Computational statistical physics: The example of hard spheres

Lectures at the 16th Chris Engelbrecht Summer School in Theoretical Physics, Drakensberg, KwaZulu-Natal, South Africa

Third part: Modern Algorithms

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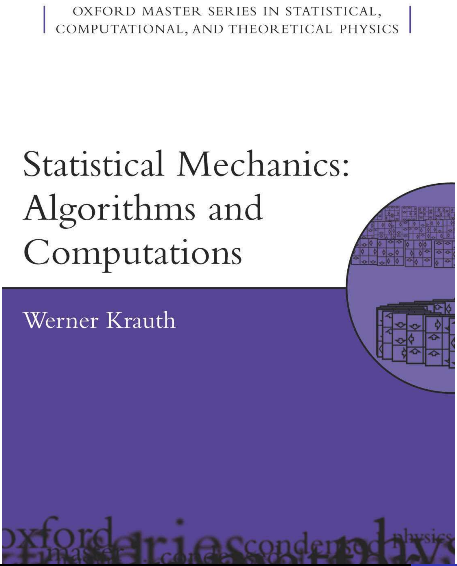
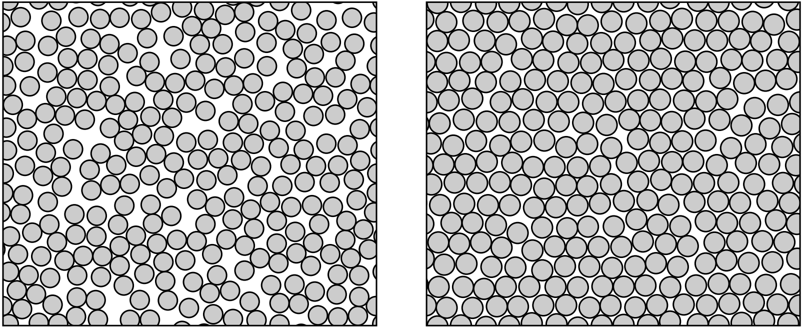
26 January 2005

Computational statistical physics: the example of hard spheres



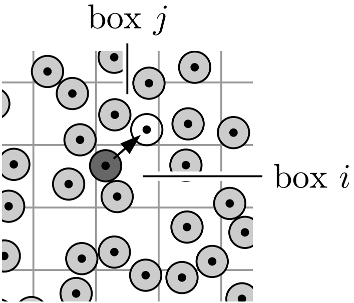
Paris, France, June 4th, 2004, Nº 3

Large systems of hard spheres



- Liquid–Solid phase transition in dimensions 2 or higher.

Complexity of the Markov-chain algorithm



- Use of boxes imposes itself for $N \gg 100$ (production phase of program)
- useful in all *local* problems

Data structures

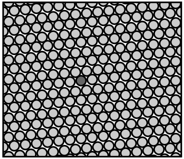
Have choice between

- occupation tables ('chemist's cabinets')
- Linked lists ('butcher's hooks'))

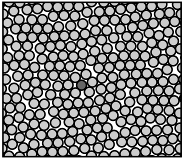
Allows to handle

- interaction partners
- move of particle

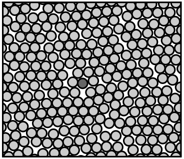
Convergence problems of the local algorithm



