Ordinary differential equations

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Chemical Process Intensification, Eindhoven University of Technology Implicit methods, Systems of ODEs and **Boudary Value Problems**

Today's outline

- Implicit methods Backward Euler Implicit midpoint method

Consider the ODE:

$$\frac{dy}{dx} = f(x, y(x)) \qquad \text{with} \qquad y(x = 0) = y_0$$

First order approximation of derivative: $\frac{dy}{dx} = \frac{y_{i+1} - y_i}{\Delta x}$.

Where to evaluate the function f?

- Evaluation at x_i : Explicit Euler method (forward Euler)
- 2 Evaluation at x_{i+1} : Implicit Euler method (backward Euler)

Problems with Euler's method: instability – forward Euler

Explicit Euler method (forward Euler):

- Use values at x_i: $\frac{y_{i+1}-y_i}{\Delta x}=f(x_i,y_i)\Rightarrow y_{i+1}=y_i+hf(x_i,y_i).$
- This is an explicit equation for y_{i+1} in terms of y_i .
- It can give instabilities with large function values.

Consider the first order batch reactor:

$$\frac{dc}{dt} = -kc \Rightarrow c_{i+1} = c_i - k \frac{c_i}{\Delta t} \Rightarrow \frac{c_{i+1}}{c_i} = 1 - k \Delta t$$

It follows that unphysical results are obtained for $k\Delta t > 1!!$

Stability requirement

$$k\Delta t < 1$$

(but probably accuracy requirements are more stringent here!)

Implicit Euler method (backward Euler):

- Use values at x_{i+1} :
 - $\frac{y_{i+1}-y_i}{\Delta x} = f(x_{i+1}, y_{i+1}) \Rightarrow y_{i+1} = y_i + hf(x_{i+1}, y_{i+1}).$
- This is an implicit equation for y_{i+1} , because it also depends on terms of y_{i+1} .

Consider the first order batch reactor:

$$\frac{dc}{dt} = -kc \Rightarrow c_{i+1} = c_i - kc_{i+1}\Delta t \Rightarrow \frac{c_{i+1}}{c_i} = \frac{1}{1 + k\Delta t}$$

This equation does never give unphysical results! The implicit Euler method is *unconditionally stable* (but maybe not very accurate or efficient).

Semi-implicit Euler method

Usually f is a non-linear function of y, so that linearization is required (recall Newton's method).

$$\frac{dy}{dx} = f(y) \Rightarrow y_{i+1} = y_i + hf(y_{i+1}) \quad \text{using} \quad f(y_{i+1}) = f(y_i) + \frac{df}{dy} \Big|_i (y_{i+1} - y_i) + \dots$$

$$\Rightarrow y_{i+1} = y_i + h \left[f(y_i) + \frac{df}{dy} \Big|_i (y_{i+1} - y_i) \right]$$

$$\Rightarrow \left(1 - h \frac{df}{dy} \Big|_i \right) y_{i+1} = \left(1 - h \frac{df}{dy} \Big|_i \right) y_i + hf(y_i)$$

$$\Rightarrow$$
 $y_{i+1} = y_i + h \left(1 - h \frac{df}{dy}\Big|_i\right)^{-1} f(y_i)$

For the case that f(x, y(x)) we could add the variable x as an additional variable $y_{n+1} = x$. Or add one fully implicit Euler step (which avoids the computation of $\frac{\partial f}{\partial x}$):

$$y_{i+1} = y_i + hf(x_{i+1}, y_{i+1}) \Rightarrow y_{i+1} = y_i + h\left(1 - h\left.\frac{df}{dy}\right|_i\right)^{-1} f(x_{i+1}, y_i)$$

Semi-implicit Euler method - example

Second order reaction in a batch reactor:

$$\frac{dc}{dt}=-kc^2$$
 with $c_0=1~\rm{mol}~m^{-3},~k=1~m^3~\rm{mol}^{-1}~s^{-1},~t_{end}=2~\rm{s}$ Analytical solution: $c(t)=\frac{c_0}{1+kc_0t}$

Define
$$f = -kc^2$$
, then $\frac{df}{dc} = -2kc \Rightarrow c_{i+1} = c_i - \frac{hkc_i^2}{1+2hkc_i}$.

