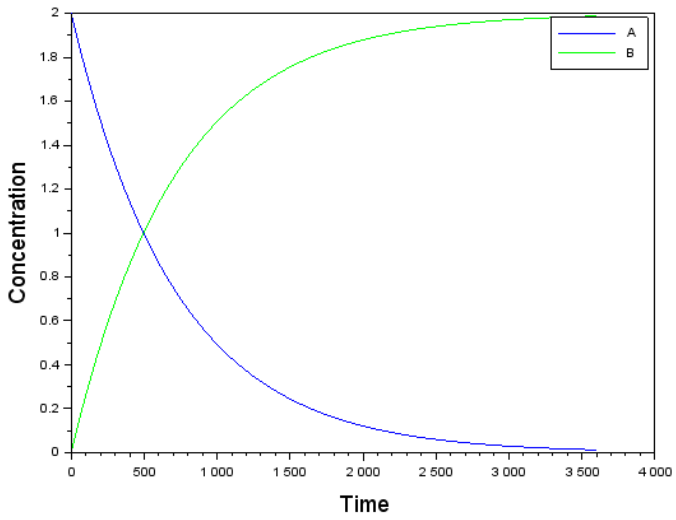
You could copy&paste this code into Scilab

```
// Scilab & chemical kinetics - intro to ode function
// A first-order reaction
// A=>B
// A0 = 2 mol/L
// B0 = 0 mol/L
// k=1.4e-3 1/s
// t = 0 - 3600s

// How to calculate concentration of the reagents dunring the reaction time?

// Approach 1: using of analytical solution (integral form)
```

$$time = 0 \ldots 3600$$

$$[A] = [A]_0 e^{-kt}$$

```
A0 = 2
B0 = 0
k = 1.4e-3
t = linspace(0, 3600)
A = A0*exp(-k*t)
B = A0 - A

plot(t,A,'b')
plot(t,B,'g')
xlabel("Time")
ylabel("Concentration")
legend(["A";"B"])
```



```
// Scilab & chemical kinetics - intro to ode function
// First-order reaction
// A=>B
// A0 = 2 mol/L
// B0 = 0 mol/L
// k=1.4e-3 1/s
// t = 0 - 3600s

// Approach 2: numerical integration of ODE

function dy=model(t, y)

  //our chemical species
  A = y(1)
  B = y(2)

  //our chemical kinetics equations
  dAdt = -k*A
  dBdt = k*A
  dy = [dAdt, dBdt]

endfunction

A0 = 2
B0 = 0
k = 1.4e-3
t = linspace(0, 3600)

//initial conditions (IC)
y0 = [A0; B0]
t0 = 0

y = ode(y0, t0, t, model)

A=y(1,:)
B=y(2,:)
plot(t,A,'b')
plot(t,B,'g')
```

$$A \rightarrow B$$

$$\frac{d[A]}{dt} = -kt$$

$$\frac{d[B]}{dt} = kt$$

$time = 0 \ldots 3600$

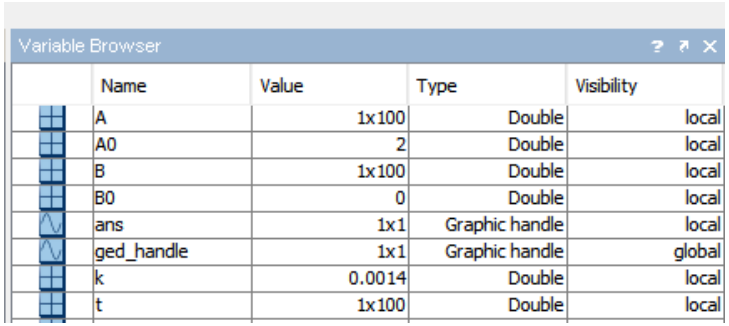
Must be always provided to ode function

The heart, calling **ode** function:
ordinary differential equation solver

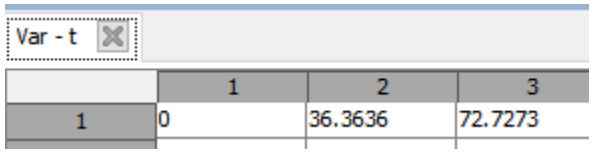
Selecting first and second row of y vector,
here A and B concentations

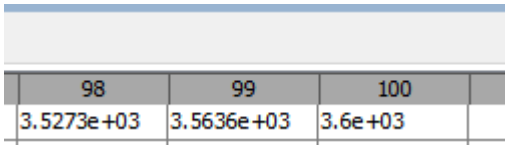
Please remember that variables: t, A and B are vectors!

Use „Variable browser” to check it



Anatomy of „t” variable: it is a 100 elements vector of values from 0 to 3600 (check linspace function in Scilab manual)

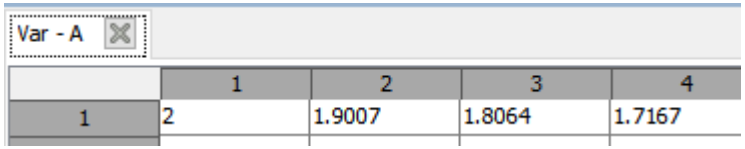


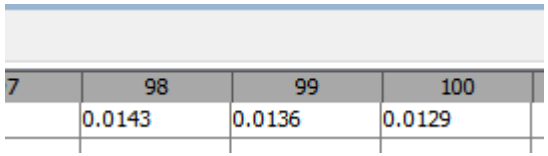


Indices

[A] at time = 0
first element: index 1
A(0)

[A] at time = 3600
last element: index 100
A(100)





Indices

Variable „A” content

Index = 1

Index = 4

Calculation results interpretation cont.

Variable: t

1	2	3	4	...
0	36.36	72.72	109.09	

Variable: A

1	2	3	4	...
2	1.9	1.8	1.71	

Variable: B

1	2	3	4	...
0	0.099	0.19	0.28	

t(0) = 0
A(0) = 2
B(0) = 0

t(4) = 109.09
A(4) = 1.71
B(4) = 0.28

At time 0 [A]=2 and [B]=0

At time 109.09 [A]=1.71 and [B]=0.28