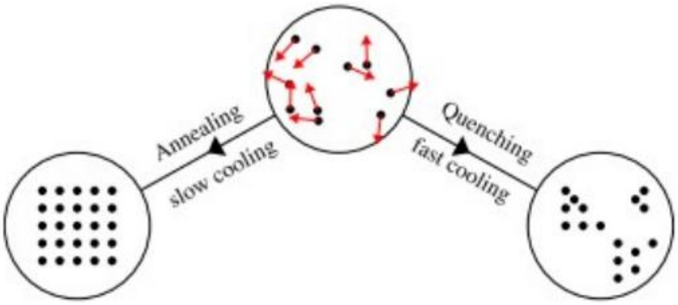
10 - Simulated annealing, main principles and the Metropolis rule

- Inspired by nature (by physics and metallorgy more specifically)
- Annealing is a process by which a sample is cooled down slowly -> finds global min
- Quench it is a quick cooling down -> finds local min
- Fitness function is called energy function

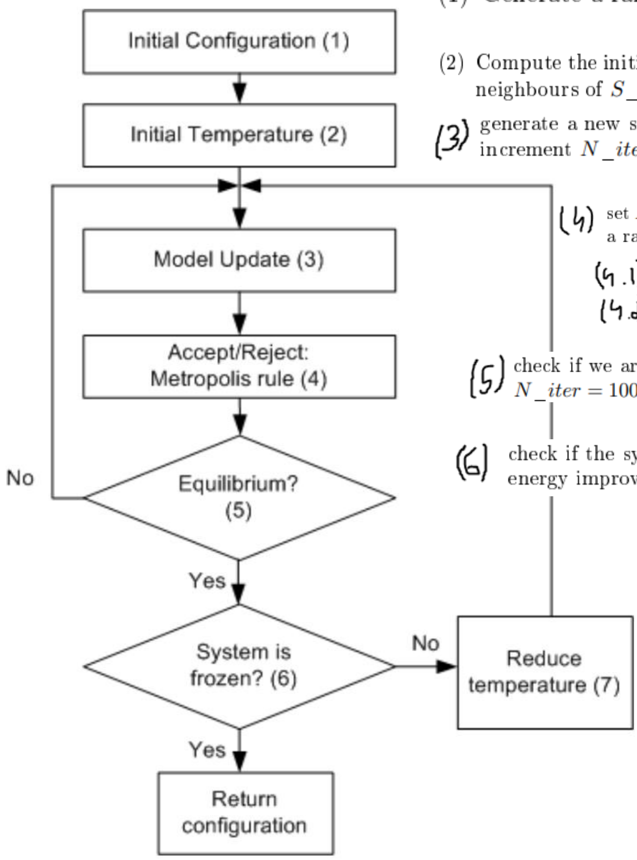
Nature minimizes energy with theses processes, and we want to capture this same property with our algorithm



- ➔ We start with high temperature, in this state the system explores many possible states
- ➔ When the temperature starts to cool down the system is "trapped" does exploitation process

The hope is to have found the global min with the use of both exploration and exploitation

Algorithm:



(1) Generate a random state S, let's call it $S\_current$

(2) Compute the initial temperature: $e^{\frac{-\langle \triangle E \rangle}{T_0}} = 0.5$, where $\langle \triangle E \rangle$ is the average energy change of 100 (random) neighbours of $S\_current$

(3) generate a new state, let this state be a random neighbour of our current state, let's call it S_new, and increment N_iter++

(4) set $P = min(1, e^{\frac{-\triangle E}{T}})$, where $\triangle E = E(S\_new) - E(S\_current)$, and T the current temperature, generate a random number r between 0 and 1:

(4.1) if $r < P$, we set the $S\_current = S\_new$, and increment $N\_accept++$

(4.2) if $r > P$, we keen our current state

(5) check if we are at an equilibrium state. We are at an equilibrium state if either $N\_accept = 12 * n$ or $N\_iter = 100 * n$

(6) check if the system is frozen. A system is frozen if for the last three temperature changes there were no energy improvements

(7) **Temperature Reduction:** Use the following simple rule:

$$T_{k+1} = 0.9 T_k$$

The current state at the last step -> is the one we return

Metropolis rule:

(4) set $P = min(1, e^{\frac{-\triangle E}{T}})$, where $\triangle E = E(S\_new) - E(S\_current)$, and T the current temperature, generate a random number r between 0 and 1:

(4.1) if $r < P$, we set the $S\_current = S\_new$, and increment $N\_accept++$

(4.2) if $r > P$, we keen our current state

The metropolis rule makes sure we always accept a lower energy state:

- Because: E(S_new) – E(S_curr) < 0 => E(S_new) < E(S_curr)
- And when E(S_new) – E(S_curr) < 0 => P = 1, we accept the new state with probability P=1

If the state is of worse energy:

- Because: E(S_new) – E(S_curr) > 0 => E(S_new) > E(S_curr)
- Then there is a chance we accept it still, the higher the temperature, the higher chance to accepting it