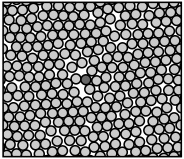
$i = 0$



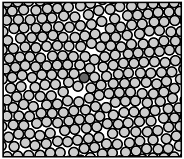
$i/N = 1000$



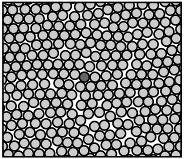
$i/N = 2000$



$i/N = 3000$

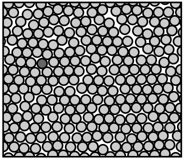


$i/N = 4000$



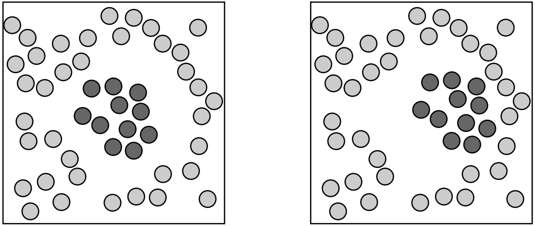
$i/N = 5000$

$\ldots$



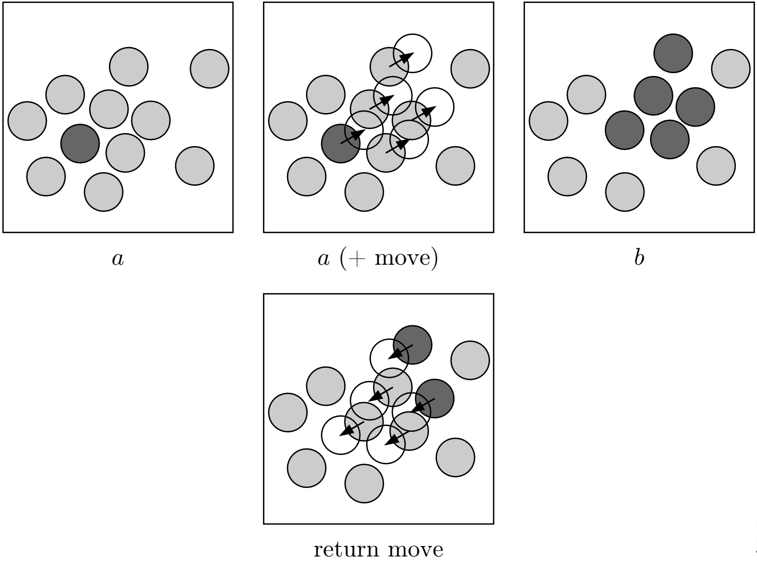
$i/N = 100000000$

Collective moves



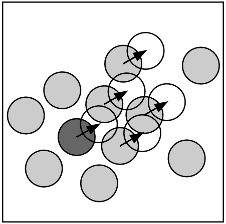
a *b*

- satisfy detailed balance?
- identify clusters?

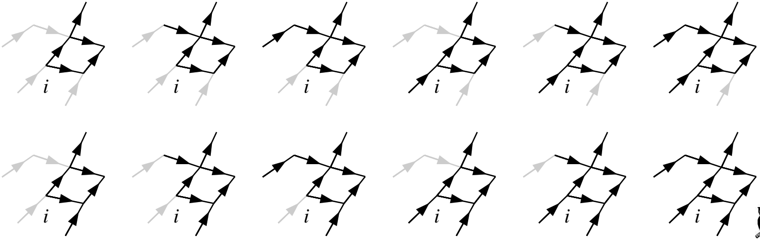


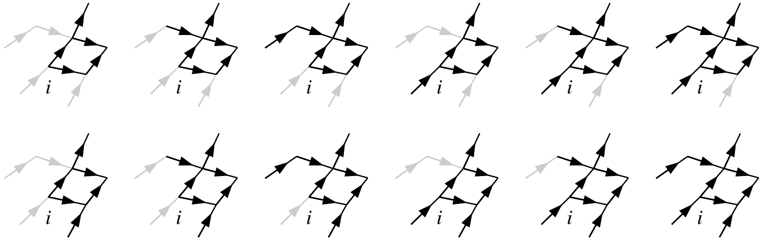
a
a (+ move)
b
return move

Avalanches–full analysis



a (+ move)

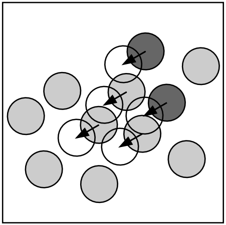




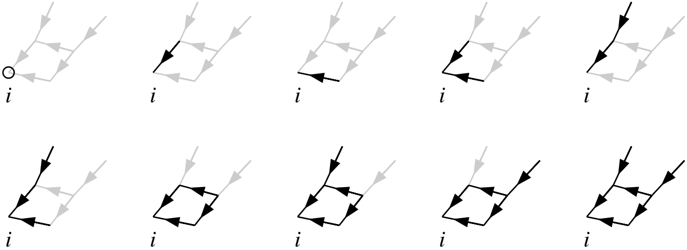
- Implies that the a priori probability of move $a \to b$ is $1/12$.

