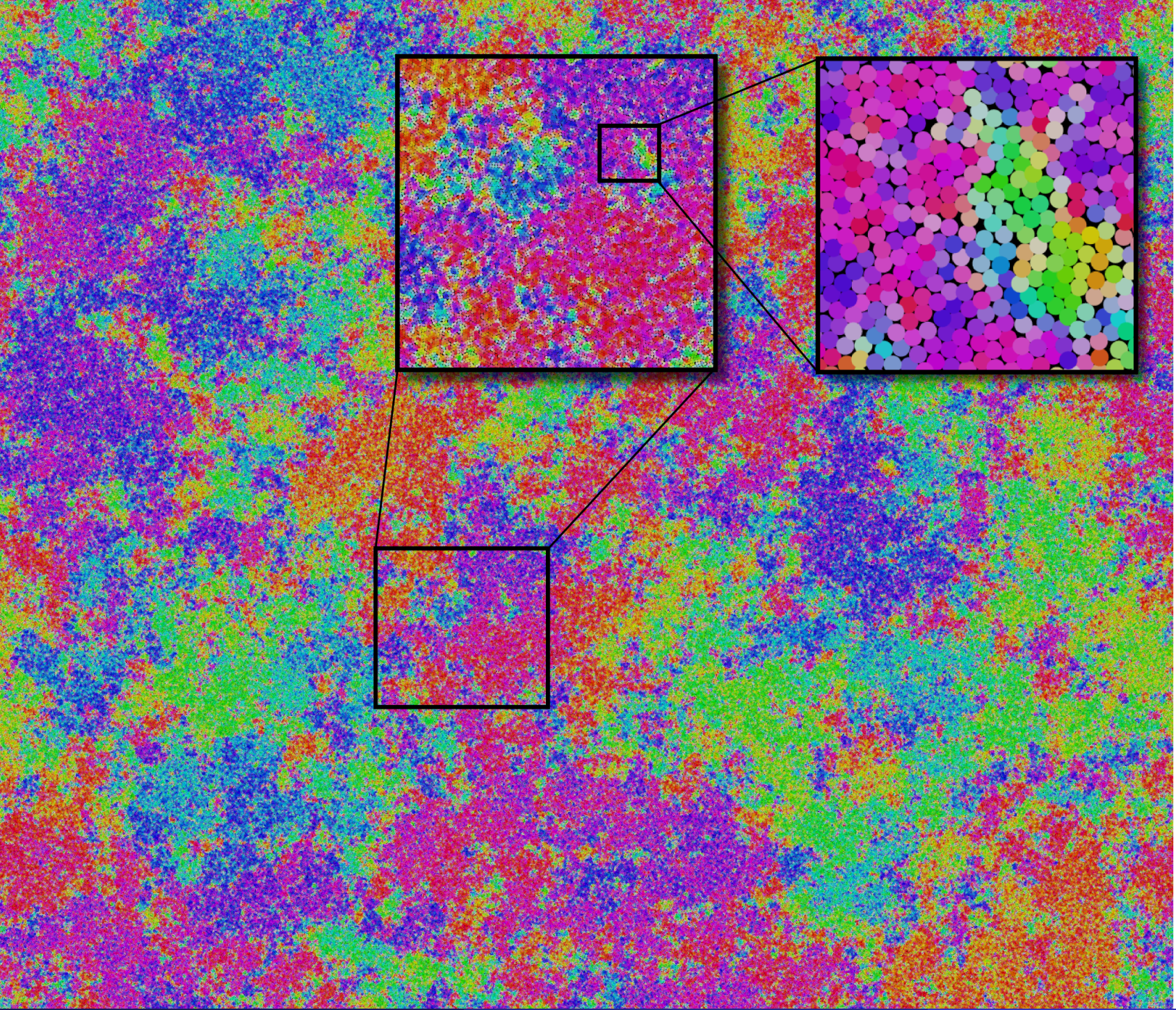


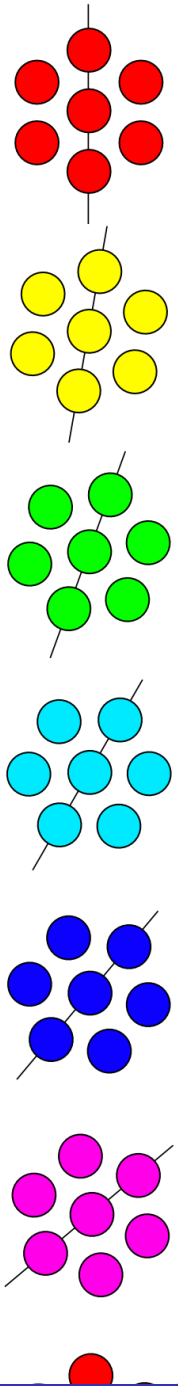
Long-range EC
Kapfer & Krauth 2016, 2017

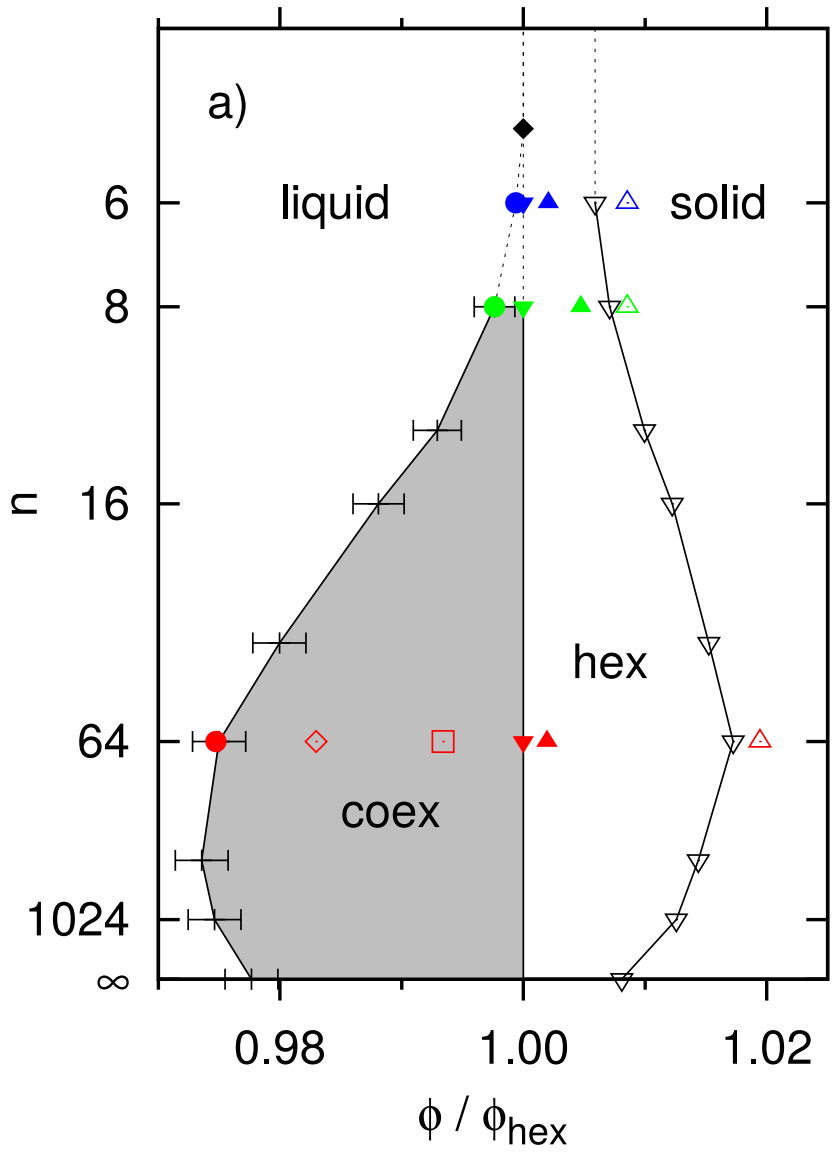
Soft-disk EC

Michel, Kapfer, Krauth 2014,
Kapfer & Krauth 2015

Hard-disk EC
Bernard & Krauth 2009/11






a)
liquid
solid
hex
coex
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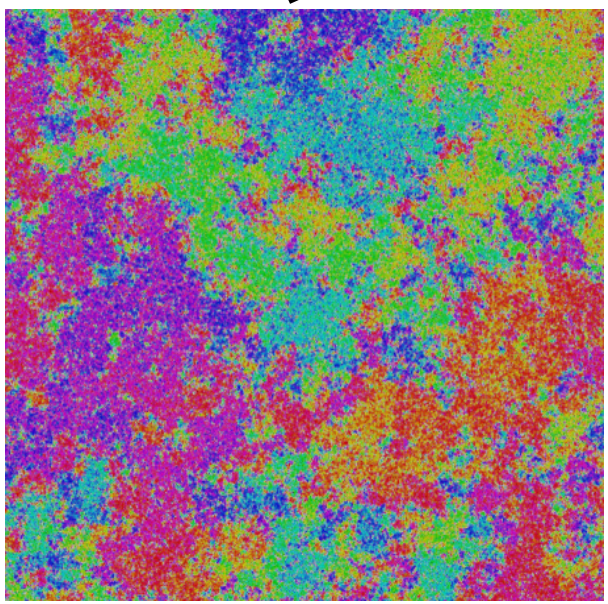
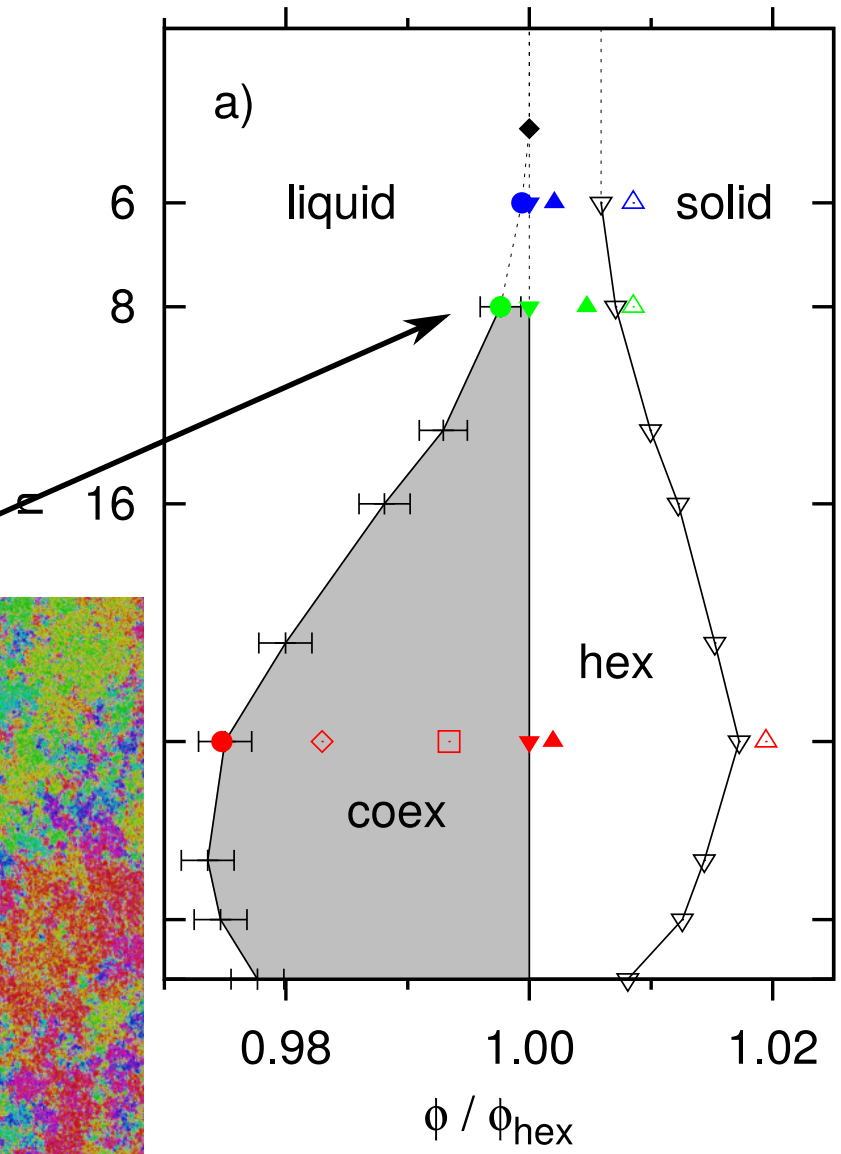
64
1024
∞
n
0.98
1.00
1.02
ϕ / ϕhex

