Zero Order

```
> restart;with( DEtools ):with( plots ):with (linalg):
> ode_1:=diff(ca(t),t)=-k_1;ode_2:=diff(cb(t),t)=(k_1);
```

$$ode\_1 := \frac{d}{dt}\, ca(t) = -k\_1$$

$$ode\_2 := \frac{d}{dt}\, cb(t) = k\_1 \tag{1.1}$$

```
> dsolve({ode_1,ca(0)=ca0},ca(t));
```

$$ca(t) = -k\_1\, t + ca0$$

```
> dsolve({ode_2,cb(0)=cb0},cb(t));
```

$$cb(t) = k\_1\, t + cb0$$

```
> sol:= dsolve({ode_1,ca(0)=ca0,ode_2,cb(0)=cb0},{ca(t),cb(t)});
```

$$sol := \{ca(t) = -k\_1\, t + ca0,\ cb(t) = k\_1\, t + cb0\}$$

```
> k_1:=1:nsol := dsolve({ode_1,ca(0)=1,ode_2,cb(0)=0}, type=
  numeric, output=listprocedure);#assign(nsol);f:=eval(ca(t),
  sol);f(t=1);
```

nsol := [*t* = **proc**(*t*) ... **end proc**, *ca*(*t*) = **proc**(*t*) ... **end proc**, *cb*(*t*) = **proc**(*t*)

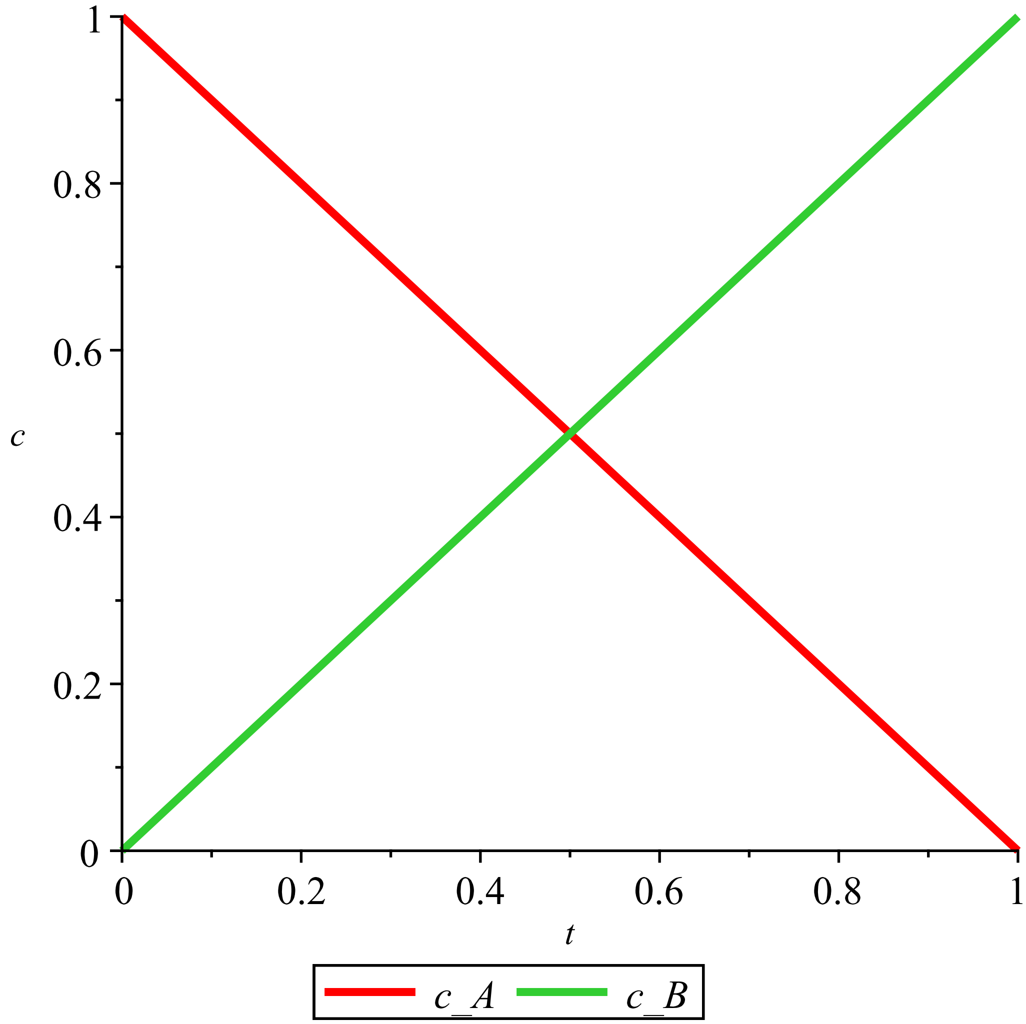
...

end proc]

```
> nsol(1);
```

$$[t(1) = 1.,\ ca(t)(1) = 6.93889390390723\ 10^{-18},\ cb(t)(1) = 1.] \tag{1.2}$$

```
> odeplot(nsol,[[t,ca(t)],[t,cb(t)]],0..1,labels=[t,c],legend=
  [c_A,c_B],thickness=3);
```



>

Prvniho radu A ->B

```
> restart;with( DEtools ):with( plots ):with (linalg):
```

```
> ode_1:=diff(ca(t),t)=-k_1*ca(t);
```

$$ode\_1 := \frac{d}{dt}\, ca(t) = -k\_1\, ca(t)$$

```
> ode_2:=diff(cb(t),t)=(k_1)*ca(t);
```

$$ode\_2 := \frac{d}{dt}\, cb(t) = k\_1\, ca(t)$$

```
> dsolve({ode_1,ca(0)=ca0},ca(t));
```

$$ca(t) = ca0\, e^{-k\_1\, t}$$

```
> dsolve({ode_2,cb(0)=cb0},cb(t));
```

$$cb(t) = \int_0^t k\_1\, ca(\_z1)\, d\_z1 + cb0$$

```
> sol:= dsolve({ode_1,ca(0)=ca0,ode_2,cb(0)=cb0},{ca(t),cb(t)});
```

$$sol := \{ca(t) = ca0\, e^{-k\_1\, t}, cb(t) = -ca0\, e^{-k\_1\, t} + ca0 + cb0\}$$

```
> k_1:=1:nsol := dsolve({ode_1,ca(0)=1,ode_2,cb(0)=0}, type=
  numeric, output=listprocedure);#assign(nsol);f:=eval(ca(t),
  sol);f(t=1);
```

nsol := [*t* = **proc**(*t*) ... **end proc**, *ca*(*t*) = **proc**(*t*) ... **end proc**, *cb*(*t*) = **proc**(*t*)

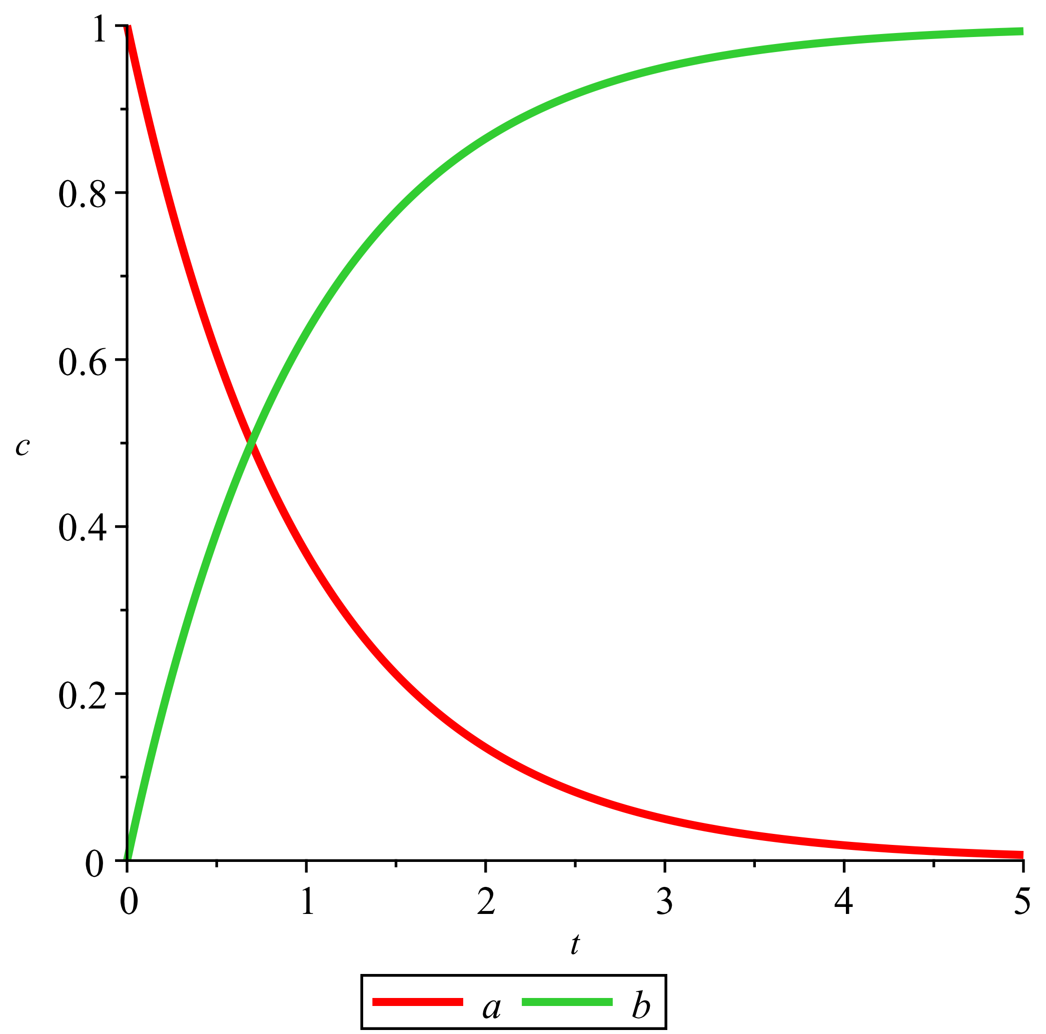
...

