PHYS516 ASSIGNMENT 7 — RANDOM WALK AND POISSON PROCESS

Due: Monday, April 26, 2021

The purpose of this assignment is to gain hands-on experience in stochastic simulations based on random walks and Poisson processes.

Assignment: Submit answers to ONE of the following three Monte Carlo (MC) simulations — (I) stock price; (II) quantum MC; and (III) kinetic MC.

Part I — Stock-Price Simulation

1. Write a program that performs MC simulations of a stock price, S, as a function of time, t, assuming that S follows a discrete stochastic equation,
$$dS = \mu S dt + \sigma S \varepsilon \sqrt{dt},$$
where dt is the time discretization unit and ε is a random variable following the normal distribution with unit variance (*cf.* the Box-Muller algorithm in assignment 2). If the stock price becomes 0, let us assume that the company is bankrupt and you have lost all your investment.

2. Let us measure the time in years, and choose dt = 0.00274 year (~ 1 day). Suppose that the expected return from the stock is 14% per annum (μ = 0.14) and the standard deviation of the return is 20% per annum (σ = 0.20). Starting stock price is \$20.0. Run MC simulations for 1 year (365 steps). Plot the stock price as a function of time.

3. Repeat MC simulations 1,000 times with the same parameters but with different random-number seeds. Plot the distribution of the stock price at step 365.

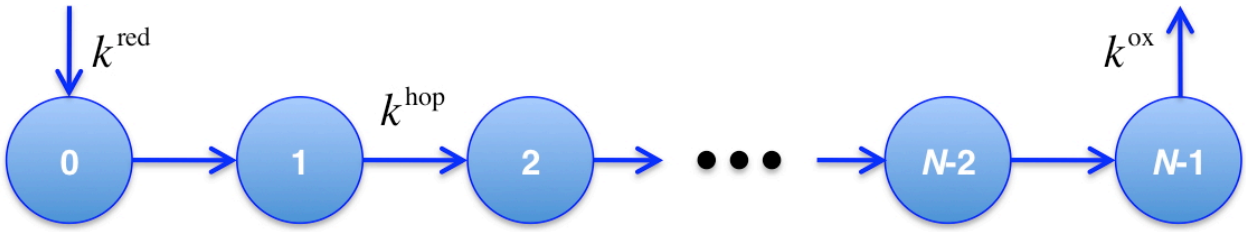
Part II — Quantum Monte Carlo Simulation

1. Write a program that performs diffusion quantum Monte Carlo (QMC) simulation of a one-dimensional electron wave function in a harmonic potential, $V(x) = x^2/2$ (in the atomic unit) following the lecture note on "Quantum Monte Carlo simulation".

2. Run the program for the initial number of walkers N_0 = 50, unit random-walk length ds = 0.1, and the number of Monte Carlo steps per walker *mcs* = 500, and plot the resulting histogram of random walkers. Before the *mcs* MC steps, you perform *nequil* = 0.4×500 = 200 MC steps to equilibrate random walkers but do not include the equilibration MC steps in the histogram.

Part III — Kinetic Monte Carlo Simulation

1. Write a program that performs kinetic Monte Carlo (KMC) simulation of electron transfer on a one-dimensional chain of redox molecules as an asymmetric simple exclusion process, following the lecture slides on "Kinetic Monte Carlo Simulation of Electron Transfer."



2. Run the program for the number of molecules $N = 20$, the electron hopping rate $k^{hop} = 10^9$ s^{-1}, and the number of KMC steps $Max\_step = 10^6$. Run two simulations with the reduction and oxidation rates, $(k^{red}, k^{ox}) = (1\times10^7$ s^{-1}, 2×10^7 s^{-1}) and (2×10^7 s^{-1}, 1×10^7 s^{-1}). For each of the two simulations, plot the occupation $occ(i)$ averaged over all KMC steps as a function of the molecular ID i ($i \in [0, N\text{-}1]$).

Submit your source code and the plot for the simulation of your choice.