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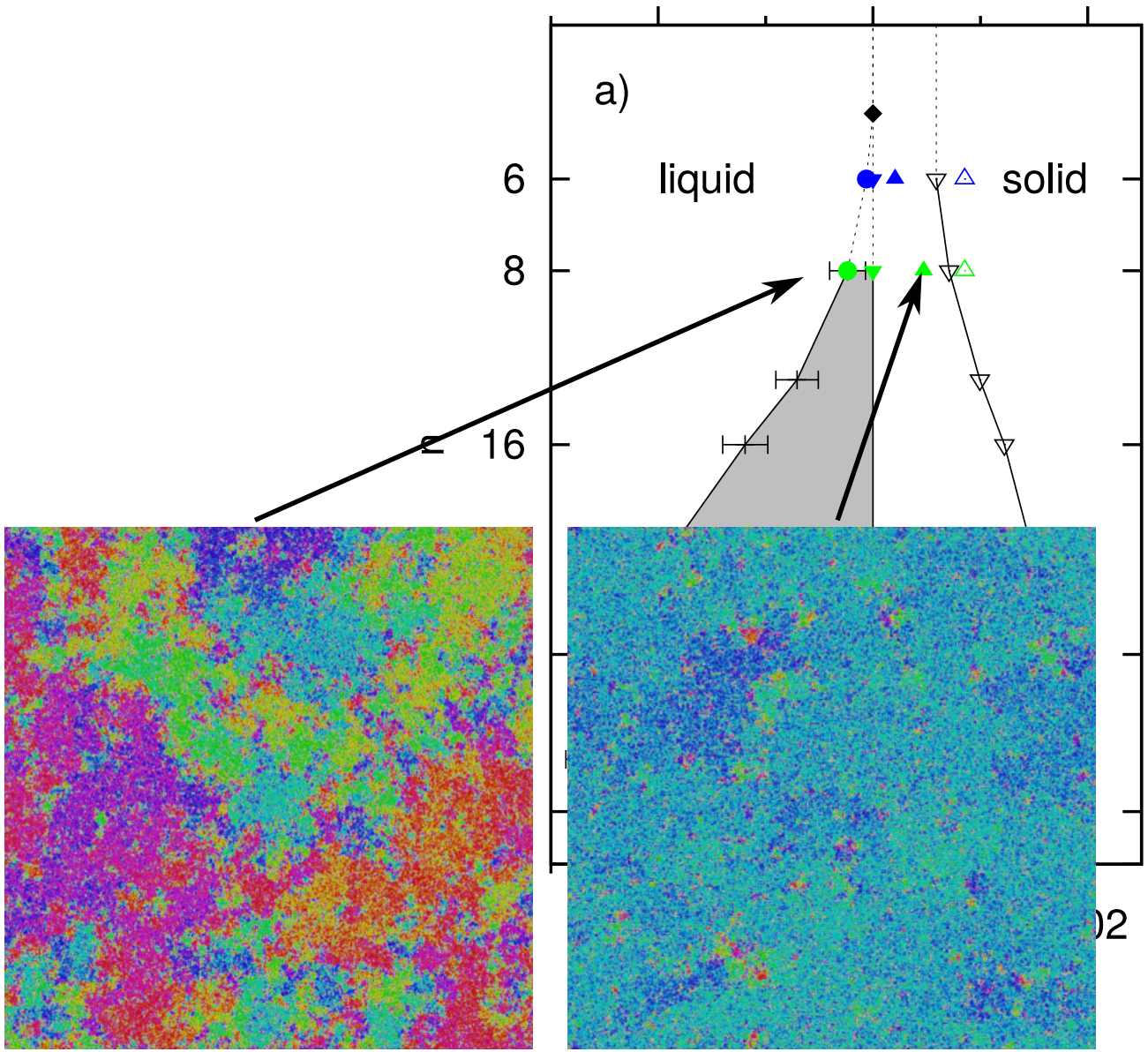
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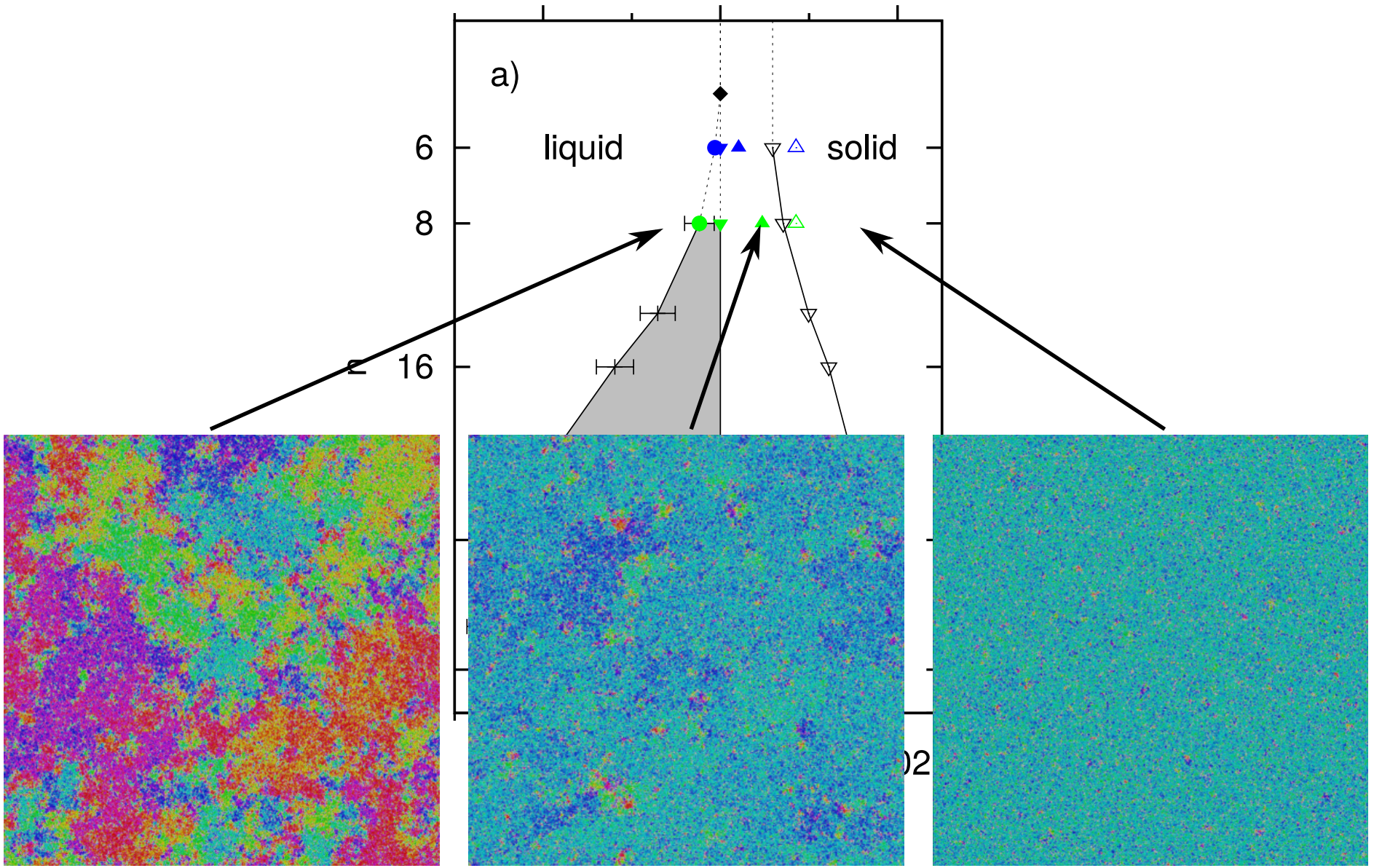
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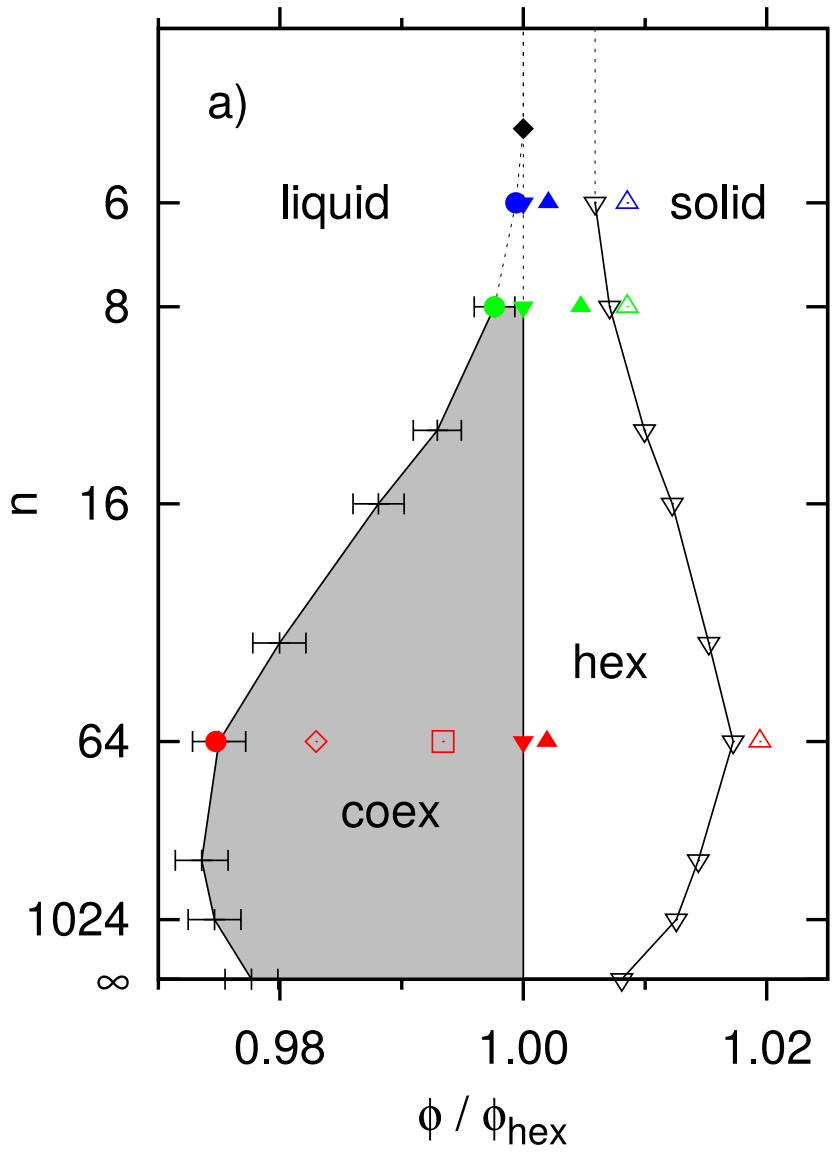
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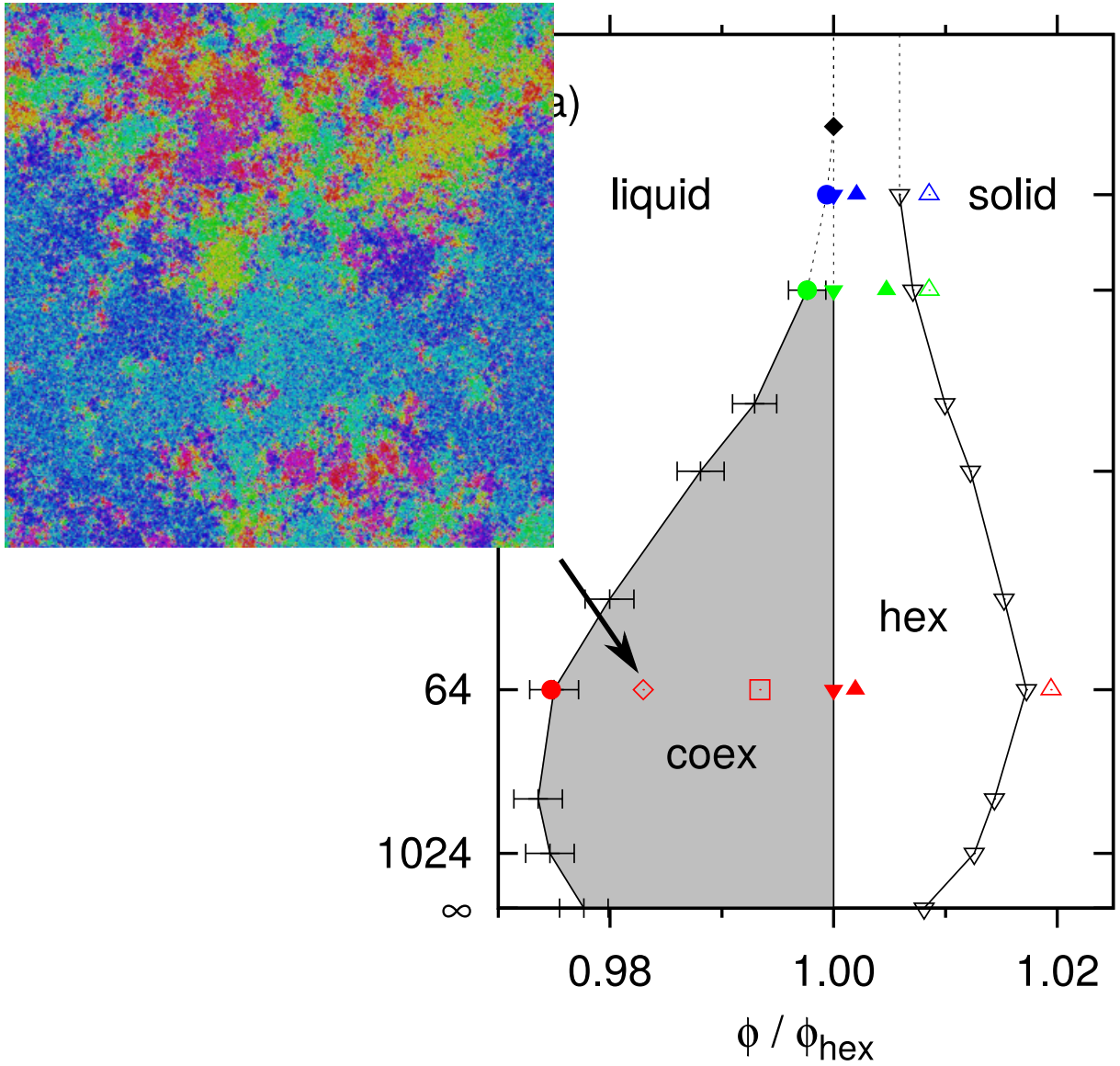
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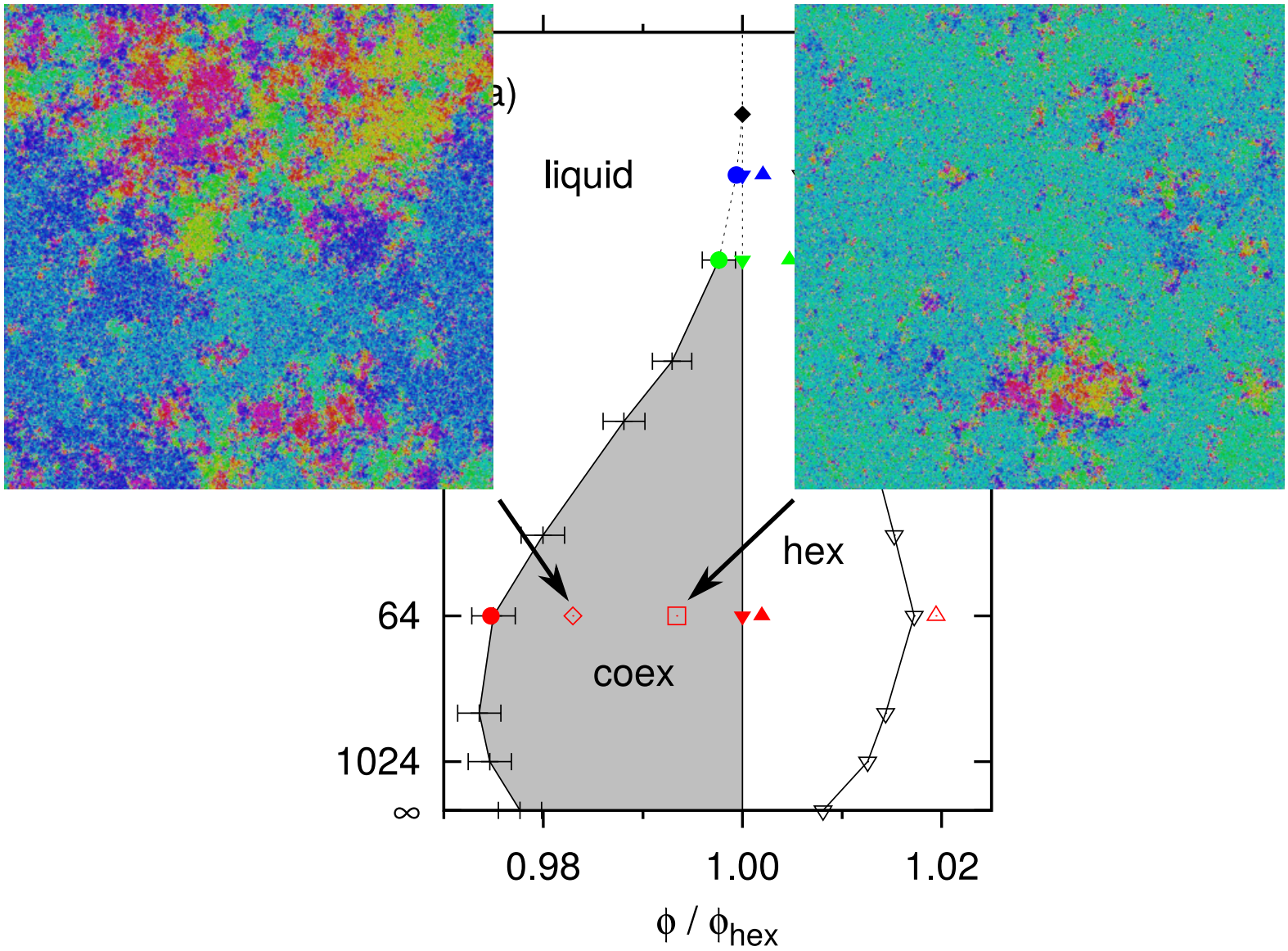
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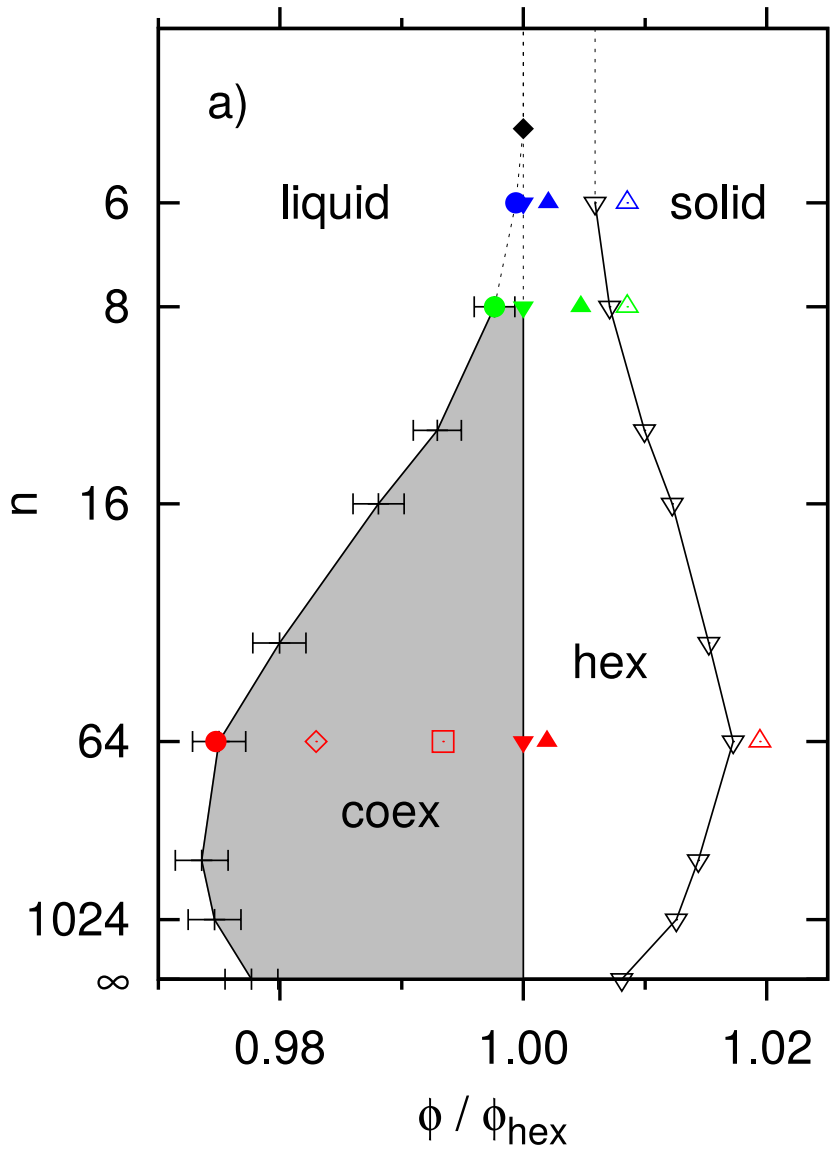
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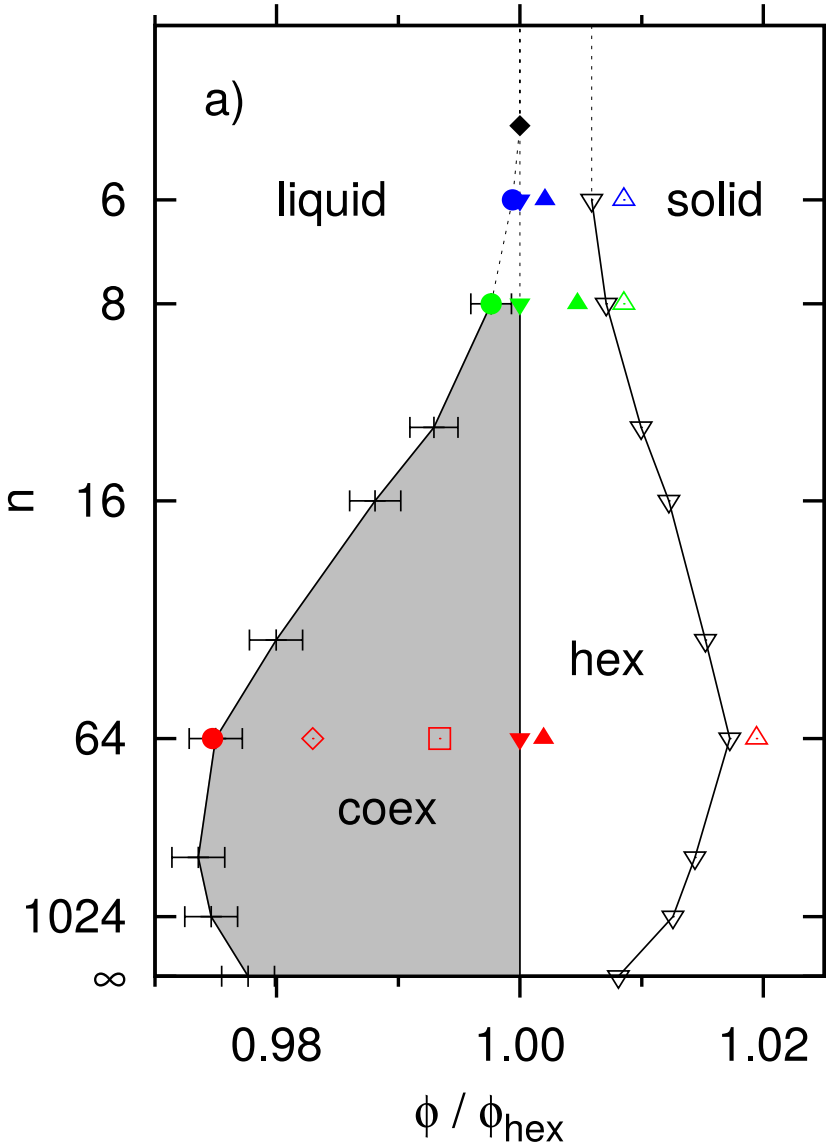
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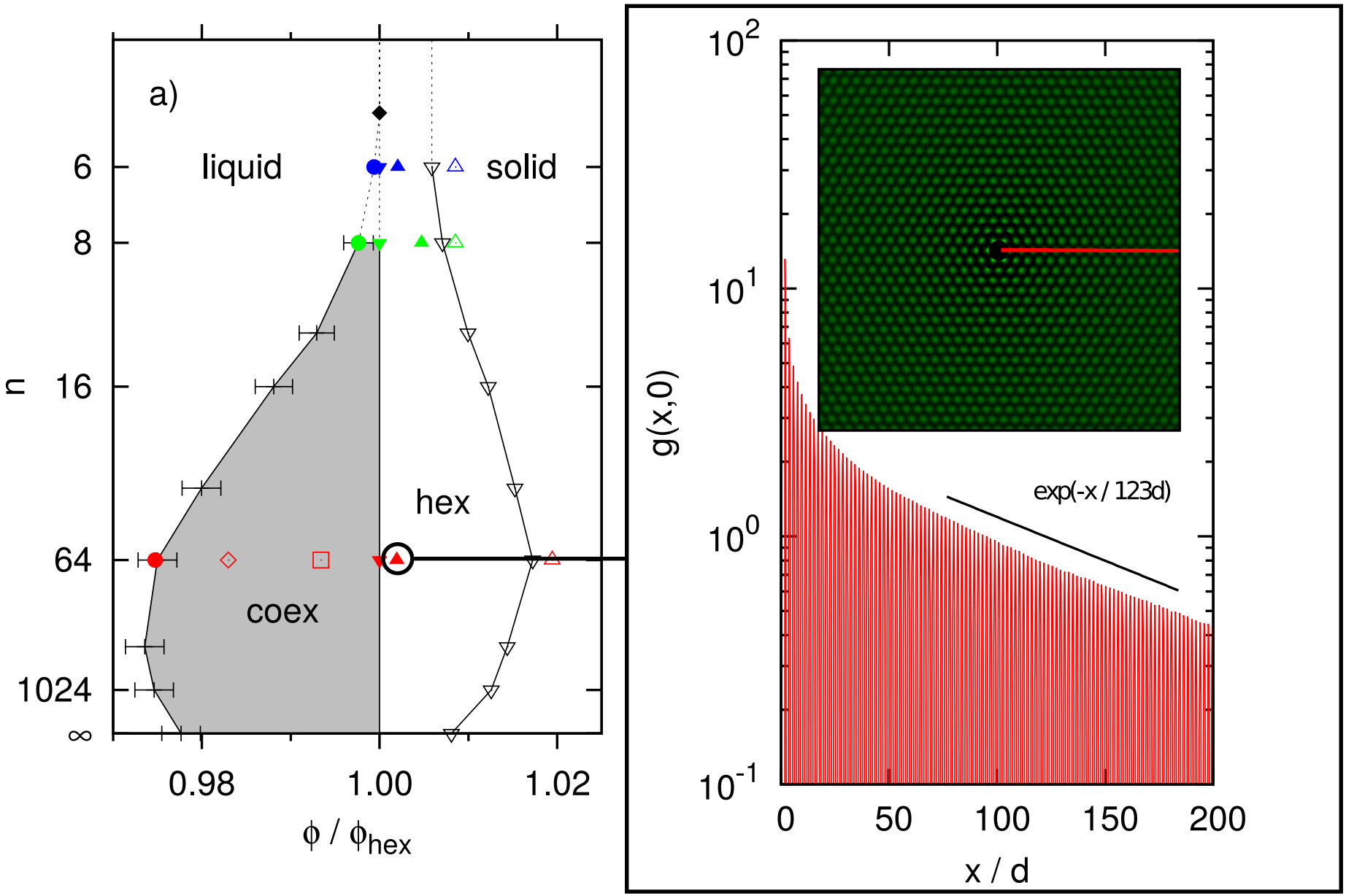
a)
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16
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1024
∞
0.98
1.00
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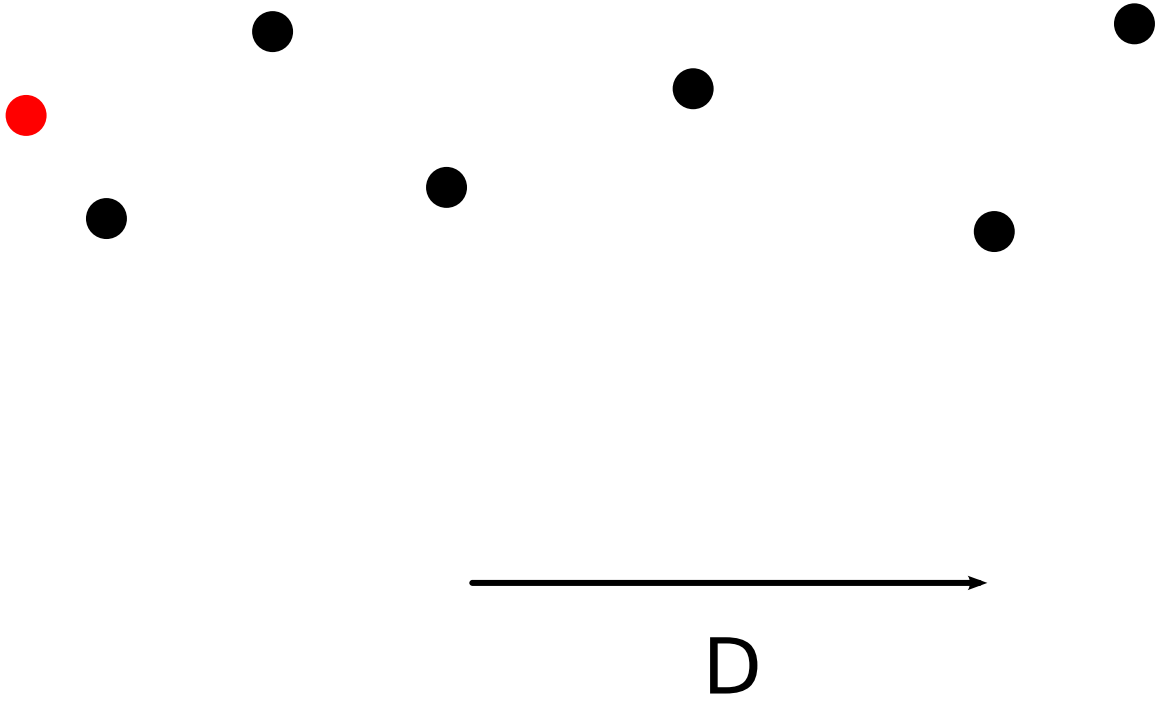
ϕ / ϕhex
g(x,0)
10^2
10^1
10^0
10^-1
exp(-x / 123d)
0
50
100
150
200
x / d

