Exercice 3 - Chemical reaction

In this exercie we will modelize the kinetic of chemical reaction. The kinetic of chemical reaction means to follow the concentration of species X_i as function of a time. Let's take the reaction:

$$R_1 : \ X \xrightarrow{c} Z \tag{1}$$

the reaction-rate equation is

$$\frac{dX}{dt} = -cX \tag{2}$$

- give the solution of eq. 2.

Implementation

In the code the values of species concentration are stored in array *ptr_spec. To allocate the memory to this array you need to declare the number of species in input_file by the keyword "species".

You can see that the read_event routine is already write. In event file you will declare two thing:

1. the initial value of species concentration. You declare the keyword "Init_species" following to number of species. The line after used to give the concentration values.
2. The chemical reaction possible in your system. With the keyword "Number_of_reaction" you define the number of reaction... After the "id" reaction you give for each reaction:
   (a) the minimum value for each species you need to make the reaction (initial state)
   (b) The difference between the final and initial state of the number of species
   (c) The rate parameter of the reaction

   To illustrate, let's take the reaction $\overline{X_1} + 2X_2 \rightarrow X_3$, the reaction declaration will be, with the "id":

   1 1 2 0 0 $-$ 2 1 0.02

   we need $1X_1$ and $2X_2$ and the line on X_1 means constante. Then we finish with $-2X_2$ and $1X_3$. The rate parameter is 0.02.

The system will be represented by just one site in which the reaction will occur. In input file you declare a 1D system with 1 site. In the event_rate_calc routine you will store the total rate of the system in array *ptr_rate and the rate of each reaction in *ptr_event_rate. The rate is computed as $h_\mu c_\mu$ where h_μ is the number of molecular reactant combinaisons for reaction R_μ and c_μ is the rate parameter. In the reaction R_1, $h_1 = X$. Warning, the reaction occurs if the initial_state conditions are met.

We will use the First reaction algorithm then in choose_event routine you need to compute the time associate to each reaction as

$$t_\mu = -\frac{\ln(\lambda_\mu)}{r_\mu} \tag{3}$$

where λ_μ is a random number associate to reaction R_μ. Once chosen, in event_applied routine we use the *ptr_f_state array to change the concentration value in *ptr_spec. Simply add for each species i the values of ptr_f_state[i]. Finally in routine analyse we store in ptr_prop[i] the concentration values of specieX_i.

Validation

In first step we will validate the implementation by comparing the result about the reation R_1. Run the simulation for an initial concentration $X_0 = 10000$ and $c_1 = 0.5$. Use "fort.100" to plot in the same graph the concentration as function of time and the solution of the eq. 2. Plot also the standart deviation around the result of the simulaiton $X(t) \pm \Delta(t)$ with

$$\Delta(t) = \left[X_0 e^{-c_1 t}\left(1 - e^{-c_1 t}\right)\right]^{1/2} \tag{4}$$

Appication

- We see now an other group of reaction:

$$\begin{array}{ll} R_1: & \overline{X} + Y \xrightarrow{c_1} 2Y \\ R_2: & 2Y \xrightarrow{c_2} Z \end{array} \tag{5}$$

  We are interesting in the concentration evolution of specie Y. The reaction-rate equation is

$$\frac{\partial Y}{\partial t} = c_1 XY - c_2 Y^2 \tag{6}$$

  this equation have two solution for the steady state $Y_{s1} = 0$ and $Y_{s2} = \frac{c_1}{c_2} X$. We will run the simulation with $c_1 X = 5$ and $c_2 = 0.005$. Find the stable and unstable solution.

In reaction 5 the factor h use to compute the rate of the reaction change. For the reaction R_1, $h_1 = XY$ and for R_2, $h_2 = Y(Y-1)$. **Build a routine which give you the good value of h_i as funciton of chemical reaction.**

- The third group of reaction (Lokta reaction):

$$\begin{array}{ll} R_1: & \overline{X} + Y_1 \xrightarrow{c_1} 2Y_1 \\ R_2: & Y_1 + Y_2 \xrightarrow{c_2} 2Y_2 \\ R_3: & Y_2 \xrightarrow{c_3} Z \end{array} \tag{7}$$

  From these reactions give the reaction-rate equation of species Y_1 and Y_2 and provide the analytic solution. With $c_1 = 0.0001$, $c_2 = 0.01$ and $c_3 = 10$ run the simulation from the steady state. What is the particularity of this group of reactions.