

# Bioengineering 499C: Systems and Synthetic Biology

April 15, 2008

Homework Assignment #2A

Due: 22<sup>th</sup> April 2008

Points awarded for each question are indicated in square brackets. Return assignment with your name clearly indicated at the top of your answer sheet. [Total points: 50]

## [10] Question 1.

Consider the simple differential equation:

$$\frac{dy}{dt} = -20y$$

For reference, the analytical solution to this equation is given by:

$$y = y_0 e^{-20t}$$

Where  $y_0$  is the value of  $y$  at time = 0.

Solve the above differential equation using the Euler method and compare your numerical solution to the analytical one.

Use an initial condition,  $y(0) = 1$  and simulate from  $t = 0$  to  $t = 1.0$ .

Study the effect of varying the step size  $h$  on the nature of the solution. Try  $h = 0.01$ ;  $h = 0.05$ ;  $h = 0.06$ ;  $h = 0.09$ ; and  $h = 0.11$ . Explain why the solution becomes progressively unstable at higher steps sizes

Without changing the Euler method itself, suggest a strategy that you could use to ensure that the solution you get resembles the true solution.

## [20] Question 2.

The Lorenz attractor is a very simple differential equation model that describes convection in the atmosphere. The model exhibits very complex chaotic behavior and is a model that can be used to test differential equation solvers.

Use the Euler method to solve the set of equations that describes the Lorenz attractor.

$$\frac{dx}{dt} = 10(y - x)$$

$$\frac{dy}{dt} = x(28 - z) - y$$

$$\frac{dz}{dt} = xy - \frac{8z}{3}$$

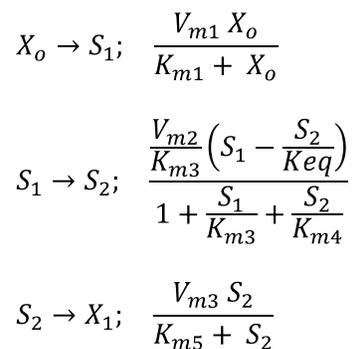
Set the initial conditions for the simulation to  $x = 0.1$ ;  $y = 0.1$ ; and  $z = 0.1$ . Plot the trajectories of  $x$ ,  $y$ , and  $z$  versus time. Use a time range from 0 to 40.

[20] **Question 3.**

There are many packages now available that provide built-in support for solving differential equations. For many projects later in the term, we will be using a package called Jarnac, an application that is part of the SBW suite of software. The advantage to using Jarnac over something like Matlab or R, is that Jarnac will accept models described as a list of reactions and corresponding rate laws from which it will automatically generate the differential equations. This reduces the likelihood of introducing errors and allows models to be very quickly prototyped for testing.

You can obtain a copy of SBW from [www.sys-bio.org](http://www.sys-bio.org). Scroll part of the way down the screen until you see the download section.

Using the Jarnac usage notes provided on the 499 Wiki, enter the following model into Jarnac and use it to carry out a time course simulation.



The text format for the model is given below (cut and paste as needed):

```
$Xo -> S1; Vm1*Xo/(Km1 + Xo);  
S1 -> S2; (Vm2/Km3)*(S1 - S2/Keq2)/(1 + S1/Km3 + S2/Km4);  
S2 -> $X1; Vm3*S2/(Km5 + S2);
```

Let  $X_o$  and  $X_1$  be boundary species. Let  $S_1$  and  $S_2$  be state variables, that is species that are allowed to change during the simulation. Set  $X_1 = 0$  and  $X_o = 6$ . Set the kinetic constants to:

$$V_{m1} = 3; \quad K_{m1} = 0.4; V_{m2} = 2; \quad K_{m3} = 0.23; K_{m4} = 0.77; Keq = 6.7; V_{m3} = 7.8; \quad K_{m5} = 1.2$$

Carry out a time course simulation for  $t = 0$  to 10 time units. Plot  $S_1$  and  $S_2$  against time. Increase the  $V_{max}$  of the second enzyme to 5.0. Carry out the simulation again and plot the same variables again.

You will observe a marked difference in behavior between the two simulations. Explain this difference using your knowledge of enzyme kinetics.

Footnote: If you would like a Matlab function of the model, run the model first to load it into the Jarnac memory then go to the SBW menu and select Translate Any and pick the Matlab translation.