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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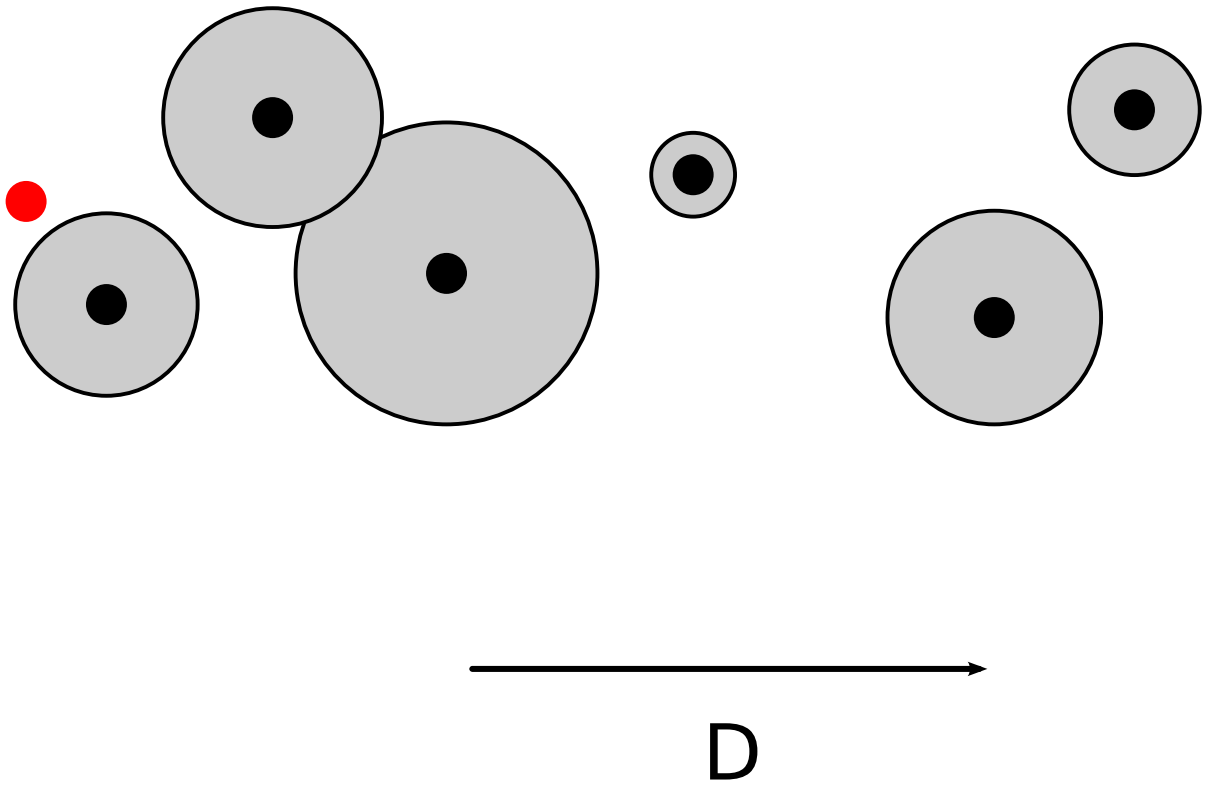

