Modelling Grain Growth

Using the Metropolis Algorithm

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Outline

Grains and Grain Growth

- Most materials are polycrystalline
- Grains grow.

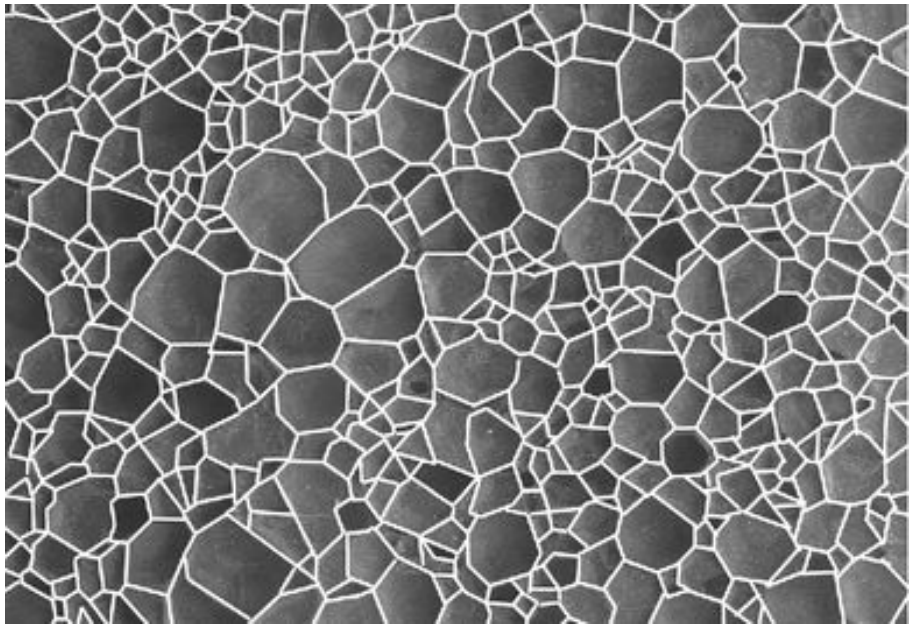


Image from literature[1]

[1] Morfa et al., "Virtual modeling of polycrystalline structures of materials using particle packing algorithms and Laguerre cells".

