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Exercise 2

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Question 1: Slow and Fast Time Scales

In the lecture we encountered the terms slow, fast and relevant time scales and their implications on the numerics. To get a better feeling for that we consider the following simple system, the reversible isomerization reaction: $S_1 \underset{c_2}{\overset{c_1}{\rightleftharpoons}} S_2$, where S_1 and S_2 are the two isomeric species and c_1 and c_2 are the corresponding reaction rates. Let x_T denote the constant total number of molecules of the two species, and $x(t)$ the time-varying number of S_1.

a) Derive the ODE describing the system in terms of $x(t)$ and x_T and solve the system analytically. Assume that $x(0) = x_0$.

b) Let us assume the solution of the ODE is given by

$$x(t) = \frac{c_2 x_T}{c_1 + c_2} + \left(x_0 - \frac{c_2 x_T}{c_1 + c_2} \right) e^{-(c_1+c_2)t}. \tag{1}$$

What is the asymptotic value of this equation? What determines whether this system is considered stiff?

c) Solve the ODE model numerically with the explicit Euler method. Assume that $c_1 = c_2 = 1$, $x_T = 2 \times 10^5$ and $x_0 = 0.8 \times 10^5$. Play with different time step sizes between 0.1 and 1.5. What do you observe? What constraints do you suggest for the time step?

d) Try to derive the general (i.e. independent of concrete values for c_1, c_2, x_T and x_0) stability criterion of the Euler scheme given this system. What is the maximum time step size?
Hint: Define a recurrence formula for the numerical error e_n based on the difference between the Euler scheme and the Taylor expansion about t_{n-1} of the analytical solution of the system, and derive the necessary and sufficient conditions for the convergence of the error.

Question 2: Time Scales in the QS system

Consider the submodel for the binding of LuxR / AHL-n-mer to DNA found in the 2005 draft of the QS model, Section 2.1.

a) Explain the derivation of the binding probability $P(A)$. Are the assumptions on the different time scales reasonable?

b) In the latter part of the section the model is further simplified using time scale arguments. Familiarize yourself with the meaning of the different variables. Why can we discard most of the variables?

Question 3: Flows, Reservoirs and Causality Diagrams of the QS model

In the 2005 draft of the QS model, Section 2.1., the model of the pathway inside the cell is described in great detail.

a) Formulate the pathway model within the cell in terms of reservoirs and flows. Assume polymerization of AHL/LuxR only takes place up to the dimer state (y_2). Draw the causality diagram of the described system.

b) Re-do the exercise for the simplified system in the 2006 publication. What are the key properties that have been conserved between the models?