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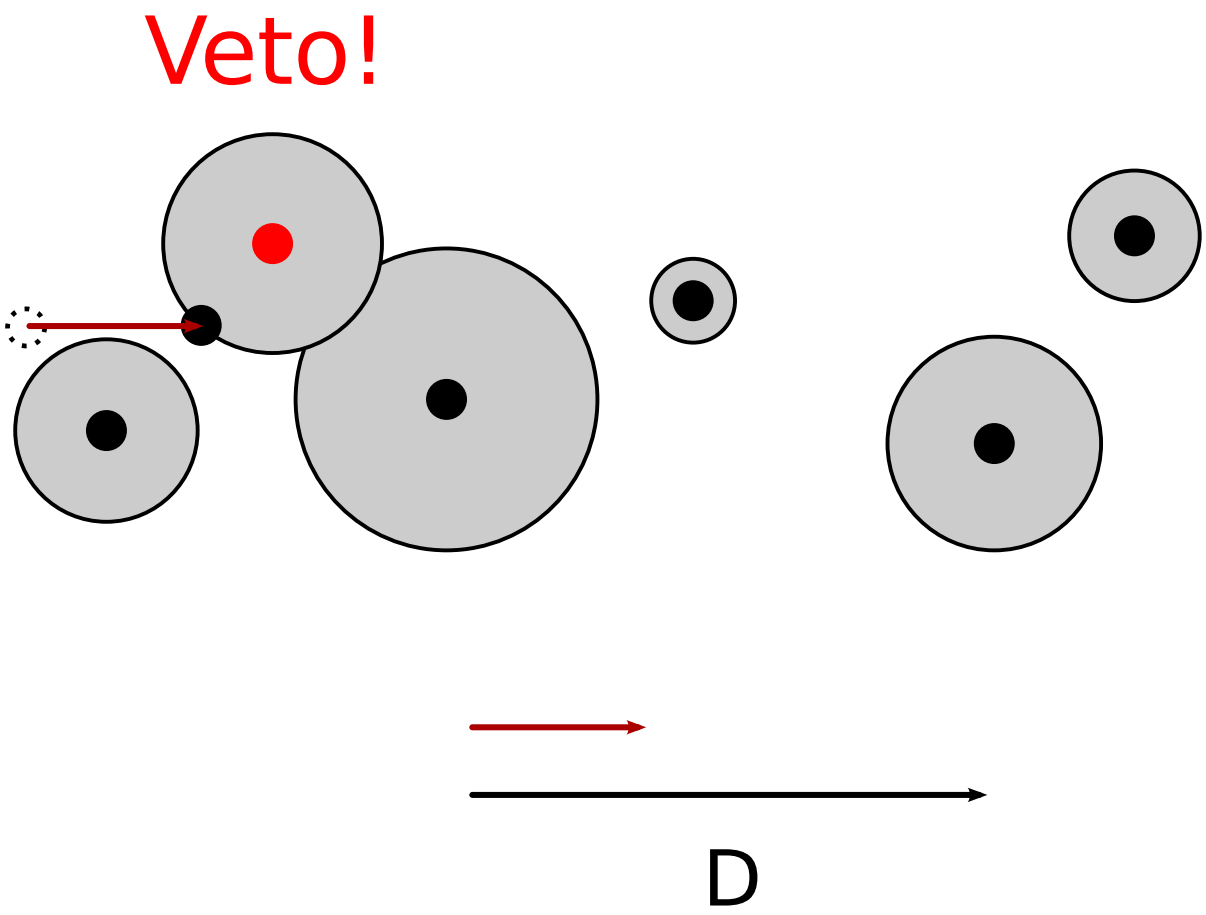

