CR11: first assessment

Deadline: 1st November
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1 Binding equilibrium

Consider the system $A + B \rightleftharpoons AB$ discussed in class.

Question 1. Rewrite the simulation algorithm so as to implement the 'next reaction' method, *i.e.* at each iteration of the loop, the timer of the reaction that is *not* fired is maintained with an appropriate rescaling.

2 The prozone effect

Let us introduce a new molecule C which can also combine with B according to $B+C \rightleftharpoons BC$. Let us further assume that formation of AB is *independent* of formation of BC. This means that A can also combine with BC to form ABC; and that AB can be combined with C, also forming ABC.

The full system of reactions is:

$$\begin{array}{rcl} A + B & \rightleftharpoons & AB \\ A + BC & \rightleftharpoons & ABC \\ B + C & \rightleftharpoons & BC \\ AB + C & \rightleftharpoons & ABC \end{array}$$

Use $k_f := 0.005$ and $k_b := 0.1$ as the forward and backward rate constants for all the reactions.

Question 2. Write the 'direct method' simulation algorithm for this new system, *i.e.* generating two random numbers per iteration: one to choose the reaction to fire; and the other to choose the time advance.

Question 3. Fix the initial conditions for A and C as $N_A := 1000$ and $N_C := 1000$. Run the system with initial conditions for B as (i) $N_B := 500$; (ii) $N_B := 1000$; and (iii) $N_B := 2000$. (NB: N_{AB}, N_{BC} and N_{ABC} are all initially 0.)

What is (roughly) the *equilibrium* value for N_{ABC} in each of these three cases? Can you explain this result?

Question 4. Let us add one final (irreversible) reaction

$$\rightarrow B$$

with rate constant $k := 0.1$. This reaction introduces a new B *ex nihilo*. Its activity is *state-independent*; its value is always 0.1.

Add this reaction to your simulation algorithm. Starting with $N_B := 0$, verify that the total number of Bs in the system, *i.e.* $B+AB+BC+ABC$, grows linearly with time (it should be roughly $t/10$ since, on average, one B is created every 10 time units).

Plot the total number of Bs [x-axis] vs ABC [y-axis]. What does this curve tell us? Why does this conclusion depend on the rate constant k being reasonably small?