Mathematical Biology, *Kazanci*

Homework Assignment 4 *(due 4/16/09)*

1. Consider the reaction system

$$A + B \rightleftharpoons C$$

with initial conditions $A = XY$, $B = 50$, $C = 0$ and reaction rates $k_1 = 0.1$, $k_2 = 1$ where XY are the last two digits of your uga-ID (810-??-??XX). Codes for simulating this reaction system using three different stochastic methods are given on the course website.

   (a) Modify langevinODE.m to create a code that uses Euler method (deterministic, ODE) to simulate this reaction system, named eulerABC.m. Find the steady state values for A, B and C using this ODE simulation. Replace the initial conditions in all four codes with these steady state values. With these new initial conditions, you should get straight lines (for concentrations) for ODE, and noisy lines for stochastic simulations. Run all four codes (with the new initial conditions), print and hand-in a graph for each of them.

   (b) Note that if you run the stochastic simulations long enough, their mean should give you the steady state values; and the variations should be roughly equal. To verify this result, add a line to print the mean and the variance of the concentration of molecule C in the three codes based on stochastic methods. Run and print the mean and variance for each stochastic method. Write your observations.

   (c) Now increase *time* from 2 to 40 and repeat part (b). How close are the mean and variances? Compare the efficiency of the three stochastic methods.

   (d) Write down the advantages and disadvantages of each stochastic method.

2. Consider the following chemical reaction system (Lotka):

$$\begin{aligned} R + A &\rightarrow 2A \quad k_1 \\ A + B &\rightarrow 2B \quad k_2 \\ B &\rightarrow P \quad k_3 \end{aligned}$$

Amount of molecule R is kept constant in the following reaction system, and P is the product. The rates are given as $k_1[R] = 5$, $k_2 = 0.1$ and $k_3 = 5$.

   (a) Derive the ODE for this system. Find all fixed points and analyze their stability.

   (b) Modify all four codes to simulate this reaction system. Let initial conditions be $A = 30$, $B = 30$ and choose appropriate step-lengths. Print the codes, and two plots for each method: temporal evolution ($A$and B vs $time$) and state space (A vs B). E-mail -mail only the codes to `caner@uga.edu`. [1]

[1] Your HW should contain 4 graphs and 4 codes for 1(a), and 8 graphs and 4 codes for 2(b). Please organize your HW clearly, title each graph and do not include extra codes/graphs. Please e-mail only the codes for 2(b) to `caner@uga.edu`.