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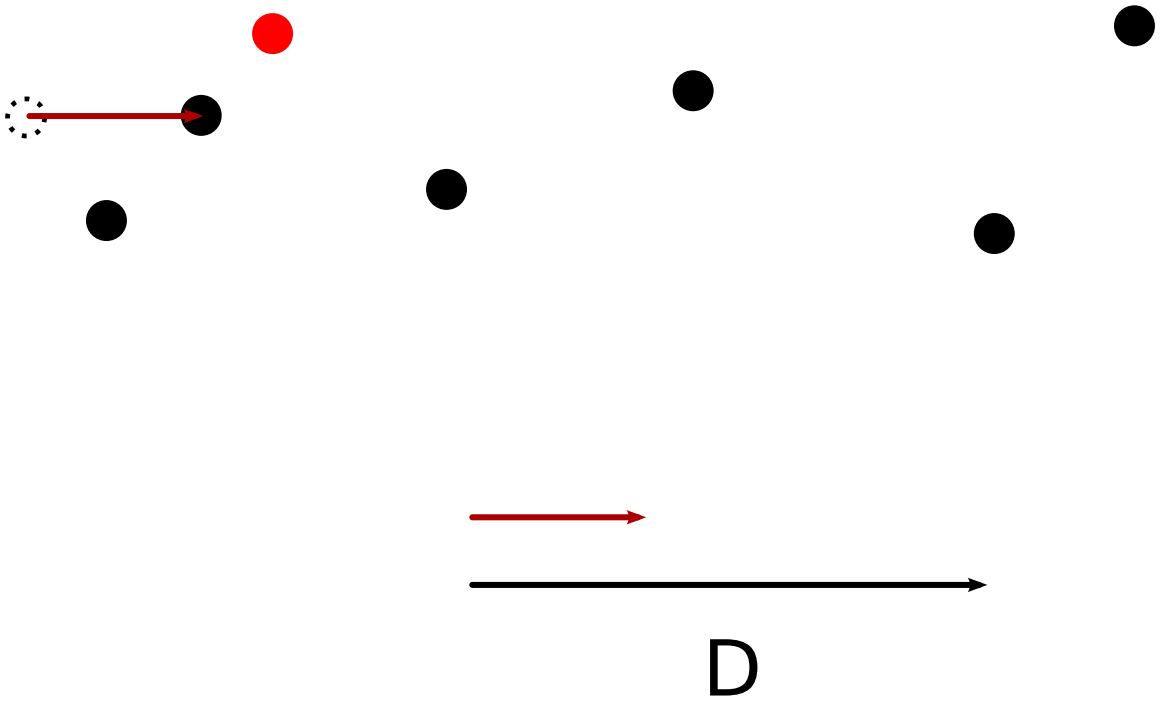

