BEBI5009 Homework4

Due 12/01/2016: before class(9:10am)

1. Consider the reaction network

$$A \xrightarrow{k_1} B + C \qquad\qquad B + C \xrightarrow{k_{-1}} A$$

(a) Suppose that the system starts with two molecules of A, one molecule of B, and no molecules of C, that is $(N_A, N_B, N_C) = (2, 1, 0)$. Determine the set of possible states the system can adopt and write the chemical master equation that describes the corresponding probability distribution.

(b) Take $k_1 = 1$ (time^{-1}) and $k_{-1} = 1$ (time^{-1}), and solve for the steady-state probability distribution.

(c) Simulate sample paths of N_A, N_B, and N_C using stochastic simulation algorithm (SSA).
Set the initial condition of N_A, N_B, and N_C=(2,1,0) or (10, 5, 0) or (100, 50, 0)
R1: A → B+C propensity: $k_1 N_A$
R2: B+C → A propensity $k_{-1} N_B N_C$

Note1: To calculate the waiting time, you will need to generate values of a random variable distributed according to an exponential distribution.
You could simply generate a random variable U drawn from the uniform distribution on the unit interval (0, 1), and $T=-\ln(U)/\lambda$ will be an exponential random variable, where λ is the rate parameter of the exponential distribution. In this example, λ would be the sum of the reaction propensities.
Another way to generate exponential random number is to use Matlab function **exprnd(μ)**, where μ is the mean of the exponential distribution $\mu=1/\lambda$.

Note2: You might need to change the value of k_1 and k_{-1} for different initial conditions due to the volume changes. Use (k_1, k_{-1}) = (1,1), (1, 1/5) and (1, 1/50) (time^{-1}) for I.C.= (2,1,0) , (10, 5, 0) , and (100, 50, 0).

(d) Set the initial condition of N_A, N_B, and N_C=(2, 1, 0). Analyzed the statistics of your ensemble, and compare to the steady state probability distribution in (b).

(e) Write down a deterministic model for the chemical reaction following the mass action law. Simulate the concentration changes of A, B C with the parameter $k_1 = 1$ (s^{-1}) and $k_{-1} = 1$ ($mM^{-1}\ s^{-1}$). Set initial concentrations [A],[B],[C] as 2,1, and 0mM. Compare simulation results in (c).