Ν	ζ	$rac{\zeta_{ ext{numerical}} - \zeta_{ ext{analytical}}}{\zeta_{ ext{analytical}}}$	$r = rac{\log\left(rac{\epsilon_i}{\epsilon_{i-1}} ight)}{\log\left(rac{N_{i-1}}{N_i} ight)}$
20	0.654066262	1.89×10^{-2}	
40	0.660462687	9.31×10^{-3}	1.02220
80	0.663589561	4.62×10^{-3}	1.01162
160	0.665134433	2.30×10^{-3}	1.00594
320	0.665902142	1.15×10^{-3}	1.00300

Second order implicit method: Implicit midpoint method

Implicit midpoint rule	Explicit midpoint rule
(second order)	(modified Euler method)
$y_{i+1} = y_i + hf\left(x_i + \frac{1}{2}h, \frac{1}{2}(y_i + y_{i+1})\right)$	$y_{i+1} = y_i + hf(x_i + \frac{1}{2}h, y_i + \frac{1}{2}hk_1)$

in case f(y) then:

$$f\left(\frac{1}{2}(y_i+y_{i+1})\right) = f_i + \frac{df}{dy}\Big|_i \left(\frac{1}{2}(y_i+y_{i+1})-y_i\right) = f_i + \frac{1}{2} \frac{df}{dy}\Big|_i (y_{i+1}-y_i)$$

Implicit midpoint rule reduces to:

$$y_{i+1} = y_i + hf_i + \frac{h}{2} \left. \frac{df}{dy} \right|_i (y_{i+1} - y_i)$$

$$\Rightarrow \left(1 - \frac{h}{2} \left. \frac{df}{dy} \right|_i \right) y_{i+1} = \left(1 - \frac{h}{2} \left. \frac{df}{dy} \right|_i \right) y_i + hf_i$$

$$\Rightarrow y_{i+1} = y_i + h \left(1 - \frac{h}{2} \frac{df}{dy} \Big|_i \right)^{-1} f_i$$

Implicit midpoint method — example

Second order reaction in a batch reactor:

$$\frac{dc}{dt}=-kc^2$$
 with $c_0=1$ mol m⁻³, $k=1$ m³ mol⁻¹ s⁻¹, $t_{\rm end}=2$ s (Analytical solution: $c(t)=\frac{c_0}{1+kc_0t}$).

Define $f = -kc^2$, then $\frac{df}{dc} = -2kc$.

Substitution:

$$c_{i+1} = c_i + h \left(1 - \frac{h}{2} \cdot (-2kc_i) \right)^{-1} \cdot (-kc_i^2)$$

$$= c_i - \frac{hkc_i^2}{1 + hkc_i} = \frac{c_i + hkc_i^2 - hkc_i^2}{1 + hkc_i} \Rightarrow c_{i+1} = \frac{c_i}{1 + hkc_i}$$

You will find that this method is exact for all step sizes h because of the quadratic source term!

Implicit midpoint method — example

Second order reaction in a batch reactor:

 $\frac{dc}{dt}=-kc^2$ with $c_0=1$ mol m⁻³, k=1 m³ mol⁻¹ s⁻¹, $t_{\rm end}=2$ s Analytical solution: $c(t)=\frac{c_0}{1+kc_0t}$

$$c_{i+1} = \frac{c_i}{1 + hkc_i}$$

N	ζ	$rac{\zeta_{ ext{numerical}} - \zeta_{ ext{analytical}}}{\zeta_{ ext{analytical}}}$	$r = rac{\log\left(rac{\epsilon_i}{\epsilon_{i-1}} ight)}{\log\left(rac{N_{i-1}}{N_i} ight)}$
20	0.6666666667	1.665×10^{-16}	
40	0.6666666667	0	
80	0.6666666667	0	
160	0.6666666667	0	
320	0.6666666667	0	

Third order reaction in a batch reactor: $\frac{dc}{dt} = -kc^3$ Analytical solution: $c(t) = \frac{c_0}{\sqrt{1+2kc_0^2t}}$

$$c_{i+1} = c_i - \frac{hkc_i^3}{1 + \frac{3}{2}hkc_i^2}$$

Ν	ζ	$rac{\zeta_{ ext{numerical}} - \zeta_{ ext{analytical}}}{\zeta_{ ext{analytical}}}$	$r = rac{\log\left(rac{\epsilon_i}{\epsilon_{i-1}} ight)}{\log\left(rac{N_{i-1}}{N_i} ight)}$
20	0.5526916174	1.71×10^{-4}	
40	0.5527633731	4.17×10^{-5}	2.041
80	0.5527807304	1.03×10^{-5}	2.021
160	0.5527849965	2.55×10^{-6}	2.011
320	0.5527860538	6.34×10^{-7}	2.005

