

Metropolis Monte Carlo

Simulates Location of Ions

both the mean and the variance

- 1) Start with Configuration A , with computed energy E_A
- 2) Move an ion to location B , with computed energy E_B
- 3) If spheres do not overlap, energy is 0.
If sphere overlap energy is ∞ .
- 4) If $E_B < E_A$: accept the new configuration.
- 5) If $E_B > E_A$: accept the new configuration

with probability $\exp\{-(E_B - E_A)/k_B T\}$

Key idea

Instead of choosing configurations from uniform distribution, then weighting them with $\exp(-E/k_B T)$, MMC chooses them with a Boltzmann probability and weights them evenly