end proc]

```
> nsol(1);
```

$[t(1) = 1., ca(t)(1) = 0.367879361988637, cb(t)(1) = 0.632120638011363]$ **(2.1)**

```
> odeplot(nsol,[[t,ca(t)],[t,cb(t)]],0..5,labels=[t,c],legend=[a,
  b],thickness=3);
```



Reakce druheho radu 2A->B

```
> restart;with( DEtools ):with( plots ):with (linalg ):
> ode_1:=diff(ca(t),t)=-k_1*(ca(t))^2;
```

$$ode\_1 := \frac{d}{dt}\, ca(t) = -k\_1\, ca(t)^2$$

```
> ode_2:=diff(cb(t),t)=(k_1)*(ca(t))^2;
```

$$ode\_2 := \frac{d}{dt}\, cb(t) = k\_1\, ca(t)^2$$

```
> dsolve({ode_1,ca(0)=ca0},ca(t));
```

$$ca(t) = \frac{ca0}{1 + k\_1\, t\, ca0}$$

```
> dsolve({ode_2,cb(0)=ca0},cb(t));
```

$$cb(t) = \int_0^t k\_1\, ca(\_z1)^2\, d\_z1 + ca0$$

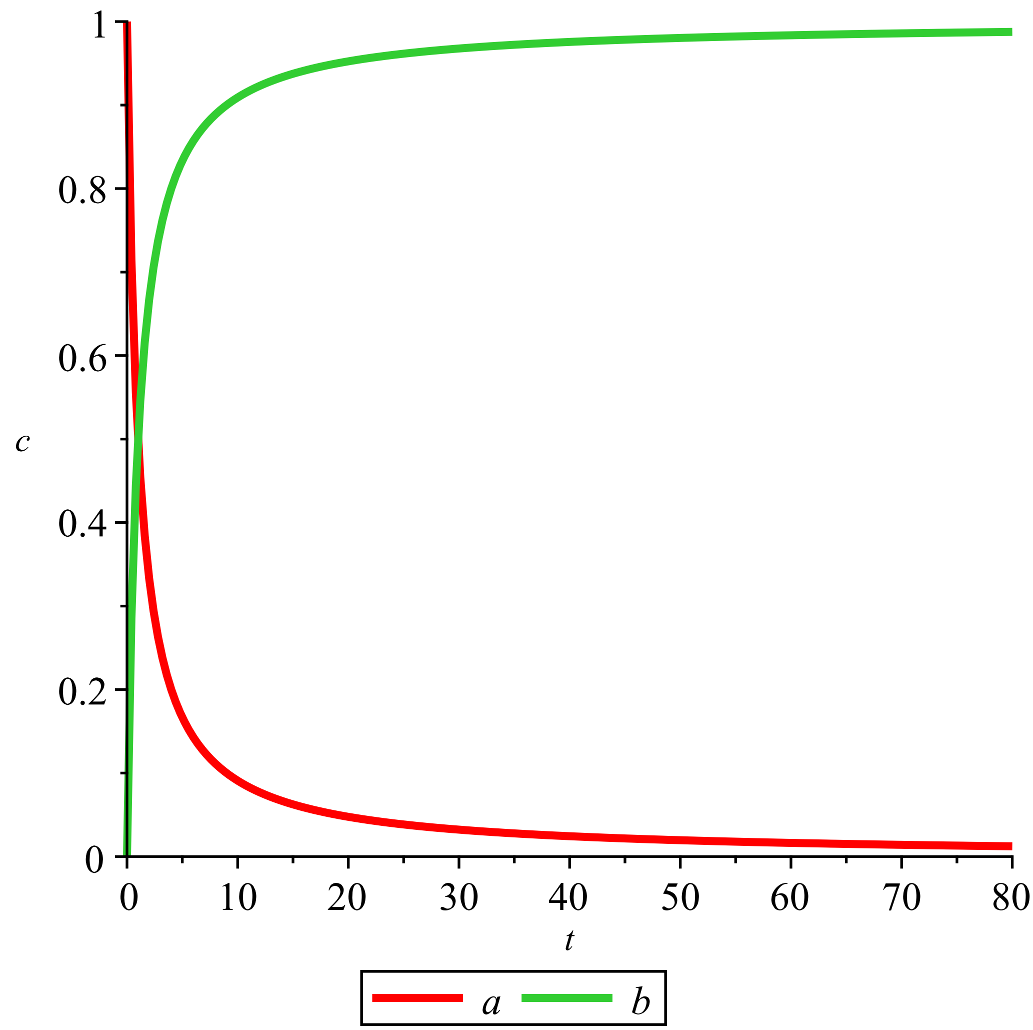
```
> dsolve({ode_1,ca(0)=ca0,ode_2,cb(0)=cb0},{ca(t),cb(t)});
```

$$\left\{ ca(t) = \frac{1}{k\_1\, t + \frac{1}{ca0}},\ cb(t) = -\frac{1}{k\_1\, t + \frac{1}{ca0}} + ca0 + cb0 \right\}$$

```
> k_1:=1:nsol := dsolve({ode_1,ca(0)=1,ode_2,cb(0)=0}, type=
  numeric);
```

$nsol :=$ **proc**(x_rkf45) ... **end proc**

```
> odeplot(nsol,[[t,ca(t)],[t,cb(t)]],0..80,labels=[t,c],legend=
  [a,b],thickness=3);
```



Reakce druheho radu A+B->C

```
> restart;with( DEtools ):with( plots ):with (linalg ):
> ode_1:=diff(ca(t),t)=-k_1*(ca(t))*(cb(t));
```

$$ode\_1 := \frac{d}{dt}\, ca(t) = -k\_1\, ca(t)\, cb(t)$$

```
> ode_2:=diff(cb(t),t)=-k_1*(ca(t))*(cb(t));
```

$$ode\_2 := \frac{d}{dt}\, cb(t) = -k\_1\, ca(t)\, cb(t)$$

```
> ode_3:=diff(cc(t),t)=k_1*(ca(t))*(cb(t));
```

$$ode\_3 := \frac{d}{dt}\, cc(t) = k\_1\, ca(t)\, cb(t) \tag{4.1}$$

```
> dsolve({ode_1,ca(0)=ca0},ca(t));
```

$$ca(t) = ca0\, e^{\int_0^t (-k\_1\, cb(\_z1))\, d\_z1}$$

```
> dsolve({ode_2,cb(0)=ca0},cb(t));
```

$$cb(t) = ca0\, e^{\int_0^t (-k\_1\, ca(\_z1))\, d\_z1}$$

```
> dsolve({ode_1,ca(0)=ca0,ode_2,cb(0)=cb0,ode_3,cc(0)=cc0},{ca(t),cb(t),cc(t)});
```

$$\Bigg\{ ca(t) = \Bigg(\left(e^{I\pi\_Z1\sim}\right)^2 e^{t(-cb0\,k\_1 + k\_1\,ca0)}\, e^{\frac{\left(\ln\left(\frac{ca0}{cb0\,k\_1}\right) + 2 I \pi\_Z2\sim\right)(-cb0\,k\_1 + k\_1\,ca0)}{k\_1(-cb0 + ca0)}} (-cb0\,k\_1$$

$$+ k\_1\,ca0)\Bigg) \Bigg/ \Bigg(-1$$

$$+ k\_1\, e^{t(-cb0\,k\_1 + k\_1\,ca0)}\, e^{\frac{\left(\ln\left(\frac{ca0}{cb0\,k\_1}\right) + 2 I \pi\_Z2\sim\right)(-cb0\,k\_1 + k\_1\,ca0)}{k\_1(-cb0 + ca0)}}\Bigg), cb(t) =$$

$$-\Bigg(\Bigg(\Bigg(\left(e^{I\pi\_Z1\sim}\right)^2 (-cb0\,k\_1$$

$$+ k\_1\,ca0)^2\, e^{t(-cb0\,k\_1 + k\_1\,ca0)}\, e^{\frac{\left(\ln\left(\frac{ca0}{cb0\,k\_1}\right) + 2 I \pi\_Z2\sim\right)(-cb0\,k\_1 + k\_1\,ca0)}{k\_1(-cb0 + ca0)}}\Bigg) \Bigg/ \Bigg(-1$$

$$+ k\_1\, e^{t\,(-cb0\,k\_1 + k\_1\,ca0)}\, e^{\frac{\left(\ln\left(\frac{ca0}{cb0\,k\_1}\right) + 2\,I\,\pi\,\_Z2\sim\right)(-cb0\,k\_1 + k\_1\,ca0)}{k\_1\,(-cb0 + ca0)}}\Bigg)$$

$$a0)\; e^{-\frac{\left(\ln\left(\frac{ca0}{cb0\,k\_1}\right) + 2\,I\,\pi\,\_Z2\sim\right)(-cb0\,k\_1 + k\_1\,ca0)}{k\_1\,(-cb0 + ca0)}}\Bigg)^2\Bigg)\Bigg(-1$$

$$+ k\_1\, e^{t\,(-cb0\,k\_1 + k\_1\,ca0)}\, e^{\frac{\left(\ln\left(\frac{ca0}{cb0\,k\_1}\right) + 2\,I\,\pi\,\_Z2\sim\right)(-cb0\,k\_1 + k\_1\,ca0)}{k\_1\,(-cb0 + ca0)}}\Bigg)\Bigg/$$

$$\Bigg(k\_1\,\left(e^{I\,\pi\,\_Z1\sim}\right)^2 e^{t\,(-cb0\,k\_1 + k\_1\,ca0)}\, e^{\frac{\left(\ln\left(\frac{ca0}{cb0\,k\_1}\right) + 2\,I\,\pi\,\_Z2\sim\right)(-cb0\,k\_1 + k\_1\,ca0)}{k\_1\,(-cb0 + ca0)}}\,(-cb0\,k\_1$$

$$+ k\_1\,ca0)\Bigg),\; cc(t) =$$

$$-\Bigg(\left(e^{I\,\pi\,\_Z1\sim}\right)^2 e^{t\,(-cb0\,k\_1 + k\_1\,ca0)}\, e^{\frac{\left(\ln\left(\frac{ca0}{cb0\,k\_1}\right) + 2\,I\,\pi\,\_Z2\sim\right)(-cb0\,k\_1 + k\_1\,ca0)}{k\_1\,(-cb0 + ca0)}}\,(-cb0\,k\_1$$

