

Simple Example: ABC reactor

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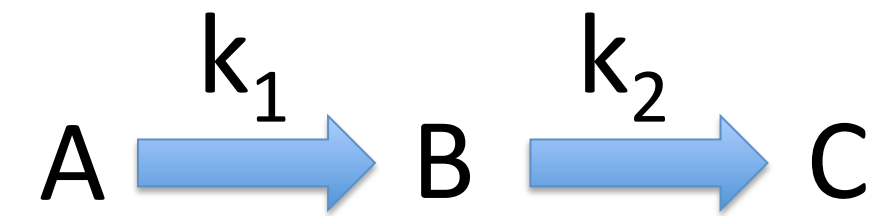
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Simple Example: ABC reactor

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:

$$\frac{dA}{dt} = -k_1 A$$

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

$$\frac{dC}{dt} = k_2 B$$

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;

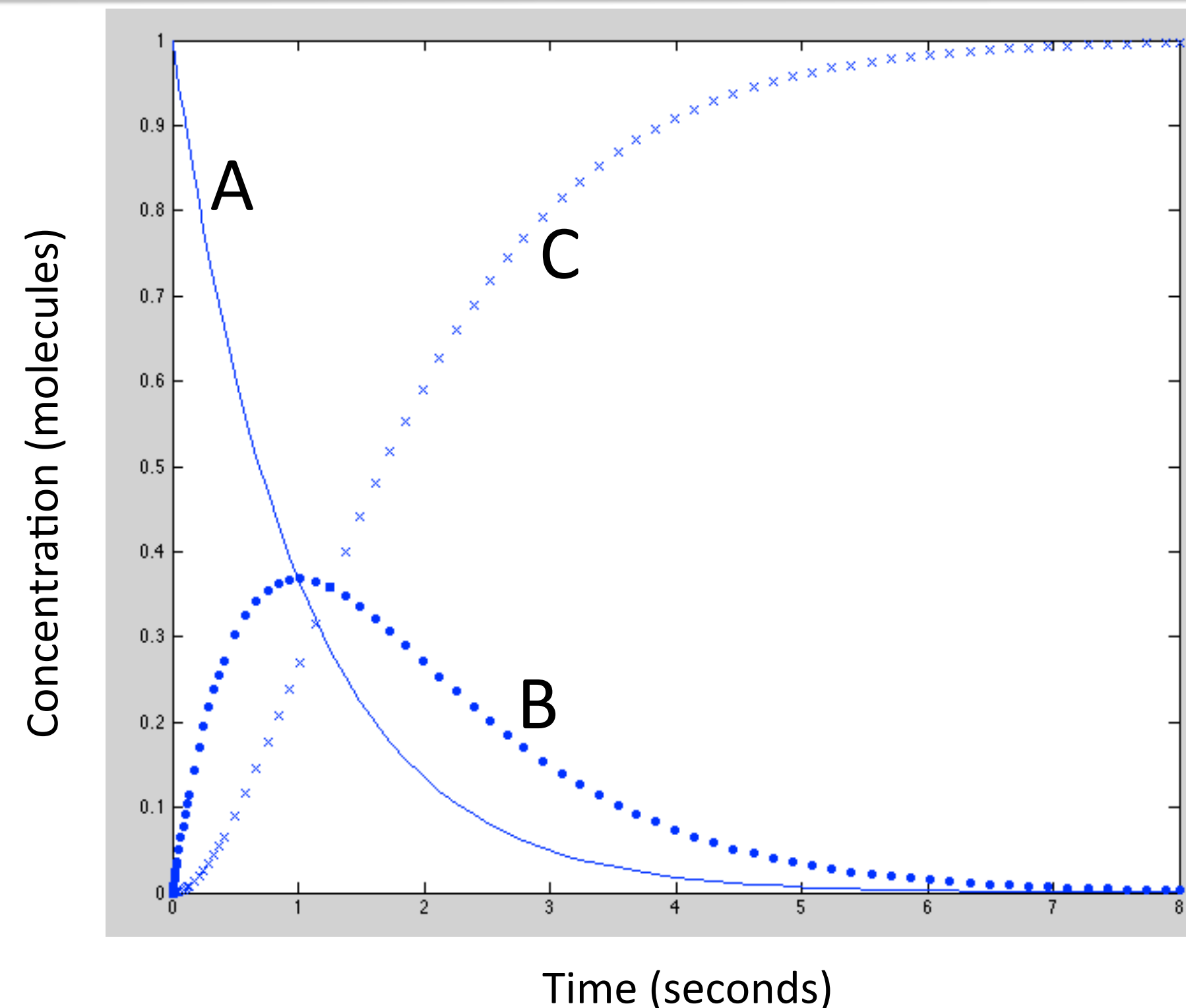
%Intial concentrations
A = 1;  B=0;  C=0;

%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



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Version 1.3, 3 November 2008

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