- Systems of ODEs Solution methods for systems of ODEs Solving systems of ODEs in Matlab Stiff systems of ODEs

A system of ODEs is specified using vector notation:

$$\frac{d\mathbf{y}}{dx} = \mathbf{f}(x, \mathbf{y}(x))$$

for

$$\frac{dy_1}{dx} = f_1(x, y_1(x), y_2(x)) \quad \text{or} \quad f_1(x, y_1, y_2)$$

$$\frac{dy_2}{dx} = f_2(x, y_1(x), y_2(x)) \quad \text{or} \quad f_2(x, y_1, y_2)$$

The solution techniques discussed before can also be used to solve systems of equations.

Systems of ODEs: Explicit methods

Forward Euler method

$$\mathbf{y}_{i+1} = \mathbf{y}_i + h\mathbf{f}(\mathbf{x}_i, \mathbf{y}_i)$$

Improved Euler method (classical RK2)

$$\mathbf{y}_{i+1} = \mathbf{y}_i + \frac{h}{2}(\mathbf{k}_1 + \mathbf{k}_2)$$
 using $\mathbf{k}_1 = \mathbf{f}(x_i, \mathbf{y}_i)$
 $\mathbf{k}_2 = \mathbf{f}(x_i + h, \mathbf{y}_i + h\mathbf{k}_1)$

Modified Euler method (midpoint rule)

$$\mathbf{y}_{i+1} = \mathbf{y}_i + h\mathbf{k}_2$$
 using $\mathbf{k}_1 = \mathbf{f}(x_i, \mathbf{y}_i)$
 $\mathbf{k}_2 = \mathbf{f}(x_i + \frac{h}{2}, \mathbf{y}_i + \frac{h}{2}\mathbf{k}_1)$

Systems of ODEs: Explicit methods

Classical fourth order Runge-Kutta method (RK4)

$$\mathbf{y}_{i+1} = \mathbf{y}_i + h\left(\frac{\mathbf{k}_1}{6} + \frac{1}{3}\left(\mathbf{k}_2 + \mathbf{k}_3\right) + \frac{\mathbf{k}_4}{6}\right)$$

$$\mathbf{k}_1 = \mathbf{f}(x_i, \mathbf{y}_i)$$

$$\mathbf{k}_2 = \mathbf{f}(x_i + \frac{h}{2}, \mathbf{y}_i + \frac{h}{2}\mathbf{k}_1)$$
using
$$\mathbf{k}_3 = \mathbf{f}(x_i + \frac{h}{2}, \mathbf{y}_i + \frac{h}{2}\mathbf{k}_2)$$

$$\mathbf{k}_4 = \mathbf{f}(x_i + h, \mathbf{y}_i + h\mathbf{k}_3)$$

Solving systems of ODEs in Matlab is completely analogous to solving a single ODE:

- 1 Create a function that specifies the ODEs. This function returns the $\frac{dy}{dx}$ vector.
- 2 Initialise solver variables and settings (e.g. step size, initial conditions, tolerance), in a separate script. Initial conditions and tolerances should be given per-equation, i.e. as a vector.
- 3 Call the ODE solver function, using a function handle to the ODE function described in point 1.
 - The ODE solver will return the vector for the independent variable, and a solution matrix, with a column as the solution for each equation in the system.

```
We solve the system: \frac{dx_1}{dt} = -x_1 - x_2, \frac{dx_2}{dt} = x_1 - 2x_2
```

Create an ODE function

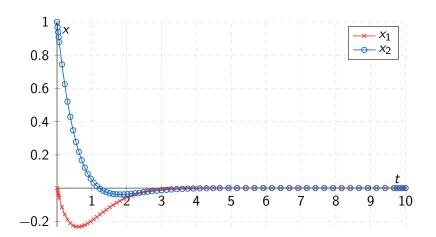
```
function [dxdt] = myODEFunction(t,x)
dxdt(1) = -x(1) - x(2);
dxdt(2) = x(1) - 2*x(2);
dxdt=dxdt'; % Transpose to column vector
return
```