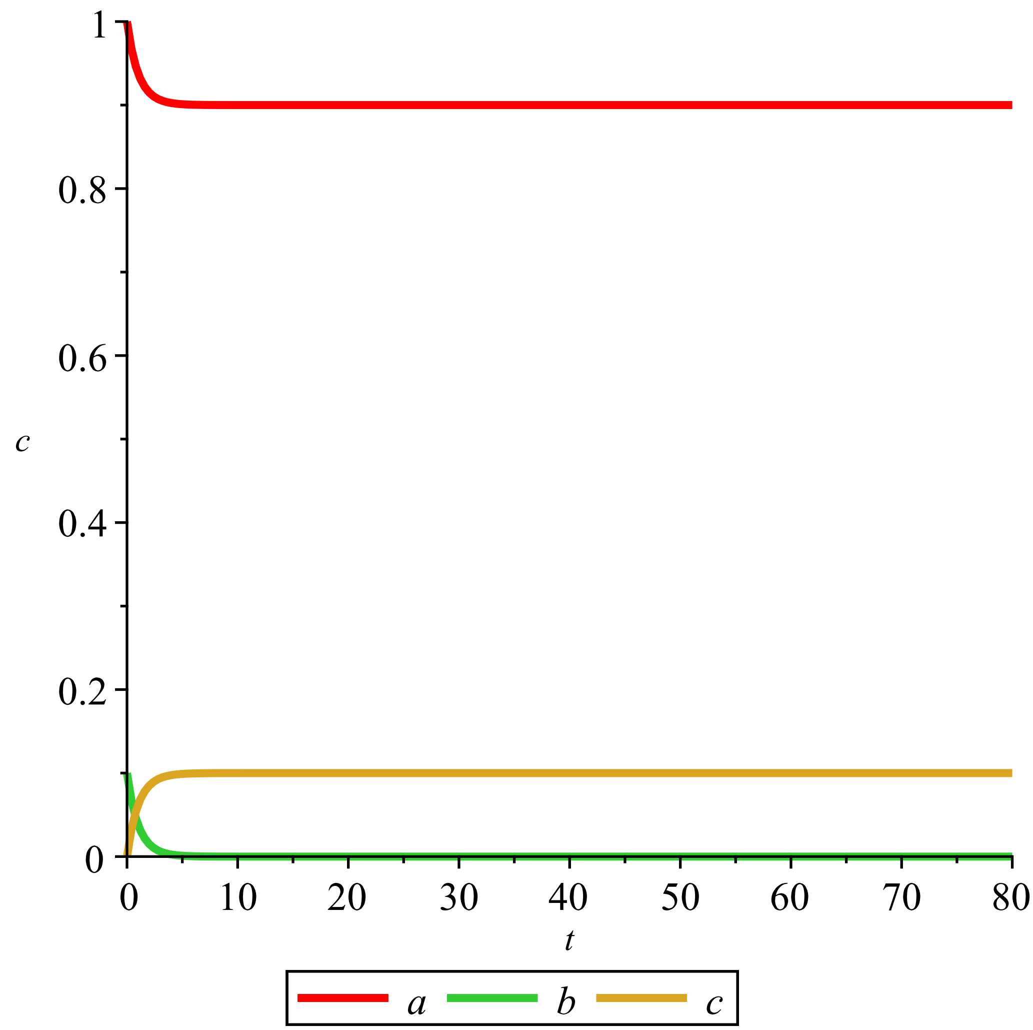
$$+ k\_1\,ca0)\Bigg)\Bigg/\Bigg(-1$$

$$+ k\_1\, e^{t\,(-cb0\,k\_1 + k\_1\,ca0)}\, e^{\frac{\left(\ln\left(\frac{ca0}{cb0\,k\_1}\right) + 2\,I\,\pi\,\_Z2\sim\right)(-cb0\,k\_1 + k\_1\,ca0)}{k\_1\,(-cb0 + ca0)}}\Bigg) + ca0 + cc0\Bigg\}$$

```
> k_1:=1:nsol := dsolve({ode_1,ca(0)=1,ode_2,cb(0)=.1,ode_3,cc(0)
=0}, type=numeric);
```

$$nsol := \textbf{proc}(x\_rkf45)\ \ldots\ \textbf{end proc}$$

```
> odeplot(nsol,[[t,ca(t)],[t,cb(t)],[t,cc(t)]],0..80,labels=[t,
c],legend=[a,b,c],thickness=3);
```



Srovnání prvního a druhého ádu

```
> restart;with( DEtools ):with( plots ):with (linalg):
> ode_1:=diff(ca(t),t)=-k_1*ca(t);
```

$$ode\_1 := \frac{d}{dt}\, ca(t) = -k\_1\, ca(t)$$

```
> ode_2:=diff(cb(t),t)=-1*(k_1)*(cb(t))^2;
```

$$ode\_2 := \frac{d}{dt}\, cb(t) = -\ln(2)\, cb(t)^2$$

```
> dsolve({ode_1,ca(0)=ca0},ca(t));
```

$$ca(t) = ca0\, 2^{-t}$$

```
> dsolve({ode_2,cb(0)=cb0},cb(t));
```

$$cb(t) = \frac{cb0}{1 + \ln(2)\, t\, cb0}$$

```
> sol:= dsolve({ode_1,ca(0)=ca0,ode_2,cb(0)=cb0},{ca(t),cb(t)});
```

$$sol := \left\{ ca(t) = ca0\, 2^{-t},\ cb(t) = \frac{1}{\ln(2)\, t + \frac{1}{cb0}} \right\}$$

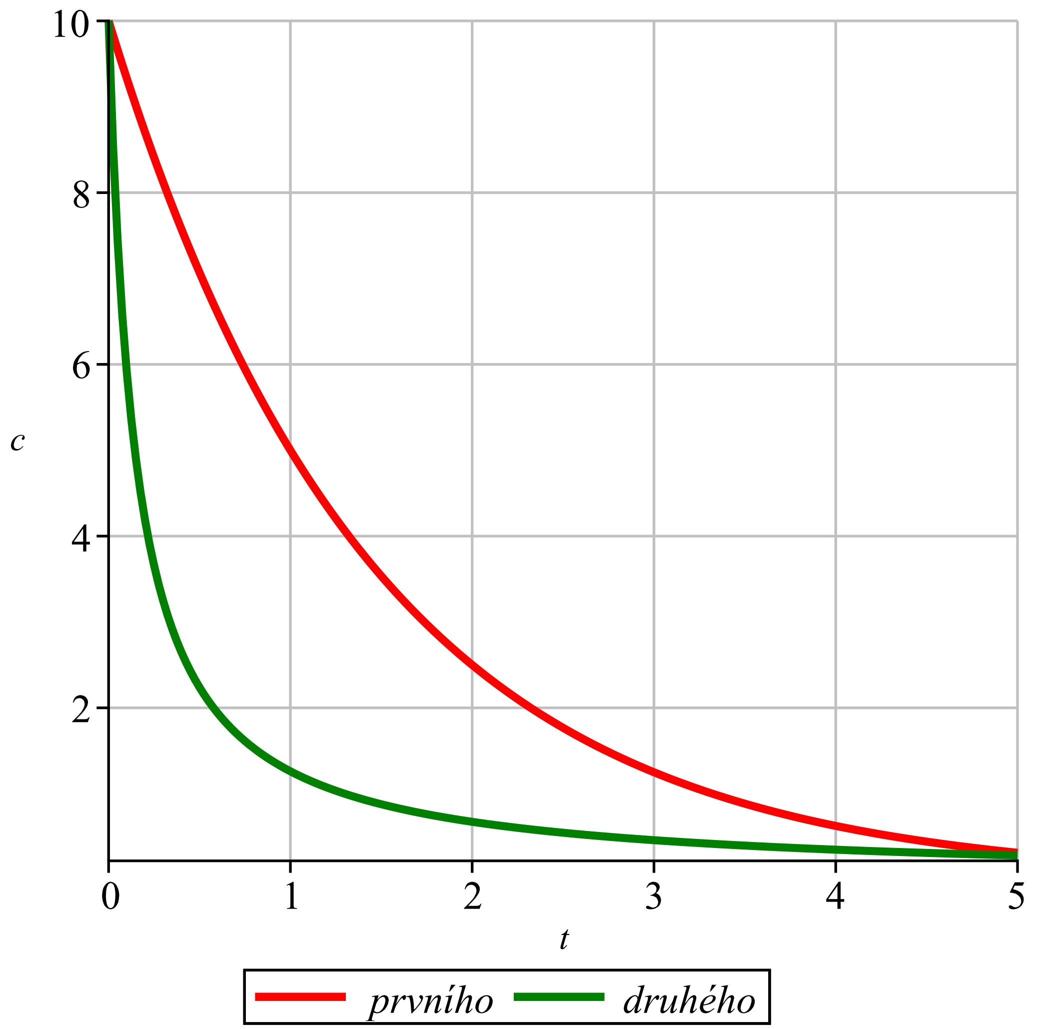
```
> k_1:=log(2):nsol := dsolve({ode_1,ca(0)=10,ode_2,cb(0)=10},
  type=numeric, output=listprocedure);#assign(nsol);f:=eval(ca
  (t), sol);f(t=1);
```

