Biological Computation 20.181
Homework 11

Note: If your grade on this assignment increases your HW average then it will be weighted as two assignments, otherwise it will be weighted as a single assignment.

Part 1. Accompanying this assignment is some python code that implements an incomplete version of Mike Gibson's "Next Reaction Method" for computing the exact behavior of discrete chemical systems (nextrxn.py). To complete the program you'll need to add a small bit of code that computes the updated time for reactions whose substrate abundances change in response to the execution of another reaction. The needed formula is:

t_new = (a_old/a_new)*(t_old-t_current)+t_current

where,
t_new is the updated reaction time,
t_old is the old reaction time
a_old is the old reaction propensity,
a_new is the new reaction propensity, and
t_current is the current system time.

(Note: Variable names provided above are not the *exact* ones used in the code.)

Part 2. Take a look at the two input files (switch.rxns and switch.spcs); these files define a simple bistable switch device [a switch is a device that stores information in one of two (or more) states]. Complete the switch.rxns input file by adding rate propensities, **c**, for all second order reactions as being near the diffusion limit, converting from a bulk second-order binding rate of 1E9/M/sec. You'll need to use a system volume of 1E-15L.

Parts 3. Use your completed Next Reaction solver to compute the expected behavior of the bistable switch for 15 minutes of simulated time. Plot the output.

Bonus. If your bistable switch system starts in a HIGH A / LOW B state, will the system remain in this state forever? Why or why not?