

Numerical Solutions

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%%python3

import numpy as np
from scipy.integrate import odeint
import matplotlib.pyplot as plt

def rxn1st(C,t,*k):

    r1=k[0]*C[0] #k[0]*(concentration of A)

    dAdt=-r1 #rate of change of A decreased by forward reaction and increased by reverse
    dBdt=r1 #rate of change of B increased by forward reaction and decreased by reverse

    return(dAdt,dBdt)

t=np.linspace(0,10,101) #the first number is the beginning point, the second number is the ending point
C0=[1,0] #initial concentrations of A and B
k1=1
k2=0
k=[k1]
C=odeint(rxn1st,C0,t,(k1,k2))

cA=C[:,0] #define cA to give the concentration from the first (zeroth) column of the C array
cB=C[:,1] #define cB to give the concentration from the second column of the C array
```

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