nsol := [*t* = **proc**(*t*) ... **end proc**, *ca*(*t*) = **proc**(*t*) ... **end proc**, *cb*(*t*) = **proc**(*t*)
...
end proc]

```
> %nsol(1);
```

nsol(1) **(5.1)**

```
> odeplot(nsol,[[t,ca(t)],[t,cb(t)]],0..5,labels=[t,c],color=
  ["Red","Green"],axis=[gridlines=[5,thickness=0,color=gray]
  ],legend=[prvního,druhého],thickness=3);
```




```
> restart;a:=0.1;t:=1;k:=log(2);prv:=a*exp(-k*t);evalf(%);druh:=
  a/(1+2*a*k*t);evalf(%);
```

$$a := 0.1$$
$$t := 1$$
$$k := \ln(2)$$

$$prv := 0.05000000000$$

$$0.05000000000$$

$$druh := \frac{0.1}{0.2\ \ln(2) + 1}$$

$$0.08782488564 \qquad (5.2)$$

```
> restart;t:=10;k:=log(2);a*exp(-k*t)=a/(1+1*a*k*t);solve(%,a);1/
(2*log(2));evalf(%);
```

$$t := 10$$

$$k := \ln(2)$$

$$\frac{a}{1024} = \frac{a}{10\ a \ln(2) + 1}$$

$$0,\ \frac{1023}{10 \ln(2)}$$

$$\frac{1}{2 \ln(2)}$$

$$0.7213475205 \qquad (5.3)$$

Paralelni reakce A->B,A->C

```
> restart;with( DEtools ):with( plots ):with (linalg ):
> ode_1:=diff(ca(t),t)=-(k_1+k_2)*ca(t);
```

$$ode\_1 := \frac{d}{dt}\ ca(t) = -(k\_1 + k\_2)\ ca(t)$$

```
> ode_2:=diff(cb(t),t)=(k_1)*ca(t);
```

$$ode\_2 := \frac{d}{dt}\ cb(t) = k\_1\ ca(t)$$

```
> ode_3:=diff(cc(t),t)=(k_2)*ca(t);
```

$$ode\_3 := \frac{d}{dt}\ cc(t) = k\_2\ ca(t)$$

```
> dsolve({ode_1,ca(0)=ca0,ode_2,cb(0)=cb0,ode_3,cc(0)=cc0},{ca
(t),cb(t),cc(t)});
```

$$\left\{ca(t) = ca0\ e^{-(k\_1 + k\_2)\ t},\ cb(t) = -\frac{k\_1\ ca0\ e^{-(k\_1 + k\_2)\ t}}{k\_1 + k\_2} + \frac{k\_1\ ca0 + cb0\ k\_1 + cb0\ k\_2}{k\_1 + k\_2},\ cc(t) = -\frac{k\_2\ ca0\ e^{-(k\_1 + k\_2)\ t}}{k\_1 + k\_2} + \frac{k\_2\ ca0 + cc0\ k\_1 + cc0\ k\_2}{k\_1 + k\_2}\right\}$$

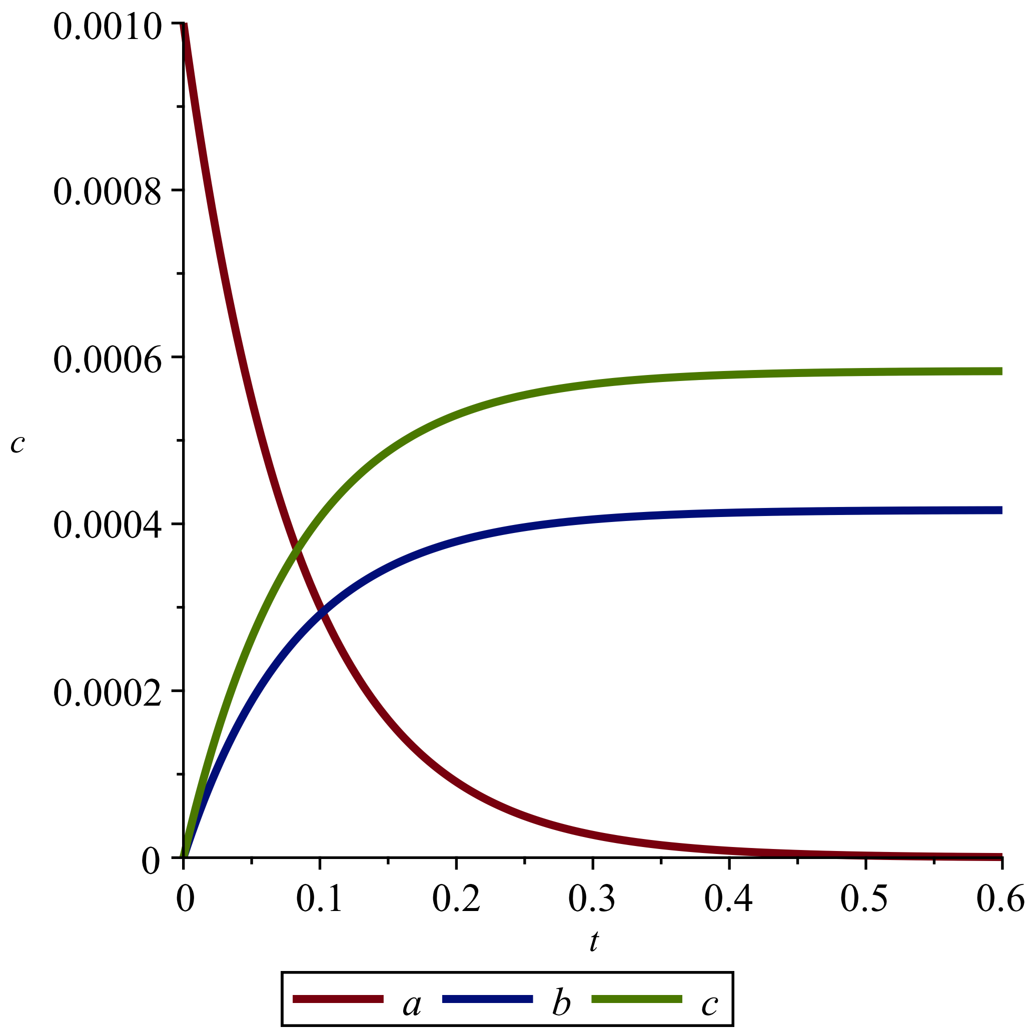
```
> dsolve({ode_2,cb(0)=cb0},cb(t));
```

$$cb(t) = \int_0^t k\_1\ ca(\_z1)\ d\_z1 + cb0$$

```
> k_1:=5:k_2:=7:nsol := dsolve({ode_1,ca(0)=.001,ode_2,cb(0)=0,
ode_3,cc(0)=0}, type=numeric);
```

$$nsol := \mathbf{proc}(x\_rkf45)\ \ldots\ \mathbf{end\ proc}$$

```
> odeplot(nsol,[[t,ca(t)],[t,cb(t)],[t,cc(t)]],0..6e-1,labels=[t,
  c],legend=[a,b,c],thickness=3);
```



Nasledne reakce

```
> restart;with( DEtools ):with( plots ):with (linalg):
> ode_1:=diff(ca(t),t)=-k_1*ca(t);
```

$$ode\_1 := \frac{d}{dt}\, ca(t) = -k\_1\, ca(t)$$

```
> ode_2:=diff(cb(t),t)=k_1*ca(t)-k_2*cb(t);
```

$$ode\_2 := \frac{d}{dt}\, cb(t) = k\_1\, ca(t) - k\_2\, cb(t)$$

```
> ode_3:=diff(cc(t),t)=k_2*cb(t);
```

$$ode\_3 := \frac{d}{dt}\, cc(t) = k\_2\, cb(t)$$

```
> dsolve({ode_1,ca(0)=ca0},ca(t));
```

$$ca(t) = ca0\, e^{-k\_1\, t}$$

```
> dsolve({ode_2,cb(0)=cb0},cb(t));
```

$$cb(t) = \left(\int_0^t k\_1\, ca(\_z1)\, e^{k\_2\,\_z1}\, d\_z1 + cb0\right) e^{-k\_2\, t}$$

```
> dsolve({ode_3,cc(0)=cc0},cc(t));
```

