1. Consider the following reaction:

$$A \rightleftharpoons_{k=}^{k+} B$$

What is the probability that:

- (a) A molecule of A becomes B over a short time step  $\Delta t$ ?
- (b) A molecule of A remains A over the time step?
- (c) A molecule of B becomes A over the time step?
- (d) A molecule of B remains B over the time step?
- 2. Construct an excel spreadsheet that lets you calculate a single "move" for the equations above. However you set it up, make sure that you can easily change: A(t), B(t),  $k_+$ ,  $k_-$  and  $\Delta t$ .
- 3. Start with [A] = 100 and [B] = 0,  $k_+ = 100$   $s^{-1}$  and  $k_- = 100$   $s^{-1}$ . Try values of  $\Delta t$  from 0 to very large.
  - (a) What happens to  $A(t + \Delta t)$  and  $B(t + \Delta t)$  as a function of  $\Delta t$ ?
  - (b) Can you understand what is going on for large  $\Delta t$ ?
  - (c) What is a "resonable" value of  $\Delta t$  for your analysis?
- 4. Choose a "reasonable" value for  $\Delta t$  from your analysis above.
  - (a) What happens to the concentration of A and B?
  - (b) Does this make sense, chemically?
  - (c) What is the value of A(t) + B(t) and  $A(t + \Delta t) + B(t + \Delta t)$ ?
  - (d) What physical property of the reaction does this capture?
- 5. Use  $A(t + \Delta t)$  and  $B(t + \Delta t)$  as inputs to the equations.
  - (a) What happens to the concentrations of A and B?
  - (b) What is the sum of the concentrations of A and B?
- 6. Run the equations 15 times, taking the output each time as the input for the next step. Save your values for [A] and [B] at each step. Make a graph of these against step. What do you observe?
- 7. Bonus: Write these equations in *matrix* form.
- 8. Bonus 2: Write a matrix describing

$$A \rightleftharpoons B \rightarrow C$$