Computer Simulations in Stat. Phys. Sheet 01 Peter Gispert

3|a) detailed balance: $\frac{W_{ij}}{W_{ji}} = e^{-\beta(E_j - E_i)} = e^{-\beta\Delta E}$

Metropolis: $W_{ij} = \min\{1, e^{-\beta\Delta E}\}$. Prove detailed balance:

If $\Delta E \leq 0$: $e^{-\beta\Delta E} \geq 1 \Rightarrow W_{ij} = 1$ and $e^{\beta\Delta E} \leq 1 \rightarrow W_{ji} = e^{\beta\Delta E}$

$\Rightarrow \frac{W_{ij}}{W_{ji}} = e^{-\beta\Delta E}$

If $\Delta E > 0$: $e^{-\beta\Delta E} < 1 \rightarrow W_{ij} = e^{-\beta\Delta E}$ and $e^{\beta\Delta E} > 1 \Rightarrow W_{ji} = 1$

$\Rightarrow \frac{W_{ij}}{W_{ji}} = e^{-\beta\Delta E}$

b) Heat bath algorithm: $W_{ij} = \frac{e^{-\beta\Delta E}}{e^{-\beta\Delta E}+1} \Rightarrow W_{ji} = \frac{e^{\beta\Delta E}}{e^{\beta\Delta E}+1}$

$$\frac{W_{ij}}{W_{ji}} = \frac{e^{-\beta\Delta E}}{e^{-\beta\Delta E}+1}\,\frac{e^{\beta\Delta E}+1}{e^{\beta\Delta E}} = \frac{1}{1+e^{\beta\Delta E}}\,\frac{e^{\beta\Delta E}+1}{e^{\beta\Delta E}} = e^{-\beta\Delta E}$$

c) $V(\vec{r}_1, \vec{r}_2) = \begin{cases} 0 & |\vec{r}_1 - \vec{r}_2| \geq \sigma \\ \infty & |\vec{r}_1 - \vec{r}_2| < \sigma \end{cases}$

Assume that the system starts in a configuration with no pairwise overlap, i.e. with $E = 0$. Then:

$$\Delta E = \begin{cases} \infty, & \exists\, k \neq l : |\vec{r}_k - \vec{r}_l| < \sigma \\ 0, & \text{otherwise} \end{cases}$$

$\rightarrow$ If $\Delta E = \infty$ (i.e. $\exists\, k \neq l : |\vec{r}_k - \vec{r}_l| < \sigma$), then $e^{-\beta\Delta E} = 0$.

$\Rightarrow W_{ij} = 0$ and $W_{ji} = 1$

Otherwise ($\Delta E = 0$): $e^{-\beta\Delta E} = 1 \Rightarrow W_{ij} = 1$, $W_{ji} = 1$.

$\Rightarrow$ It is not allowed to jump into a disk configuration with some pairwise overlap (probability 0). Any other transition will be accepted (probability 1)

4|a) At low temperatures almost all spins align eventually. Big domains with the same spin-orientation form and absorb small fluctuations. Whereas at high temperatures the spin orientation is almost random. There are no big domains and the total magnetisation is approximately zero.

3| a) While at $T = 2.5K$ the total magnetisation fluctuates around 0, it reaches a non-zero value of $|m| \approx 0.8$ (and fluctuates around it) at $T = 2K$. Thus, the phase transition is between 2K and 2.5K. For an infinite 2D lattice the exact value is $T_c \approx 2.27K$.

Compared to the single-spin-flip algorithm (Metropolis) the Wolff algorithm flips multiple spins at the same time. At low temperatures (below the phase transition) the Metropolis algorithm takes a long time to flip entire domains. This is because at the domain boundary a spin flip often does not reduce the energy. Here, the Wolff algorithm is much more efficient because it can attack entire domains within one step, which amounts to big energy gains. At high temperatures, domains become smaller and contain only a couple of spins in most cases. Here, it might be advantageous to apply the single-spin-flip algorithm because domains only form due to statistical fluctuations, but barely systematically.

b) pseudo-code: single-spin-flip algorithm:

1. Choose a (potentially random) start configuration
2. Choose a single spin and consider its flip: $S_i \to -S_i$
3. Compute the change in energy ΔE and the corresponding transition probability $W(\Delta E)$
4. Choose a random number $r \sim \text{Unif}_{[0,1]}$:
   If $r < W(\Delta E)$ accept the spinflip, otherwise reject it
5. Repeat from 2 or terminate (according to some criterion).

→ in general $\Delta E = -J\left[(-S_i)\sum_{\substack{\text{nearest}\\\text{neighbours } j}} S_j - S_i \sum_{\substack{\text{nearest}\\\text{neighbours } j}} S_j\right] = 2 S_i \sum_{\substack{\text{nearest}\\\text{neighbours}}} S_j$

1D: each spin has two nearest neighbours: $S_i \in \{\pm 1\}$

$$\Delta E = -J\left[(-S_i)(S_{i-1} + S_{i+1}) - S_i(S_{i-1} + S_{i+1})\right] = 2J\, S_i(S_{i-1} + S_{i+1}) \in \{0, \pm 4J\}$$

2D: each spin has four nearest neighbours (on a square lattice)

$$\Delta E = 2J\, S_{ij}(S_{i-1,j} + S_{i+1,j} + S_{i,j-1} + S_{i,j+1}) \in \{0, \pm 4J, \pm 8J\}$$