$$cc(t) = \int_0^t k\_2\, cb(\_z1)\, d\_z1 + cc0$$

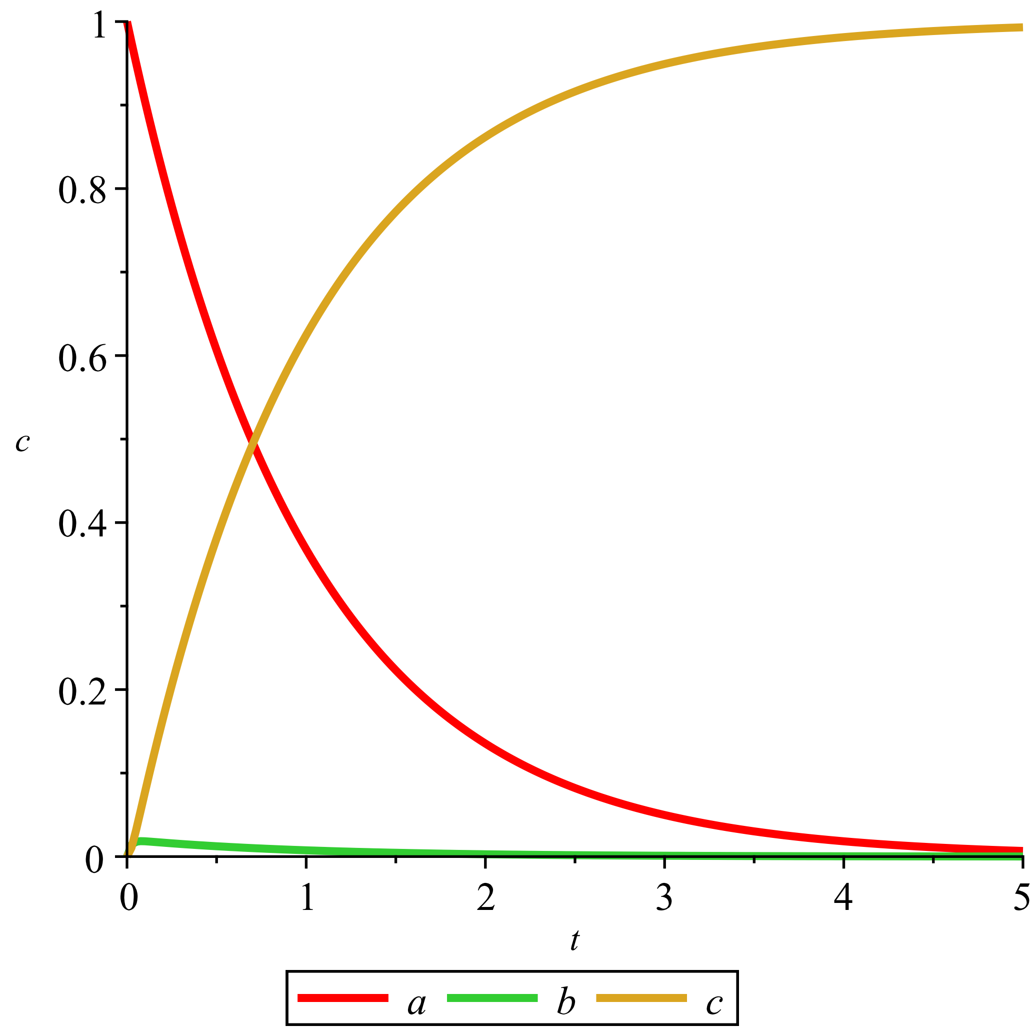
```
> dsolve({ode_1,ca(0)=ca0,ode_2,cb(0)=cb0,ode_3,cc(0)=cc0},{ca
  (t),cb(t),cc(t)});
```

$$\left\{ ca(t) = ca0\, e^{-k\_1\, t},\ cb(t) = \frac{1}{k\_1 - k\_2}\left(\left(\frac{(-k\_2\, cb0 + k\_1\, ca0 + cb0\, k\_1)\, k\_1}{k\_1 - k\_2} - \frac{(-k\_2\, cb0 + k\_1\, ca0 + cb0\, k\_1)\, k\_2}{k\_1 - k\_2}\right) e^{-k\_2\, t}\right) - \frac{k\_1\, ca0\, e^{-k\_1\, t}}{k\_1 - k\_2},\ cc(t) = \frac{1}{k\_1 - k\_2}\left(e^{-k\_1\, t}\, ca0\, k\_2 - \frac{e^{-k\_2\, t}\, (-k\_2\, cb0 + k\_1\, ca0 + cb0\, k\_1)\, k\_1}{k\_1 - k\_2} + \frac{e^{-k\_2\, t}\, (-k\_2\, cb0 + k\_1\, ca0 + cb0\, k\_1)\, k\_2}{k\_1 - k\_2} + (cc0 + ca0 + cb0)\, k\_1 - (cc0 + ca0 + cb0)\, k\_2\right)\right\}$$

```
> k_1:=1:k_2:=50:nsol := dsolve({ode_1,ca(0)=1,ode_2,cb(0)=0,
  ode_3,cc(0)=0}, type=numeric);
```

$nsol :=$ **proc**(x_rkf45) ... **end proc**

```
> odeplot(nsol,[[t,ca(t)],[t,cb(t)],[t,cc(t)]],0..5,labels=[t,c],
  legend=[a,b,c],thickness=3);
```




```
> 
```

Vratná reakce A <--> B

```
> restart;with( DEtools ):with( plots ):with (linalg):
> ode_1:=diff(ca(t),t)=-k_1*(ca(t))+k_2*cb(t);
```

$$ode\_1 := \frac{d}{dt}\ ca(t) = -k\_1\ ca(t) + k\_2\ cb(t)$$

```
> ode_2:=diff(cb(t),t)=(k_1)*ca(t)-k_2*cb(t);
```

$$ode\_2 := \frac{d}{dt}\ cb(t) = k\_1\ ca(t) - k\_2\ cb(t)$$

```
> dsolve({ode_1,ca(0)=ca0},ca(t));
```

$$ca(t) = \left(\int_0^t k\_2\ cb(\_z1)\ e^{k\_1\ \_z1}\ d\_z1 + ca0\right) e^{-k\_1\ t}$$

```
> dsolve({ode_2,cb(0)=cb0},cb(t));
```

$$cb(t) = \left(\int_0^t k\_1\, ca(\_z1)\, e^{k\_2\,\_z1}\, d\_z1 + cb0 \right) e^{-k\_2\, t}$$

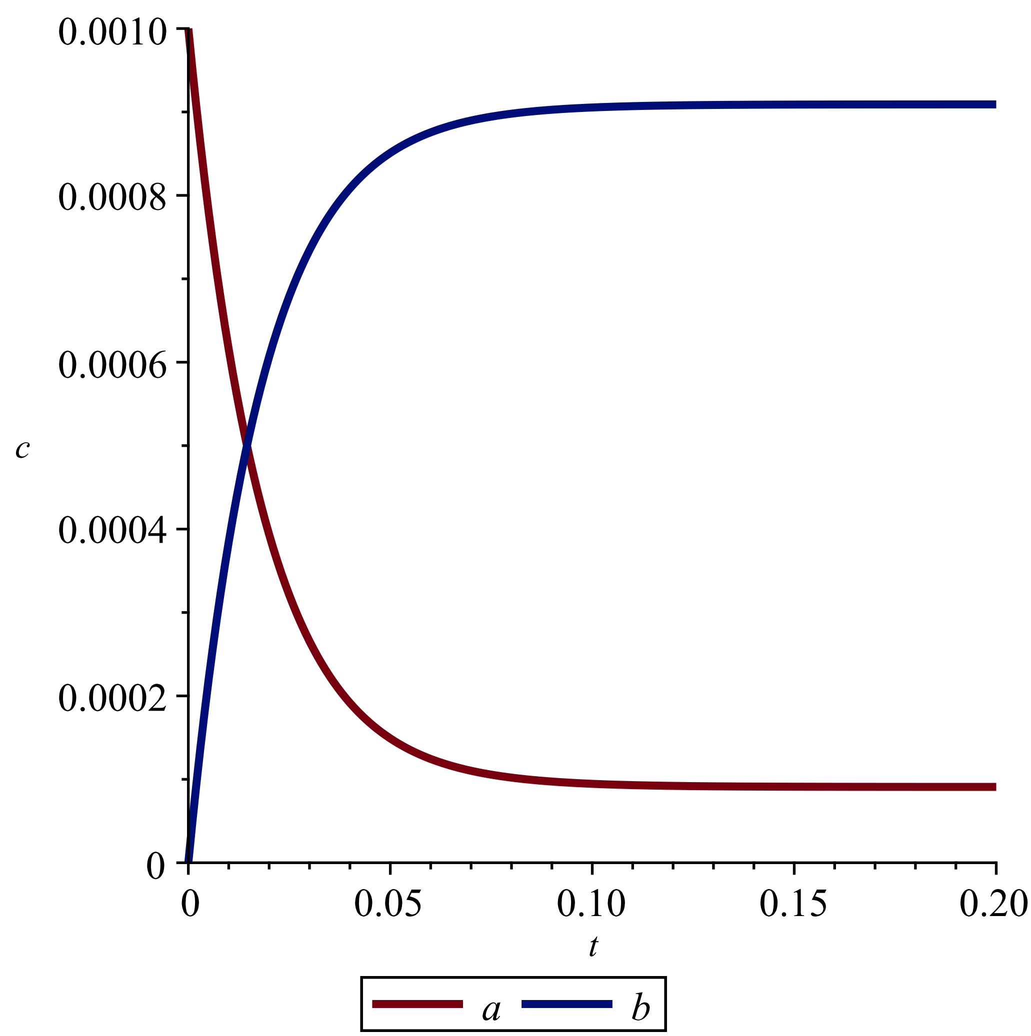
```
> dsolve({ode_1,ca(0)=ca0,ode_2,cb(0)=cb0},{ca(t),cb(t)});
```

$$\left\{ ca(t) = \frac{k\_2\,(ca0 + cb0)}{k\_1 + k\_2} + \frac{(k\_1\, ca0 - k\_2\, cb0)\, e^{-(k\_1 + k\_2)\, t}}{k\_1 + k\_2},\; cb(t) = -\frac{\frac{(k\_1\, ca0 - k\_2\, cb0)\, e^{-(k\_1 + k\_2)\, t}\, k\_2}{k\_1 + k\_2} - \frac{k\_2\,(ca0 + cb0)\, k\_1}{k\_1 + k\_2}}{k\_2} \right\}$$

```
> k_1:=50:k_2:=5:nsol := dsolve({ode_1,ca(0)=0.001,ode_2,cb(0)=0}
  , type=numeric);
```

