# TP 4 : Kinetic Monte-Carlo ($KMC$)

Cours de modélisation numérique

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## Introduction

In this TP, we will implement the chemical reaction seen as an example during the lessons, trough the *Kinetic Monte-Carlo KMC* method.

## Model

Consider two interacting chemical species $A$ and $B$ of initial quantities $A_0$ and $B_0$, and let the reaction rates be $k_1 \geq 0$ and $k_2 \geq 0$ such that :

$$A \xrightarrow{k_1} B \qquad\qquad B \xrightarrow{k_2} A \tag{1}$$

It can be shown that the evolution of these quantities is given by the following equations :

$$A(t) = \frac{k_2(A_0 + B_0)}{k_1 + k_2} + \frac{A_0 k_1 - B_0 k_2}{k_1 + k_2} e^{-(k_1+k_2)t} \tag{2}$$

$$B(t) = \frac{k_1(A_0 + B_0)}{k_1 + k_2} - \frac{A_0 k_1 - B_0 k_2}{k_1 + k_2} e^{-(k_1+k_2)t} \tag{3}$$

We propose to simulate the evolution of the system using a Monte Carlo method. For this purpose, $A$ and $B$ will be discretised for example in a number of molecules. The algorithm will have to, at each time step $\Delta t$, iterate over the number $N = A + B$ of molecules present in the system and :

— Draw with probability $p(A) = \frac{A}{N}$ a molecule $A$, or $p(B) = \frac{B}{N}$ a molecule $B$.

— If species $A$ is drawn, one carries out reaction $A \to B$ with probability $k_1 \Delta t$.

— If species $B$ is drawn,one carries out reaction $B \to A$ with probability $k_2 \Delta t$.

Note that the choice of parameters must be such that $k_1 \Delta t \leq 1$ and $k_2 \Delta t \leq 1$ are satisfied.

Write a `Python` code implementing this algorithm and test it for different values of $A_0, B_0, k_1, k_2, \Delta t$. You can use the `random.uniform()` function, which returns a random number between 0 and 1.

Compare your results with the expected value for the analytical solution when $t \to \infty$.