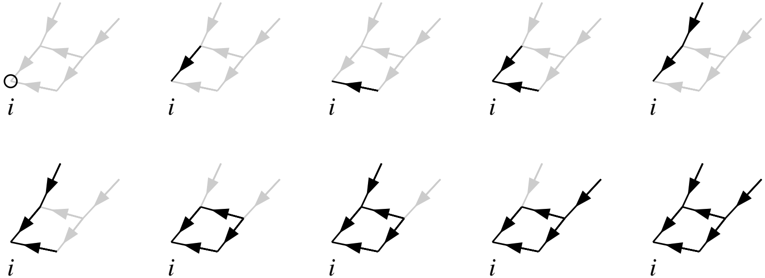
$$\mathcal{A}(a \to b) = \frac{1}{12}$$

Avalanches–full analysis (return move)



return move

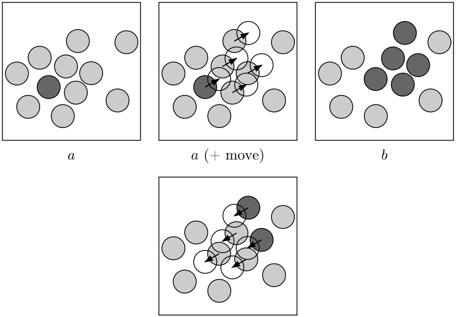




- Implies that the a priori probability of the return move $b \to a$ is $1/10$.

$$\mathcal{A}(a \to b) = \frac{1}{12}$$

Avalanches (conclusion)

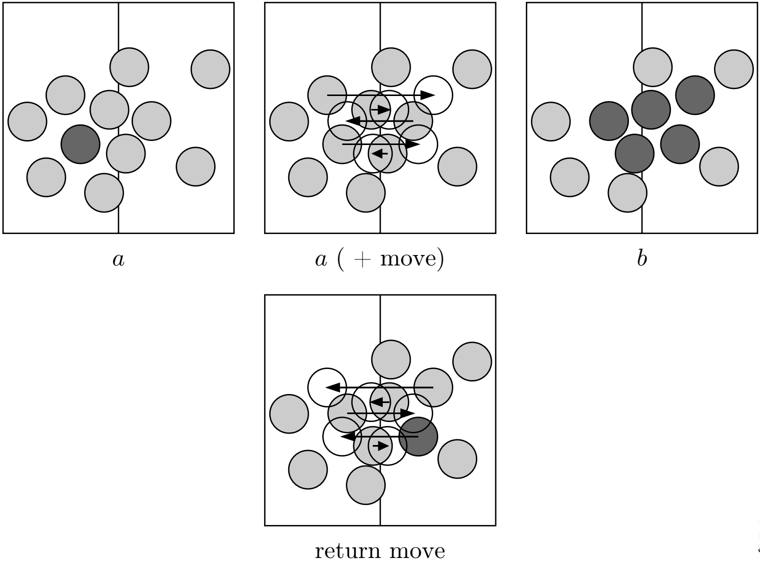


a | a (+ move) | b | return move

- Accept move $a \to b$ with probability

$$p(a \to b) = \min\left[1, \frac{12}{10}\right]$$

Pivot Cluster algorithm



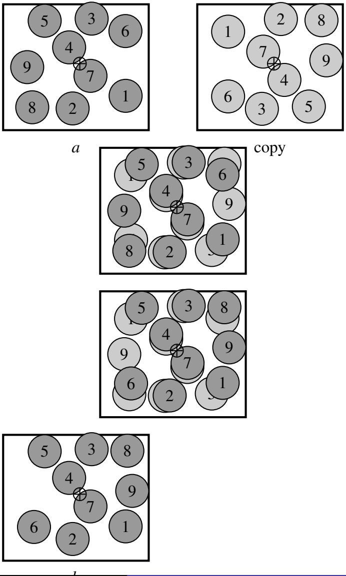
Pivot Cluster algorithm (properties)