$nsol := \mathbf{proc}(x\_rkf45)\ \ldots\ \mathbf{end\ proc}$

```
> odeplot(nsol,[[t,ca(t)],[t,cb(t)]],0..2e-1,labels=[t,c],legend=
  [a,b],thickness=3);
```




```
>
```

Vratná reakce 2A <--> B

```
> restart;with( DEtools ):with( plots ):with (linalg):
```

```
> ode_1:=diff(ca(t),t)=-k_1*(ca(t))^2+k_2*cb(t);
```

$$ode\_1 := \frac{d}{dt}\, ca(t) = -k\_1\, ca(t)^2 + k\_2\, cb(t)$$

```
> ode_2:=diff(cb(t),t)=(k_1)*(ca(t))^2-k_2*cb(t);
```

$$ode\_2 := \frac{d}{dt}\, cb(t) = k\_1\, ca(t)^2 - k\_2\, cb(t)$$

```
> dsolve({ode_1,ca(0)=ca0},ca(t));
> dsolve({ode_2,cb(0)=cb0},cb(t));
```

$$cb(t) = \left(\int_0^t k\_1\, ca(\_z1)^2\, e^{k\_2\, \_z1}\, d\_z1 + cb0\right) e^{-k\_2\, t}$$

```
> dsolve({ode_1,ca(0)=ca0,ode_2,cb(0)=cb0},{ca(t),cb(t)});
```

$$\Big\{ ca(t) = \frac{1}{2\, k\_1} \left(\frac{1}{2} \left(\tanh\Big(\Big(\Big((4\, I\, \pi\, \_Z1\sim + 2 \ln\big(RootOf\big((ca0^2\, k\_1^2 - cb0\, k\_1\, k\_2)\, \_Z^4 \right.\right.$$

$$+ (2\, ca0^2\, k\_1^2 + 4\, ca0\, k\_1\, k\_2 + 2\, cb0\, k\_1\, k\_2 + k\_2^2)\, \_Z^2 + ca0^2\, k\_1^2$$

$$- cb0\, k\_1\, k\_2\big)\big)\Big)\, RootOf\big((ca0^2\, k\_1^2 - cb0\, k\_1\, k\_2)\, \_Z^4 + (2\, ca0^2\, k\_1^2$$

$$+ 4\, ca0\, k\_1\, k\_2 + 2\, cb0\, k\_1\, k\_2 + k\_2^2)\, \_Z^2 + ca0^2\, k\_1^2 - cb0\, k\_1\, k\_2\big)^2$$

$$- 4\, I\, \pi\, \_Z1\sim - 2 \ln\big(RootOf\big((ca0^2\, k\_1^2 - cb0\, k\_1\, k\_2)\, \_Z^4 + (2\, ca0^2\, k\_1^2$$

$$+ 4\, ca0\, k\_1\, k\_2 + 2\, cb0\, k\_1\, k\_2 + k\_2^2)\, \_Z^2 + ca0^2\, k\_1^2 - cb0\, k\_1\, k\_2\big)\big)\Big)$$

$\sqrt{4}\,\sqrt{k\_2\,(4\,ca0\,k\_1+4\,cb0\,k\_1+k\_2)}\,\Big)\Big/\Big(4\,\Big(2\,RootOf\big(\big(ca0^2\,k\_1^2$

$-cb0\,k\_1\,k\_2\big)\,\_Z^4+\big(2\,ca0^2\,k\_1^2+4\,ca0\,k\_1\,k\_2+2\,cb0\,k\_1\,k\_2+k\_2^2\big)\,\_Z^2$

$+ca0^2\,k\_1^2-cb0\,k\_1\,k\_2\big)^2\,ca0\,k\_1+RootOf\big(\big(ca0^2\,k\_1^2-cb0\,k\_1\,k\_2\big)\,\_Z^4$

$+\big(2\,ca0^2\,k\_1^2+4\,ca0\,k\_1\,k\_2+2\,cb0\,k\_1\,k\_2+k\_2^2\big)\,\_Z^2+ca0^2\,k\_1^2$

$-cb0\,k\_1\,k\_2\big)^2\,k\_2+2\,ca0\,k\_1+k\_2\Big)\Big)$

$+\dfrac{t\,\sqrt{4}\,\sqrt{k\_2\,(4\,ca0\,k\_1+4\,cb0\,k\_1+k\_2)}}{4}\Bigg)$

$\sqrt{4}\,\sqrt{k\_2\,(4\,ca0\,k\_1+4\,cb0\,k\_1+k\_2)}\Bigg)-k\_2\Bigg),\ cb(t)=$

$-\dfrac{1}{4\,k\_1\,k\_2}\Bigg(\tanh\Bigg(\dfrac{1}{4}\Big(\sqrt{4}\,\sqrt{k\_2\,(4\,ca0\,k\_1+4\,cb0\,k\_1+k\_2)}\,\Big(\Big(\Big(4\,\mathrm{I}\,\pi\,\_Z1\sim$

$+2\,\ln\big(RootOf\big(\big(ca0^2\,k\_1^2-cb0\,k\_1\,k\_2\big)\,\_Z^4+\big(2\,ca0^2\,k\_1^2+4\,ca0\,k\_1\,k\_2$

$+2\,cb0\,k\_1\,k\_2+k\_2^2\big)\,\_Z^2+ca0^2\,k\_1^2-cb0\,k\_1\,k\_2\big)\big)\Big)\,RootOf\big(\big(ca0^2\,k\_1^2$

$-cb0\,k\_1\,k\_2\big)\,\_Z^4+\big(2\,ca0^2\,k\_1^2+4\,ca0\,k\_1\,k\_2+2\,cb0\,k\_1\,k\_2+k\_2^2\big)\,\_Z^2$

$+ca0^2\,k\_1^2-cb0\,k\_1\,k\_2\big)^2-4\,\mathrm{I}\,\pi\,\_Z1\sim-2\,\ln\big(RootOf\big(\big(ca0^2\,k\_1^2$

$-cb0\,k\_1\,k\_2\big)\,\_Z^4+\big(2\,ca0^2\,k\_1^2+4\,ca0\,k\_1\,k\_2+2\,cb0\,k\_1\,k\_2+k\_2^2\big)\,\_Z^2$

$+ca0^2\,k\_1^2-cb0\,k\_1\,k\_2\big)\big)\Big)\Big/\Big(2\,RootOf\big(\big(ca0^2\,k\_1^2-cb0\,k\_1\,k\_2\big)\,\_Z^4$

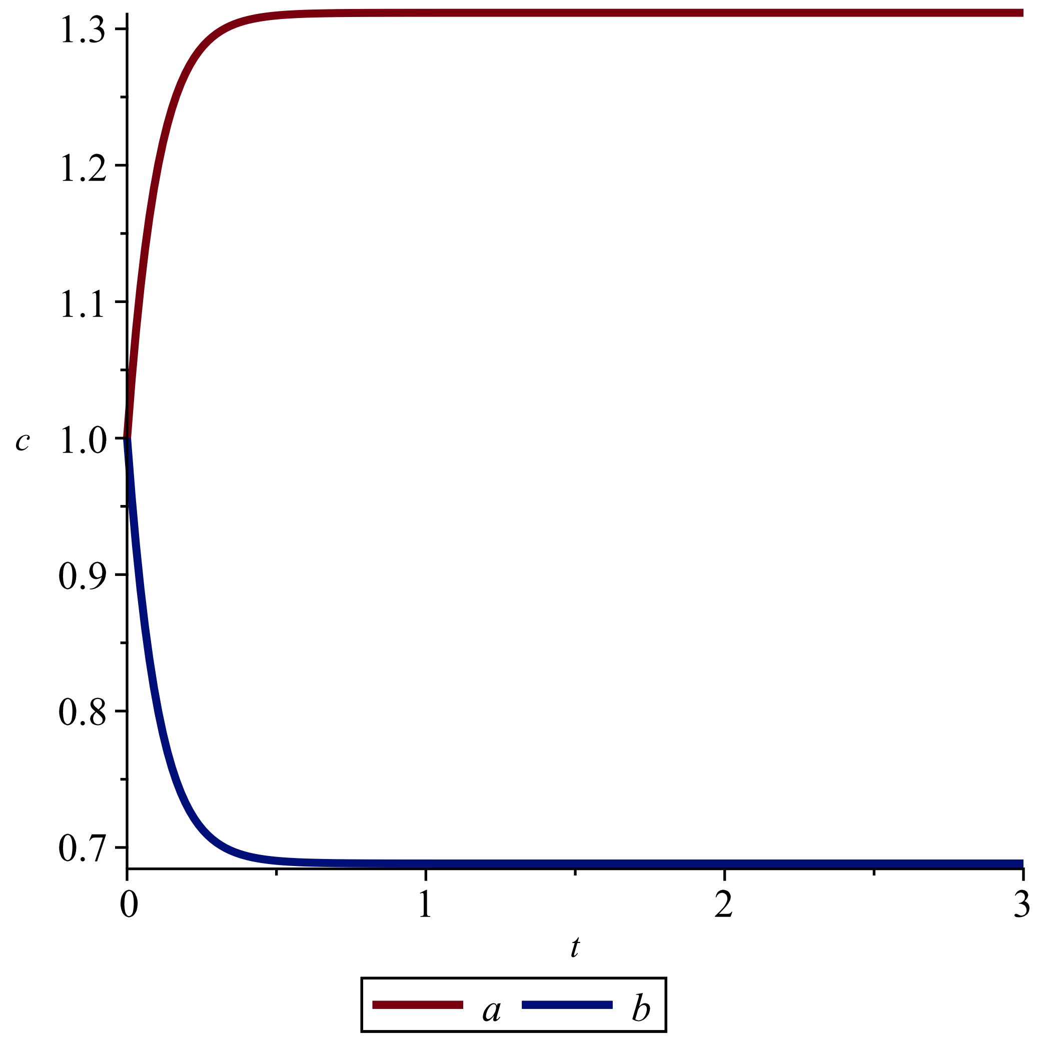
$+\big(2\,ca0^2\,k\_1^2+4\,ca0\,k\_1\,k\_2+2\,cb0\,k\_1\,k\_2+k\_2^2\big)\,\_Z^2+ca0^2\,k\_1^2$

