Homework for Yang Cao's Section

due on Oct 13th, 2011

1. Consider a set of chemical reactions given below

$$\begin{aligned} \emptyset &\xrightarrow{c_0} S_1 \\ S_1 &\xrightarrow{c_1} \emptyset \\ S_1 + S_1 &\underset{c_3}{\overset{c_2}{\rightleftharpoons}} S_2 \\ S_2 &\xrightarrow{c_4} \emptyset. \end{aligned} \tag{1}$$

   Write down the reaction rate equations. Describe what will happen when time goes to ∞. Verify your description by showing a solution trajectory of this system in Matlab from $t = 0$ to $t = 10$ with the following parameters:

$$c_0 = 1000, \quad c_1 = 1, \quad c_2 = 0.002, \quad c_3 = 0.5, \quad c_4 = 0.04,$$

   and initial state $x_1(0) = 10,000$, $x_2(0) = 0$.

2. **The Brusselator.** The following hypothetical reaction mechanism was first proposed by Prigogine and Lefever, working in Brussels in 1968:

$$\begin{aligned} A &\longrightarrow X \\ B + X &\longrightarrow Y + D \\ 2X + Y &\longrightarrow 3X \\ X &\longrightarrow E \end{aligned} \tag{2}$$

   It is assumed that the concentrations of A, B, D and E are kept artificially constant, so that only X and Y vary with time.

   (a) Using the law of mass action, write the kinetic equations for $d[X]/dt$ and $d[Y]/dt$.

   (b) Let $x = [X]/X_0$, $y = [Y]/Y_0$, $\tau = t/t_0$. Choose X_0, Y_0, t_0 so that

$$\frac{dx}{d\tau} = \alpha - (\beta + 1)x + x^2 y, \quad \frac{dy}{d\tau} = \beta x - x^2 y. \tag{3}$$

   (c) Draw phase plane portraits for $\alpha = 1$ and $\beta = 1, 2, 3$.

3. **Schlögl model.** The Schlögl model is famous for its bistable steady-state distribution. The reactions are

$$\begin{aligned} B_1 + 2X &\underset{c_2}{\overset{c_1}{\rightleftharpoons}} 3X, \\ B_2 &\underset{c_4}{\overset{c_3}{\rightleftharpoons}} X, \end{aligned} \tag{4}$$

where B_1 and B_2 denote buffered species whose respective molecular populations N_1 and N_2 are assumed to remain essentially constant over the time interval of interest. There is only one time-varying species, X; the state change vectors are $v_1 = v_3 = 1$, $v_2 = v_4 = -1$; and the propensity functions are

$$\begin{aligned} a_1(x) &= \tfrac{c_1}{2} N_1 x(x-1), \\ a_2(x) &= \tfrac{c_2}{6} x(x-1)(x-2), \\ a_3(x) &= c_3 N_2, \\ a_4(x) &= c_4 x. \end{aligned} \tag{5}$$

For some values of the parameters this model has two stable states, and that is the case for the parameter values we have chosen here:

$$\begin{gathered} c_1 = 3\times 10^{-7}, \quad c_2 = 10^{-4}, \quad c_3 = 10^{-3}, \quad c_4 = 3.5, \\ N_1 = 1\times 10^5, \quad N_2 = 2\times 10^5. \end{gathered} \tag{6}$$

In the following questions, we assume the initial condition is at $X(0) = 250$.

(a) Write down the Chemical Master Equation for the model.

(b) Write down the reaction rate equations and simulate the equation in matlab.

(c) Write a program to run the SSA simulation and compare the result with the reaction rate equations result. You need to show at least five different trajectories.

4. The Lotka-Volterra system consists of three reaction channels and two species:

$$\begin{aligned} S_1 &\xrightarrow{c_1} S_1 + S_1, \\ S_1 + S_2 &\xrightarrow{c_2} S_2 + S_2, \\ S_2 &\xrightarrow{c_3} \mathit{Decayed}. \end{aligned} \tag{7}$$

with rate constants: $c_1 = 10,\ c_2 = 0.01,\ c_3 = 10$ and initial conditions $x_1(0) = x_2(0) = 1000$. Write down the reaction rate equations and simulate the equation in matlab. Write a program to run the SSA simulation and compare the result with the reaction rate equation result.