

# Homework for Yang Cao's Section

due on Oct 13th, 2011

1. Consider a set of chemical reactions given below



Write down the reaction rate equations. Describe what will happen when time goes to  $\infty$ . 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:



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

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

- (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



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

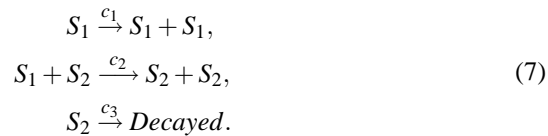
$$\begin{aligned} a_1(x) &= \frac{c_1}{2} N_1 x(x-1), \\ a_2(x) &= \frac{c_2}{6} x(x-1)(x-2), \\ a_3(x) &= c_3 N_2, \\ a_4(x) &= c_4 x. \end{aligned} \quad (5)$$

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:

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

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

- Write down the Chemical Master Equation for the model.
  - 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 equations result. You need to show at least five different trajectories.
4. The Lotka-Volterra system consists of three reaction channels and two species:



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.