$$- cb0\,k\_1\,k\_2)^2\,ca0\,k\_1 + RootOf\big((ca0^2\,k\_1^2 - cb0\,k\_1\,k\_2)\,\_Z^4$$
$$+ (2\,ca0^2\,k\_1^2 + 4\,ca0\,k\_1\,k\_2 + 2\,cb0\,k\_1\,k\_2 + k\_2^2)\,\_Z^2 + ca0^2\,k\_1^2$$
$$- cb0\,k\_1\,k\_2)^2\,k\_2 + 2\,ca0\,k\_1 + k\_2) + t\big)\big)\big)$$
$$\sqrt{4}\,\sqrt{k\_2\,(4\,ca0\,k\_1 + 4\,cb0\,k\_1 + k\_2)}\,k\_2 - k\_2\,(4\,ca0\,k\_1 + 4\,cb0\,k\_1 + k\_2)$$
$$- k\_2^2)\}$$

```
> k_1:=2:k_2:=5:nsol := dsolve({ode_1,ca(0)=1,ode_2,cb(0)=1},
  type=numeric);
```

$$nsol := \textbf{proc}(x\_rkf45)\ \ldots\ \textbf{end proc}$$

```
> odeplot(nsol,[[t,ca(t)],[t,cb(t)]],0..3,labels=[t,c],legend=[a,
  b],thickness=3);
```



ešení využívající piblížení

Reakce druheho ádu A+B->C, pevedená na pseudoprvní ád

```
> restart;with( DEtools ):with( plots ):with (linalg ):
```

```
> ode_1:=diff(ca(t),t)=-k_1*(ca(t))*(cb(t));
```

$$ode\_1 := \frac{d}{dt}\, ca(t) = -k\_1\, ca(t)\, cb(t)$$

```
> ode_2:=diff(cb(t),t)=-k_1*(ca(t))*(cb(t));
```

$$ode\_2 := \frac{d}{dt}\, cb(t) = -k\_1\, ca(t)\, cb(t)$$

```
> ode_3:=diff(cc(t),t)=k_1*(ca(t))*(cb(t));
```

$$ode\_3 := \frac{d}{dt}\, cc(t) = k\_1\, ca(t)\, cb(t) \qquad (10.1.1)$$

```
> dsolve({ode_1,ca(0)=ca0},ca(t));
```

$$ca(t) = ca0\, e^{\int_0^t (-k\_1\, cb(\_z1))\, d\_z1}$$

```
> dsolve({ode_2,cb(0)=ca0},cb(t));
```

$$cb(t) = ca0\, e^{\int_0^t (-k\_1\, ca(\_z1))\, d\_z1}$$

```
> dsolve({ode_1,ca(0)=ca0,ode_2,cb(0)=cb0,ode_3,cc(0)=cc0},{ca
(t),cb(t),cc(t)});
```

$$\Bigg\{ ca(t) = \Bigg(\left(e^{I\pi\_Z1\sim}\right)^2 e^{t(-cb0\, k\_1 + k\_1\, ca0)}\, e^{\frac{\left(\ln\left(\frac{ca0}{cb0\, k\_1}\right) + 2\, I\pi\_Z2\sim\right)(-cb0\, k\_1 + k\_1\, ca0)}{k\_1(-cb0 + ca0)}} \Big($$

$$-cb0\, k\_1 + k\_1\, ca0\Big)\Bigg) \Bigg/ \Bigg(-1$$

$$+ k\_1\, e^{t(-cb0\, k\_1 + k\_1\, ca0)}\, e^{\frac{\left(\ln\left(\frac{ca0}{cb0\, k\_1}\right) + 2\, I\pi\_Z2\sim\right)(-cb0\, k\_1 + k\_1\, ca0)}{k\_1(-cb0 + ca0)}} \Bigg), cb(t) =$$

$$- \left(\left(\left(\left(e^{I \pi \_Z1\sim} \right)^2 (-cb0\, k\_1 \right.\right.\right.\right.$$

$$\left. + k\_1\, ca0)^2 e^{t(-cb0\, k\_1 + k\_1\, ca0)} e^{\frac{\left(\ln\left(\frac{ca0}{cb0\, k\_1} \right) + 2 I \pi \_Z2\sim \right)(-cb0\, k\_1 + k\_1\, ca0)}{k\_1(-cb0 + ca0)}} \right) \Big/ \left(-1 \right.$$

$$\left. + k\_1\, e^{t(-cb0\, k\_1 + k\_1\, ca0)} e^{\frac{\left(\ln\left(\frac{ca0}{cb0\, k\_1} \right) + 2 I \pi \_Z2\sim \right)(-cb0\, k\_1 + k\_1\, ca0)}{k\_1(-cb0 + ca0)}} \right)$$

$$k\_1\, ca0)\; e^{\frac{\left(\ln\left(\frac{ca0}{cb0\, k\_1} \right) + 2 I \pi \_Z2\sim \right)(-cb0\, k\_1 + k\_1\, ca0)}{k\_1(-cb0 + ca0)}} \Bigg)^2 \Bigg) \Big/ \left(-1 \right.$$

$$\left.\left. + k\_1\, e^{t(-cb0\, k\_1 + k\_1\, ca0)} e^{\frac{\left(\ln\left(\frac{ca0}{cb0\, k\_1} \right) + 2 I \pi \_Z2\sim \right)(-cb0\, k\_1 + k\_1\, ca0)}{k\_1(-cb0 + ca0)}} \right) \right) \Big/$$

$$\left(k\_1 \left(e^{I \pi \_Z1\sim} \right)^2 e^{t(-cb0\, k\_1 + k\_1\, ca0)} e^{\frac{\left(\ln\left(\frac{ca0}{cb0\, k\_1} \right) + 2 I \pi \_Z2\sim \right)(-cb0\, k\_1 + k\_1\, ca0)}{k\_1(-cb0 + ca0)}} \right. ($$

$$\left. -cb0\, k\_1 + k\_1\, ca0) \right), cc(t) =$$

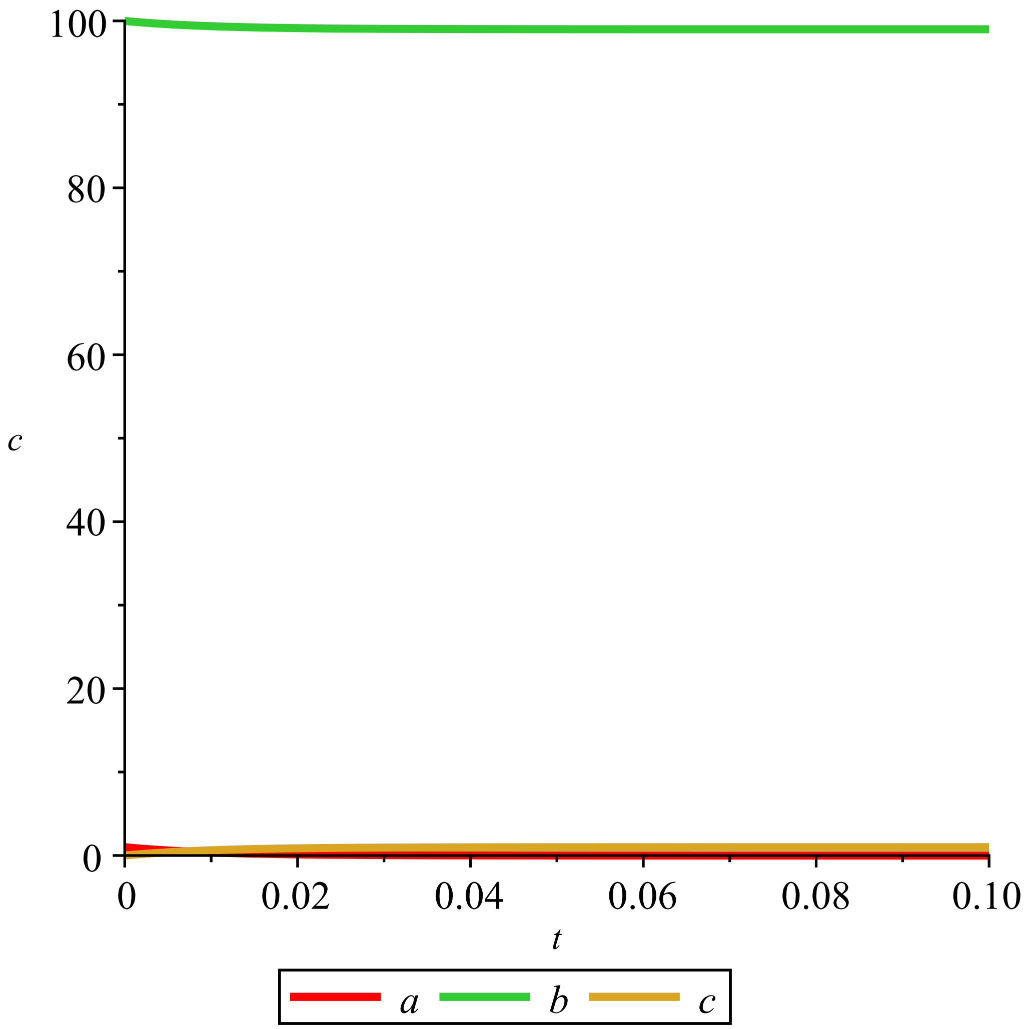
$$- \left(\left(e^{I \pi \_Z1\sim} \right)^2 e^{t(-cb0\, k\_1 + k\_1\, ca0)} e^{\frac{\left(\ln\left(\frac{ca0}{cb0\, k\_1} \right) + 2 I \pi \_Z2\sim \right)(-cb0\, k\_1 + k\_1\, ca0)}{k\_1(-cb0 + ca0)}} (-cb0\, k\_1 \right.$$