- each move its own inverse!
- random reflection, point transformations, etc
- Acceptance probability = 1

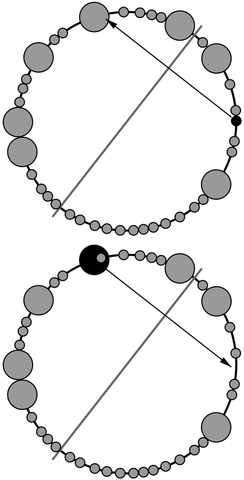
Pivot cluster algorithm (implementation)

procedure `pocket-disks`
input $\{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$
$\mathcal{T} \leftarrow$ random symmetry operation
$i \leftarrow$ `Nran`$[1, N]$ (random initial particle)
$\mathcal{P} \leftarrow \{i\}$
$\mathcal{A} \leftarrow \{1, \ldots, N\} \setminus \{i\}$
while $(\mathcal{P} \neq \{\})$ **do**
$\quad\left\{\begin{array}{l} i \leftarrow \text{any element of } \mathcal{P} \\ \mathcal{P} \leftarrow \mathcal{P} \setminus \{i\} \\ \mathbf{x}_i \leftarrow \mathcal{T}(\mathbf{x}_i) \\ \textbf{for } \forall\, j \in \mathcal{A} \textbf{ do} \\ \quad \left\{\begin{array}{l} \textbf{if } (j \cap i) \\ \quad \left\{\begin{array}{l} \mathcal{A} \leftarrow \mathcal{A} \setminus \{j\} \\ \mathcal{P} \leftarrow \mathcal{P} \cup \{j\} \end{array}\right. \end{array}\right. \end{array}\right.$
output $\{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$

alternative representation of pivot cluster algorithm



Algorithm in one dimension



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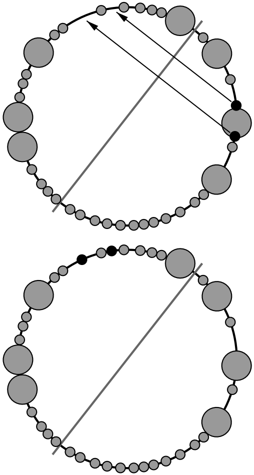
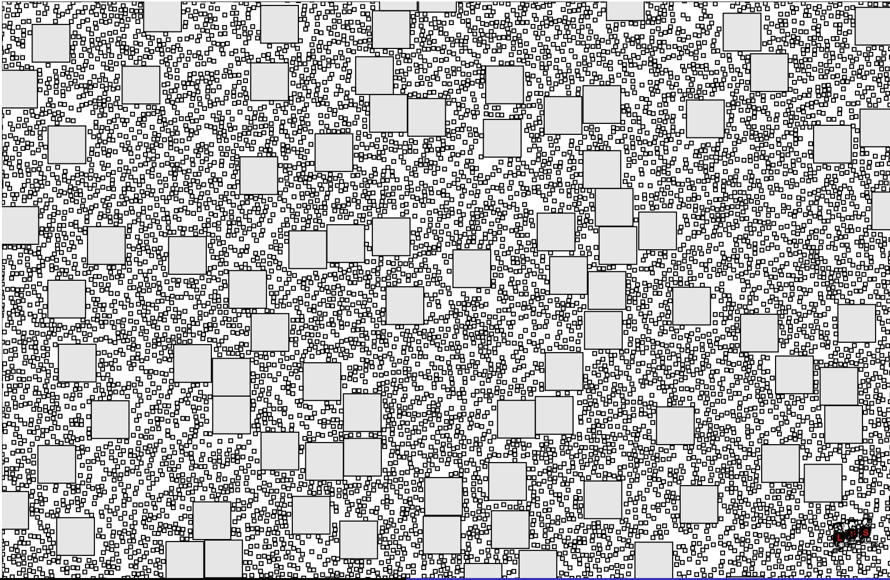
Algorithm in one dimension

- . . . (continued from last frame)



Binary mixture (detail)



Binary mixtures