

PHYS 516: Methods of Computational Physics
ASSIGNMENT 1- Writing like a Computational Scientist

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1 Part 1- Theoretical Foundation of Metropolis Foundation

Consider a set of N states, $\Gamma_1, \Gamma_2, \dots, \Gamma_N$ and let the probability to find the system in the m -th state, Γ_m , be ρ_m . Prove that the probability distribution is a fixed point of the metropolis transition matrix defined below, i.e., $\Pi\rho = \rho$.

$$(\text{Metropolis transition matrix})\pi_{mn} = \begin{cases} \alpha_{mn} & \rho_m \geq \rho_n, m \neq n \\ \frac{\rho_m}{\rho_n} \alpha_{mn} & \rho_m < \rho_n, m \neq n \\ 1 - \sum_{m' \neq n} \pi_{m'n} & m = n \end{cases}$$

Here, π_{mn} are elements of the matrix Π , ρ_m are the elements of vector ρ , and α_{mn} are elements of a symmetric attempt matrix, i.e., $\alpha_{mn} = \alpha_{nm}$.

2 Solution