Dynamic simulation of microbial growth

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Operating conditions:

$s_f := 200$ ... Feed substrate concentration

$D := 0.1$ ... Dilution rate

Constitutive relations:

$\mu_m := 0.3$ ... maximum specific growth rate

$K := 50$ ... Michaelis-Menten constant

$A := 0.004$ ... constant part of yield coefficient

$B := 0.001$ ... linear part of yield coefficient

$\mu(s) := \frac{\mu_m \cdot s}{K + s}$ ... Monod specific growth rate

$Y(s) := A + B \cdot s$ ... yield coefficient

Dynamic Equations:

$$dxdt(x, s) := (\mu(s) - D) \cdot x$$

$$dsdt(x, s) := D \cdot \left(s_f - s\right) - \frac{\mu(s)}{Y(s)} \cdot x$$

Combine individual functions into a vector function suitable for MathCAD's "rkfixed"

$$ydot(t, y) := \begin{pmatrix} dxdt\left(y_0, y_1\right) \\ dsdt\left(y_0, y_1\right) \end{pmatrix}$$

Initial conditions: $x_0 := 0.5$ $s_0 := 30$

$y_{initial} := \begin{pmatrix} x_0 \\ s_0 \end{pmatrix}$ ... biomass ... substrate

Solve both sets of ODEs from $t_0 := 0$ to $t_f := 100$ in $nstep := 1000$

$$yout := rkfixed\left(y_{initial}, t_0, t_f, nstep, ydot\right)$$

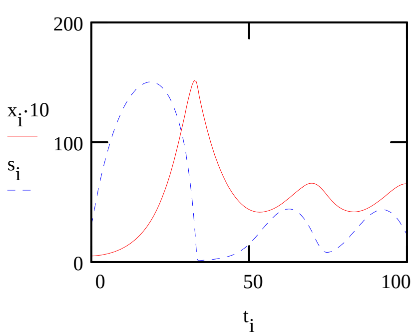
Extract each variable from columns of "yout"

$t := yout^{\langle 0 \rangle}$ $x := yout^{\langle 1 \rangle}$ $s := yout^{\langle 2 \rangle}$

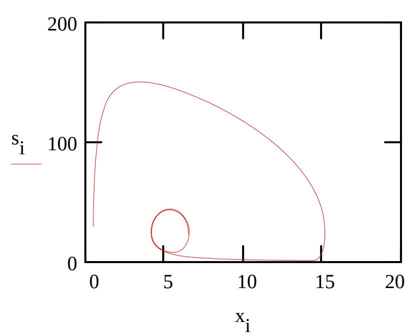
A sample of numbers:

$x_{nstep} = 6.523$ $s_{nstep} = 22.745$

Plots of state variables $i := 0 .. last(t)$



Phase diagram



Solve the same ODEs with the Euler's method in "nstep" steps

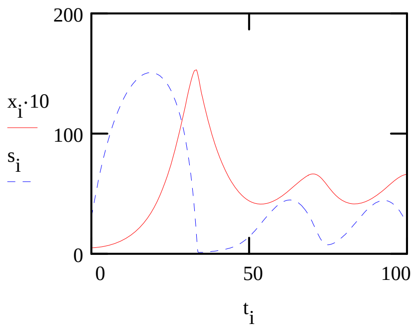
$i := 0 .. nstep$

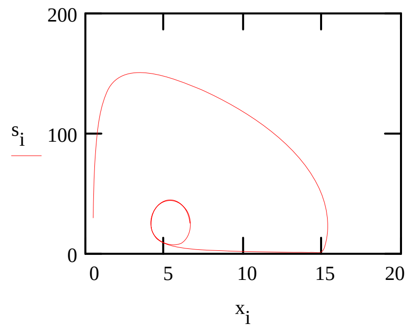
$h := \frac{t_f - t_0}{nstep}$ ... step size

$t_i := i \cdot h$

$x_0 := x_0 \qquad s_0 := s_0$ ... Initial conditions

$\begin{pmatrix} x_{i+1} \\ s_{i+1} \end{pmatrix} := \begin{pmatrix} x_i + dxdt(x_i, s_i) \cdot h \\ s_i + dsdt(x_i, s_i) \cdot h \end{pmatrix}$ ... Euler's method of integration
(Note: coupled equations must be grouped together in a vector.)





For this problem, results from the Runge-Kutta's method and Euler's method are almost indistinguishable.

Extra: Integration by Runge-Kutta's 4th-Order Method without calling "rkfixed"

Slopes for the x & s dynamic equations evaluated at 4 different intermediate points ...

$kx_1(x, s) := dxdt(x, s)$ ... 1st slope at the lhs of the step

$ks_1(x, s) := dsdt(x, s)$

$kx_2(x, s) := dxdt(x + 0.5 \cdot h \cdot kx_1(x, s), s + 0.5 \cdot h \cdot ks_1(x, s))$ ... 2nd slope at the midpoint of the step

$ks_2(x, s) := dsdt(x + 0.5 \cdot h \cdot kx_1(x, s), s + 0.5 \cdot h \cdot ks_1(x, s))$

$kx_3(x, s) := dxdt(x + 0.5 \cdot h \cdot kx_2(x, s), s + 0.5 \cdot h \cdot ks_2(x, s))$ ... 3rd slope at the midpoint of the step

$ks_3(x, s) := dsdt(x + 0.5 \cdot h \cdot kx_2(x, s), s + 0.5 \cdot h \cdot ks_2(x, s))$

$kx_4(x, s) := dxdt(x + h \cdot kx_3(x, s), s + h \cdot ks_3(x, s))$ ... 4th slope at the rhs of the step

$ks_4(x, s) := dsdt(x + h \cdot kx_3(x, s), s + h \cdot ks_3(x, s))$

Average slope in the interval ...

$kx_{ave}(x, s) := \frac{1}{6} \cdot (kx_1(x, s) + 2 \cdot kx_2(x, s) + 2 \cdot kx_3(x, s) + kx_4(x, s))$

$ks_{ave}(x, s) := \frac{1}{6} \cdot (ks_1(x, s) + 2 \cdot ks_2(x, s) + 2 \cdot ks_3(x, s) + ks_4(x, s))$

Compare some numbers:

A sample from Euler's Method:

$x_{nstep} = 6.624 \qquad s_{nstep} = 25.043$

Integration based on the average slope (similar to Euler's Method) ...

$t_i := i \cdot h$

$x_0 := x0$ $s_0 := s0$ ... Initial conditions

$$\begin{pmatrix} x_{i+1} \\ s_{i+1} \end{pmatrix} := \begin{pmatrix} x_i + kx_{ave}(x_i, s_i) \cdot h \\ s_i + ks_{ave}(x_i, s_i) \cdot h \end{pmatrix}$$

A sample from RK Method:

$x_{nstep} = 6.523$ $s_{nstep} = 22.745$