Create a solution script

```
options = odeset('RelTol',1e-4,'AbsTol',[1e-4 1e-4]);
[t,x] = ode45(@myODEfunction,tspan,x_init,options);
```

Solving systems of ODEs in Matlab: example

Plot the solution:



Solving systems of ODEs in Matlab: repeated notes

A few notes on working with ode45 and other solvers. If we want to give additional arguments (e.g. a, b and c) to our ODE function, we can list them in the function line:

```
function [dxdt] = myODE(t,x,a,b,c)
```

The additional arguments can now be set in the solver script by adding them after the options:

```
[t,x] = ode45(@myODE,tspan,x_0,options,a,b,c);
```

 Of course, in the solver script, the variables do not need to be called a, b and c:

```
[t,x] = ode45(@myODE,tspan,x_0,options,k1,phi,V);
```

 These variables may be of any type (vectors, matrix, struct). Especially a struct is useful to carry many values in 1 variable.

Systems of ODEs: Implicit methods

Backward Euler method

$$\mathbf{y}_{i+1} = \mathbf{y}_i + h \left(1 - h \left. \frac{d\mathbf{f}}{d\mathbf{y}} \right|_i \right)^{-1} \mathbf{f}(\mathbf{y}_i)$$

Implicit midpoint method

$$\mathbf{y}_{i+1} = \mathbf{y}_i + h \left(1 - \frac{h}{2} \left. \frac{d\mathbf{f}}{d\mathbf{y}} \right|_i \right)^{-1} \mathbf{f}(\mathbf{y}_i)$$

Stiff systems of ODEs

A system of ODEs can be stiff and require a different solution method. For example:

$$\frac{dc_1}{dt} = 998c_1 + 1998c_2 \qquad \frac{dc_2}{dt} = -999c_1 - 1999c_2$$

with boundary conditions $c_1(t=0)=1$ and $c_2(t=0)=0$. The analytical solution is:

$$c_1 = 2e^{-t} - e^{-1000t}$$
 $c_2 = -e^{-t} + e^{-1000t}$

For the explicit method we require $\Delta t < 10^{-3}$ despite the fact that the term is completely negligible, but essential to keep stability.

The "disease" of stiff equations: we need to follow the solution on the shortest length scale to maintain stability of the integration, although accuracy requirements would allow a much larger time step.

Forward Euler (explicit)

$$\begin{aligned} &\frac{c_{1,i+1} - c_{1,i}}{dt} = 998c_{1,i} + 1998c_{2,i} \\ &\frac{c_{2,i+1} - c_{2,i}}{dt} = -999c_{1,i} - 1999c_{2,i} \\ &\Rightarrow \frac{c_{1,i+1} = (1 + 998\Delta t)c_{1,i} + 1998\Delta tc_{2,i}}{c_{2,i+1} = -999\Delta tc_{1,i} + (1 - 1999\Delta t)c_{2,i}} \end{aligned}$$

Backward Euler (implicit)

$$\begin{aligned} &\frac{dc_{1,i+1} - c_{1,i+1}}{dt} = 998c_{1,i+1} + 1998c_{2,i+1} \\ &\frac{dc_{2,i+1} - c_{2,i+1}}{dt} = -999c_{1,i+1} - 1999c_{2,i+1} \\ &\Rightarrow \frac{(1 - 998\Delta t)c_{1,i+1} - 1998\Delta tc_{2,i} = c_{1,i}}{999\Delta tc_{1,i+1} + (1 + 999\Delta t)c_{2,i+1} = c_{2,i}} \end{aligned}$$

$$A\boldsymbol{c}_{i+1} = \boldsymbol{c}_i$$
 with $A = \begin{pmatrix} 1 - 998\Delta t & -1998\Delta t \\ 999\Delta t & 1 + 1999\Delta t \end{pmatrix}$ and $\boldsymbol{b} = \begin{pmatrix} c_{1,i} \\ c_{2,i} \end{pmatrix}$

Demonstration with example

Backward Euler (implicit)
$$A\boldsymbol{c}_{i+1} = \boldsymbol{c}_i$$
 with $A = \begin{pmatrix} 1 - 998\Delta t & -1998\Delta t \\ 999\Delta t & 1 + 1999\Delta t \end{pmatrix}$ and $\boldsymbol{b} = \begin{pmatrix} c_{1,i} \\ c_{2,i} \end{pmatrix}$

