Simulationstechnik A
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Exercise 3 - Chemical Langevin Equation

For all our exercises, we will consider the following system consisting of substrate S_1, enzyme S_2, complex S_3 and product S_4:

$$S_1 + S_2 \xrightarrow{c_1} S_3$$
$$S_3 \xrightarrow{c_2} S_1 + S_2$$
$$S_3 \xrightarrow{c_3} S_4 + S_2$$

It is often referred to as Michaelis Menten Kinetics and will serve as a manageable system to train techniques and algorithms from the lecture.

1. **From τ-Leaping to the Chemical Langevin Equation (CLE) and beyond**
   For τ-Leaping, the number of triggered reactions is given by a Poisson random variable $\mathcal{P}$.
   a) What happens to a random variable $\mathcal{P}$ that is Poisson-distributed with a very large mean (and equal variance)?
   b) How do you modify the τ-Leaping code in order to create a solver for the CLE?
   c) What do you observe when varying τ?
   d) How could you further modify your code to solve the Reaction Rate Equation (RRE)?
   e) How does the solution look like for different numbers of traces and τ?

2. **An Overview**

	CME	Gillespie	τ-Leaping	CLE	RRE
Overall accuracy					
Approximations (stacked)					
Quality of solution					
Conditions to control the error (stacked)					
Type of solution					
Algorithmic complexity					