The Metropolis Algorithm

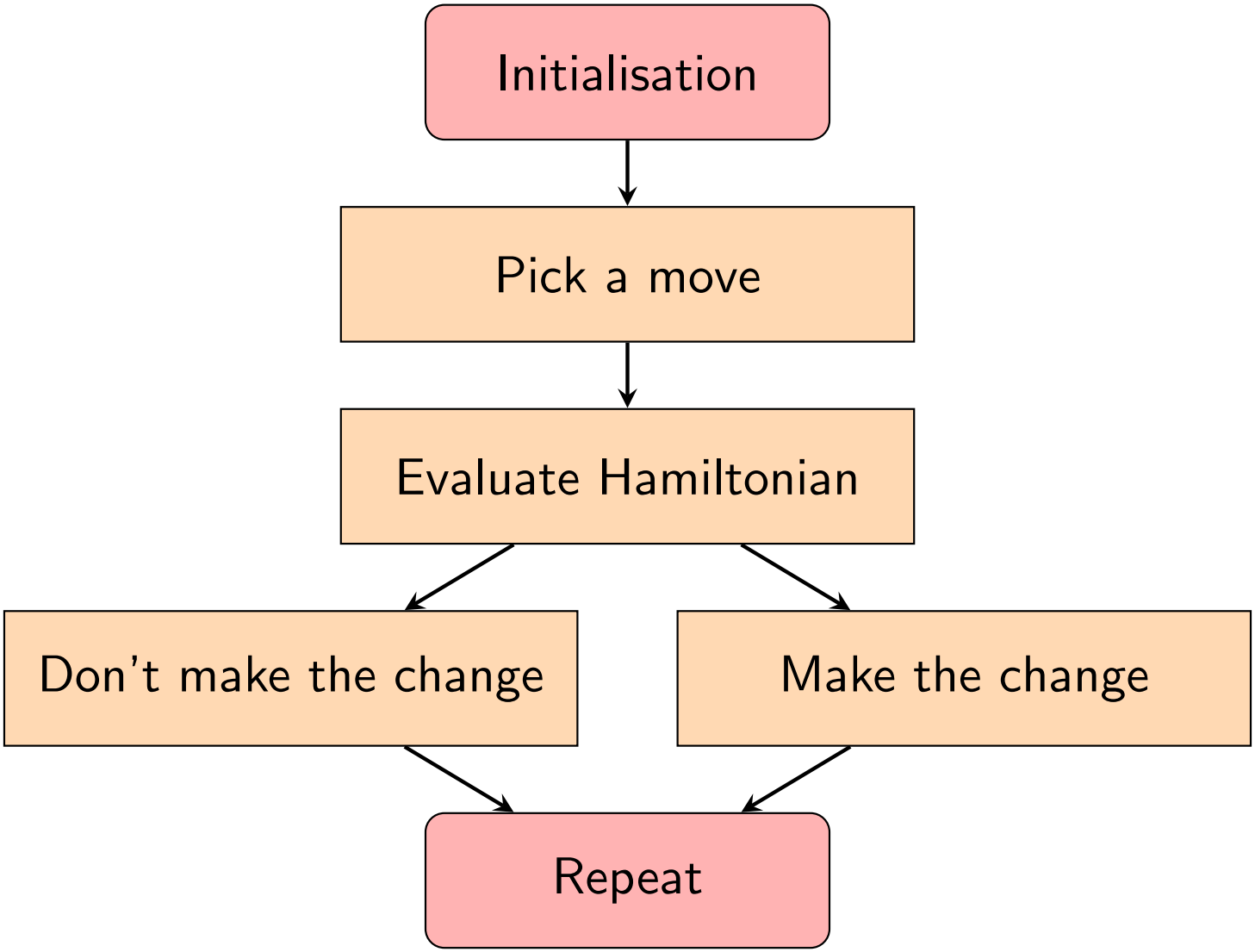
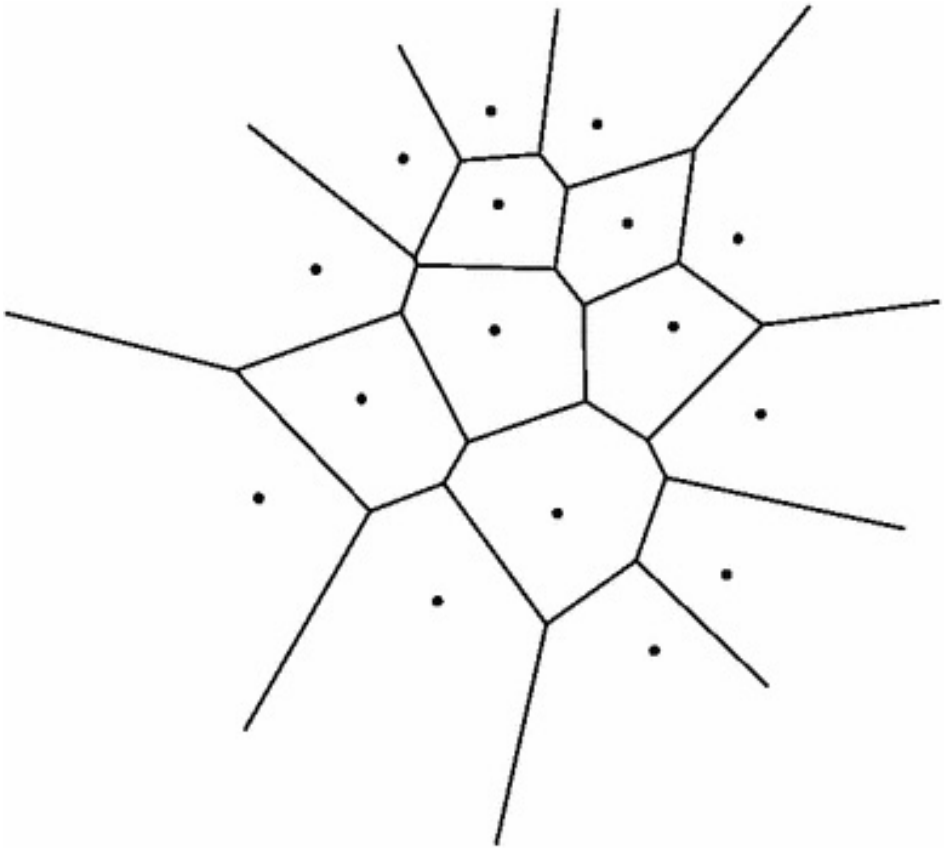


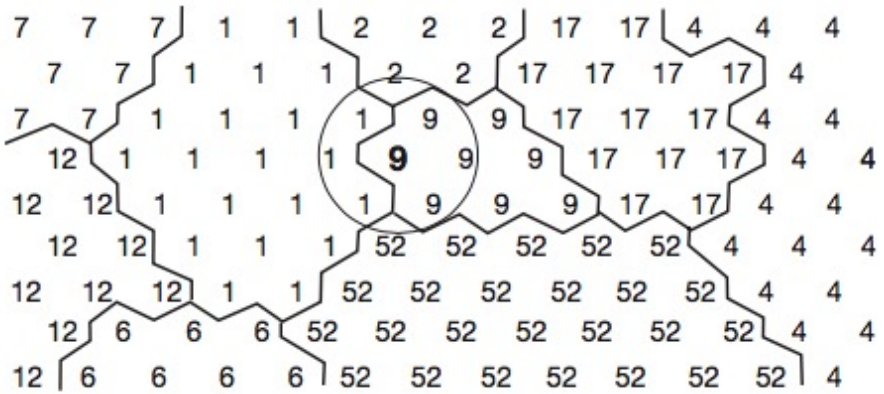
Figure: Metropolis Algorithm

The Potts Model

- States represent orientation
- Very similar to the Ising Model
- Initialisation?