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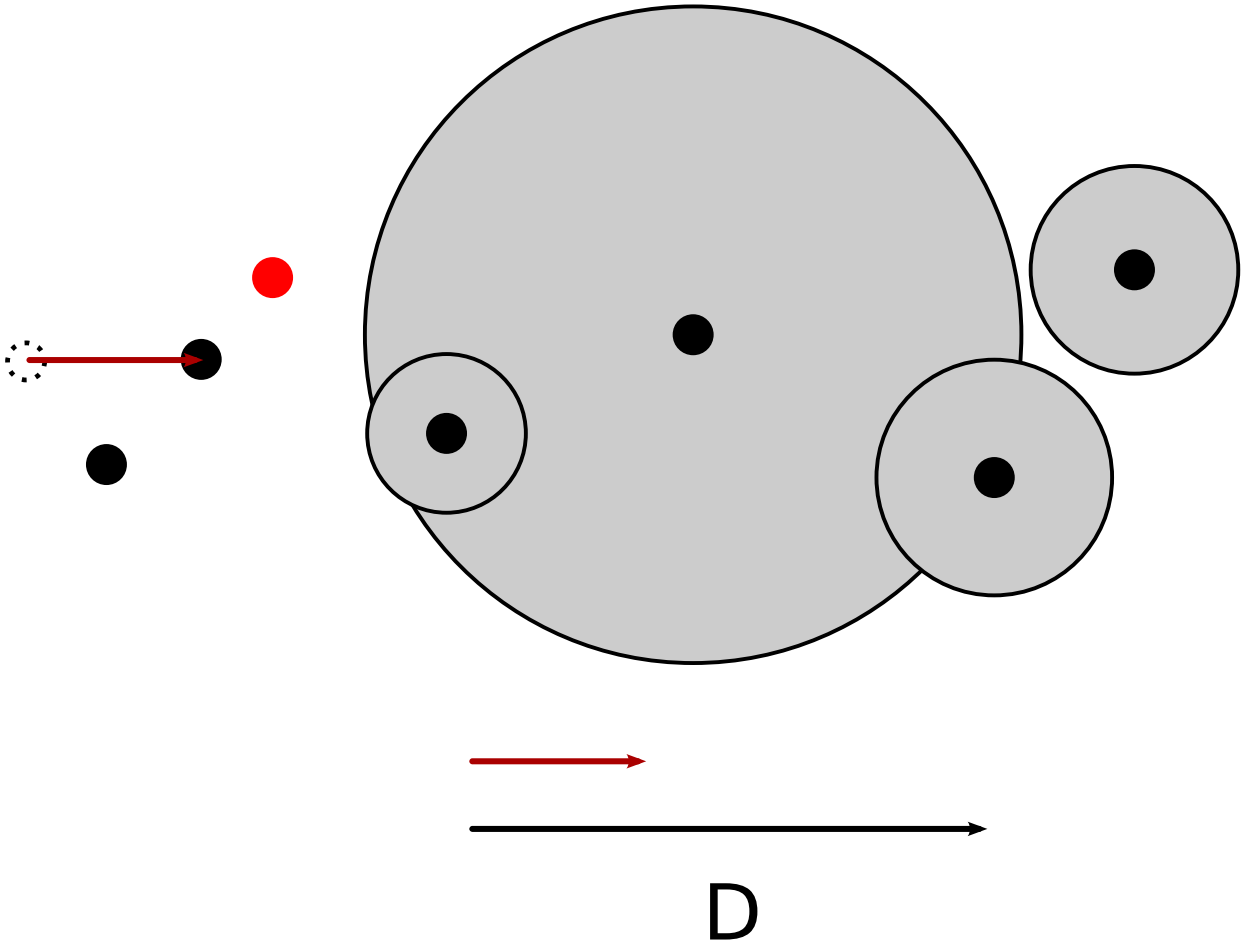

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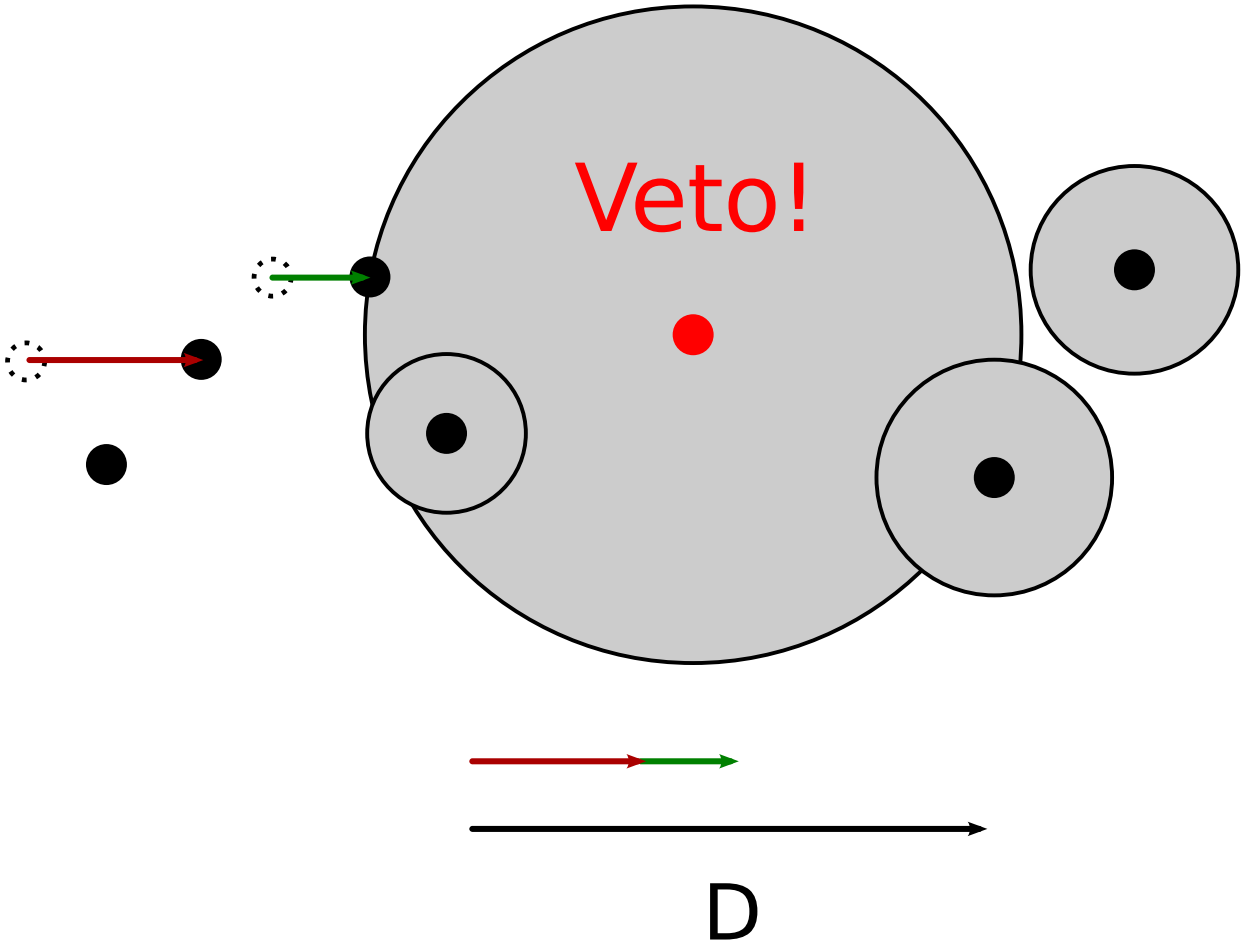

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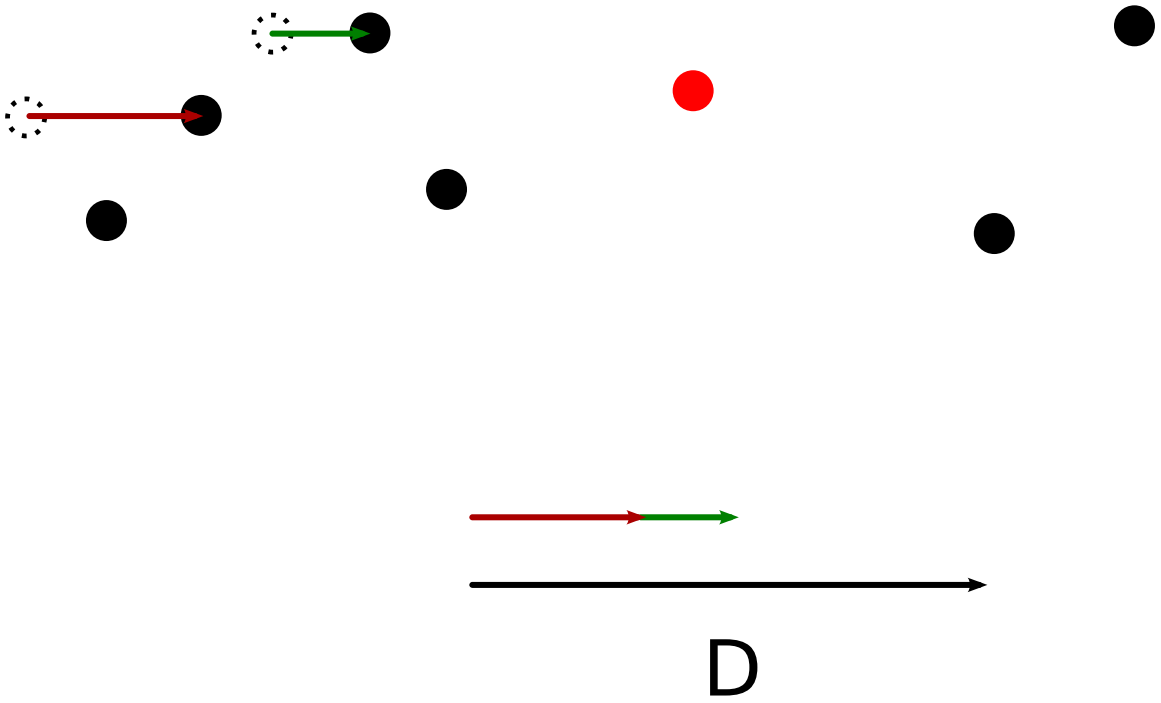

