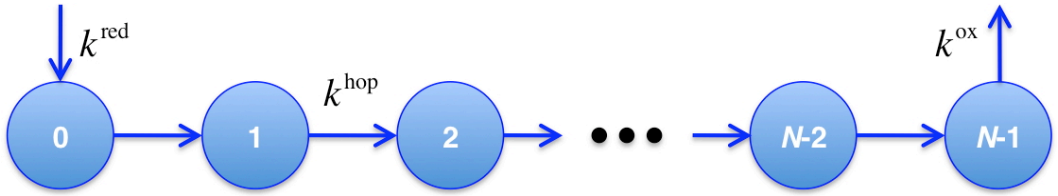
PHYS516 ASSIGNMENT 6—KINETIC MONTE CARLO SIMULATION

Due: Monday, April 18, 2016

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 as well as the plots.