Cramers rule:

Cramers rule:
$$c_{1,i+1} = \frac{\begin{vmatrix} c_{1,i} & -1998\Delta t \\ c_{2,i} & 1+1999\Delta t \end{vmatrix}}{\det \begin{vmatrix} A \end{vmatrix}} = \frac{\frac{(1+1999\Delta t)c_{1,i}+1998\Delta tc_{2,i}}{(1-998\Delta t)(1+1999\Delta t)+1998\cdot999\Delta t^2}}{\frac{1-998\Delta t}{c_{2,i}}}{\det \begin{vmatrix} A \end{vmatrix}} = \frac{\frac{-999\Delta tc_{1,i}+(1-998\Delta t)c_{2,i}}{(1-998\Delta t)(1+1999\Delta t)+1998\cdot999\Delta t^2}}$$

Forward Euler: $\Delta t \leq 0.001$ for stability

Backward Euler: always stable, even for $\Delta t > 100$ (but then not very accurate!)

Demonstration with example

Cure for stiff problems: use implicit methods! To find out whether your system is stiff: check whether one of the eigenvalues have an imaginary part

Matlab offers a stabilized solver, ode15s, for stiff problems.

$$\frac{dc_1}{dt} = 998c_1 + 1998c_2 \quad \frac{dc_2}{dt} = -999c_1 - 1999c_2, \ c_1(0) = 1, \ c_2(0) = 0$$

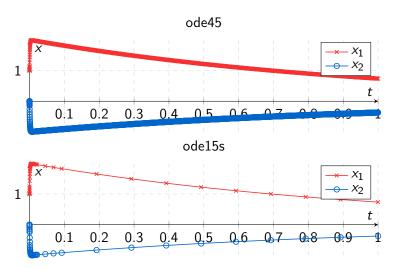
Create the ode function

```
function [dcdt] = stiff_ode(t,c)
dcdt = zeros(2,1); % Pre-allocation
dcdt(1) = 998 * c(1) + 1998*c(2);
dcdt(2) = -999 * c(1) - 1999*c(2);
return
```

Compare the resolution of the solutions

```
subplot (2,1,1);
ode45(@stiff_ode, [0 1], [1 0]);
subplot(2,1,2);
ode15s(@stiff_ode, [0 1], [1 0]);
```

Implicit methods in Matlab



The explicit solver requires 1245 data points (default settings), the implicit solver requires just 48!

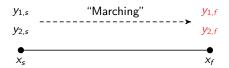
Boundary value problems 000000000

- Boundary value problems Shooting method

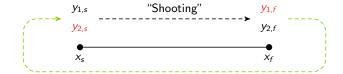
The nature of boundary conditions determines the appropriate numerical method. Classification into 2 main categories:

Initial value problems (IVP) We know the values of all y_i at some starting position x_s , and it is desired to find the values of y_i at some final point x_f .

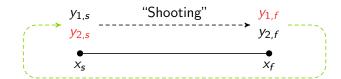
Boundary value problems 00000000



Boundary value problems (BVP) Boundary conditions are specified at more than one x. Typically, some of the BC are specified at x_s and the remainder at x_f .



How to solve a BVP using the shooting method:



Boundary value problems 000000000

- Define the system of ODEs
- Provide an initial guess for the unknown boundary condition
- Solve the system and compare the resulting boundary condition to the expected value
- Adjust the guessed boundary value, and solve again. Repeat until convergence.
 - Of course, you can subtract the expected value from the computed value at the boundary, and use a non-linear root finding method

BVP: example in Excel

Consider a chemical reaction in a liquid film layer of thickness δ :

$$\mathcal{D} \frac{d^2c}{dx^2} = k_Rc$$
 with $c(x=0) = C_{A,i,L} = 1$ (interface concentration) $c(x=\delta) = 0$ (bulk concentration)

Boundary value problems 000000000

Question: compute the concentration profile in the film layer.