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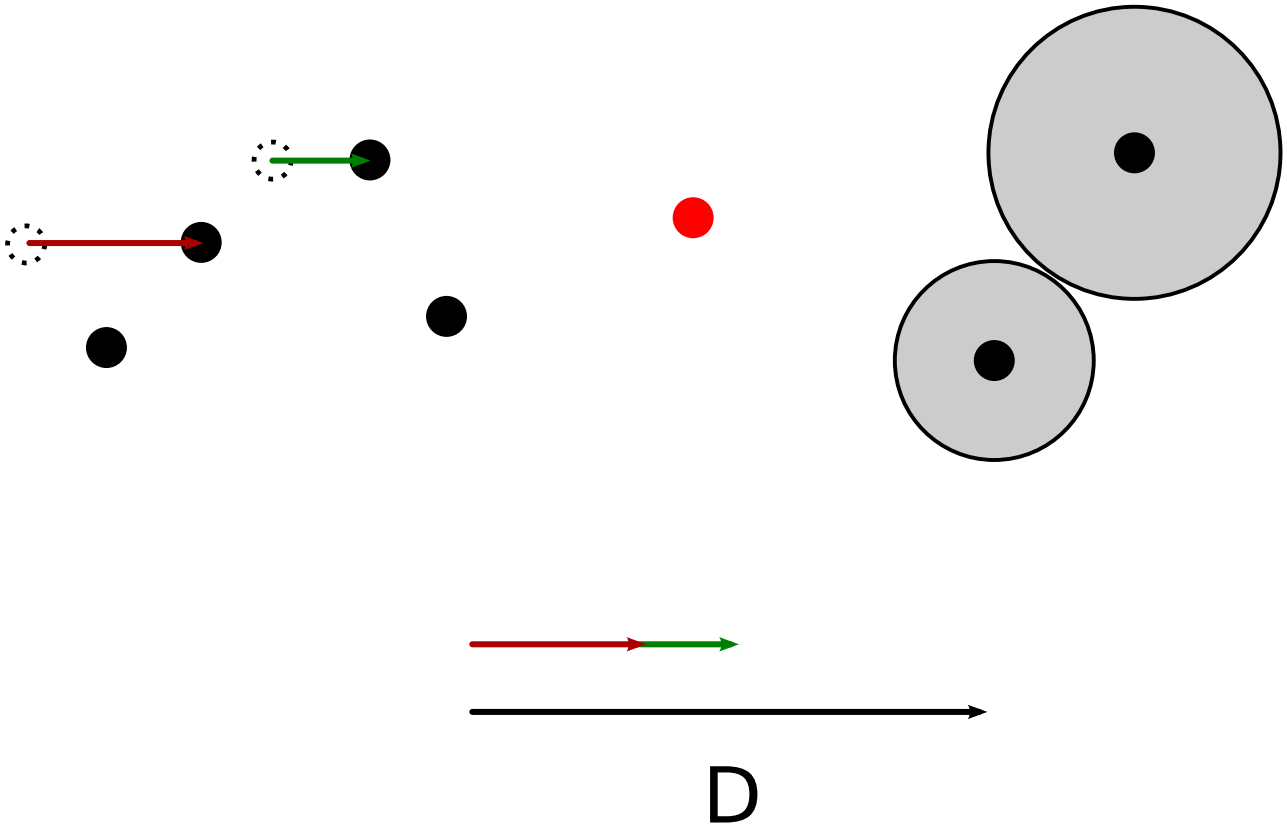

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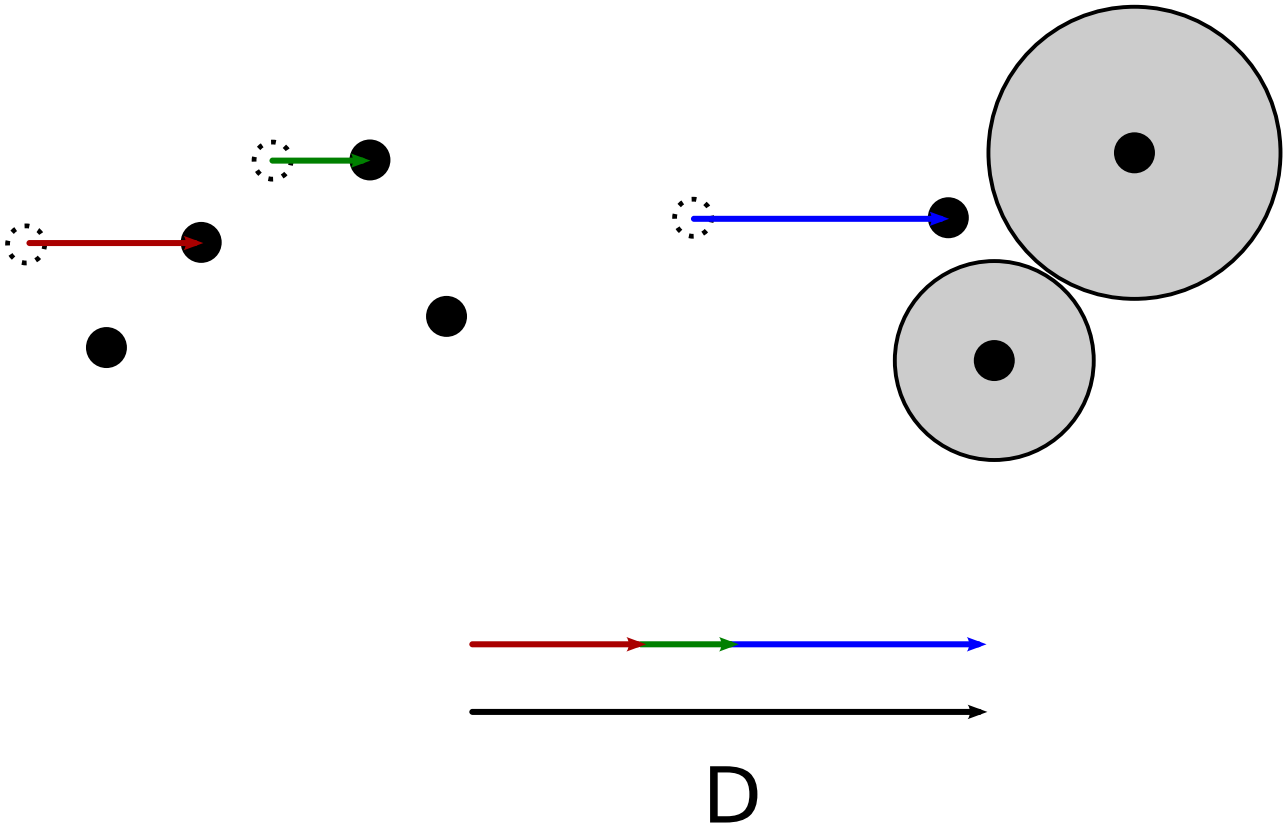

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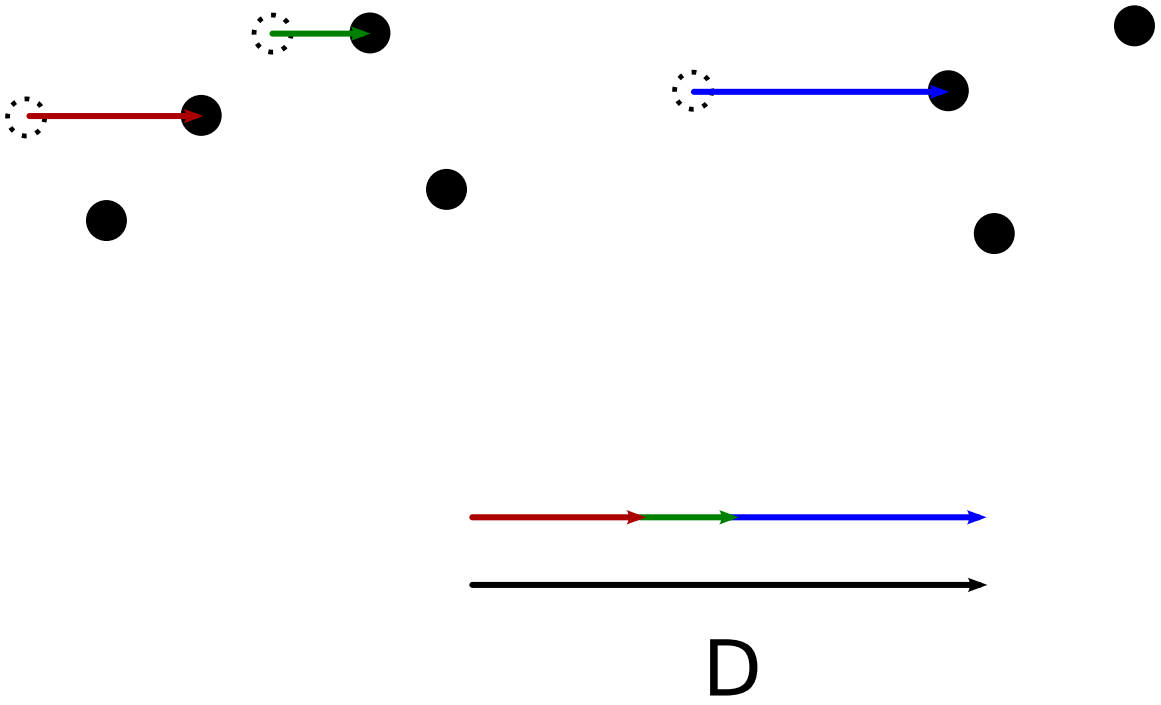

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Recipe for an Event-chain algorithm

