Oberwolfach Seminar
Mathematical Modelling in Systems Biology
Nov 19-25, 2017

Task 1 (Michaelis-Menten kinetics)
The names *Michaelis-Menten* are associated with a system involving four species: a substrate, S, an enzyme, E, a complex, C, and a product, P. The reactions may be written

$$E + S \underset{k_2}{\overset{k_1}{\rightleftharpoons}} C \xrightarrow{k_3} E + P.$$

Overall, the enzyme converts substrate into product. It does this by binding with the substrate to form the enzyme-substrate complex. A molecule of this complex may simply dissociate back into enzyme and product. Or it may dissociate into the product (an altered version of the substrate) and the enzyme. This model rules out the possibility of reversibility – product and enzyme cannot recombine to form the complex. Although simple, the Michaelis-Menten system deals with an extremely important mechanism and hence has been very widely studied.

For the reeaction-rate equations, we use concentration based data

$$\begin{pmatrix} S(0) \\ E(0) \\ C(0) \\ P(0) \end{pmatrix} = \begin{pmatrix} y_1(0) \\ y_2(0) \\ y_3(0) \\ y_4(0) \end{pmatrix} \begin{pmatrix} 5 \cdot 10^{-7} M \\ 2 \cdot 10^{-7} M \\ 0M \\ 0M \end{pmatrix}, k_1 = 10^6, k_2 = 10^{-4},\ k_3 = 10^{-1},$$

within a volume of $vol = 10^{-15}$ litres. This corresponds to molecular data of

$$\begin{pmatrix} X_1(0) \\ X_2(0) \\ X_3(0) \\ X_4(0) \end{pmatrix} = \begin{pmatrix} \lfloor 5 \cdot 10^{-7} n_A\, vol \rfloor \\ \lfloor 2 \cdot 10^{-7} n_A\, vol \rfloor \\ 0 \\ 0 \end{pmatrix}, k_1 = \frac{10^6}{n_A\, vol}, k_2 = 10^{-4},\ k_3 = 10^{-1},$$

where $\lfloor \cdot \rfloor$ denotes rounding to the nearest integer. We will simulate reactions until the time exceeds $t = 50$.

(a) Implement the SSA for this system.
(b) Implement the Euler-Maruyama method on the CLE for the same system, with a stepsize $\tau = 0.2$.
(c) Formulate and solve the RREs. You might need to specify a more stringent absolute tolerance for the ODE solver.
(d) Derive the Michaelis-Menten equations by assuming $C' = 0$ (called *quasi steady state assumption*) and compare the simulation results with the original RRE solution for various values of the reaction rate constants.