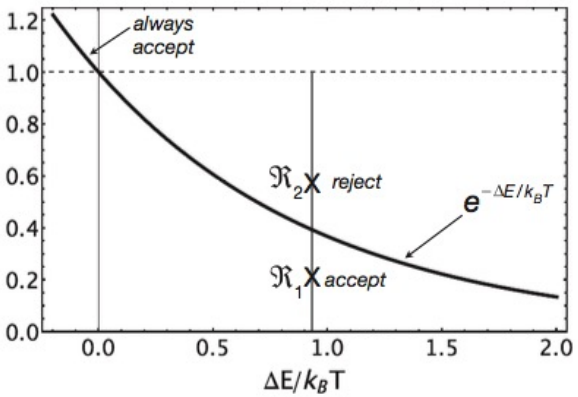
The Potts Model



$$\Delta E = -J\Sigma_{j=1}^{N}(\delta_{S_i,S_j} - 1)$$

$$p = \exp \frac{-\Delta E}{k_B T}$$

The Potts Model



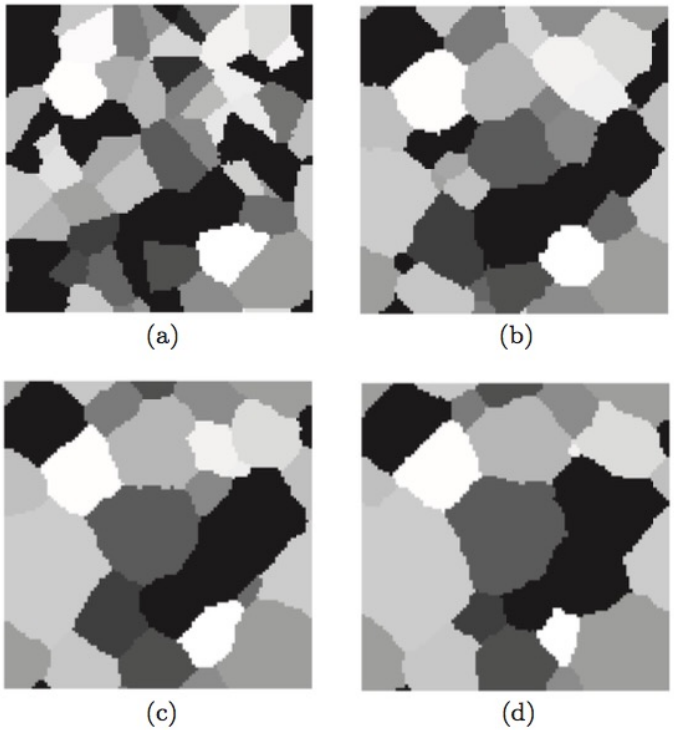


Figure 10.5 Three microstructures from a MC Potts model study of normal "grain growth". (a) $t = 1$, (b) $t = 350$, (c) $t = 700$, and (d) $t = 1000$. The data for the figures are courtesy of A. D. Rollett. Visualization by the ParaView graphics package [265].

Images from Prof. Richard LeSar's book.[2]

[2] LeSar, *Introduction to Computational Materials Science: Fundamentals to Applications*.

Data Structures and Complexity

Data Structures:

- Data structure depends on flavour of lattice
- Can be an array for square lattices
- Structures (C) or objects (Python) for triangular lattices

Complexity:

- Complexity?
- Choice of "Monte Carlo time step"
- $\mathcal{O}$(neighbours) $\times$ # iterations

References I

LeSar, Richard. *Introduction to Computational Materials Science: Fundamentals to Applications*. Cambridge University Press, 2013. DOI: 10.1017/CBO9781139033398.

Morfa, Carlos Recarey et al. "Virtual modeling of polycrystalline structures of materials using particle packing algorithms and Laguerre cells". In: *Computational Particle Mechanics* 5.2 (2018), pp. 213–226. ISSN: 2196-4386. DOI: 10.1007/s40571-017-0164-5. URL: https://doi.org/10.1007/s40571-017-0164-5.

Thank You!