Three ingredients

- **Lifted Markov chain**
  extend physical configuration space (*particle coordinates*)
  by artificial variables *direction of motion* and *active particle*
  persistence $\Rightarrow$ **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

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? **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:

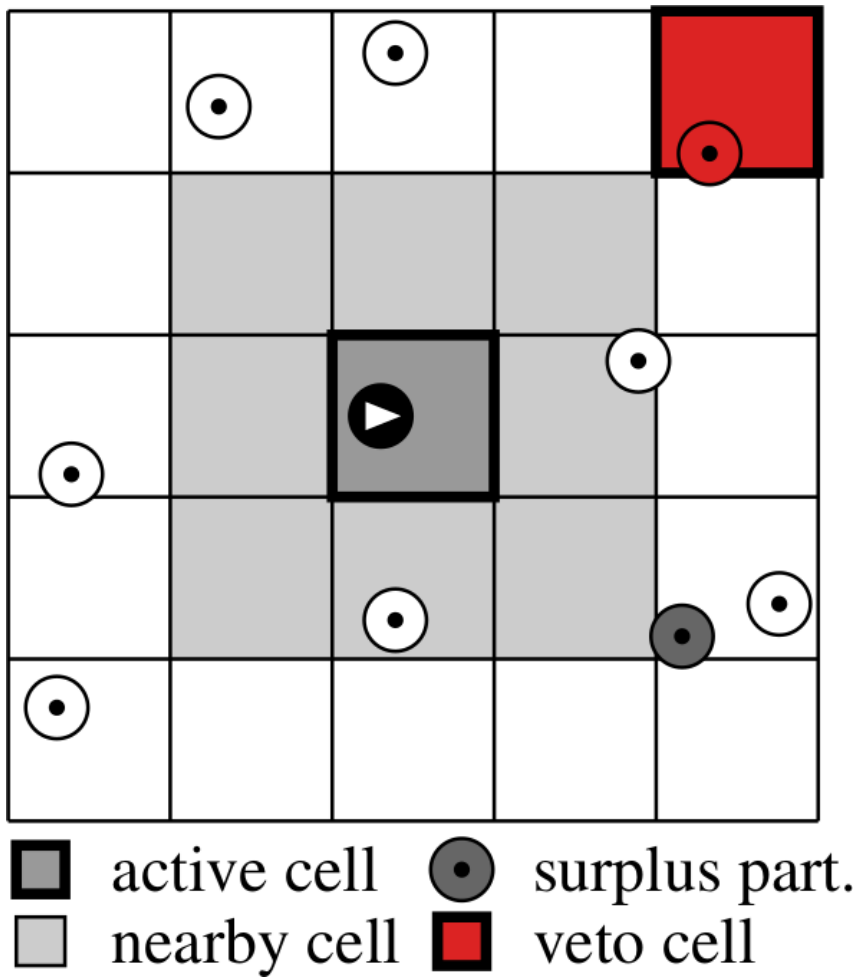
e.g. Walker's alias method, $\mathcal{O}(1)$

If vetoing cell contains a particle:

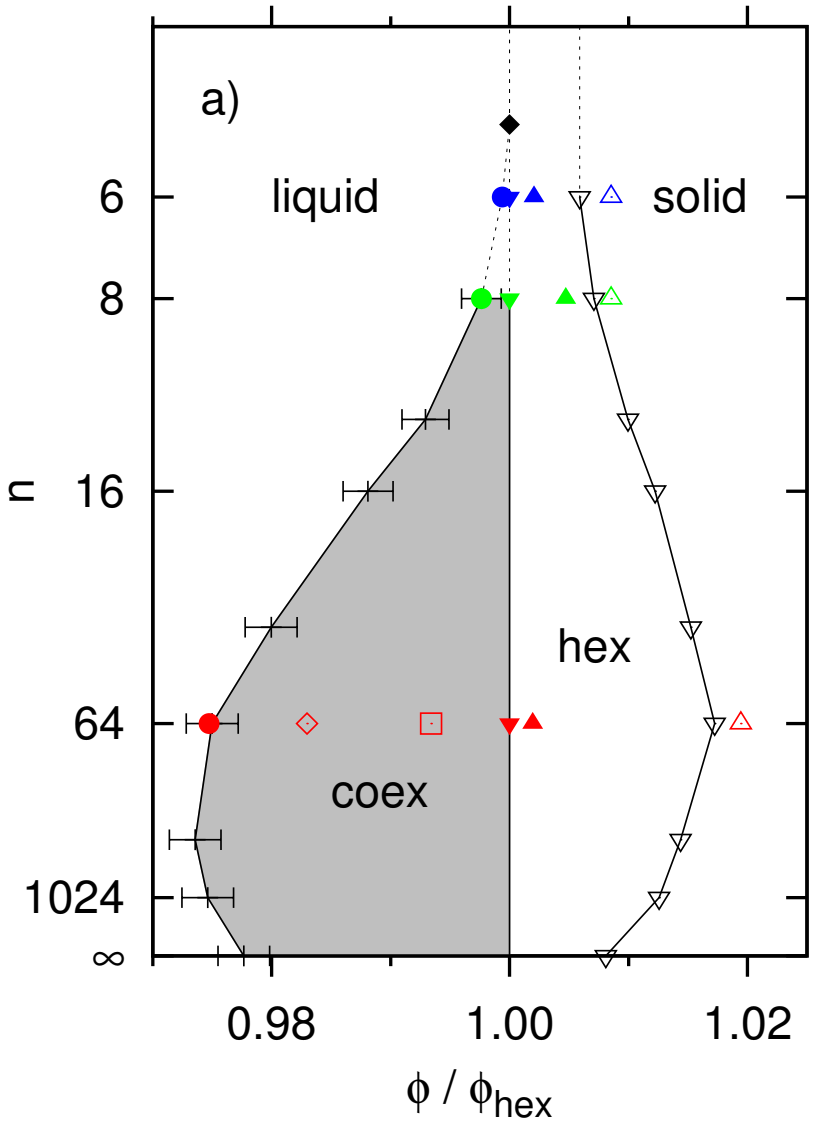
With probability q/Q:

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

Soft-disk EC

Michel, Kapfer, Krauth 2014,
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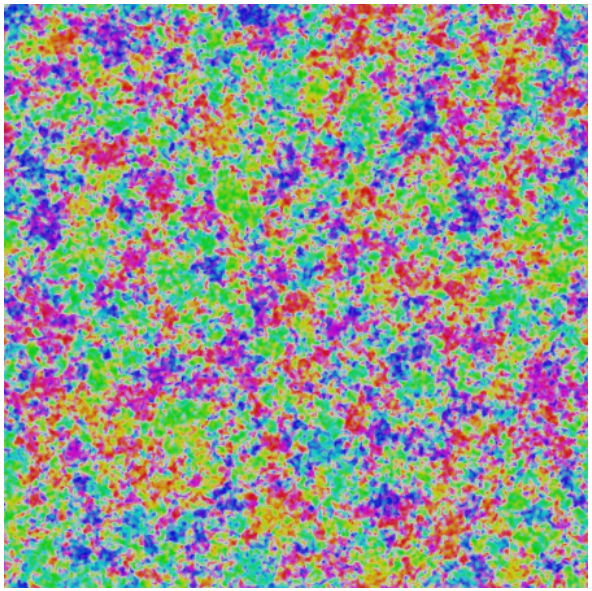
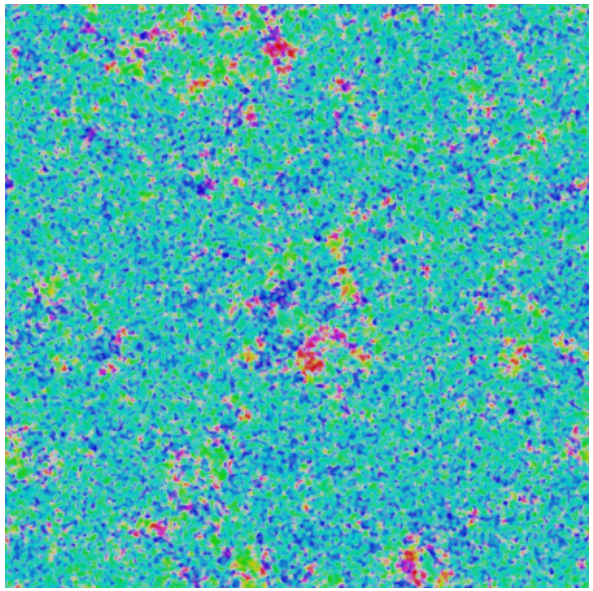
Hard-disk EC
Bernard & Krauth 2009/11

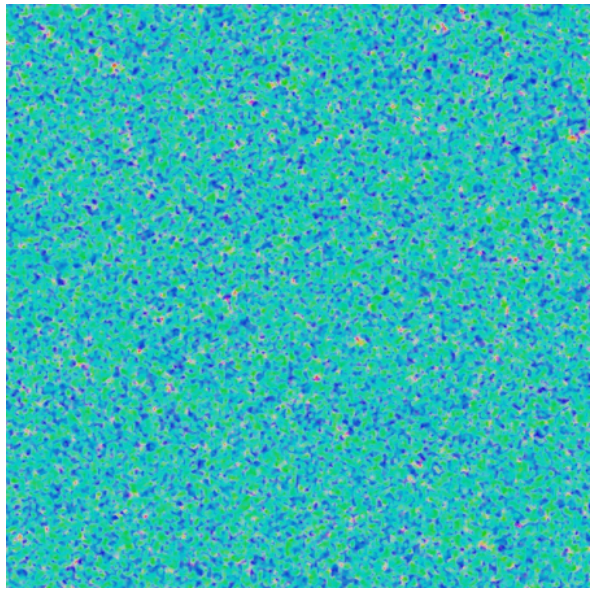
Soft disks with $U = 1/r^3$ interactions



liquid



hexatic



solid

Summary

- **Hexatic/liquid coexistence** for short-range repulsive forces in 2D
  Continuous transition (**classical KTHNY**) for softer / long-ranged
- Lifting, Factorized Metropolis, Infinitesimal moves
  allow to construct new MCMC algorithms of the Event-chain type

  Global balance, zero-rejection, cooperative, event-driven
- 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?

Collaborators

Werner Krauth,
Manon Michel (ENS)

Code

https://github.com/cell-veto/

Papers

Event-chain: PRE **94**, 031302 (2016)
& JCP **140**, 054116 (2014)
2D melting: PRL **114**, 035702 (2015)