mathematik
fakultät8

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)?

   The random variable becomes a normally distributed random variable (and keeps its mean and variance)

   b) How do you modify the τ-Leaping code in order to create a solver for the CLE?

   Exchange the expression that calculates the number of triggered reactions according to Higham.
   Then, introduce a rounding operator that does not change the state but only enables a proper visualization.

   c) What do you observe when varying τ?

   Larger time steps lead to a better approximation!
   This can be explained using the premises needed for CLE: The mean of a Poisson distributed random variable must be large so that it can be properly approximated by a Gaussian random variable. Otherwise the error is very large.

   d) How could you further modify your code to solve the Reaction Rate Equation (RRE)?

   Ignore each of the three random terms when calculating the number of triggered reactions.

e) How does the solution look like for different numbers of traces and τ?

All traces are identical because there is no random behavior implemented at all: We again obtain a deterministic method that only returns one trajectory through state space.

2. An Overview

	CME	Gillespie	τ-Leaping	CLE	RRE
Overall accuracy	very high	high	ok	low	very low
Approximations (stacked)	time discretization	mean of several traces to approximate sol.	several reactions are combined (Poisson) and time steps lengthen	Poisson for large means becomes Gaussian	Ignore the stoch. part completely
Quality of solution	exact sol. for small dt	arbitrarily good approximation of exact solution for many traces	modelling error that can be controlled using small τ	always modelling error	even larger modelling error
Conditions to control the error (stacked)	small dt	many traces	$\frac{da_j(X(t))}{dt}$ small $\forall j$	$a_j(X(t))\tau$ large $\forall j$	just accept the error...
Type of solution	discrete state discrete time deterministic	discrete state discrete time (but no control of dt) stochastic	discrete state discrete time stochastic	continuous state discrete time stochastic	continuous state discrete time deterministic
Algorithmic complexity	very high	high	ok	low	very low