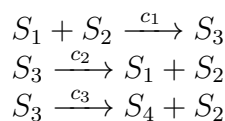


## Exercise 1 - Chemical Master Equation

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



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. **Defining state-transition vectors  $\nu_j$  and the propensity function  $a_j(X(t))$**   
Each chemical reaction  $j$  is defined by a state-transition vector  $\nu_j$  and a propensity function  $a_j(X(t))$  depending on the system state  $X$  at time  $t$ . While the first indicates the change induced by the specific reaction, the latter describes the frequency in which reaction  $j$  is likely to occur.

- a) Determine the state-change vectors  $\nu_1$ ,  $\nu_2$  and  $\nu_3$ .
- b) Determine the propensity functions  $a_1(X(t))$ ,  $a_2(X(t))$  and  $a_3(X(t))$  for a given system state  $X(t)$ .

2. **System reduction**

The system state  $X$  seems to be four-dimensional.

- a) Show, that its actual dimension is lower than that by using conservation laws.
- b) How are  $\nu_j$  and  $a_j(X(t))$   $j = 1, 2, 3$  defined now?

3. **The Chemical Master Equation**

Everything is set up to solve the system now. This actually means that we are interested in knowing the probability  $P(X(t), t)$  of our System being in state  $X(t)$  at time  $t$  for all possible states and times.

- a) Each probability density (and therefore also  $P(X(t), t)$ ) must be normalized. State, how this normalization criterion is mathematically defined for  $P(X(t), t)$ .
- b) Derive the Chemical Master Equation (CME), the differential equation whose solution is  $P(X(t), t)$

#### 4. Implementing the System

We will now implement, solve and visualize the system.

- a) Define the state-transition vectors and propensity functions in the provided code.
- b) How could you solve the CME derived in 3b) numerically? Implement your idea.
- c) Determine the algorithmic complexity of your solution.
- d) How could you visualize the solution  $P(X(t), t)$ ? Implement your idea.