Molecular and Neural Computation (CSE P 590)
Homework 5

1. **Gillespie Algorithm**
   You can find Gillespie's original paper on SSA here:
   http://pubs.acs.org/doi/pdf/10.1021/j100540a008

   a. Using your favorite programming language (MATLAB, Mathematica, Python, R, C++, …), implement SSA for the reactions in Equations 38a-c in Gillespie's paper. Use the reaction rates and initial conditions described in Figure 8 to produce a plot similar to Figure 8a.
   Note: In Equation 38a, $\bar{X}$ is assumed to be constant over time. Equivalently, you can consider the reaction in Equation 38a to be the following unimolecular reaction,

   $$Y_1 \xrightarrow{\bar{X}\cdot c_1} 2Y_1$$

   b. The following reaction is a course grained model for protein production and degradation:

   $$\emptyset \xrightarrow{1.5} A \xrightarrow{0.075} \emptyset$$

   Implement SSA for this reaction starting with [A]=0. Simulate the system from time t=0 to time t=100. Repeat the simulation 50 times, and compute the mean and variance at times t=0,1,2,…,100. On a single graph, plot:
   - A few stochastic trajectories of your choice.
   - The mean trajectory
   - The mean trajectory ±1 standard deviation
   - The expected number of [A] computed from mass action kinetics

   c. ***Extra Credit.*** Tau-leaping and the Gibson & Bruck are faster methods for stochastic simulation. Choose one of these methods to implement, and simulate the system from part (a).

2. **gro**
   Download gro here:
   http://depts.washington.edu/soslab/gro/

   In the examples directory you'll find a program "chemotaxis.gro". Run the example, and make the following modifications:
   - Remove the signal from the center of the screen (e.g. set *true* to *false* in the main loop).
   - Add a new cell state variable *emit* to *program p()*.
   - Add guarded commands that encode the following behaviors:

- While *emit*=1, the cell should be green and emit signal *s* at a dose of 50.
- While *emit*=0, the cell should not be green, and should not emit signal *s*.
- Non-emitting cells should become emitting cells at some small rate (e.g. 0.0001).
- Emitting cells should be come non-emitting at some small rate (e.g. 0.001).

Play with the rate parameters. In a few sentences, describe what the system does. Turn in your gro code.

3. **Pattern Formation Review**
   You might find the UW Proxy Bookmarklet useful for this review:
   http://www.lib.washington.edu/help/proxyTools.html

   Search google scholar (or select from the list below) for an article involving cellular pattern formation that interests you. Summarize the results of the research, why you find it interesting, and suggest some ways you might use the technology. Make a concise summary (approximately half a page).

   Here are some papers to get you started:

   - *An Externally Tunable Band Pass Filter* (Sohka et al., 2006) http://www.pnas.org/content/early/2009/06/04/0901246106
   - *A Synthetic Genetic Edge Detection Program* (Tabor et al., 2009) http://www.cell.com/abstract/S0092-8674(09)00509-1
   - *A synchronized quorum of genetic clocks* (Danino et al., 2010) http://www.nature.com/nature/journal/v463/n7279/full/nature08753.html
   - *Sequential Establishment of Stripe Patterns in an Expanding Cell Population* (Liu et al., 2011). http://www.sciencemag.org/content/334/6053/238.abstract