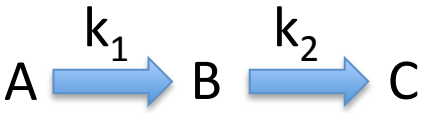
Simple Example: ABC reactor

Importance: This is conceptually what is going on in the more complex software

Substance A becomes B at a rate of k_1 with units of 1/second

Substance B becomes C at a rate of k_2 with units of 1/second



The differential equations that describe the change in concentrations can be expressed as:

$$\frac{dA}{dt} = -k_1 A \qquad \frac{dB}{dt} = k_1 A - k_2 B \qquad \frac{dC}{dt} = k_2 B$$

Here the variables A,B,C represent the concentration of each substance with units of molecules

We can integrate to find a solution using a simple iterative procedure.

```
%Reaction rates
k1 = 1;       k2 = 1;

%Intial concentrations
A = 1;   B=0;    C=0;

%dt is our time-step
dt = 0.01;
time = 0:dt:8;

%Iterative loop
for i=1:length(time)-1
    dAdt = -k1*A(i);
    dBdt = k1*A(i)-k2*B(i);
    dCdt = k2*B(i);
    A = [A   A(i)+dAdt*dt];
    B = [B   B(i)+dBdt*dt];
    C = [C   C(i)+dCdt*dt];
end
```

Here we calculate the values from the above equations

Here we add the value of substance at next time-step to the list