Batch chemical reactor:
Reversible, consecutive reaction:

$A \rightleftharpoons B \rightleftharpoons C$

Concentrations of species A,B,C (Ca,Cb,Cc)
as a function of time, t:
Initial value problem - system of first ODE:

$$\frac{d}{dt}Ca = -k1 \cdot Ca + k2 \cdot Cb$$
$$\frac{d}{dt}Cb = -(k3 + k2) \cdot Cb + k4 \cdot Cc + k1 \cdot Ca$$
$$\frac{d}{dt}Ca = -k4 \cdot Cc + k3 \cdot Cb$$

$t = 0$

$Ca(t) = Ca0 \quad Cb(t) = Cb0 \quad Cc(0) = Cc0$

Reaction rate constants:

$k1 := 3$
$k2 := 0.1$
$k3 := 2$
$k4 := 0.04$

Interval of integration and initial concentrations:

$t0 := 0$
$tmax := 1.5$

$Ca0 := 1$
$Cb0 := 0$
$Cc0 := 0$

SOLVING

Vector ov initial values:

$$x0 := \begin{pmatrix} Ca0 \\ Cb0 \\ Cc0 \end{pmatrix}$$

LHS of system of firs orde ODE:

$$f := \begin{pmatrix} -k1 \cdot x_1 + k2 \cdot x_2 \\ -(k3 + k2) \cdot x_2 + k4 \cdot x_3 + k1 \cdot x_1 \\ -k4 \cdot x_3 + k3 \cdot x_2 \end{pmatrix}$$

$f(t, x) := f$

Fifth-order Runge-Kutta method with adaptive step

$x := x0$ A Cauchy problem

$t_1 := t0$ Start Point

$T := tmax$ Segment length

$\varepsilon := 10^{-3}$ Precision

$n := 100$

$h := \frac{tmax - t0}{n}$

for $j := t_1 + h, j \le T + t_1 + h, j := j + h$

$tx := col(x, cols(x))$

$k1 := \frac{h}{3} \cdot eval(f(j, tx))$

$k2 := \frac{h}{3} \cdot eval\left(f\left(j + \frac{h}{3}, tx + k1\right)\right)$

$k3 := \frac{h}{3} \cdot eval\left(f\left(j + \frac{h}{3}, tx + \frac{k1 + k2}{2}\right)\right)$

$k4 := \frac{h}{3} \cdot eval\left(f\left(j + \frac{h}{2}, tx + \frac{3 \cdot k1 + 9 \cdot k3}{8}\right)\right)$

$k5 := \frac{h}{3} \cdot eval\left(f\left(j + h, tx + \frac{3 \cdot k1 - 9 \cdot k3}{2} + 6 \cdot k4\right)\right)$

$\delta := k1 - \frac{9}{2} \cdot k3 + 4 \cdot k4 - \frac{1}{2} \cdot k5$

if $(|min(\delta)| \le 5 \cdot \varepsilon) \wedge (|max(\delta)| \le 5 \cdot \varepsilon)$

$x := augment\left(x, tx + \frac{1}{2} \cdot (k1 + 4 \cdot k4 + k5)\right)$

$steps_{1, cols(x)} := j$

$h := h \cdot 2$

else

$j := j - h$

$h := \frac{h}{2}$

$result := stack(steps, x)$

$cols(result) = 10$ Number of values

Data analysis

$X := steps^T$

$Y1 := row(x, 1)^T \quad Y2 := row(x, 2)^T \quad Y3 := row(x, 3)^T$

$time := t0, t0 + \frac{tmax - t0}{20} .. tmax$

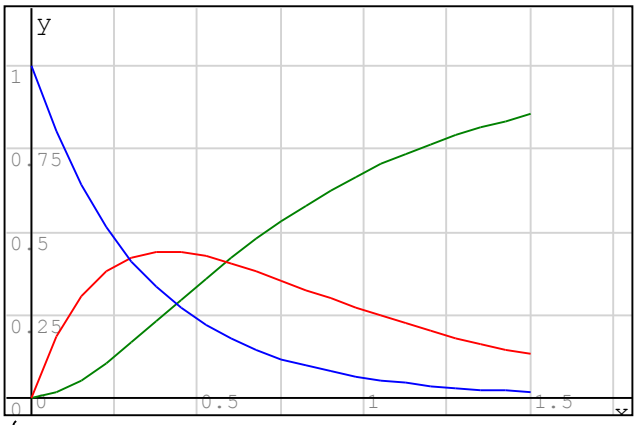
for $j \in 1 .. length(time)$

$A_j := cinterp(X, Y1, time_j)$

$B_j := cinterp(X, Y2, time_j)$

$C_j := cinterp(X, Y3, time_j)$

$A := augment(time, A) \quad B := augment(time, B) \quad C := augment(time, C)$



A
B
C

Concentration profiles:
A - reactant (blue)
B - Intermediear has the maximum (red)
C - product (green)

Concentrations at the end of reaction:

Ca := cinterp(X, Y1, tmax) Ca = 0.0174

Cb := cinterp(X, Y2, tmax) Cb = 0.1303

Cc := cinterp(X, Y3, tmax) Cc = 0.8523

End: