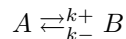


1. Consider the following reaction:



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  $[B] = 0$ ,  $k_+ = 100 \text{ s}^{-1}$  and  $k_- = 100 \text{ s}^{-1}$ . 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 “reasonable” value of  $\Delta t$  for your analysis? Can you come up with a rule-of-thumb for a useful  $\Delta t$ ?
  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. What happens if you set  $k_- = 10 \text{ s}^{-1}$ ? Does this match what you would expect chemically?
  8. Bonus 1: Write these equations in *matrix* form.
  9. Bonus 2: Write a matrix describing