Step 1: Define the system of ODEs

This second-order ODE can be rewritten as a system of first-order ODEs, if we define the flux q as:

$$q = -\mathcal{D}\frac{dc}{dx}$$

Now, we find:

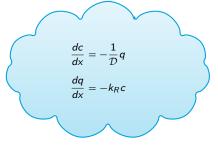
$$\frac{dc}{dx} = -\frac{1}{\mathcal{D}}q$$

$$\frac{dq}{dx} = -k_R c$$

BVP: example in Excel

Solving the two first-order ODEs in Excel. First, the cells with constants:

	Α	В	С
1	CAiL	1	mol/m3
2	D	1e-8	m2/s
3	kR	10	1/s
4	delta	1e-4	m
5	N	100	
6	dx	=B4/B5	



Boundary value problems

Now, we program the forward Euler (explicit) schemes for c and q below:

	А	В	С
10	х	С	q
11	0	=B1	10
12	=A11+\$B\$6	=B11+\$B\$6*(-1/\$B\$2*C11)	=C11+\$B\$6*(-\$B\$3*B11)
13	=A12+\$B\$6	=B12+\$B\$6*(-1/\$B\$2*C12)	=C12+\$B\$6*(-\$B\$3*B12)
111	=A110+\$B\$6	=B110+\$B\$6*(-1/\$B\$2*C110)	=C110+\$B\$6*(-\$B\$3*B110)

BVP: example in Excel

We now have profiles for c and q as a function of position x.

Boundary value problems 000000000

- The concentration $c(x = \delta)$ depends (eventually) on the boundary condition at the interface q(x=0)
- We can use the solver to change q(x = 0) such that the concentration at the bulk meets our requirement: $c(x = \delta) = 0$

Boundary value problems

We first program the system of ODEs in a separate function:

$$\frac{dc}{dx} = -\frac{1}{\mathcal{D}}q$$
$$\frac{dq}{dx} = -k_R c$$

```
function [dxdt] = BVPODE(t,x,ps)
dxdt(1)=-1/ps.D*x(2);
dxdt(2)=-ps.kR*x(1);
dxdt=dxdt';
return
```

Note that we pass a variable (type: struct) that contains required parameters: ps.

The ODE function is solved via ode45, after setting a number of initial and boundary conditions:

Boundary value problems 0000000000

```
function f = RunBVP(bcq,ps)
[x,cq] = ode45(@BVPODE,[0 ps.delta],[1 bcq], [], ps);
f = cq(end, 1) - 0;
plotyy(x,cq(:,1),x,cq(:,2));
return:
```

Note the following:

- We use the interval $0 < x < \delta$
- Boundary conditions are given as: c(x = 0) = 1 and q(x = 0) = bcq, which is given as an argument to the function (i.e. changable from 'outside'!)
- The function returns f, the difference between the computed and desired concentration at $x = \delta$.

Finally, we should solve the system so that we obtain the right boundary condition q = bcq such that $c(x = \delta) = 0$. We can use the built-in function fzero to do this

Boundary value problems 000000000

```
% Parameter definition
ps.D=1e-8;
ps.kR=10;
ps.delta=1e-4;
% Solve for flux boundary condition (initial guess: 0)
opt = optimset('Display', 'iter');
flux = fzero(@RunBVP,0,opt,ps);
```

Boundary value problems 000000000

BVP example: analytical solution

Compare with the analytical solution:

$$q=k_L E_A C_{A,i,L}$$
 with $E_A=rac{Ha}{ anh Ha}$ (Enhancement factor) $Ha=rac{\sqrt{k_R \mathcal{D}}}{k_L}$ (Hatta number) $k_L=rac{\mathcal{D}}{\delta}$ (mass transfer coefficient)

- - Solving systems of ODEs in Matlab
- Conclusion

Other methods

Other explicit methods:

 Burlisch-Stoer method (Richardson extrapolation + modified midpoint method)

Other implicit methods:

- Rosenbrock methods (higher order implicit Runge-Kutta methods)
- Predictor-corrector methods

Summary

- Several solution methods and their derivation were discussed:
 - Explicit solution methods: Euler, Improved Euler, Midpoint method, RK45
 - Implicit methods: Implicit Euler and Implicit midpoint method
 - A few examples of their spreadsheet implementation were shown
- We have paid attention to accuracy and instability, rate of convergence and step size
- Systems of ODEs can be solved by the same algorithms. Stiff problems should be treated with care.
- An example of solving ODEs with Matlab was demonstrated.