Molecular and Neural Computation (CSE P 590) Homework 3

1. Mass Action Kinetics

For the following two chemical reaction networks, write down the mass action kinetics. Note that the symbol \emptyset is used to denote spontaneous creation or degradation into untracked waste, and you do not need to write a differential equation describing its dynamics. When \emptyset appears as a reactant, the rate of production of the products is simply the rate of the reaction (as though the "species" \emptyset is at a constant concentration of 1). When \emptyset appears as a product, the reactants disappear and nothing is produced.

a.

$$\emptyset \xrightarrow{k_1} A$$

$$A \xrightarrow{k_2} \emptyset$$

b.

Rabbit
$$\xrightarrow{\alpha}$$
 2 Rabbit Rabbit + Fox $\xrightarrow{\beta}$ 2 Fox Fox $\xrightarrow{\gamma}$ \emptyset

c. Write a chemical reaction network with species X, Y, and Z, and reaction rates k_1 , k_2 , k_3 , and k_4 , that has the following mass action kinetics:

$$\frac{d}{dt}[X] = k_5 - [X](k_1[Y] + k_4)$$

$$\frac{d}{dt}[Y] = -[Y](k_1[X] + k_2[Z])$$

$$\frac{d}{dt}[Z] = k_1[X][Y] - k_3[Z]^2$$

2. Visual DSD

For this problem, you will use VisualDSD to simulate a reaction network implemented in DNA using strand displacement. The VisualDSD tutorial, user manual, and simulation environment can be found here: http://research.microsoft.com/en-us/projects/dna/.

- a. Simulate the two-gate cascade illustrated on page 11 of the Module 5 slides in VisualDSD. Use default parameters for binding and unbinding rates. Initialize your system with the following species counts:
 - *Gate* = 100 and *Input* = 50
 - Gate = 1000 and Input = 500

You should turn in your VisualDSD code and a screen shot of your plots.

b. **Extra Credit.** Use AND and OR gates from pages 19-36 of the Module 5 slides to implement any two-layer cascaded logic circuit of your choosing. Your circuit should include at least two gates, and have at least two layers. Show that you can generate the truth table for your circuit in VisualDSD. You should turn in your VisualDSD code and a screen shot of your plots.

3. Nano Crafter game

For this problem, go to

http://games.cs.washington.edu/DNA_New/versions/csep590/index.html and play the Nano Crafter DNA game. The aim of Nano Crafter is to introduce basic concepts for engineering chemical reaction networks with DNA. The game is in pre-alpha (*please do not share this link*).

Play as far as you can or want to, and write 1-3 sentences to answer the following questions. We will share your feedback with the Nano Crafter development team.

- 1. What did you like? (give one or two examples)
- 2. What didn't you like? (give one or two examples)
- 3. Were there any levels, aspects of gameplay, or game physics, were particularly confusing?
- 4. Do you feel like this game improved your understanding of DNA strand displacement?
- 5. Was the game fun?