$$+ k\_1\, ca0) \Bigg) \Bigg/ \Bigg(-1 + k\_1\, e^{t(-cb0\, k\_1 + k\_1\, ca0)}\, e^{\frac{\left(\ln\left(\frac{ca0}{cb0\, k\_1}\right) + 2\, I\, \pi\, \_Z2\sim\right)(-cb0\, k\_1 + k\_1\, ca0)}{k\_1\,(-cb0 + ca0)}} \Bigg) + ca0 + cc0 \Bigg\}$$

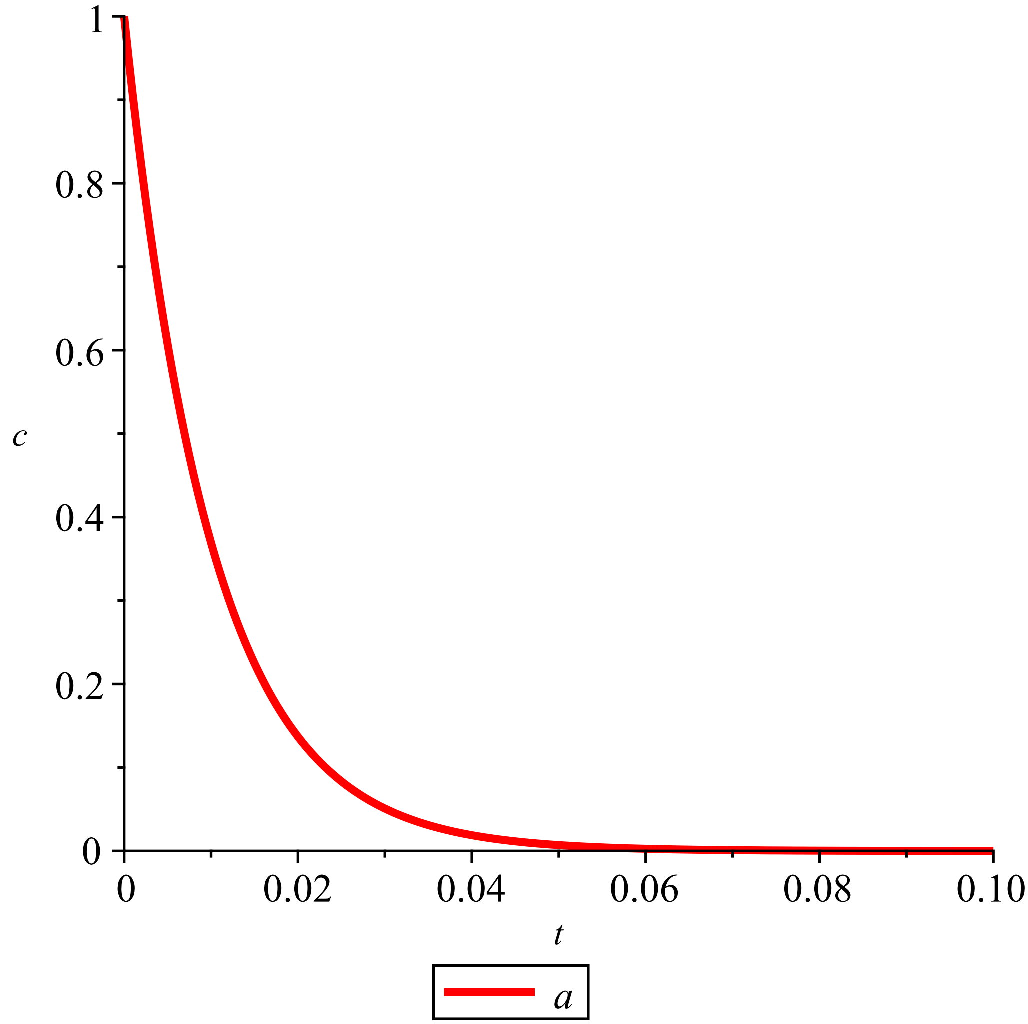
```
> k_1:=1:nsol := dsolve({ode_1,ca(0)=1,ode_2,cb(0)=100,ode_3,
  cc(0)=0}, type=numeric);
```

nsol := **proc**(*x_rkf45*) ... **end proc**

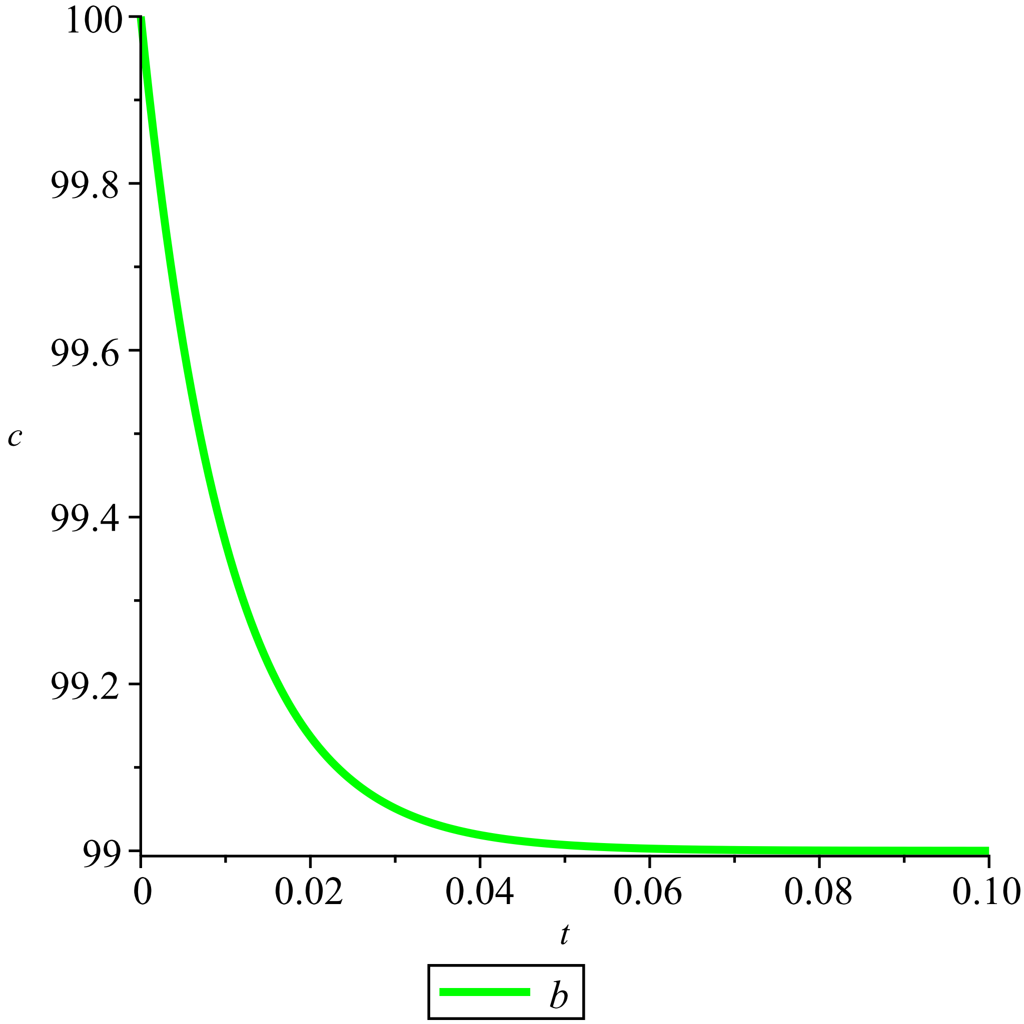
```
> odeplot(nsol,[[t,ca(t)],[t,cb(t)],[t,cc(t)]],0..0.1,labels=
  [t,c],legend=[a,b,c],thickness=3);
```




```
> odeplot(nsol,[[t,ca(t)]],0..0.1,labels=[t,c],legend=[a],
  thickness=3);
```




```
> odeplot(nsol,[[t,cb(t)]],0..0.1,labels=[t,c],legend=[b],
  thickness=3,color=[green]);
```


100
99.8
99.6
c
99.4
99.2
99
0
0.02
0.04
0.06
0.08
0.10
t
b