Chemistry 4010 Fall 2019
Final Examination

Time allowed: 3 hours

Marks: 60

Handwritten notes are allowed. No printed or mechanically reproduced materials of any kind are permitted.

Software allowed: text editor, XPPAUT, MAPLE, OCTAVE, calculator. If any other software is found to be in use during this exam, you will receive a grade of zero.

Answers are to be written in the exam booklets provided. If your answer involves the use of software, make sure to describe the calculation, providing a clear outline of the steps as well as the results of key steps. You need not reproduce every command. If the output of a calculation is a graph, you should provide a reasonable sketch of the graph, and label the axes.

Make sure that each answer is clearly marked with the section and question number.

Choice: Several of the sections of this exam give you choices of questions to answer. There is no extra credit for answering more questions than required in a given section. If you attempt more than the required number, make sure it is clear which one(s) I should mark by crossing out extra answers. I will not mark more than the required number of questions in each section.

Similarly, if a question has options, there is no extra credit for doing more work, so don't waste time doing more work than is required for full credit.

Good luck!

1 Answer *one* question in this section.

Value of this section: 5 marks

1. What is a canard explosion? Support your answer with a sketch of the bifurcation diagram of a system with a canard.

2. A Boolean model of a two gene network has the following evolution equations:

$$x_1^{(i+1)} = \text{not } x_2^{(i)}$$
$$x_2^{(i+1)} = \text{not } x_1^{(i)}$$

   (The superscript indices represent the time step. A Boolean network is essentially a map over Boolean variables.)

   Let the state be represented by the binary "word" (or vector, if you prefer) $(x_1 x_2)$. Draw a complete state transition graph. Name the type(s) of attractor of this network.

3. What is a symplectic numerical method? Why are symplectic methods important? Name one method that is symplectic, and one that is not.

2 Answer *one* question in this section.

Value of this section: 5 marks

1. Explain briefly what the time evolution operator of a dynamical system is, and give three properties of this operator.

2. What is a Poisson bracket? What is the Poisson bracket used for?

3. What is Tikhonov's theorem? Make sure to give all relevant conditions.

3 Answer *three* questions in this section.

Value of this section: 30 marks

Note: It is generally unnecessary to rescale equations in this section unless the question specifically requires it.

1. The following is a simple model of a laser:

$$\frac{d\phi}{dt} = G\phi N - k\phi,$$
$$\frac{dN}{dt} = -G\phi N - fN + p.$$

In these equations, ϕ is the number of coherent photons in the laser cavity, and N is the number of excited atoms. The coherent photons add to their number by stimulating coherent emission from excited atoms, the $G\phi N$ term, with G being the laser gain. The $k\phi$ term corresponds to loss of laser photons from various processes, including the laser beam that emerges from the device. The constant p is the "pump strength", i.e. a measure of the rate at which energy is put into the device to excite the atoms, while the fN term corresponds to loss of atomic excitation in collisions or incoherent emission. All of the parameters of this model are positive quantities.

Find all equilibrium points, and carry out a linear stability analysis. Identify any bifurcations discovered.

2. Find the fixed points of the map

$$x_{n+1} = \lambda\sqrt{x_n(1-x_n)}$$

and analyze their stability. Note that only values $0 \leq \lambda \leq 2$ are of interest. (Outside of this range, iterations of this map may generate complex values.)

3. Determine the stability of the equilibrium point of the system

$$\dot{x} = xy,$$
$$\dot{y} = x^2 - y$$

using centre-manifold theory.

4. Determine the stability of the equilibrium point of the exciplex mechanism

$$2\,\mathrm{X} \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} \mathrm{C},$$
$$\mathrm{C} \xrightarrow{k_2} \mathrm{X} + \mathrm{P}$$

by phase-plane analysis.

5. For the chemical system of question 4, obtain a condition for the validity of the steady-state approximation using a scaling argument. Would it generally be possible to design experiments for which this condition would be realized?

4 Answer *two* questions in this section.

Value of this section: 20 marks

1. Calculate the Lyapunov exponent of the map

$$x_{n+1} = \lambda\sqrt{x_n(1-x_n)}$$

when $\lambda = 2$. What can you conclude from the value of the Lyapunov exponent? In your answer, although you do not need to give every command used, make sure to outline the key steps of the calculation.

Note: The following MATLAB/OCTAVE functions may be useful:

`abs()`	absolute value
`log()`	natural logarithm
`mean()`	mean or average

2. The following are dimensionless equations for a simplified form of the Gray-Scott model, a classic chemical oscillator model:

$$\dot{x} = \mu - \kappa x - xy^2,$$
$$\dot{y} = \kappa x + xy^2 - y.$$

Carry out a numerical bifurcation analysis of this model using μ as the control parameter. Make sure to give all details of your calculation (including numerical parameters). Provide a sketch of the bifurcation diagram. Give the value of μ at any bifurcations you find, and identify the type of bifurcation.

Notes and hints: In order to observe oscillations, we must have $\kappa < \frac{1}{8}$, so choose a value of κ accordingly. What equilibrium point(s) does the model have when $\mu = 0$?

3. Lü and Chen have studied the following system:

$$\begin{aligned}\dot{x} &= a(y-x),\\ \dot{y} &= -xz + cy,\\ \dot{z} &= xy - bz.\end{aligned}$$

Chaos is found for a wide range of parameters, in particular $a = 35$, $b = 3$, $c = 20$.

(a) Integrate these equations in XPPAUT. Note that you must use nonzero initial conditions since $(0, 0, 0)$ is an equilibrium point. Find a time step size such that the attractor looks smooth. Sketch the attractor (perhaps in an (x, z) projection) and report the value of the step size you used. [3 marks]

Notes: I want the attractor, and not transient behavior. I don't need a very precise sketch of the attractor.

(b) At these parameters, like the Lorenz attractor, this system has a simple next-amplitude map in the variable z. Compute this map and provide a sketch of your result. [4 marks]

Reminder: After doing the calculation and setting up XPPAUT to display the result, you may need to force a redraw in order to actually see the map.

(c) You can draw next-amplitude maps whenever the time series of a variable has minima and maxima. What would a next-amplitude map for a simple limit cycle look like? What would happen to this map after passing through a period-doubling bifurcation? [3 marks]

Have a pleasant and restful Christmas break.