Chemistry 5850 Summer 2004 Assignment 12

Weight of this assignment: 58 marks

1. The Lotka-Volterra model has been given both chemical and population dynamics interpretations. It consists of the following mass-action steps:

$$\mathrm{R} \xrightarrow{k_r} a\mathrm{R} \qquad \mathrm{R} + \mathrm{F} \xrightarrow{k_e} b\mathrm{F} \qquad \mathrm{F} \xrightarrow{k_d}$$

   The first step describes the net reproductive rate of a prey population (e.g. rabbits). In the second reaction, the prey are eaten by the predators (e.g. foxes), which supports an increase in the predator population. In the absence of prey, the predators die (third reaction).

   The differential equations for this model can be written in the dimensionless form

$$\dot{r} = r(1-f), \qquad \dot{f} = \mu f(r-1).$$

   (a) Carry out a linearized stability analysis of this model in the absence of diffusion. [5 marks]

   (b) Show that

$$\chi = \mu \ln r + \ln f - \mu r - f$$

   is a first integral. Conclude that the system displays conservative oscillations. [3 marks]

   (c) Add diffusion terms to the Lotka-Volterra equations. (Don't forget to set one of the diffusion constants to 1 to get a dimensionless form.) Carry out a stability analysis of this model. Do the diffusion terms alter the stability in any way? [20 marks]

2. Our analysis of the Brusselator with diffusion separates the behavior into three regions:

   (a) a region in which we expect to see a stable homogeneous steady state,

   (b) a region in which we expect to see limit-cycle-like behavior, and

   (c) a region in which we expect to see Turing patterns.

   Using `xpp`, carry out a simulation in each of these three regions. Show your results in the form of a space-time plot. Also attach a copy of your `xpp` input file to your report. [30 marks]

   Hints: You probably won't get anything sensible unless you use initial conditions which are nonuniform. Start by playing around with the Brusselator without diffusion to get a sense of the time scale of the oscillations. This will give you some idea of how long to integrate for. One or two hundred mesh points should be enough. However, the smaller you make Δx, the smaller you also need Δt to be, so don't go overboard. The value of Δx to choose or, equivalently, of the size of the simulation domain, is a tricky issue, but quite important in the Turing regime. Once you have picked values of a, b and D, go back to the equation involving k which determines the Turing bifurcation condition, and find a value of k such that the inequality is obeyed. The wavelength corresponding to this k is $2\pi/k$. Pick a size for your simulation domain which is 5–10 times larger than the wavelength.

Terry will be delivering a lecture as part of his course requirement next Thursday, July 29. The final test will be on Tuesday, August 3. To accommodate both Terry's lecture preparation and your studying, the return date for this assignment will therefore be flexible. You can turn it in anytime up to 5:00 p.m. on Thursday, August 5. I will even accept solutions to individual questions submitted at different times. If you turn in a solution before the test, I will return your marked question within one business day. If you turn in solutions sufficiently early, you will therefore be able to see my comments before the test. On the other hand, if you decide that your time is better spent preparing for the test in other ways, you can set the assignment aside until later. I do encourage you to look at the assignment, even if you don't have time to complete it before the test.

The test will again include a mixture of conceptual questions and problems. The balance may be slightly more toward conceptual questions this time than it was last time.