MATH 319, Fall 2013, Assignment 4

Due date: Friday, October 11

Name (printed): ____________________________

UW Student ID Number: ____________________________

Discussion Section: (circle)

Liu Liu:	**301**	**302**	**303**	**304**
Huanyu Wen:	**305**	**306**	**323**	**324**
Dongfei Pei:	**325**	**326**	**329**	
Kai Hsu:	**327**	**328**		

Instructions

1. Fill out this cover page **completely** and affix it to the front of your submitted assignment.
2. **Staple** your assignment together and answer the questions in the order they appear on the assignment sheet.
3. You are encouraged to collaborate on assignment problems but you must write up your assignment independently. **Copying is strictly forbidden!**

Correctness
/20

Completeness
/5

Total:	/25
Bonus:	/3

Applications, Numerical Methods

Suggested problems:

Section 2.3: 1-5, 13-19
Section 2.7: 1-4, 11-19
Section 8.3: 1-15

Problems for submission:

Section 2.3: 3, 5(a)
Section 2.7: 3(a,b)
Section 8.3: 3(a) (compare with *exact* solution as well)
(Justify your answers for full marks!)

1. Consider the reversible chemical reaction

$$X + Y \underset{\beta}{\overset{\alpha}{\rightleftarrows}} 2X$$

where X and Y are chemical species (i.e. molecules). Assuming the solution is well-stirred, it is reasonable to model the reaction rate by the *law of mass action*, which says the rate of a reaction is proportional to the product of the reactant concentrations. For example, the reaction rate of the forward reaction $X + Y \overset{\alpha}{\to} 2X$ would be $\alpha[X][Y] = \alpha xy$ where α is a proportionality constant. The differential equation governing the concentration of X can then be given by

$$\frac{dx}{dt} = \alpha xy - \beta x^2, \; x(0) = x_0. \tag{1}$$

(*Note:* This equation cannot be solved directly because it depends on a second variable, y, which depends on t.)

(a) Note that the variables x and y are related by the *conservation* relationship $x + y = C$ (that is to say, the total amount of X and Y remains constant over time). Use this relationship to rewrite the RHS of (1) so that it only depends on x (i.e. eliminate y from the equation).

(b) Solve the initial value problem found in part (a) for $x(t)$ with the values $\alpha = \beta = C = x_0 = 1$.

(c) Use the conservation relationship to solve for $y(t)$.

(d) Describe the long-term behavior of $x(t)$ and $y(t)$. How does this depend on the initial conditions? Does this make sense in the context of the physical problem? (*Hint:* Note that the initial conditions are related by $x_0 + y_0 = C$.)

2. Consider the irreversible chemical reaction

$$X \rightarrow Y$$

subject to continuous inflow and outflow of X and Y (constant inflow can be modeled by a constant, while outflow is typically assumed to be proportional to the current concentration, x or y, respectively). This can be modeled by the *system* of first-order differential equations

$$\begin{aligned} \frac{dx}{dt} &= \alpha - \beta x, \qquad & x(0) = x_0 \\ \frac{dy}{dt} &= \gamma + \delta x - \eta y, \qquad & y(0) = y_0 \end{aligned}$$

where $\alpha, \beta, \gamma, \delta, \eta > 0$ are constants. (*Note:* Positive signs corresponds to terms of inflow, while negative signs correspond to terms of outflow.)

(a) Solve this differential equation for the parameter values $\alpha = \beta = \gamma = \delta = 1$, $\eta = 2$, $x_0 = 0$ and $y_0 = 1$. [**Hint:** Solve the equation for x first, and then substitute it into the equation for y.]

(b) What are the limiting values (i.e. $t \rightarrow \infty$) of the concentrations?

Bonus! Adapt the MATLAB code given online to perform the forward Euler method for the system in Question #2(a) with $\Delta t = 0.1$ and $\Delta t = 0.01$ over the range $t = 0$ to $t = 5$. Print off the results of the numerical simulations of both the x and y variables. Also include plots of the real solutions found in Question # 2(a), for comparison. *Note:* You will need to modify the code to keep track of *two* independent variables, x and y, which both depend on t. In general, for a system of two variables

$$\begin{aligned} \frac{dx}{dt} &= f_1(x, y, t) \\ \frac{dy}{dt} &= f_2(x, y, t) \end{aligned}$$

the forward Euler method is given by

$$\begin{aligned} x_{n+1} &= x_n + f_1(x_n, y_n, t_n)\Delta t \\ y_{n+1} &= y_n + f_2(x_n, y_n, t_n)\Delta t \\ t_{n+1} &= t_n + \Delta t. \end{aligned}$$